Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2026 – 08:05 AM EDT

PDB ID	:	2BCC / pdb_00002bcc
Title	:	STIGMATELLIN-BOUND CYTOCHROME BC1 COMPLEX FROM CHICKEN
Authors	:	Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.I.; Kim, K.K.; Hung, L.W.; Crofts, A.R.; Berry, E.A.; Kim, S.H.
Deposited on	:	1998-09-18
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

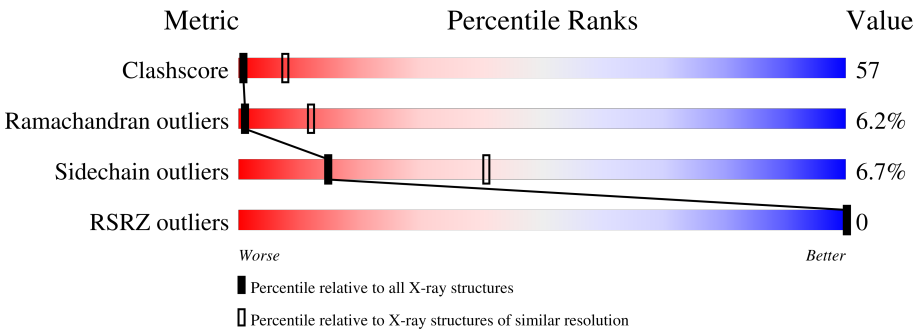
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	33% 56% 10% • •
2	B	422	32% 52% 11% • • •
3	C	380	25% 56% 17% •
4	D	241	34% 54% 11% •
5	E	196	31% 54% 14% •
6	F	109	43% 39% 10% 8%

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Mol	Chain	Length	Quality of chain
7	G	81	28% 53% 11%
8	H	78	40% 44% 15%
9	I	33	61% 39%
10	J	62	32% 48% 10% 5% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	PEE	C	384	X	-	-	-
13	PEE	E	198	X	-	-	-
16	HEC	D	243	X	-	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 15754 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3423	2147	601	657	18	0	0	0

- Molecule 2 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	406	2994	1878	518	591	7	0	0	0

- Molecule 3 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	379	3002	2013	473	504	12	0	0	0

- Molecule 4 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1899	1214	326	345	14	0	0	0

- Molecule 5 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1512	953	266	285	8	0	0	0

- Molecule 6 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	100	875	557	153	162	3	0	0	0

- Molecule 7 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	78	626	411	114	100	1	0	0	0

- Molecule 8 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	66	490	301	88	96	5	0	0	0

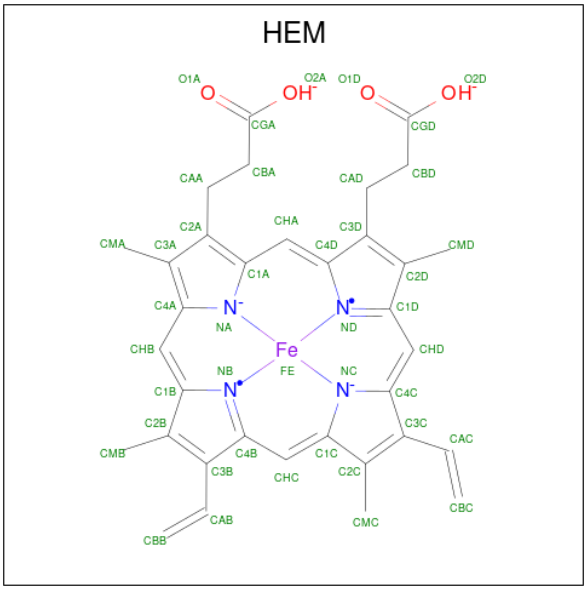
- Molecule 9 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	33	159	92	33	34	0	0	0

- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

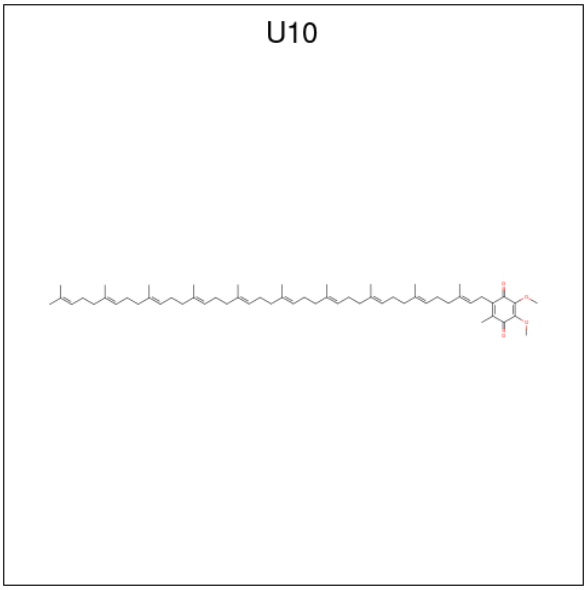
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	59	459	299	78	82	0	0	0

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



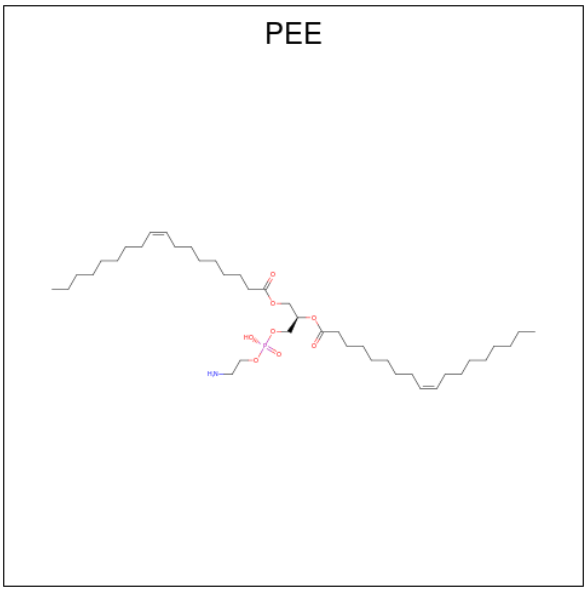
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
11	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
11	C	1	43	34	1	4	4	0	0

- Molecule 12 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



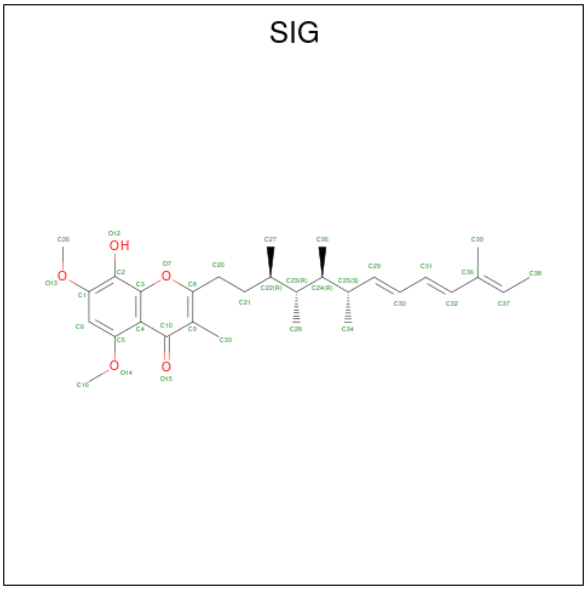
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	C	1	29	25	4	0	0

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



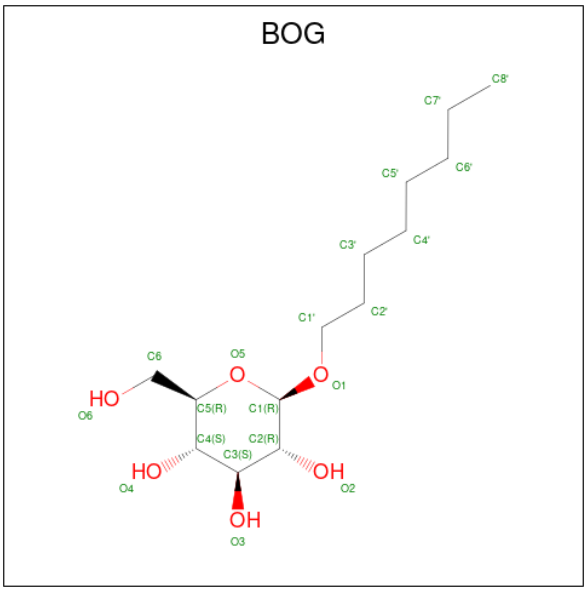
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
13	C	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
13	E	1	49	39	1	8	1	0	0

- Molecule 14 is STIGMATELLIN (CCD ID: SIG) (formula: $C_{30}H_{42}O_5$).



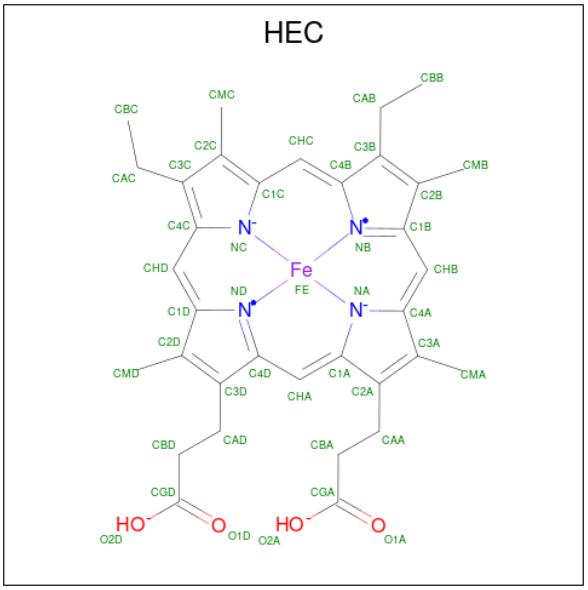
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	O				
14	C	1	35	30	5			0	0

- Molecule 15 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



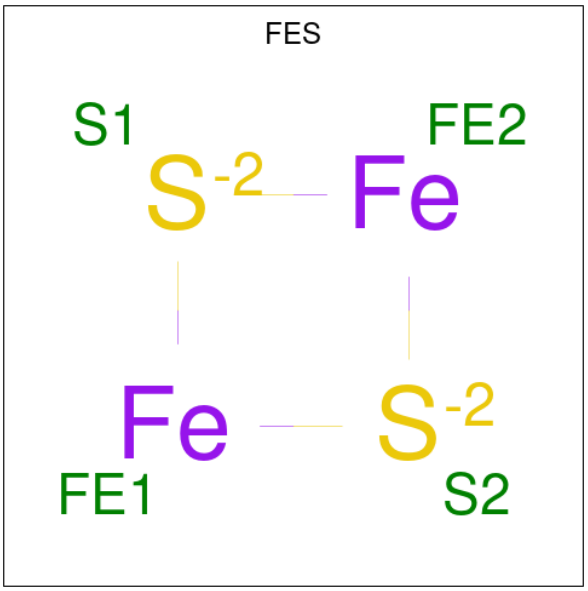
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	D	1	20	14	6	0	0

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
16	D	1	43	34	1	4	4	0	0

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



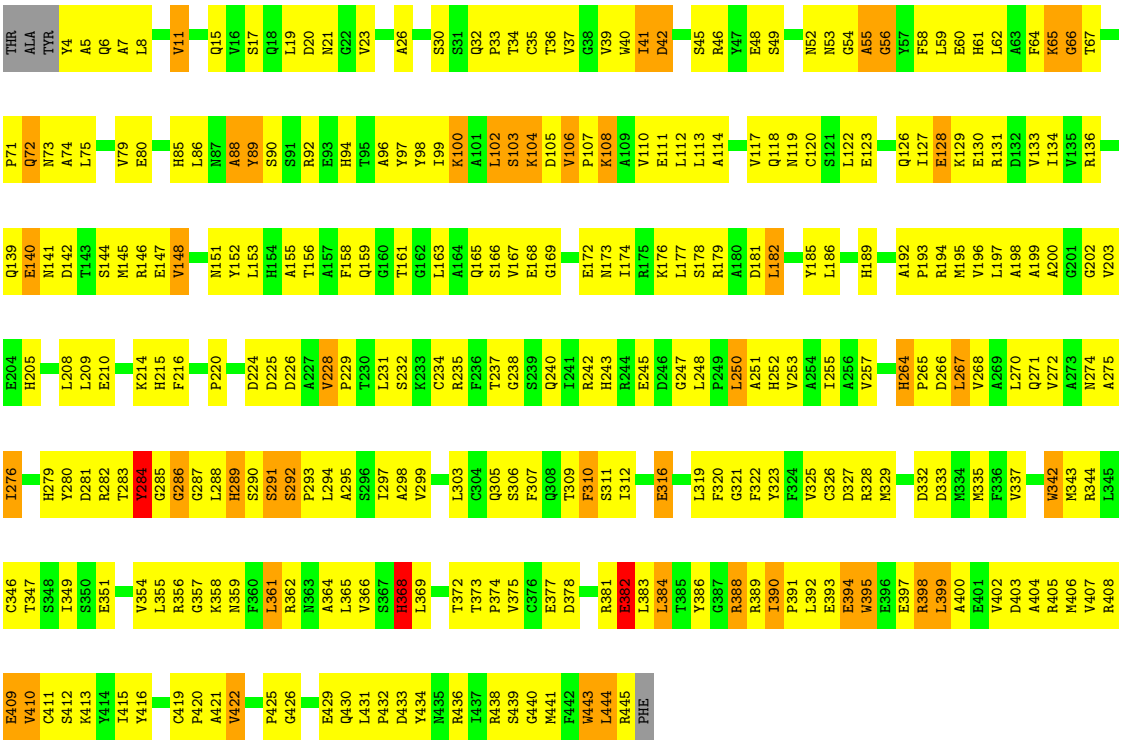
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
17	E	1	4	2	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

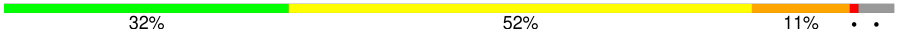
• Molecule 1: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

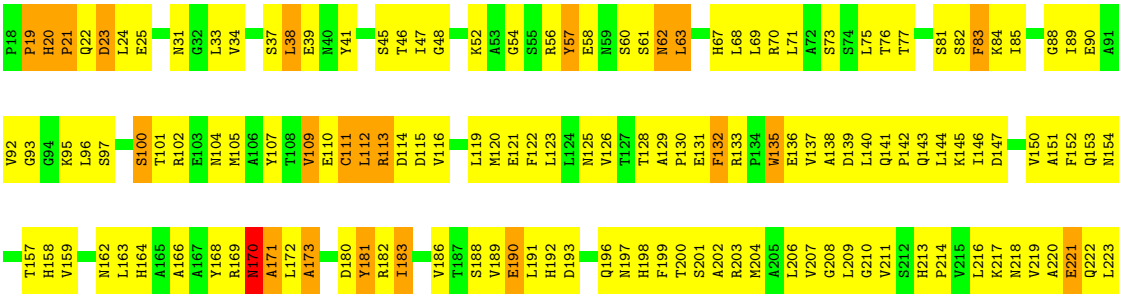
Chain A:

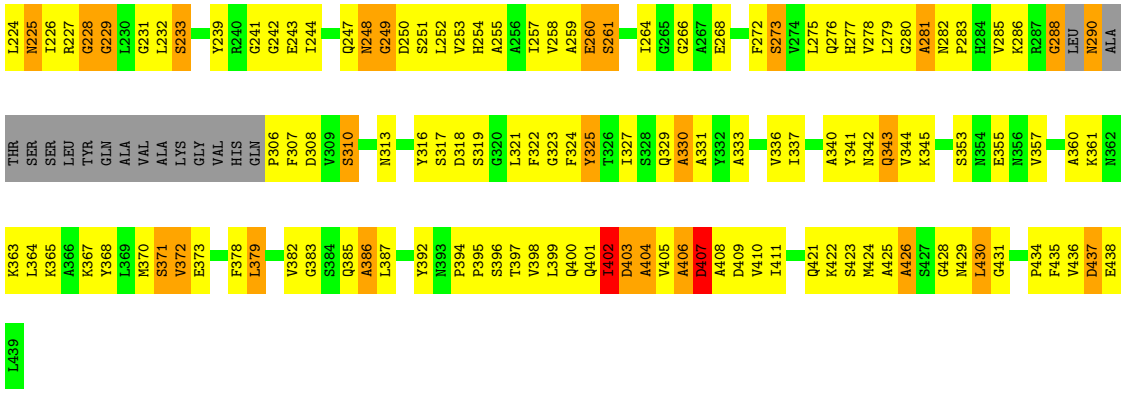


• Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain B:

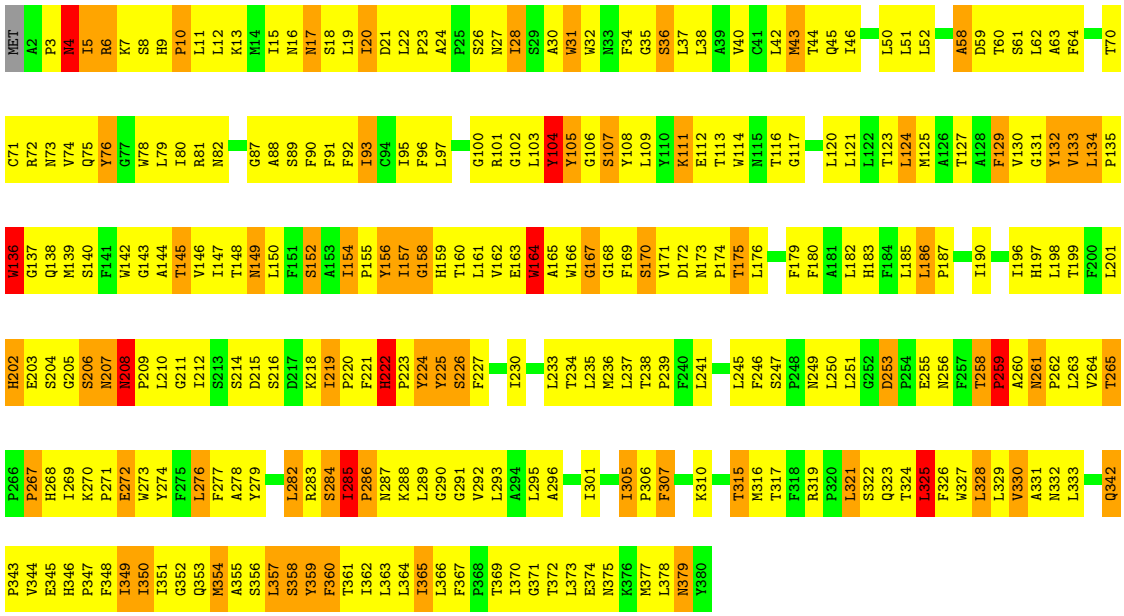






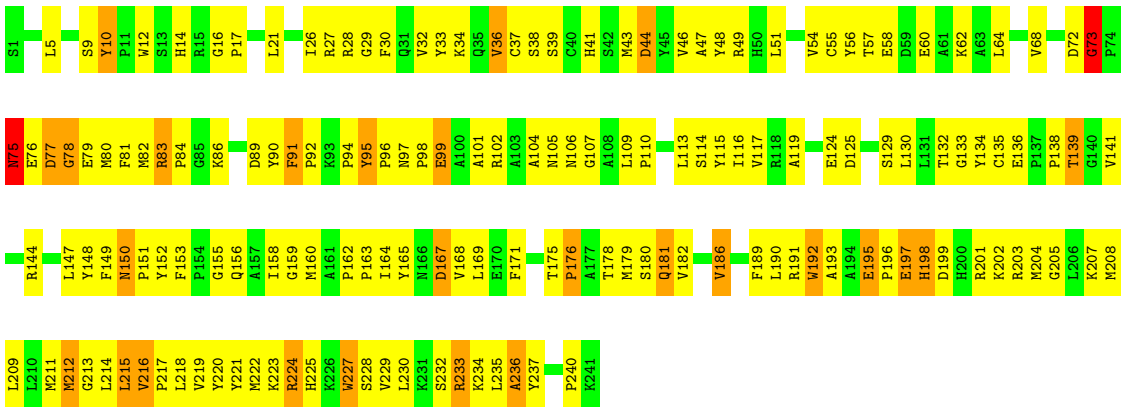
- Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain C: 25% 56% 17%



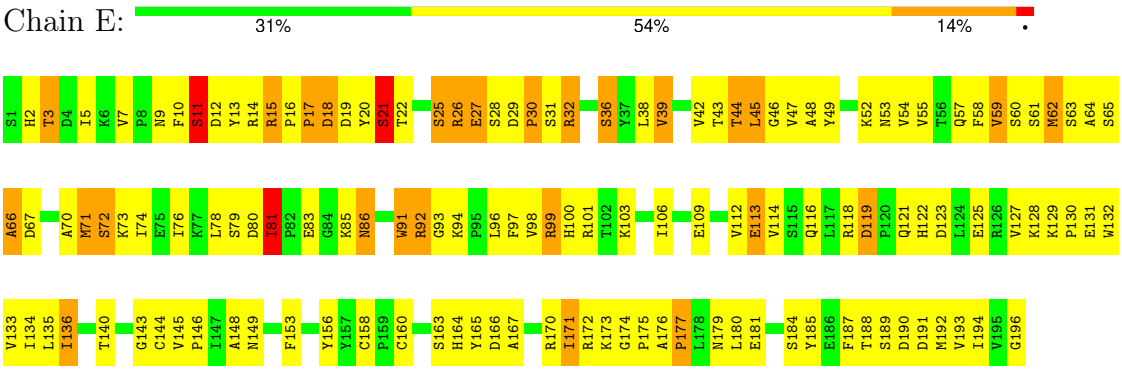
- Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain D: 34% 54% 11%



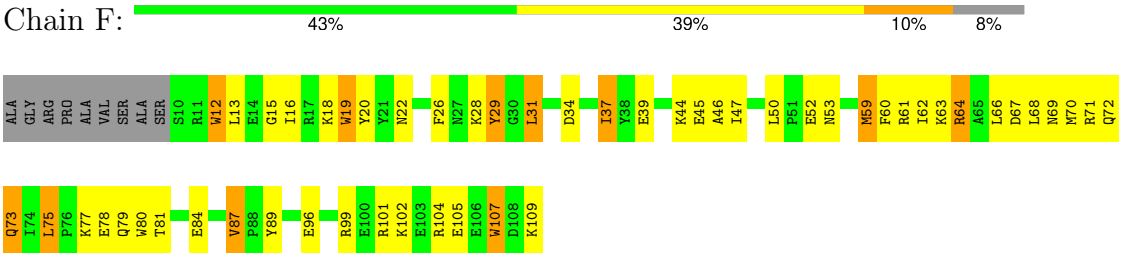
• Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain E:



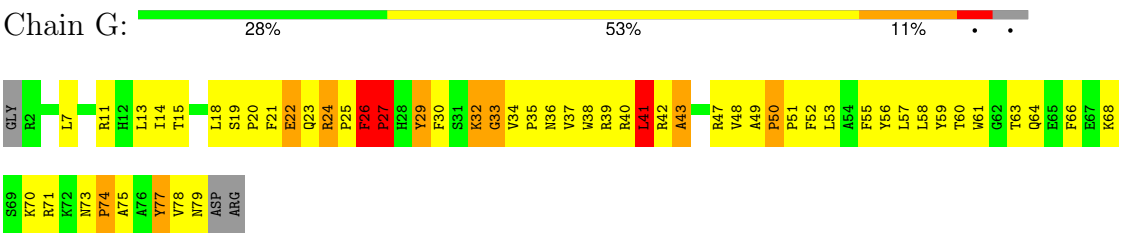
• Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain F:



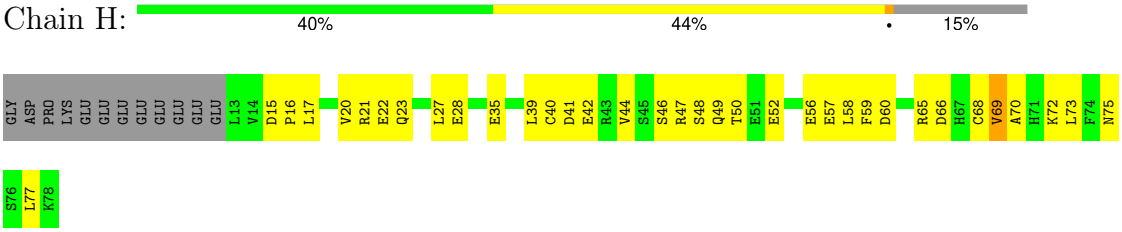
• Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain G:



• Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain H:

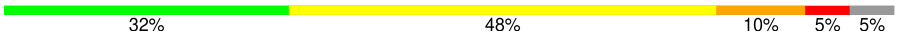


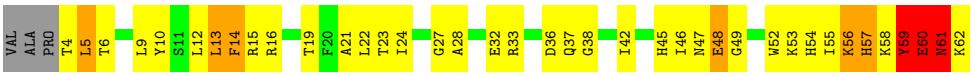
• Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain I:

• Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain J:


32%
48%
10%
5%
5%


VAL
ALA
PRO
T4
L5
T6
L9
Y10
S11
L12
L13
F14
R15
R16
T19
F20
A21
L22
T23
I24
G27
A28
E32
R33
D36
Q37
G38
I42
H45
I46
N47
E48
G49
W52
K53
H54
I55
K56
H57
K58
Y59
E60
N61
K62

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	173.46Å 182.45Å 241.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.50 12.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	85.6 (12.00-3.50) 70.6 (12.00-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.01Å)	Xtriage
Refinement program	CNS 0.1	Depositor
R, R_{free}	0.284 , 0.317 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 101.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.29$, $< L^2 > = 0.12$	Xtriage
Estimated twinning fraction	0.229 for k,h,-l	Xtriage
F_o,F_c correlation	0.65	EDS
Total number of atoms	15754	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SIG, HEM, HEC, FES, BOG, U10, PEE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.57	0/3495	1.22	44/4742 (0.9%)
2	B	0.55	1/3046 (0.0%)	1.11	19/4132 (0.5%)
3	C	0.67	0/3104	1.26	44/4252 (1.0%)
4	D	0.66	0/1960	1.33	30/2665 (1.1%)
5	E	0.57	0/1548	1.23	18/2095 (0.9%)
6	F	0.64	0/896	1.14	6/1206 (0.5%)
7	G	0.66	0/648	2.63	9/882 (1.0%)
8	H	0.55	0/495	0.96	1/669 (0.1%)
10	J	0.70	1/470 (0.2%)	1.20	6/635 (0.9%)
All	All	0.61	2/15662 (0.0%)	1.30	177/21278 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
10	J	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	288	GLY	CA-C	7.52	1.57	1.52
10	J	60	GLU	CA-C	5.09	1.59	1.52

