Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 04:06 am BST

PDB ID	:	2CD8 / pdb_00002cd8
Title	:	Crystal structure of YC-17-bound cytochrome P450 PikC (CYP107L1)
Authors	:	Yermalitskaya, L.I.; Kim, Y.; Sherman, D.H.; Waterman, M.R.; Podust, L.M.
Deposited on	:	2006-01-20
Resolution	:	1.70 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 (i)) were used in the production of this report:

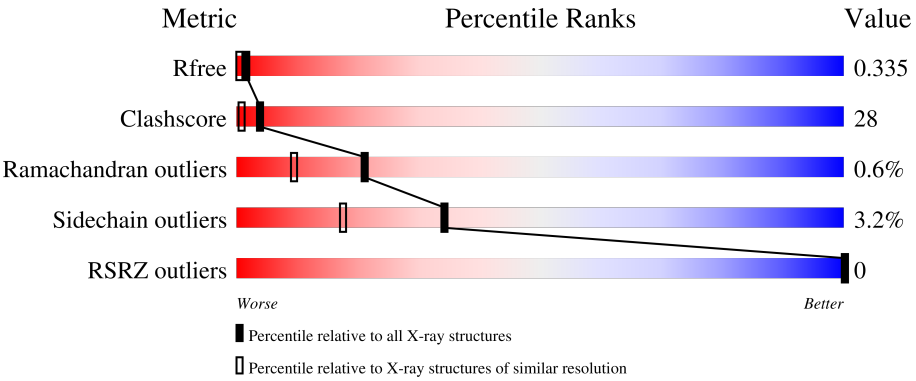
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.70 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))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	436	49% 38% · 10%
1	B	436	50% 36% · 10%

2 Entry composition (i)

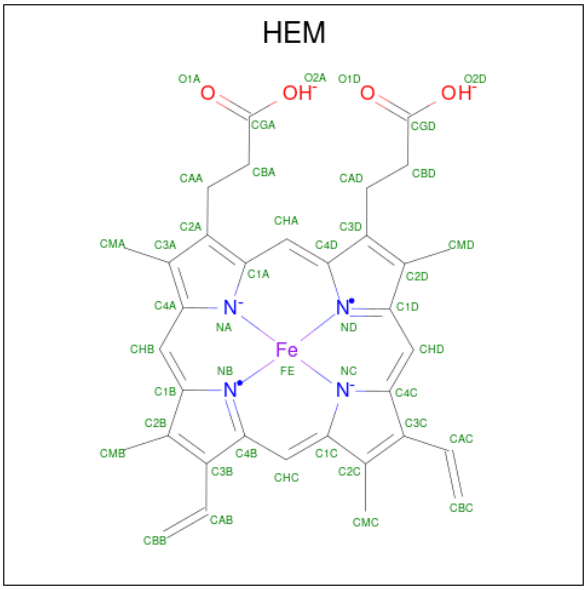
There are 4 unique types of molecules in this entry. The entry contains 6456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYTOCHROME P450 MONOOXYGENASE.

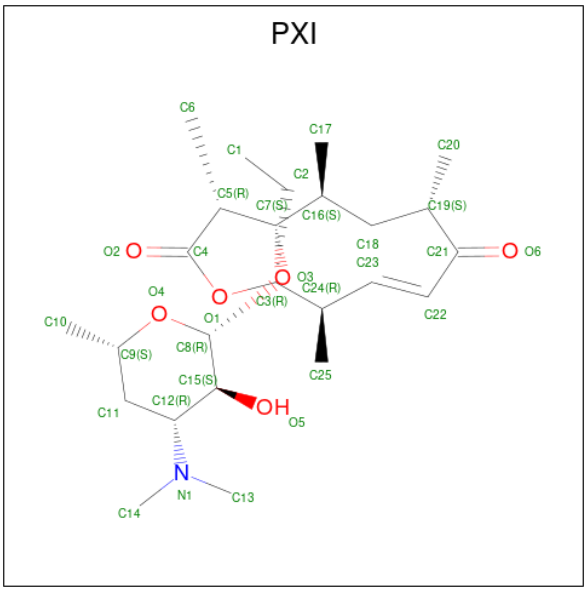
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	1
			3024	1904	543	564	13			
1	B	393	Total	C	N	O	S	0	0	1
			3027	1910	545	559	13			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is 4-{[4-(DIMETHYLAMINO)-3-HYDROXY-6-METHYLTETRAHYDRO-2H-PYRAN-2-YL]OXY}-12-ETHYL-3,5,7,11-TETRAMETHYLOXACYCLODODEC-9-ENE-2,8-DIONE (CCD ID: PXI) (formula: $C_{25}H_{43}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 32 25 1 6	0	0
3	B	1	Total C N O 32 25 1 6	0	0

- Molecule 4 is water.

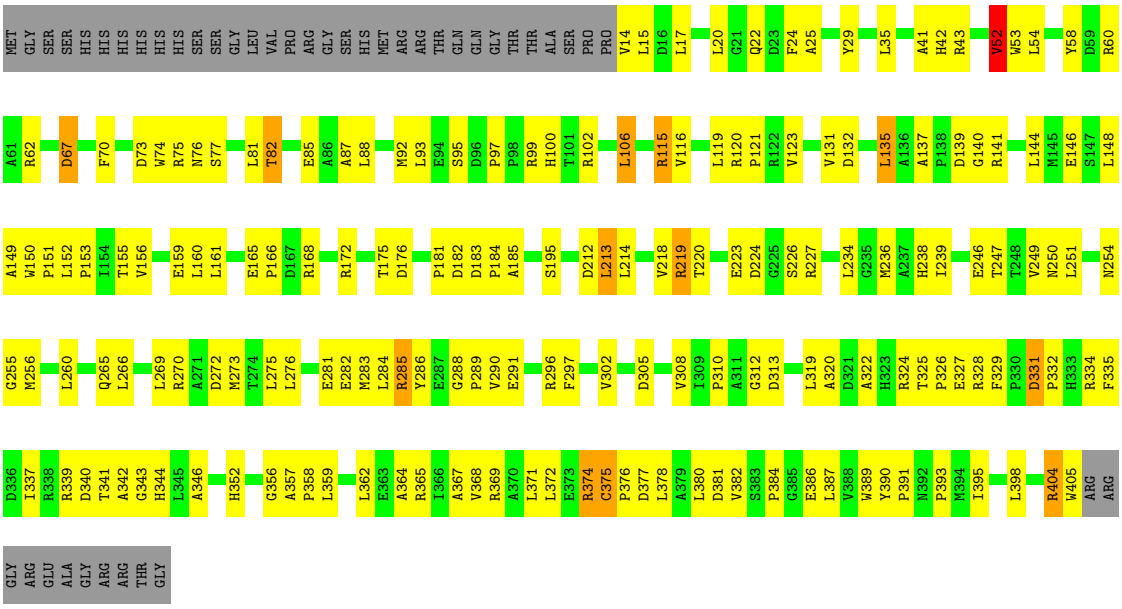
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	139	Total O 139 139	0	0
4	B	116	Total O 116 116	0	0

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.

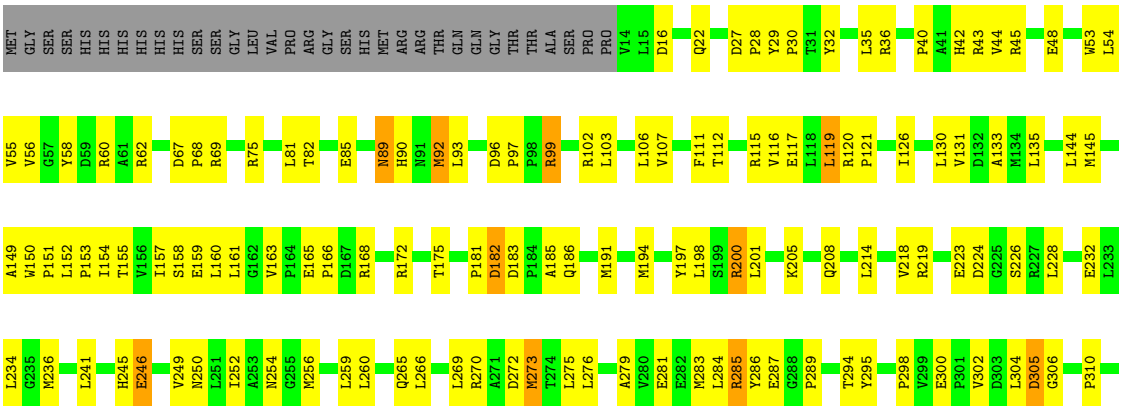
• Molecule 1: CYTOCHROME P450 MONOOXYGENASE

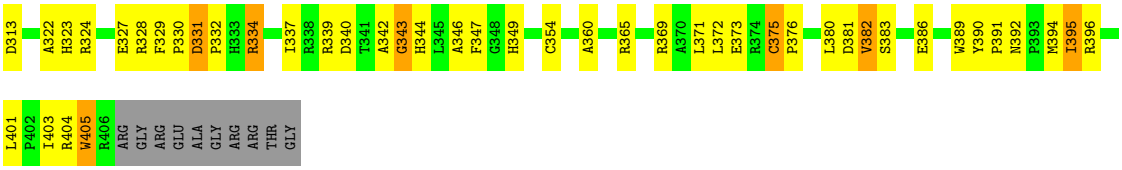
Chain A:



• Molecule 1: CYTOCHROME P450 MONOOXYGENASE

Chain B:




D313
A322
H323
R324
E327
R328
F329
P330
D331
P332
H333
R334
I337
R338
R339
D340
T341
A342
G343
H344
L345
A346
F347
G348
H349
C354
A360
R365
R369
A370
L371
L372
E373
R374
C375
P376
L380
D381
V382
S383
E386
W389
Y390
P391
N392
P393
M394
I395
R396
L401
P402
I403
R404
W405
R406
ARG
GLY
ARG
GLU
ALA
GLY
ARG
ARG
THR
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.40Å 92.10Å 67.57Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	39.84 – 1.70 39.84 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.6 (39.84-1.70) 96.7 (39.84-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.290 , 0.333 0.293 , 0.335	Depositor DCC
R_{free} test set	8535 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 21.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6456	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: PXI, HEM

