Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 06:33 AM EDT

PDB ID	:	1Z11
Title	:	Crystal Structure of Human Microsomal P450 2A6 with Methoxsalen Bound
Authors	:	Yano, J.K.; Hsu, M.H.; Griffin, K.J.; Stout, C.D.; Johnson, E.F.
Deposited on	:	2005-03-02
Resolution	:	2.05 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:

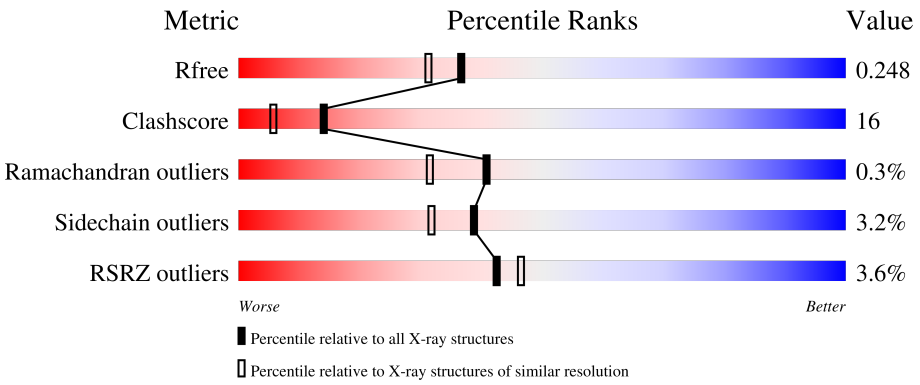
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	4% 78% 19%
1	B	476	5% 66% 30%
1	C	476	2% 73% 22%
1	D	476	3% 70% 25%

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
3	8MO	A	501	-	-	X	-
3	8MO	B	501	-	-	X	-
3	8MO	C	501	-	-	X	-
3	8MO	D	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15779 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, family 2, subfamily A, polypeptide 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	467	3780	2426	656	680	18	0	0	0
1	B	464	3757	2412	650	677	18	0	0	0
1	C	464	3751	2408	648	677	18	0	0	0
1	D	464	3751	2408	648	677	18	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	SEE REMARK 999	UNP P11509
A	24	ALA	-	SEE REMARK 999	UNP P11509
A	25	LYS	-	SEE REMARK 999	UNP P11509
A	26	LYS	-	SEE REMARK 999	UNP P11509
A	27	THR	-	SEE REMARK 999	UNP P11509
A	28	SER	-	SEE REMARK 999	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	-	SEE REMARK 999	UNP P11509
B	24	ALA	-	SEE REMARK 999	UNP P11509
B	25	LYS	-	SEE REMARK 999	UNP P11509
B	26	LYS	-	SEE REMARK 999	UNP P11509
B	27	THR	-	SEE REMARK 999	UNP P11509
B	28	SER	-	SEE REMARK 999	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	-	SEE REMARK 999	UNP P11509

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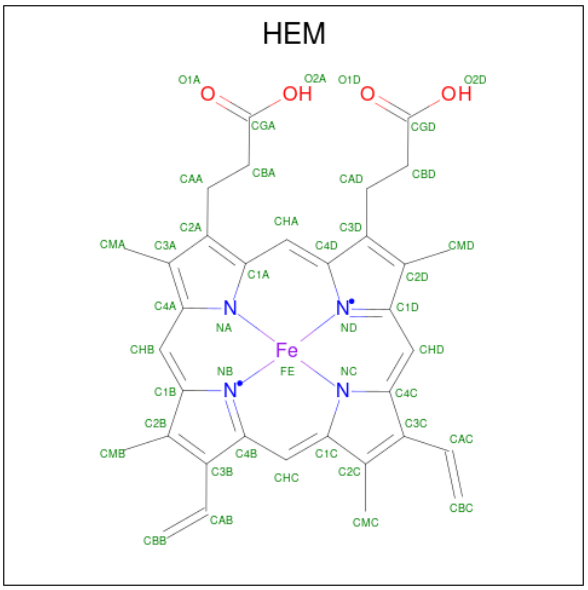
Chain	Residue	Modelled	Actual	Comment	Reference
C	24	ALA	-	SEE REMARK 999	UNP P11509
C	25	LYS	-	SEE REMARK 999	UNP P11509
C	26	LYS	-	SEE REMARK 999	UNP P11509
C	27	THR	-	SEE REMARK 999	UNP P11509
C	28	SER	-	SEE REMARK 999	UNP P11509
C	495	HIS	-	expression tag	UNP P11509
C	496	HIS	-	expression tag	UNP P11509
C	497	HIS	-	expression tag	UNP P11509
C	498	HIS	-	expression tag	UNP P11509
D	23	MET	-	SEE REMARK 999	UNP P11509
D	24	ALA	-	SEE REMARK 999	UNP P11509
D	25	LYS	-	SEE REMARK 999	UNP P11509
D	26	LYS	-	SEE REMARK 999	UNP P11509
D	27	THR	-	SEE REMARK 999	UNP P11509
D	28	SER	-	SEE REMARK 999	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 PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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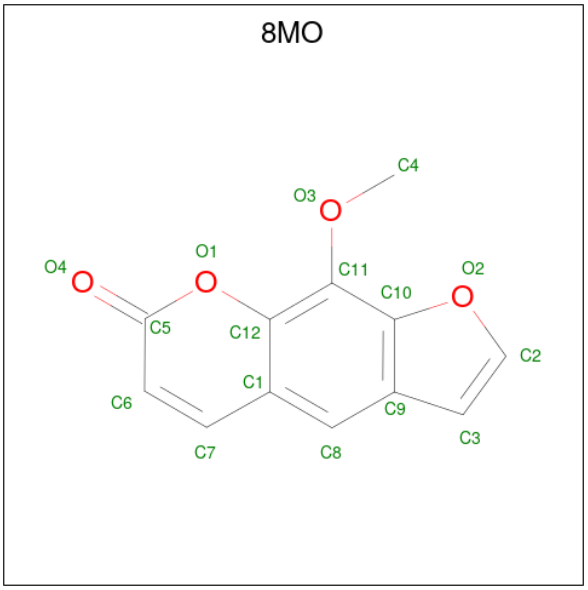
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is METHOXSALEN (three-letter code: 8MO) (formula: $C_{12}H_8O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	16	12	4	0	0
			Total	C	O		
3	B	1	16	12	4	0	0
			Total	C	O		
3	C	1	16	12	4	0	0
			Total	C	O		
3	D	1	16	12	4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	148	148	148	0	0
			Total	O		
4	B	107	107	107	0	0

