Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:00 AM UTC

PDB ID	:	2FDV / pdb_00002fdv
Title	:	Microsomal P450 2A6 with the inhibitor N-Methyl(5-(pyridin-3-yl)furan-2-yl)methanamine bound
Authors	:	Yano, J.K.; Stout, C.D.; Johnson, E.F.
Deposited on	:	2005-12-14
Resolution	:	1.65 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 ⓘ 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 ⓘ) were used in the production of this report:

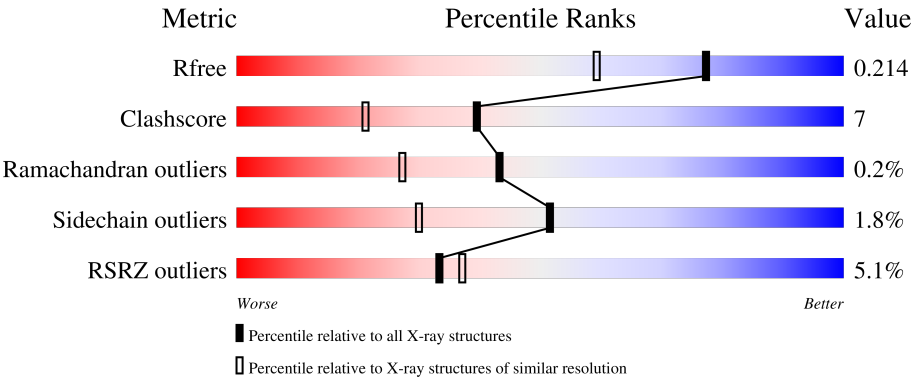
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	476	3% 83% 14%
1	B	476	9% 80% 16%
1	C	476	2% 82% 14%
1	D	476	6% 80% 17%

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
5	EDO	C	2004	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16747 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 2A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3760	2414	650	678	18			
1	B	465	Total	C	N	O	S	0	0	0
			3767	2418	653	678	18			
1	C	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	D	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	cloning artifact	UNP P11509
A	24	ALA	-	cloning artifact	UNP P11509
A	25	LYS	-	cloning artifact	UNP P11509
A	26	LYS	-	cloning artifact	UNP P11509
A	27	THR	-	cloning artifact	UNP P11509
A	28	SER	-	cloning artifact	UNP P11509
A	495	HIS	-	expression tag	UNP P11509
A	496	HIS	-	expression tag	UNP P11509
A	497	HIS	-	expression tag	UNP P11509
A	498	HIS	-	expression tag	UNP P11509
B	23	MET	-	cloning artifact	UNP P11509
B	24	ALA	-	cloning artifact	UNP P11509
B	25	LYS	-	cloning artifact	UNP P11509
B	26	LYS	-	cloning artifact	UNP P11509
B	27	THR	-	cloning artifact	UNP P11509
B	28	SER	-	cloning artifact	UNP P11509
B	495	HIS	-	expression tag	UNP P11509
B	496	HIS	-	expression tag	UNP P11509
B	497	HIS	-	expression tag	UNP P11509
B	498	HIS	-	expression tag	UNP P11509
C	23	MET	-	cloning artifact	UNP P11509

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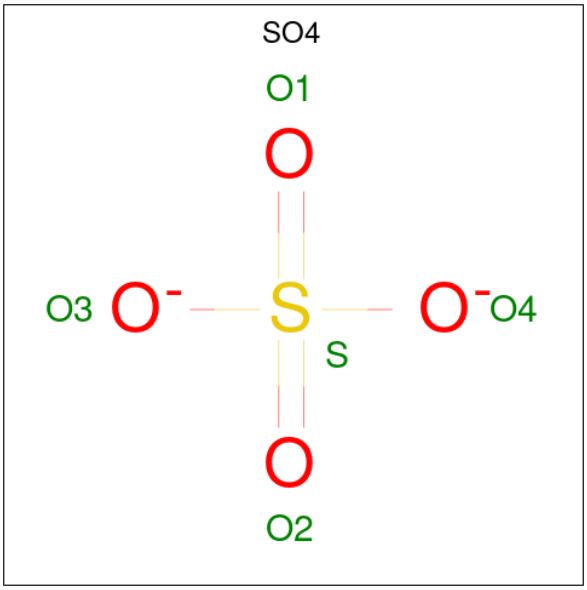
Chain	Residue	Modelled	Actual	Comment	Reference
C	24	ALA	-	cloning artifact	UNP P11509
C	25	LYS	-	cloning artifact	UNP P11509
C	26	LYS	-	cloning artifact	UNP P11509
C	27	THR	-	cloning artifact	UNP P11509
C	28	SER	-	cloning artifact	UNP P11509
C	495	HIS	-	expression tag	UNP P11509
C	496	HIS	-	expression tag	UNP P11509
C	497	HIS	-	expression tag	UNP P11509
C	498	HIS	-	expression tag	UNP P11509
D	23	MET	-	cloning artifact	UNP P11509
D	24	ALA	-	cloning artifact	UNP P11509
D	25	LYS	-	cloning artifact	UNP P11509
D	26	LYS	-	cloning artifact	UNP P11509
D	27	THR	-	cloning artifact	UNP P11509
D	28	SER	-	cloning artifact	UNP P11509
D	495	HIS	-	expression tag	UNP P11509
D	496	HIS	-	expression tag	UNP P11509
D	497	HIS	-	expression tag	UNP P11509
D	498	HIS	-	expression tag	UNP P11509

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

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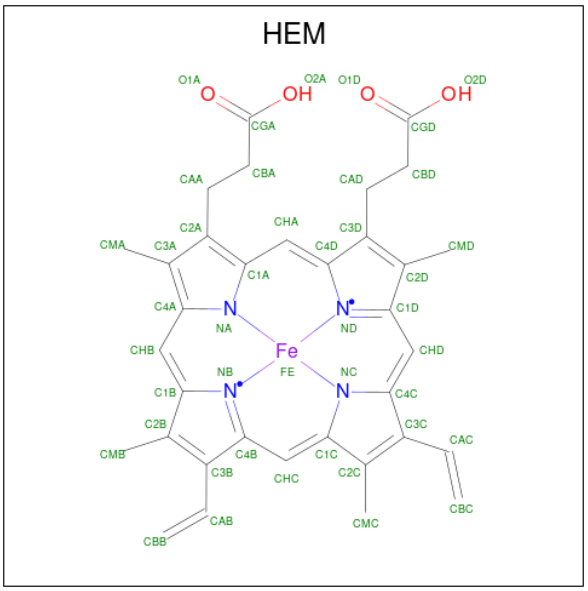
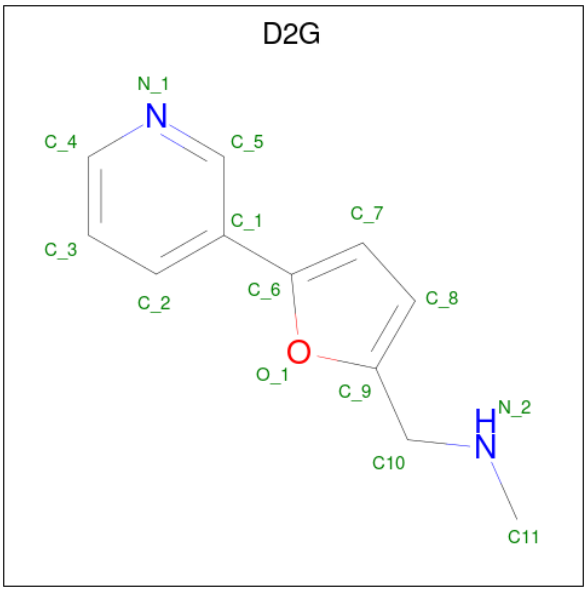
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



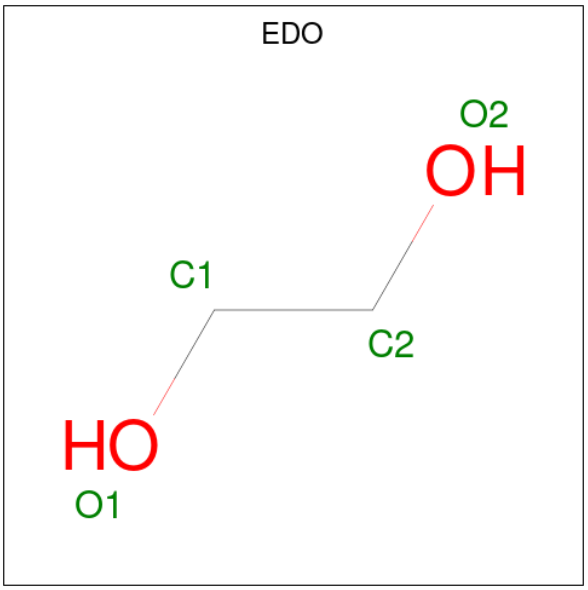
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	D	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 4 is N-METHYL(5-(PYRIDIN-3-YL)FURAN-2-YL)METHANAMINE (CCD ID: D2G) (formula: $C_{11}H_{12}N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 11 2 1	0	0
4	B	1	Total C N O 14 11 2 1	0	0
4	C	1	Total C N O 14 11 2 1	0	0
4	D	1	Total C N O 14 11 2 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

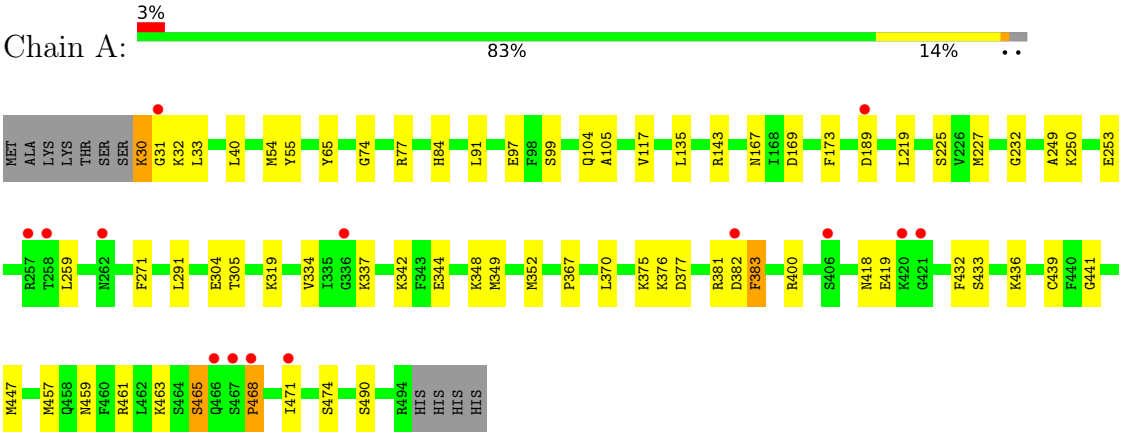
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	411	Total O 411 411	0	0
6	B	255	Total O 255 255	0	0
6	C	417	Total O 417 417	0	0
6	D	354	Total O 354 354	0	0

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.