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	0.50	1/3092 (0.0%)	1.01	17/4219 (0.4%)
1	B	0.46	1/3097 (0.0%)	1.01	15/4228 (0.4%)
All	All	0.48	2/6189 (0.0%)	1.01	32/8447 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	TRP	C-N	-5.91	1.25	1.33
1	A	404	ARG	C-N	-5.62	1.25	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	390	TYR	CA-C-N	7.83	127.11	118.97
1	B	390	TYR	C-N-CA	7.83	127.11	118.97
1	B	168	ARG	N-CA-C	7.70	119.31	111.07
1	B	295	TYR	N-CA-C	6.60	120.06	110.42
1	A	82	THR	N-CA-C	-6.54	102.09	110.53
1	B	92	MET	N-CA-C	6.54	119.24	111.33
1	A	226	SER	N-CA-C	-6.36	105.34	113.23
1	B	208	GLN	N-CA-C	-6.34	100.53	110.36
1	A	331	ASP	CA-C-N	6.23	125.91	119.56
1	A	331	ASP	C-N-CA	6.23	125.91	119.56
1	A	140	GLY	N-CA-C	-6.16	106.42	115.30
1	A	251	LEU	N-CA-C	-5.74	104.94	111.14
1	B	96	ASP	CA-C-N	-5.62	114.59	120.38
1	B	96	ASP	C-N-CA	-5.62	114.59	120.38
1	A	213	LEU	N-CA-C	5.60	118.92	111.75
1	B	375	CYS	CA-C-N	5.55	126.78	119.84
1	B	375	CYS	C-N-CA	5.55	126.78	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	VAL	N-CA-C	5.53	115.28	108.53
1	B	89	ASN	N-CA-C	5.50	119.86	113.20
1	A	67	ASP	CA-C-N	5.50	125.02	119.19
1	A	67	ASP	C-N-CA	5.50	125.02	119.19
1	A	97	PRO	N-CA-C	-5.25	105.43	110.47
1	A	390	TYR	CA-C-N	5.24	125.05	119.28
1	A	390	TYR	C-N-CA	5.24	125.05	119.28
1	B	75	ARG	N-CA-C	-5.23	106.73	113.01
1	A	92	MET	N-CA-C	5.23	117.66	111.33
1	B	331	ASP	CA-C-N	5.21	126.35	119.84
1	B	331	ASP	C-N-CA	5.21	126.35	119.84
1	A	308	VAL	N-CA-C	5.21	115.27	107.51
1	A	87	ALA	N-CA-C	-5.19	106.95	113.28
1	B	97	PRO	N-CA-C	-5.17	104.39	110.70
1	A	302	VAL	N-CA-C	5.02	114.70	106.72

There are no chirality outliers.

There are no planarity outliers.

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	3024	0	2994	179	0
1	B	3027	0	2995	171	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	32	0	43	1	0
3	B	32	0	43	5	0
4	A	139	0	0	25	0
4	B	116	0	0	17	0
All	All	6456	0	6135	350	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 28.