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	26	PHE	CA-C-N	47.84	179.63	119.84
7	G	26	PHE	C-N-CA	47.84	179.63	119.84
7	G	26	PHE	C-N-CD	-11.24	78.91	125.00
3	C	265	THR	N-CA-C	-11.04	96.16	110.07
7	G	41	LEU	N-CA-C	-10.88	97.74	111.02
4	D	76	GLU	N-CA-C	-10.88	98.72	113.30
5	E	25	SER	N-CA-C	-10.59	98.48	111.40
1	A	329	MET	N-CA-C	10.02	124.86	112.23
6	F	13	LEU	N-CA-C	-9.79	100.46	111.82
4	D	95	TYR	CA-C-N	9.56	129.80	119.28
4	D	95	TYR	C-N-CA	9.56	129.80	119.28
4	D	91	PHE	CA-C-N	9.46	130.05	119.83
4	D	91	PHE	C-N-CA	9.46	130.05	119.83
3	C	267	PRO	N-CA-C	-9.37	96.03	111.68
3	C	285	ILE	CA-C-N	9.18	131.32	119.84
3	C	285	ILE	C-N-CA	9.18	131.32	119.84
3	C	358	SER	N-CA-C	-8.92	101.47	111.82
10	J	61	ASN	N-CA-C	8.41	128.72	110.80
1	A	66	GLY	N-CA-C	8.39	121.69	112.29
1	A	305	GLN	N-CA-C	-8.25	102.09	112.90
1	A	426	GLY	CA-C-N	8.19	130.08	119.84
1	A	426	GLY	C-N-CA	8.19	130.08	119.84
7	G	27	PRO	CA-N-CD	-8.03	100.76	112.00
5	E	3	THR	N-CA-C	-7.97	103.45	113.01
2	B	278	VAL	N-CA-C	-7.93	102.53	110.62
1	A	104	LYS	N-CA-C	-7.86	102.52	113.37
1	A	228	VAL	CA-C-N	7.71	128.16	119.83
1	A	228	VAL	C-N-CA	7.71	128.16	119.83
1	A	264	HIS	CA-C-N	7.62	127.67	119.28
1	A	264	HIS	C-N-CA	7.62	127.67	119.28
10	J	59	TYR	N-CA-C	-7.61	100.94	113.50
4	D	44	ASP	N-CA-C	7.57	120.49	111.33
5	E	143	GLY	N-CA-C	7.48	126.39	115.32
3	C	328	LEU	N-CA-C	-7.46	103.09	111.07
6	F	87	VAL	N-CA-C	7.44	115.56	107.60
3	C	226	SER	N-CA-C	-7.40	103.16	111.07
5	E	18	ASP	N-CA-C	-7.38	102.24	113.89
4	D	77	ASP	N-CA-C	-7.37	102.56	113.61
1	A	20	ASP	N-CA-C	-7.31	103.29	113.37
2	B	281	ALA	N-CA-C	-7.22	102.95	112.34
5	E	114	VAL	N-CA-C	7.19	120.04	111.05
3	C	20	ILE	N-CA-C	-7.19	98.86	108.35
7	G	24	ARG	CA-C-N	7.16	127.77	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	24	ARG	C-N-CA	7.16	127.77	119.47
1	A	248	LEU	CA-C-N	7.12	126.64	119.24
1	A	248	LEU	C-N-CA	7.12	126.64	119.24
10	J	14	PHE	N-CA-C	7.10	120.06	111.82
3	C	288	LYS	N-CA-C	-7.06	103.28	110.97
3	C	208	ASN	CA-C-N	6.98	128.56	119.84
3	C	208	ASN	C-N-CA	6.98	128.56	119.84
3	C	104	TYR	N-CA-C	6.95	121.07	111.55
2	B	60	SER	N-CA-C	-6.91	102.97	111.33
1	A	416	TYR	N-CA-C	6.75	120.42	110.30
8	H	69	VAL	N-CA-C	-6.74	102.94	110.62
2	B	327	ILE	N-CA-C	-6.64	98.72	108.54
2	B	379	LEU	N-CA-C	-6.64	104.44	112.54
3	C	134	LEU	N-CA-C	6.60	121.73	112.75
6	F	79	GLN	N-CA-C	6.50	120.81	113.01
3	C	143	GLY	N-CA-C	-6.50	104.62	112.49
4	D	9	SER	N-CA-C	6.50	119.11	108.52
1	A	419	CYS	CA-C-N	6.48	126.43	120.21
1	A	419	CYS	C-N-CA	6.48	126.43	120.21
3	C	107	SER	N-CA-C	-6.48	104.47	112.38
1	A	410	VAL	N-CA-C	6.47	116.51	110.42
3	C	6	ARG	N-CA-C	-6.46	105.04	113.17
4	D	62	LYS	N-CA-C	-6.46	103.93	110.97
2	B	173	ALA	N-CA-C	-6.45	105.16	113.16
5	E	59	VAL	N-CA-C	-6.35	106.75	111.90
1	A	368	HIS	N-CA-C	-6.35	104.23	112.23
4	D	212	MET	N-CA-C	-6.35	103.49	111.11
3	C	129	PHE	N-CA-C	-6.32	104.02	111.03
1	A	88	ALA	N-CA-C	6.29	116.75	107.88
1	A	140	GLU	N-CA-C	-6.25	103.18	111.24
2	B	329	GLN	N-CA-C	-6.22	102.32	110.53
7	G	29	TYR	N-CA-C	-6.22	101.73	110.50
2	B	273	SER	N-CA-C	-6.21	104.50	111.28
3	C	206	SER	N-CA-C	-6.18	102.81	110.41
4	D	139	THR	N-CA-C	6.17	118.51	110.43
4	D	119	ALA	N-CA-C	-6.13	105.08	113.30
1	A	11	VAL	CA-C-N	6.08	126.10	119.90
1	A	11	VAL	C-N-CA	6.08	126.10	119.90
10	J	57	HIS	N-CA-C	6.08	120.77	113.23
3	C	276	LEU	N-CA-C	6.06	118.38	111.11
4	D	110	PRO	CA-C-N	6.05	126.40	119.92
4	D	110	PRO	C-N-CA	6.05	126.40	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	276	ILE	N-CA-C	6.01	116.07	110.42
7	G	32	LYS	N-CA-C	-5.99	106.62	114.04
5	E	44	THR	N-CA-C	-5.98	104.09	111.33
3	C	132	TYR	N-CA-C	-5.96	104.86	111.71
2	B	336	VAL	N-CA-C	5.95	116.61	110.36
1	A	415	ILE	CB-CA-C	-5.92	106.68	111.71
4	D	114	SER	N-CA-C	-5.92	104.80	112.68
3	C	136	TRP	N-CA-C	5.92	119.56	111.39
3	C	104	TYR	CA-CB-CG	-5.90	103.28	113.90
1	A	74	ALA	N-CA-C	5.90	117.38	111.07
3	C	222	HIS	N-CA-C	5.89	122.84	109.81
3	C	253	ASP	CA-C-N	5.89	125.58	119.64
3	C	253	ASP	C-N-CA	5.89	125.58	119.64
10	J	53	LYS	N-CA-C	-5.85	104.91	111.28
2	B	403	ASP	N-CA-C	-5.78	104.67	110.97
5	E	39	VAL	N-CA-C	-5.76	104.71	110.30
3	C	261	ASN	CA-C-N	5.76	125.46	119.82
3	C	261	ASN	C-N-CA	5.76	125.46	119.82
2	B	188	SER	N-CA-C	-5.74	105.11	111.71
3	C	225	TYR	N-CA-C	5.72	119.08	111.75
2	B	54	GLY	N-CA-C	5.67	117.71	110.96
2	B	100	SER	N-CA-C	5.67	118.70	109.06
3	C	35	GLY	N-CA-C	-5.65	99.79	113.18
3	C	37	LEU	N-CA-C	-5.64	105.05	111.14
2	B	231	GLY	N-CA-C	5.61	120.89	113.37
4	D	195	GLU	N-CA-C	5.60	118.06	108.82
5	E	81	ILE	CA-C-N	5.58	125.89	119.92
5	E	81	ILE	C-N-CA	5.58	125.89	119.92
1	A	98	TYR	N-CA-C	5.57	117.87	109.23
2	B	93	GLY	N-CA-C	-5.57	104.38	114.46
3	C	365	ILE	N-CA-C	5.56	120.90	109.34
5	E	80	ASP	N-CA-C	-5.56	105.76	112.54
1	A	390	ILE	CA-C-N	5.53	125.29	119.76
1	A	390	ILE	C-N-CA	5.53	125.29	119.76
3	C	285	ILE	N-CA-C	-5.53	96.94	108.88
4	D	167	ASP	N-CA-C	5.52	119.83	113.38
6	F	29	TYR	N-CA-C	-5.51	106.56	113.28
2	B	402	ILE	N-CA-C	-5.51	105.00	111.00
4	D	186	VAL	CB-CA-C	-5.50	104.93	111.81
3	C	325	LEU	N-CA-C	-5.49	104.69	111.33
1	A	144	SER	N-CA-C	-5.47	101.34	109.11
5	E	103	LYS	N-CA-C	-5.46	105.22	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	183	ILE	N-CA-C	5.46	116.09	110.36
10	J	48	GLU	N-CA-C	5.42	118.20	110.24
3	C	186	LEU	N-CA-C	5.41	120.84	113.16
4	D	227	TRP	N-CA-C	5.39	117.91	111.71
1	A	32	GLN	CA-C-N	5.38	126.56	119.84
1	A	32	GLN	C-N-CA	5.38	126.56	119.84
5	E	99	ARG	N-CA-C	5.38	118.17	109.40
1	A	284	TYR	N-CA-C	5.38	122.25	110.80
2	B	426	ALA	N-CA-C	5.37	117.93	108.75
3	C	36	SER	N-CA-C	-5.34	105.45	111.28
3	C	17	ASN	N-CA-C	-5.33	105.83	114.09
3	C	315	THR	N-CA-C	-5.32	103.87	110.41
4	D	150	ASN	CA-C-N	5.31	125.12	119.28
4	D	150	ASN	C-N-CA	5.31	125.12	119.28
2	B	310	SER	N-CA-C	5.29	116.05	108.74
1	A	89	TYR	N-CA-C	5.29	116.32	108.60
1	A	189	HIS	N-CA-C	5.27	119.98	113.50
1	A	415	ILE	N-CA-C	5.27	116.43	111.48
4	D	83	ARG	CA-C-N	5.27	125.27	119.90
4	D	83	ARG	C-N-CA	5.27	125.27	119.90
5	E	91	TRP	N-CA-C	5.26	116.95	108.32
4	D	215	LEU	CA-C-N	-5.26	116.93	120.24
4	D	215	LEU	C-N-CA	-5.26	116.93	120.24
1	A	310	PHE	N-CA-C	5.26	116.51	108.52
3	C	305	ILE	CA-C-N	5.26	124.92	119.56
3	C	305	ILE	C-N-CA	5.26	124.92	119.56
1	A	264	HIS	N-CA-C	5.24	117.16	109.71
3	C	360	PHE	N-CA-C	5.20	117.62	111.33
1	A	394	GLU	N-CA-C	-5.20	104.54	111.24
4	D	73	GLY	CA-C-N	5.19	125.13	119.78
4	D	73	GLY	C-N-CA	5.19	125.13	119.78
1	A	400	ALA	N-CA-C	-5.18	106.74	113.16
3	C	93	ILE	N-CA-C	-5.17	104.85	110.23
5	E	21	SER	N-CA-C	5.17	121.81	110.80
3	C	154	ILE	CA-C-N	5.15	125.08	119.78
3	C	154	ILE	C-N-CA	5.15	125.08	119.78
1	A	176	LYS	N-CA-C	5.13	120.66	113.02
1	A	439	SER	N-CA-C	-5.12	107.10	113.19
3	C	203	GLU	N-CA-C	-5.10	105.61	111.07
4	D	10	TYR	CA-C-N	5.08	129.62	120.88
4	D	10	TYR	C-N-CA	5.08	129.62	120.88
5	E	92	ARG	N-CA-C	5.08	118.44	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	50	LEU	CA-C-N	5.07	125.07	119.90
6	F	50	LEU	C-N-CA	5.07	125.07	119.90
1	A	42	ASP	N-CA-C	-5.07	104.51	111.81
1	A	106	VAL	CA-C-N	5.06	124.23	118.97
1	A	106	VAL	C-N-CA	5.06	124.23	118.97
4	D	216	VAL	N-CA-CB	5.05	113.68	110.50
5	E	119	ASP	CA-C-N	5.04	126.14	119.84
5	E	119	ASP	C-N-CA	5.04	126.14	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	76	TYR	Sidechain
10	J	59	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3423	0	3286	381	0
2	B	2994	0	2906	359	0
3	C	3002	0	3036	463	0
4	D	1899	0	1822	227	0
5	E	1512	0	1483	183	0
6	F	875	0	839	76	0
7	G	626	0	591	91	0
8	H	490	0	445	62	0
9	I	159	0	46	20	0
10	J	459	0	424	57	0
11	C	86	0	60	19	0
12	C	29	0	33	9	0
13	C	49	0	70	7	0
13	E	49	0	70	4	0
14	C	35	0	42	12	0
15	D	20	0	28	1	0
16	D	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	E	4	0	0	1	0
All	All	15754	0	15211	1768	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (1768) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:TRP:HB2	3:C:175:THR:HB	1.22	1.17
1:A:36:THR:HG22	1:A:100:LYS:HB3	1.22	1.17
2:B:280:GLY:H	2:B:283:PRO:HD2	1.06	1.16
4:D:132:THR:HA	4:D:179:MET:HE2	1.32	1.08
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.36	1.05
10:J:57:HIS:HB2	10:J:61:ASN:C	1.84	1.03
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.39	1.02
7:G:60:THR:HG22	7:G:64:GLN:HE21	1.19	1.01
3:C:354:MET:HE2	3:C:354:MET:HA	1.44	1.00
3:C:52:LEU:HD13	3:C:80:ILE:HG22	1.43	0.99
2:B:337:ILE:HD11	2:B:434:PRO:HD2	1.41	0.99
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.27	0.98
1:A:349:ILE:HG22	1:A:408:ARG:HG3	1.45	0.97
3:C:138:GLN:NE2	3:C:261:ASN:H	1.62	0.97
4:D:158:ILE:HG22	4:D:160:MET:H	1.30	0.96
5:E:16:PRO:HG2	5:E:32:ARG:HH12	1.30	0.96
3:C:166:TRP:HB2	3:C:175:THR:CB	1.95	0.95
3:C:138:GLN:HE21	3:C:260:ALA:HA	1.32	0.95
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.49	0.94
3:C:207:ASN:O	3:C:208:ASN:HB3	1.66	0.93
3:C:327:TRP:HA	3:C:330:VAL:HG12	1.48	0.93
2:B:209:LEU:HG	2:B:379:LEU:HD23	1.51	0.93
3:C:138:GLN:HE22	3:C:261:ASN:H	1.03	0.93
7:G:26:PHE:HD1	7:G:26:PHE:H	1.17	0.92
5:E:13:TYR:O	5:E:14:ARG:HD3	1.69	0.92
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.49	0.92
1:A:297:ILE:HG21	1:A:337:VAL:HG11	1.52	0.91
3:C:43:MET:HA	3:C:43:MET:HE2	1.50	0.91
3:C:107:SER:HB3	11:C:382:HEM:HBD1	1.52	0.91
5:E:101:ARG:HH22	5:E:127:VAL:HG21	1.36	0.91
1:A:245:GLU:HG3	7:G:11:ARG:HG2	1.50	0.91
3:C:202:HIS:CE1	12:C:383:U10:O2	2.24	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:TRP:CB	3:C:175:THR:HB	2.02	0.91
3:C:238:THR:OG1	4:D:212:MET:HG3	1.70	0.90
2:B:280:GLY:N	2:B:283:PRO:HD2	1.85	0.90
4:D:130:LEU:HD11	4:D:158:ILE:HD11	1.52	0.90
3:C:120:LEU:HB3	11:C:382:HEM:HBB2	1.51	0.90
3:C:172:ASP:H	3:C:175:THR:HG23	1.37	0.90
2:B:76:THR:HG22	2:B:82:SER:H	1.37	0.90
5:E:16:PRO:HG2	5:E:32:ARG:NH1	1.87	0.90
1:A:391:PRO:HG2	1:A:394:GLU:HB2	1.53	0.89
5:E:72:SER:O	5:E:196:GLY:HA3	1.69	0.89
1:A:152:TYR:OH	5:E:5:ILE:HD12	1.73	0.88
1:A:250:LEU:HD21	1:A:325:VAL:HG13	1.54	0.88
3:C:261:ASN:HD21	3:C:264:VAL:HG23	1.35	0.88
4:D:224:ARG:HH22	7:G:27:PRO:HG3	1.34	0.88
5:E:9:ASN:ND2	5:E:11:SER:HB3	1.89	0.88
1:A:166:SER:OG	5:E:3:THR:HG23	1.73	0.87
4:D:75:ASN:HB2	4:D:77:ASP:H	1.39	0.87
1:A:250:LEU:C	1:A:250:LEU:HD22	1.98	0.87
4:D:83:ARG:NH1	4:D:86:LYS:HG3	1.89	0.86
1:A:333:ASP:O	1:A:337:VAL:HG23	1.73	0.86
2:B:199:PHE:C	2:B:204:MET:HE3	2.01	0.86
2:B:25:GLU:HB2	2:B:213:HIS:ND1	1.90	0.86
4:D:165:TYR:O	4:D:168:VAL:HG23	1.76	0.85
2:B:122:PHE:O	2:B:126:VAL:HG23	1.77	0.85
3:C:283:ARG:HG3	3:C:283:ARG:O	1.77	0.85
3:C:342:GLN:NE2	3:C:343:PRO:HD2	1.90	0.85
4:D:132:THR:HA	4:D:179:MET:CE	2.07	0.84
2:B:92:VAL:HG11	2:B:115:ASP:HB3	1.57	0.84
2:B:399:LEU:HA	2:B:402:ILE:HG22	1.59	0.84
1:A:281:ASP:HB3	1:A:284:TYR:HE1	1.41	0.84
2:B:280:GLY:H	2:B:283:PRO:CD	1.87	0.83
3:C:272:GLU:OE1	3:C:272:GLU:N	2.10	0.83
5:E:122:HIS:O	5:E:125:GLU:HG2	1.76	0.83
10:J:56:LYS:O	10:J:60:GLU:HB2	1.78	0.83
3:C:142:TRP:CE3	3:C:265:THR:HG22	2.13	0.83
4:D:54:VAL:HG21	4:D:192:TRP:CZ3	2.14	0.83
2:B:154:ASN:O	2:B:157:THR:HG22	1.79	0.82
2:B:258:VAL:HG13	2:B:322:PHE:H	1.44	0.82
5:E:47:VAL:HG21	13:E:198:PEE:H24	1.60	0.82
10:J:57:HIS:O	10:J:61:ASN:N	2.13	0.82
3:C:31:TRP:CZ3	13:C:384:PEE:H17	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:ASN:HB2	6:F:69:ASN:HD22	1.44	0.82
3:C:245:LEU:O	4:D:201:ARG:HD3	1.79	0.82
8:H:47:ARG:HD3	8:H:48:SER:H	1.41	0.82
3:C:317:THR:HG23	13:C:384:PEE:O2P	1.80	0.81
2:B:69:LEU:HD12	2:B:105:MET:HE1	1.59	0.81
3:C:316:MET:HE3	3:C:322:SER:OG	1.81	0.81
3:C:316:MET:SD	3:C:319:ARG:HG3	2.19	0.81
4:D:158:ILE:HG22	4:D:159:GLY:N	1.94	0.81
2:B:62:ASN:C	2:B:62:ASN:HD22	1.89	0.81
2:B:143:GLN:OE1	2:B:146:ILE:HD11	1.80	0.81
5:E:29:ASP:C	5:E:31:SER:H	1.88	0.81
5:E:62:MET:HG3	5:E:63:SER:H	1.46	0.81
5:E:189:SER:OG	5:E:192:MET:HB2	1.81	0.80
1:A:33:PRO:HG2	1:A:34:THR:H	1.46	0.80
2:B:62:ASN:HD22	2:B:63:LEU:N	1.79	0.80
3:C:295:LEU:HD21	14:C:385:SIG:H273	1.63	0.80
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.17	0.80
1:A:56:GLY:HA2	1:A:185:TYR:CE2	2.17	0.80
3:C:120:LEU:CB	11:C:382:HEM:HBB2	2.11	0.79
3:C:342:GLN:HE21	3:C:342:GLN:HA	1.46	0.79
5:E:9:ASN:HD21	5:E:11:SER:HB3	1.46	0.79
1:A:90:SER:O	1:A:167:VAL:HG11	1.83	0.79
1:A:382:GLU:HG2	1:A:389:ARG:HA	1.62	0.79
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.18	0.79
1:A:49:SER:H	1:A:52:ASN:HB3	1.47	0.79
2:B:248:ASN:HD22	2:B:249:GLY:N	1.81	0.79
3:C:325:LEU:CD2	3:C:362:ILE:HG23	2.11	0.79
2:B:357:VAL:HG12	2:B:361:LYS:HD2	1.65	0.78
3:C:325:LEU:HD13	3:C:367:PHE:CD1	2.18	0.78
4:D:75:ASN:HD22	4:D:75:ASN:N	1.82	0.78
1:A:444:LEU:H	1:A:444:LEU:HD12	1.48	0.78
3:C:172:ASP:H	3:C:175:THR:CG2	1.95	0.78
1:A:361:LEU:HD13	1:A:399:LEU:HD22	1.66	0.78
1:A:65:LYS:NZ	9:I:311:UNK:HA	1.99	0.77
6:F:60:PHE:HD1	7:G:13:LEU:HD22	1.48	0.77
1:A:240:GLN:HB3	1:A:422:VAL:HG12	1.67	0.77
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.14	0.77
3:C:319:ARG:NH2	3:C:371:GLY:HA2	2.00	0.77
3:C:327:TRP:HA	3:C:330:VAL:CG1	2.14	0.77
1:A:142:ASP:OD1	5:E:2:HIS:HB3	1.85	0.76
4:D:57:THR:HB	4:D:60:GLU:HB2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.67	0.76
2:B:120:MET:HE2	2:B:219:VAL:HG11	1.67	0.76
3:C:138:GLN:NE2	3:C:261:ASN:N	2.33	0.76
4:D:55:CYS:HG	4:D:56:TYR:HD1	1.33	0.76
4:D:230:LEU:HB3	6:F:70:MET:HE3	1.67	0.76
10:J:57:HIS:HA	10:J:60:GLU:C	2.09	0.76
1:A:42:ASP:HB2	1:A:384:LEU:HD21	1.66	0.76
2:B:24:LEU:HD23	2:B:24:LEU:H	1.50	0.76
4:D:30:PHE:CE2	4:D:64:LEU:HD21	2.20	0.76
7:G:78:VAL:C	7:G:79:ASN:HD22	1.93	0.76
4:D:164:ILE:HD11	4:D:182:VAL:HG22	1.66	0.76
6:F:68:LEU:HD21	6:F:75:LEU:HD13	1.68	0.76
1:A:102:LEU:C	1:A:104:LYS:H	1.94	0.76
2:B:146:ILE:HG13	2:B:147:ASP:N	2.01	0.75
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.67	0.75
2:B:258:VAL:HG12	2:B:259:ALA:N	2.01	0.75
1:A:237:THR:HG23	7:G:22:GLU:HG2	1.69	0.75
2:B:159:VAL:HG21	2:B:254:HIS:HB3	1.66	0.75
4:D:224:ARG:NH2	7:G:27:PRO:HG3	2.00	0.75
1:A:85:HIS:HA	9:I:314:UNK:HG1	1.67	0.75
2:B:260:GLU:O	2:B:261:SER:HB3	1.86	0.75
4:D:165:TYR:CE1	4:D:168:VAL:HG22	2.22	0.75
2:B:258:VAL:HG13	2:B:322:PHE:N	2.01	0.75
4:D:164:ILE:HD11	4:D:182:VAL:HG13	1.68	0.75
1:A:240:GLN:CB	1:A:422:VAL:HG12	2.17	0.74
2:B:341:TYR:OH	2:B:422:LYS:HE3	1.87	0.74
3:C:101:ARG:HD2	3:C:101:ARG:C	2.12	0.74
2:B:257:ILE:O	2:B:323:GLY:HA3	1.87	0.74
3:C:350:ILE:HD13	3:C:350:ILE:N	2.02	0.74
1:A:106:VAL:HG21	1:A:203:VAL:HG13	1.69	0.74
1:A:286:GLY:C	1:A:288:LEU:H	1.93	0.74
1:A:288:LEU:HD13	2:B:83:PHE:HA	1.70	0.74
3:C:73:ASN:O	5:E:66:ALA:HB3	1.88	0.74
7:G:29:TYR:O	7:G:30:PHE:HB2	1.88	0.74
1:A:67:THR:HB	1:A:119:ASN:O	1.86	0.74
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.23	0.73
3:C:131:GLY:HA2	3:C:134:LEU:HD13	1.69	0.73
4:D:225:HIS:HA	7:G:25:PRO:HB3	1.69	0.73
3:C:206:SER:OG	12:C:383:U10:H3M1	1.87	0.73
5:E:10:PHE:O	5:E:11:SER:O	2.05	0.73
1:A:250:LEU:HD21	1:A:325:VAL:CG1	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:VAL:HG22	2:B:119:LEU:HD11	1.68	0.73
3:C:31:TRP:O	3:C:101:ARG:HG3	1.87	0.73
3:C:172:ASP:O	3:C:175:THR:HG23	1.89	0.73
1:A:349:ILE:CG2	1:A:408:ARG:HG3	2.19	0.73
1:A:145:MET:HB2	1:A:252:HIS:NE2	2.03	0.73
2:B:264:ILE:HG12	2:B:316:TYR:O	1.89	0.73
2:B:337:ILE:HD11	2:B:434:PRO:CD	2.19	0.73
1:A:240:GLN:NE2	1:A:242:ARG:HE	1.87	0.72
1:A:153:LEU:HD23	1:A:153:LEU:C	2.13	0.72
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.54	0.72
7:G:29:TYR:HD1	7:G:30:PHE:CD1	2.07	0.72
1:A:252:HIS:HB3	1:A:323:TYR:HE1	1.55	0.72
2:B:243:GLU:OE2	2:B:436:VAL:HG22	1.89	0.72
3:C:350:ILE:HD13	3:C:350:ILE:H	1.53	0.72
5:E:45:LEU:HD11	10:J:28:ALA:HA	1.71	0.72
1:A:88:ALA:HB1	1:A:96:ALA:O	1.89	0.72
2:B:19:PRO:C	2:B:21:PRO:HD3	2.14	0.72
4:D:21:LEU:HD13	4:D:26:ILE:HD11	1.72	0.72
3:C:104:TYR:CZ	3:C:316:MET:HB2	2.24	0.72
3:C:145:THR:O	3:C:149:ASN:HB2	1.90	0.72
5:E:52:LYS:C	5:E:52:LYS:HD3	2.14	0.72
2:B:89:ILE:HD13	2:B:96:LEU:HB2	1.72	0.72
3:C:138:GLN:NE2	3:C:260:ALA:HA	2.05	0.72
3:C:7:LYS:O	3:C:13:LYS:HD2	1.90	0.71
1:A:103:SER:C	1:A:105:ASP:H	1.97	0.71
3:C:120:LEU:CG	11:C:382:HEM:HBB2	2.20	0.71
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.19	0.71
1:A:35:CYS:HA	1:A:372:THR:HG21	1.72	0.71
1:A:250:LEU:HD13	1:A:250:LEU:N	2.05	0.71
3:C:142:TRP:CD2	3:C:265:THR:HG22	2.26	0.71
5:E:16:PRO:CG	5:E:32:ARG:HH12	2.02	0.71
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.72	0.71
2:B:273:SER:O	2:B:276:GLN:HB3	1.90	0.71
1:A:178:SER:HB2	1:A:181:ASP:OD1	1.91	0.71
1:A:291:SER:HB2	1:A:356:ARG:NH2	2.05	0.71
2:B:46:THR:HG22	2:B:110:GLU:HB2	1.72	0.71
2:B:250:ASP:O	2:B:252:LEU:HD23	1.89	0.71
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.73	0.71
3:C:226:SER:O	3:C:230:ILE:HG13	1.90	0.71
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.21	0.71
5:E:71:MET:O	5:E:73:LYS:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:C	1:A:21:ASN:H	1.97	0.71
1:A:349:ILE:HG22	1:A:408:ARG:CG	2.21	0.70
2:B:169:ARG:O	2:B:170:ASN:HB3	1.90	0.70
2:B:109:VAL:HG13	2:B:119:LEU:HD21	1.72	0.70
3:C:378:LEU:O	3:C:379:ASN:HB2	1.91	0.70
4:D:32:VAL:HG11	4:D:186:VAL:HG22	1.73	0.70
1:A:291:SER:O	1:A:292:SER:C	2.34	0.70
6:F:31:LEU:HD23	6:F:31:LEU:H	1.57	0.70
3:C:127:THR:HG22	3:C:186:LEU:HB3	1.72	0.70
3:C:327:TRP:CE3	3:C:330:VAL:HG11	2.26	0.70
2:B:62:ASN:C	2:B:62:ASN:ND2	2.48	0.70
3:C:12:LEU:HD23	3:C:12:LEU:O	1.91	0.70
1:A:45:SER:HA	1:A:48:GLU:HG3	1.72	0.69
1:A:276:ILE:CD1	1:A:349:ILE:HD11	2.23	0.69
3:C:261:ASN:HD21	3:C:264:VAL:CG2	2.02	0.69
5:E:140:THR:OG1	5:E:177:PRO:HD2	1.90	0.69
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.22	0.69
5:E:62:MET:HG3	5:E:63:SER:N	2.06	0.69
2:B:286:LYS:CB	2:B:343:GLN:HG3	2.23	0.69
3:C:319:ARG:CZ	3:C:374:GLU:HB2	2.22	0.69
2:B:128:THR:C	2:B:130:PRO:HD3	2.17	0.69
3:C:70:THR:HA	3:C:74:VAL:HG23	1.74	0.69
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.75	0.69
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.27	0.69
3:C:325:LEU:HD11	3:C:366:LEU:HB3	1.74	0.69
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.75	0.69
3:C:13:LYS:O	3:C:17:ASN:HB2	1.93	0.69
2:B:166:ALA:HB1	2:B:242:GLY:C	2.18	0.68
3:C:120:LEU:HG	11:C:382:HEM:HBB2	1.75	0.68
8:H:17:LEU:HD11	8:H:21:ARG:NE	2.07	0.68
3:C:27:ASN:HB2	6:F:69:ASN:ND2	2.07	0.68
3:C:222:HIS:O	3:C:223:PRO:C	2.34	0.68
8:H:17:LEU:HD11	8:H:21:ARG:HE	1.57	0.68
1:A:102:LEU:HD12	1:A:102:LEU:H	1.58	0.68
4:D:28:ARG:HD2	4:D:171:PHE:CE2	2.28	0.68
1:A:102:LEU:HD12	1:A:102:LEU:N	2.08	0.68
10:J:54:HIS:O	10:J:57:HIS:CD2	2.47	0.68
1:A:4:TYR:O	1:A:7:ALA:N	2.26	0.68
1:A:388:ARG:H	1:A:388:ARG:HD3	1.58	0.68
5:E:29:ASP:O	5:E:32:ARG:N	2.26	0.68
1:A:65:LYS:HZ2	9:I:311:UNK:HA	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:SER:O	2:B:85:ILE:HG22	1.94	0.68
3:C:27:ASN:ND2	3:C:208:ASN:OD1	2.23	0.68
4:D:102:ARG:NH1	4:D:109:LEU:HB2	2.08	0.68
3:C:104:TYR:CE2	3:C:316:MET:HB2	2.29	0.68
3:C:120:LEU:HB3	11:C:382:HEM:CBB	2.22	0.68
8:H:73:LEU:O	8:H:73:LEU:HD23	1.94	0.68
2:B:162:ASN:HB3	2:B:244:ILE:HD11	1.75	0.67
3:C:142:TRP:CZ3	3:C:265:THR:HG22	2.29	0.67
1:A:156:THR:HA	5:E:7:VAL:HG21	1.75	0.67
4:D:83:ARG:HH12	4:D:86:LYS:HG3	1.59	0.67
3:C:348:PHE:O	3:C:350:ILE:N	2.28	0.67
6:F:16:ILE:O	6:F:19:TRP:HB3	1.94	0.67
1:A:36:THR:HG22	1:A:100:LYS:CB	2.14	0.67
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.29	0.67
1:A:382:GLU:HG2	1:A:389:ARG:HD2	1.75	0.67
1:A:354:VAL:HG11	1:A:404:ALA:HA	1.76	0.67
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.30	0.67
5:E:160:CYS:HB2	17:E:197:FES:S2	2.35	0.67
1:A:399:LEU:C	1:A:399:LEU:HD12	2.19	0.66
1:A:438:ARG:O	1:A:438:ARG:HD3	1.96	0.66
2:B:168:TYR:CE2	2:B:172:LEU:HD23	2.30	0.66
6:F:59:MET:HA	6:F:59:MET:CE	2.25	0.66
8:H:35:GLU:O	8:H:39:LEU:HD13	1.95	0.66
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.59	0.66
3:C:245:LEU:O	4:D:201:ARG:CD	2.44	0.66
3:C:350:ILE:H	3:C:350:ILE:CD1	2.08	0.66
2:B:56:ARG:NH2	2:B:318:ASP:OD2	2.29	0.66
2:B:370:MET:O	2:B:373:GLU:HG3	1.96	0.66
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.78	0.66
1:A:307:PHE:CD1	1:A:307:PHE:C	2.73	0.66
5:E:43:THR:O	5:E:47:VAL:HG23	1.94	0.66
8:H:69:VAL:O	8:H:73:LEU:HB2	1.95	0.66
2:B:96:LEU:HD23	2:B:97:SER:N	2.10	0.66
3:C:123:THR:O	3:C:127:THR:HG23	1.96	0.66
3:C:131:GLY:CA	3:C:134:LEU:HD13	2.25	0.66
1:A:243:HIS:O	1:A:425:PRO:HA	1.96	0.66
1:A:433:ASP:OD1	1:A:436:ARG:HG2	1.96	0.66
2:B:19:PRO:C	2:B:21:PRO:CD	2.69	0.66
3:C:133:VAL:CG1	3:C:144:ALA:HB2	2.24	0.66
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.77	0.66
3:C:146:VAL:HG23	3:C:147:ILE:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:93:GLY:O	5:E:94:LYS:HE3	1.96	0.66
10:J:13:LEU:HD12	10:J:13:LEU:N	2.11	0.66
3:C:222:HIS:HB3	3:C:223:PRO:HD2	1.78	0.65
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.30	0.65
4:D:180:SER:HB3	8:H:15:ASP:OD1	1.96	0.65
1:A:297:ILE:CG2	1:A:337:VAL:HG11	2.25	0.65
4:D:75:ASN:ND2	4:D:79:GLU:O	2.27	0.65
10:J:59:TYR:O	10:J:60:GLU:HG3	1.96	0.65
1:A:94:HIS:NE2	1:A:381:ARG:HG2	2.11	0.65
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.09	0.65
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.31	0.65
1:A:252:HIS:HD1	1:A:325:VAL:HG22	1.61	0.65
2:B:379:LEU:O	2:B:379:LEU:HD13	1.96	0.65
3:C:131:GLY:O	3:C:134:LEU:HB2	1.96	0.65
4:D:153:PHE:CG	4:D:158:ILE:HG12	2.31	0.65
10:J:55:ILE:O	10:J:57:HIS:N	2.29	0.65
2:B:61:SER:O	2:B:62:ASN:ND2	2.29	0.65
3:C:9:HIS:HB3	3:C:12:LEU:HB3	1.77	0.65
1:A:106:VAL:O	1:A:110:VAL:HG23	1.97	0.65
3:C:282:LEU:HD13	3:C:282:LEU:O	1.95	0.65
5:E:16:PRO:O	5:E:18:ASP:N	2.25	0.65
5:E:26:ARG:O	5:E:27:GLU:HG3	1.96	0.65
1:A:159:GLN:HE21	5:E:7:VAL:HG11	1.62	0.65
2:B:137:VAL:HG23	2:B:138:ALA:N	2.11	0.65
2:B:272:PHE:O	2:B:276:GLN:N	2.29	0.65
1:A:403:ASP:OD2	1:A:405:ARG:HB3	1.97	0.65
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.79	0.65
2:B:101:THR:HG22	2:B:102:ARG:N	2.12	0.65
4:D:186:VAL:O	4:D:189:PHE:HB3	1.96	0.65
10:J:42:ILE:O	10:J:46:ILE:HG13	1.97	0.65
1:A:343:MET:HE2	1:A:343:MET:HA	1.80	0.64
2:B:385:GLN:O	2:B:387:LEU:N	2.30	0.64
3:C:233:LEU:CD1	3:C:237:LEU:HD22	2.27	0.64
2:B:170:ASN:ND2	2:B:170:ASN:C	2.55	0.64
3:C:235:LEU:O	3:C:239:PRO:HD3	1.98	0.64
4:D:43:MET:HE2	4:D:91:PHE:HE2	1.61	0.64
8:H:73:LEU:HD23	8:H:73:LEU:C	2.22	0.64
1:A:100:LYS:HE3	2:B:370:MET:CE	2.27	0.64
1:A:286:GLY:C	1:A:288:LEU:N	2.56	0.64
1:A:293:PRO:O	1:A:297:ILE:N	2.26	0.64
3:C:301:ILE:HD11	3:C:364:LEU:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:THR:HG21	1:A:235:ARG:H	1.61	0.64
3:C:349:ILE:HG22	3:C:350:ILE:HD13	1.79	0.64
4:D:44:ASP:O	4:D:90:TYR:HD2	1.80	0.64
1:A:291:SER:O	1:A:293:PRO:N	2.31	0.64
4:D:75:ASN:N	4:D:75:ASN:ND2	2.42	0.64
4:D:182:VAL:O	4:D:186:VAL:HG23	1.96	0.64
1:A:250:LEU:C	1:A:250:LEU:CD2	2.71	0.64
1:A:389:ARG:HD2	1:A:390:ILE:H	1.63	0.64
2:B:76:THR:CG2	2:B:82:SER:H	2.11	0.64
3:C:36:SER:O	3:C:40:VAL:HG23	1.97	0.64
3:C:347:PRO:HG3	7:G:66:PHE:CD1	2.32	0.64
3:C:354:MET:HA	3:C:354:MET:CE	2.22	0.64
2:B:33:LEU:HD21	2:B:223:LEU:HD23	1.80	0.64
3:C:130:VAL:HG12	3:C:183:HIS:HB2	1.79	0.64
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.79	0.64
6:F:12:TRP:HA	6:F:12:TRP:CE3	2.32	0.64
1:A:15:GLN:HB3	1:A:205:HIS:ND1	2.13	0.64
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.27	0.64
3:C:20:ILE:O	3:C:21:ASP:HB2	1.97	0.64
3:C:261:ASN:ND2	3:C:264:VAL:HG23	2.11	0.64
4:D:75:ASN:ND2	4:D:75:ASN:H	1.96	0.64
4:D:102:ARG:HH11	4:D:109:LEU:HB2	1.62	0.64
4:D:178:THR:O	4:D:182:VAL:HG12	1.98	0.64
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.80	0.64
2:B:258:VAL:HG12	2:B:259:ALA:H	1.63	0.64
5:E:29:ASP:O	5:E:31:SER:N	2.30	0.64
2:B:361:LYS:O	2:B:365:LYS:HG3	1.98	0.64
3:C:282:LEU:HD23	3:C:295:LEU:HB2	1.80	0.64
5:E:16:PRO:HD3	7:G:22:GLU:O	1.98	0.64
1:A:443:TRP:C	1:A:445:ARG:H	2.06	0.63
4:D:218:LEU:O	4:D:222:MET:HG3	1.98	0.63
1:A:146:ARG:HH21	9:I:206:UNK:CB	2.12	0.63
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.62	0.63
2:B:217:LYS:C	2:B:219:VAL:H	2.07	0.63
3:C:148:THR:HG21	3:C:166:TRP:CE3	2.33	0.63
5:E:113:GLU:OE2	5:E:116:GLN:HG3	1.98	0.63
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.62	0.63
3:C:238:THR:OG1	4:D:212:MET:CG	2.44	0.63
4:D:165:TYR:CD1	4:D:168:VAL:HG22	2.33	0.63
1:A:382:GLU:OE2	1:A:390:ILE:HB	1.98	0.63
1:A:436:ARG:HD3	3:C:223:PRO:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.28	0.63
1:A:61:HIS:HD2	1:A:134:ILE:HG12	1.63	0.63
1:A:102:LEU:O	1:A:104:LYS:N	2.31	0.63
1:A:290:SER:O	1:A:291:SER:C	2.42	0.63
3:C:113:THR:HG21	3:C:201:LEU:HA	1.81	0.63
4:D:54:VAL:HG11	4:D:192:TRP:CH2	2.33	0.63
5:E:5:ILE:HD13	7:G:14:ILE:CD1	2.29	0.63
7:G:60:THR:HG22	7:G:64:GLN:NE2	2.03	0.63
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.34	0.63
2:B:248:ASN:HD22	2:B:248:ASN:C	2.04	0.63
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.13	0.63
1:A:235:ARG:HD3	5:E:21:SER:H	1.64	0.63
1:A:245:GLU:HG2	1:A:247:GLY:H	1.64	0.63
2:B:258:VAL:CG1	2:B:322:PHE:H	2.10	0.63
5:E:101:ARG:NH2	5:E:127:VAL:HG21	2.13	0.63
4:D:218:LEU:HD11	5:E:42:VAL:HG12	1.80	0.62
3:C:61:SER:C	3:C:62:LEU:HD22	2.23	0.62
3:C:253:ASP:OD1	3:C:255:GLU:N	2.31	0.62
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.34	0.62
10:J:59:TYR:N	10:J:59:TYR:CD1	2.67	0.62
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.35	0.62
5:E:5:ILE:HD13	7:G:14:ILE:HD13	1.82	0.62
5:E:62:MET:O	5:E:64:ALA:O	2.17	0.62
1:A:444:LEU:O	1:A:445:ARG:O	2.17	0.62
3:C:16:ASN:OD1	3:C:16:ASN:O	2.16	0.62
1:A:15:GLN:HB3	1:A:205:HIS:CE1	2.35	0.62
2:B:228:GLY:O	2:B:229:GLY:C	2.42	0.62
2:B:243:GLU:CD	2:B:436:VAL:HG22	2.24	0.62
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.64	0.62
3:C:18:SER:C	3:C:19:LEU:HD12	2.24	0.62
3:C:27:ASN:HD22	6:F:69:ASN:ND2	1.97	0.62
3:C:325:LEU:HD13	3:C:367:PHE:HD1	1.65	0.62
4:D:95:TYR:HE2	4:D:104:ALA:HB3	1.63	0.62
7:G:71:ARG:NE	8:H:56:GLU:OE2	2.32	0.62
2:B:258:VAL:HG11	2:B:321:LEU:CB	2.28	0.62
3:C:52:LEU:HD13	3:C:80:ILE:CG2	2.25	0.62
1:A:295:ALA:O	1:A:298:ALA:HB3	2.00	0.62
3:C:325:LEU:HD22	3:C:362:ILE:HG23	1.81	0.62
3:C:373:LEU:HD23	3:C:373:LEU:C	2.24	0.62
7:G:29:TYR:HA	7:G:33:GLY:HA3	1.80	0.62
10:J:57:HIS:HB2	10:J:61:ASN:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:O	1:A:26:ALA:HA	2.01	0.61
1:A:86:LEU:HD13	1:A:99:ILE:HG13	1.82	0.61
1:A:151:ASN:ND2	5:E:2:HIS:NE2	2.48	0.61
6:F:59:MET:HA	6:F:59:MET:HE3	1.81	0.61
8:H:66:ASP:HA	8:H:69:VAL:CG2	2.30	0.61
2:B:280:GLY:C	2:B:282:ASN:N	2.56	0.61
4:D:158:ILE:CG2	4:D:159:GLY:N	2.63	0.61
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.35	0.61
1:A:85:HIS:O	1:A:99:ILE:HA	2.00	0.61
1:A:297:ILE:HG22	1:A:303:LEU:HD11	1.82	0.61
3:C:43:MET:HA	3:C:43:MET:CE	2.27	0.61
3:C:377:MET:CE	6:F:20:TYR:HB2	2.26	0.61
6:F:60:PHE:CD1	7:G:13:LEU:HD22	2.33	0.61
1:A:267:LEU:O	1:A:271:GLN:HB2	2.01	0.61
4:D:144:ARG:HG3	4:D:147:LEU:HD23	1.83	0.61
2:B:38:LEU:HD23	2:B:378:PHE:HZ	1.64	0.61
5:E:32:ARG:C	5:E:32:ARG:HD3	2.26	0.61
2:B:276:GLN:OE1	2:B:313:ASN:HB3	2.00	0.61
3:C:71:CYS:SG	3:C:81:ARG:HD3	2.40	0.61
3:C:101:ARG:C	3:C:101:ARG:CD	2.74	0.61
3:C:362:ILE:HA	3:C:366:LEU:HD23	1.82	0.61
4:D:79:GLU:O	4:D:80:MET:C	2.44	0.61
1:A:106:VAL:N	1:A:107:PRO:HD2	2.16	0.61
4:D:5:LEU:HB2	8:H:59:PHE:CD1	2.36	0.61
10:J:57:HIS:HB2	10:J:61:ASN:CA	2.30	0.61
6:F:12:TRP:HA	6:F:12:TRP:HE3	1.65	0.61
7:G:57:LEU:HD22	7:G:57:LEU:H	1.65	0.61
7:G:77:TYR:CE1	8:H:52:GLU:HB2	2.35	0.61
1:A:293:PRO:O	1:A:294:LEU:C	2.44	0.60
1:A:264:HIS:HD2	1:A:266:ASP:HB2	1.65	0.60
3:C:201:LEU:O	3:C:204:SER:O	2.19	0.60
8:H:47:ARG:HD3	8:H:48:SER:N	2.15	0.60
1:A:235:ARG:HB2	5:E:21:SER:HA	1.84	0.60
2:B:96:LEU:HD23	2:B:96:LEU:C	2.25	0.60
3:C:344:VAL:HG23	3:C:344:VAL:O	2.00	0.60
4:D:21:LEU:HD13	4:D:26:ILE:CD1	2.30	0.60
4:D:130:LEU:HD11	4:D:158:ILE:CD1	2.29	0.60
10:J:57:HIS:CE1	10:J:62:LYS:C	2.79	0.60
1:A:255:ILE:HA	1:A:421:ALA:O	2.02	0.60
2:B:162:ASN:HB3	2:B:244:ILE:CD1	2.31	0.60
3:C:198:LEU:HD13	12:C:383:U10:H1M2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:ILE:CD1	3:C:364:LEU:HD11	2.31	0.60
3:C:319:ARG:HH22	3:C:371:GLY:HA2	1.64	0.60
10:J:13:LEU:HA	10:J:19:THR:CG2	2.31	0.60
1:A:436:ARG:HD3	3:C:223:PRO:CD	2.31	0.60
2:B:100:SER:OG	2:B:105:MET:HG2	2.01	0.60
2:B:399:LEU:CA	2:B:402:ILE:HG22	2.32	0.60
3:C:222:HIS:HB3	3:C:223:PRO:CD	2.31	0.60
4:D:117:VAL:HG12	4:D:191:ARG:NH2	2.16	0.60
10:J:55:ILE:C	10:J:57:HIS:H	2.09	0.60
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.47	0.60
2:B:426:ALA:HB1	2:B:430:LEU:HD21	1.83	0.60
3:C:319:ARG:NH1	3:C:374:GLU:HB2	2.16	0.60
5:E:148:ALA:O	5:E:149:ASN:HB2	2.02	0.60
5:E:163:SER:OG	5:E:175:PRO:HD2	2.00	0.60
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.69	0.60
3:C:3:PRO:HG2	3:C:4:ASN:H	1.67	0.60
3:C:147:ILE:O	3:C:150:LEU:HB3	2.01	0.60
3:C:307:PHE:N	3:C:307:PHE:CD1	2.69	0.60
1:A:40:TRP:CH2	1:A:377:GLU:HA	2.35	0.60
2:B:132:PHE:CE2	2:B:191:LEU:HB3	2.37	0.60
2:B:137:VAL:CG2	2:B:138:ALA:N	2.65	0.60
4:D:78:GLY:O	4:D:79:GLU:HG3	2.02	0.60
1:A:64:PHE:CE1	1:A:86:LEU:HG	2.37	0.59
2:B:128:THR:HG21	2:B:223:LEU:HD12	1.84	0.59
3:C:342:GLN:NE2	3:C:342:GLN:HA	2.16	0.59
5:E:106:ILE:HG12	5:E:130:PRO:O	2.02	0.59
1:A:145:MET:CB	1:A:252:HIS:CD2	2.84	0.59
2:B:101:THR:HB	2:B:104:ASN:OD1	2.02	0.59
2:B:109:VAL:HG13	2:B:119:LEU:CD2	2.31	0.59
3:C:377:MET:HE2	6:F:20:TYR:CB	2.28	0.59
5:E:184:SER:O	5:E:196:GLY:N	2.29	0.59
8:H:57:GLU:CD	8:H:57:GLU:H	2.11	0.59
1:A:46:ARG:HD2	1:A:163:LEU:HD21	1.83	0.59
2:B:58:GLU:HB3	2:B:62:ASN:HD21	1.67	0.59
2:B:95:LYS:HB2	2:B:110:GLU:HG2	1.84	0.59
2:B:150:VAL:O	2:B:153:GLN:HG3	2.02	0.59
2:B:368:TYR:O	2:B:372:VAL:HG23	2.00	0.59
4:D:32:VAL:O	4:D:36:VAL:HG13	2.02	0.59
5:E:65:SER:C	5:E:67:ASP:H	2.10	0.59
2:B:241:GLY:HA3	2:B:421:GLN:HE21	1.67	0.59
3:C:107:SER:CB	11:C:382:HEM:HBD1	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:50:PRO:HG2	7:G:51:PRO:HD2	1.82	0.59
3:C:230:ILE:HG21	13:E:198:PEE:H26	1.84	0.59
4:D:30:PHE:HE2	4:D:64:LEU:HD21	1.65	0.59
3:C:149:ASN:O	3:C:152:SER:HB3	2.03	0.59
3:C:289:LEU:HG	3:C:293:LEU:CD2	2.33	0.59
5:E:81:ILE:HD13	5:E:98:VAL:HG12	1.84	0.59
1:A:378:ASP:O	1:A:382:GLU:HB2	2.02	0.59
2:B:402:ILE:HD13	2:B:402:ILE:C	2.27	0.59
3:C:289:LEU:HG	3:C:293:LEU:HD23	1.83	0.59
4:D:158:ILE:HG22	4:D:159:GLY:H	1.67	0.59
4:D:164:ILE:HD11	4:D:182:VAL:CG2	2.32	0.59
10:J:57:HIS:CA	10:J:60:GLU:C	2.74	0.59
4:D:211:MET:HG3	15:D:242:BOG:H5'1	1.85	0.59
3:C:272:GLU:H	3:C:272:GLU:CD	1.96	0.59
4:D:149:PHE:CE1	4:D:156:GLN:HB3	2.38	0.59
5:E:26:ARG:C	5:E:28:SER:H	2.10	0.59
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.03	0.59
1:A:288:LEU:HD13	2:B:83:PHE:CA	2.32	0.59
2:B:166:ALA:HB1	2:B:242:GLY:HA3	1.85	0.59
2:B:255:ALA:O	2:B:325:TYR:HA	2.02	0.59
3:C:238:THR:CG2	4:D:212:MET:HG3	2.32	0.59
5:E:9:ASN:ND2	5:E:11:SER:H	2.01	0.59
5:E:45:LEU:O	5:E:48:ALA:HB3	2.03	0.59
1:A:85:HIS:CA	9:I:314:UNK:HG1	2.33	0.58
3:C:27:ASN:HD22	6:F:69:ASN:HD22	1.50	0.58
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.84	0.58
2:B:109:VAL:CG2	2:B:119:LEU:HD11	2.33	0.58
3:C:271:PRO:HB3	14:C:385:SIG:C2	2.33	0.58
3:C:321:LEU:HD12	3:C:374:GLU:HG2	1.85	0.58
4:D:95:TYR:CE2	4:D:101:ALA:HA	2.38	0.58
4:D:134:TYR:O	4:D:135:CYS:HB3	2.03	0.58
4:D:230:LEU:HB3	6:F:70:MET:CE	2.34	0.58
5:E:11:SER:OG	5:E:12:ASP:N	2.36	0.58
1:A:103:SER:C	1:A:105:ASP:N	2.59	0.58
2:B:101:THR:HG22	2:B:102:ARG:H	1.68	0.58
3:C:283:ARG:O	3:C:284:SER:HB3	2.03	0.58
4:D:224:ARG:NH1	7:G:25:PRO:O	2.36	0.58
6:F:61:ARG:HH11	6:F:61:ARG:HG3	1.68	0.58
2:B:170:ASN:C	2:B:170:ASN:HD22	2.11	0.58
1:A:146:ARG:NH2	9:I:206:UNK:CB	2.67	0.58
1:A:291:SER:HB2	1:A:356:ARG:HH22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ARG:HG3	2:B:114:ASP:N	2.19	0.58
1:A:153:LEU:CD2	1:A:319:LEU:HD13	2.33	0.58
1:A:242:ARG:O	7:G:14:ILE:HA	2.03	0.58
1:A:391:PRO:CG	1:A:394:GLU:HB2	2.29	0.58
2:B:397:THR:HA	2:B:400:GLN:HB3	1.86	0.58
3:C:6:ARG:HA	3:C:12:LEU:HD22	1.85	0.58
3:C:78:TRP:CG	4:D:197:GLU:HG2	2.37	0.58
7:G:25:PRO:O	7:G:26:PHE:C	2.47	0.58
1:A:272:VAL:O	1:A:275:ALA:HB3	2.03	0.58
1:A:351:GLU:O	1:A:354:VAL:HG22	2.03	0.58
10:J:55:ILE:C	10:J:57:HIS:N	2.62	0.58
1:A:85:HIS:CB	9:I:314:UNK:HG1	2.33	0.58
1:A:250:LEU:N	1:A:250:LEU:CD1	2.66	0.58
2:B:357:VAL:HG12	2:B:361:LYS:CD	2.33	0.58
4:D:181:GLN:HG2	8:H:77:LEU:HD22	1.84	0.58
6:F:18:LYS:O	6:F:22:ASN:ND2	2.37	0.58
3:C:332:ASN:HD21	3:C:359:TYR:CA	2.16	0.58
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.03	0.57
2:B:193:ASP:O	2:B:197:ASN:ND2	2.37	0.57
3:C:104:TYR:O	3:C:105:TYR:CD2	2.57	0.57
4:D:233:ARG:O	6:F:71:ARG:NH2	2.37	0.57
2:B:199:PHE:CA	2:B:204:MET:HE3	2.33	0.57
2:B:285:VAL:O	2:B:285:VAL:HG12	2.03	0.57
3:C:3:PRO:O	3:C:5:ILE:HG13	2.04	0.57
3:C:307:PHE:N	3:C:307:PHE:HD1	2.02	0.57
3:C:346:HIS:N	3:C:347:PRO:HD2	2.19	0.57
2:B:400:GLN:O	2:B:404:ALA:HB2	2.05	0.57
3:C:92:PHE:CZ	3:C:124:LEU:HD13	2.39	0.57
3:C:323:GLN:HE21	7:G:47:ARG:HD3	1.69	0.57
1:A:45:SER:HA	1:A:48:GLU:CG	2.35	0.57
1:A:75:LEU:O	1:A:79:VAL:HG23	2.05	0.57
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.04	0.57
2:B:402:ILE:HD13	2:B:402:ILE:O	2.04	0.57
3:C:370:ILE:O	3:C:374:GLU:HG3	2.04	0.57
5:E:85:LYS:HG2	5:E:86:ASN:N	2.19	0.57
6:F:101:ARG:HA	6:F:104:ARG:HE	1.69	0.57
3:C:325:LEU:HD21	3:C:362:ILE:HG23	1.87	0.57
4:D:218:LEU:HD22	5:E:39:VAL:HG13	1.86	0.57
4:D:233:ARG:HB3	6:F:71:ARG:HH21	1.70	0.57
10:J:21:ALA:O	10:J:24:ILE:N	2.37	0.57
3:C:206:SER:OG	12:C:383:U10:C3M	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:32:LYS:C	7:G:35:PRO:HD2	2.29	0.57
2:B:258:VAL:CG1	2:B:259:ALA:N	2.68	0.57
3:C:43:MET:O	3:C:44:THR:C	2.48	0.57
4:D:28:ARG:HD2	4:D:171:PHE:CD2	2.40	0.57
4:D:212:MET:O	4:D:216:VAL:HG22	2.04	0.57
5:E:9:ASN:HD21	5:E:11:SER:CB	2.18	0.57
5:E:109:GLU:CG	5:E:167:ALA:HB3	2.35	0.57
10:J:57:HIS:C	10:J:60:GLU:H	2.13	0.57
1:A:250:LEU:HD13	1:A:250:LEU:H	1.67	0.57
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.68	0.57
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.86	0.57
2:B:219:VAL:C	2:B:221:GLU:H	2.13	0.57
2:B:250:ASP:C	2:B:252:LEU:H	2.13	0.57
6:F:31:LEU:HD23	6:F:31:LEU:N	2.18	0.57
1:A:159:GLN:NE2	5:E:7:VAL:HG11	2.19	0.56
3:C:28:ILE:HG23	3:C:32:TRP:HB2	1.87	0.56
10:J:13:LEU:N	10:J:13:LEU:CD1	2.68	0.56
1:A:152:TYR:CZ	5:E:5:ILE:HD12	2.38	0.56
1:A:343:MET:O	1:A:347:THR:HG22	2.05	0.56
2:B:213:HIS:N	2:B:214:PRO:HD2	2.20	0.56
5:E:45:LEU:CD1	10:J:28:ALA:HA	2.34	0.56
1:A:45:SER:HA	1:A:48:GLU:CD	2.29	0.56
1:A:59:LEU:HD11	1:A:186:LEU:HD11	1.87	0.56
1:A:72:GLN:O	1:A:73:ASN:C	2.47	0.56
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.86	0.56
1:A:250:LEU:CD2	1:A:325:VAL:HG13	2.31	0.56
1:A:270:LEU:HG	1:A:320:PHE:CE2	2.40	0.56
2:B:76:THR:HG22	2:B:82:SER:N	2.13	0.56
2:B:202:ALA:HB3	2:B:229:GLY:HA2	1.85	0.56
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.40	0.56
2:B:385:GLN:CD	2:B:392:TYR:HA	2.29	0.56
2:B:405:VAL:HG12	2:B:406:ALA:N	2.19	0.56
3:C:182:LEU:HD22	14:C:385:SIG:H381	1.87	0.56
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.87	0.56
3:C:282:LEU:HD13	3:C:282:LEU:C	2.29	0.56
3:C:342:GLN:HB3	3:C:348:PHE:CE2	2.41	0.56
3:C:358:SER:O	3:C:362:ILE:HG13	2.05	0.56
3:C:366:LEU:H	3:C:366:LEU:HD22	1.70	0.56
5:E:153:PHE:HD2	5:E:172:ARG:NH1	2.04	0.56
1:A:250:LEU:HB2	1:A:326:CYS:O	2.06	0.56
3:C:22:LEU:HD21	12:C:383:U10:H3M2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:TYR:CD1	3:C:209:PRO:HA	2.40	0.56
4:D:178:THR:OG1	4:D:181:GLN:HB2	2.05	0.56
3:C:223:PRO:O	3:C:227:PHE:HD2	1.87	0.56
5:E:26:ARG:O	5:E:28:SER:N	2.31	0.56
9:I:310:UNK:O	9:I:311:UNK:C	2.53	0.56
1:A:23:VAL:HG23	1:A:192:ALA:CB	2.36	0.56
2:B:111:CYS:O	2:B:112:LEU:HB3	2.06	0.56
2:B:143:GLN:OE1	2:B:146:ILE:CD1	2.53	0.56
2:B:169:ARG:O	2:B:170:ASN:CB	2.53	0.56
5:E:60:SER:C	5:E:62:MET:H	2.14	0.56
5:E:94:LYS:HE2	5:E:94:LYS:HA	1.87	0.56
3:C:319:ARG:NH2	3:C:374:GLU:OE2	2.38	0.56
4:D:153:PHE:CD2	4:D:158:ILE:HG12	2.41	0.56
1:A:159:GLN:OE1	5:E:15:ARG:NH2	2.35	0.56
2:B:132:PHE:CD2	2:B:191:LEU:HB3	2.41	0.56
3:C:133:VAL:HG11	3:C:144:ALA:HB2	1.87	0.56
3:C:293:LEU:O	3:C:296:ALA:HB3	2.06	0.56
4:D:97:ASN:OD1	4:D:99:GLU:HG2	2.06	0.56
4:D:215:LEU:O	4:D:219:VAL:HG22	2.05	0.56
5:E:85:LYS:HG2	5:E:86:ASN:H	1.71	0.56
6:F:84:GLU:CD	6:F:84:GLU:H	2.14	0.56
1:A:145:MET:HB3	1:A:252:HIS:HD2	1.71	0.56
3:C:219:ILE:HD13	4:D:230:LEU:HD11	1.88	0.56
6:F:28:LYS:O	6:F:75:LEU:HB2	2.06	0.56
1:A:108:LYS:HA	1:A:108:LYS:HE3	1.88	0.56
2:B:61:SER:C	2:B:63:LEU:H	2.13	0.56
2:B:113:ARG:O	2:B:116:VAL:HG23	2.06	0.56
2:B:168:TYR:HB2	2:B:173:ALA:CB	2.25	0.56
2:B:272:PHE:HA	2:B:275:LEU:HB3	1.87	0.56
2:B:397:THR:O	2:B:401:GLN:HG2	2.05	0.56
3:C:369:THR:C	3:C:371:GLY:N	2.60	0.56
1:A:346:CYS:HB3	1:A:411:CYS:CB	2.36	0.55
2:B:150:VAL:HG23	2:B:151:ALA:N	2.21	0.55
3:C:104:TYR:CZ	3:C:316:MET:CB	2.88	0.55
3:C:261:ASN:ND2	3:C:264:VAL:CG2	2.67	0.55
4:D:55:CYS:SG	4:D:56:TYR:HD1	2.29	0.55
5:E:171:ILE:HD12	5:E:172:ARG:H	1.71	0.55
10:J:13:LEU:HA	10:J:19:THR:HG21	1.87	0.55
1:A:145:MET:HA	1:A:148:VAL:CG1	2.35	0.55
1:A:366:VAL:C	1:A:368:HIS:H	2.14	0.55
2:B:409:ASP:O	2:B:411:ILE:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:ASN:O	3:C:5:ILE:HB	2.05	0.55
3:C:166:TRP:C	3:C:166:TRP:CD1	2.84	0.55
3:C:233:LEU:O	3:C:237:LEU:HB2	2.05	0.55
3:C:278:ALA:HB1	3:C:295:LEU:HD11	1.86	0.55
4:D:192:TRP:CD1	4:D:193:ALA:N	2.75	0.55
1:A:391:PRO:O	1:A:394:GLU:N	2.38	0.55
2:B:130:PRO:HB3	2:B:132:PHE:CE1	2.42	0.55
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.37	0.55
9:I:313:UNK:CB	9:I:314:UNK:CD	2.84	0.55
1:A:266:ASP:C	1:A:268:VAL:N	2.63	0.55
1:A:438:ARG:HD3	1:A:438:ARG:C	2.32	0.55
2:B:399:LEU:HA	2:B:402:ILE:CG2	2.32	0.55
3:C:283:ARG:O	3:C:283:ARG:CG	2.51	0.55
6:F:12:TRP:HB3	6:F:15:GLY:H	1.71	0.55
8:H:17:LEU:HD13	8:H:73:LEU:HD11	1.88	0.55
3:C:75:GLN:O	3:C:76:TYR:HB2	2.07	0.55
3:C:345:GLU:HB3	3:C:347:PRO:HD2	1.86	0.55
4:D:218:LEU:CD1	5:E:42:VAL:HG12	2.37	0.55
10:J:57:HIS:C	10:J:59:TYR:H	2.13	0.55
3:C:173:ASN:N	3:C:174:PRO:HD2	2.22	0.55
4:D:75:ASN:H	4:D:79:GLU:H	1.53	0.55
7:G:42:ARG:O	7:G:43:ALA:HB2	2.07	0.55
8:H:72:LYS:HA	8:H:75:ASN:ND2	2.22	0.55
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.87	0.55
3:C:92:PHE:O	3:C:95:ILE:HG22	2.06	0.55
4:D:147:LEU:C	4:D:148:TYR:CD1	2.85	0.55
4:D:164:ILE:HD11	4:D:182:VAL:CG1	2.34	0.55
1:A:266:ASP:O	1:A:268:VAL:N	2.40	0.55
3:C:202:HIS:CE1	12:C:383:U10:H1M1	2.42	0.55
3:C:323:GLN:NE2	7:G:47:ARG:HD3	2.22	0.55
5:E:57:GLN:C	5:E:59:VAL:H	2.14	0.55
7:G:78:VAL:C	7:G:79:ASN:ND2	2.62	0.55
10:J:14:PHE:CD1	10:J:14:PHE:N	2.71	0.55
1:A:100:LYS:HE3	2:B:370:MET:HE2	1.89	0.55
2:B:140:LEU:C	2:B:142:PRO:HD2	2.32	0.55
5:E:62:MET:O	5:E:63:SER:C	2.49	0.55
5:E:122:HIS:H	5:E:125:GLU:CD	2.15	0.55
1:A:250:LEU:HD22	1:A:251:ALA:N	2.21	0.55
1:A:297:ILE:HG21	1:A:337:VAL:CG1	2.32	0.55
4:D:164:ILE:CD1	4:D:182:VAL:HG13	2.37	0.55
1:A:19:LEU:C	1:A:21:ASN:N	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:CE2	1:A:319:LEU:HD21	2.42	0.54
1:A:4:TYR:C	1:A:6:GLN:N	2.61	0.54
1:A:365:LEU:HD21	1:A:395:TRP:CD1	2.42	0.54
2:B:406:ALA:O	2:B:407:ASP:C	2.50	0.54
3:C:295:LEU:CD2	14:C:385:SIG:H273	2.35	0.54
1:A:344:ARG:HA	1:A:347:THR:HG22	1.89	0.54
2:B:24:LEU:H	2:B:24:LEU:CD2	2.19	0.54
2:B:25:GLU:CB	2:B:213:HIS:ND1	2.67	0.54
3:C:42:LEU:HD22	3:C:190:ILE:HG22	1.88	0.54
3:C:130:VAL:HA	3:C:133:VAL:HG23	1.90	0.54
3:C:230:ILE:CG2	13:E:198:PEE:H26	2.37	0.54
1:A:443:TRP:C	1:A:445:ARG:N	2.64	0.54
2:B:129:ALA:N	2:B:130:PRO:HD3	2.23	0.54
2:B:260:GLU:O	2:B:261:SER:CB	2.56	0.54
2:B:370:MET:O	2:B:372:VAL:N	2.38	0.54
3:C:127:THR:CG2	3:C:186:LEU:HB3	2.37	0.54
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.25	0.54
4:D:144:ARG:CZ	4:D:147:LEU:HD21	2.37	0.54
4:D:218:LEU:HD11	5:E:42:VAL:CG1	2.37	0.54
2:B:68:LEU:HD23	2:B:186:VAL:HG11	1.89	0.54
3:C:166:TRP:O	3:C:167:GLY:C	2.51	0.54
8:H:73:LEU:CD2	8:H:77:LEU:HD11	2.38	0.54
1:A:373:THR:HB	1:A:374:PRO:CD	2.38	0.54
1:A:42:ASP:HB3	1:A:194:ARG:HB3	1.89	0.54
3:C:166:TRP:CA	3:C:175:THR:HB	2.37	0.54
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.90	0.54
4:D:43:MET:HE3	4:D:46:VAL:CG2	2.27	0.54
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.42	0.54
5:E:32:ARG:HG3	5:E:32:ARG:HH11	1.72	0.54
5:E:96:LEU:HD12	5:E:135:LEU:O	2.08	0.54
8:H:16:PRO:O	8:H:20:VAL:HG23	2.08	0.54
10:J:4:THR:O	10:J:5:LEU:C	2.49	0.54
2:B:281:ALA:O	2:B:285:VAL:HB	2.07	0.54
3:C:270:LYS:O	3:C:270:LYS:HG3	2.06	0.54
1:A:445:ARG:NH1	10:J:16:ARG:HG2	2.23	0.54
2:B:52:LYS:HB2	2:B:203:ARG:HB2	1.90	0.54
3:C:130:VAL:HG12	3:C:131:GLY:N	2.23	0.54
5:E:190:ASP:N	5:E:190:ASP:OD1	2.40	0.54
2:B:31:ASN:HB3	2:B:201:SER:HB2	1.89	0.54
2:B:146:ILE:O	2:B:147:ASP:C	2.50	0.54
2:B:207:VAL:HG11	2:B:382:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:HG23	1:A:195:MET:HG2	1.90	0.53
1:A:49:SER:HB2	1:A:52:ASN:HB3	1.89	0.53
2:B:20:HIS:N	2:B:21:PRO:CD	2.71	0.53
3:C:207:ASN:C	3:C:207:ASN:HD22	2.15	0.53
1:A:61:HIS:CD2	1:A:134:ILE:HG12	2.42	0.53
2:B:171:ALA:O	2:B:172:LEU:HB3	2.09	0.53
2:B:385:GLN:C	2:B:387:LEU:H	2.16	0.53
3:C:332:ASN:HD21	3:C:359:TYR:HA	1.72	0.53
1:A:65:LYS:N	1:A:65:LYS:HD2	2.23	0.53
3:C:332:ASN:ND2	3:C:359:TYR:HA	2.23	0.53
4:D:43:MET:CE	4:D:46:VAL:HG21	2.26	0.53
7:G:53:LEU:O	7:G:56:TYR:HB3	2.08	0.53
1:A:294:LEU:O	1:A:298:ALA:N	2.38	0.53
2:B:24:LEU:HD23	2:B:24:LEU:N	2.22	0.53
2:B:120:MET:O	2:B:121:GLU:C	2.51	0.53
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.41	0.53
7:G:77:TYR:CZ	8:H:52:GLU:HB2	2.44	0.53
10:J:12:LEU:O	10:J:19:THR:HG21	2.09	0.53
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.42	0.53
5:E:9:ASN:CG	5:E:11:SER:HB3	2.32	0.53
2:B:429:ASN:C	2:B:431:GLY:H	2.17	0.53
4:D:47:ALA:HB1	4:D:89:ASP:O	2.08	0.53
5:E:14:ARG:O	5:E:15:ARG:C	2.52	0.53
5:E:20:TYR:O	5:E:21:SER:O	2.27	0.53
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.39	0.53
1:A:290:SER:N	2:B:90:GLU:OE1	2.40	0.53
2:B:198:HIS:HD2	2:B:203:ARG:HH22	1.57	0.53
3:C:113:THR:HG22	3:C:201:LEU:N	2.24	0.53
3:C:142:TRP:HA	3:C:145:THR:OG1	2.08	0.53
4:D:181:GLN:HE21	4:D:181:GLN:C	2.16	0.53
5:E:52:LYS:HD3	5:E:52:LYS:O	2.08	0.53
1:A:410:VAL:O	1:A:413:LYS:HB3	2.09	0.53
2:B:166:ALA:HB1	2:B:242:GLY:CA	2.38	0.53
2:B:333:ALA:O	2:B:337:ILE:HG12	2.09	0.53
3:C:81:ARG:NH1	11:C:381:HEM:O2D	2.42	0.53
4:D:27:ARG:NH2	10:J:59:TYR:CE2	2.77	0.53
8:H:40:CYS:O	8:H:44:VAL:HG23	2.09	0.53
1:A:145:MET:CB	1:A:252:HIS:NE2	2.72	0.53
1:A:264:HIS:CD2	1:A:266:ASP:HB2	2.44	0.53
1:A:391:PRO:HG2	1:A:394:GLU:CB	2.34	0.53
2:B:372:VAL:O	2:B:372:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:VAL:HG23	3:C:147:ILE:H	1.72	0.53
4:D:27:ARG:NH2	10:J:59:TYR:HE2	2.07	0.53
1:A:362:ARG:HG3	1:A:399:LEU:HD11	1.91	0.53
1:A:444:LEU:O	1:A:445:ARG:C	2.52	0.53
2:B:131:GLU:O	2:B:132:PHE:C	2.51	0.53
2:B:202:ALA:CB	2:B:229:GLY:HA2	2.39	0.53
3:C:283:ARG:O	3:C:284:SER:CB	2.57	0.53
1:A:172:GLU:OE1	1:A:172:GLU:HA	2.07	0.52
1:A:444:LEU:H	1:A:444:LEU:CD1	2.21	0.52
2:B:141:GLN:N	2:B:142:PRO:HD2	2.25	0.52
2:B:242:GLY:O	2:B:423:SER:HA	2.08	0.52
3:C:3:PRO:HG2	3:C:4:ASN:N	2.24	0.52
4:D:224:ARG:HB3	4:D:224:ARG:HH11	1.74	0.52
7:G:26:PHE:HD1	7:G:26:PHE:N	1.96	0.52
1:A:104:LYS:HG2	1:A:104:LYS:O	2.10	0.52
1:A:120:CYS:O	1:A:122:LEU:HG	2.09	0.52
1:A:159:GLN:OE1	1:A:237:THR:HG21	2.09	0.52
1:A:252:HIS:ND1	1:A:325:VAL:HG22	2.25	0.52
1:A:287:GLY:HA2	1:A:299:VAL:HG11	1.92	0.52