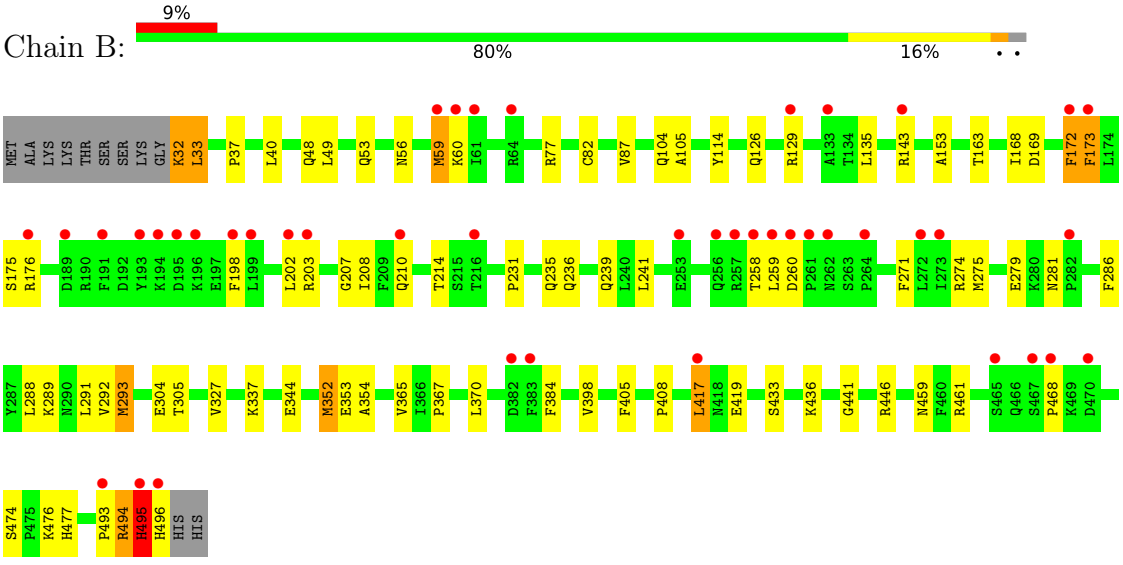
• Molecule 1: Cytochrome P450 2A6

Chain A:



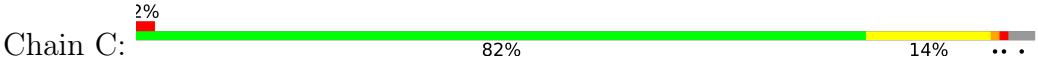
• Molecule 1: Cytochrome P450 2A6

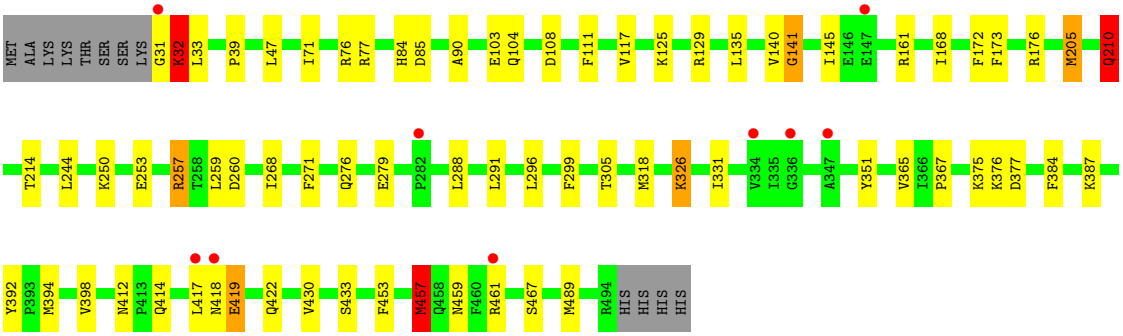
Chain B:



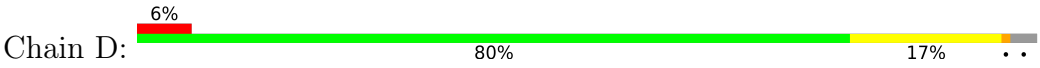
• Molecule 1: Cytochrome P450 2A6

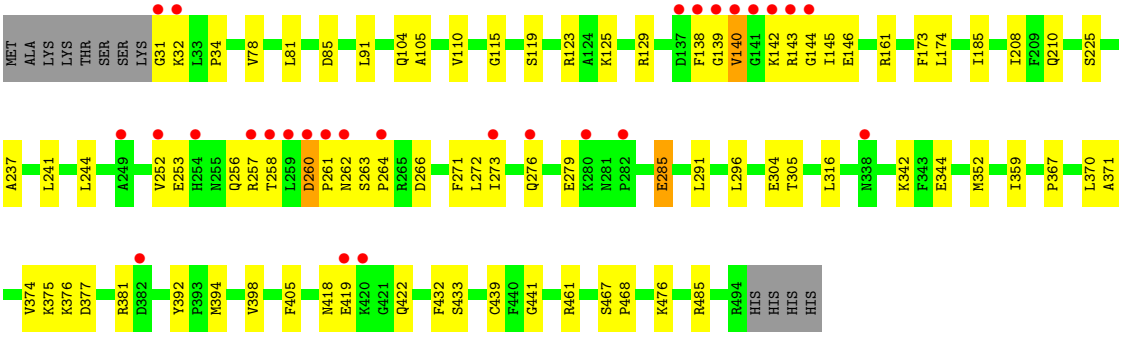
Chain C:





• Molecule 1: Cytochrome P450 2A6





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.93Å 157.43Å 103.90Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	33.80 – 1.65 33.80 – 1.65	Depositor EDS
% Data completeness (in resolution range)	88.0 (33.80-1.65) 92.5 (33.80-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.188 , 0.220 0.184 , 0.214	Depositor DCC
R_{free} test set	13799 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16747	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: SO4, HEM, D2G, EDO

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	1.23	6/3851 (0.2%)	1.24	25/5186 (0.5%)
1	B	1.09	8/3860 (0.2%)	1.23	26/5200 (0.5%)
1	C	1.25	8/3842 (0.2%)	1.23	18/5175 (0.3%)
1	D	1.22	10/3842 (0.3%)	1.21	20/5175 (0.4%)
All	All	1.20	32/15395 (0.2%)	1.23	89/20736 (0.4%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	34	PRO	CA-C	9.23	1.56	1.51
1	A	349	MET	SD-CE	-8.63	1.57	1.79
1	D	237	ALA	CA-CB	7.28	1.64	1.53
1	B	293	MET	SD-CE	-6.79	1.62	1.79
1	D	352	MET	SD-CE	-6.24	1.64	1.79
1	C	71	ILE	N-CA	6.23	1.53	1.46
1	A	457	MET	SD-CE	5.98	1.94	1.79
1	B	275	MET	SD-CE	-5.92	1.64	1.79
1	C	457	MET	SD-CE	5.90	1.94	1.79
1	B	327	VAL	CA-CB	5.88	1.61	1.54
1	D	81	LEU	N-CA	5.77	1.53	1.46
1	C	205	MET	SD-CE	-5.76	1.65	1.79
1	B	352	MET	SD-CE	-5.75	1.65	1.79
1	D	34	PRO	C-O	5.74	1.29	1.25
1	C	318	MET	SD-CE	5.72	1.93	1.79
1	D	78	VAL	CA-CB	5.68	1.63	1.54
1	A	334	VAL	CA-CB	5.63	1.62	1.54
1	A	352	MET	SD-CE	-5.63	1.65	1.79
1	A	227	MET	SD-CE	-5.57	1.65	1.79
1	B	153	ALA	CA-CB	5.52	1.61	1.53
1	D	110	VAL	CA-CB	5.45	1.61	1.54
1	D	405	PHE	CA-C	-5.44	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	398	VAL	N-CA	5.41	1.52	1.46
1	C	394	MET	CG-SD	5.38	1.94	1.80
1	B	114	TYR	N-CA	5.25	1.51	1.45
1	B	59	MET	SD-CE	-5.23	1.66	1.79
1	B	87	VAL	CA-CB	5.16	1.60	1.54
1	C	489	MET	SD-CE	5.11	1.92	1.79
1	C	268	ILE	CA-CB	5.09	1.60	1.54
1	A	447	MET	SD-CE	5.04	1.92	1.79
1	C	90	ALA	CA-CB	5.04	1.61	1.53
1	D	394	MET	CG-SD	5.03	1.93	1.80

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	304	GLU	N-CA-C	8.77	120.92	111.36
1	B	494	ARG	N-CA-C	-7.86	103.84	113.19
1	C	104	GLN	N-CA-C	-7.53	94.78	107.80
1	D	104	GLN	N-CA-C	-7.41	94.99	107.80
1	A	436	LYS	N-CA-C	7.00	119.94	111.82
1	A	370	LEU	N-CA-C	-6.99	97.81	109.07
1	C	461	ARG	N-CA-C	-6.97	98.87	109.95
1	B	459	ASN	N-CA-C	6.77	121.62	113.23
1	B	279	GLU	N-CA-C	6.76	119.51	111.33
1	B	436	LYS	N-CA-C	6.66	120.66	112.54
1	D	370	LEU	N-CA-C	-6.65	98.86	109.76
1	D	304	GLU	N-CA-C	6.53	119.40	111.82
1	A	169	ASP	N-CA-C	-6.52	100.17	109.24
1	A	259	LEU	N-CA-C	6.52	119.81	110.10
1	D	173	PHE	N-CA-C	-6.50	104.27	111.36
1	B	474	SER	N-CA-C	-6.48	101.14	110.08
1	C	419	GLU	N-CA-C	-6.46	104.33	111.82
1	B	260	ASP	CA-C-N	6.46	127.91	119.84
1	B	260	ASP	C-N-CA	6.46	127.91	119.84
1	A	104	GLN	N-CA-C	-6.41	95.06	107.44
1	C	173	PHE	N-CA-C	-6.27	104.44	111.28
1	B	173	PHE	N-CA-C	-6.22	104.42	111.14
1	B	40	LEU	N-CA-C	-6.22	102.25	110.40
1	C	288	LEU	N-CA-C	6.19	118.54	111.11
1	A	84	HIS	N-CA-C	6.18	118.56	111.02
1	B	33	LEU	N-CA-C	-6.18	101.21	110.24
1	B	169	ASP	N-CA-C	-6.14	100.33	109.42
1	C	365	VAL	N-CA-C	6.14	116.88	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	MET	N-CA-C	6.10	117.60	111.07
1	B	370	LEU	N-CA-C	-5.99	99.94	109.76
1	A	377	ASP	N-CA-C	-5.98	101.56	110.23
1	D	371	ALA	N-CA-C	5.93	118.60	110.24
1	A	232	GLY	CA-C-N	5.91	126.32	119.47
1	A	232	GLY	C-N-CA	5.91	126.32	119.47
1	B	281	ASN	N-CA-C	-5.87	101.08	109.24
1	D	398	VAL	N-CA-C	-5.84	105.15	110.82
1	C	459	ASN	N-CA-C	5.84	120.13	112.89
1	C	84	HIS	N-CA-C	5.77	118.03	111.11
1	D	91	LEU	CA-C-N	-5.74	117.28	123.08
1	D	91	LEU	C-N-CA	-5.74	117.28	123.08
1	D	85	ASP	N-CA-C	5.73	117.20	111.07
1	A	367	PRO	N-CA-C	5.70	121.34	113.65
1	A	219	LEU	N-CA-C	-5.66	105.19	111.36
1	C	398	VAL	N-CA-C	-5.64	105.35	110.82
1	B	231	PRO	N-CA-C	-5.56	103.07	111.41
1	D	260	ASP	CA-C-N	5.55	126.78	119.84
1	D	260	ASP	C-N-CA	5.55	126.78	119.84
1	C	367	PRO	N-CA-C	5.54	120.83	113.57
1	B	461	ARG	N-CA-C	-5.51	101.19	109.95
1	C	111	PHE	N-CA-C	5.48	117.34	111.36
1	D	285	GLU	N-CA-C	-5.48	106.59	113.28
1	C	141	GLY	N-CA-C	-5.47	108.08	115.36
1	C	210	GLN	CB-CG-CD	5.44	121.85	112.60
1	B	288	LEU	N-CA-C	5.41	117.88	111.33
1	D	105	ALA	N-CA-C	5.40	117.17	111.28
1	C	392	TYR	CB-CA-C	-5.38	104.85	110.33
1	B	367	PRO	N-CA-C	5.36	120.88	113.65
1	C	85	ASP	N-CA-C	5.35	117.11	111.28
1	B	398	VAL	N-CA-C	-5.34	105.92	111.58
1	A	173	PHE	N-CA-C	-5.33	105.55	111.36
1	A	304	GLU	N-CA-C	5.30	117.13	111.36
1	D	367	PRO	N-CA-C	5.29	120.79	113.65
1	A	459	ASN	N-CA-C	5.28	119.78	113.23
1	A	419	GLU	N-CA-C	5.26	117.76	111.71
1	C	117	VAL	N-CA-C	5.26	115.92	110.82
1	A	91	LEU	N-CA-C	5.23	117.89	111.82
1	D	381	ARG	CA-C-N	-5.20	114.02	122.65
1	D	381	ARG	C-N-CA	-5.20	114.02	122.65
1	B	104	GLN	N-CA-C	-5.19	97.42	107.44
1	A	334	VAL	N-CA-C	5.18	116.65	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	495	HIS	N-CA-C	-5.18	102.43	113.20
1	D	377	ASP	N-CA-C	-5.17	102.40	110.10
1	C	259	LEU	N-CA-C	5.16	117.72	110.23
1	A	474	SER	N-CA-C	-5.14	102.74	110.24
1	B	105	ALA	N-CA-C	5.13	116.88	111.28
1	B	365	VAL	N-CA-C	5.13	117.46	111.05
1	D	461	ARG	N-CA-C	-5.11	101.82	109.95
1	A	461	ARG	N-CA-C	-5.10	101.84	109.95
1	A	105	ALA	N-CA-C	5.08	116.82	111.28
1	B	441	GLY	N-CA-C	-5.08	106.93	115.62
1	A	337	LYS	N-CA-C	5.08	119.57	113.17
1	B	259	LEU	N-CA-C	5.07	117.64	110.50
1	C	260	ASP	N-CA-C	-5.02	98.42	109.11
1	D	359	ILE	N-CA-C	-5.02	105.65	110.72
1	A	383	PHE	N-CA-C	-5.02	102.36	110.14
1	B	87	VAL	N-CA-C	5.02	115.24	110.42
1	A	65	TYR	N-CA-C	5.02	119.67	113.50
1	A	74	GLY	N-CA-C	-5.01	102.11	112.34
1	D	392	TYR	CB-CA-C	-5.01	104.61	110.17