All (350) 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)
1:A:285:ARG:HH11	1:A:285:ARG:HB3	1.09	1.09
1:B:119:LEU:HD13	1:B:160:LEU:HD11	1.51	0.92
1:A:285:ARG:HB3	1:A:285:ARG:NH1	1.84	0.92
1:B:40:PRO:HG3	1:B:305:ASP:HB2	1.54	0.89
1:B:150:TRP:HB3	1:B:151:PRO:HD3	1.52	0.88
1:A:329:PHE:O	1:A:332:PRO:HG3	1.76	0.85
1:A:265:GLN:HE21	1:A:337:ILE:H	1.21	0.83
1:B:16:ASP:HA	1:B:45:ARG:HB3	1.58	0.82
1:B:382:VAL:HG22	1:B:383:SER:H	1.43	0.82
1:A:175:THR:CG2	1:A:246:GLU:HG2	2.11	0.81
1:B:102:ARG:O	1:B:106:LEU:HD13	1.81	0.80
1:B:152:LEU:HB3	1:B:153:PRO:HD3	1.61	0.80
1:B:250:ASN:HB3	4:B:2076:HOH:O	1.81	0.79
1:A:95:SER:CB	1:A:99:ARG:HD2	2.13	0.79
1:B:107:VAL:HG22	4:B:2044:HOH:O	1.83	0.79
1:B:181:PRO:HB2	1:B:186:GLN:HB3	1.63	0.78
1:A:95:SER:HB3	1:A:99:ARG:HH11	1.49	0.77
1:B:197:TYR:HD1	1:B:200:ARG:HH12	1.30	0.77
1:A:95:SER:HB2	1:A:99:ARG:HD2	1.67	0.77
1:A:175:THR:HG22	1:A:246:GLU:HG2	1.67	0.77
1:B:381:ASP:OD2	1:B:404:ARG:HB3	1.85	0.77
1:A:319:LEU:HB3	4:A:2121:HOH:O	1.83	0.77
1:A:288:GLY:HA3	4:A:2102:HOH:O	1.85	0.77
1:B:22:GLN:HE22	1:B:389:TRP:H	1.30	0.77
1:A:265:GLN:NE2	1:A:337:ILE:H	1.82	0.77
1:B:35:LEU:HB3	1:B:42:HIS:CD2	2.20	0.76
1:B:395:ILE:N	1:B:395:ILE:HD12	2.00	0.76
1:A:219:ARG:O	1:A:223:GLU:HG3	1.86	0.76
1:B:131:VAL:O	1:B:135:LEU:HG	1.87	0.75
1:A:281:GLU:OE1	1:A:344:HIS:HE1	1.70	0.74
1:A:289:PRO:O	1:A:395:ILE:HD12	1.88	0.74
1:B:81:LEU:CD2	1:B:85:GLU:HB2	2.17	0.74
1:B:273:MET:HE1	1:B:276:LEU:HD23	1.69	0.73
1:B:205:LYS:HG3	1:B:214:LEU:HD12	1.71	0.73
1:A:344:HIS:HD2	1:A:346:ALA:H	1.35	0.73
1:A:327:GLU:H	1:A:327:GLU:CD	1.97	0.73
1:B:119:LEU:HD22	1:B:160:LEU:HD21	1.71	0.72
1:A:106:LEU:HD11	1:A:220:THR:HG21	1.71	0.72
1:B:120:ARG:HB3	1:B:121:PRO:HD3	1.72	0.72
1:B:85:GLU:HG2	1:B:191:MET:SD	2.29	0.72
1:B:165:GLU:HB3	1:B:166:PRO:HD3	1.73	0.71
1:A:282:GLU:HG3	1:A:335:PHE:CE1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:HIS:ND1	1:B:99:ARG:NH2	2.41	0.69
1:A:328:ARG:HG3	1:A:329:PHE:CD1	2.28	0.69
1:B:327:GLU:CD	1:B:327:GLU:H	2.00	0.69
1:B:294:THR:HA	1:B:394:MET:HE3	1.75	0.69
1:B:339:ARG:HG2	1:B:340:ASP:N	2.08	0.69
1:B:334:ARG:CZ	1:B:334:ARG:HA	2.23	0.67
1:B:329:PHE:O	1:B:332:PRO:HG3	1.95	0.67
1:B:32:TYR:HA	1:B:35:LEU:HD12	1.76	0.67
1:B:44:VAL:HG11	1:B:54:LEU:HD12	1.77	0.67
1:B:294:THR:HA	1:B:394:MET:CE	2.25	0.67
1:B:246:GLU:HG3	3:B:420:PXI:O6	1.95	0.66
1:A:250:ASN:HD22	1:A:395:ILE:HD11	1.60	0.66
1:A:324:ARG:O	1:A:326:PRO:HD3	1.96	0.66
1:B:28:PRO:HB2	1:B:32:TYR:CE1	2.31	0.65
1:A:43:ARG:HG2	4:A:2019:HOH:O	1.96	0.65
1:B:289:PRO:HA	4:B:2076:HOH:O	1.96	0.65
1:B:144:LEU:HD21	1:B:256:MET:HG3	1.77	0.65
1:A:120:ARG:HB3	1:A:121:PRO:HD3	1.79	0.65
1:B:376:PRO:HG2	1:B:405:TRP:HB2	1.78	0.65
1:B:331:ASP:N	1:B:332:PRO:HD3	2.12	0.64
1:B:182:ASP:OD1	1:B:186:GLN:NE2	2.30	0.64
1:B:145:MET:HA	1:B:149:ALA:HB3	1.79	0.64
1:A:165:GLU:HB3	1:A:166:PRO:HD3	1.79	0.64
1:A:62:ARG:HG2	1:A:62:ARG:HH11	1.62	0.63
1:B:310:PRO:HG2	1:B:313:ASP:OD2	1.98	0.63
1:B:265:GLN:HE21	1:B:337:ILE:H	1.45	0.63
1:B:81:LEU:HD23	1:B:85:GLU:HB2	1.80	0.63
1:B:376:PRO:HG2	1:B:405:TRP:O	1.99	0.63
1:A:150:TRP:CE2	1:A:172:ARG:HD2	2.33	0.63
1:A:22:GLN:HE22	1:A:389:TRP:H	1.46	0.63
1:A:255:GLY:O	1:A:283:MET:HE2	1.98	0.63
1:A:139:ASP:O	1:A:141:ARG:HG3	2.00	0.62
1:B:224:ASP:C	1:B:226:SER:H	2.08	0.61
1:B:254:ASN:ND2	4:B:2076:HOH:O	2.33	0.61
1:A:29:TYR:HE2	1:A:320:ALA:HB1	1.65	0.61
1:A:137:ALA:C	1:A:139:ASP:H	2.08	0.61
1:A:266:LEU:C	1:A:266:LEU:HD13	2.26	0.61
1:A:339:ARG:NE	4:A:2117:HOH:O	2.31	0.61
1:B:69:ARG:HD3	4:B:2020:HOH:O	2.01	0.60
1:A:132:ASP:OD1	1:A:374:ARG:NH1	2.34	0.60
1:A:285:ARG:HD2	1:A:329:PHE:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:VAL:HG11	1:B:54:LEU:CD1	2.32	0.60
1:B:103:LEU:HD21	4:B:2075:HOH:O	2.01	0.60
1:B:214:LEU:O	1:B:218:VAL:HG23	2.01	0.60
1:A:115:ARG:HB2	1:A:115:ARG:NH1	2.17	0.60
1:B:276:LEU:CD1	1:B:365:ARG:HG2	2.31	0.59
1:B:58:TYR:HD1	1:B:322:ALA:HB1	1.67	0.59
1:A:260:LEU:HD21	1:A:378:LEU:HG	1.85	0.59
1:B:197:TYR:HA	1:B:200:ARG:NH1	2.18	0.59
1:A:282:GLU:OE1	1:A:285:ARG:NH1	2.35	0.59
1:B:92:MET:HE1	4:B:2044:HOH:O	2.02	0.59
1:B:286:TYR:CD2	1:B:287:GLU:HG2	2.37	0.58
1:B:256:MET:HE2	1:B:371:LEU:CD1	2.34	0.58
1:A:266:LEU:HD13	1:A:266:LEU:O	2.04	0.58
1:A:165:GLU:HA	1:A:168:ARG:NE	2.18	0.57
1:A:285:ARG:NH2	4:A:2117:HOH:O	2.36	0.57
1:B:150:TRP:CZ2	1:B:172:ARG:HB2	2.39	0.57
1:A:29:TYR:CE2	1:A:320:ALA:HB1	2.40	0.57
1:A:135:LEU:N	1:A:135:LEU:HD23	2.20	0.57
1:A:276:LEU:HD11	1:A:365:ARG:HB3	1.87	0.57
1:A:328:ARG:HG3	1:A:329:PHE:CE1	2.40	0.56
1:B:276:LEU:HD13	1:B:276:LEU:C	2.30	0.56
1:A:35:LEU:HB3	1:A:42:HIS:CD2	2.40	0.56
1:A:135:LEU:HD12	1:A:374:ARG:CZ	2.35	0.56
1:A:310:PRO:HG2	1:A:313:ASP:CG	2.30	0.56
1:B:214:LEU:HD13	1:B:218:VAL:HG23	1.88	0.56
1:B:260:LEU:HB3	1:B:380:LEU:HG	1.86	0.56
1:B:285:ARG:NH2	1:B:332:PRO:O	2.35	0.56
1:A:250:ASN:O	1:A:254:ASN:HB2	2.06	0.56
1:A:152:LEU:HB3	1:A:153:PRO:HD3	1.87	0.56
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.71	0.56
1:B:382:VAL:HG22	1:B:383:SER:N	2.19	0.56
1:B:82:THR:OG1	1:B:85:GLU:HG3	2.06	0.56
1:B:298:PRO:HD2	1:B:313:ASP:O	2.06	0.56
1:A:255:GLY:C	1:A:283:MET:HE2	2.31	0.55
1:A:376:PRO:HG2	1:A:377:ASP:H	1.71	0.55
1:B:245:HIS:O	1:B:249:VAL:HG23	2.05	0.55
1:A:150:TRP:O	1:A:153:PRO:HD2	2.06	0.55
1:B:133:ALA:HB3	4:B:2052:HOH:O	2.06	0.55
1:A:273:MET:HE3	1:A:369:ARG:HG3	1.89	0.55
1:B:69:ARG:CZ	1:B:302:VAL:HG13	2.37	0.55
1:B:250:ASN:O	1:B:254:ASN:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:THR:HG23	4:A:2139:HOH:O	2.07	0.55
1:B:344:HIS:HD2	1:B:346:ALA:H	1.54	0.55
1:B:112:THR:O	1:B:116:VAL:HG13	2.07	0.54
1:B:285:ARG:NH2	1:B:324:ARG:HD3	2.22	0.54
1:B:200:ARG:HH11	1:B:200:ARG:HB2	1.72	0.54
1:B:62:ARG:NH1	1:B:349:HIS:NE2	2.55	0.54
1:A:17:LEU:HA	1:A:20:LEU:HD12	1.90	0.54
1:A:341:THR:O	1:A:342:ALA:C	2.51	0.54
1:A:344:HIS:CD2	1:A:346:ALA:HB3	2.42	0.54
1:A:352:HIS:NE2	4:A:2125:HOH:O	2.34	0.54
1:B:360:ALA:HB1	2:B:419:HEM:CBB	2.38	0.54
1:A:82:THR:OG1	1:A:85:GLU:HG3	2.08	0.53
1:B:81:LEU:HD21	1:B:85:GLU:HB2	1.89	0.53
1:B:150:TRP:O	1:B:153:PRO:HD2	2.08	0.53
1:A:88:LEU:HD21	1:A:195:SER:HB2	1.89	0.53
1:A:156:VAL:O	1:A:160:LEU:HG	2.09	0.53
1:A:181:PRO:C	1:A:183:ASP:H	2.17	0.53
1:A:181:PRO:HB2	1:A:183:ASP:O	2.08	0.53
1:B:60:ARG:CZ	1:B:304:LEU:HD22	2.39	0.53
1:B:175:THR:HG23	1:B:246:GLU:OE2	2.09	0.53
1:A:73:ASP:CG	1:A:75:ARG:HE	2.18	0.52
1:A:155:THR:O	1:A:159:GLU:HG3	2.09	0.52
1:A:357:ALA:HB3	1:A:358:PRO:HD3	1.91	0.52
1:B:394:MET:C	1:B:395:ILE:HD12	2.34	0.52
1:A:381:ASP:HB2	1:A:404:ARG:HB3	1.91	0.52
1:B:310:PRO:HG2	1:B:313:ASP:CG	2.34	0.52
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.24	0.52
1:A:272:ASP:HB3	1:A:275:LEU:CD1	2.39	0.52
1:A:331:ASP:N	1:A:332:PRO:HD3	2.24	0.52
1:A:247:THR:O	1:A:289:PRO:HG3	2.09	0.52
1:A:282:GLU:OE1	1:A:282:GLU:HA	2.09	0.52
1:B:194:MET:O	1:B:198:LEU:HG	2.09	0.52
1:A:175:THR:HG22	1:A:246:GLU:CG	2.39	0.52
1:B:22:GLN:NE2	1:B:389:TRP:H	2.05	0.52
1:A:290:VAL:HG12	1:A:319:LEU:HD12	1.91	0.52
1:B:183:ASP:OD1	1:B:185:ALA:HB3	2.10	0.52
1:B:48:GLU:N	4:B:2011:HOH:O	2.42	0.51
1:B:161:LEU:HD13	1:B:241:LEU:HG	1.92	0.51
1:A:260:LEU:HB3	1:A:380:LEU:HG	1.93	0.51
1:B:327:GLU:HB3	4:B:2091:HOH:O	2.10	0.51
1:A:41:ALA:HA	1:A:54:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:PRO:HG3	4:B:2115:HOH:O	2.09	0.51
1:A:381:ASP:HA	1:A:404:ARG:HH11	1.76	0.51
1:A:328:ARG:NE	4:A:2113:HOH:O	2.43	0.51
1:A:256:MET:HE2	1:A:371:LEU:HD13	1.92	0.51
1:A:250:ASN:HB2	1:A:289:PRO:HB3	1.92	0.51
1:A:405:TRP:N	4:A:2137:HOH:O	2.44	0.51
1:B:150:TRP:CB	1:B:151:PRO:HD3	2.35	0.51
1:A:74:TRP:CE3	1:A:81:LEU:HG	2.46	0.51
1:B:272:ASP:HB3	1:B:275:LEU:HG	1.92	0.50
1:A:183:ASP:C	1:A:185:ALA:H	2.18	0.50
1:A:339:ARG:HG2	1:A:340:ASP:N	2.24	0.50
1:A:364:ALA:O	1:A:368:VAL:HG23	2.11	0.50