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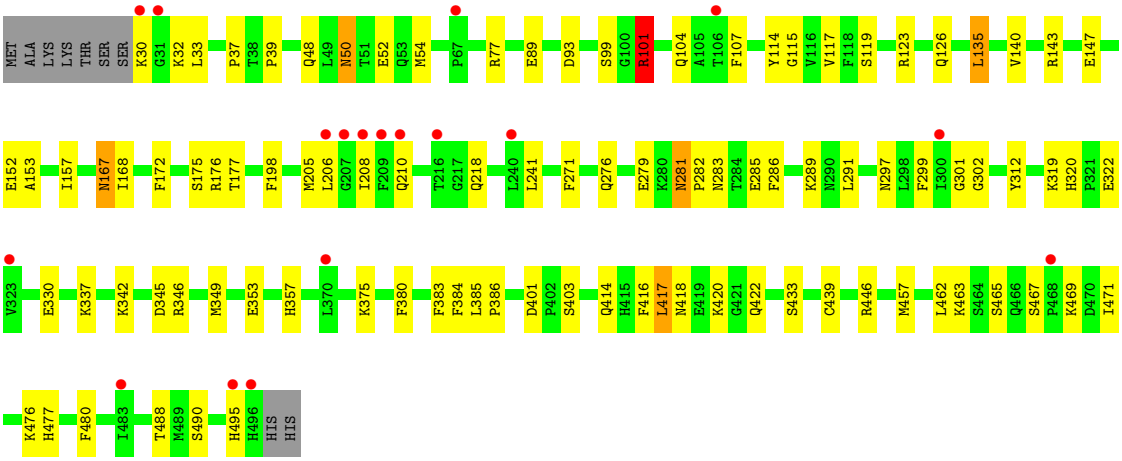
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	119	119	119	0	0
			Total	O		
4	D	130	130	130	0	0

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.

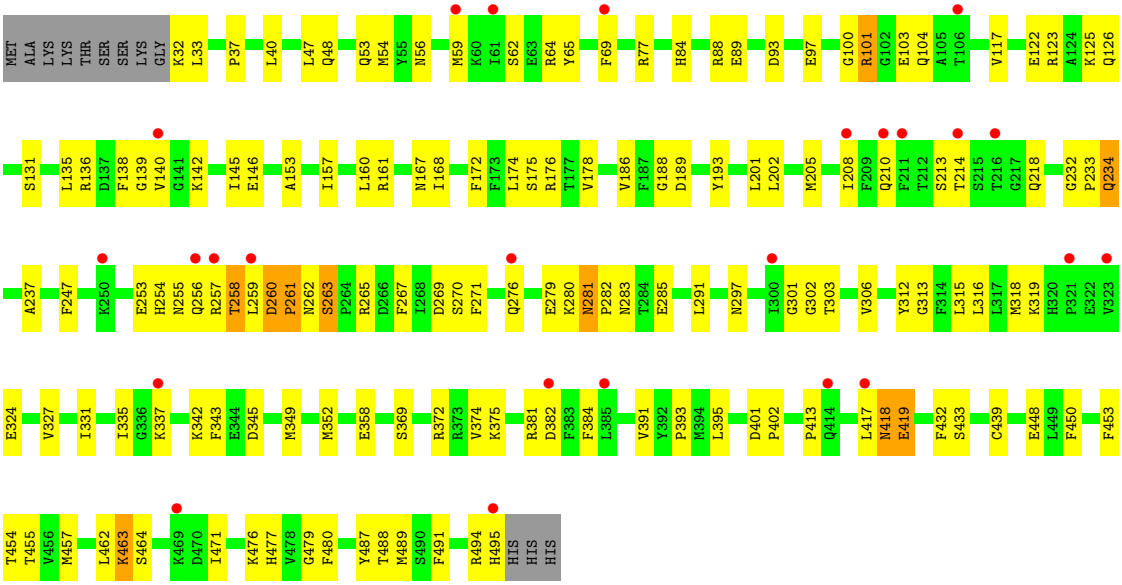
• Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6

Chain A:



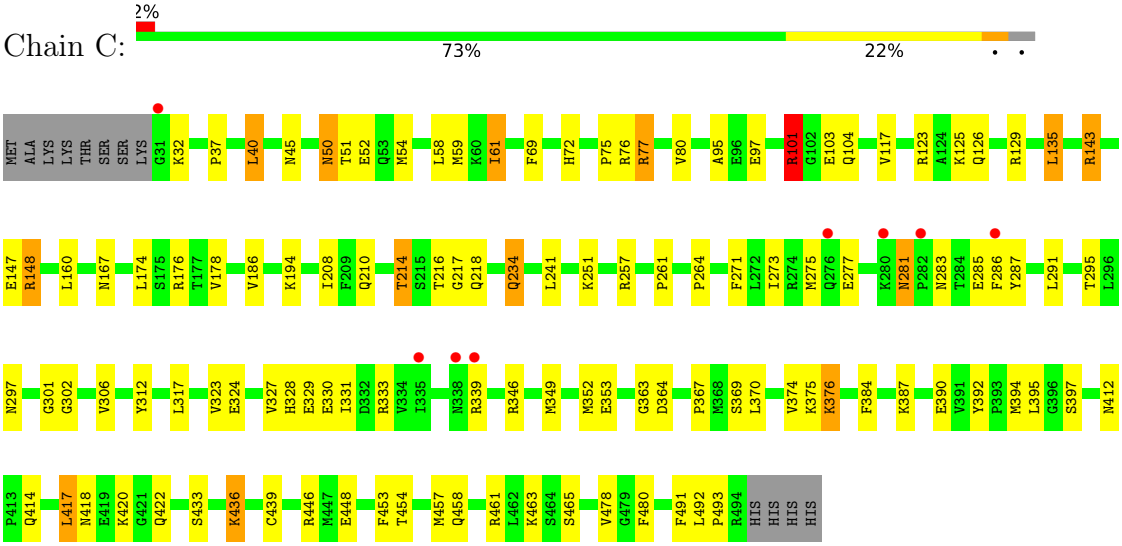
• Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6