2:B:143:GLN:CD	2:B:146:ILE:HD11	2.33	0.52
2:B:361:LYS:NZ	2:B:403:ASP:O	2.42	0.52
2:B:395:PRO:C	2:B:398:VAL:HG12	2.35	0.52
4:D:180:SER:HB2	8:H:17:LEU:HB2	1.91	0.52
1:A:102:LEU:C	1:A:104:LYS:N	2.62	0.52
2:B:24:LEU:HG	2:B:24:LEU:O	2.09	0.52
2:B:248:ASN:C	2:B:248:ASN:ND2	2.63	0.52
3:C:105:TYR:HA	3:C:315:THR:HA	1.91	0.52
3:C:155:PRO:O	3:C:156:TYR:HB2	2.10	0.52
3:C:271:PRO:HB3	14:C:385:SIG:C3	2.39	0.52
3:C:325:LEU:HD12	3:C:370:ILE:HG13	1.90	0.52
5:E:119:ASP:HB3	5:E:179:ASN:CG	2.35	0.52
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.49	0.52
1:A:4:TYR:CG	2:B:113:ARG:HB3	2.44	0.52
1:A:36:THR:CG2	1:A:100:LYS:HB3	2.16	0.52
2:B:353:SER:C	2:B:355:GLU:H	2.17	0.52
3:C:277:PHE:CG	3:C:278:ALA:N	2.76	0.52
5:E:28:SER:O	5:E:31:SER:HB3	2.08	0.52
8:H:68:CYS:O	8:H:69:VAL:C	2.53	0.52
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.45	0.52
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.45	0.52
1:A:397:GLU:O	1:A:398:ARG:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:GLN:C	2:B:387:LEU:N	2.66	0.52
3:C:101:ARG:HE	3:C:102:GLY:CA	2.22	0.52
3:C:105:TYR:CE1	3:C:209:PRO:HA	2.44	0.52
3:C:207:ASN:C	3:C:207:ASN:ND2	2.65	0.52
5:E:52:LYS:C	5:E:52:LYS:CD	2.82	0.52
7:G:63:THR:O	7:G:64:GLN:C	2.52	0.52
1:A:100:LYS:HG3	2:B:370:MET:HE1	1.92	0.52
2:B:330:ALA:O	2:B:333:ALA:HB2	2.08	0.52
3:C:107:SER:HB3	11:C:382:HEM:CBD	2.32	0.52
3:C:351:ILE:HG23	7:G:58:LEU:HD21	1.90	0.52
1:A:173:ASN:O	1:A:177:LEU:HG	2.09	0.52
2:B:21:PRO:HG2	2:B:21:PRO:O	2.09	0.52
2:B:57:TYR:CD1	2:B:57:TYR:N	2.78	0.52
2:B:111:CYS:SG	2:B:116:VAL:HA	2.50	0.52
2:B:406:ALA:O	2:B:408:ALA:N	2.43	0.52
3:C:28:ILE:HB	3:C:225:TYR:OH	2.10	0.52
3:C:31:TRP:CZ3	13:C:384:PEE:C13	2.89	0.52
3:C:136:TRP:CD1	3:C:176:LEU:HD13	2.44	0.52
4:D:29:GLY:HA2	4:D:32:VAL:HG12	1.92	0.52
5:E:123:ASP:O	5:E:127:VAL:HG22	2.09	0.52
2:B:258:VAL:CG1	2:B:259:ALA:H	2.22	0.52
2:B:405:VAL:CG1	2:B:409:ASP:OD1	2.57	0.52
3:C:169:PHE:O	3:C:170:SER:HB3	2.09	0.52
3:C:262:PRO:C	3:C:263:LEU:HD12	2.35	0.52
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.44	0.52
5:E:65:SER:C	5:E:67:ASP:N	2.67	0.52
1:A:146:ARG:NH2	9:I:206:UNK:HA	2.24	0.52
1:A:250:LEU:CD2	1:A:325:VAL:CG1	2.87	0.52
2:B:92:VAL:CG1	2:B:115:ASP:HB3	2.35	0.52
2:B:96:LEU:C	2:B:96:LEU:CD2	2.83	0.52
2:B:227:ARG:O	2:B:229:GLY:N	2.43	0.52
2:B:395:PRO:HA	2:B:398:VAL:HG11	1.92	0.52
3:C:222:HIS:CB	3:C:223:PRO:CD	2.86	0.52
6:F:26:PHE:O	6:F:31:LEU:HD23	2.10	0.52
7:G:60:THR:O	7:G:61:TRP:C	2.52	0.52
2:B:146:ILE:HG13	2:B:147:ASP:H	1.72	0.52
2:B:290:ASN:CB	2:B:306:PRO:HD2	2.39	0.52
3:C:342:GLN:HB3	3:C:348:PHE:CD2	2.44	0.52
4:D:217:PRO:HG2	4:D:218:LEU:H	1.75	0.52
7:G:56:TYR:O	7:G:59:TYR:HB3	2.10	0.52
7:G:73:ASN:O	7:G:75:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:95:TYR:CE2	4:D:104:ALA:HB3	2.44	0.51
4:D:139:THR:HG23	8:H:41:ASP:OD1	2.10	0.51
5:E:136:ILE:HG22	5:E:136:ILE:O	2.10	0.51
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.75	0.51
1:A:257:VAL:HG22	1:A:320:PHE:O	2.11	0.51
1:A:276:ILE:HD11	1:A:349:ILE:HD11	1.90	0.51
1:A:409:GLU:OE1	1:A:409:GLU:HA	2.09	0.51
2:B:112:LEU:O	2:B:113:ARG:C	2.54	0.51
2:B:310:SER:O	2:B:324:PHE:HB2	2.10	0.51
9:I:203:UNK:O	9:I:204:UNK:C	2.58	0.51
2:B:385:GLN:NE2	2:B:392:TYR:HA	2.25	0.51
3:C:95:ILE:HG23	3:C:96:PHE:N	2.25	0.51
4:D:117:VAL:CG1	4:D:191:ARG:HH21	2.22	0.51
5:E:21:SER:O	5:E:22:THR:HB	2.09	0.51
5:E:171:ILE:HD12	5:E:172:ARG:N	2.25	0.51
8:H:50:THR:HG22	8:H:52:GLU:H	1.75	0.51
1:A:100:LYS:CB	1:A:100:LYS:HZ2	2.24	0.51
2:B:89:ILE:HD11	2:B:96:LEU:HD12	1.91	0.51
3:C:372:THR:HA	3:C:375:ASN:HD22	1.74	0.51
4:D:192:TRP:CD1	4:D:192:TRP:C	2.86	0.51
8:H:42:GLU:O	8:H:46:SER:HB3	2.11	0.51
1:A:136:ARG:O	1:A:139:GLN:N	2.43	0.51
3:C:95:ILE:HD13	3:C:121:LEU:CD1	2.40	0.51
3:C:131:GLY:N	3:C:134:LEU:HD13	2.26	0.51
4:D:57:THR:HB	4:D:60:GLU:CB	2.40	0.51
4:D:178:THR:HG21	8:H:16:PRO:HD2	1.93	0.51
5:E:21:SER:OG	5:E:22:THR:N	2.42	0.51
1:A:127:ILE:O	1:A:129:LYS:N	2.44	0.51
1:A:389:ARG:HD2	1:A:390:ILE:N	2.25	0.51
2:B:147:ASP:O	2:B:150:VAL:HG22	2.09	0.51
2:B:264:ILE:C	2:B:266:GLY:H	2.18	0.51
3:C:261:ASN:ND2	3:C:264:VAL:HB	2.25	0.51
3:C:327:TRP:HE3	3:C:330:VAL:HG11	1.75	0.51
5:E:62:MET:CG	5:E:63:SER:H	2.22	0.51
10:J:32:GLU:O	10:J:33:ARG:C	2.53	0.51
1:A:106:VAL:HB	1:A:107:PRO:CD	2.41	0.51
3:C:261:ASN:HD22	3:C:264:VAL:HB	1.74	0.51
3:C:377:MET:HE3	6:F:16:ILE:CG2	2.41	0.51
4:D:32:VAL:CG1	4:D:186:VAL:HG22	2.40	0.51
1:A:153:LEU:HD22	1:A:319:LEU:HD13	1.92	0.51
2:B:198:HIS:HD2	2:B:203:ARG:NH2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:LYS:HE2	2:B:403:ASP:OD1	2.11	0.51
2:B:406:ALA:C	2:B:408:ALA:N	2.66	0.51
3:C:276:LEU:O	3:C:279:TYR:HB3	2.10	0.51
5:E:10:PHE:CD2	7:G:18:LEU:HD21	2.45	0.51
3:C:369:THR:O	3:C:370:ILE:C	2.54	0.51
5:E:32:ARG:HD3	5:E:32:ARG:O	2.11	0.51
7:G:57:LEU:HD22	7:G:57:LEU:N	2.24	0.51
3:C:103:LEU:HD13	3:C:103:LEU:C	2.35	0.51
10:J:57:HIS:CB	10:J:61:ASN:C	2.72	0.51
1:A:7:ALA:O	1:A:11:VAL:HG23	2.11	0.50
1:A:120:CYS:HB3	1:A:122:LEU:CD2	2.42	0.50
1:A:266:ASP:C	1:A:268:VAL:H	2.18	0.50
1:A:434:TYR:O	1:A:438:ARG:HB2	2.11	0.50
2:B:217:LYS:O	2:B:219:VAL:N	2.44	0.50
14:C:385:SIG:H353	14:C:385:SIG:H201	1.93	0.50
4:D:116:ILE:HG23	4:D:117:VAL:N	2.26	0.50
5:E:129:LYS:HB2	5:E:187:PHE:CZ	2.47	0.50
1:A:346:CYS:HB3	1:A:411:CYS:HB2	1.92	0.50
1:A:365:LEU:HD21	1:A:395:TRP:CB	2.41	0.50
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.42	0.50
3:C:222:HIS:CG	3:C:223:PRO:N	2.77	0.50
3:C:362:ILE:N	3:C:366:LEU:HD23	2.26	0.50
4:D:46:VAL:HG12	4:D:47:ALA:N	2.25	0.50
8:H:17:LEU:HD21	8:H:21:ARG:CZ	2.41	0.50
8:H:17:LEU:O	8:H:21:ARG:HG3	2.11	0.50
1:A:26:ALA:O	1:A:198:ALA:HA	2.10	0.50
4:D:213:GLY:O	4:D:217:PRO:HG3	2.10	0.50
1:A:36:THR:HG21	1:A:373:THR:OG1	2.12	0.50
1:A:228:VAL:HG13	1:A:228:VAL:O	2.10	0.50
2:B:162:ASN:O	2:B:163:LEU:C	2.54	0.50
3:C:30:ALA:C	3:C:32:TRP:H	2.19	0.50
3:C:32:TRP:HZ2	3:C:207:ASN:HB3	1.76	0.50
4:D:26:ILE:HD13	4:D:192:TRP:HB3	1.93	0.50
4:D:215:LEU:HD11	5:E:47:VAL:CG2	2.42	0.50
5:E:128:LYS:HB2	5:E:187:PHE:HE2	1.75	0.50
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.12	0.50
6:F:70:MET:C	6:F:70:MET:SD	2.95	0.50
6:F:89:TYR:C	6:F:89:TYR:CD1	2.90	0.50
1:A:33:PRO:O	1:A:103:SER:OG	2.28	0.50
1:A:114:ALA:HA	1:A:216:PHE:CE1	2.47	0.50
3:C:219:ILE:HB	3:C:224:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:HIS:HA	10:J:60:GLU:CA	2.41	0.50
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.42	0.50
2:B:82:SER:O	2:B:85:ILE:CG2	2.60	0.50
3:C:187:PRO:HG2	11:C:381:HEM:HMC3	1.94	0.50
3:C:324:THR:O	3:C:325:LEU:C	2.55	0.50
4:D:117:VAL:CG1	4:D:191:ARG:NH2	2.75	0.50
5:E:112:VAL:HG21	5:E:170:ARG:NH2	2.26	0.50
1:A:4:TYR:HB2	2:B:113:ARG:CB	2.42	0.50
1:A:394:GLU:O	1:A:395:TRP:C	2.54	0.50
3:C:167:GLY:HA2	3:C:174:PRO:HB2	1.94	0.50
3:C:269:ILE:HG22	14:C:385:SIG:H263	1.94	0.50
5:E:148:ALA:HA	5:E:156:TYR:CD1	2.47	0.50
2:B:436:VAL:C	2:B:438:GLU:H	2.19	0.50
3:C:12:LEU:HD23	3:C:12:LEU:C	2.37	0.50
3:C:347:PRO:HG3	7:G:66:PHE:HD1	1.76	0.50
4:D:195:GLU:HG3	4:D:195:GLU:O	2.11	0.50
1:A:85:HIS:HA	9:I:314:UNK:CG	2.37	0.50
1:A:105:ASP:O	1:A:106:VAL:C	2.55	0.50
2:B:171:ALA:O	2:B:172:LEU:CB	2.60	0.50
3:C:133:VAL:HG13	3:C:144:ALA:HB2	1.92	0.50
3:C:167:GLY:H	3:C:175:THR:CB	2.24	0.50
3:C:234:THR:HG22	13:E:198:PEE:H31	1.94	0.50
4:D:41:HIS:HB3	4:D:113:LEU:HD13	1.93	0.50
4:D:54:VAL:HG13	4:D:55:CYS:N	2.27	0.50
5:E:106:ILE:HD11	5:E:131:GLU:HA	1.93	0.50
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.94	0.49
2:B:209:LEU:O	2:B:211:VAL:HG13	2.12	0.49
4:D:117:VAL:HG23	4:D:190:LEU:HB3	1.93	0.49
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.46	0.49
4:D:216:VAL:N	4:D:217:PRO:HD2	2.27	0.49
1:A:46:ARG:NH2	1:A:232:SER:O	2.43	0.49
2:B:31:ASN:HB3	2:B:201:SER:CB	2.41	0.49
5:E:14:ARG:O	7:G:24:ARG:HG2	2.12	0.49
4:D:124:GLU:O	4:D:125:ASP:C	2.55	0.49
1:A:92:ARG:NH1	1:A:165:GLN:O	2.45	0.49
1:A:245:GLU:CG	7:G:11:ARG:HG2	2.35	0.49
2:B:133:ARG:HD3	2:B:135:TRP:CH2	2.48	0.49
2:B:316:TYR:HB2	2:B:319:SER:O	2.13	0.49
3:C:45:GLN:CB	11:C:381:HEM:HAB	2.43	0.49
3:C:131:GLY:H	3:C:134:LEU:HD13	1.78	0.49
8:H:15:ASP:O	8:H:17:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HH12	1:A:166:SER:HA	1.77	0.49
1:A:365:LEU:HD13	1:A:392:LEU:HD22	1.93	0.49
2:B:24:LEU:HD21	2:B:392:TYR:CD2	2.47	0.49
2:B:38:LEU:C	2:B:38:LEU:HD12	2.37	0.49
2:B:150:VAL:CG2	2:B:151:ALA:N	2.75	0.49
3:C:101:ARG:NH1	11:C:382:HEM:O2A	2.32	0.49
4:D:237:TYR:HB2	6:F:60:PHE:CG	2.47	0.49
5:E:65:SER:O	5:E:67:ASP:N	2.45	0.49
5:E:97:PHE:O	5:E:134:ILE:HG23	2.13	0.49
8:H:15:ASP:C	8:H:17:LEU:N	2.68	0.49
1:A:86:LEU:HB2	1:A:99:ILE:HG12	1.94	0.49
1:A:298:ALA:HA	1:A:303:LEU:HD12	1.95	0.49
1:A:332:ASP:O	1:A:333:ASP:C	2.53	0.49
1:A:354:VAL:HG23	1:A:355:LEU:N	2.26	0.49
1:A:381:ARG:O	1:A:382:GLU:C	2.56	0.49
2:B:111:CYS:C	2:B:112:LEU:HD23	2.37	0.49
2:B:135:TRP:CD1	2:B:135:TRP:H	2.30	0.49
3:C:31:TRP:CE3	13:C:384:PEE:H13	2.47	0.49
3:C:101:ARG:HE	3:C:102:GLY:N	2.09	0.49
3:C:362:ILE:CA	3:C:366:LEU:HD23	2.42	0.49
5:E:25:SER:O	5:E:28:SER:HB3	2.13	0.49
8:H:17:LEU:HD13	8:H:73:LEU:CD1	2.43	0.49
1:A:34:THR:HA	1:A:102:LEU:HA	1.94	0.49
1:A:444:LEU:C	1:A:445:ARG:O	2.53	0.49
2:B:137:VAL:C	2:B:139:ASP:N	2.63	0.49
3:C:327:TRP:CA	3:C:330:VAL:HG12	2.32	0.49
7:G:36:ASN:O	7:G:40:ARG:HG3	2.13	0.49
1:A:178:SER:O	1:A:179:ARG:C	2.55	0.49
2:B:318:ASP:O	2:B:319:SER:HB2	2.12	0.49
2:B:353:SER:C	2:B:355:GLU:N	2.68	0.49
3:C:70:THR:HA	3:C:74:VAL:CG2	2.41	0.49
3:C:282:LEU:C	3:C:282:LEU:CD1	2.86	0.49
4:D:10:TYR:N	4:D:10:TYR:CD1	2.81	0.49
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.48	0.49
4:D:132:THR:CA	4:D:179:MET:HE2	2.24	0.49
7:G:49:ALA:O	7:G:50:PRO:C	2.51	0.49
1:A:436:ARG:HH22	3:C:20:ILE:HG22	1.77	0.49
2:B:67:HIS:O	2:B:70:ARG:HB3	2.12	0.49
2:B:152:PHE:HA	2:B:157:THR:HG21	1.94	0.49
3:C:109:LEU:C	3:C:111:LYS:H	2.21	0.49
3:C:220:PRO:HG2	3:C:223:PRO:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:VAL:HB	3:C:349:ILE:HD11	1.95	0.49
6:F:61:ARG:HG3	6:F:61:ARG:NH1	2.28	0.49
7:G:25:PRO:HG2	7:G:26:PHE:HD1	1.77	0.49
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.46	0.49
7:G:73:ASN:O	7:G:74:PRO:C	2.56	0.49
1:A:443:TRP:O	1:A:445:ARG:N	2.36	0.49
2:B:429:ASN:O	2:B:431:GLY:N	2.46	0.49
4:D:37:CYS:C	4:D:39:SER:H	2.21	0.49
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.95	0.49
4:D:235:LEU:CD1	6:F:64:ARG:HA	2.43	0.49
7:G:34:VAL:N	7:G:35:PRO:CD	2.76	0.49
1:A:403:ASP:OD1	1:A:406:MET:HB2	2.13	0.48
3:C:60:THR:HG23	3:C:136:TRP:CZ3	2.48	0.48
3:C:81:ARG:HH11	3:C:81:ARG:HG3	1.77	0.48
3:C:163:GLU:HB3	3:C:169:PHE:CD1	2.48	0.48
3:C:215:ASP:HB3	7:G:7:LEU:HB3	1.93	0.48
3:C:285:ILE:HG23	3:C:291:GLY:HA2	1.95	0.48
4:D:215:LEU:HD11	5:E:47:VAL:HG23	1.95	0.48
1:A:100:LYS:HZ2	1:A:100:LYS:HB2	1.79	0.48
1:A:152:TYR:HA	1:A:155:ALA:HB3	1.94	0.48
3:C:100:GLY:O	3:C:101:ARG:C	2.56	0.48
3:C:133:VAL:O	3:C:136:TRP:HD1	1.96	0.48
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.48	0.48
1:A:45:SER:HB3	1:A:167:VAL:HA	1.96	0.48
1:A:88:ALA:HB2	1:A:97:TYR:HA	1.95	0.48
1:A:369:LEU:HD22	1:A:375:VAL:HA	1.95	0.48
1:A:374:PRO:O	1:A:377:GLU:HB3	2.13	0.48
3:C:87:GLY:O	3:C:88:ALA:C	2.56	0.48
2:B:111:CYS:C	2:B:112:LEU:CD2	2.87	0.48
2:B:280:GLY:O	2:B:281:ALA:C	2.56	0.48
2:B:399:LEU:O	2:B:402:ILE:HG22	2.14	0.48
3:C:42:LEU:CD2	3:C:190:ILE:HG22	2.43	0.48
3:C:127:THR:HG22	3:C:186:LEU:CB	2.41	0.48
3:C:238:THR:CB	4:D:212:MET:HG3	2.43	0.48
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.94	0.48
1:A:85:HIS:CG	9:I:314:UNK:HG1	2.49	0.48
2:B:84:LYS:O	2:B:88:GLY:N	2.44	0.48
3:C:167:GLY:CA	3:C:174:PRO:HB2	2.44	0.48
3:C:196:ILE:O	3:C:199:THR:HB	2.14	0.48
3:C:361:THR:C	3:C:363:LEU:N	2.71	0.48
4:D:44:ASP:O	4:D:90:TYR:CD2	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:HB	5:E:193:VAL:HG13	1.94	0.48
1:A:240:GLN:HB2	1:A:422:VAL:HG12	1.93	0.48
2:B:219:VAL:C	2:B:221:GLU:N	2.71	0.48
3:C:157:ILE:O	3:C:161:LEU:HB2	2.12	0.48
3:C:361:THR:HA	3:C:365:ILE:HG22	1.95	0.48
1:A:4:TYR:O	1:A:5:ALA:C	2.56	0.48
1:A:58:PHE:HD1	1:A:58:PHE:O	1.97	0.48
3:C:139:MET:HB2	3:C:256:ASN:OD1	2.14	0.48
3:C:283:ARG:NH2	3:C:342:GLN:O	2.46	0.48
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.96	0.48
6:F:101:ARG:CB	6:F:104:ARG:HH21	2.27	0.48
1:A:30:SER:O	1:A:202:GLY:HA2	2.13	0.48
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.44	0.48
2:B:113:ARG:HG3	2:B:114:ASP:H	1.77	0.48
2:B:225:ASN:C	2:B:226:ILE:HG13	2.38	0.48
4:D:214:LEU:O	4:D:217:PRO:HG2	2.14	0.48
5:E:83:GLU:HG3	5:E:100:HIS:NE2	2.29	0.48
10:J:61:ASN:O	10:J:62:LYS:CB	2.62	0.48
1:A:46:ARG:HG2	1:A:231:LEU:HD13	1.94	0.48
1:A:438:ARG:C	1:A:438:ARG:CD	2.87	0.48
2:B:22:GLN:O	2:B:23:ASP:C	2.57	0.48
3:C:19:LEU:HD12	3:C:19:LEU:N	2.28	0.48
3:C:235:LEU:C	3:C:237:LEU:H	2.22	0.48
4:D:98:PRO:HG2	4:D:99:GLU:OE2	2.13	0.48
5:E:55:VAL:O	5:E:59:VAL:HG23	2.13	0.48
2:B:275:LEU:O	2:B:279:LEU:HB2	2.13	0.48
3:C:138:GLN:NE2	3:C:138:GLN:HA	2.28	0.48
3:C:219:ILE:HD13	4:D:230:LEU:CD1	2.43	0.48
3:C:285:ILE:N	3:C:286:PRO:HD3	2.29	0.48
4:D:165:TYR:H	4:D:168:VAL:CG2	2.26	0.48
4:D:232:SER:HB2	7:G:23:GLN:OE1	2.14	0.48
5:E:136:ILE:HB	5:E:181:GLU:HB3	1.94	0.48
3:C:182:LEU:CD2	14:C:385:SIG:H381	2.44	0.47
3:C:342:GLN:HE21	3:C:342:GLN:CA	2.11	0.47
4:D:51:LEU:O	4:D:54:VAL:HG12	2.14	0.47
2:B:111:CYS:SG	2:B:119:LEU:HD23	2.54	0.47
3:C:295:LEU:O	3:C:296:ALA:C	2.56	0.47
5:E:15:ARG:NH1	5:E:19:ASP:HB3	2.29	0.47
5:E:62:MET:CG	5:E:63:SER:N	2.77	0.47
8:H:73:LEU:HD21	8:H:77:LEU:HD11	1.96	0.47
1:A:253:VAL:HG11	1:A:335:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLY:CA	1:A:299:VAL:HG11	2.44	0.47
2:B:89:ILE:CD1	2:B:96:LEU:HD12	2.44	0.47
2:B:259:ALA:O	2:B:260:GLU:C	2.58	0.47
4:D:158:ILE:HG22	4:D:160:MET:N	2.14	0.47
4:D:235:LEU:O	4:D:236:ALA:HB2	2.15	0.47
5:E:171:ILE:HG12	5:E:176:ALA:HB3	1.96	0.47
2:B:82:SER:C	2:B:85:ILE:HG22	2.39	0.47
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.43	0.47
2:B:170:ASN:HD22	2:B:170:ASN:N	2.12	0.47
2:B:250:ASP:O	2:B:251:SER:HB3	2.15	0.47
4:D:147:LEU:HD22	4:D:147:LEU:N	2.29	0.47
8:H:50:THR:HG22	8:H:52:GLU:N	2.29	0.47
1:A:382:GLU:O	1:A:386:TYR:N	2.43	0.47
2:B:69:LEU:CD1	2:B:105:MET:HE1	2.38	0.47
2:B:170:ASN:O	2:B:171:ALA:C	2.57	0.47
2:B:288:GLY:O	2:B:290:ASN:CB	2.63	0.47
3:C:148:THR:HB	3:C:166:TRP:CZ3	2.49	0.47
3:C:167:GLY:H	3:C:175:THR:CA	2.27	0.47
7:G:25:PRO:HG2	7:G:26:PHE:CD1	2.49	0.47
10:J:36:ASP:O	10:J:37:GLN:C	2.56	0.47
10:J:57:HIS:C	10:J:59:TYR:N	2.72	0.47
1:A:145:MET:HA	1:A:148:VAL:HG13	1.96	0.47
1:A:152:TYR:O	1:A:155:ALA:HB3	2.13	0.47
1:A:253:VAL:HG11	1:A:335:MET:CE	2.45	0.47
2:B:137:VAL:C	2:B:139:ASP:H	2.22	0.47
3:C:32:TRP:CZ3	3:C:209:PRO:HD3	2.49	0.47
3:C:198:LEU:HD21	11:C:382:HEM:CMA	2.44	0.47
6:F:67:ASP:OD1	6:F:71:ARG:CZ	2.62	0.47
7:G:40:ARG:O	7:G:41:LEU:C	2.56	0.47
1:A:306:SER:HB2	9:I:206:UNK:CB	2.45	0.47
1:A:344:ARG:CA	1:A:347:THR:HG22	2.45	0.47
2:B:71:LEU:C	2:B:73:SER:H	2.22	0.47
2:B:192:HIS:O	2:B:196:GLN:HG3	2.14	0.47
2:B:209:LEU:O	2:B:211:VAL:N	2.48	0.47
2:B:225:ASN:O	2:B:226:ILE:HG13	2.14	0.47
2:B:250:ASP:O	2:B:252:LEU:CD2	2.59	0.47
3:C:92:PHE:CZ	3:C:124:LEU:CD1	2.97	0.47
3:C:162:VAL:O	3:C:164:TRP:N	2.42	0.47
3:C:356:SER:O	3:C:357:LEU:HB2	2.14	0.47
5:E:153:PHE:CD2	5:E:172:ARG:HG3	2.49	0.47
1:A:265:PRO:O	1:A:268:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:LEU:O	2:B:211:VAL:HG22	2.15	0.47
3:C:78:TRP:CD2	3:C:79:LEU:N	2.83	0.47
5:E:26:ARG:C	5:E:28:SER:N	2.73	0.47
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.50	0.47
7:G:29:TYR:O	7:G:30:PHE:CB	2.59	0.47
1:A:40:TRP:CZ3	1:A:377:GLU:CD	2.93	0.47
13:C:384:PEE:H12	6:F:69:ASN:OD1	2.15	0.47
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.96	0.47
4:D:228:SER:O	4:D:229:VAL:C	2.58	0.47
5:E:42:VAL:O	5:E:45:LEU:HB3	2.15	0.47
1:A:431:LEU:HD23	1:A:432:PRO:N	2.30	0.47
1:A:436:ARG:HH11	3:C:223:PRO:HD2	1.80	0.47
2:B:277:HIS:CE1	2:B:364:LEU:CD2	2.97	0.47
3:C:27:ASN:CB	6:F:69:ASN:HD22	2.20	0.47
3:C:233:LEU:C	3:C:233:LEU:HD13	2.40	0.47
3:C:295:LEU:HD11	14:C:385:SIG:H273	1.97	0.47
4:D:75:ASN:ND2	4:D:79:GLU:H	2.13	0.47
5:E:113:GLU:CD	5:E:116:GLN:HG3	2.40	0.47
7:G:57:LEU:O	7:G:58:LEU:C	2.58	0.47
1:A:64:PHE:C	1:A:66:GLY:H	2.23	0.46
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.97	0.46
1:A:235:ARG:HD3	5:E:21:SER:N	2.28	0.46
2:B:436:VAL:C	2:B:438:GLU:N	2.72	0.46
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.50	0.46
7:G:71:ARG:NH2	8:H:60:ASP:OD2	2.49	0.46
1:A:420:PRO:HD3	1:A:441:MET:HG3	1.96	0.46
2:B:24:LEU:HD11	2:B:392:TYR:CG	2.49	0.46
2:B:371:SER:C	2:B:372:VAL:HG23	2.40	0.46
3:C:40:VAL:HG11	3:C:233:LEU:HD21	1.96	0.46
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.51	0.46
3:C:346:HIS:O	3:C:347:PRO:C	2.58	0.46
3:C:353:GLN:HA	3:C:356:SER:HB3	1.97	0.46
4:D:197:GLU:O	4:D:198:HIS:C	2.58	0.46
5:E:18:ASP:HB3	5:E:28:SER:OG	2.15	0.46
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.50	0.46
1:A:391:PRO:C	1:A:393:GLU:N	2.72	0.46
2:B:82:SER:O	2:B:85:ILE:HG22	2.15	0.46
2:B:166:ALA:O	2:B:242:GLY:HA3	2.15	0.46
3:C:156:TYR:C	3:C:158:GLY:H	2.23	0.46
4:D:138:PRO:HD3	8:H:58:LEU:CD2	2.46	0.46
8:H:15:ASP:C	8:H:17:LEU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:73:LEU:C	8:H:73:LEU:CD2	2.88	0.46
1:A:250:LEU:CD2	1:A:251:ALA:N	2.77	0.46
2:B:307:PHE:CD2	2:B:308:ASP:N	2.83	0.46
2:B:307:PHE:CG	2:B:308:ASP:N	2.80	0.46
3:C:167:GLY:N	3:C:175:THR:HG22	2.31	0.46
4:D:29:GLY:O	4:D:30:PHE:C	2.58	0.46
4:D:165:TYR:CZ	4:D:168:VAL:HG22	2.50	0.46
5:E:57:GLN:O	5:E:59:VAL:N	2.47	0.46
7:G:78:VAL:O	7:G:78:VAL:HG12	2.15	0.46
10:J:49:GLY:N	10:J:54:HIS:ND1	2.61	0.46
2:B:144:LEU:O	2:B:145:LYS:C	2.59	0.46
2:B:248:ASN:HD21	2:B:428:GLY:CA	2.26	0.46
2:B:275:LEU:O	2:B:275:LEU:HD12	2.15	0.46
3:C:211:GLY:CA	3:C:315:THR:HG23	2.46	0.46
5:E:13:TYR:C	5:E:14:ARG:HD3	2.38	0.46
5:E:175:PRO:O	5:E:176:ALA:C	2.58	0.46
10:J:52:TRP:O	10:J:56:LYS:N	2.45	0.46
1:A:64:PHE:O	1:A:75:LEU:HD23	2.15	0.46
1:A:161:THR:HG21	1:A:235:ARG:N	2.29	0.46
1:A:408:ARG:O	1:A:409:GLU:C	2.58	0.46
3:C:95:ILE:CG2	3:C:96:PHE:N	2.78	0.46
3:C:168:GLY:O	3:C:169:PHE:HD1	1.98	0.46
5:E:188:THR:CG2	5:E:194:ILE:HD12	2.45	0.46
1:A:436:ARG:HD3	3:C:223:PRO:HG3	1.98	0.46
3:C:102:GLY:HA2	3:C:107:SER:HB2	1.97	0.46
3:C:113:THR:O	3:C:197:HIS:CE1	2.69	0.46
7:G:26:PHE:N	7:G:26:PHE:CD1	2.68	0.46
1:A:39:VAL:HG22	1:A:41:ILE:HD13	1.98	0.46
1:A:120:CYS:HB3	1:A:122:LEU:HD21	1.97	0.46
2:B:62:ASN:O	2:B:63:LEU:C	2.58	0.46
2:B:170:ASN:O	2:B:171:ALA:O	2.33	0.46
2:B:217:LYS:C	2:B:219:VAL:N	2.70	0.46
3:C:147:ILE:O	3:C:150:LEU:CB	2.63	0.46
3:C:158:GLY:C	3:C:160:THR:N	2.71	0.46
3:C:210:LEU:HB3	3:C:212:ILE:HG12	1.97	0.46
5:E:32:ARG:HH22	7:G:25:PRO:HD2	1.81	0.46
5:E:36:SER:OG	7:G:21:PHE:HE1	1.99	0.46
1:A:106:VAL:HG13	1:A:208:LEU:HD13	1.98	0.46
1:A:399:LEU:HA	1:A:402:VAL:HG23	1.97	0.46
2:B:92:VAL:O	2:B:92:VAL:HG12	2.14	0.46
2:B:342:ASN:O	2:B:345:LYS:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:ASN:HB3	11:C:382:HEM:O1D	2.16	0.46
3:C:220:PRO:O	3:C:221:PHE:C	2.58	0.46
3:C:234:THR:HB	4:D:216:VAL:HG12	1.97	0.46
4:D:227:TRP:O	4:D:228:SER:C	2.58	0.46
4:D:233:ARG:HB3	6:F:71:ARG:NH2	2.30	0.46
5:E:25:SER:C	5:E:26:ARG:O	2.56	0.46
10:J:13:LEU:HG	10:J:23:THR:HG21	1.98	0.46
1:A:197:LEU:HD23	1:A:216:PHE:HE2	1.80	0.46
2:B:47:ILE:HG22	2:B:48:GLY:N	2.31	0.46
4:D:113:LEU:N	4:D:113:LEU:HD12	2.30	0.46
5:E:25:SER:O	5:E:26:ARG:O	2.34	0.46
5:E:38:LEU:O	5:E:42:VAL:HG23	2.16	0.46
8:H:44:VAL:C	8:H:46:SER:H	2.23	0.46
1:A:158:PHE:O	1:A:159:GLN:C	2.59	0.45
2:B:38:LEU:HG	2:B:38:LEU:O	2.15	0.45
3:C:15:ILE:C	3:C:17:ASN:H	2.25	0.45
3:C:46:ILE:O	3:C:50:LEU:HB2	2.16	0.45
3:C:146:VAL:CG2	3:C:147:ILE:N	2.78	0.45
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.43	0.45
3:C:287:ASN:OD1	3:C:289:LEU:N	2.49	0.45
3:C:373:LEU:C	3:C:373:LEU:CD2	2.89	0.45
4:D:234:LYS:HE2	5:E:10:PHE:CE1	2.50	0.45
1:A:366:VAL:C	1:A:368:HIS:N	2.74	0.45
2:B:405:VAL:CG1	2:B:406:ALA:N	2.79	0.45
2:B:424:MET:HG2	2:B:425:ALA:N	2.31	0.45
4:D:149:PHE:CE2	4:D:151:PRO:HD3	2.51	0.45
5:E:45:LEU:HD21	10:J:28:ALA:N	2.30	0.45
6:F:29:TYR:HB2	6:F:31:LEU:HD21	1.98	0.45
1:A:129:LYS:O	1:A:133:VAL:HG23	2.15	0.45
1:A:430:GLN:O	1:A:430:GLN:HG2	2.16	0.45
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.98	0.45
2:B:280:GLY:C	2:B:282:ASN:H	2.24	0.45
3:C:154:ILE:O	3:C:158:GLY:HA3	2.16	0.45
5:E:78:LEU:HD22	5:E:132:TRP:CE2	2.52	0.45
5:E:118:ARG:NH1	5:E:174:GLY:O	2.38	0.45
7:G:55:PHE:O	7:G:56:TYR:C	2.60	0.45
1:A:4:TYR:HB2	2:B:113:ARG:HB3	1.97	0.45
2:B:152:PHE:HA	2:B:157:THR:CG2	2.47	0.45
2:B:372:VAL:O	2:B:378:PHE:HB2	2.16	0.45
2:B:405:VAL:HG11	2:B:409:ASP:CG	2.41	0.45
3:C:72:ARG:NE	4:D:115:TYR:OH	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:VAL:CG1	3:C:183:HIS:HB2	2.47	0.45
3:C:346:HIS:ND1	3:C:346:HIS:C	2.74	0.45
3:C:369:THR:O	3:C:371:GLY:N	2.49	0.45
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.51	0.45
4:D:81:PHE:CD1	4:D:81:PHE:C	2.94	0.45
4:D:213:GLY:O	4:D:217:PRO:CD	2.64	0.45
4:D:235:LEU:HD12	6:F:64:ARG:HA	1.98	0.45
5:E:29:ASP:N	5:E:30:PRO:HD2	2.31	0.45
5:E:76:ILE:O	5:E:193:VAL:HG12	2.17	0.45
5:E:128:LYS:HB2	5:E:187:PHE:CE2	2.52	0.45
1:A:33:PRO:CG	1:A:34:THR:H	2.20	0.45
1:A:245:GLU:C	1:A:247:GLY:H	2.24	0.45
1:A:349:ILE:HD12	1:A:407:VAL:HG11	1.99	0.45
2:B:277:HIS:HB2	2:B:360:ALA:HB1	1.99	0.45
2:B:437:ASP:OD1	2:B:438:GLU:HG3	2.16	0.45
3:C:277:PHE:CD2	3:C:278:ALA:N	2.85	0.45
3:C:350:ILE:HA	3:C:353:GLN:HE21	1.81	0.45
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.51	0.45
4:D:113:LEU:N	4:D:113:LEU:CD1	2.80	0.45
4:D:116:ILE:HG12	16:D:243:HEC:HMA3	1.99	0.45
6:F:29:TYR:HB2	6:F:31:LEU:CD2	2.46	0.45
7:G:71:ARG:CZ	8:H:56:GLU:OE2	2.65	0.45
1:A:356:ARG:O	1:A:357:GLY:C	2.59	0.45
1:A:436:ARG:HD3	3:C:223:PRO:CG	2.47	0.45
2:B:135:TRP:CD1	2:B:135:TRP:N	2.84	0.45
3:C:101:ARG:HE	3:C:102:GLY:HA2	1.81	0.45
3:C:354:MET:O	3:C:357:LEU:HB3	2.16	0.45
3:C:361:THR:O	3:C:362:ILE:C	2.57	0.45
4:D:232:SER:O	4:D:233:ARG:O	2.34	0.45
6:F:96:GLU:HA	6:F:96:GLU:OE1	2.16	0.45
1:A:153:LEU:C	1:A:153:LEU:CD2	2.86	0.45
1:A:210:GLU:O	1:A:214:LYS:HB2	2.17	0.45
1:A:346:CYS:HB2	1:A:412:SER:HB3	1.99	0.45
3:C:59:ASP:O	3:C:60:THR:C	2.60	0.45
3:C:121:LEU:HD11	3:C:125:MET:HE3	1.99	0.45
3:C:166:TRP:O	3:C:167:GLY:O	2.34	0.45
7:G:18:LEU:O	7:G:19:SER:C	2.59	0.45
2:B:56:ARG:NH1	2:B:172:LEU:HD13	2.32	0.45
2:B:137:VAL:CG2	2:B:138:ALA:H	2.30	0.45
2:B:181:TYR:CE1	2:B:182:ARG:CG	2.99	0.45
5:E:109:GLU:CD	5:E:167:ALA:HB3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:SER:O	1:A:295:ALA:HB3	2.17	0.45
3:C:160:THR:O	3:C:161:LEU:C	2.60	0.45
4:D:34:LYS:O	4:D:34:LYS:HG2	2.15	0.45
4:D:57:THR:HG22	4:D:58:GLU:N	2.32	0.45
4:D:195:GLU:HG3	4:D:198:HIS:HB2	1.98	0.45
5:E:134:ILE:HD12	5:E:185:TYR:CD1	2.52	0.45
1:A:127:ILE:HG22	1:A:128:GLU:N	2.32	0.45
2:B:24:LEU:HD11	2:B:392:TYR:CD2	2.51	0.45
2:B:200:THR:HG22	2:B:226:ILE:HG21	1.99	0.45
2:B:225:ASN:O	2:B:226:ILE:CG1	2.65	0.45
3:C:82:ASN:HD22	3:C:82:ASN:N	2.15	0.45
3:C:101:ARG:HD2	3:C:101:ARG:O	2.16	0.45
3:C:120:LEU:O	3:C:121:LEU:C	2.59	0.45
3:C:323:GLN:O	3:C:326:PHE:HB3	2.17	0.45
4:D:37:CYS:O	4:D:39:SER:N	2.50	0.45
5:E:16:PRO:CD	7:G:22:GLU:O	2.65	0.45
6:F:71:ARG:O	6:F:72:GLN:HB2	2.17	0.45
1:A:178:SER:O	1:A:182:LEU:HD23	2.17	0.44
3:C:285:ILE:O	3:C:285:ILE:HG13	2.17	0.44
12:C:383:U10:H8	12:C:383:U10:C1M	2.47	0.44
4:D:72:ASP:O	4:D:73:GLY:O	2.34	0.44
4:D:168:VAL:O	4:D:168:VAL:HG12	2.17	0.44
6:F:12:TRP:CE3	6:F:12:TRP:CA	3.00	0.44
1:A:23:VAL:HG23	1:A:192:ALA:HB1	1.99	0.44
3:C:89:SER:O	3:C:90:PHE:C	2.60	0.44
3:C:238:THR:N	3:C:239:PRO:CD	2.80	0.44
3:C:349:ILE:CG2	3:C:350:ILE:HD13	2.44	0.44
3:C:359:TYR:HD2	3:C:360:PHE:CE1	2.34	0.44
4:D:102:ARG:NH1	4:D:109:LEU:CB	2.77	0.44
4:D:167:ASP:C	4:D:169:LEU:N	2.75	0.44
5:E:15:ARG:HA	5:E:16:PRO:HD3	1.79	0.44
6:F:78:GLU:H	6:F:78:GLU:CD	2.25	0.44
6:F:102:LYS:HB3	6:F:102:LYS:HE2	1.72	0.44
10:J:5:LEU:O	10:J:6:THR:C	2.61	0.44
10:J:57:HIS:CE1	10:J:62:LYS:OXT	2.70	0.44
1:A:65:LYS:HZ1	9:I:311:UNK:HA	1.77	0.44
1:A:100:LYS:HG3	2:B:370:MET:CE	2.48	0.44
1:A:382:GLU:CG	1:A:389:ARG:HA	2.39	0.44
3:C:139:MET:HE2	3:C:255:GLU:HB3	1.99	0.44
3:C:282:LEU:HD22	3:C:291:GLY:C	2.43	0.44
3:C:295:LEU:CG	14:C:385:SIG:H273	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:33:TYR:HA	4:D:37:CYS:SG	2.58	0.44
7:G:77:TYR:C	7:G:79:ASN:H	2.24	0.44
3:C:95:ILE:HD13	3:C:121:LEU:HD12	2.00	0.44
3:C:148:THR:C	3:C:150:LEU:N	2.72	0.44
3:C:349:ILE:HG22	3:C:350:ILE:N	2.32	0.44
5:E:121:GLN:HA	5:E:125:GLU:OE2	2.17	0.44
10:J:48:GLU:HA	10:J:54:HIS:CE1	2.53	0.44
1:A:294:LEU:O	1:A:298:ALA:HB2	2.18	0.44
2:B:157:THR:HG23	2:B:158:HIS:N	2.32	0.44
2:B:241:GLY:HA3	2:B:421:GLN:NE2	2.32	0.44
3:C:154:ILE:HG22	3:C:157:ILE:HG22	2.00	0.44
3:C:247:SER:O	3:C:250:LEU:HB2	2.17	0.44
3:C:267:PRO:O	3:C:268:HIS:HB2	2.17	0.44
5:E:43:THR:O	5:E:44:THR:C	2.61	0.44
10:J:13:LEU:HA	10:J:19:THR:HG22	1.98	0.44
1:A:140:GLU:O	1:A:142:ASP:N	2.51	0.44
1:A:290:SER:HB3	2:B:90:GLU:OE1	2.18	0.44
3:C:172:ASP:CG	3:C:173:ASN:H	2.25	0.44
3:C:225:TYR:O	3:C:226:SER:C	2.58	0.44
3:C:241:LEU:C	4:D:208:MET:HE2	2.43	0.44
5:E:109:GLU:HG3	5:E:167:ALA:HB3	1.99	0.44
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.53	0.44
7:G:57:LEU:H	7:G:57:LEU:CD2	2.31	0.44
10:J:21:ALA:O	10:J:22:LEU:C	2.60	0.44
1:A:111:GLU:HB2	1:A:215:HIS:CD2	2.52	0.44
1:A:153:LEU:HD21	1:A:319:LEU:HD13	1.98	0.44
1:A:322:PHE:C	1:A:322:PHE:CD1	2.95	0.44
2:B:102:ARG:NE	2:B:164:HIS:CD2	2.86	0.44
2:B:112:LEU:HD23	2:B:112:LEU:N	2.33	0.44
2:B:171:ALA:C	2:B:173:ALA:H	2.26	0.44
3:C:22:LEU:HD12	3:C:23:PRO:HD2	1.99	0.44
3:C:30:ALA:O	3:C:32:TRP:N	2.51	0.44
4:D:95:TYR:CG	4:D:101:ALA:HB2	2.52	0.44
6:F:71:ARG:O	6:F:72:GLN:CB	2.65	0.44
6:F:107:TRP:C	6:F:109:LYS:H	2.25	0.44
8:H:72:LYS:HA	8:H:75:ASN:HD21	1.81	0.44
10:J:38:GLY:O	10:J:42:ILE:HG13	2.18	0.44
10:J:52:TRP:O	10:J:56:LYS:HB2	2.18	0.44
1:A:358:LYS:O	1:A:359:ASN:C	2.60	0.44
2:B:213:HIS:O	2:B:213:HIS:HD2	2.01	0.44
2:B:258:VAL:CG1	2:B:322:PHE:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:TYR:HA	11:C:381:HEM:HAA2	2.00	0.44
3:C:179:PHE:O	3:C:180:PHE:C	2.61	0.44
3:C:271:PRO:HG2	3:C:276:LEU:HD23	2.00	0.44
2:B:253:VAL:HG12	2:B:254:HIS:N	2.33	0.44
2:B:424:MET:HE3	2:B:436:VAL:CG1	2.48	0.44
3:C:133:VAL:HG13	3:C:140:SER:O	2.18	0.44
3:C:148:THR:HG22	3:C:162:VAL:HG13	2.00	0.44
3:C:162:VAL:C	3:C:164:TRP:H	2.26	0.44
4:D:221:TYR:CD2	5:E:39:VAL:HG21	2.52	0.44
7:G:24:ARG:HA	7:G:25:PRO:HD2	1.57	0.44
7:G:36:ASN:O	7:G:37:VAL:C	2.60	0.44
8:H:50:THR:CG2	8:H:52:GLU:H	2.31	0.44
2:B:207:VAL:HG12	2:B:208:GLY:N	2.33	0.43
3:C:45:GLN:HB3	11:C:381:HEM:HAB	2.00	0.43
3:C:130:VAL:HA	3:C:133:VAL:CG2	2.47	0.43
3:C:142:TRP:CE2	3:C:265:THR:HG22	2.52	0.43
3:C:342:GLN:HE21	3:C:343:PRO:CD	2.13	0.43
4:D:29:GLY:O	4:D:32:VAL:HG12	2.18	0.43
4:D:148:TYR:CD1	4:D:148:TYR:N	2.86	0.43
5:E:188:THR:HG21	5:E:194:ILE:HD12	2.00	0.43
1:A:158:PHE:CZ	1:A:319:LEU:HD21	2.53	0.43
1:A:166:SER:HG	5:E:3:THR:HG23	1.78	0.43
1:A:252:HIS:HB3	1:A:323:TYR:CE1	2.44	0.43
2:B:89:ILE:CD1	2:B:96:LEU:HB2	2.45	0.43
2:B:325:TYR:OH	9:I:119:UNK:HA	2.18	0.43
3:C:38:LEU:HD21	3:C:95:ILE:N	2.34	0.43
3:C:289:LEU:O	3:C:290:GLY:C	2.60	0.43
4:D:78:GLY:C	4:D:79:GLU:HG3	2.43	0.43
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.52	0.43
4:D:139:THR:C	4:D:141:VAL:H	2.26	0.43
7:G:38:TRP:C	7:G:40:ARG:N	2.73	0.43
8:H:17:LEU:HD21	8:H:21:ARG:NH2	2.33	0.43
8:H:47:ARG:HD2	8:H:49:GLN:H	1.83	0.43
1:A:228:VAL:HA	1:A:229:PRO:HD2	1.82	0.43
3:C:214:SER:HA	6:F:66:LEU:HD11	2.01	0.43
4:D:197:GLU:O	4:D:199:ASP:N	2.51	0.43
5:E:76:ILE:HD13	5:E:98:VAL:HG21	2.00	0.43
6:F:73:GLN:OE1	7:G:36:ASN:ND2	2.51	0.43
6:F:104:ARG:O	6:F:105:GLU:C	2.61	0.43
8:H:22:GLU:O	8:H:23:GLN:C	2.61	0.43
1:A:17:SER:OG	1:A:209:LEU:CD2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:CA	1:A:48:GLU:HG3	2.46	0.43
1:A:54:GLY:O	1:A:55:ALA:C	2.61	0.43
1:A:399:LEU:C	1:A:399:LEU:CD1	2.90	0.43
1:A:431:LEU:HD23	1:A:431:LEU:C	2.43	0.43
2:B:279:LEU:HD11	2:B:344:VAL:HG13	2.00	0.43
3:C:132:TYR:O	3:C:135:PRO:HD2	2.17	0.43
3:C:328:LEU:HD12	3:C:328:LEU:HA	1.83	0.43
4:D:28:ARG:CD	4:D:171:PHE:CD2	3.01	0.43
5:E:11:SER:O	5:E:12:ASP:C	2.61	0.43
7:G:38:TRP:C	7:G:40:ARG:H	2.25	0.43
1:A:126:GLN:O	1:A:130:GLU:HG2	2.19	0.43
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.83	0.43
1:A:281:ASP:O	1:A:284:TYR:CD1	2.71	0.43
12:C:383:U10:H161	12:C:383:U10:H121	1.89	0.43
4:D:233:ARG:C	6:F:71:ARG:HH22	2.27	0.43
5:E:148:ALA:HB2	5:E:156:TYR:HE1	1.82	0.43
10:J:13:LEU:CD1	10:J:13:LEU:H	2.31	0.43
1:A:53:ASN:HD22	1:A:54:GLY:N	2.15	0.43
1:A:156:THR:CA	5:E:7:VAL:HG21	2.47	0.43
1:A:365:LEU:HD21	1:A:395:TRP:CG	2.53	0.43
2:B:111:CYS:SG	2:B:119:LEU:CD2	3.07	0.43
4:D:230:LEU:CB	6:F:70:MET:HE3	2.43	0.43
5:E:171:ILE:HD11	5:E:173:LYS:O	2.18	0.43
1:A:35:CYS:HB2	1:A:200:ALA:O	2.17	0.43
1:A:294:LEU:HG	1:A:307:PHE:CE2	2.54	0.43
3:C:19:LEU:C	3:C:20:ILE:HG13	2.42	0.43
3:C:329:LEU:O	3:C:330:VAL:C	2.60	0.43
5:E:11:SER:C	5:E:13:TYR:N	2.72	0.43
6:F:73:GLN:HA	7:G:39:ARG:HH12	1.83	0.43
3:C:134:LEU:HD21	3:C:180:PHE:HD1	1.83	0.43
3:C:164:TRP:CD1	3:C:164:TRP:C	2.96	0.43
3:C:261:ASN:ND2	3:C:264:VAL:CB	2.82	0.43
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.89	0.43
1:A:310:PHE:CE1	1:A:322:PHE:N	2.87	0.43
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.83	0.43
2:B:45:SER:OG	2:B:116:VAL:HG21	2.18	0.43
2:B:130:PRO:CB	2:B:132:PHE:CE1	3.02	0.43
2:B:170:ASN:O	2:B:173:ALA:HB3	2.19	0.43
2:B:253:VAL:CG1	2:B:254:HIS:N	2.81	0.43
2:B:371:SER:O	2:B:372:VAL:HG23	2.19	0.43
4:D:138:PRO:HD3	8:H:58:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:243:HEC:HMC3	16:D:243:HEC:HBC3	2.01	0.43
5:E:83:GLU:HG3	5:E:100:HIS:CE1	2.53	0.43
3:C:5:ILE:HA	3:C:8:SER:OG	2.19	0.43
3:C:9:HIS:HA	3:C:10:PRO:HD2	1.83	0.43
3:C:58:ALA:O	3:C:59:ASP:HB2	2.19	0.43
3:C:108:TYR:HB2	3:C:306:PRO:HG3	2.00	0.43
3:C:171:VAL:HA	3:C:175:THR:HG21	2.01	0.43
3:C:210:LEU:HD23	3:C:210:LEU:HA	1.76	0.43
3:C:321:LEU:O	3:C:322:SER:C	2.62	0.43
4:D:235:LEU:HD22	6:F:63:LYS:HE2	2.00	0.43
5:E:26:ARG:O	5:E:27:GLU:CG	2.67	0.43
7:G:52:PHE:O	7:G:53:LEU:C	2.60	0.43
7:G:71:ARG:NH2	8:H:56:GLU:OE2	2.52	0.43
8:H:35:GLU:O	8:H:39:LEU:CD1	2.67	0.43
1:A:19:LEU:HB2	1:A:21:ASN:HB3	2.00	0.42
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.81	0.42
1:A:327:ASP:O	1:A:328:ARG:C	2.62	0.42
3:C:250:LEU:HB3	3:C:251:LEU:HD12	2.01	0.42
1:A:108:LYS:O	1:A:112:LEU:HG	2.19	0.42
2:B:189:VAL:O	2:B:191:LEU:N	2.52	0.42
3:C:88:ALA:O	3:C:91:PHE:HB3	2.19	0.42
3:C:366:LEU:HD22	3:C:366:LEU:N	2.33	0.42
4:D:47:ALA:HB2	4:D:90:TYR:HA	2.02	0.42
4:D:105:ASN:O	4:D:107:GLY:N	2.52	0.42
4:D:153:PHE:HB2	4:D:158:ILE:HD11	2.01	0.42
5:E:57:GLN:C	5:E:59:VAL:N	2.77	0.42
5:E:153:PHE:CD2	5:E:172:ARG:NH1	2.87	0.42
7:G:71:ARG:HH21	8:H:56:GLU:CG	2.32	0.42
1:A:120:CYS:CB	1:A:122:LEU:HD21	2.50	0.42
1:A:224:ASP:O	1:A:225:ASP:C	2.62	0.42
3:C:24:ALA:O	3:C:218:LYS:HA	2.20	0.42
3:C:43:MET:CE	3:C:43:MET:CA	2.96	0.42
3:C:129:PHE:CE1	3:C:147:ILE:HD12	2.54	0.42
3:C:162:VAL:C	3:C:164:TRP:N	2.77	0.42
5:E:91:TRP:O	5:E:94:LYS:O	2.37	0.42
6:F:101:ARG:O	6:F:102:LYS:C	2.61	0.42
1:A:127:ILE:C	1:A:129:LYS:N	2.75	0.42
1:A:274:ASN:O	1:A:309:THR:HG21	2.20	0.42
2:B:22:GLN:O	2:B:23:ASP:O	2.37	0.42
2:B:120:MET:O	2:B:123:LEU:N	2.52	0.42
2:B:258:VAL:HA	2:B:322:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:GLY:O	3:C:160:THR:N	2.52	0.42
3:C:350:ILE:O	3:C:351:ILE:C	2.61	0.42
4:D:217:PRO:O	4:D:220:TYR:HB3	2.19	0.42
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.18	0.42
6:F:45:GLU:OE1	6:F:45:GLU:HA	2.19	0.42
8:H:66:ASP:HA	8:H:69:VAL:HG23	2.00	0.42
10:J:46:ILE:O	10:J:46:ILE:HG22	2.20	0.42
1:A:5:ALA:O	1:A:8:LEU:HB2	2.20	0.42
2:B:226:ILE:HG22	2:B:227:ARG:N	2.34	0.42
2:B:277:HIS:HD2	2:B:363:LYS:CB	2.32	0.42
3:C:20:ILE:O	3:C:21:ASP:CB	2.63	0.42
3:C:101:ARG:NE	3:C:102:GLY:N	2.67	0.42
3:C:221:PHE:C	3:C:221:PHE:CD1	2.97	0.42
3:C:349:ILE:HG22	3:C:353:GLN:NE2	2.35	0.42
4:D:158:ILE:CG2	4:D:159:GLY:H	2.27	0.42
6:F:31:LEU:N	6:F:31:LEU:CD2	2.81	0.42
6:F:39:GLU:O	6:F:44:LYS:HE3	2.19	0.42
8:H:27:LEU:O	8:H:28:GLU:C	2.61	0.42
8:H:57:GLU:OE1	8:H:57:GLU:N	2.43	0.42
1:A:283:THR:HG21	9:I:114:UNK:CB	2.48	0.42
2:B:39:GLU:HG3	2:B:41:TYR:CD1	2.54	0.42
2:B:340:ALA:O	2:B:344:VAL:HG23	2.19	0.42
3:C:92:PHE:O	3:C:93:ILE:C	2.61	0.42
3:C:163:GLU:OE1	3:C:169:PHE:CE1	2.73	0.42
1:A:39:VAL:HG22	1:A:41:ILE:CD1	2.49	0.42
1:A:280:TYR:CG	1:A:281:ASP:N	2.88	0.42
1:A:372:THR:O	1:A:373:THR:C	2.63	0.42
1:A:429:GLU:OE1	7:G:7:LEU:HD23	2.20	0.42
3:C:27:ASN:HA	6:F:70:MET:HB2	2.01	0.42
3:C:89:SER:C	3:C:91:PHE:N	2.76	0.42
3:C:129:PHE:CD1	3:C:147:ILE:HD12	2.54	0.42
3:C:148:THR:C	3:C:150:LEU:H	2.27	0.42
4:D:16:GLY:HA2	4:D:17:PRO:HD2	1.83	0.42
4:D:155:GLY:C	4:D:156:GLN:NE2	2.78	0.42
4:D:218:LEU:CD2	5:E:39:VAL:HG13	2.48	0.42
5:E:14:ARG:O	5:E:15:ARG:O	2.37	0.42
5:E:53:ASN:O	5:E:54:VAL:C	2.63	0.42
5:E:148:ALA:HB2	5:E:156:TYR:CE1	2.55	0.42
7:G:68:LYS:C	7:G:70:LYS:H	2.27	0.42
10:J:9:LEU:O	10:J:13:LEU:HB2	2.19	0.42
1:A:268:VAL:O	1:A:272:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ARG:C	1:A:440:GLY:H	2.27	0.42
2:B:371:SER:O	2:B:372:VAL:CG2	2.67	0.42
2:B:397:THR:HA	2:B:400:GLN:CB	2.49	0.42
2:B:435:PHE:HD1	2:B:438:GLU:OE2	2.03	0.42
3:C:111:LYS:HE3	3:C:307:PHE:CE1	2.55	0.42
3:C:111:LYS:HE3	3:C:307:PHE:HE1	1.85	0.42
3:C:170:SER:O	3:C:171:VAL:C	2.63	0.42
3:C:187:PRO:HG2	11:C:381:HEM:CMC	2.50	0.42
3:C:331:ALA:O	3:C:332:ASN:C	2.61	0.42
4:D:98:PRO:HG2	4:D:99:GLU:H	1.85	0.42
4:D:134:TYR:CD1	4:D:162:PRO:HG3	2.55	0.42
8:H:15:ASP:O	8:H:16:PRO:C	2.62	0.42
9:I:205:UNK:O	9:I:207:UNK:N	2.53	0.42
10:J:57:HIS:CB	10:J:61:ASN:O	2.67	0.42
1:A:240:GLN:HB2	1:A:422:VAL:CG1	2.50	0.42
1:A:240:GLN:OE1	1:A:434:TYR:HB2	2.20	0.42
1:A:362:ARG:CG	1:A:399:LEU:HD11	2.49	0.42
1:A:436:ARG:HA	1:A:436:ARG:HD2	1.84	0.42
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.55	0.42
4:D:234:LYS:O	7:G:15:THR:HA	2.19	0.42
6:F:96:GLU:OE1	6:F:99:ARG:NE	2.53	0.42
8:H:68:CYS:C	8:H:70:ALA:N	2.76	0.42
1:A:46:ARG:NH1	1:A:316:GLU:OE2	2.43	0.42
1:A:59:LEU:CD1	1:A:186:LEU:HD11	2.49	0.42
2:B:395:PRO:CA	2:B:398:VAL:HG12	2.48	0.42
4:D:68:VAL:HG21	4:D:92:PRO:HG2	2.02	0.42
4:D:95:TYR:HA	4:D:96:PRO:HD3	1.73	0.42
5:E:16:PRO:HA	5:E:17:PRO:HD2	1.90	0.42
5:E:134:ILE:HD12	5:E:185:TYR:CG	2.55	0.42
7:G:49:ALA:N	7:G:50:PRO:HD2	2.35	0.42
1:A:163:LEU:HG	1:A:234:CYS:SG	2.60	0.41
1:A:237:THR:O	1:A:238:GLY:C	2.62	0.41
3:C:27:ASN:CA	6:F:70:MET:HB2	2.50	0.41
3:C:116:THR:O	3:C:117:GLY:C	2.62	0.41
3:C:166:TRP:C	3:C:166:TRP:HD1	2.27	0.41
3:C:361:THR:C	3:C:366:LEU:HD23	2.45	0.41
3:C:364:LEU:N	3:C:364:LEU:HD12	2.35	0.41
4:D:202:LYS:O	4:D:203:ARG:C	2.59	0.41
5:E:171:ILE:N	5:E:179:ASN:OD1	2.46	0.41
7:G:77:TYR:C	7:G:79:ASN:N	2.78	0.41
8:H:44:VAL:C	8:H:46:SER:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:107:UNK:HA	9:I:115:UNK:O	2.20	0.41
1:A:64:PHE:O	1:A:66:GLY:N	2.52	0.41
1:A:279:HIS:HA	1:A:307:PHE:CE1	2.55	0.41
2:B:146:ILE:CG1	2:B:147:ASP:N	2.79	0.41
2:B:180:ASP:O	2:B:182:ARG:N	2.54	0.41
2:B:268:GLU:O	2:B:268:GLU:HG2	2.19	0.41
3:C:282:LEU:HD22	3:C:291:GLY:O	2.19	0.41
4:D:54:VAL:HG21	4:D:192:TRP:CE3	2.55	0.41
4:D:204:MET:O	4:D:205:GLY:C	2.61	0.41
10:J:45:HIS:C	10:J:47:ASN:H	2.28	0.41
1:A:89:TYR:CD1	1:A:89:TYR:C	2.98	0.41
1:A:311:SER:O	1:A:312:ILE:C	2.63	0.41
1:A:343:MET:HE2	1:A:343:MET:CA	2.48	0.41
1:A:438:ARG:C	1:A:440:GLY:N	2.77	0.41
2:B:111:CYS:SG	2:B:112:LEU:N	2.92	0.41
2:B:264:ILE:HD11	2:B:317:SER:HA	2.01	0.41
2:B:394:PRO:C	2:B:396:SER:N	2.78	0.41
3:C:95:ILE:HD13	3:C:121:LEU:HD13	2.01	0.41
3:C:123:THR:O	3:C:124:LEU:C	2.62	0.41
3:C:125:MET:HB3	14:C:385:SIG:H281	2.02	0.41
3:C:131:GLY:O	3:C:134:LEU:N	2.46	0.41
3:C:162:VAL:O	3:C:165:ALA:N	2.53	0.41
3:C:167:GLY:HA3	3:C:174:PRO:CG	2.50	0.41
3:C:167:GLY:HA3	3:C:175:THR:HG22	2.01	0.41
4:D:175:THR:HA	4:D:176:PRO:HD3	1.82	0.41
8:H:72:LYS:O	8:H:75:ASN:ND2	2.54	0.41
1:A:169:GLY:O	5:E:3:THR:HG21	2.20	0.41
2:B:33:LEU:HD23	2:B:220:ALA:HB1	2.02	0.41
2:B:189:VAL:O	2:B:190:GLU:C	2.63	0.41
2:B:221:GLU:HG3	2:B:222:GLN:N	2.36	0.41
2:B:353:SER:OG	2:B:355:GLU:HB3	2.20	0.41
2:B:378:PHE:CD1	2:B:378:PHE:C	2.98	0.41
3:C:51:LEU:HD12	3:C:51:LEU:HA	1.74	0.41
3:C:103:LEU:HD12	3:C:326:PHE:CE1	2.56	0.41
3:C:104:TYR:O	3:C:105:TYR:CG	2.73	0.41
3:C:137:GLY:O	3:C:138:GLN:C	2.61	0.41
3:C:224:TYR:HB3	4:D:227:TRP:CZ2	2.54	0.41
3:C:249:ASN:O	3:C:250:LEU:C	2.61	0.41
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.49	0.41
3:C:355:ALA:O	3:C:357:LEU:N	2.53	0.41
3:C:369:THR:C	3:C:371:GLY:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:171:ILE:HG23	5:E:171:ILE:O	2.18	0.41
8:H:47:ARG:CD	8:H:48:SER:N	2.82	0.41
3:C:30:ALA:C	3:C:32:TRP:N	2.76	0.41
13:C:384:PEE:O5	7:G:48:VAL:HG21	2.19	0.41
4:D:150:ASN:O	4:D:156:GLN:HA	2.21	0.41
4:D:151:PRO:HB2	8:H:59:PHE:HE1	1.84	0.41
16:D:243:HEC:HBB3	16:D:243:HEC:CMB	2.50	0.41
5:E:78:LEU:HD13	5:E:132:TRP:NE1	2.34	0.41
6:F:64:ARG:HB3	6:F:64:ARG:HH11	1.85	0.41
10:J:54:HIS:O	10:J:57:HIS:NE2	2.53	0.41
1:A:46:ARG:CD	1:A:231:LEU:HD13	2.50	0.41
1:A:65:LYS:N	1:A:65:LYS:CD	2.83	0.41
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.66	0.41
1:A:364:ALA:O	1:A:365:LEU:C	2.63	0.41
2:B:150:VAL:HA	2:B:153:GLN:HG3	2.01	0.41
2:B:277:HIS:CE1	2:B:364:LEU:HD21	2.56	0.41
2:B:399:LEU:C	2:B:401:GLN:N	2.78	0.41
2:B:436:VAL:HG23	2:B:437:ASP:N	2.36	0.41
3:C:253:ASP:OD1	3:C:253:ASP:C	2.63	0.41
5:E:129:LYS:HA	5:E:130:PRO:HD3	1.87	0.41
10:J:23:THR:O	10:J:27:GLY:N	2.46	0.41
1:A:382:GLU:HG2	1:A:390:ILE:H	1.85	0.41
2:B:111:CYS:O	2:B:112:LEU:CB	2.68	0.41
2:B:248:ASN:ND2	2:B:249:GLY:N	2.61	0.41
2:B:330:ALA:O	2:B:333:ALA:CB	2.68	0.41
3:C:27:ASN:CG	3:C:27:ASN:O	2.62	0.41
3:C:64:PHE:CE2	3:C:259:PRO:HG3	2.56	0.41
3:C:113:THR:CG2	3:C:201:LEU:HA	2.48	0.41
3:C:246:PHE:O	4:D:201:ARG:NH1	2.54	0.41
6:F:34:ASP:O	6:F:37:ILE:HG13	2.21	0.41
3:C:31:TRP:HZ3	13:C:384:PEE:H22	1.86	0.41
3:C:112:GLU:O	3:C:113:THR:C	2.63	0.41
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.03	0.41
4:D:113:LEU:HA	4:D:116:ILE:HB	2.02	0.41
4:D:228:SER:HB2	7:G:23:GLN:CD	2.46	0.41
10:J:10:TYR:CD1	10:J:10:TYR:C	2.97	0.41
1:A:23:VAL:N	1:A:192:ALA:HB1	2.34	0.41
1:A:39:VAL:O	1:A:39:VAL:HG13	2.20	0.41
1:A:59:LEU:O	1:A:60:GLU:C	2.62	0.41
2:B:101:THR:CG2	2:B:102:ARG:N	2.81	0.41
2:B:135:TRP:O	2:B:136:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:HIS:CD2	2:B:203:ARG:NH2	2.88	0.41
2:B:277:HIS:CD2	2:B:363:LYS:HB2	2.56	0.41
2:B:409:ASP:OD1	2:B:409:ASP:N	2.54	0.41
2:B:436:VAL:O	2:B:438:GLU:N	2.54	0.41
3:C:26:SER:HA	3:C:219:ILE:HD11	2.02	0.41
3:C:34:PHE:CZ	3:C:97:LEU:HD13	2.56	0.41
3:C:167:GLY:HA3	3:C:174:PRO:HG2	2.02	0.41
3:C:319:ARG:HH22	3:C:371:GLY:CA	2.30	0.41
3:C:321:LEU:HB2	3:C:374:GLU:CD	2.46	0.41
14:C:385:SIG:H23	14:C:385:SIG:H343	1.79	0.41
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.55	0.41
5:E:32:ARG:NH2	7:G:25:PRO:HD2	2.36	0.41
6:F:34:ASP:OD1	6:F:34:ASP:N	2.54	0.41
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.56	0.41
7:G:68:LYS:C	7:G:70:LYS:N	2.79	0.41
1:A:64:PHE:CZ	1:A:86:LEU:HG	2.56	0.41
1:A:253:VAL:O	1:A:323:TYR:HA	2.21	0.41
1:A:289:HIS:C	1:A:290:SER:O	2.61	0.41
2:B:105:MET:CE	2:B:107:TYR:HE1	2.32	0.41
2:B:200:THR:HG22	2:B:226:ILE:CG2	2.51	0.41
2:B:331:ALA:C	2:B:333:ALA:H	2.29	0.41
2:B:394:PRO:C	2:B:396:SER:H	2.29	0.41
2:B:403:ASP:O	2:B:404:ALA:C	2.64	0.41
3:C:27:ASN:ND2	6:F:69:ASN:HD22	2.18	0.41
4:D:21:LEU:CD1	4:D:192:TRP:HB2	2.51	0.41
4:D:86:LYS:N	4:D:89:ASP:OD1	2.49	0.41
5:E:46:GLY:O	5:E:49:TYR:HB3	2.21	0.41
5:E:60:SER:C	5:E:62:MET:N	2.79	0.41
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.56	0.41
5:E:163:SER:HA	5:E:174:GLY:HA3	2.03	0.41
1:A:53:ASN:C	1:A:53:ASN:ND2	2.79	0.40
1:A:56:GLY:CA	1:A:185:TYR:CE2	2.97	0.40
1:A:79:VAL:O	1:A:80:GLU:C	2.63	0.40
1:A:388:ARG:HD3	1:A:388:ARG:N	2.31	0.40
2:B:61:SER:C	2:B:63:LEU:N	2.78	0.40
2:B:250:ASP:C	2:B:252:LEU:N	2.77	0.40
2:B:280:GLY:O	2:B:282:ASN:N	2.54	0.40
3:C:9:HIS:O	3:C:11:LEU:N	2.54	0.40
3:C:50:LEU:HD12	11:C:381:HEM:HBC1	2.02	0.40
3:C:139:MET:O	3:C:140:SER:C	2.64	0.40
4:D:47:ALA:O	4:D:48:TYR:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:116:ILE:HG21	4:D:190:LEU:HD13	2.01	0.40
8:H:47:ARG:CD	8:H:48:SER:H	2.22	0.40
1:A:65:LYS:NZ	9:I:311:UNK:CA	2.77	0.40
1:A:192:ALA:N	1:A:193:PRO:HD2	2.35	0.40
1:A:365:LEU:HD21	1:A:395:TRP:HB3	2.03	0.40
2:B:34:VAL:HG11	2:B:386:ALA:O	2.21	0.40
2:B:77:THR:CB	2:B:125:ASN:HB3	2.51	0.40
3:C:13:LYS:HE2	3:C:17:ASN:ND2	2.36	0.40
3:C:172:ASP:N	3:C:175:THR:HG23	2.19	0.40
3:C:211:GLY:HA3	3:C:315:THR:HG23	2.03	0.40
3:C:285:ILE:CG2	3:C:291:GLY:HA2	2.51	0.40
3:C:295:LEU:HD12	3:C:295:LEU:HA	1.82	0.40
4:D:160:MET:HB2	16:D:243:HEC:C1D	2.50	0.40
4:D:207:LYS:O	4:D:211:MET:HG2	2.21	0.40
5:E:15:ARG:HH11	5:E:19:ASP:HB3	1.86	0.40
5:E:29:ASP:C	5:E:31:SER:N	2.60	0.40
5:E:81:ILE:HD13	5:E:98:VAL:CG1	2.51	0.40
8:H:15:ASP:HA	8:H:16:PRO:HD2	1.97	0.40
1:A:405:ARG:HG2	1:A:405:ARG:HH11	1.85	0.40
2:B:37:SER:O	2:B:38:LEU:CB	2.69	0.40
2:B:47:ILE:HD11	2:B:116:VAL:HG12	2.03	0.40
2:B:83:PHE:O	2:B:84:LYS:C	2.64	0.40
2:B:206:LEU:O	2:B:216:LEU:HD21	2.21	0.40
2:B:268:GLU:HG2	2:B:272:PHE:HE1	1.86	0.40
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.89	0.40
3:C:106:GLY:C	3:C:108:TYR:N	2.73	0.40
3:C:202:HIS:NE2	12:C:383:U10:H1M1	2.35	0.40
3:C:292:VAL:O	3:C:295:LEU:HB3	2.22	0.40
3:C:327:TRP:HB2	7:G:51:PRO:HG3	2.03	0.40
4:D:160:MET:HB2	16:D:243:HEC:C2D	2.51	0.40
6:F:46:ALA:O	6:F:47:ILE:C	2.63	0.40
6:F:87:VAL:HG23	6:F:87:VAL:O	2.21	0.40
8:H:66:ASP:HA	8:H:69:VAL:HB	2.04	0.40
1:A:40:TRP:CE3	1:A:96:ALA:HB2	2.57	0.40
1:A:110:VAL:HA	1:A:113:LEU:HD12	2.03	0.40
1:A:147:GLU:O	1:A:148:VAL:C	2.64	0.40
1:A:346:CYS:HB3	1:A:411:CYS:HB3	2.03	0.40
2:B:222:GLN:C	2:B:224:LEU:N	2.79	0.40
3:C:114:TRP:HE3	11:C:382:HEM:HMD1	1.87	0.40
3:C:129:PHE:C	3:C:130:VAL:O	2.63	0.40
3:C:163:GLU:HB3	3:C:169:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:147:LEU:N	4:D:147:LEU:CD2	2.84	0.40
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.85	0.40
7:G:73:ASN:C	7:G:75:ALA:N	2.78	0.40
7:G:79:ASN:ND2	7:G:79:ASN:N	2.69	0.40
1:A:40:TRP:N	1:A:40:TRP:CD1	2.89	0.40
2:B:232:LEU:O	2:B:233:SER:C	2.65	0.40
2:B:367:LYS:O	2:B:371:SER:HB2	2.21	0.40
3:C:91:PHE:CE1	3:C:124:LEU:HG	2.56	0.40
3:C:222:HIS:O	3:C:224:TYR:N	2.55	0.40
3:C:310:LYS:HB3	3:C:372:THR:HG23	2.04	0.40
4:D:47:ALA:C	4:D:49:ARG:N	2.78	0.40
4:D:78:GLY:O	4:D:79:GLU:CG	2.68	0.40
4:D:195:GLU:OE2	4:D:201:ARG:NH2	2.55	0.40
8:H:69:VAL:CG1	8:H:73:LEU:HD12	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	440/446 (99%)	337 (77%)	85 (19%)	18 (4%)	2 19
2	B	404/422 (96%)	295 (73%)	78 (19%)	31 (8%)	1 8
3	C	377/380 (99%)	278 (74%)	68 (18%)	31 (8%)	0 8
4	D	239/241 (99%)	194 (81%)	34 (14%)	11 (5%)	2 17
5	E	194/196 (99%)	151 (78%)	28 (14%)	15 (8%)	1 8
6	F	98/109 (90%)	84 (86%)	12 (12%)	2 (2%)	6 32
7	G	76/81 (94%)	52 (68%)	18 (24%)	6 (8%)	1 8
8	H	64/78 (82%)	56 (88%)	7 (11%)	1 (2%)	7 36
10	J	57/62 (92%)	32 (56%)	20 (35%)	5 (9%)	0 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1949/2015 (97%)	1479 (76%)	350 (18%)	120 (6%)	1 12