1:A:319:LEU:HD13	4:A:2121:HOH:O	2.10	0.50
1:A:324:ARG:HA	1:A:332:PRO:HB3	1.94	0.50
1:A:346:ALA:HA	4:A:2121:HOH:O	2.11	0.50
1:B:347:PHE:HB3	1:B:354:CYS:HB3	1.94	0.50
1:B:260:LEU:HA	1:B:266:LEU:HD22	1.94	0.50
1:B:246:GLU:CD	1:B:246:GLU:H	2.20	0.49
1:B:273:MET:HE2	1:B:369:ARG:CZ	2.42	0.49
1:A:276:LEU:HD11	1:A:365:ARG:CB	2.42	0.49
1:A:334:ARG:CZ	1:A:335:PHE:O	2.60	0.49
1:B:281:GLU:OE1	1:B:344:HIS:HE1	1.95	0.49
1:B:304:LEU:C	1:B:306:GLY:H	2.20	0.49
1:B:395:ILE:N	1:B:395:ILE:CD1	2.71	0.49
1:A:224:ASP:OD2	1:A:227:ARG:HB2	2.12	0.49
1:A:234:LEU:HD23	4:A:2038:HOH:O	2.13	0.49
1:A:246:GLU:OE1	1:A:246:GLU:HA	2.13	0.49
1:B:256:MET:HE2	1:B:371:LEU:HD12	1.95	0.49
1:A:67:ASP:HB3	1:A:70:PHE:HD1	1.78	0.49
1:B:181:PRO:C	1:B:183:ASP:N	2.69	0.49
1:B:252:ILE:O	1:B:256:MET:HG2	2.13	0.49
1:B:150:TRP:NE1	1:B:172:ARG:HG3	2.28	0.48
1:B:89:ASN:HB3	3:B:420:PXI:H141	1.94	0.48
1:A:352:HIS:HB2	4:A:2123:HOH:O	2.13	0.48
1:B:181:PRO:C	1:B:183:ASP:H	2.20	0.48
1:A:82:THR:HB	4:A:2073:HOH:O	2.12	0.48
1:B:276:LEU:HD11	1:B:365:ARG:HG2	1.95	0.48
1:A:135:LEU:HD12	1:A:374:ARG:NH2	2.29	0.48
1:A:272:ASP:HB3	1:A:275:LEU:HD11	1.95	0.48
1:B:155:THR:HG22	1:B:159:GLU:OE2	2.13	0.48
1:A:25:ALA:HB2	1:A:391:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:O	1:B:161:LEU:HB2	2.14	0.47
1:B:158:SER:HB3	1:B:163:VAL:HB	1.97	0.47
1:B:381:ASP:HB2	1:B:403:ILE:C	2.39	0.47
1:A:153:PRO:HB2	4:A:2061:HOH:O	2.14	0.47
1:A:328:ARG:O	1:A:328:ARG:HD3	2.14	0.47
1:B:373:GLU:OE1	1:B:373:GLU:N	2.47	0.47
1:A:150:TRP:NE1	1:A:172:ARG:HD2	2.29	0.47
1:A:389:TRP:CZ2	1:A:398:LEU:HD21	2.49	0.47
1:B:115:ARG:HG3	4:B:2047:HOH:O	2.15	0.47
1:B:256:MET:HE2	1:B:371:LEU:HD13	1.95	0.47
1:A:359:LEU:HD23	2:A:419:HEM:HBC2	1.95	0.47
1:B:144:LEU:HD23	1:B:401:LEU:HD23	1.96	0.47
1:B:198:LEU:HB2	1:B:234:LEU:CD1	2.44	0.47
1:B:40:PRO:O	1:B:55:VAL:HA	2.15	0.47
1:B:165:GLU:C	1:B:165:GLU:CD	2.83	0.47
1:B:35:LEU:HB3	1:B:42:HIS:HD2	1.72	0.47
1:A:344:HIS:HD2	1:A:346:ALA:N	2.09	0.46
1:A:381:ASP:HA	1:A:404:ARG:NH1	2.30	0.46
1:A:339:ARG:NH2	4:A:2117:HOH:O	2.48	0.46
1:A:62:ARG:HG2	1:A:62:ARG:NH1	2.29	0.46
1:A:266:LEU:CD2	1:A:372:LEU:HD11	2.45	0.46
1:A:290:VAL:CG1	1:A:319:LEU:HD12	2.45	0.46
1:A:43:ARG:O	1:A:43:ARG:HG3	2.15	0.46
1:B:334:ARG:HA	1:B:334:ARG:NH1	2.31	0.46
1:A:285:ARG:HH12	1:A:286:TYR:HB2	1.81	0.46
1:A:384:PRO:O	1:A:387:LEU:HB2	2.15	0.46
1:B:126:ILE:O	1:B:130:LEU:HG	2.15	0.46
1:A:369:ARG:NH2	4:A:2130:HOH:O	2.48	0.46
1:B:81:LEU:HD21	1:B:85:GLU:CB	2.45	0.46
1:B:150:TRP:HE3	1:B:151:PRO:HG3	1.80	0.46
1:A:150:TRP:HB3	1:A:151:PRO:HD3	1.98	0.46
1:A:137:ALA:C	1:A:139:ASP:N	2.74	0.46
1:A:144:LEU:HD21	1:A:256:MET:HG3	1.98	0.46
1:A:284:LEU:HB3	1:A:346:ALA:CB	2.46	0.46
1:B:150:TRP:HB3	1:B:151:PRO:CD	2.34	0.45
1:B:93:LEU:HB3	4:B:2036:HOH:O	2.15	0.45
1:B:119:LEU:O	1:B:120:ARG:C	2.58	0.45
1:A:343:GLY:O	1:A:344:HIS:C	2.59	0.45
1:B:67:ASP:HA	1:B:68:PRO:HD3	1.84	0.45
1:A:148:LEU:HD21	1:A:367:ALA:HB1	1.99	0.45
1:B:191:MET:HG2	3:B:420:PXI:H101	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ASP:OD1	1:A:184:PRO:HD2	2.17	0.45
1:B:106:LEU:CD1	4:B:2042:HOH:O	2.64	0.45
1:A:291:GLU:HB3	1:A:393:PRO:O	2.17	0.44
1:A:382:VAL:HG22	1:A:386:GLU:HB3	1.98	0.44
1:B:27:ASP:O	1:B:30:PRO:HD2	2.16	0.44
1:A:58:TYR:HA	1:A:322:ALA:HB1	1.99	0.44
1:B:328:ARG:NH2	1:B:343:GLY:HA3	2.33	0.44
1:A:161:LEU:HD13	1:A:213:LEU:HB3	1.98	0.44
1:B:328:ARG:HG3	1:B:328:ARG:HH11	1.83	0.44
1:A:148:LEU:C	1:A:151:PRO:HD2	2.43	0.44
1:A:165:GLU:HA	1:A:168:ARG:CZ	2.47	0.44
1:A:305:ASP:OD1	1:A:305:ASP:O	2.35	0.44
1:B:43:ARG:CZ	1:B:53:TRP:HZ2	2.31	0.44
1:B:154:ILE:N	4:B:2056:HOH:O	2.43	0.44
1:A:272:ASP:O	1:A:275:LEU:HD12	2.17	0.44
1:A:389:TRP:CD2	1:A:398:LEU:HD23	2.53	0.44
1:B:36:ARG:HA	1:B:56:VAL:CG2	2.48	0.44
1:B:219:ARG:O	1:B:223:GLU:HG3	2.18	0.44
1:A:149:ALA:O	1:A:249:VAL:HG22	2.18	0.44
1:B:228:LEU:HD12	1:B:232:GLU:CB	2.48	0.44
1:B:391:PRO:O	1:B:392:ASN:C	2.61	0.44
1:A:15:LEU:HD11	1:A:20:LEU:HD11	1.99	0.44
1:B:36:ARG:HA	1:B:56:VAL:HG23	1.99	0.44
1:B:259:LEU:HG	1:B:266:LEU:HB2	2.00	0.44
1:B:273:MET:O	1:B:276:LEU:HB2	2.17	0.44
1:A:266:LEU:HD21	1:A:372:LEU:HD11	2.00	0.43
1:A:346:ALA:CB	4:A:2102:HOH:O	2.65	0.43
1:B:300:GLU:O	1:B:302:VAL:HG23	2.18	0.43
1:A:116:VAL:HG12	1:A:362:LEU:HD22	2.00	0.43
1:A:102:ARG:NH1	1:A:227:ARG:O	2.51	0.43
1:A:182:ASP:O	1:A:183:ASP:HB2	2.19	0.43
1:A:358:PRO:HD2	4:A:2127:HOH:O	2.17	0.43
1:A:131:VAL:O	1:A:135:LEU:HG	2.18	0.43
1:A:165:GLU:HA	1:A:168:ARG:CD	2.49	0.43
1:B:331:ASP:N	1:B:332:PRO:CD	2.79	0.43
1:B:152:LEU:CB	1:B:153:PRO:HD3	2.37	0.43
1:B:214:LEU:HD13	1:B:218:VAL:CG2	2.49	0.43
1:B:279:ALA:O	1:B:283:MET:HG3	2.18	0.43
1:B:281:GLU:HA	1:B:284:LEU:HD12	1.99	0.43
1:A:296:ARG:HG3	1:A:296:ARG:HH11	1.84	0.43
1:A:334:ARG:NH1	1:A:335:PHE:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLY:HA2	4:A:2127:HOH:O	2.18	0.43
1:A:375:CYS:HA	1:A:376:PRO:HD2	1.86	0.43
1:B:111:PHE:CE2	2:B:419:HEM:HBC1	2.54	0.43
1:B:285:ARG:O	1:B:323:HIS:HB3	2.18	0.43
1:A:236:MET:O	1:A:239:ILE:HG22	2.19	0.43
1:A:52:VAL:HG23	1:A:53:TRP:N	2.32	0.43
1:A:100:HIS:CD2	1:A:352:HIS:CE1	3.07	0.43
1:B:285:ARG:HH21	1:B:324:ARG:HD3	1.84	0.43
1:A:41:ALA:C	1:A:42:HIS:CG	2.96	0.42
1:A:183:ASP:CG	1:A:184:PRO:HD2	2.44	0.42
1:B:382:VAL:HG21	1:B:386:GLU:OE1	2.19	0.42
1:A:214:LEU:O	1:A:218:VAL:HG23	2.19	0.42
1:A:269:LEU:HD11	1:A:276:LEU:HA	2.01	0.42
1:B:29:TYR:HB2	1:B:30:PRO:HD3	2.01	0.42
1:B:224:ASP:C	1:B:226:SER:N	2.74	0.42
1:B:369:ARG:NH1	1:B:373:GLU:OE2	2.52	0.42
1:B:342:ALA:N	4:B:2098:HOH:O	2.52	0.42
1:A:14:VAL:N	4:A:2001:HOH:O	2.52	0.42
1:A:95:SER:HB3	1:A:99:ARG:HD2	1.96	0.42
1:A:115:ARG:HB2	1:A:115:ARG:HH11	1.84	0.42
1:A:183:ASP:C	1:A:185:ALA:N	2.78	0.42
1:B:32:TYR:O	1:B:35:LEU:HB2	2.20	0.42
1:B:85:GLU:HB3	3:B:420:PXI:H132	2.00	0.42
1:A:270:ARG:NH2	1:A:375:CYS:O	2.53	0.42
1:B:265:GLN:NE2	1:B:337:ILE:HG12	2.35	0.42
1:B:375:CYS:HA	1:B:376:PRO:HD2	1.90	0.42
1:A:131:VAL:CG1	1:A:374:ARG:HD3	2.50	0.41
1:A:150:TRP:N	1:A:151:PRO:CD	2.83	0.41
1:B:102:ARG:O	1:B:106:LEU:CD1	2.60	0.41
1:B:85:GLU:O	3:B:420:PXI:H143	2.20	0.41
1:A:325:THR:HG22	1:A:327:GLU:OE1	2.19	0.41
1:B:372:LEU:HB2	1:B:373:GLU:OE1	2.20	0.41
1:A:119:LEU:O	1:A:123:VAL:HG23	2.20	0.41
1:A:334:ARG:NH2	1:A:335:PHE:O	2.53	0.41
1:B:254:ASN:ND2	1:B:396:ARG:O	2.48	0.41
1:B:266:LEU:O	1:B:270:ARG:HG3	2.20	0.41
1:B:272:ASP:HB3	1:B:275:LEU:CD1	2.51	0.41
1:B:117:GLU:HG3	1:B:117:GLU:O	2.21	0.41
1:A:20:LEU:HB3	1:A:24:PHE:HB2	2.03	0.41
1:A:77:SER:HB2	1:A:297:PHE:CD2	2.56	0.41
1:A:328:ARG:HA	4:A:2113:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:HG13	1:B:161:LEU:HD12	2.03	0.41
1:A:43:ARG:HA	1:A:52:VAL:O	2.21	0.40
1:A:116:VAL:HA	4:A:2054:HOH:O	2.21	0.40
1:A:212:ASP:HA	4:A:2064:HOH:O	2.19	0.40
1:A:290:VAL:HG13	3:A:420:PXI:H252	2.02	0.40
1:A:324:ARG:HA	1:A:332:PRO:CB	2.52	0.40
1:A:339:ARG:CZ	4:A:2117:HOH:O	2.67	0.40
1:B:201:LEU:O	1:B:205:LYS:HG2	2.21	0.40
1:A:76:ASN:O	1:A:312:GLY:HA2	2.22	0.40
1:A:331:ASP:O	1:A:334:ARG:HB3	2.20	0.40
1:B:330:PRO:O	1:B:331:ASP:C	2.64	0.40
1:B:92:MET:HE2	1:B:92:MET:HB3	1.95	0.40
1:B:161:LEU:CD1	1:B:241:LEU:HG	2.52	0.40
1:B:165:GLU:N	1:B:166:PRO:CD	2.84	0.40
1:B:269:LEU:HD11	1:B:276:LEU:HA	2.03	0.40
1:A:93:LEU:HA	2:A:419:HEM:O1D	2.21	0.40
1:A:175:THR:HG21	1:A:246:GLU:HG2	1.96	0.40
1:A:282:GLU:OE1	1:A:282:GLU:CA	2.70	0.40
1:B:48:GLU:HB2	4:B:2011:HOH:O	2.20	0.40
1:A:273:MET:HE1	1:A:369:ARG:HA	2.03	0.40
1:B:276:LEU:HD11	1:B:365:ARG:CB	2.52	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	390/436 (89%)	360 (92%)	28 (7%)	2 (0%)	24 12
1	B	391/436 (90%)	350 (90%)	38 (10%)	3 (1%)	16 5
All	All	781/872 (90%)	710 (91%)	66 (8%)	5 (1%)	21 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	382	VAL
1	A	374	ARG
1	B	273	MET
1	A	375	CYS
1	B	343	GLY