Chain B:



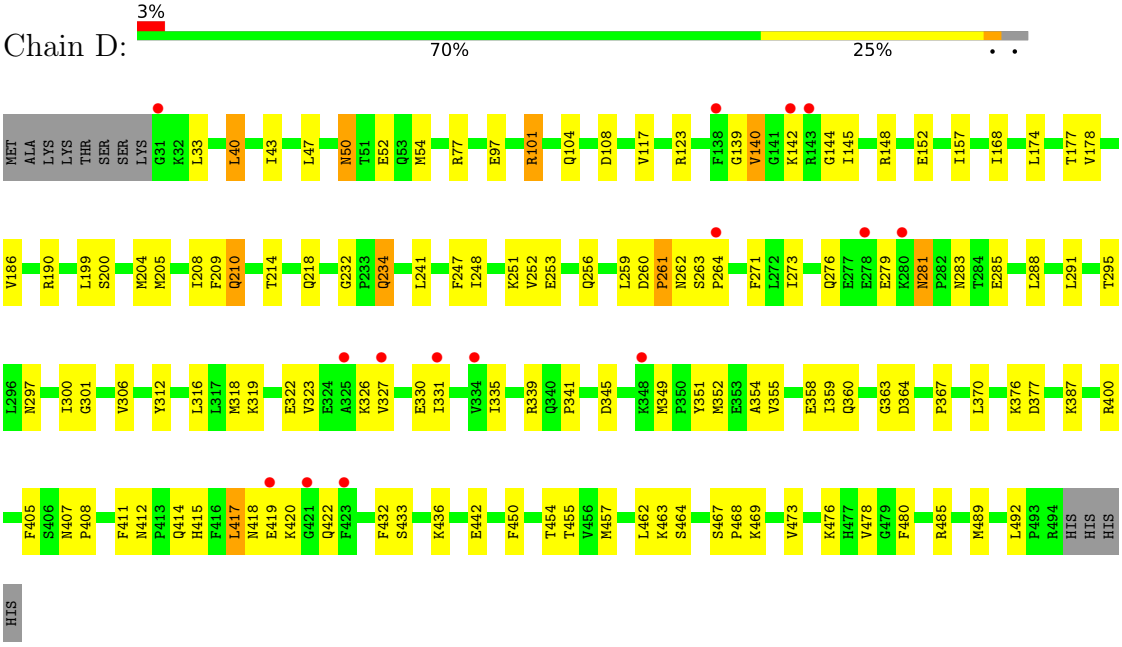
• Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6

Chain C:



• Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.66Å 159.03Å 103.88Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 49.35 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-2.05) 93.9 (49.35-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.05Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.261 0.209 , 0.248	Depositor DCC
R_{free} test set	5674 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15779	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: HEM, 8MO

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	0.54	0/3873	0.68	3/5216 (0.1%)
1	B	0.51	0/3849	0.67	2/5185 (0.0%)
1	C	0.50	0/3842	0.67	2/5175 (0.0%)
1	D	0.50	0/3842	0.67	1/5175 (0.0%)
All	All	0.51	0/15406	0.67	8/20751 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	A	101	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	104	GLN	N-CA-C	-6.41	93.70	111.00
1	B	104	GLN	N-CA-C	-5.66	95.73	111.00
1	B	101	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	104	GLN	N-CA-C	-5.38	96.46	111.00
1	C	101	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	104	GLN	N-CA-C	-5.03	97.41	111.00

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	3780	0	3761	83	0
1	B	3757	0	3738	137	0
1	C	3751	0	3734	138	0
1	D	3751	0	3734	119	0
2	A	43	0	30	5	0
2	B	43	0	30	4	0
2	C	43	0	30	5	0
2	D	43	0	30	2	0
3	A	16	0	8	9	0
3	B	16	0	8	9	0
3	C	16	0	8	6	0
3	D	16	0	8	7	0
4	A	148	0	0	2	0
4	B	107	0	0	3	0
4	C	119	0	0	3	0
4	D	130	0	0	6	0
All	All	15779	0	15119	476	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 16.