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	3760	0	3747	38	0
1	B	3767	0	3745	57	0
1	C	3751	0	3734	52	0
1	D	3751	0	3734	56	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	43	0	30	4	0
3	B	43	0	30	1	0
3	C	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	43	0	30	2	0
4	A	14	0	11	2	0
4	B	14	0	11	2	0
4	C	14	0	11	1	0
4	D	14	0	11	2	0
5	A	4	0	6	0	0
5	C	20	0	30	9	0
5	D	4	0	6	0	0
6	A	411	0	0	4	0
6	B	255	0	0	9	0
6	C	417	0	0	10	0
6	D	354	0	0	2	0
All	All	16747	0	15166	204	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 7.

All (204) 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:C:108:ASP:HA	5:C:2004:EDO:H22	1.22	1.11
5:C:2004:EDO:H11	6:C:2808:HOH:O	1.58	1.04
1:C:108:ASP:CA	5:C:2004:EDO:H22	1.91	0.99
1:B:176:ARG:HD3	1:B:198:PHE:CE2	2.00	0.96
1:B:59:MET:HE1	1:B:82:CYS:SG	2.09	0.92
1:C:453:PHE:O	1:C:457:MET:HG2	1.71	0.91
1:D:418:ASN:HD21	1:D:422:GLN:HE21	1.13	0.90
1:C:108:ASP:HB2	5:C:2004:EDO:O1	1.70	0.90
1:C:31:GLY:O	1:C:32:LYS:HB2	1.72	0.89
1:A:30:LYS:HG3	1:A:32:LYS:H	1.37	0.89
1:B:344:GLU:HG3	6:B:2549:HOH:O	1.74	0.88
1:A:189:ASP:HB2	6:A:2881:HOH:O	1.74	0.87
1:A:30:LYS:HG2	1:A:382:ASP:O	1.76	0.85
1:B:236:GLN:HG2	6:B:2614:HOH:O	1.78	0.84
1:B:203:ARG:NH1	1:B:203:ARG:HB3	1.93	0.82
1:C:210:GLN:HG2	6:C:2873:HOH:O	1.78	0.82
1:B:292:VAL:HG12	1:B:293:MET:HE2	1.61	0.81
1:B:59:MET:HA	1:B:59:MET:HE2	1.64	0.80
1:C:257:ARG:HG2	1:C:257:ARG:HH11	1.48	0.78
1:B:305:THR:HG23	6:B:2714:HOH:O	1.82	0.78
1:C:32:LYS:HA	1:C:32:LYS:HE2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:GLN:O	1:D:279:GLU:HG3	1.84	0.77
1:D:140:VAL:H	1:D:145:ILE:HB	1.49	0.77
1:A:99:SER:OG	1:A:375:LYS:HE3	1.84	0.77
1:B:176:ARG:HD3	1:B:198:PHE:CD2	2.20	0.76
1:C:210:GLN:CD	6:C:2606:HOH:O	2.28	0.76
1:C:32:LYS:HA	1:C:32:LYS:CE	2.16	0.74
1:B:33:LEU:HD21	1:B:77:ARG:HD2	1.70	0.74
1:C:412:ASN:HD21	1:C:414:GLN:HB2	1.52	0.73
1:C:276:GLN:O	1:C:279:GLU:HG3	1.91	0.71
1:D:305:THR:HG23	6:D:2236:HOH:O	1.90	0.71
1:A:225:SER:HB2	1:D:225:SER:HB2	1.71	0.71
1:B:48:GLN:NE2	6:B:2724:HOH:O	2.23	0.71
1:B:203:ARG:HB3	1:B:203:ARG:HH11	1.53	0.70
1:D:342:LYS:HE3	1:D:344:GLU:OE2	1.91	0.70
1:C:125:LYS:NZ	1:C:129:ARG:NH2	2.40	0.69
1:A:30:LYS:HG3	1:A:31:GLY:N	2.07	0.69
1:B:32:LYS:HD2	1:B:384:PHE:HB2	1.75	0.68
1:C:39:PRO:O	5:C:2001:EDO:H22	1.94	0.68
1:B:129:ARG:NH1	6:B:2676:HOH:O	2.27	0.68
1:D:161:ARG:HG3	1:D:161:ARG:HH11	1.58	0.68
1:B:176:ARG:CZ	1:B:202:LEU:HB2	2.24	0.67
1:B:235:GLN:O	1:B:239:GLN:HG2	1.96	0.66
1:D:271:PHE:CD2	1:D:291:LEU:HB2	2.31	0.66
1:C:125:LYS:HZ3	1:C:129:ARG:NH2	1.93	0.65
1:A:305:THR:HG21	4:A:501:D2G:H112	1.78	0.65
1:D:305:THR:HG21	4:D:501:D2G:H112	1.79	0.65
1:D:256:GLN:HG3	1:D:272:LEU:CD1	2.28	0.64
1:B:203:ARG:HH11	1:B:203:ARG:CB	2.10	0.64
1:C:32:LYS:HD3	1:C:384:PHE:HB3	1.79	0.64
1:D:418:ASN:HD21	1:D:422:GLN:NE2	1.92	0.63
1:C:161:ARG:HD2	6:C:2865:HOH:O	1.98	0.62
1:C:108:ASP:HA	5:C:2004:EDO:C2	2.15	0.61
1:C:257:ARG:HH11	1:C:257:ARG:CG	2.13	0.61
1:A:348:LYS:NZ	6:A:2907:HOH:O	2.30	0.61
1:B:176:ARG:NE	1:B:176:ARG:HA	2.16	0.61
1:A:30:LYS:HG3	1:A:32:LYS:N	2.13	0.61
1:B:493:PRO:C	1:B:495:HIS:H	2.07	0.60
1:A:342:LYS:HG3	1:A:344:GLU:HG2	1.83	0.60
1:A:342:LYS:HE3	1:A:344:GLU:OE1	2.01	0.60
1:B:305:THR:HG21	4:B:501:D2G:H112	1.83	0.60
1:D:264:PRO:HG3	1:D:273:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.83	0.58
1:D:342:LYS:CE	1:D:344:GLU:OE2	2.51	0.58
1:B:172:PHE:O	1:B:176:ARG:HG2	2.03	0.58
1:C:31:GLY:N	6:C:2901:HOH:O	2.36	0.58
1:D:271:PHE:CE2	1:D:291:LEU:HB2	2.39	0.58
1:B:210:GLN:O	1:B:214:THR:HG23	2.04	0.57
1:B:143:ARG:HG3	6:B:2636:HOH:O	2.04	0.57
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.87	0.57
1:B:59:MET:HE2	1:B:59:MET:CA	2.34	0.56
1:D:115:GLY:O	1:D:119:SER:HB3	2.05	0.56
1:D:260:ASP:OD2	1:D:262:ASN:HB2	2.04	0.56
1:C:125:LYS:NZ	1:C:129:ARG:HH22	2.04	0.55
1:B:176:ARG:NH2	1:B:202:LEU:HB2	2.22	0.55
1:B:493:PRO:C	1:B:495:HIS:N	2.65	0.54
5:C:2006:EDO:H22	6:C:2606:HOH:O	2.06	0.54
1:D:139:GLY:HA2	1:D:142:LYS:HG2	1.90	0.54
1:D:374:VAL:CG1	1:D:376:LYS:O	2.55	0.54
1:B:236:GLN:NE2	6:B:2614:HOH:O	2.33	0.54
1:A:465:SER:HB3	6:B:2675:HOH:O	2.07	0.54
1:A:305:THR:HG23	6:A:2598:HOH:O	2.08	0.54
1:B:176:ARG:NH1	1:B:198:PHE:O	2.41	0.53
1:C:32:LYS:HD3	1:C:384:PHE:CB	2.39	0.53
1:D:253:GLU:O	1:D:257:ARG:HG2	2.09	0.53
1:D:256:GLN:HG3	1:D:272:LEU:HD13	1.89	0.53
1:A:30:LYS:CG	1:A:31:GLY:N	2.71	0.53
1:B:32:LYS:HB3	1:B:384:PHE:HB3	1.89	0.52
1:C:161:ARG:NH1	6:C:2865:HOH:O	2.39	0.52
1:C:108:ASP:HB2	5:C:2004:EDO:C1	2.39	0.52
1:A:33:LEU:HD21	1:A:77:ARG:NE	2.25	0.51
1:A:249:ALA:O	1:A:253:GLU:HG3	2.09	0.51
1:C:331:ILE:CD1	1:C:457:MET:HB2	2.39	0.51
1:C:418:ASN:HB3	1:C:422:GLN:H	1.76	0.51
1:D:138:PHE:CE1	1:D:266:ASP:HA	2.46	0.51
1:D:145:ILE:HD13	1:D:185:ILE:HD11	1.93	0.51
1:B:176:ARG:HA	1:B:176:ARG:HE	1.75	0.51
1:B:208:ILE:HD13	1:B:241:LEU:HG	1.93	0.50
1:D:140:VAL:H	1:D:145:ILE:CB	2.21	0.50
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.93	0.50
1:B:337:LYS:HE2	1:B:496:HIS:NE2	2.26	0.50
1:A:433:SER:HB3	3:A:500:HEM:HBA1	1.93	0.50
1:D:264:PRO:HG3	1:D:273:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LYS:CE	1:A:344:GLU:OE1	2.60	0.50
1:D:433:SER:HB3	3:D:500:HEM:HBA1	1.94	0.50
1:A:143:ARG:HD3	6:A:2872:HOH:O	2.11	0.49
1:D:142:LYS:HG3	1:D:144:GLY:H	1.77	0.49
1:D:31:GLY:C	1:D:32:LYS:HD3	2.37	0.49
1:B:446:ARG:HG3	1:B:446:ARG:NH1	2.27	0.49
1:C:108:ASP:CB	5:C:2004:EDO:H22	2.43	0.49
1:C:326:LYS:HB2	1:C:351:TYR:CE2	2.48	0.49
1:B:354:ALA:HB2	1:B:417:LEU:HD13	1.94	0.49
1:D:210:GLN:NE2	6:D:2204:HOH:O	2.29	0.49