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	316/355 (89%)	306 (97%)	10 (3%)	34	17
1	B	314/355 (88%)	304 (97%)	10 (3%)	34	17
All	All	630/710 (89%)	610 (97%)	20 (3%)	34	17

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	60	ARG
1	A	106	LEU
1	A	115	ARG
1	A	135	LEU
1	A	146	GLU
1	A	176	ASP
1	A	219	ARG
1	A	238	HIS
1	A	285	ARG
1	B	99	ARG
1	B	119	LEU
1	B	182	ASP
1	B	200	ARG
1	B	236	MET
1	B	246	GLU
1	B	285	ARG
1	B	305	ASP

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Mol	Chain	Res	Type
1	B	334	ARG
1	B	395	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	188	GLN
1	A	208	GLN
1	A	250	ASN
1	A	265	GLN
1	A	344	HIS
1	B	22	GLN
1	B	42	HIS
1	B	208	GLN
1	B	238	HIS
1	B	265	GLN
1	B	344	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
2	HEM	B	419	-	50,50,50	1.41	10 (20%)	66,82,82	1.45	9 (13%)
3	PXI	A	420	-	33,33,33	1.87	7 (21%)	40,47,47	2.08	9 (22%)
3	PXI	B	420	-	33,33,33	2.03	5 (15%)	40,47,47	2.11	12 (30%)
2	HEM	A	419	-	50,50,50	1.56	10 (20%)	66,82,82	1.00	4 (6%)

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
2	HEM	B	419	-	-	1/14/54/54	-
3	PXI	A	420	-	-	16/43/59/59	0/1/2/2
3	PXI	B	420	-	-	15/43/59/59	0/1/2/2
2	HEM	A	419	-	-	1/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	420	PXI	C19-C21	6.45	1.62	1.51
3	B	420	PXI	C16-C7	5.87	1.63	1.53
3	A	420	PXI	C19-C21	5.70	1.61	1.51
3	A	420	PXI	C16-C7	4.59	1.61	1.53
3	A	420	PXI	C24-C3	4.01	1.63	1.53
3	B	420	PXI	C24-C3	3.85	1.62	1.53
2	A	419	HEM	CBC-CAC	3.26	1.46	1.30
2	B	419	HEM	CAC-C3C	-3.22	1.38	1.47
2	A	419	HEM	CBB-CAB	3.16	1.45	1.30
2	A	419	HEM	FE-ND	3.06	2.04	1.94
2	A	419	HEM	CMB-C2B	3.03	1.57	1.50
3	A	420	PXI	C11-C9	2.95	1.57	1.51
3	B	420	PXI	C11-C9	2.85	1.56	1.51
2	A	419	HEM	C1A-NA	2.80	1.45	1.39
2	B	419	HEM	CBB-CAB	2.62	1.43	1.30
3	B	420	PXI	O4-C9	2.53	1.49	1.44
2	A	419	HEM	C1A-C2A	2.52	1.49	1.44
2	B	419	HEM	CHB-C1B	2.51	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	419	HEM	CAB-C3B	-2.45	1.40	1.47
2	B	419	HEM	CBC-CAC	2.44	1.42	1.30
2	B	419	HEM	CHA-C4D	2.42	1.43	1.38
2	A	419	HEM	C1B-C2B	2.38	1.49	1.44
2	B	419	HEM	C1A-C2A	2.31	1.49	1.44
3	A	420	PXI	C5-C4	-2.28	1.46	1.51
2	B	419	HEM	CMC-C2C	2.20	1.55	1.50
2	A	419	HEM	CAC-C3C	-2.12	1.41	1.47
2	A	419	HEM	C4A-NA	2.10	1.43	1.39
2	A	419	HEM	O2A-CGA	-2.09	1.23	1.30
3	A	420	PXI	C15-C12	2.06	1.58	1.53
2	B	419	HEM	C1B-C2B	2.06	1.48	1.44
2	B	419	HEM	FE-NB	2.03	2.01	1.94
3	A	420	PXI	O4-C9	2.01	1.48	1.44

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	420	PXI	C3-O1-C4	7.61	129.32	117.89
3	B	420	PXI	C3-O1-C4	6.88	128.21	117.89
3	A	420	PXI	O3-C7-C5	-6.01	100.68	111.14
3	B	420	PXI	O3-C7-C5	-5.49	101.59	111.14
2	B	419	HEM	CAA-C2A-C1A	4.82	134.38	124.89
3	B	420	PXI	C7-C5-C4	3.57	117.30	110.01
3	A	420	PXI	C7-C5-C4	3.35	116.86	110.01
2	B	419	HEM	CAD-C3D-C4D	3.24	130.32	124.66
2	B	419	HEM	C4B-C3B-C2B	-3.19	104.58	107.11
2	B	419	HEM	CAC-C3C-C4C	3.18	132.59	124.90
2	B	419	HEM	CAA-C2A-C3A	-3.11	119.95	127.07
3	B	420	PXI	C10-C9-C11	-3.06	108.59	113.40
3	B	420	PXI	O1-C3-C2	2.97	111.67	106.92
3	B	420	PXI	C6-C5-C7	-2.85	106.46	112.92
3	B	420	PXI	C25-C24-C23	-2.85	103.10	109.99
2	B	419	HEM	CAD-C3D-C2D	-2.82	122.62	127.88
2	A	419	HEM	C4A-NA-C1A	-2.78	102.62	105.35
3	A	420	PXI	O3-C8-O4	2.72	118.26	110.67
2	A	419	HEM	C3B-C2B-C1B	-2.71	104.47	106.49
3	A	420	PXI	C25-C24-C23	-2.69	103.48	109.99
3	B	420	PXI	C13-N1-C12	-2.59	105.33	113.11
3	B	420	PXI	O3-C8-O4	2.57	117.85	110.67
2	B	419	HEM	CAC-C3C-C2C	-2.53	120.25	128.60
3	A	420	PXI	C6-C5-C7	-2.49	107.27	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	420	PXI	C10-C9-C11	-2.47	109.53	113.40
2	A	419	HEM	C3A-C4A-NA	2.43	113.77	110.08
3	A	420	PXI	C13-N1-C12	-2.41	105.87	113.11
2	B	419	HEM	CHC-C1C-C2C	-2.38	120.49	125.48
3	A	420	PXI	O1-C3-C2	2.28	110.56	106.92
3	B	420	PXI	C19-C21-C22	2.25	123.95	118.29
3	B	420	PXI	C9-C11-C12	-2.25	106.52	110.46
2	A	419	HEM	CMD-C2D-C1D	2.13	128.28	125.04
3	B	420	PXI	C8-C15-C12	-2.11	105.73	109.19
2	B	419	HEM	C3B-C2B-C1B	2.09	108.04	106.49

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	420	PXI	C23-C24-C3-O1
3	A	420	PXI	C11-C12-N1-C13
3	A	420	PXI	C11-C12-N1-C14
3	A	420	PXI	C15-C12-N1-C13
3	A	420	PXI	C15-C12-N1-C14
3	A	420	PXI	C16-C18-C19-C21
3	B	420	PXI	C23-C24-C3-O1
3	B	420	PXI	C11-C12-N1-C13
3	B	420	PXI	C11-C12-N1-C14
3	B	420	PXI	C15-C12-N1-C13
3	B	420	PXI	C15-C12-N1-C14
3	A	420	PXI	O4-C8-O3-C7
3	B	420	PXI	O4-C8-O3-C7
3	A	420	PXI	C22-C23-C24-C25
3	B	420	PXI	C22-C23-C24-C25
3	B	420	PXI	O6-C21-C22-C23
3	B	420	PXI	C6-C5-C7-O3
3	A	420	PXI	C19-C21-C22-C23
3	B	420	PXI	C19-C21-C22-C23
3	B	420	PXI	C16-C18-C19-C21
3	A	420	PXI	C25-C24-C3-C2
3	A	420	PXI	C25-C24-C3-O1
3	B	420	PXI	C16-C18-C19-C20
3	A	420	PXI	O6-C21-C22-C23
2	B	419	HEM	C2B-C3B-CAB-CBB
3	A	420	PXI	C23-C24-C3-C2
3	B	420	PXI	C23-C24-C3-C2