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
1	A	284	TYR
2	B	19	PRO
2	B	20	HIS
2	B	23	ASP
2	B	38	LEU
2	B	113	ARG
2	B	132	PHE
2	B	170	ASN
2	B	171	ALA
2	B	228	GLY
2	B	233	SER
2	B	290	ASN
2	B	410	VAL
3	C	5	ILE
3	C	111	LYS
3	C	167	GLY
3	C	208	ASN
3	C	222	HIS
3	C	284	SER
3	C	349	ILE
3	C	357	LEU
4	D	73	GLY
4	D	75	ASN
4	D	198	HIS
4	D	233	ARG
5	E	11	SER
5	E	21	SER
5	E	58	PHE
5	E	72	SER
7	G	27	PRO
7	G	43	ALA
10	J	5	LEU
10	J	56	LYS
10	J	61	ASN
1	A	65	LYS
1	A	128	GLU

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Mol	Chain	Res	Type
1	A	289	HIS
1	A	291	SER
2	B	210	GLY
2	B	218	ASN
2	B	229	GLY
2	B	261	SER
2	B	372	VAL
2	B	386	ALA
2	B	430	LEU
3	C	58	ALA
3	C	164	TRP
3	C	170	SER
4	D	38	SER
4	D	78	GLY
4	D	106	ASN
4	D	236	ALA
5	E	15	ARG
5	E	17	PRO
5	E	26	ARG
5	E	66	ALA
7	G	33	GLY
1	A	55	ALA
1	A	56	GLY
1	A	72	GLN
1	A	103	SER
1	A	141	ASN
1	A	267	LEU
1	A	285	GLY
2	B	63	LEU
2	B	111	CYS
2	B	181	TYR
2	B	190	GLU
2	B	330	ALA
2	B	371	SER
2	B	407	ASP
3	C	31	TRP
3	C	105	TYR
3	C	207	ASN
3	C	286	PRO
5	E	30	PRO
6	F	53	ASN
10	J	60	GLU