1:D:140:VAL:HA	1:D:145:ILE:HG21	1.94	0.48
1:B:305:THR:CG2	4:B:501:D2G:H112	2.42	0.48
1:D:140:VAL:CA	1:D:145:ILE:HG21	2.43	0.48
1:A:55:TYR:CZ	1:A:400:ARG:NH2	2.82	0.48
1:C:168:ILE:HD12	1:C:168:ILE:O	2.13	0.48
1:B:433:SER:HB3	3:B:500:HEM:HBA1	1.95	0.48
1:B:33:LEU:CD2	1:B:77:ARG:HD2	2.42	0.48
1:A:30:LYS:HD3	1:A:32:LYS:HB2	1.95	0.47
1:B:33:LEU:HD21	1:B:77:ARG:CD	2.42	0.47
1:C:433:SER:HB3	3:C:500:HEM:HBA1	1.95	0.47
1:A:189:ASP:C	1:A:189:ASP:OD1	2.57	0.47
1:C:76:ARG:NH2	1:C:103:GLU:HG3	2.30	0.46
1:A:97:GLU:HG3	1:A:376:LYS:HE3	1.97	0.46
1:D:125:LYS:NZ	1:D:129:ARG:HH21	2.13	0.46
1:D:374:VAL:HG12	1:D:376:LYS:O	2.15	0.46
1:B:207:GLY:O	1:B:210:GLN:HG2	2.15	0.46
1:D:208:ILE:HD13	1:D:241:LEU:CD2	2.46	0.46
1:D:260:ASP:O	1:D:262:ASN:N	2.49	0.46
1:B:258:THR:HG22	1:B:258:THR:O	2.16	0.46
1:D:244:LEU:HB3	1:D:296:LEU:HD11	1.97	0.46
1:D:342:LYS:HB2	1:D:342:LYS:HE2	1.51	0.46
1:D:432:PHE:HB3	1:D:439:CYS:HB3	1.98	0.45
1:A:463:LYS:HB3	1:A:490:SER:OG	2.15	0.45
1:A:99:SER:OG	1:A:375:LYS:CE	2.59	0.45
1:C:168:ILE:HD12	1:C:168:ILE:C	2.41	0.45
1:D:142:LYS:HG3	1:D:144:GLY:N	2.32	0.45
1:D:260:ASP:C	1:D:262:ASN:H	2.24	0.45
1:A:468:PRO:HA	1:A:471:ILE:HD12	1.98	0.45
1:D:467:SER:O	1:D:468:PRO:C	2.58	0.45
3:A:500:HEM:HMB1	3:A:500:HEM:HBB2	1.98	0.45
1:C:244:LEU:HB3	1:C:296:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ILE:CD1	1:D:185:ILE:HD11	2.47	0.45
1:B:163:THR:HG21	1:B:168:ILE:HD13	1.98	0.45
1:B:175:SER:OG	1:B:202:LEU:HD13	2.17	0.45
1:C:210:GLN:O	1:C:214:THR:HG23	2.18	0.45
1:D:256:GLN:HG3	1:D:272:LEU:HD11	1.99	0.45
1:A:30:LYS:HE3	1:A:383:PHE:CE2	2.51	0.44
1:C:250:LYS:HE3	1:C:253:GLU:OE2	2.17	0.44
1:B:176:ARG:HE	1:B:176:ARG:CA	2.29	0.44
1:D:342:LYS:HE2	1:D:344:GLU:HG2	1.99	0.44
1:C:430:VAL:HA	6:C:2572:HOH:O	2.18	0.44
1:D:305:THR:CG2	4:D:501:D2G:H112	2.45	0.44
1:B:126:GLN:HE21	1:B:126:GLN:HB3	1.62	0.44
1:C:271:PHE:HB3	1:C:291:LEU:HD13	2.00	0.44
1:B:176:ARG:NE	1:B:176:ARG:CA	2.81	0.43
1:B:352:MET:HB2	1:B:352:MET:HE2	1.81	0.43
1:C:419:GLU:H	1:C:419:GLU:CD	2.24	0.43
1:C:250:LYS:HD2	1:C:250:LYS:HA	1.66	0.43
1:D:161:ARG:HG3	1:D:161:ARG:NH1	2.30	0.43
1:D:260:ASP:C	1:D:262:ASN:N	2.76	0.43
1:B:203:ARG:NH1	1:B:203:ARG:CB	2.71	0.43
1:C:140:VAL:HA	1:C:145:ILE:HG21	2.01	0.43
1:C:141:GLY:HA2	6:C:2706:HOH:O	2.18	0.43
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.53	0.43
1:D:143:ARG:HA	1:D:146:GLU:HB3	2.00	0.43
1:A:30:LYS:CG	1:A:32:LYS:H	2.20	0.43
1:C:257:ARG:CG	1:C:257:ARG:NH1	2.77	0.42
1:B:494:ARG:O	1:B:495:HIS:HB2	2.18	0.42
1:C:412:ASN:ND2	1:C:414:GLN:HB2	2.28	0.42
1:C:205:MET:CE	1:C:299:PHE:CE2	3.03	0.42
1:B:37:PRO:HB2	1:B:48:GLN:NE2	2.35	0.42
1:A:319:LYS:HD2	1:A:468:PRO:O	2.18	0.42
1:B:405:PHE:O	1:B:408:PRO:HD3	2.20	0.42
1:B:476:LYS:HG2	1:B:477:HIS:CD2	2.54	0.42
1:A:441:GLY:HA3	3:A:500:HEM:C3C	2.55	0.42
1:D:257:ARG:O	1:D:258:THR:HG23	2.20	0.42
1:D:271:PHE:CB	1:D:291:LEU:HD13	2.49	0.42
1:B:49:LEU:O	6:B:2664:HOH:O	2.22	0.41
1:A:40:LEU:HD21	1:C:47:LEU:HD11	2.02	0.41
1:A:117:VAL:HG22	3:A:500:HEM:HAD1	2.02	0.41
1:A:381:ARG:O	1:A:382:ASP:HB2	2.20	0.41
1:D:208:ILE:HD13	1:D:241:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PHE:HB3	1:B:291:LEU:HD13	2.01	0.41
1:C:305:THR:HG23	6:C:2774:HOH:O	2.18	0.41
1:D:441:GLY:HA3	3:D:500:HEM:C3C	2.54	0.41
1:C:376:LYS:O	1:C:377:ASP:C	2.64	0.41
1:B:53:GLN:HB3	1:B:56:ASN:HB2	2.01	0.41
1:C:33:LEU:HD11	1:C:77:ARG:CZ	2.51	0.41
1:A:305:THR:CG2	4:A:501:D2G:H112	2.50	0.41
1:B:446:ARG:HG3	1:B:446:ARG:HH11	1.85	0.41
1:C:326:LYS:HE3	1:C:351:TYR:CE1	2.55	0.41
1:D:266:ASP:C	1:D:266:ASP:OD1	2.62	0.41
1:A:271:PHE:HB3	1:A:291:LEU:HD13	2.03	0.41
1:B:274:ARG:NH1	1:B:286:PHE:CE2	2.89	0.40
1:C:172:PHE:O	1:C:176:ARG:HG3	2.22	0.40
1:C:375:LYS:O	1:C:387:LYS:HG3	2.21	0.40
1:B:168:ILE:HD12	1:B:173:PHE:CE1	2.56	0.40
1:A:418:ASN:OD1	1:A:418:ASN:C	2.64	0.40
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.56	0.40
1:A:432:PHE:HB3	1:A:439:CYS:HB3	2.03	0.40
1:C:305:THR:HG21	4:C:501:D2G:H112	2.03	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	463/476 (97%)	453 (98%)	10 (2%)	0	100	100
1	B	463/476 (97%)	451 (97%)	12 (3%)	0	100	100
1	C	462/476 (97%)	453 (98%)	8 (2%)	1 (0%)	43	27
1	D	462/476 (97%)	448 (97%)	12 (3%)	2 (0%)	30	15
All	All	1850/1904 (97%)	1805 (98%)	42 (2%)	3 (0%)	43	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	32	LYS
1	D	140	VAL
1	D	261	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	412/422 (98%)	406 (98%)	6 (2%)	57	37
1	B	413/422 (98%)	403 (98%)	10 (2%)	43	20
1	C	411/422 (97%)	403 (98%)	8 (2%)	50	28
1	D	411/422 (97%)	405 (98%)	6 (2%)	57	37
All	All	1647/1688 (98%)	1617 (98%)	30 (2%)	51	30

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	135	LEU
1	A	167	ASN
1	A	250	LYS
1	A	465	SER
1	A	468	PRO
1	B	32	LYS
1	B	60	LYS
1	B	135	LEU
1	B	172	PHE
1	B	289	LYS
1	B	353	GLU
1	B	417	LEU
1	B	419	GLU
1	B	468	PRO
1	B	495	HIS
1	C	32	LYS

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Mol	Chain	Res	Type
1	C	135	LEU
1	C	210	GLN
1	C	257	ARG
1	C	326	LYS
1	C	417	LEU
1	C	457	MET
1	C	467	SER
1	D	174	LEU
1	D	252	VAL
1	D	263	SER
1	D	316	LEU
1	D	375	LYS
1	D	419	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	72	HIS
1	A	466	GLN
1	B	53	GLN
1	B	56	ASN
1	B	72	HIS
1	B	126	GLN
1	B	150	GLN
1	B	210	GLN
1	B	320	HIS
1	B	407	ASN
1	C	72	HIS
1	C	242	GLN
1	C	276	GLN
1	C	297	ASN
1	C	338	ASN
1	C	409	GLN
1	D	53	GLN
1	D	56	ASN
1	D	72	HIS
1	D	236	GLN
1	D	297	ASN
1	D	320	HIS
1	D	422	GLN

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)