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Mol	Chain	Res	Type	Atoms
3	A	420	PXI	C16-C18-C19-C20
3	B	420	PXI	C25-C24-C3-O1
3	A	420	PXI	C17-C16-C18-C19
2	A	419	HEM	C3A-C2A-CAA-CBA
3	A	420	PXI	C7-C16-C18-C19
3	B	420	PXI	C4-C5-C7-C16

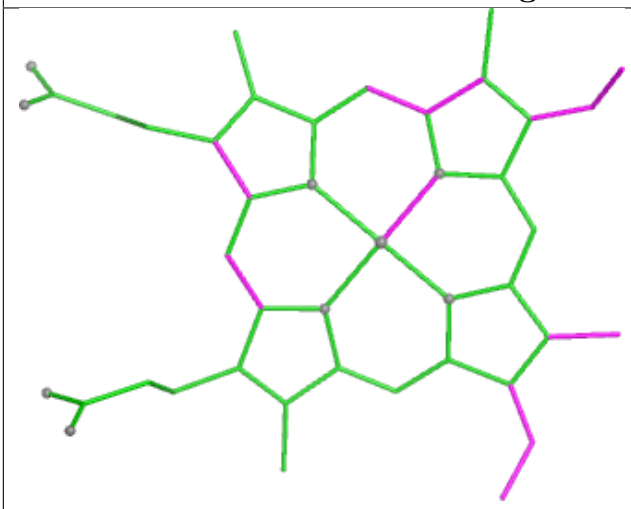
There are no ring outliers.

4 monomers are involved in 10 short contacts:

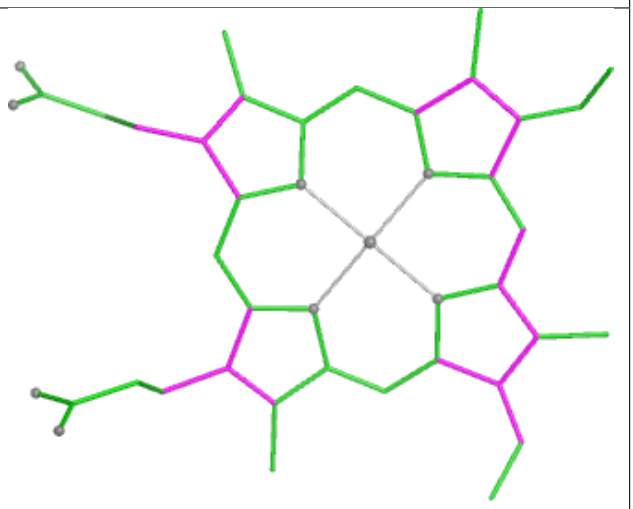
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	419	HEM	2	0
3	A	420	PXI	1	0
3	B	420	PXI	5	0
2	A	419	HEM	2	0

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.

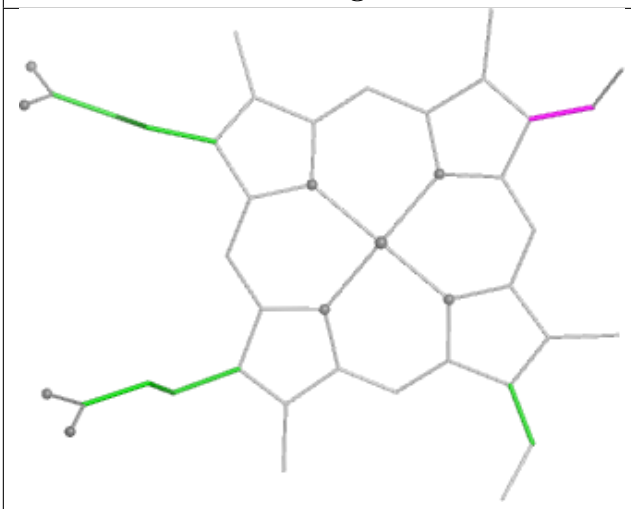
Ligand HEM B 419



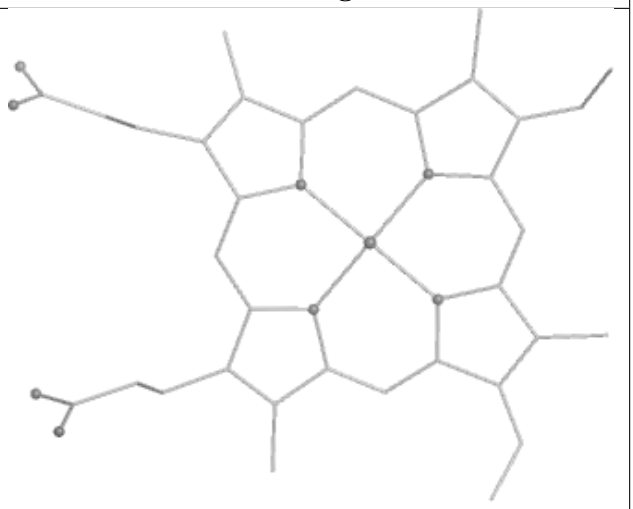
Bond lengths



Bond angles

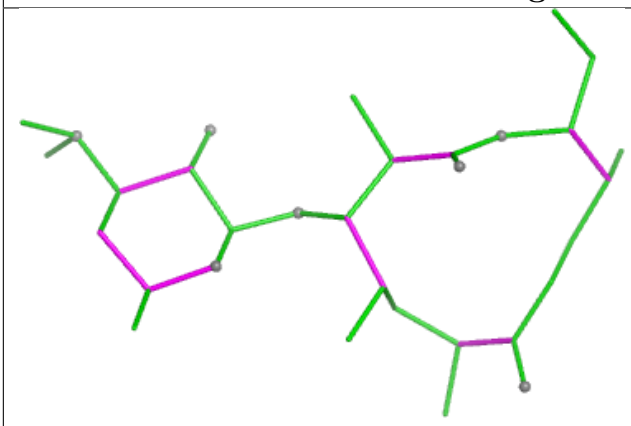


Torsions



Rings

Ligand PXI A 420



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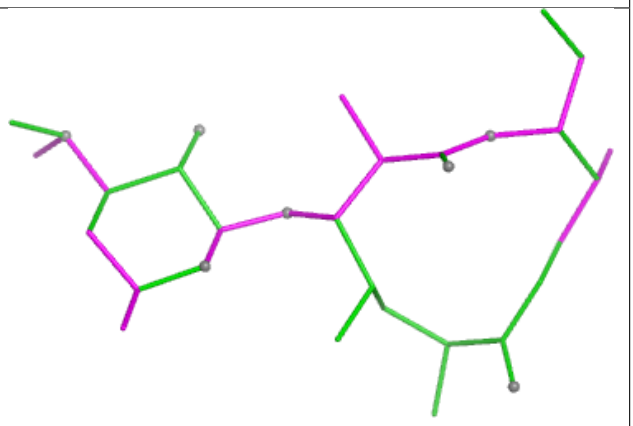

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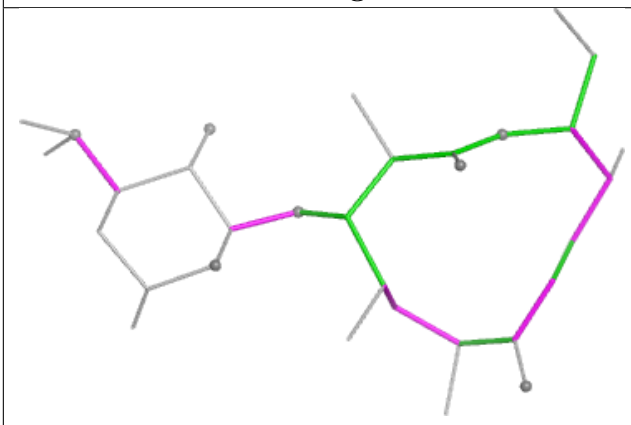

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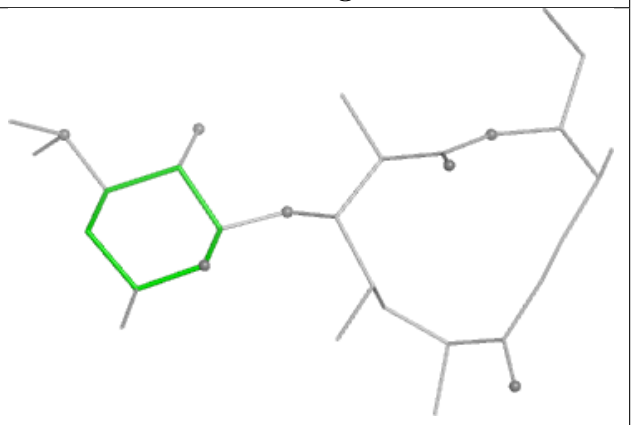
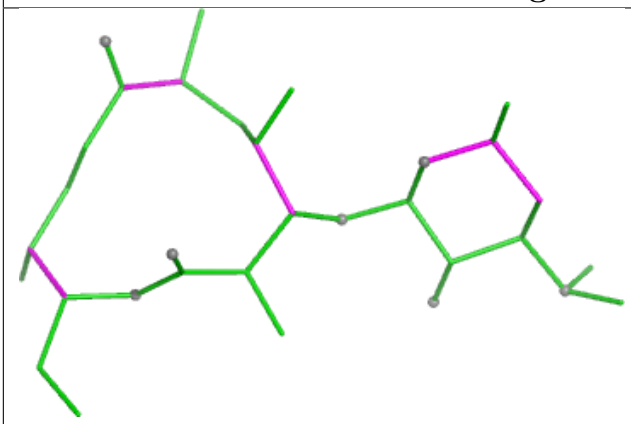
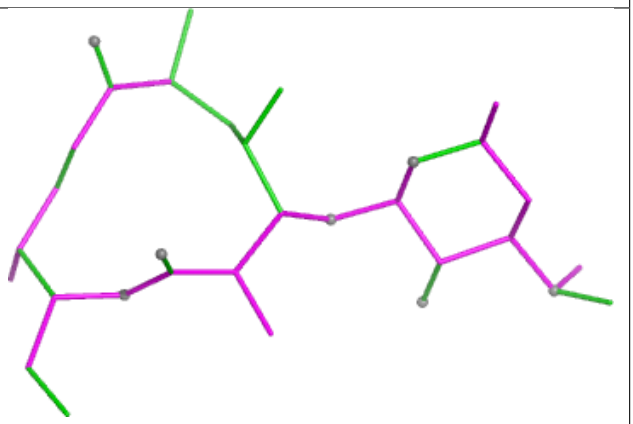