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Mol	Chain	Res	Type
1	A	71	PRO
1	A	292	SER
2	B	83	PHE
2	B	260	GLU
2	B	406	ALA
3	C	4	ASN
3	C	63	ALA
3	C	156	TYR
3	C	159	HIS
3	C	224	TYR
3	C	379	ASN
4	D	240	PRO
5	E	27	GLU
5	E	61	SER
1	A	286	GLY
1	A	382	GLU
1	A	398	ARG
2	B	404	ALA
3	C	10	PRO
3	C	202	HIS
3	C	321	LEU
3	C	359	TYR
5	E	62	MET
5	E	70	ALA
7	G	74	PRO
8	H	65	ARG
10	J	15	ARG
3	C	274	TYR
4	D	176	PRO
5	E	71	MET
5	E	177	PRO
6	F	19	TRP
2	B	249	GLY
3	C	158	GLY
3	C	205	GLY
3	C	352	GLY
7	G	26	PHE
3	C	157	ILE
3	C	259	PRO
4	D	133	GLY
7	G	50	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/376 (96%)	336 (94%)	23 (6%)	16	42
2	B	307/336 (91%)	291 (95%)	16 (5%)	21	47
3	C	326/329 (99%)	298 (91%)	28 (9%)	10	33
4	D	201/207 (97%)	189 (94%)	12 (6%)	17	44
5	E	165/169 (98%)	153 (93%)	12 (7%)	13	38
6	F	90/98 (92%)	81 (90%)	9 (10%)	7	28
7	G	60/72 (83%)	55 (92%)	5 (8%)	10	34
8	H	51/74 (69%)	51 (100%)	0	100	100
10	J	41/52 (79%)	39 (95%)	2 (5%)	22	48
All	All	1600/1713 (93%)	1493 (93%)	107 (7%)	15	41