20 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	$\#\|Z\| > 2$
4	D2G	A	501	3	15,15,15	1.70	5 (33%)	17,19,19	1.29	3 (17%)
5	EDO	C	2004	-	3,3,3	1.41	0	2,2,2	0.95	0
5	EDO	C	2001	-	3,3,3	1.39	0	2,2,2	0.21	0
4	D2G	D	501	3	15,15,15	1.77	4 (26%)	17,19,19	1.41	3 (17%)
5	EDO	A	2003	-	3,3,3	1.77	1 (33%)	2,2,2	0.27	0
5	EDO	D	2007	-	3,3,3	0.52	0	2,2,2	1.19	0
4	D2G	C	501	3	15,15,15	1.31	2 (13%)	17,19,19	0.68	0
5	EDO	C	2002	-	3,3,3	0.48	0	2,2,2	0.73	0
2	SO4	A	2504	-	4,4,4	0.56	0	6,6,6	0.31	0
3	HEM	A	500	4,1	50,50,50	1.95	17 (34%)	67,82,82	1.18	8 (11%)
3	HEM	B	500	4,1	50,50,50	2.31	22 (44%)	67,82,82	1.26	9 (13%)
2	SO4	B	2506	-	4,4,4	0.66	0	6,6,6	0.37	0
5	EDO	C	2006	-	3,3,3	0.88	0	2,2,2	0.46	0
2	SO4	C	2508	-	4,4,4	0.57	0	6,6,6	0.15	0
2	SO4	A	2503	-	4,4,4	0.62	0	6,6,6	0.12	0
4	D2G	B	501	3	15,15,15	1.67	4 (26%)	17,19,19	1.19	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEM	C	500	4,1	50,50,50	2.18	21 (42%)	67,82,82	1.22	5 (7%)
2	SO4	A	2502	-	4,4,4	0.60	0	6,6,6	0.23	0
3	HEM	D	500	4,1	50,50,50	2.30	21 (42%)	67,82,82	1.04	6 (8%)
5	EDO	C	2005	-	3,3,3	1.38	0	2,2,2	0.29	0

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
5	EDO	D	2007	-	-	0/1/1/1	-
4	D2G	C	501	3	-	1/7/7/7	0/2/2/2
5	EDO	C	2006	-	-	0/1/1/1	-
5	EDO	C	2002	-	-	1/1/1/1	-
4	D2G	A	501	3	-	1/7/7/7	0/2/2/2
5	EDO	C	2004	-	-	0/1/1/1	-
5	EDO	C	2001	-	-	1/1/1/1	-
3	HEM	C	500	4,1	-	1/14/54/54	-
3	HEM	D	500	4,1	-	1/14/54/54	-
4	D2G	D	501	3	-	1/7/7/7	0/2/2/2
5	EDO	C	2005	-	-	0/1/1/1	-
5	EDO	A	2003	-	-	0/1/1/1	-
3	HEM	A	500	4,1	-	3/14/54/54	-
3	HEM	B	500	4,1	-	1/14/54/54	-
4	D2G	B	501	3	-	1/7/7/7	0/2/2/2

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	HEM	C4D-ND	-5.46	1.30	1.40
3	D	500	HEM	FE-NB	4.83	2.09	1.94
3	C	500	HEM	FE-ND	4.53	2.08	1.94
3	D	500	HEM	CMD-C2D	4.52	1.60	1.50
3	D	500	HEM	C3C-C4C	-4.20	1.38	1.46
3	B	500	HEM	FE-ND	4.18	2.07	1.94
4	D	501	D2G	C_2-C_1	4.14	1.45	1.39
3	B	500	HEM	C1B-NB	-4.10	1.33	1.40
3	D	500	HEM	FE-NA	4.10	2.08	1.95
3	C	500	HEM	C4D-ND	-4.05	1.33	1.40
3	C	500	HEM	C1C-NC	-4.05	1.32	1.39
3	B	500	HEM	CMC-C2C	4.01	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	500	HEM	C1D-ND	-4.01	1.31	1.38
3	A	500	HEM	CBB-CAB	3.85	1.48	1.30
3	B	500	HEM	C3C-C4C	-3.84	1.39	1.46
3	B	500	HEM	FE-NB	3.80	2.06	1.94
3	C	500	HEM	CMC-C2C	3.60	1.58	1.50
3	C	500	HEM	CMA-C3A	3.58	1.58	1.50
3	D	500	HEM	C4A-NA	-3.49	1.33	1.39
3	B	500	HEM	C1C-C2C	-3.48	1.38	1.45
3	D	500	HEM	C1B-NB	-3.47	1.34	1.40
3	A	500	HEM	FE-ND	3.45	2.05	1.94
3	C	500	HEM	FE-NB	3.43	2.05	1.94
3	B	500	HEM	C1D-ND	-3.39	1.32	1.38
3	B	500	HEM	FE-NA	3.39	2.06	1.95
3	D	500	HEM	FE-ND	3.37	2.05	1.94
3	D	500	HEM	C3B-C4B	-3.37	1.38	1.44
3	D	500	HEM	C1C-C2C	-3.34	1.38	1.45
4	D	501	D2G	C_5-C_1	3.31	1.44	1.39
3	A	500	HEM	CMA-C3A	3.30	1.57	1.50
3	A	500	HEM	FE-NB	3.28	2.05	1.94
3	C	500	HEM	CBD-CAD	3.20	1.63	1.51
3	C	500	HEM	CBB-CAB	3.18	1.45	1.30
3	D	500	HEM	C1D-ND	-3.12	1.32	1.38
4	A	501	D2G	C_5-C_1	3.06	1.44	1.39
4	B	501	D2G	C_1-C_6	-3.05	1.41	1.48
3	B	500	HEM	C3B-C2B	3.04	1.43	1.37
3	A	500	HEM	C4B-NB	-3.04	1.32	1.38
3	A	500	HEM	CMC-C2C	3.03	1.57	1.50
3	D	500	HEM	CBB-CAB	3.03	1.44	1.30
4	B	501	D2G	C_2-C_1	3.02	1.44	1.39
3	B	500	HEM	CBB-CAB	2.98	1.44	1.30
3	A	500	HEM	C4D-ND	-2.96	1.35	1.40
3	A	500	HEM	FE-NA	2.96	2.04	1.95
3	B	500	HEM	C1A-NA	-2.91	1.34	1.39
3	D	500	HEM	FE-NC	2.85	2.04	1.95
3	D	500	HEM	C3C-C2C	2.84	1.42	1.37
3	C	500	HEM	FE-NC	2.83	2.04	1.95
3	B	500	HEM	C4B-NB	-2.78	1.33	1.38
3	A	500	HEM	CBD-CGD	2.76	1.57	1.50
3	A	500	HEM	C1B-C2B	-2.75	1.38	1.44
3	C	500	HEM	CAC-C3C	-2.74	1.40	1.47
3	D	500	HEM	CAC-C3C	-2.74	1.40	1.47
3	D	500	HEM	C3B-C2B	2.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	CMD-C2D	2.67	1.56	1.50
3	D	500	HEM	CMB-C2B	2.66	1.56	1.50
3	B	500	HEM	C4A-NA	-2.66	1.34	1.39
3	A	500	HEM	C3C-C4C	-2.65	1.41	1.46
3	C	500	HEM	C1B-NB	-2.65	1.35	1.40
3	B	500	HEM	C3C-C2C	2.62	1.42	1.37
3	A	500	HEM	C1D-ND	-2.62	1.33	1.38
3	D	500	HEM	C1C-NC	-2.59	1.34	1.39
3	C	500	HEM	O2A-CGA	-2.58	1.22	1.30
3	C	500	HEM	CHD-C4C	2.57	1.43	1.38
3	C	500	HEM	C4B-NB	-2.56	1.33	1.38
4	A	501	D2G	C_2-C_1	2.56	1.43	1.39
4	C	501	D2G	C_2-C_1	2.55	1.43	1.39
3	A	500	HEM	FE-NC	2.54	2.03	1.95
3	A	500	HEM	CAC-C3C	-2.49	1.40	1.47
3	D	500	HEM	CMA-C3A	2.46	1.55	1.50
3	C	500	HEM	C4D-C3D	-2.43	1.40	1.45
3	B	500	HEM	CMB-C2B	2.42	1.55	1.50
4	B	501	D2G	O_1-C_6	2.42	1.43	1.38
3	A	500	HEM	CHB-C1B	2.42	1.43	1.38
3	B	500	HEM	O2A-CGA	-2.41	1.22	1.30
4	A	501	D2G	C_3-C_2	2.40	1.43	1.38
3	D	500	HEM	O2A-CGA	-2.40	1.22	1.30
3	C	500	HEM	C3B-C4B	-2.39	1.40	1.44
4	B	501	D2G	C_5-C_1	2.35	1.42	1.39
3	C	500	HEM	C1D-C2D	-2.33	1.39	1.44
3	B	500	HEM	CBC-CAC	2.31	1.41	1.30
3	D	500	HEM	C1A-C2A	-2.29	1.40	1.44
4	A	501	D2G	C_1-C_6	-2.29	1.42	1.48
3	B	500	HEM	C1A-C2A	-2.27	1.40	1.44
3	B	500	HEM	C4D-C3D	-2.26	1.41	1.45
3	C	500	HEM	CMD-C2D	2.24	1.55	1.50
3	C	500	HEM	O2D-CGD	-2.21	1.23	1.30
5	A	2003	EDO	O2-C2	2.21	1.53	1.42
4	A	501	D2G	C10-C_9	2.16	1.53	1.48
3	B	500	HEM	CMA-C3A	2.16	1.55	1.50
4	D	501	D2G	C_1-C_6	-2.15	1.43	1.48
3	A	500	HEM	CHD-C4C	2.13	1.42	1.38
3	D	500	HEM	C4B-NB	-2.12	1.34	1.38
3	C	500	HEM	FE-NA	2.12	2.02	1.95
3	B	500	HEM	FE-NC	2.12	2.02	1.95
4	D	501	D2G	C_3-C_2	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	D2G	C_1-C_6	-2.03	1.43	1.48

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	500	HEM	O2A-CGA-CBA	3.76	125.87	114.00
3	B	500	HEM	CHD-C4C-NC	-3.35	120.81	124.45
3	A	500	HEM	O2A-CGA-CBA	3.23	124.21	114.00
3	B	500	HEM	C3B-C4B-NB	3.19	111.76	109.47
3	B	500	HEM	O2A-CGA-CBA	3.17	124.01	114.00
4	B	501	D2G	C_4-N_1-C_5	3.12	122.32	116.85
3	B	500	HEM	C4B-C3B-C2B	-3.00	104.52	107.28
3	C	500	HEM	C3B-C4B-NB	2.98	111.61	109.47
4	D	501	D2G	C_6-O_1-C_9	-2.96	105.35	106.93
3	C	500	HEM	CHD-C4C-NC	-2.75	121.46	124.45
4	D	501	D2G	O_1-C_6-C_7	2.74	111.49	109.39
4	A	501	D2G	C_6-O_1-C_9	-2.73	105.47	106.93
3	D	500	HEM	O2A-CGA-CBA	2.56	122.10	114.00
3	B	500	HEM	C3B-C2B-C1B	-2.50	104.53	106.41
3	C	500	HEM	O1A-CGA-CBA	-2.50	115.15	123.09
3	B	500	HEM	C1B-NB-C4B	2.36	108.00	105.21
3	D	500	HEM	C1B-NB-C4B	2.31	107.94	105.21
3	B	500	HEM	C4D-ND-C1D	2.29	107.92	105.21
3	A	500	HEM	O1A-CGA-CBA	-2.28	115.87	123.09
4	A	501	D2G	C_3-C_2-C_1	-2.21	118.19	120.36
3	D	500	HEM	C3B-C2B-C1B	-2.20	104.76	106.41
4	D	501	D2G	C_3-C_2-C_1	-2.20	118.21	120.36
3	A	500	HEM	CHB-C1B-NB	-2.18	121.67	124.37
3	D	500	HEM	C3B-C4B-NB	2.18	111.03	109.47
3	D	500	HEM	CHD-C4C-NC	-2.17	122.09	124.45
3	A	500	HEM	C4D-ND-C1D	2.15	107.76	105.21
3	A	500	HEM	CHD-C4C-NC	-2.15	122.11	124.45
3	A	500	HEM	O2D-CGD-CBD	2.12	120.71	114.00
3	B	500	HEM	O1A-CGA-CBA	-2.10	116.43	123.09
3	A	500	HEM	CHC-C1C-NC	-2.07	122.20	124.45
3	B	500	HEM	CHC-C1C-NC	-2.07	122.20	124.45
3	D	500	HEM	C4D-ND-C1D	2.05	107.64	105.21
4	A	501	D2G	O_1-C_6-C_7	2.05	110.96	109.39
3	C	500	HEM	CHB-C1B-NB	-2.03	121.86	124.37
3	A	500	HEM	C4B-C3B-C2B	-2.01	105.44	107.28