Rings

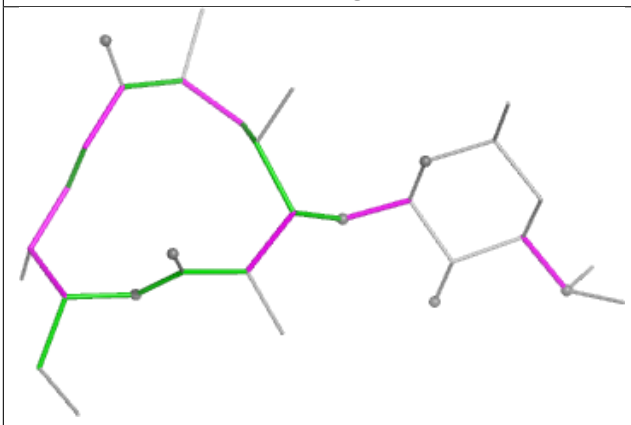
Ligand PXI B 420



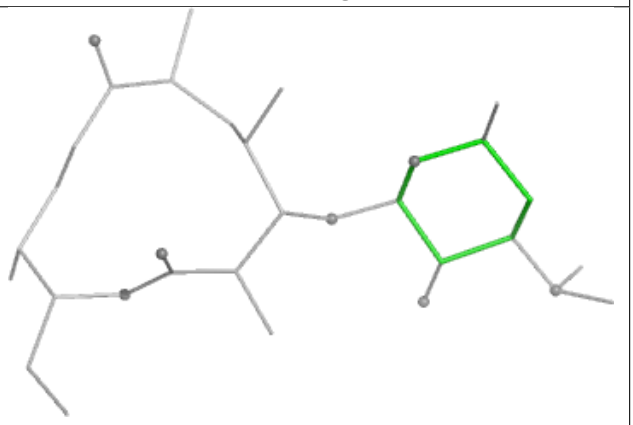
Bond lengths



Bond angles

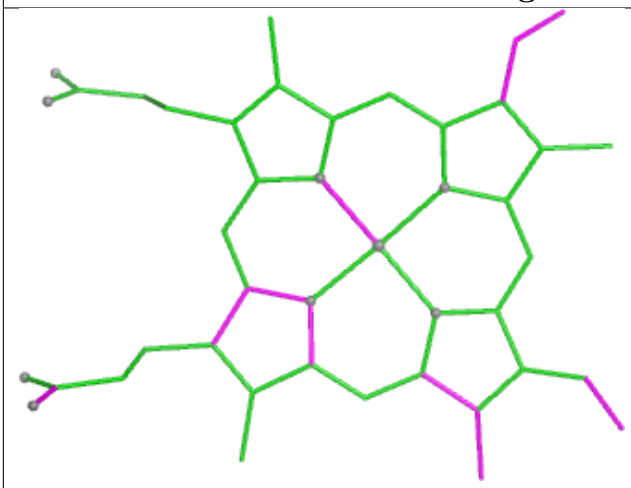


Torsions

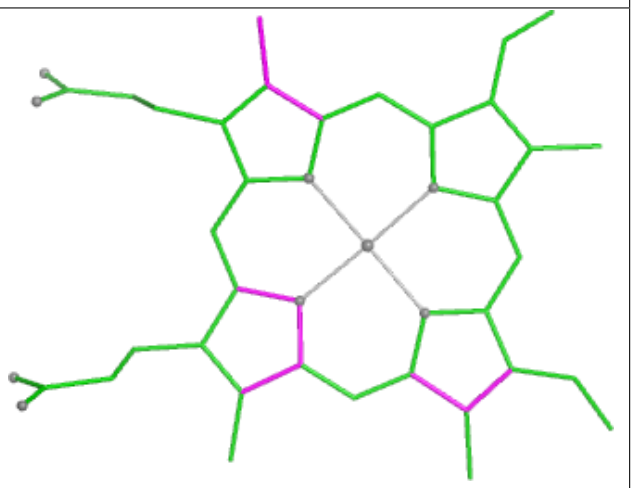


Rings

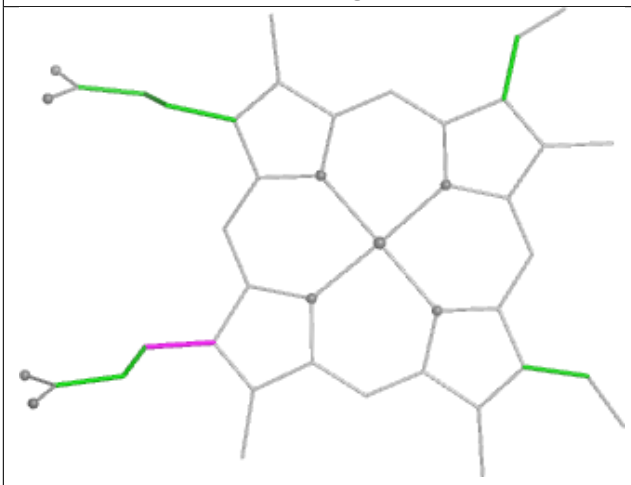
Ligand HEM A 419



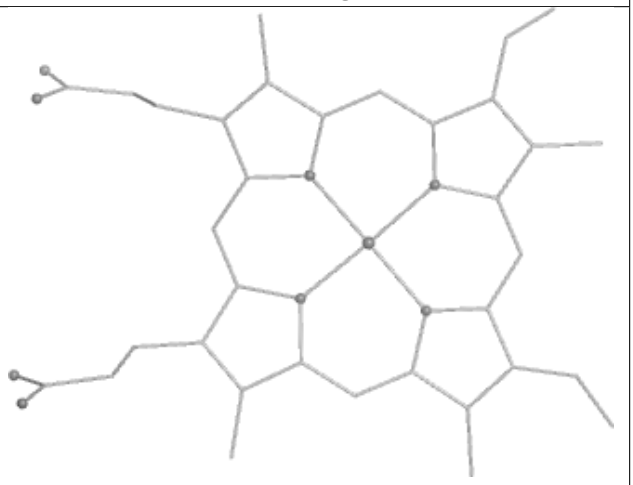
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	392/436 (89%)	-1.27	0	100	100	12, 20, 31, 41	0
1	B	393/436 (90%)	-1.21	0	100	100	12, 24, 36, 41	0
All	All	785/872 (90%)	-1.24	0	100	100	12, 22, 35, 41	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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.

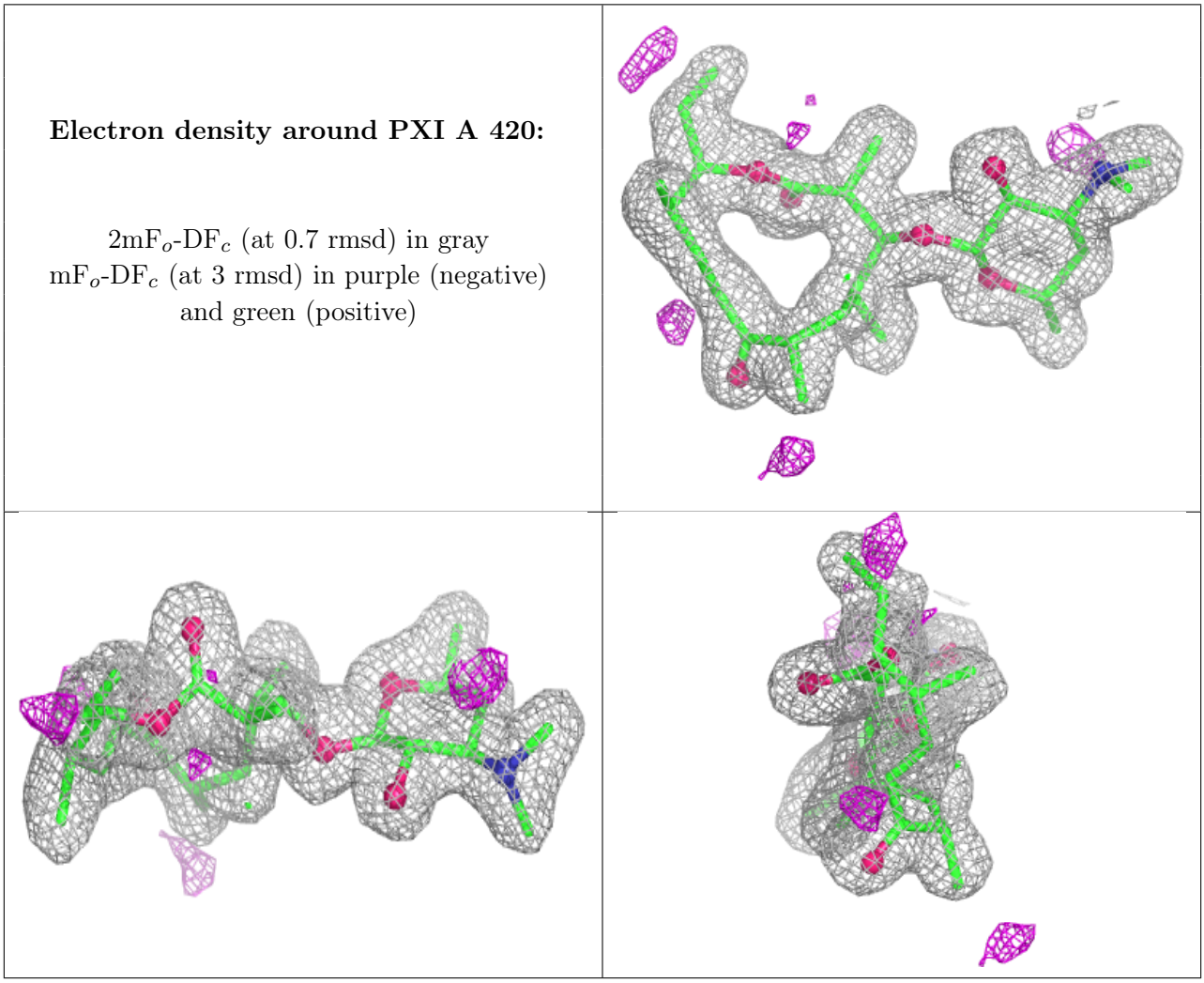
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PXI	A	420	32/32	0.99	0.03	13,19,23,25	0
3	PXI	B	420	32/32	0.99	0.03	14,20,24,26	0
2	HEM	A	419	43/43	1.00	0.02	6,13,17,18	0
2	HEM	B	419	43/43	1.00	0.02	10,15,18,19	0

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.