All (476) 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:32:LYS:HB3	1:C:384:PHE:HB3	1.28	1.15
1:B:318:MET:HE1	1:B:489:MET:HB2	1.27	1.06
1:C:54:MET:HG3	1:C:218:GLN:HE21	1.27	0.97
1:B:352:MET:HE3	1:B:454:THR:HG22	1.49	0.94
1:B:54:MET:HG3	1:B:218:GLN:HE21	1.32	0.94
1:C:214:THR:HG22	1:C:217:GLY:H	1.31	0.94
1:C:375:LYS:HB3	1:C:376:LYS:HE2	1.51	0.93
1:C:45:ASN:HD22	1:C:72:HIS:H	1.01	0.93
1:B:234:GLN:H	1:B:234:GLN:NE2	1.68	0.92
1:C:234:GLN:H	1:C:234:GLN:HE21	1.01	0.92
1:A:420:LYS:HB3	1:A:422:GLN:HE21	1.37	0.89
1:B:117:VAL:HG21	3:B:501:8MO:H43	1.54	0.89
1:C:32:LYS:HE2	1:C:384:PHE:HB2	1.53	0.89
1:C:143:ARG:HE	1:C:147:GLU:HG3	1.36	0.89
1:D:418:ASN:HD22	1:D:422:GLN:HB2	1.37	0.89
1:A:33:LEU:HD21	1:A:77:ARG:HD2	1.53	0.87
1:D:54:MET:HG3	1:D:218:GLN:HE21	1.40	0.87
1:C:234:GLN:H	1:C:234:GLN:NE2	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLN:H	1:B:234:GLN:HE21	1.17	0.86
1:A:30:LYS:HD3	1:A:32:LYS:HD2	1.59	0.85
1:A:54:MET:HG3	1:A:218:GLN:HE21	1.41	0.84
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.44	0.81
1:C:61:ILE:HD11	1:C:69:PHE:CD1	2.17	0.80
1:B:318:MET:HE3	1:B:462:LEU:HB3	1.64	0.79
1:C:418:ASN:HD22	1:C:422:GLN:HB2	1.47	0.78
1:C:234:GLN:HE21	1:C:234:GLN:N	1.80	0.78
1:B:135:LEU:HG	1:B:140:VAL:HG21	1.66	0.78
1:C:352:MET:HE3	1:C:454:THR:HG22	1.65	0.78
1:B:318:MET:CE	1:B:489:MET:HB2	2.12	0.77
1:D:412:ASN:HD21	1:D:414:GLN:HB2	1.48	0.77
1:D:418:ASN:ND2	1:D:422:GLN:HB2	1.99	0.77
1:C:143:ARG:NE	1:C:147:GLU:HG3	2.00	0.77
1:C:412:ASN:OD1	1:C:414:GLN:HB2	1.85	0.76
1:D:322:GLU:O	1:D:326:LYS:HG2	1.84	0.76
1:C:251:LYS:NZ	1:C:251:LYS:HB3	2.00	0.76
1:B:375:LYS:HE2	4:B:576:HOH:O	1.85	0.75
1:B:259:LEU:HD12	1:B:260:ASP:H	1.51	0.75
1:C:125:LYS:HE2	1:C:129:ARG:NH2	2.02	0.75
1:C:45:ASN:ND2	1:C:72:HIS:H	1.82	0.74
1:D:264:PRO:HG3	1:D:273:ILE:CD1	2.18	0.73
1:C:125:LYS:HE2	1:C:129:ARG:HH22	1.54	0.73
1:C:59:MET:HE3	1:C:397:SER:HB3	1.70	0.73
1:B:318:MET:HE1	1:B:489:MET:CB	2.14	0.72
1:A:281:ASN:ND2	1:A:283:ASN:H	1.85	0.72
1:A:322:GLU:OE2	1:A:322:GLU:N	2.21	0.71
1:C:59:MET:CE	1:C:397:SER:HB3	2.20	0.71
1:D:186:VAL:HG11	1:D:295:THR:HG23	1.72	0.70
1:D:234:GLN:NE2	1:D:234:GLN:H	1.90	0.70
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.73	0.70
1:D:50:ASN:HD22	1:D:52:GLU:H	1.37	0.70
1:D:50:ASN:ND2	1:D:52:GLU:H	1.89	0.70
1:B:480:PHE:CZ	3:B:501:8MO:H8	2.25	0.69
1:D:271:PHE:CE2	1:D:291:LEU:HB2	2.27	0.69
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.73	0.69
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.28	0.69
1:D:139:GLY:HA2	1:D:142:LYS:HE3	1.73	0.69
1:C:45:ASN:HD22	1:C:72:HIS:N	1.85	0.68
1:B:262:ASN:O	1:B:263:SER:HB2	1.94	0.68
1:D:140:VAL:H	1:D:145:ILE:HB	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:TYR:HB3	1:C:394:MET:HE2	1.75	0.68
1:D:412:ASN:ND2	1:D:414:GLN:HB2	2.08	0.68
1:C:330:GLU:OE1	1:C:349:MET:HB3	1.93	0.68
1:A:101:ARG:HD2	1:A:117:VAL:O	1.94	0.68
1:D:462:LEU:HD22	1:D:489:MET:HE1	1.76	0.68
1:C:346:ARG:HG2	1:C:353:GLU:OE1	1.94	0.67
1:C:117:VAL:HG21	3:C:501:8MO:H42	1.76	0.67
1:C:186:VAL:CG1	1:C:295:THR:HG23	2.24	0.67
1:B:117:VAL:CG2	3:B:501:8MO:H43	2.24	0.67
1:B:265:ARG:HB2	1:B:269:ASP:OD1	1.93	0.67
1:C:32:LYS:HB3	1:C:384:PHE:CB	2.16	0.67