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	D2G	C_9-C10-N_2-C11
4	C	501	D2G	C_9-C10-N_2-C11
4	D	501	D2G	C_9-C10-N_2-C11
5	C	2001	EDO	O1-C1-C2-O2
5	C	2002	EDO	O1-C1-C2-O2
4	A	501	D2G	C_9-C10-N_2-C11
3	A	500	HEM	CAA-CBA-CGA-O1A
3	B	500	HEM	CAA-CBA-CGA-O1A
3	C	500	HEM	CAA-CBA-CGA-O1A
3	D	500	HEM	CAA-CBA-CGA-O1A
3	A	500	HEM	CAD-CBD-CGD-O1D
3	A	500	HEM	CAD-CBD-CGD-O2D

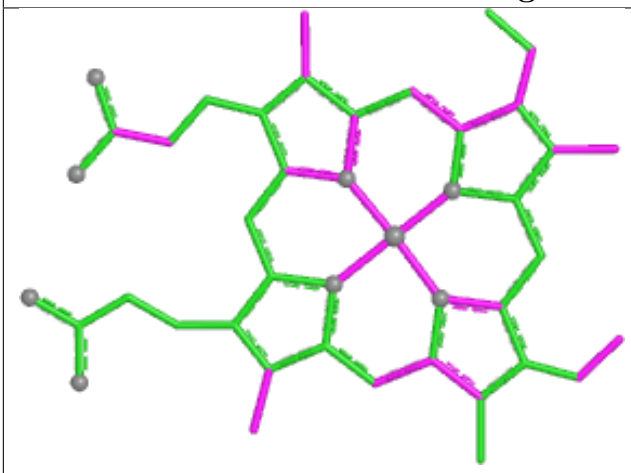
There are no ring outliers.

11 monomers are involved in 24 short contacts:

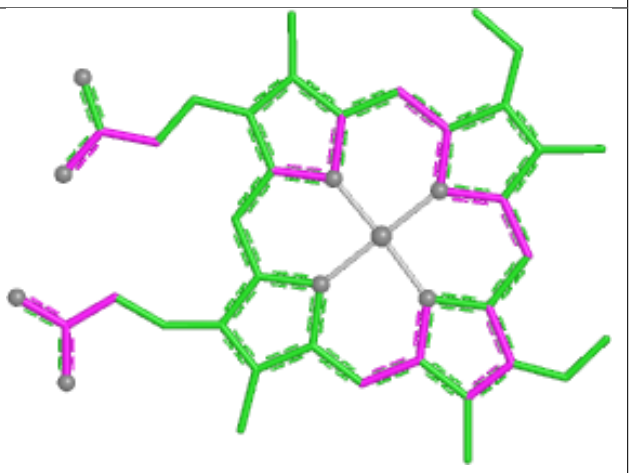
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	D2G	2	0
5	C	2004	EDO	7	0
5	C	2001	EDO	1	0
4	D	501	D2G	2	0
4	C	501	D2G	1	0
3	A	500	HEM	4	0
3	B	500	HEM	1	0
5	C	2006	EDO	1	0
4	B	501	D2G	2	0
3	C	500	HEM	1	0
3	D	500	HEM	2	0

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.