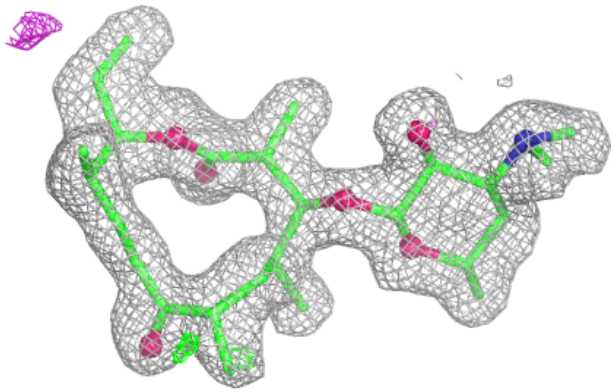
Electron density around PXI A 420:

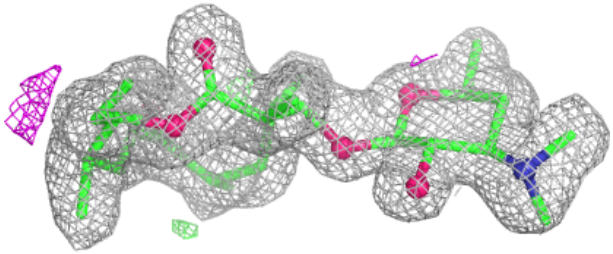
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

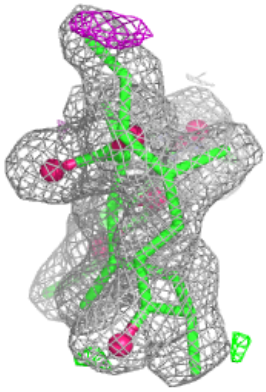


Electron density around PXI B 420:

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

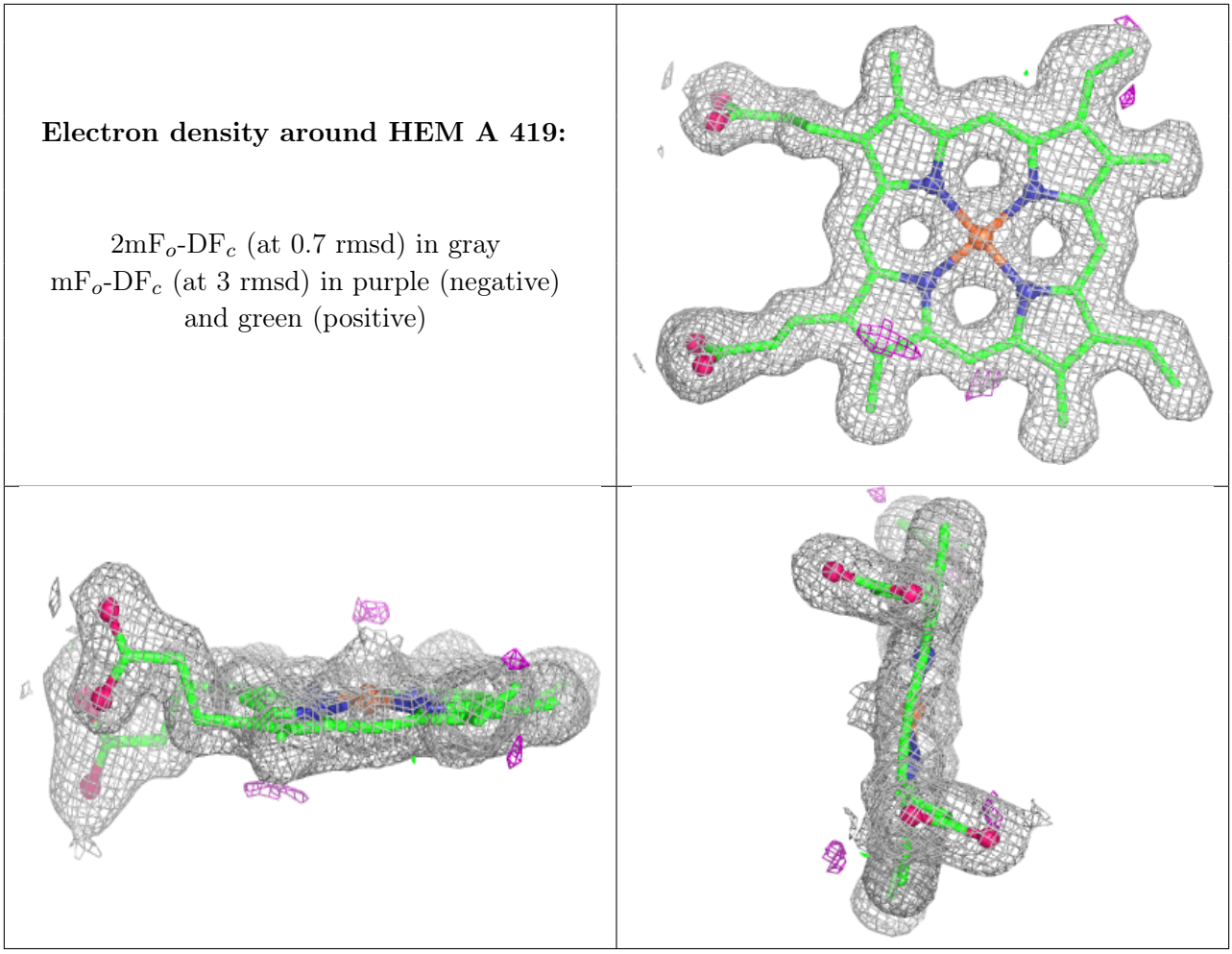






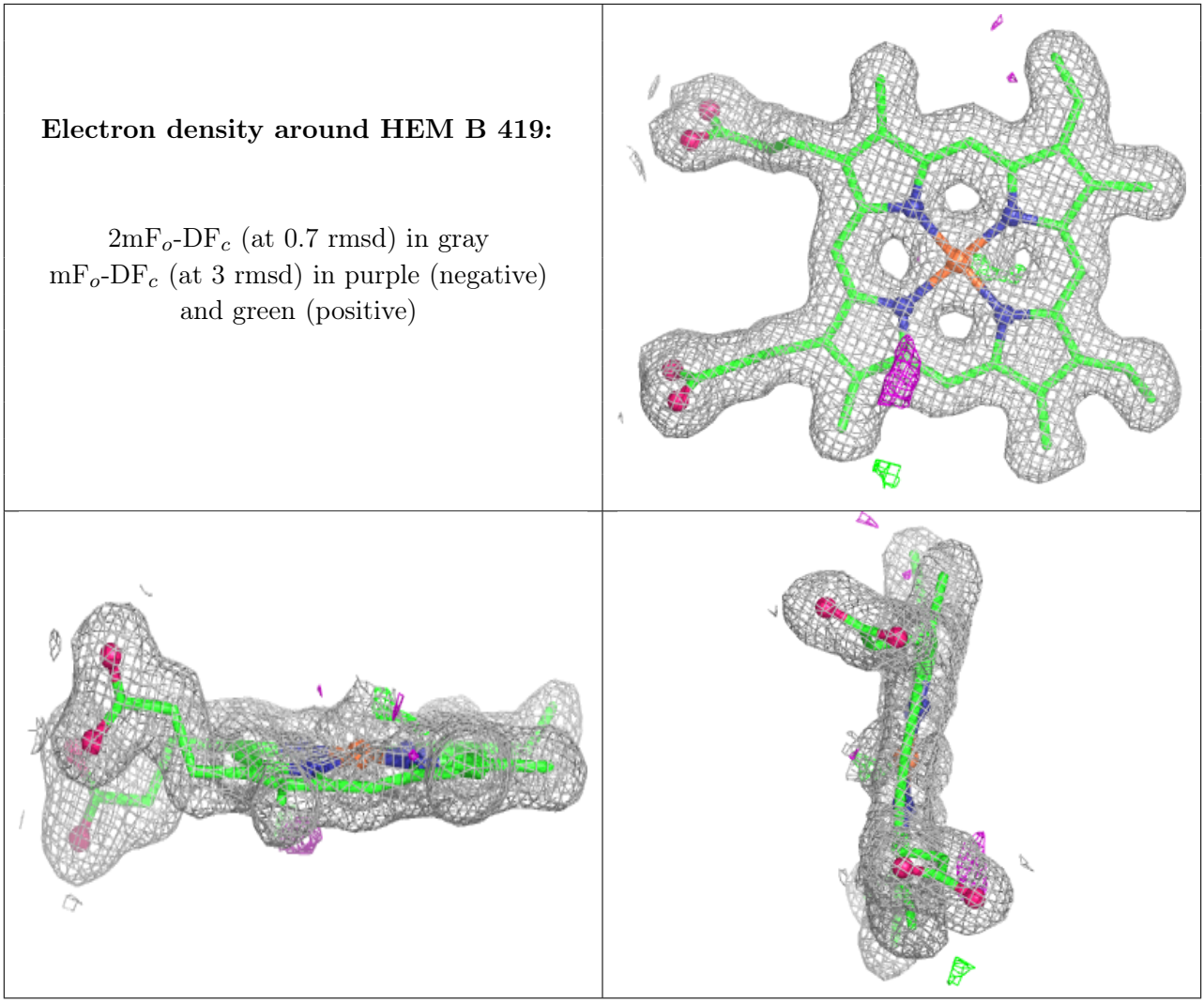
Electron density around HEM A 419:

$2mF_o$-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 B 419:

$2mF_o$-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.