1:C:352:MET:CE	1:C:454:THR:HG22	2.25	0.67
1:D:331:ILE:HG12	1:D:349:MET:HE1	1.76	0.67
1:A:276:GLN:HA	1:A:279:GLU:HG3	1.77	0.67
1:D:276:GLN:HB3	4:D:597:HOH:O	1.95	0.66
1:B:254:HIS:HA	1:B:257:ARG:NH1	2.09	0.66
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.60	0.66
1:B:33:LEU:HD21	1:B:77:ARG:HD2	1.78	0.66
1:C:58:LEU:HD13	1:C:394:MET:HE3	1.77	0.65
1:D:281:ASN:ND2	1:D:283:ASN:H	1.95	0.65
1:D:248:ILE:O	1:D:252:VAL:HG23	1.96	0.64
1:D:271:PHE:CD2	1:D:291:LEU:HB2	2.33	0.64
1:D:480:PHE:CZ	3:D:501:8MO:H8	2.32	0.64
1:D:97:GLU:HG3	4:D:576:HOH:O	1.97	0.64
1:D:50:ASN:HD22	1:D:50:ASN:C	2.00	0.64
1:C:50:ASN:ND2	1:C:52:GLU:H	1.93	0.64
1:C:392:TYR:HB3	1:C:394:MET:CE	2.26	0.64
1:D:462:LEU:HD22	1:D:489:MET:CE	2.28	0.64
1:A:115:GLY:O	1:A:119:SER:HB3	1.98	0.64
1:C:323:VAL:O	1:C:327:VAL:HG23	1.97	0.64
1:A:135:LEU:HG	1:A:140:VAL:HG21	1.80	0.64
1:C:463:LYS:HD3	1:C:492:LEU:HD11	1.80	0.63
1:D:204:MET:O	1:D:208:ILE:HG13	1.98	0.63
1:D:360:GLN:HG2	4:D:511:HOH:O	1.99	0.63
1:D:420:LYS:HB2	1:D:422:GLN:HE21	1.63	0.63
1:B:281:ASN:C	1:B:281:ASN:HD22	2.01	0.63
1:C:208:ILE:HD13	1:C:241:LEU:HD23	1.79	0.63
1:B:324:GLU:HG3	1:B:457:MET:HE3	1.81	0.63
1:D:463:LYS:HE3	1:D:492:LEU:HD11	1.81	0.63
1:B:281:ASN:ND2	1:B:283:ASN:H	1.96	0.62
1:B:324:GLU:HG3	1:B:457:MET:CE	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:GLY:HA3	3:D:501:8MO:O3	1.99	0.62
1:A:123:ARG:HA	1:A:285:GLU:HG3	1.81	0.62
1:B:480:PHE:HZ	3:B:501:8MO:H8	1.63	0.62
1:C:375:LYS:HB3	1:C:376:LYS:CE	2.28	0.62
1:A:301:GLY:HA3	3:A:501:8MO:O3	2.00	0.62
1:D:264:PRO:HG3	1:D:273:ILE:HD12	1.81	0.62
1:C:32:LYS:HE2	1:C:384:PHE:CB	2.28	0.62
1:D:117:VAL:HG22	2:D:500:HEM:HAD1	1.82	0.62
1:B:463:LYS:HE2	1:B:463:LYS:HA	1.81	0.61
1:C:143:ARG:HE	1:C:147:GLU:CG	2.12	0.61
1:C:80:VAL:HG13	1:C:394:MET:HE2	1.82	0.61
1:C:214:THR:HG21	4:C:559:HOH:O	1.99	0.61
1:B:419:GLU:CD	1:B:419:GLU:H	2.03	0.61
1:C:478:VAL:HG12	4:C:560:HOH:O	1.99	0.61
1:C:446:ARG:HG2	1:C:446:ARG:HH11	1.66	0.61
1:D:168:ILE:O	1:D:168:ILE:HD12	2.01	0.61
1:B:64:ARG:HD3	1:B:65:TYR:CE2	2.36	0.60
1:B:494:ARG:O	1:B:495:HIS:HB2	2.01	0.60
1:C:271:PHE:CD2	1:C:291:LEU:HB2	2.36	0.60
1:D:50:ASN:HD21	1:D:52:GLU:HB3	1.65	0.60
1:D:117:VAL:HG21	3:D:501:8MO:C4	2.31	0.60
1:D:234:GLN:H	1:D:234:GLN:HE21	1.48	0.60
1:A:281:ASN:C	1:A:281:ASN:HD22	2.03	0.60
1:C:275:MET:HE3	1:C:287:TYR:HA	1.82	0.60
1:C:126:GLN:HG3	1:C:286:PHE:CE2	2.37	0.60
1:C:317:LEU:HD13	1:C:457:MET:CE	2.31	0.60
1:C:420:LYS:HD3	1:C:422:GLN:NE2	2.17	0.60
1:D:418:ASN:HD22	1:D:422:GLN:CB	2.14	0.59
1:C:80:VAL:HG13	1:C:394:MET:CE	2.32	0.59
1:D:400:ARG:NH1	4:D:559:HOH:O	2.35	0.59
1:B:201:LEU:HD11	1:B:247:PHE:CE1	2.37	0.59
1:A:420:LYS:HB3	1:A:422:GLN:NE2	2.14	0.59
1:B:64:ARG:HG2	1:B:64:ARG:HH11	1.66	0.59
1:B:381:ARG:O	1:B:382:ASP:HB2	2.01	0.59
1:C:417:LEU:HD12	1:C:422:GLN:O	2.03	0.59
1:B:297:ASN:HA	3:B:501:8MO:O4	2.02	0.59
1:C:281:ASN:HD22	1:C:281:ASN:C	2.05	0.59
1:B:318:MET:SD	1:B:464:SER:HB3	2.43	0.59
1:A:50:ASN:C	1:A:50:ASN:HD22	2.04	0.58
1:B:369:SER:HB2	1:B:395:LEU:HG	1.85	0.58
1:C:148:ARG:HE	1:C:148:ARG:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:LYS:CB	1:D:422:GLN:HE21	2.15	0.58
1:D:355:VAL:O	1:D:359:ILE:HG13	2.03	0.58
1:D:400:ARG:HG3	1:D:400:ARG:HH11	1.68	0.58