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	100	LYS
1	A	102	LEU
1	A	108	LYS
1	A	148	VAL
1	A	168	GLU
1	A	182	LEU
1	A	220	PRO
1	A	226	ASP
1	A	250	LEU
1	A	316	GLU
1	A	342	TRP
1	A	361	LEU
1	A	368	HIS
1	A	382	GLU
1	A	384	LEU
1	A	388	ARG
1	A	395	TRP

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Mol	Chain	Res	Type
1	A	399	LEU
1	A	409	GLU
1	A	422	VAL
1	A	443	TRP
1	A	444	LEU
2	B	21	PRO
2	B	57	TYR
2	B	62	ASN
2	B	109	VAL
2	B	112	LEU
2	B	135	TRP
2	B	170	ASN
2	B	221	GLU
2	B	225	ASN
2	B	247	GLN
2	B	248	ASN
2	B	325	TYR
2	B	343	GLN
2	B	402	ILE
2	B	407	ASP
2	B	437	ASP
3	C	4	ASN
3	C	28	ILE
3	C	43	MET
3	C	104	TYR
3	C	124	LEU
3	C	133	VAL
3	C	136	TRP
3	C	145	THR
3	C	149	ASN
3	C	152	SER
3	C	164	TRP
3	C	175	THR
3	C	185	LEU
3	C	208	ASN
3	C	216	SER
3	C	219	ILE
3	C	258	THR
3	C	259	PRO
3	C	272	GLU
3	C	282	LEU
3	C	285	ILE

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Mol	Chain	Res	Type
3	C	307	PHE
3	C	325	LEU
3	C	330	VAL
3	C	333	LEU
3	C	342	GLN
3	C	350	ILE
3	C	354	MET
4	D	36	VAL
4	D	75	ASN
4	D	82	MET
4	D	99	GLU
4	D	136	GLU
4	D	163	PRO
4	D	181	GLN
4	D	192	TRP
4	D	196	PRO
4	D	197	GLU
4	D	209	LEU
4	D	224	ARG
5	E	11	SER
5	E	32	ARG
5	E	36	SER
5	E	45	LEU
5	E	74	ILE
5	E	79	SER
5	E	81	ILE
5	E	86	ASN
5	E	113	GLU
5	E	136	ILE
5	E	171	ILE
5	E	191	ASP
6	F	12	TRP
6	F	31	LEU
6	F	37	ILE
6	F	59	MET
6	F	64	ARG
6	F	73	GLN
6	F	75	LEU
6	F	81	THR
6	F	107	TRP
7	G	22	GLU
7	G	26	PHE