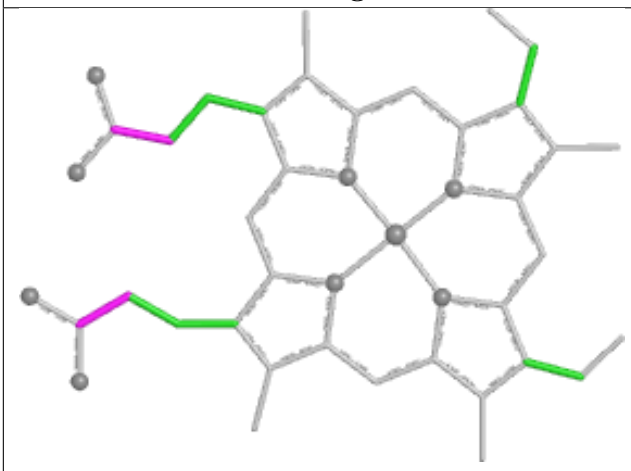
Ligand HEM A 500



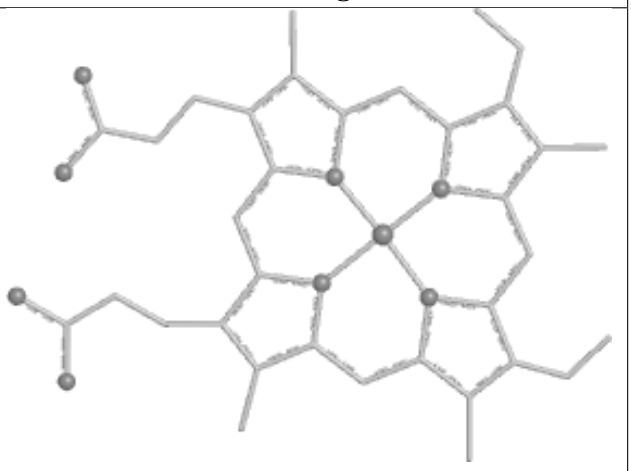
Bond lengths



Bond angles

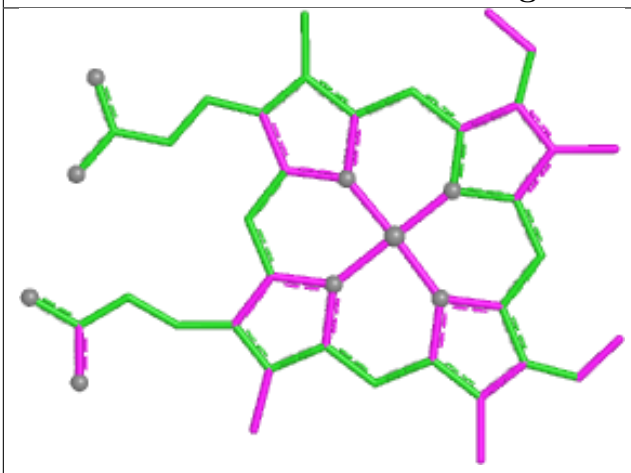


Torsions

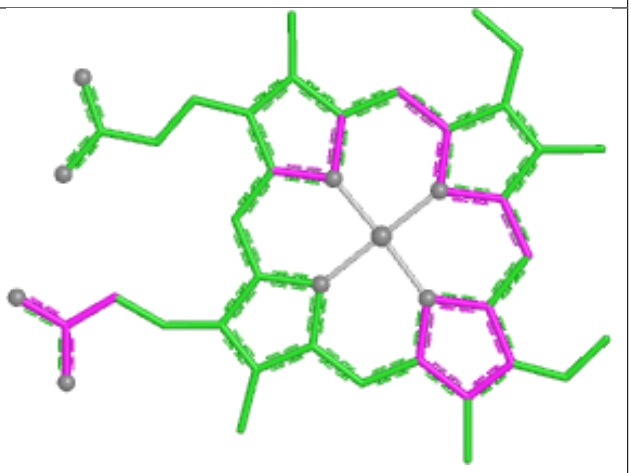


Rings

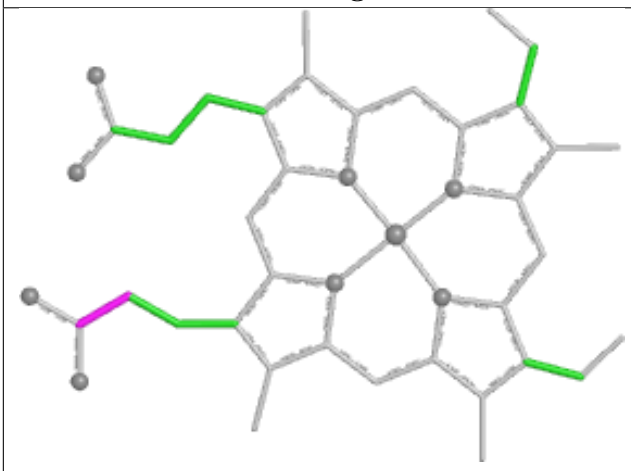
Ligand HEM B 500



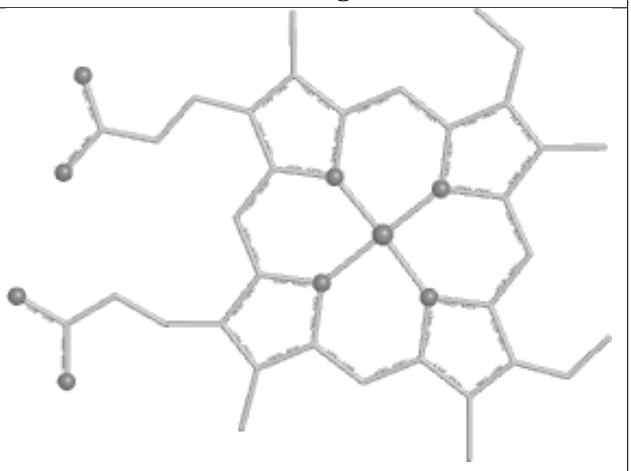
Bond lengths



Bond angles

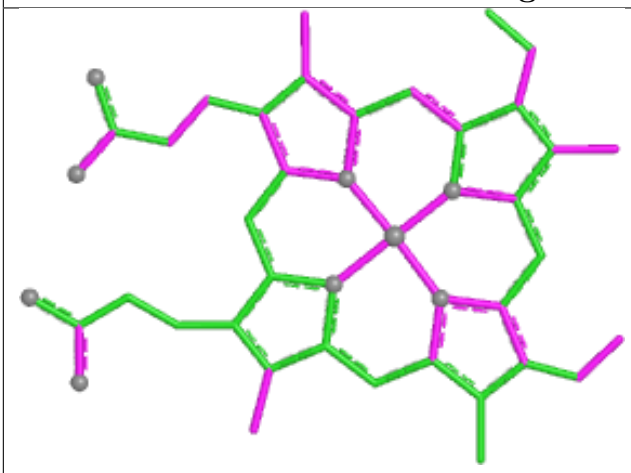


Torsions

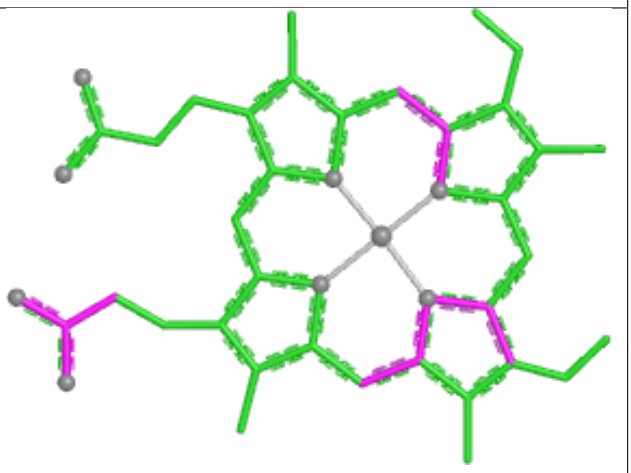


Rings

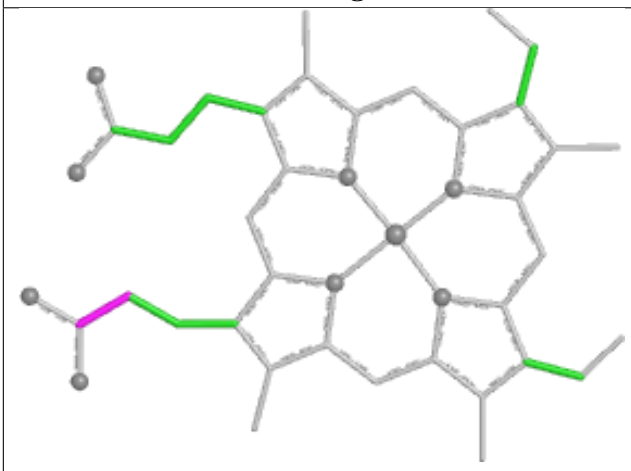
Ligand HEM C 500



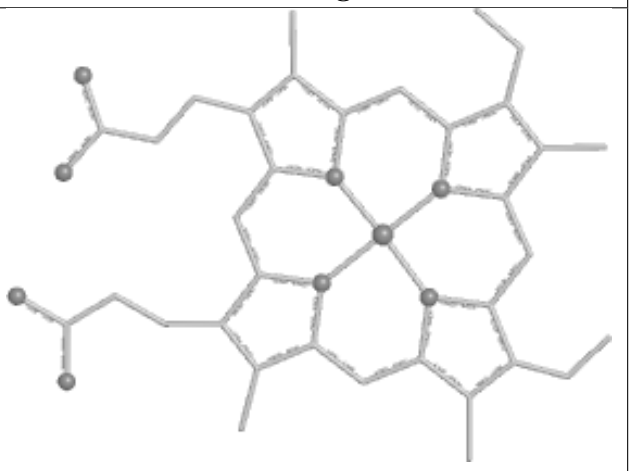
Bond lengths



Bond angles

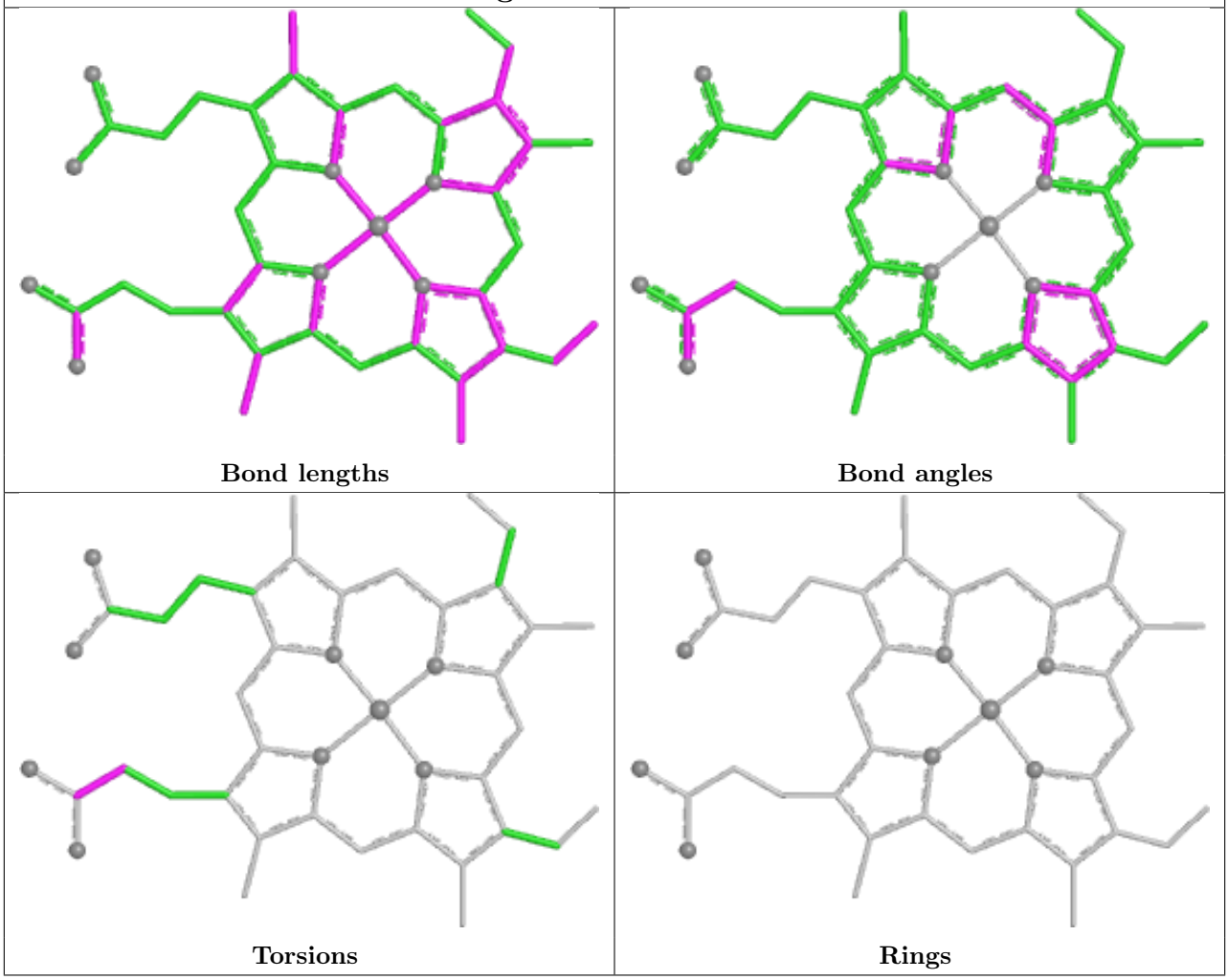


Torsions



Rings

Ligand HEM D 500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	465/476 (97%)	0.08	14 (3%)	52	57	16, 25, 41, 58	0
1	B	465/476 (97%)	0.74	44 (9%)	14	14	19, 31, 50, 67	0
1	C	464/476 (97%)	0.09	9 (1%)	66	71	16, 24, 39, 56	0
1	D	464/476 (97%)	0.24	28 (6%)	27	31	16, 25, 50, 64	0
All	All	1858/1904 (97%)	0.29	95 (5%)	33	37	16, 26, 45, 67	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	139	GLY	7.9
1	B	198	PHE	5.2
1	B	193	TYR	5.1
1	D	140	VAL	4.7
1	B	258	THR	4.5
1	D	261	PRO	4.4
1	B	496	HIS	4.3
1	B	195	ASP	4.1
1	B	261	PRO	4.0
1	D	142	LYS	4.0
1	D	143	ARG	3.9
1	D	259	LEU	3.7
1	A	31	GLY	3.7
1	B	495	HIS	3.6
1	C	418	ASN	3.5
1	B	194	LYS	3.5
1	D	273	ILE	3.5
1	D	141	GLY	3.4
1	B	202	LEU	3.3
1	D	144	GLY	3.1
1	D	258	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	199	LEU	3.1
1	D	257	ARG	3.0
1	B	273	ILE	3.0
1	B	196	LYS	2.9
1	B	262	ASN	2.9
1	C	417	LEU	2.9
1	B	467	SER	2.9
1	B	259	LEU	2.8
1	B	173	PHE	2.8
1	C	31	GLY	2.7
1	D	260	ASP	2.7
1	B	133	ALA	2.7
1	B	253	GLU	2.6
1	D	252	VAL	2.6
1	A	258	THR	2.6
1	B	417	LEU	2.6
1	B	468	PRO	2.6
1	B	257	ARG	2.6
1	C	461	ARG	2.6
1	D	276	GLN	2.5
1	B	172	PHE	2.5
1	A	189	ASP	2.5
1	B	210	GLN	2.5
1	A	382	ASP	2.5
1	A	468	PRO	2.5
1	B	260	ASP	2.4
1	D	382	ASP	2.4
1	B	383	PHE	2.4
1	C	334	VAL	2.4
1	D	338	ASN	2.4
1	B	382	ASP	2.4
1	B	470	ASP	2.4
1	B	60	LYS	2.4
1	B	176	ARG	2.4
1	C	336	GLY	2.3
1	D	264	PRO	2.3
1	B	143	ARG	2.3
1	B	64	ARG	2.3
1	B	282	PRO	2.3
1	C	282	PRO	2.3
1	B	216	THR	2.3
1	A	466	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	262	ASN	2.3
1	D	419	GLU	2.3
1	B	189	ASP	2.3
1	A	467	SER	2.2
1	D	420	LYS	2.2
1	D	31	GLY	2.2
1	D	138	PHE	2.2
1	B	465	SER	2.2
1	D	280	LYS	2.2
1	A	421	GLY	2.2
1	B	191	PHE	2.2
1	D	282	PRO	2.2
1	D	254	HIS	2.2
1	B	61	ILE	2.2
1	B	264	PRO	2.2
1	B	493	PRO	2.2
1	B	203	ARG	2.1
1	D	262	ASN	2.1
1	B	59	MET	2.1
1	B	256	GLN	2.1
1	C	347	ALA	2.1
1	D	249	ALA	2.1
1	A	336	GLY	2.1
1	D	32	LYS	2.1
1	B	272	LEU	2.1
1	C	147	GLU	2.1
1	B	129	ARG	2.1
1	A	257	ARG	2.1
1	A	471	ILE	2.1
1	D	137	ASP	2.0
1	A	406	SER	2.0
1	A	420	LYS	2.0

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)

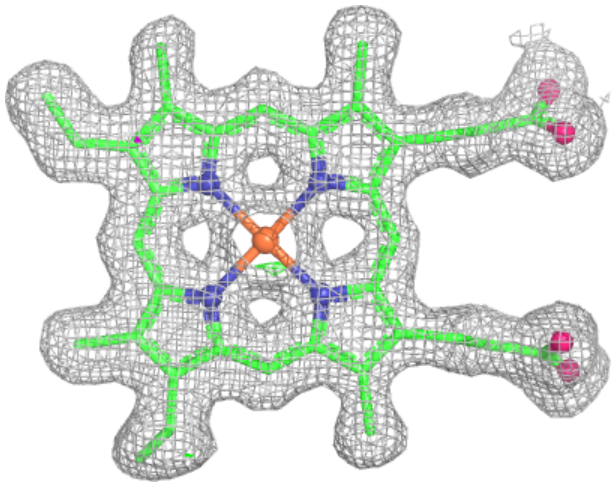
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