1:C:420:LYS:HD3	1:C:422:GLN:HE21	1.66	0.58
1:A:342:LYS:HG2	1:A:345:ASP:OD2	2.03	0.58
1:A:457:MET:HE2	1:A:457:MET:HA	1.86	0.58
1:B:32:LYS:HE2	1:B:384:PHE:HB2	1.85	0.57
1:C:178:VAL:HG13	1:C:448:GLU:OE1	2.05	0.57
1:B:40:LEU:HD21	1:D:47:LEU:HD21	1.86	0.57
1:C:339:ARG:HH11	1:C:339:ARG:HG2	1.69	0.57
1:D:335:ILE:HA	1:D:339:ARG:NH2	2.19	0.57
1:A:50:ASN:ND2	1:A:52:GLU:H	2.03	0.57
1:D:142:LYS:HZ1	1:D:144:GLY:HA3	1.70	0.56
1:B:489:MET:HE1	1:B:491:PHE:CZ	2.40	0.56
1:D:33:LEU:HD11	1:D:77:ARG:CZ	2.35	0.56
1:D:276:GLN:O	1:D:279:GLU:HG3	2.05	0.56
1:A:480:PHE:CZ	3:A:501:8MO:H8	2.41	0.56
1:C:103:GLU:HG2	1:C:390:GLU:OE2	2.06	0.56
1:D:463:LYS:CE	1:D:492:LEU:HD11	2.36	0.56
1:B:476:LYS:HE3	1:B:477:HIS:NE2	2.21	0.56
1:A:37:PRO:HB2	1:A:48:GLN:HE22	1.70	0.56
1:D:152:GLU:HG3	1:D:177:THR:HG23	1.86	0.56
1:D:480:PHE:HZ	3:D:501:8MO:H8	1.71	0.56
1:A:302:GLY:HA2	2:A:500:HEM:HMC2	1.88	0.56
1:A:476:LYS:HE3	1:A:477:HIS:NE2	2.20	0.55
1:C:251:LYS:HB3	1:C:251:LYS:HZ2	1.69	0.55
1:B:32:LYS:O	1:B:384:PHE:N	2.35	0.55
1:D:331:ILE:HG12	1:D:349:MET:CE	2.37	0.55
1:A:281:ASN:HD22	1:A:282:PRO:N	2.05	0.55
1:C:50:ASN:C	1:C:50:ASN:HD22	2.10	0.55
1:C:301:GLY:HA3	3:C:501:8MO:O3	2.06	0.55
1:B:89:GLU:CD	1:B:381:ARG:HH21	2.10	0.55
1:B:233:PRO:HD2	1:B:234:GLN:NE2	2.21	0.54
1:D:319:LYS:HD2	1:D:468:PRO:O	2.07	0.54
1:B:253:GLU:HA	1:B:256:GLN:NE2	2.23	0.54
1:A:101:ARG:CD	1:A:117:VAL:O	2.55	0.54
1:B:157:ILE:HD11	1:B:455:THR:HG22	1.90	0.54
1:D:271:PHE:CB	1:D:291:LEU:HD13	2.37	0.54
1:B:489:MET:HE1	1:B:491:PHE:CE2	2.43	0.53
1:B:37:PRO:HB2	1:B:48:GLN:OE1	2.08	0.53
1:B:40:LEU:CD2	1:D:47:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HG21	3:A:501:8MO:C4	2.38	0.53
1:C:167:ASN:ND2	1:C:465:SER:HB3	2.23	0.53
1:C:369:SER:HB2	1:C:395:LEU:HG	1.89	0.53
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.90	0.53
1:A:143:ARG:O	1:A:147:GLU:HG2	2.09	0.53
1:A:208:ILE:HD13	1:A:241:LEU:HD23	1.90	0.53
1:A:37:PRO:HB2	1:A:48:GLN:NE2	2.24	0.53
1:A:208:ILE:HD13	1:A:241:LEU:CD2	2.39	0.53
1:B:281:ASN:C	1:B:281:ASN:ND2	2.62	0.53
1:B:337:LYS:NZ	1:B:494:ARG:NH1	2.57	0.53
1:D:318:MET:SD	1:D:464:SER:HB3	2.49	0.53
1:C:186:VAL:HG11	1:C:295:THR:HG23	1.89	0.52
1:C:167:ASN:HD21	1:C:465:SER:HB3	1.72	0.52
1:D:142:LYS:NZ	1:D:144:GLY:HA3	2.25	0.52
1:A:206:LEU:HD12	4:A:602:HOH:O	2.10	0.52
1:B:117:VAL:HG22	2:B:500:HEM:HAD1	1.92	0.52
1:B:258:THR:O	1:B:258:THR:OG1	2.27	0.52
1:C:77:ARG:HG2	1:C:77:ARG:NH1	2.14	0.52
1:D:323:VAL:O	1:D:327:VAL:HG23	2.09	0.52
1:A:480:PHE:HZ	3:A:501:8MO:H8	1.74	0.52
1:C:61:ILE:HD11	1:C:69:PHE:CE1	2.45	0.52
1:C:76:ARG:CZ	1:C:103:GLU:HG3	2.40	0.52
1:D:208:ILE:HD13	1:D:241:LEU:CD2	2.40	0.52
1:B:178:VAL:HG11	1:B:306:VAL:HB	1.92	0.52
1:C:214:THR:HG23	1:C:216:THR:H	1.75	0.52
1:D:208:ILE:HD13	1:D:241:LEU:HD23	1.91	0.52
1:B:319:LYS:HD3	1:B:471:ILE:HB	1.91	0.52
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.75	0.52
1:D:400:ARG:NH1	1:D:400:ARG:HG3	2.25	0.52
1:D:407:ASN:H	1:D:415:HIS:HE1	1.58	0.52
1:A:380:PHE:O	1:A:383:PHE:HB2	2.10	0.51
1:C:271:PHE:CE2	1:C:291:LEU:HB2	2.44	0.51
1:C:281:ASN:C	1:C:281:ASN:ND2	2.64	0.51
1:D:450:PHE:O	1:D:454:THR:HG23	2.10	0.51
1:B:255:ASN:HA	1:B:265:ARG:HH22	1.75	0.51