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Mol	Chain	Res	Type
7	G	27	PRO
7	G	41	LEU
7	G	77	TYR
10	J	13	LEU
10	J	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	53	ASN
1	A	69	ASN
1	A	85	HIS
1	A	118	GLN
1	A	139	GLN
1	A	151	ASN
1	A	165	GLN
1	A	207	GLN
1	A	274	ASN
1	A	301	ASN
1	A	308	GLN
1	A	339	GLN
1	A	363	ASN
2	B	22	GLN
2	B	62	ASN
2	B	225	ASN
2	B	248	ASN
2	B	254	HIS
2	B	277	HIS
2	B	284	HIS
2	B	335	GLN
2	B	342	ASN
2	B	343	GLN
2	B	349	GLN
2	B	351	ASN
2	B	356	ASN
2	B	400	GLN
2	B	421	GLN
2	B	429	ASN
3	C	16	ASN
3	C	17	ASN
3	C	55	HIS

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Mol	Chain	Res	Type
3	C	82	ASN
3	C	86	ASN
3	C	138	GLN
3	C	207	ASN
3	C	261	ASN
3	C	323	GLN
3	C	332	ASN
3	C	342	GLN
3	C	353	GLN
4	D	31	GLN
4	D	35	GLN
4	D	75	ASN
4	D	156	GLN
4	D	225	HIS
5	E	9	ASN
5	E	57	GLN
5	E	86	ASN
6	F	69	ASN
6	F	72	GLN
7	G	64	GLN
7	G	79	ASN
8	H	75	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	PEE	C	384	-	48,48,50	2.67	11 (22%)	51,53,55	4.31	17 (33%)
15	BOG	D	242	-	20,20,20	1.14	2 (10%)	25,25,25	0.85	1 (4%)
17	FES	E	197	5	0,4,4	-	-	-		
14	SIG	C	385	-	35,36,36	3.22	14 (40%)	42,50,50	1.76	10 (23%)
11	HEM	C	382	3	50,50,50	1.61	10 (20%)	67,82,82	2.28	26 (38%)
16	HEC	D	243	4	50,50,50	1.14	2 (4%)	68,82,82	1.96	19 (27%)
11	HEM	C	381	3	50,50,50	1.48	6 (12%)	67,82,82	2.08	21 (31%)
12	U10	C	383	-	29,29,63	3.16	5 (17%)	36,38,79	2.00	11 (30%)
13	PEE	E	198	-	48,48,50	2.57	9 (18%)	51,53,55	4.34	18 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PEE	C	384	-	1/1/4/8	22/52/52/54	-
15	BOG	D	242	-	-	5/11/31/31	0/1/1/1
17	FES	E	197	5	-	-	0/1/1/1
14	SIG	C	385	-	-	16/30/30/30	0/2/2/2
11	HEM	C	382	3	-	11/14/54/54	-
16	HEC	D	243	4	1/1/3/7	10/14/54/54	-
11	HEM	C	381	3	-	6/14/54/54	-
12	U10	C	383	-	-	6/23/47/87	0/1/1/1
13	PEE	E	198	-	1/1/4/8	26/52/52/54	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	385	SIG	C24-C23	-13.33	1.47	1.55
12	C	383	U10	C13-C14	12.71	1.62	1.33
13	E	198	PEE	O5-C30	11.67	1.57	1.22
13	C	384	PEE	O5-C30	11.20	1.55	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	383	U10	C6-C1	7.41	1.48	1.35
13	C	384	PEE	O2-C10	6.33	1.52	1.34
14	C	385	SIG	C37-C36	5.60	1.37	1.33
13	C	384	PEE	C18-C19	5.37	1.62	1.31
13	C	384	PEE	C39-C38	5.08	1.60	1.31
13	E	198	PEE	O2-C10	4.96	1.48	1.34
13	E	198	PEE	C39-C38	4.94	1.59	1.31
13	E	198	PEE	C18-C19	4.85	1.59	1.31
12	C	383	U10	C7-C6	4.82	1.60	1.51
11	C	382	HEM	FE-NA	-4.52	1.80	1.95
14	C	385	SIG	O7-C8	4.39	1.41	1.36
13	C	384	PEE	C11-C10	4.22	1.63	1.50
14	C	385	SIG	C9-C8	4.11	1.42	1.34
13	E	198	PEE	C11-C10	3.72	1.61	1.50
14	C	385	SIG	C20-C8	3.69	1.59	1.49
14	C	385	SIG	O14-C5	3.66	1.43	1.37
11	C	381	HEM	CAB-C3B	-3.62	1.37	1.47
14	C	385	SIG	O13-C1	3.61	1.43	1.37
11	C	382	HEM	CAB-C3B	-3.59	1.37	1.47
12	C	383	U10	C3-C2	-3.56	1.38	1.48
14	C	385	SIG	C2-C3	3.55	1.45	1.39
13	E	198	PEE	C21-C22	-3.49	1.34	1.51
13	E	198	PEE	C42-C41	-3.40	1.34	1.51
13	C	384	PEE	C42-C41	-3.37	1.35	1.51
14	C	385	SIG	C6-C1	3.31	1.44	1.38
13	C	384	PEE	C21-C22	-3.30	1.35	1.51
13	C	384	PEE	C31-C30	-3.29	1.41	1.50
14	C	385	SIG	C21-C22	3.27	1.62	1.54
11	C	381	HEM	CAC-C3C	-3.22	1.38	1.47
13	E	198	PEE	C31-C30	-3.13	1.41	1.50
14	C	385	SIG	O7-C3	3.12	1.42	1.38
11	C	382	HEM	CAC-C3C	-3.07	1.39	1.47
14	C	385	SIG	C6-C5	3.05	1.44	1.38
11	C	382	HEM	CHB-C1B	-3.01	1.32	1.38
14	C	385	SIG	C31-C30	2.62	1.52	1.44
11	C	381	HEM	FE-NA	-2.62	1.86	1.95
11	C	382	HEM	C3B-C4B	2.61	1.50	1.44
11	C	381	HEM	CHD-C4C	-2.56	1.33	1.38
13	C	384	PEE	P-O3P	2.52	1.69	1.59
15	D	242	BOG	C4-C5	2.51	1.58	1.53
12	C	383	U10	C8-C9	2.45	1.38	1.33
15	D	242	BOG	O5-C1	2.44	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	382	HEM	CMA-C3A	2.36	1.55	1.50
11	C	382	HEM	C1B-NB	-2.33	1.36	1.40
13	C	384	PEE	C1-C2	2.29	1.58	1.50
13	E	198	PEE	O2-C2	-2.27	1.41	1.46
13	C	384	PEE	O2-C2	-2.25	1.41	1.46
11	C	381	HEM	CHA-C1A	-2.20	1.34	1.39
11	C	382	HEM	C4A-NA	-2.11	1.35	1.39
11	C	381	HEM	CHD-C1D	-2.10	1.34	1.39
16	D	243	HEC	CMA-C3A	2.09	1.55	1.50
14	C	385	SIG	C4-C5	2.09	1.44	1.40
16	D	243	HEC	C1A-NA	-2.07	1.35	1.39
11	C	382	HEM	C1D-C2D	2.05	1.48	1.44
11	C	382	HEM	CAA-C2A	2.03	1.56	1.51

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	384	PEE	O4-C10-C11	-18.59	51.07	123.78
13	E	198	PEE	O4-C10-C11	-18.55	51.22	123.78
13	E	198	PEE	O3-C30-C31	13.03	151.56	111.83
13	C	384	PEE	O3-C30-C31	12.96	151.35	111.83
13	C	384	PEE	O3-C30-O5	-11.40	95.11	123.63
13	E	198	PEE	O3-C30-O5	-11.40	95.11	123.63
13	E	198	PEE	O2-C2-C3	8.12	137.47	108.34
13	C	384	PEE	O2-C2-C3	7.77	136.21	108.34
13	E	198	PEE	O2-C10-C11	7.10	126.85	111.48
13	C	384	PEE	O2-C10-C11	6.99	126.60	111.48
13	E	198	PEE	C12-C11-C10	-6.59	89.54	113.69
13	E	198	PEE	O2-C10-O4	-6.30	108.98	123.70
13	C	384	PEE	O2-C10-O4	-6.29	109.01	123.70
13	C	384	PEE	C12-C11-C10	-6.00	91.70	113.69
11	C	381	HEM	CAD-C3D-C4D	5.60	134.46	124.70
11	C	381	HEM	CMB-C2B-C1B	5.55	133.71	125.03
11	C	382	HEM	C2B-C1B-NB	5.29	115.92	109.84
12	C	383	U10	C12-C13-C14	-5.28	115.54	127.62
16	D	243	HEC	CMD-C2D-C1D	5.16	133.10	125.03
11	C	381	HEM	C3B-C4B-NB	4.91	113.00	109.47
16	D	243	HEC	CAD-C3D-C4D	4.84	133.14	124.70
14	C	385	SIG	C39-C36-C32	-4.80	110.75	118.09
11	C	381	HEM	CAD-C3D-C2D	-4.80	118.87	127.87
13	C	384	PEE	O3-C3-C2	4.72	121.99	108.40
11	C	381	HEM	CMD-C2D-C1D	4.69	132.37	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	382	HEM	CBA-CAA-C2A	4.66	125.43	112.53
13	E	198	PEE	O3-C3-C2	4.56	121.55	108.40
11	C	382	HEM	CAA-C2A-C1A	4.55	133.82	124.94
11	C	382	HEM	CHB-C1B-NB	-4.46	118.85	124.37
14	C	385	SIG	C24-C23-C22	4.32	117.59	113.89
16	D	243	HEC	C4A-C3A-C2A	-4.08	100.92	106.97
12	C	383	U10	C1-C6-C5	-4.07	115.66	119.62
11	C	382	HEM	CHC-C4B-NB	-4.03	120.08	124.42
16	D	243	HEC	CBA-CAA-C2A	3.99	123.57	112.53
16	D	243	HEC	CAD-C3D-C2D	-3.99	120.40	127.87
16	D	243	HEC	CAC-C3C-C4C	-3.98	119.44	124.91
11	C	381	HEM	CBD-CAD-C3D	3.95	123.47	112.53
11	C	382	HEM	C3B-C2B-C1B	-3.92	103.47	106.41
12	C	383	U10	C15-C14-C16	3.89	121.98	115.23
11	C	382	HEM	CMC-C2C-C1C	3.83	131.47	124.73
11	C	382	HEM	CMB-C2B-C1B	3.82	131.00	125.03
12	C	383	U10	O2-C2-C3	-3.76	113.06	121.03
11	C	382	HEM	C3D-C4D-ND	3.71	114.24	110.17
12	C	383	U10	C15-C14-C13	-3.68	114.19	123.63
12	C	383	U10	C10-C9-C8	-3.57	114.45	123.63
16	D	243	HEC	CAA-C2A-C1A	-3.56	117.62	124.85
11	C	382	HEM	C4D-ND-C1D	-3.49	101.07	105.21
13	C	384	PEE	C42-C41-C40	3.48	130.59	113.86
13	E	198	PEE	C22-C21-C20	3.43	130.37	113.86
14	C	385	SIG	C35-C24-C23	3.41	114.25	111.03
13	E	198	PEE	C42-C41-C40	3.37	130.08	113.86
16	D	243	HEC	CMA-C3A-C4A	3.37	130.67	124.73
11	C	382	HEM	CMD-C2D-C1D	3.29	130.18	125.03
16	D	243	HEC	CMC-C2C-C1C	3.24	130.35	125.42
14	C	385	SIG	O15-C10-C9	-3.24	116.19	120.45
13	C	384	PEE	C12-C13-C14	-3.18	98.28	114.37
11	C	381	HEM	CBA-CAA-C2A	-3.18	103.73	112.53
11	C	382	HEM	C2A-C1A-NA	3.16	113.66	110.15
11	C	382	HEM	CHD-C1D-ND	-3.16	121.03	124.42
13	C	384	PEE	C22-C21-C20	3.03	128.44	113.86
13	E	198	PEE	C34-C33-C32	-3.03	99.04	114.37
11	C	382	HEM	CMC-C2C-C3C	-3.02	121.12	128.43
15	D	242	BOG	C1'-O1-C1	2.98	118.77	113.68
13	E	198	PEE	C33-C32-C31	2.95	123.95	113.13
11	C	381	HEM	C1B-NB-C4B	-2.94	101.72	105.21
13	C	384	PEE	C33-C32-C31	2.91	123.82	113.13
14	C	385	SIG	O7-C8-C9	-2.91	119.26	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	381	HEM	CMB-C2B-C3B	-2.89	121.43	128.43
11	C	382	HEM	CAD-C3D-C4D	2.87	129.69	124.70
16	D	243	HEC	CMB-C2B-C1B	2.82	129.45	125.03
11	C	381	HEM	CHC-C4B-NB	-2.82	121.39	124.42
16	D	243	HEC	C2B-C1B-NB	2.81	113.15	109.90
11	C	382	HEM	C1B-NB-C4B	-2.77	101.92	105.21
13	C	384	PEE	C34-C33-C32	-2.76	100.39	114.37
11	C	382	HEM	C4A-NA-C1A	-2.74	101.36	105.82
13	E	198	PEE	C12-C13-C14	-2.73	100.58	114.37
16	D	243	HEC	CHA-C4D-ND	-2.70	121.52	124.42
13	E	198	PEE	O5-C30-C31	-2.67	113.32	123.78
12	C	383	U10	C10-C9-C11	2.67	119.85	115.23
13	C	384	PEE	O5-C30-C31	-2.65	113.41	123.78
11	C	382	HEM	CAB-C3B-C2B	-2.64	119.84	128.43
16	D	243	HEC	CAC-C3C-C2C	2.64	131.07	126.89
11	C	381	HEM	C4D-ND-C1D	-2.64	102.08	105.21
11	C	382	HEM	CHB-C4A-C3A	-2.63	119.78	127.43
11	C	382	HEM	CAC-C3C-C4C	2.62	131.07	124.82
11	C	381	HEM	C2B-C1B-NB	2.51	112.73	109.84
13	E	198	PEE	C3-C2-C1	-2.48	106.00	111.78
13	C	384	PEE	O2-C2-C1	2.44	117.11	108.34
11	C	382	HEM	C1A-C2A-C3A	-2.43	103.11	106.87
16	D	243	HEC	C3A-C4A-NA	2.41	114.09	109.64
11	C	381	HEM	C4C-C3C-C2C	-2.40	104.74	106.81
13	E	198	PEE	C36-C35-C34	-2.38	102.32	114.37
14	C	385	SIG	C33-C9-C8	2.37	126.79	123.28
11	C	382	HEM	C3B-C4B-NB	2.36	111.16	109.47
12	C	383	U10	C3-C2-C1	2.34	122.72	118.10
14	C	385	SIG	C6-C1-C2	-2.33	118.38	120.59
14	C	385	SIG	O7-C3-C2	2.31	120.86	116.28
11	C	382	HEM	CBD-CAD-C3D	2.30	118.90	112.53
16	D	243	HEC	CHD-C1D-ND	-2.28	121.55	124.37
13	E	198	PEE	O2-C2-C1	2.28	116.52	108.34
13	C	384	PEE	C14-C15-C16	-2.25	102.99	114.37
11	C	381	HEM	C2D-C1D-ND	2.23	112.48	109.90
13	C	384	PEE	C3-C2-C1	-2.22	106.61	111.78
11	C	381	HEM	C3D-C4D-ND	2.22	112.61	110.17
11	C	382	HEM	CHA-C1A-C2A	-2.22	120.45	125.30
16	D	243	HEC	C1A-C2A-C3A	2.16	109.95	107.11
11	C	381	HEM	CHB-C4A-C3A	-2.16	121.16	127.43
11	C	382	HEM	C4C-NC-C1C	-2.16	102.31	105.82
11	C	381	HEM	CAB-C3B-C2B	-2.12	121.55	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	381	HEM	C3B-C2B-C1B	-2.09	104.84	106.41
12	C	383	U10	C8-C7-C6	2.09	117.23	112.08
16	D	243	HEC	CHB-C1B-C2B	-2.07	121.76	125.03
14	C	385	SIG	C20-C21-C22	2.06	118.31	114.46
11	C	381	HEM	CHB-C1B-NB	-2.06	121.82	124.37
16	D	243	HEC	CHC-C4B-NB	-2.05	121.83	124.37
14	C	385	SIG	C32-C36-C37	2.04	123.98	118.55
11	C	381	HEM	C4A-NA-C1A	-2.03	102.51	105.82
11	C	381	HEM	C4C-NC-C1C	-2.03	102.51	105.82
13	E	198	PEE	C14-C15-C16	-2.03	104.13	114.37
16	D	243	HEC	CMD-C2D-C3D	-2.02	120.68	126.15
11	C	382	HEM	CAC-C3C-C2C	-2.02	121.87	128.43
12	C	383	U10	C11-C9-C8	2.02	125.69	121.17
12	C	383	U10	O5-C5-C4	-2.02	116.76	121.03

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	C	384	PEE	C2
13	E	198	PEE	C2
16	D	243	HEC	NA

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	381	HEM	C2B-C3B-CAB-CBB
11	C	381	HEM	C4B-C3B-CAB-CBB
11	C	382	HEM	C1A-C2A-CAA-CBA
11	C	382	HEM	C2C-C3C-CAC-CBC
11	C	382	HEM	C4C-C3C-CAC-CBC
12	C	383	U10	C1-C6-C7-C8
12	C	383	U10	C5-C6-C7-C8
12	C	383	U10	C12-C11-C9-C10
12	C	383	U10	C14-C16-C17-C18
13	C	384	PEE	O4-C10-O2-C2
13	E	198	PEE	O4-C10-O2-C2
13	E	198	PEE	O5-C30-O3-C3
13	E	198	PEE	C31-C30-O3-C3
14	C	385	SIG	C21-C20-C8-O7
14	C	385	SIG	C21-C20-C8-C9
14	C	385	SIG	C21-C22-C23-C24
14	C	385	SIG	C21-C22-C23-C28

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Mol	Chain	Res	Type	Atoms
14	C	385	SIG	C27-C22-C23-C24
14	C	385	SIG	C27-C22-C23-C28
14	C	385	SIG	C22-C23-C24-C25
14	C	385	SIG	C22-C23-C24-C35
14	C	385	SIG	C28-C23-C24-C25
14	C	385	SIG	C28-C23-C24-C35
14	C	385	SIG	C31-C32-C36-C37
14	C	385	SIG	C31-C32-C36-C39
16	D	243	HEC	C1A-C2A-CAA-CBA
16	D	243	HEC	C3A-C2A-CAA-CBA
13	C	384	PEE	O5-C30-O3-C3
16	D	243	HEC	C4C-C3C-CAC-CBC
12	C	383	U10	C12-C11-C9-C8
13	E	198	PEE	C22-C23-C24-C25
13	C	384	PEE	C37-C38-C39-C40
13	C	384	PEE	C22-C23-C24-C25
13	C	384	PEE	C31-C30-O3-C3
13	C	384	PEE	C17-C18-C19-C20
13	E	198	PEE	C37-C38-C39-C40
16	D	243	HEC	C2B-C3B-CAB-CBB
13	E	198	PEE	C30-C31-C32-C33
16	D	243	HEC	C4B-C3B-CAB-CBB
11	C	382	HEM	C3A-C2A-CAA-CBA
15	D	242	BOG	O5-C1-O1-C1'
15	D	242	BOG	C2-C1-O1-C1'
13	C	384	PEE	C3-C2-O2-C10
13	E	198	PEE	C17-C18-C19-C20
13	E	198	PEE	C12-C13-C14-C15
13	C	384	PEE	C13-C14-C15-C16
13	E	198	PEE	C31-C32-C33-C34
13	C	384	PEE	C20-C21-C22-C23
13	E	198	PEE	C21-C22-C23-C24
13	E	198	PEE	C14-C15-C16-C17
13	E	198	PEE	C35-C36-C37-C38
15	D	242	BOG	C2'-C3'-C4'-C5'
13	E	198	PEE	C33-C34-C35-C36
15	D	242	BOG	C3'-C4'-C5'-C6'
13	E	198	PEE	C11-C12-C13-C14
13	E	198	PEE	C1-C2-C3-O3
13	E	198	PEE	C19-C20-C21-C22
13	E	198	PEE	C39-C40-C41-C42
13	C	384	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
13	C	384	PEE	C40-C41-C42-C43
13	E	198	PEE	O3P-C1-C2-O2
13	C	384	PEE	C39-C40-C41-C42
11	C	382	HEM	C3D-CAD-CBD-CGD
13	E	198	PEE	C41-C42-C43-C44
13	C	384	PEE	C41-C42-C43-C44
16	D	243	HEC	C2C-C3C-CAC-CBC
14	C	385	SIG	C20-C21-C22-C27
13	C	384	PEE	C23-C24-C25-C26
13	C	384	PEE	O3P-C1-C2-O2
13	E	198	PEE	C42-C43-C44-C45
13	C	384	PEE	O2-C2-C3-O3
13	C	384	PEE	C4-O4P-P-O1P
13	C	384	PEE	C14-C15-C16-C17
13	E	198	PEE	C36-C37-C38-C39
14	C	385	SIG	C8-C20-C21-C22
14	C	385	SIG	C29-C30-C31-C32
13	C	384	PEE	C16-C17-C18-C19
13	E	198	PEE	C20-C21-C22-C23
11	C	381	HEM	CAA-CBA-CGA-O2A
14	C	385	SIG	C20-C21-C22-C23
13	E	198	PEE	C38-C39-C40-C41
11	C	381	HEM	CAA-CBA-CGA-O1A
16	D	243	HEC	CAD-CBD-CGD-O2D
11	C	381	HEM	CAD-CBD-CGD-O2D
13	C	384	PEE	C36-C37-C38-C39
11	C	381	HEM	CAD-CBD-CGD-O1D
13	E	198	PEE	C13-C14-C15-C16
16	D	243	HEC	CAD-CBD-CGD-O1D
11	C	382	HEM	C4D-C3D-CAD-CBD
15	D	242	BOG	C4'-C5'-C6'-C7'
11	C	382	HEM	CAA-CBA-CGA-O2A
16	D	243	HEC	CAA-CBA-CGA-O2A
12	C	383	U10	C16-C17-C18-C19
11	C	382	HEM	CAD-CBD-CGD-O2D
13	E	198	PEE	C3-C2-O2-C10
11	C	382	HEM	CAA-CBA-CGA-O1A
11	C	382	HEM	C2A-CAA-CBA-CGA
16	D	243	HEC	CAA-CBA-CGA-O1A
11	C	382	HEM	CAD-CBD-CGD-O1D
13	C	384	PEE	C42-C43-C44-C45
13	C	384	PEE	O4-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	E	198	PEE	O3-C30-C31-C32

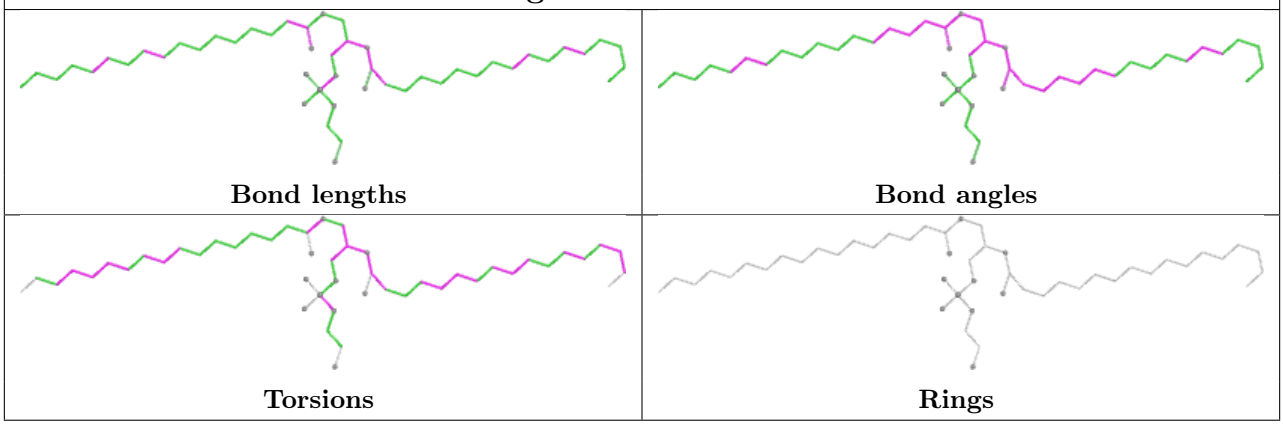
There are no ring outliers.

9 monomers are involved in 58 short contacts:

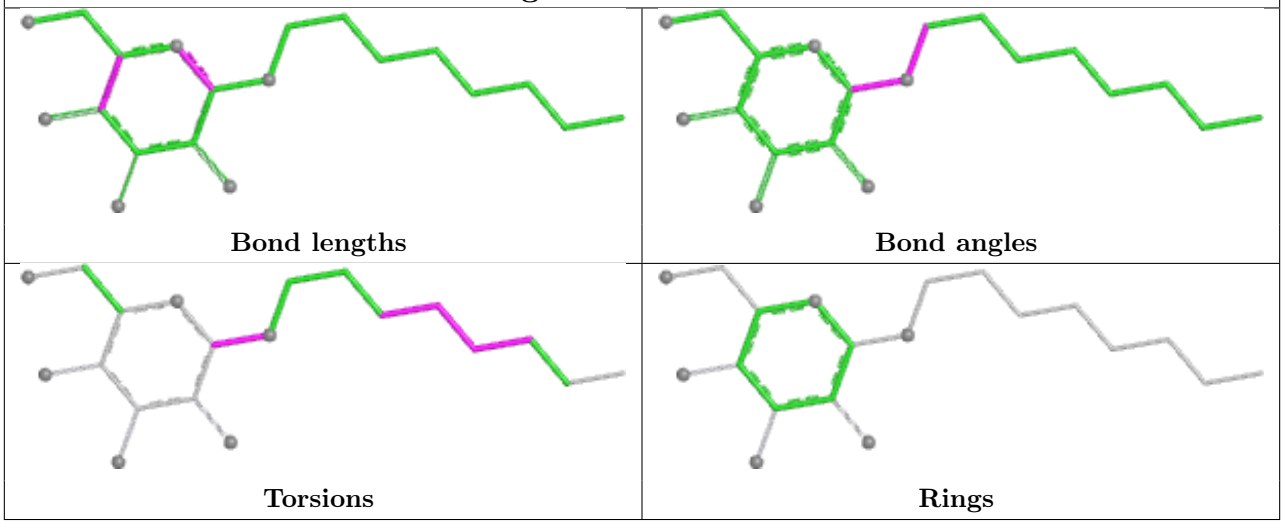
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	384	PEE	7	0
15	D	242	BOG	1	0
17	E	197	FES	1	0
14	C	385	SIG	12	0
11	C	382	HEM	12	0
16	D	243	HEC	5	0
11	C	381	HEM	7	0
12	C	383	U10	9	0
13	E	198	PEE	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