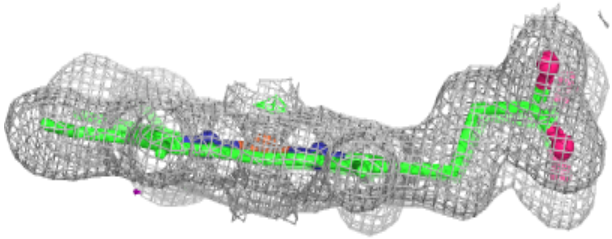
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	2508	5/5	0.67	0.13	62,62,63,65	0
2	SO4	A	2504	5/5	0.79	0.15	50,51,53,55	0
5	EDO	A	2003	4/4	0.79	0.18	34,34,35,36	0
2	SO4	B	2506	5/5	0.80	0.13	57,59,60,60	0
2	SO4	A	2502	5/5	0.82	0.12	54,55,57,57	0
2	SO4	A	2503	5/5	0.83	0.11	56,56,57,58	0
5	EDO	C	2006	4/4	0.83	0.13	34,35,36,37	0
5	EDO	D	2007	4/4	0.83	0.13	31,32,33,34	0
5	EDO	C	2002	4/4	0.85	0.17	33,35,36,39	0
5	EDO	C	2001	4/4	0.87	0.24	33,35,36,37	0
5	EDO	C	2005	4/4	0.92	0.10	36,37,38,39	0
5	EDO	C	2004	4/4	0.95	0.09	23,25,28,30	0
4	D2G	B	501	14/14	0.96	0.06	22,24,25,26	0
4	D2G	D	501	14/14	0.97	0.05	20,22,24,28	0
4	D2G	C	501	14/14	0.97	0.06	19,22,24,28	0
3	HEM	D	500	43/43	0.98	0.06	16,20,23,29	0
4	D2G	A	501	14/14	0.98	0.04	16,19,21,23	0
3	HEM	B	500	43/43	0.98	0.06	17,21,24,29	0
3	HEM	A	500	43/43	0.99	0.04	12,15,18,25	0
3	HEM	C	500	43/43	0.99	0.05	15,18,21,24	0

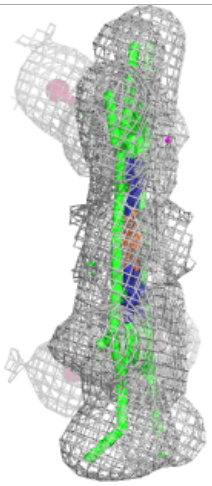
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM D 500:

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

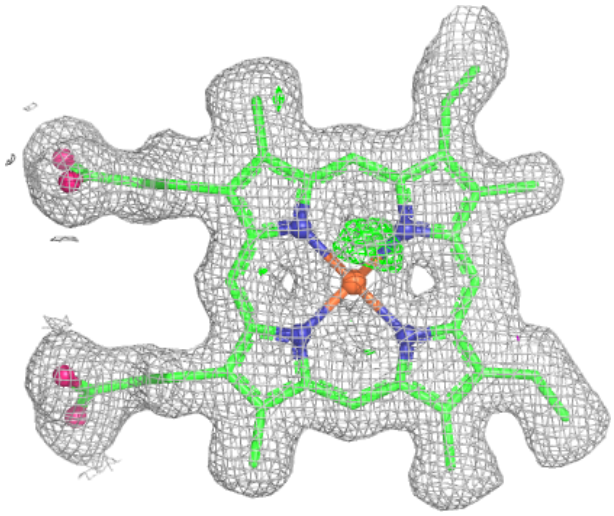


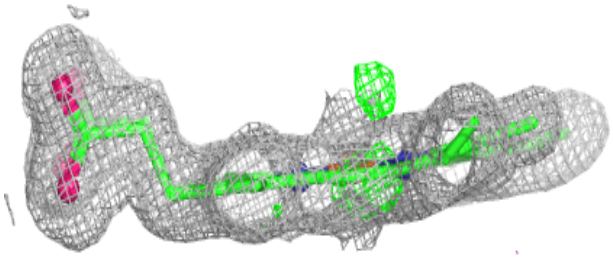


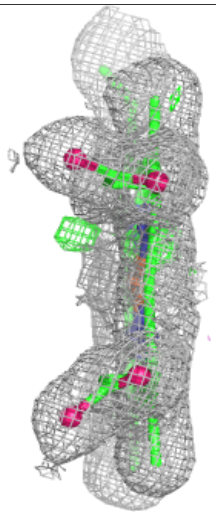


Electron density around HEM B 500:

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

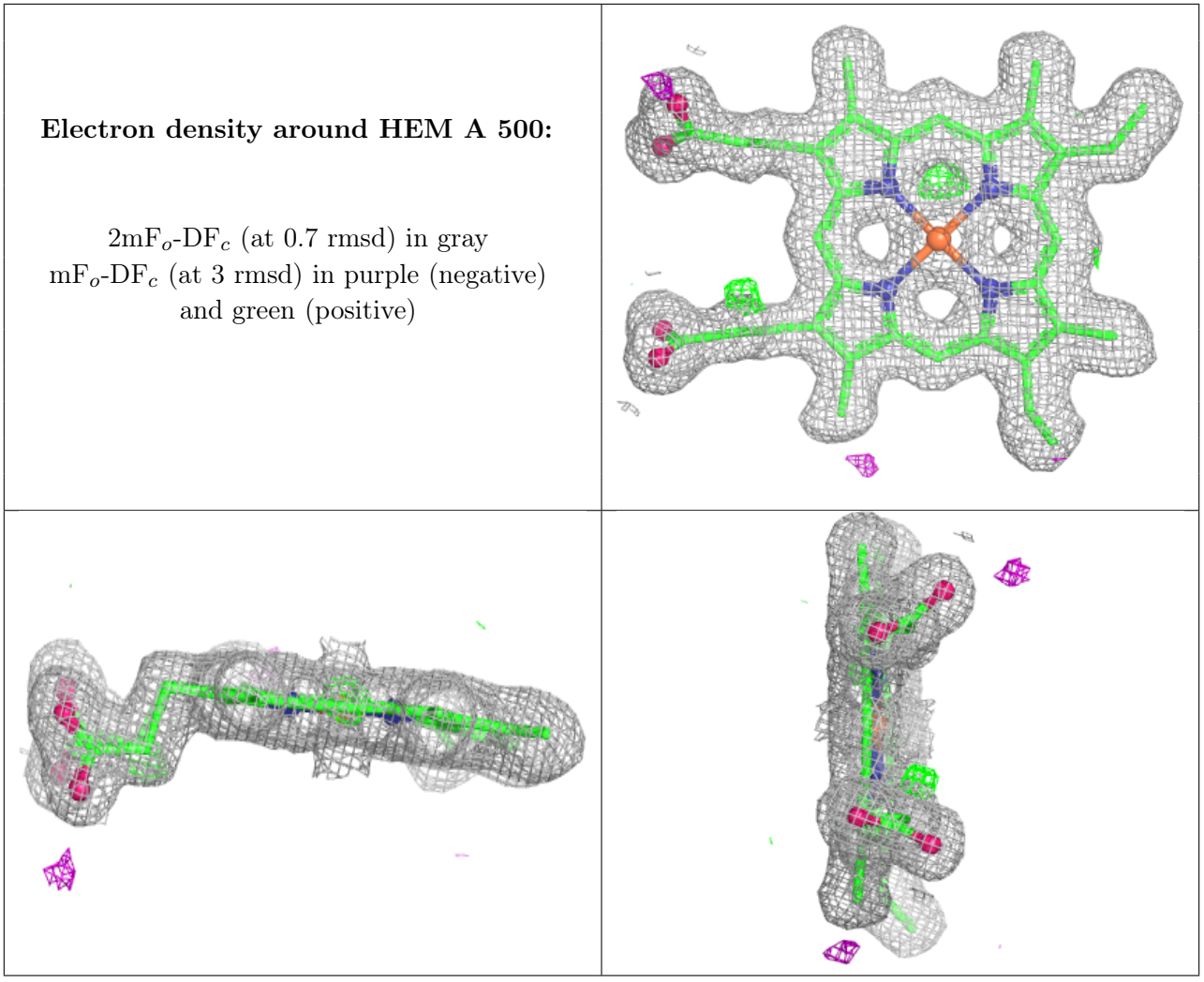






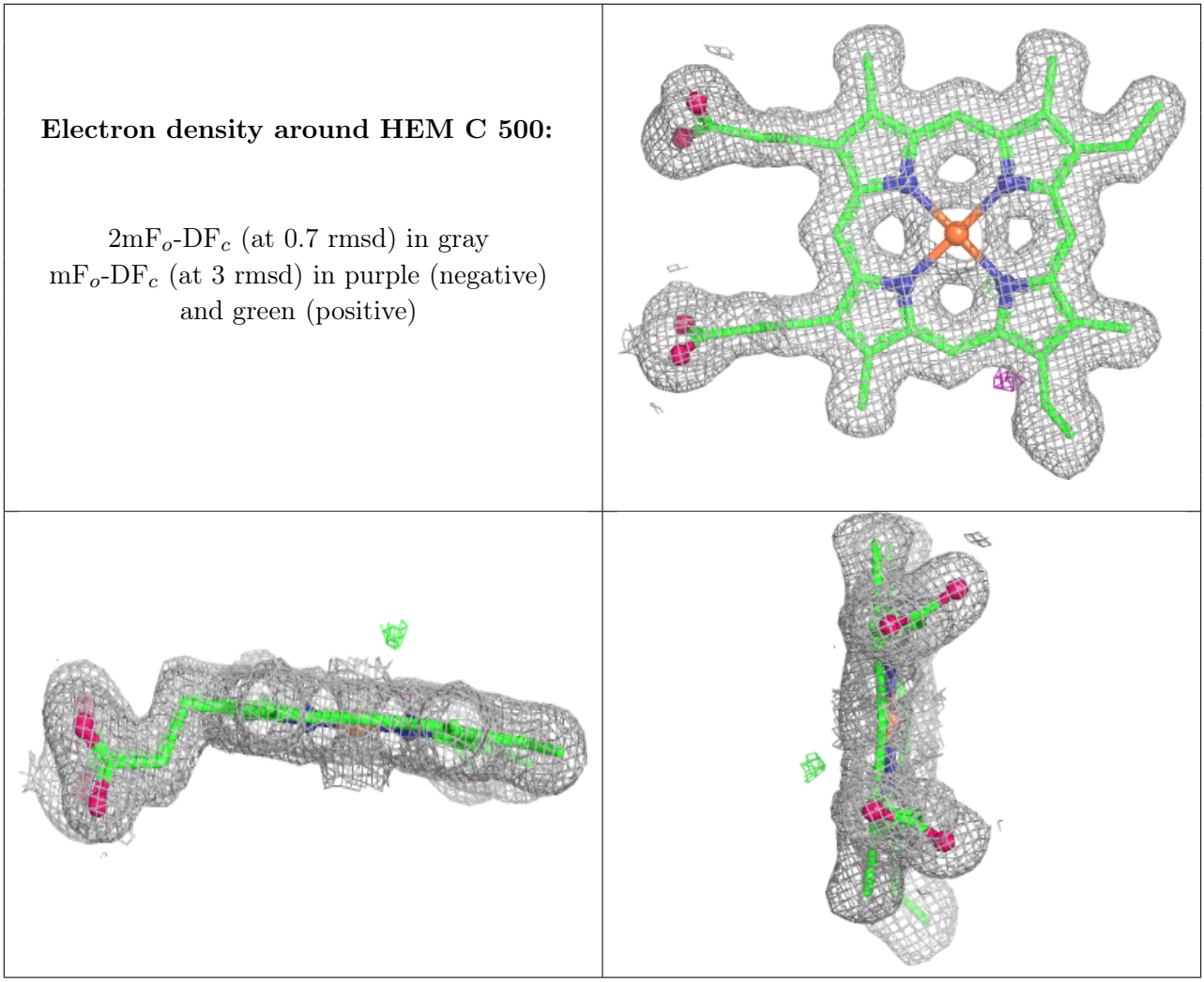
Electron density around HEM A 500:

$2mF_o$-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 500:

$2mF_o$-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

There are no such residues in this entry.