1:C:143:ARG:NE	1:C:147:GLU:CG	2.70	0.51
1:C:375:LYS:CB	1:C:376:LYS:HE2	2.33	0.51
1:C:392:TYR:HD1	1:C:394:MET:HE1	1.75	0.51
1:C:37:PRO:HD3	1:C:61:ILE:HD13	1.93	0.51
1:D:364:ASP:OD2	1:D:367:PRO:HB3	2.10	0.51
1:B:259:LEU:C	1:B:261:PRO:HD3	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LYS:HG2	1:B:345:ASP:OD2	2.10	0.51
1:B:450:PHE:O	1:B:454:THR:HG23	2.11	0.51
1:D:297:ASN:HA	3:D:501:8MO:O4	2.11	0.51
1:A:337:LYS:HG3	4:A:572:HOH:O	2.11	0.51
1:D:117:VAL:HG21	3:D:501:8MO:H43	1.92	0.51
1:D:139:GLY:CA	1:D:142:LYS:HE3	2.39	0.51
1:A:433:SER:HB3	2:A:500:HEM:HBA1	1.93	0.51
1:C:302:GLY:HA2	2:C:500:HEM:HMC2	1.92	0.51
1:B:153:ALA:O	1:B:157:ILE:HG12	2.11	0.50
1:B:210:GLN:O	1:B:214:THR:HG23	2.12	0.50
1:B:53:GLN:HG3	1:B:56:ASN:ND2	2.26	0.50
1:A:50:ASN:C	1:A:50:ASN:ND2	2.64	0.50
1:A:457:MET:HE3	1:A:462:LEU:HD11	1.93	0.50
1:D:363:GLY:O	1:D:364:ASP:C	2.50	0.50
1:D:232:GLY:HA3	1:D:234:GLN:HE22	1.75	0.50
1:D:168:ILE:HD12	1:D:168:ILE:C	2.32	0.50
1:D:200:SER:O	1:D:204:MET:HG3	2.11	0.50
1:A:89:GLU:O	1:A:93:ASP:HB2	2.12	0.50
1:A:33:LEU:HD21	1:A:77:ARG:CD	2.34	0.50
1:A:89:GLU:HA	1:A:93:ASP:OD2	2.11	0.50
1:B:122:GLU:O	1:B:126:GLN:HB2	2.12	0.50
1:D:260:ASP:O	1:D:262:ASN:N	2.44	0.50
1:D:405:PHE:O	1:D:408:PRO:HD3	2.12	0.50
1:C:261:PRO:HA	1:C:273:ILE:CD1	2.42	0.49
1:D:259:LEU:O	1:D:261:PRO:HD3	2.11	0.49
1:B:281:ASN:HD22	1:B:282:PRO:N	2.11	0.49
1:A:281:ASN:ND2	1:A:281:ASN:C	2.65	0.49
1:C:317:LEU:HD13	1:C:457:MET:HE2	1.94	0.49
1:A:117:VAL:HG21	3:A:501:8MO:H43	1.93	0.49
1:B:319:LYS:NZ	1:B:471:ILE:O	2.36	0.49
1:B:337:LYS:HZ1	1:B:494:ARG:NH1	2.11	0.49
1:A:319:LYS:HD3	1:A:471:ILE:HB	1.94	0.49
1:C:412:ASN:OD1	1:C:414:GLN:CB	2.59	0.49
1:A:463:LYS:HB3	1:A:490:SER:OG	2.13	0.49
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.78	0.49
1:A:114:TYR:CD1	1:A:289:LYS:HD3	2.48	0.49
1:B:59:MET:CE	1:B:59:MET:HA	2.43	0.49
1:B:358:GLU:HA	1:B:358:GLU:OE1	2.12	0.49
1:D:101:ARG:NH2	1:D:370:LEU:HB3	2.28	0.49
1:B:53:GLN:HG3	1:B:56:ASN:HD22	1.78	0.48
1:B:259:LEU:O	1:B:261:PRO:HD3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:LYS:HE2	1:C:376:LYS:N	2.27	0.48
1:A:297:ASN:HA	3:A:501:8MO:O4	2.13	0.48
1:C:453:PHE:O	1:C:457:MET:HG2	2.13	0.48
1:C:117:VAL:HG21	3:C:501:8MO:C4	2.43	0.48
1:B:301:GLY:HA3	3:B:501:8MO:O3	2.14	0.48
3:B:501:8MO:H42	3:B:501:8MO:O1	2.13	0.48
1:C:208:ILE:HD13	1:C:241:LEU:CD2	2.44	0.48
1:C:281:ASN:ND2	1:C:283:ASN:H	2.11	0.48
1:B:315:LEU:HD13	1:B:487:TYR:CG	2.49	0.48
1:D:101:ARG:HD2	1:D:117:VAL:O	2.13	0.48
1:B:135:LEU:O	1:B:140:VAL:HG23	2.14	0.48
1:A:384:PHE:C	1:A:385:LEU:HD12	2.34	0.48
1:C:251:LYS:NZ	1:C:251:LYS:CB	2.75	0.48
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.96	0.48
1:C:273:ILE:O	1:C:277:GLU:HG3	2.13	0.48
1:D:264:PRO:HG3	1:D:273:ILE:HD11	1.96	0.48
1:B:253:GLU:HA	1:B:256:GLN:HE21	1.79	0.47
1:B:302:GLY:HA2	2:B:500:HEM:HMC2	1.95	0.47
1:D:148:ARG:NH2	1:D:190:ARG:HD2	2.29	0.47
1:A:345:ASP:O	1:A:349:MET:HG3	2.13	0.47
1:B:62:SER:HB3	1:B:69:PHE:CE2	2.48	0.47
1:C:418:ASN:C	1:C:420:LYS:N	2.66	0.47
1:A:30:LYS:HD3	1:A:32:LYS:CD	2.36	0.47
1:B:161:ARG:HG3	1:B:161:ARG:NH1	2.29	0.47
1:B:391:VAL:O	1:B:393:PRO:HD3	2.13	0.47
1:D:117:VAL:HG21	3:D:501:8MO:H42	1.95	0.47
1:B:201:LEU:HD11	1:B:247:PHE:CD1	2.50	0.47