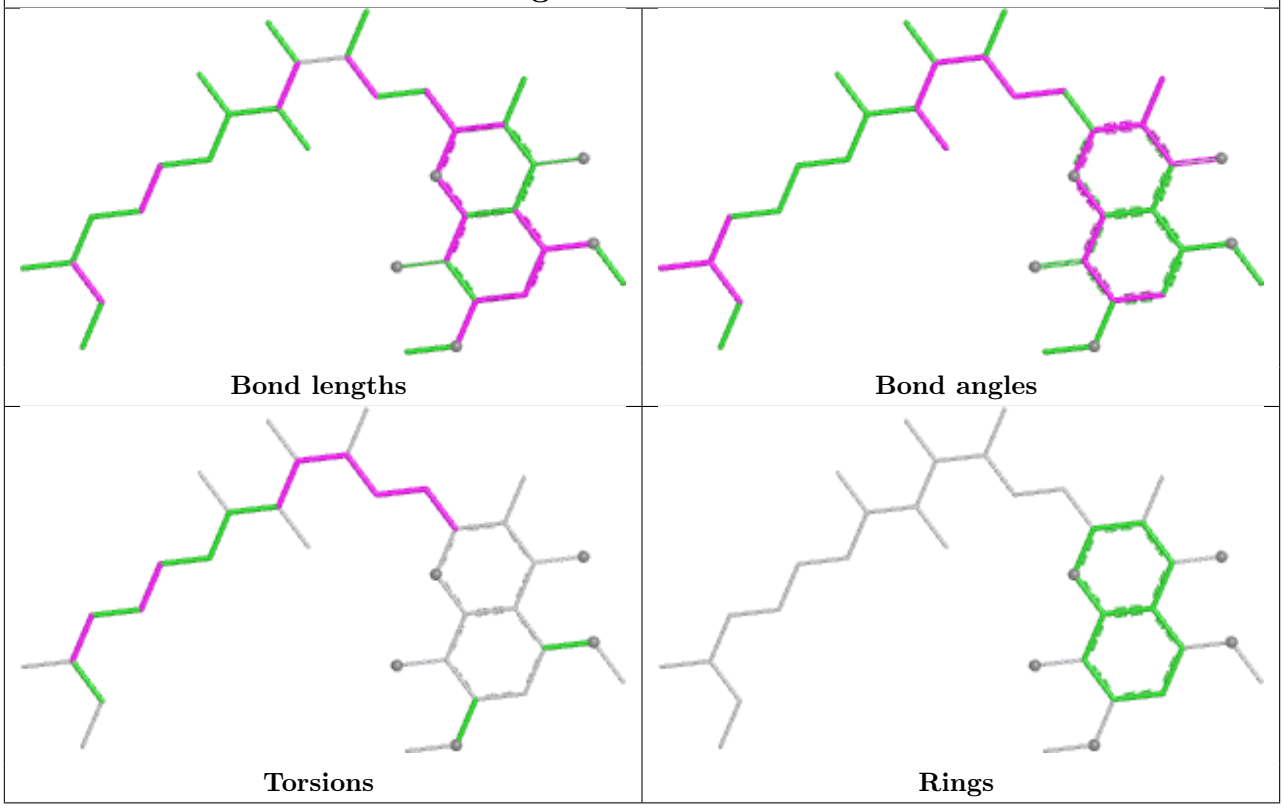
Ligand PEE C 384



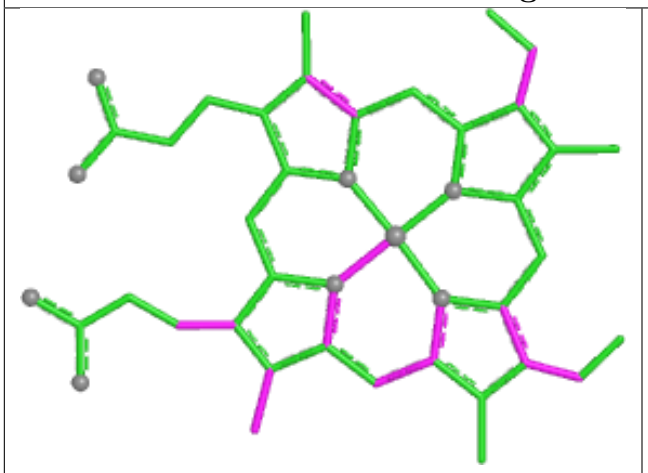
Ligand BOG D 242



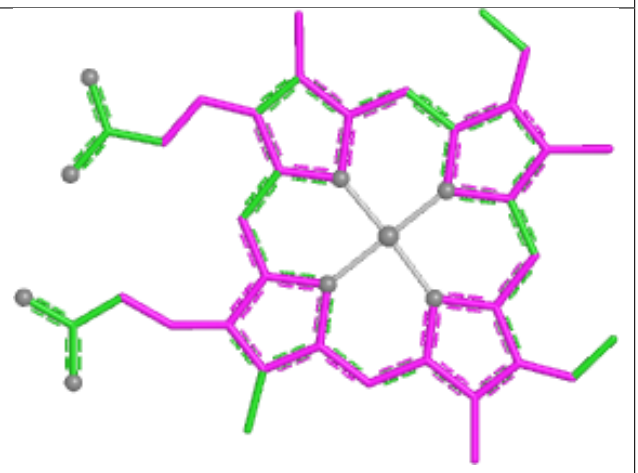
Ligand SIG C 385



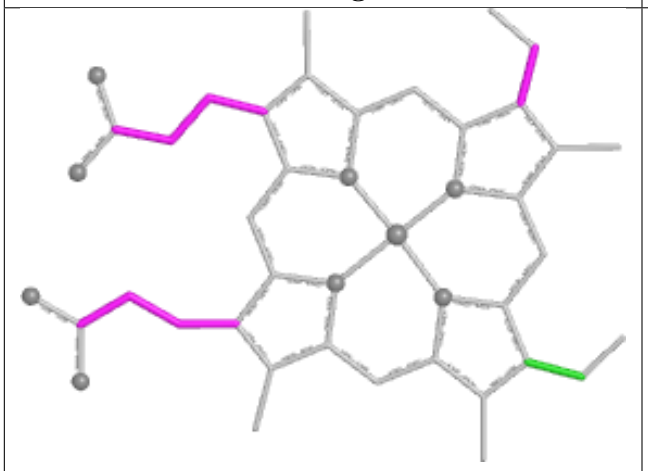
Ligand HEM C 382



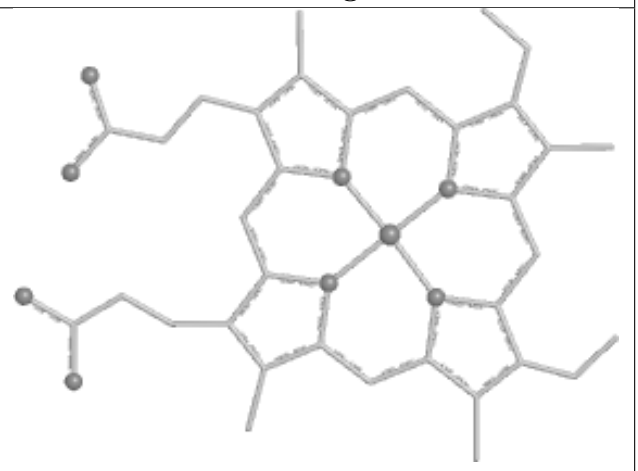
Bond lengths



Bond angles

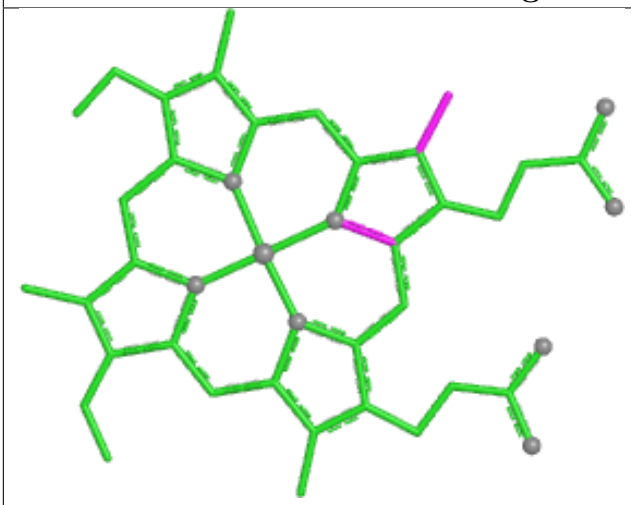


Torsions

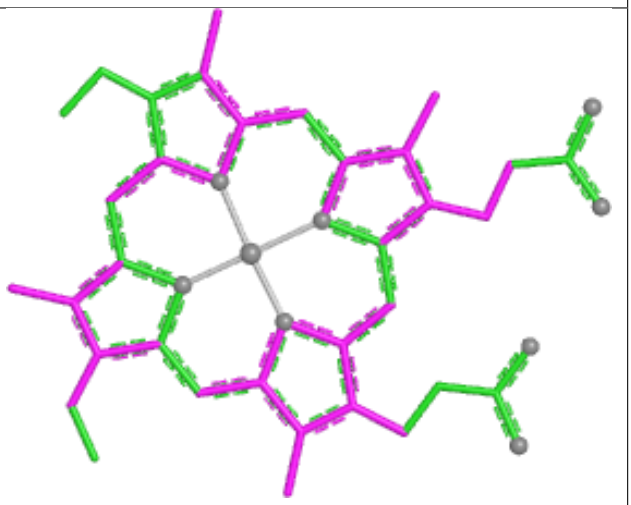


Rings

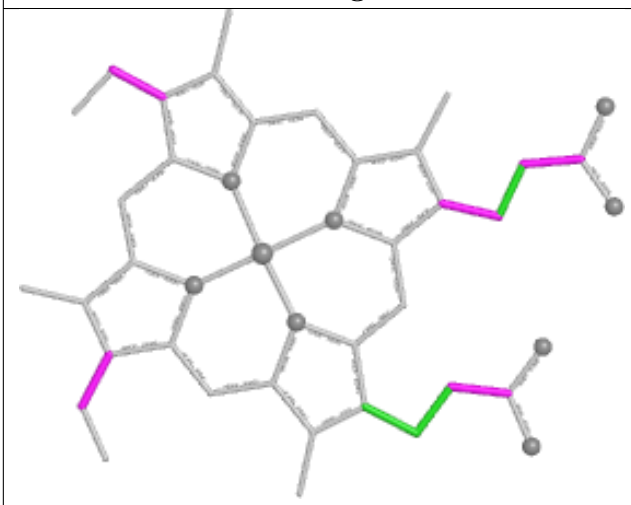
Ligand HEC D 243



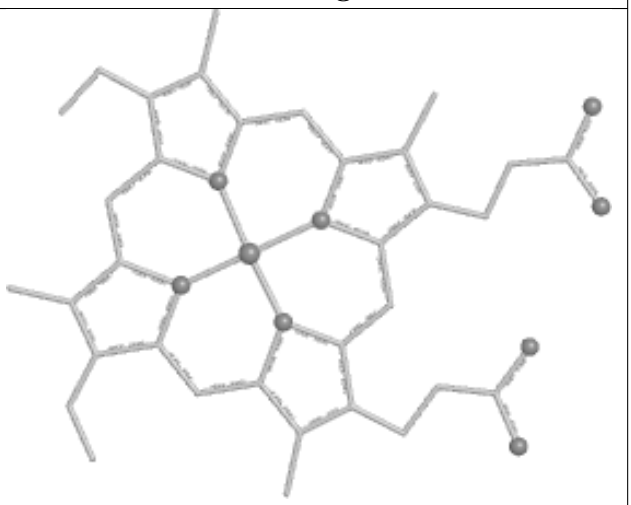
Bond lengths



Bond angles

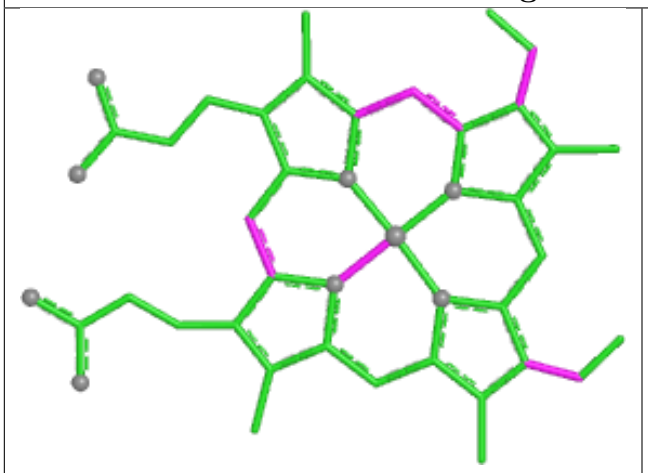


Torsions

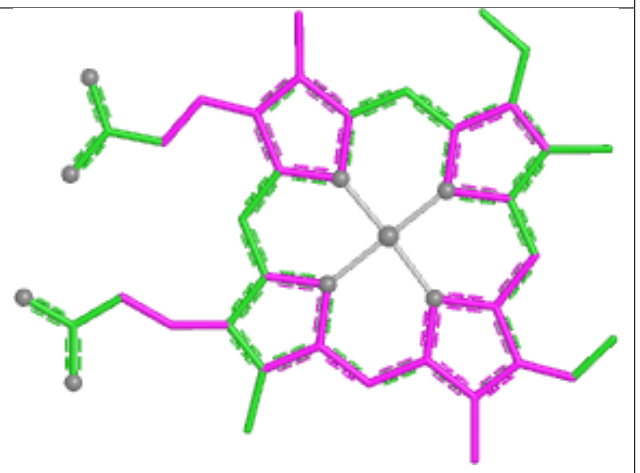


Rings

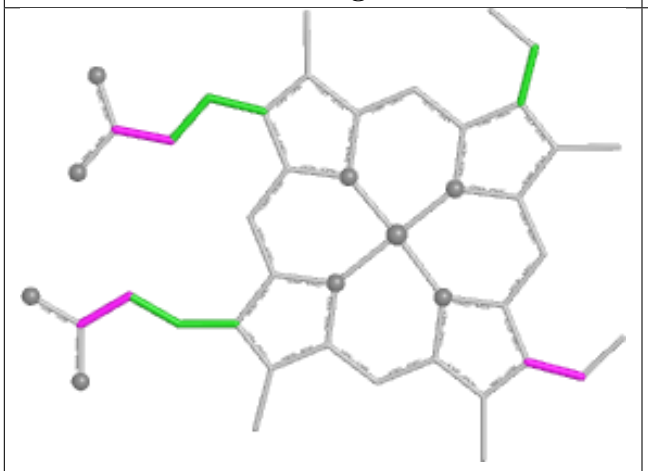
Ligand HEM C 381



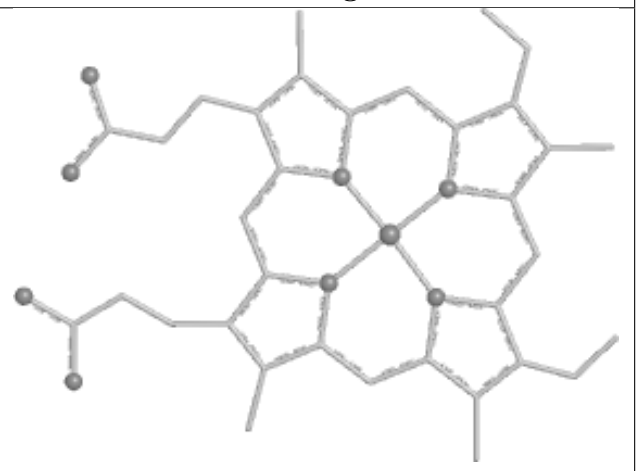
Bond lengths



Bond angles

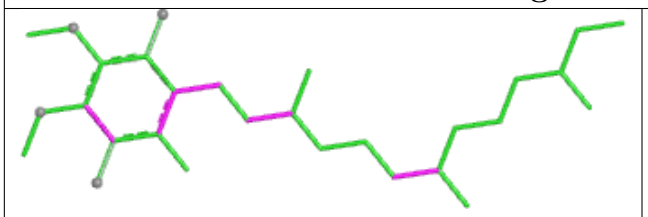


Torsions

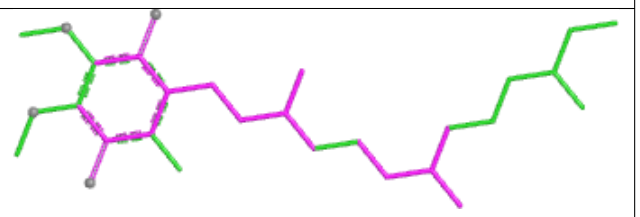


Rings

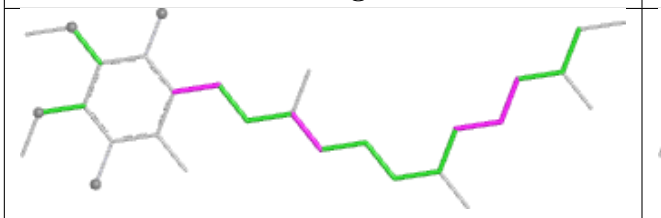
Ligand U10 C 383



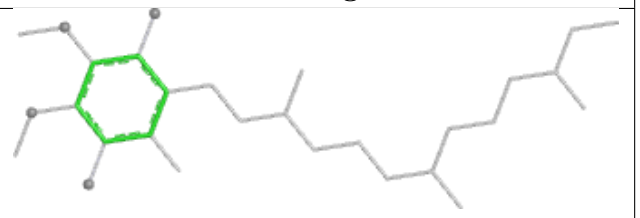
Bond lengths



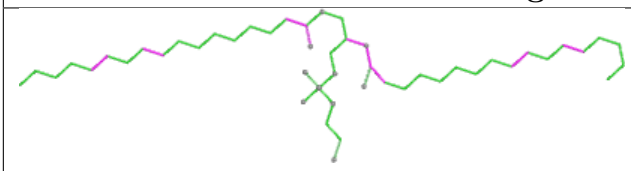
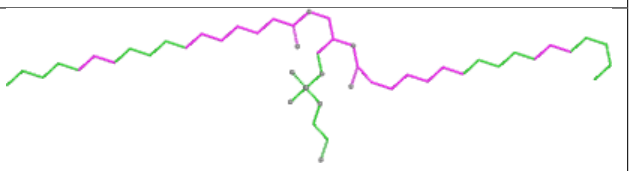
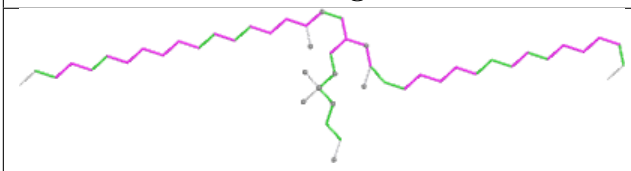
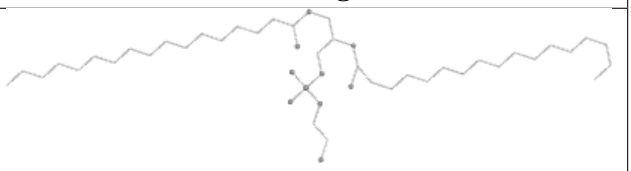
Bond angles



Torsions



Rings

Ligand PEE E 198	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	210:UNK	C	309:UNK	N	33.76
1	I	121:UNK	C	202:UNK	N	29.13

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	442/446 (99%)	-0.91	0	100	100	12, 58, 89, 100	0
2	B	406/422 (96%)	-0.78	0	100	100	36, 71, 100, 100	0
3	C	379/380 (99%)	-1.05	0	100	100	4, 32, 71, 91	0
4	D	241/241 (100%)	-0.98	0	100	100	10, 41, 77, 100	0
5	E	196/196 (100%)	-0.74	0	100	100	17, 76, 100, 100	0
6	F	100/109 (91%)	-1.04	0	100	100	18, 42, 74, 99	0
7	G	78/81 (96%)	-0.87	0	100	100	26, 54, 89, 100	0
8	H	66/78 (84%)	-0.88	0	100	100	27, 67, 86, 88	0
9	I	0/33	-	-			-	-
10	J	59/62 (95%)	-0.82	0	100	100	37, 53, 86, 100	0
All	All	1967/2048 (96%)	-0.90	0	100	100	4, 55, 98, 100	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

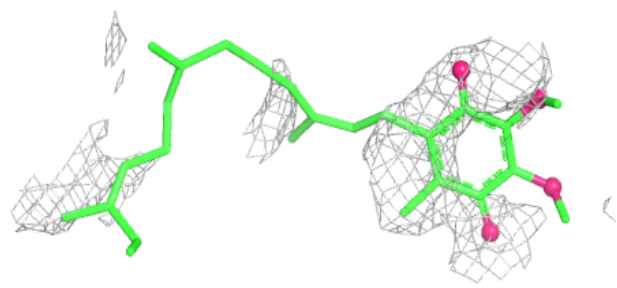
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

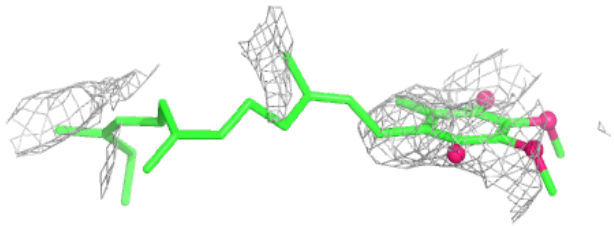
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	U10	C	383	29/63	0.97	0.12	72,88,100,100	0
15	BOG	D	242	20/20	0.97	0.11	35,68,81,81	0
13	PEE	C	384	49/51	0.98	0.08	42,58,76,87	0
11	HEM	C	382	43/43	0.99	0.05	8,20,32,41	0
13	PEE	E	198	49/51	0.99	0.08	43,80,98,100	0
14	SIG	C	385	35/35	0.99	0.05	2,17,26,29	0
11	HEM	C	381	43/43	0.99	0.05	6,24,32,43	0
16	HEC	D	243	43/43	0.99	0.05	10,21,32,35	0
17	FES	E	197	4/4	1.00	0.04	59,60,64,65	0

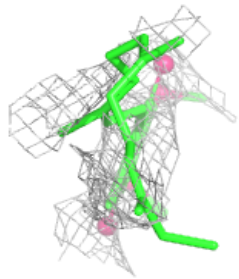
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around U10 C 383:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

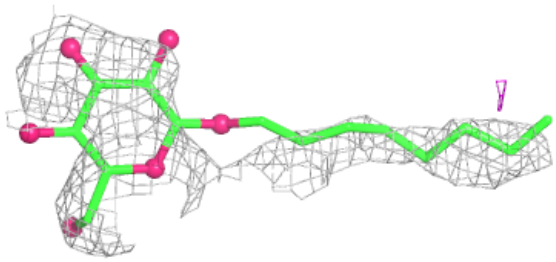


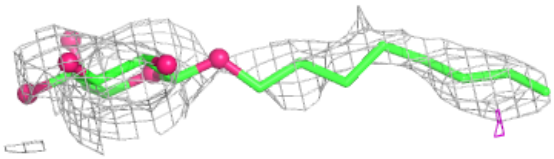


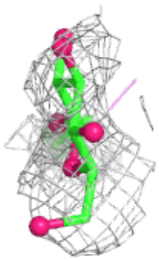


Electron density around BOG D 242:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

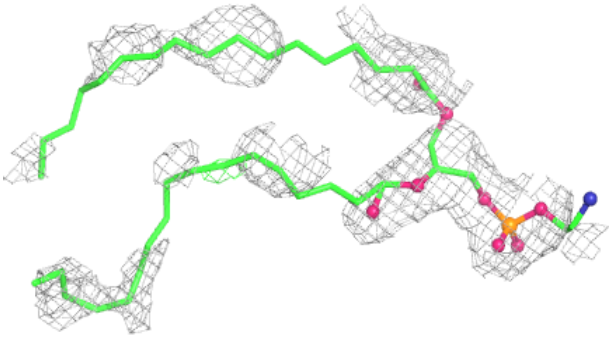


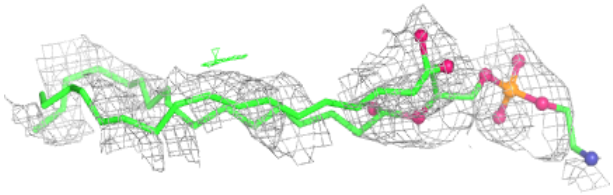




Electron density around PEE C 384:

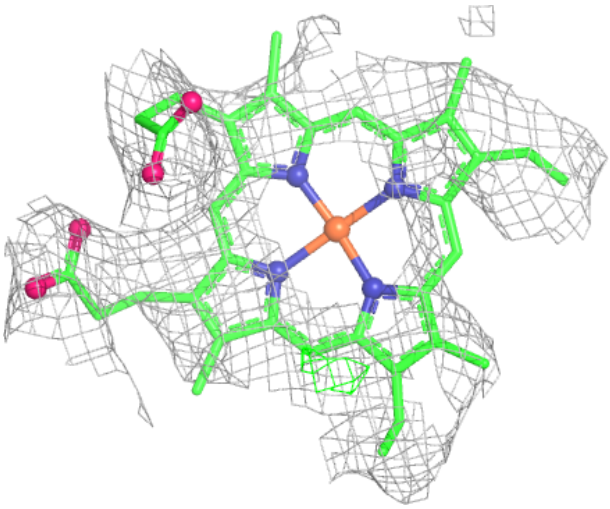
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

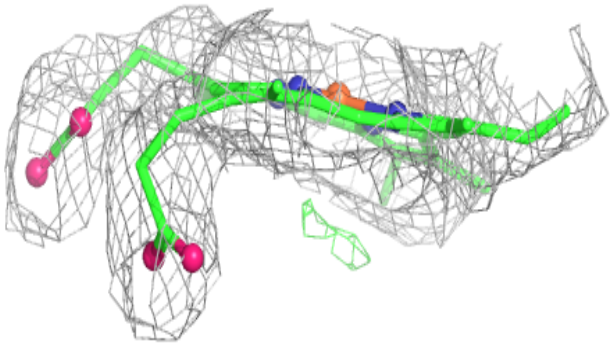




Electron density around HEM C 382:

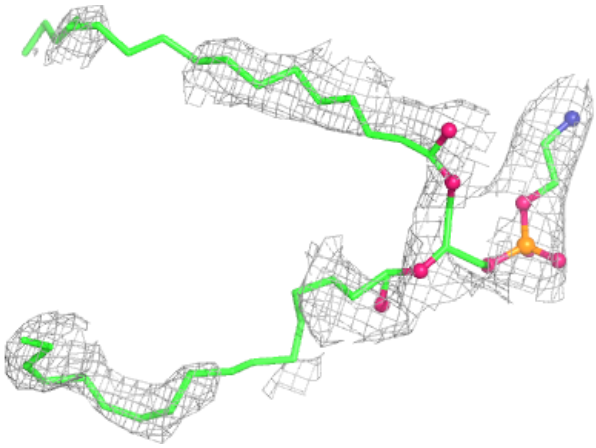
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

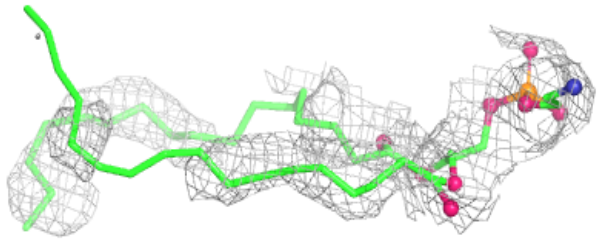


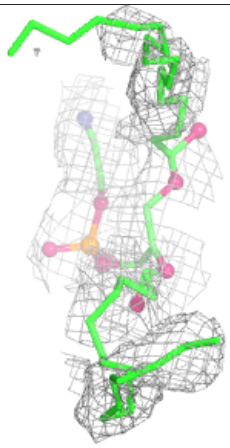


Electron density around PEE E 198:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

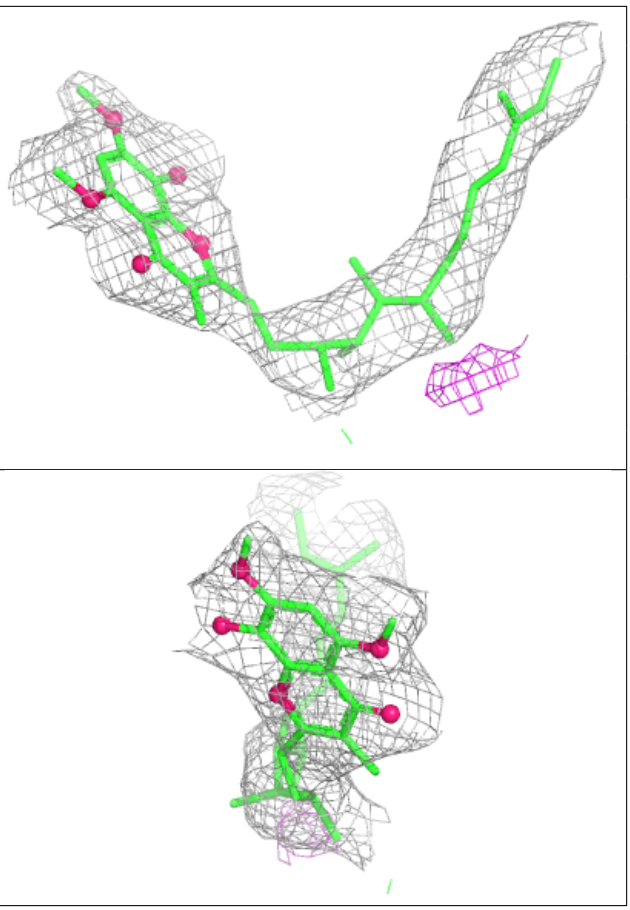


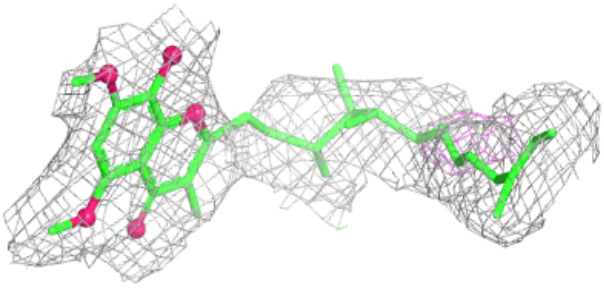




Electron density around SIG C 385:

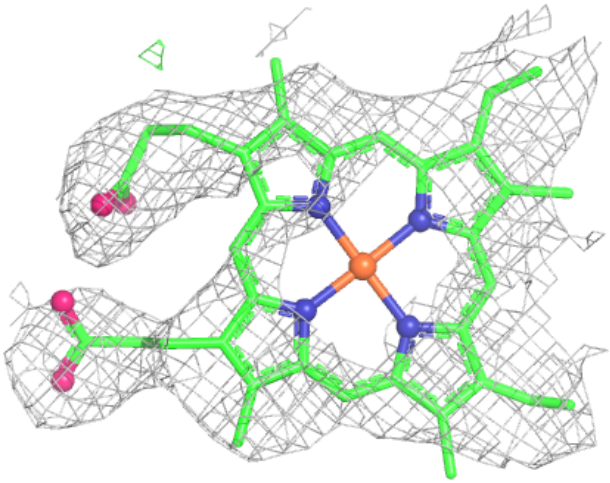
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

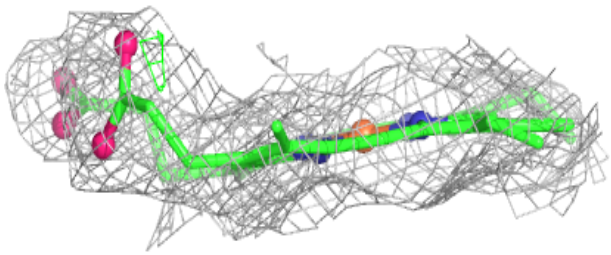


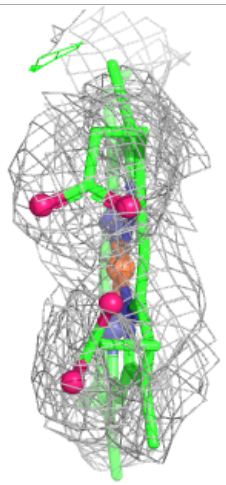


Electron density around HEM C 381:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

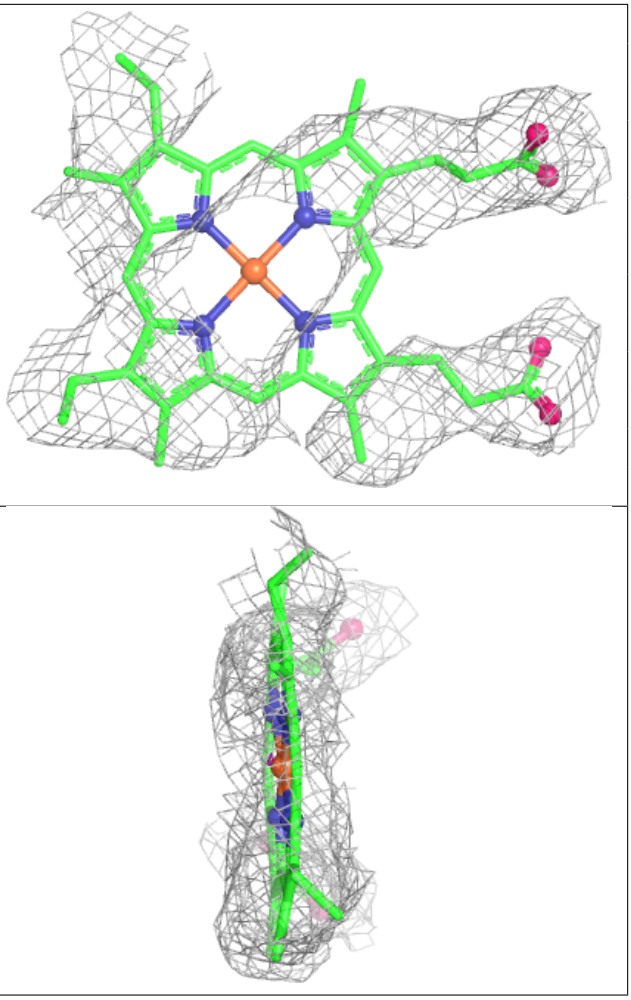






Electron density around HEC D 243:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.