1:A:107:PHE:CD2	3:A:501:8MO:H6	2.49	0.47
1:C:95:ALA:HB1	1:C:436:LYS:HD3	1.94	0.47
1:C:392:TYR:CD1	1:C:394:MET:HE1	2.49	0.47
1:D:457:MET:HE2	1:D:457:MET:HA	1.96	0.47
1:A:126:GLN:HG3	1:A:286:PHE:CE2	2.50	0.47
1:A:153:ALA:O	1:A:157:ILE:HG12	2.15	0.47
1:A:401:ASP:OD2	1:A:403:SER:HB3	2.13	0.47
1:B:280:LYS:O	1:B:282:PRO:HD3	2.15	0.47
1:D:335:ILE:HD13	1:D:341:PRO:HG3	1.96	0.47
1:B:101:ARG:CD	1:B:117:VAL:O	2.62	0.47
1:B:476:LYS:HE3	1:B:477:HIS:CD2	2.49	0.47
1:C:363:GLY:O	1:C:364:ASP:C	2.52	0.47
1:D:210:GLN:HE21	1:D:210:GLN:HB2	1.57	0.46
1:D:473:VAL:HG12	1:D:473:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:PHE:HB2	4:B:512:HOH:O	2.15	0.46
1:C:439:CYS:HB2	2:C:500:HEM:NA	2.30	0.46
1:B:117:VAL:HG21	3:B:501:8MO:C4	2.36	0.46
1:C:364:ASP:OD2	1:C:367:PRO:HB3	2.16	0.46
1:D:473:VAL:O	1:D:473:VAL:CG1	2.64	0.46
1:C:160:LEU:HD13	1:C:491:PHE:CD2	2.51	0.46
1:C:370:LEU:HD11	3:C:501:8MO:C3	2.45	0.46
1:B:188:GLY:O	1:B:189:ASP:HB2	2.16	0.46
1:B:271:PHE:CD2	1:B:291:LEU:HB2	2.51	0.46
1:B:345:ASP:O	1:B:349:MET:HG3	2.16	0.46
1:A:302:GLY:HA2	2:A:500:HEM:CMC	2.46	0.46
1:C:433:SER:HB3	2:C:500:HEM:HBA1	1.98	0.46
1:C:32:LYS:O	1:C:384:PHE:N	2.41	0.45
1:C:297:ASN:HA	3:C:501:8MO:O4	2.16	0.45
1:C:54:MET:HG3	1:C:218:GLN:NE2	2.10	0.45
1:A:457:MET:CE	1:A:462:LEU:HD21	2.47	0.45
1:C:329:GLU:OE1	1:C:333:ARG:NH2	2.49	0.45
1:B:381:ARG:O	1:B:381:ARG:HG3	2.17	0.45
1:C:458:GLN:O	1:C:458:GLN:HG2	2.16	0.45
1:B:352:MET:CE	1:B:454:THR:HG22	2.33	0.45
1:C:261:PRO:HA	1:C:273:ILE:HG12	1.97	0.45
1:C:327:VAL:O	1:C:331:ILE:HG13	2.17	0.45
1:B:84:HIS:CE1	1:B:88:ARG:HD2	2.52	0.45
1:B:327:VAL:O	1:B:331:ILE:HG13	2.16	0.45
1:C:251:LYS:HB3	1:C:251:LYS:HZ3	1.78	0.45
1:A:167:ASN:OD1	1:A:465:SER:HB3	2.17	0.45
1:B:131:SER:O	1:B:135:LEU:HB2	2.16	0.45
1:D:140:VAL:H	1:D:145:ILE:CB	2.28	0.45
1:D:178:VAL:HG11	1:D:306:VAL:HB	1.98	0.45
1:D:271:PHE:CD2	1:D:291:LEU:HD13	2.51	0.45
1:B:259:LEU:HD12	1:B:260:ASP:N	2.24	0.45
1:C:117:VAL:HG23	1:C:297:ASN:CG	2.37	0.45
1:B:186:VAL:HA	1:B:267:PHE:HB3	1.99	0.44
1:A:320:HIS:HB3	1:A:322:GLU:OE1	2.17	0.44
1:B:138:PHE:HE2	1:B:270:SER:HG	1.64	0.44
1:A:457:MET:HE3	1:A:462:LEU:HD21	1.98	0.44
1:B:40:LEU:HD12	1:B:47:LEU:HD12	1.99	0.44
1:D:101:ARG:CD	1:D:117:VAL:O	2.65	0.44
1:B:160:LEU:HD22	1:B:491:PHE:CD1	2.53	0.44
1:B:463:LYS:NZ	1:B:464:SER:O	2.44	0.44
1:C:178:VAL:HG11	1:C:306:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLN:HA	1:A:414:GLN:NE2	2.33	0.44
1:B:176:ARG:NH1	1:B:193:TYR:HB3	2.32	0.44
1:C:75:PRO:HA	4:C:555:HOH:O	2.17	0.44
1:C:461:ARG:NH1	1:C:493:PRO:O	2.50	0.44
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.53	0.44
1:B:254:HIS:O	1:B:257:ARG:HB3	2.18	0.44
1:D:205:MET:HE2	1:D:300:ILE:HA	1.98	0.44
1:D:467:SER:HB3	1:D:469:LYS:HG2	2.00	0.44
1:B:145:ILE:HD12	1:B:145:ILE:HA	1.88	0.44
1:B:178:VAL:HG13	1:B:448:GLU:OE1	2.18	0.44
1:C:76:ARG:NH2	1:C:103:GLU:HG3	2.33	0.44
1:A:281:ASN:ND2	1:A:283:ASN:N	2.62	0.43
1:A:357:HIS:CE1	1:A:446:ARG:NH2	2.86	0.43
1:C:37:PRO:CD	1:C:61:ILE:HD13	2.48	0.43
1:C:264:PRO:HB3	1:C:273:ILE:HD12	2.00	0.43
1:C:50:ASN:ND2	1:C:50:ASN:C	2.71	0.43
1:D:354:ALA:HB2	1:D:417:LEU:HD13	1.99	0.43
1:C:125:LYS:CE	1:C:129:ARG:HH22	2.29	0.43
1:C:257:ARG:HG2	1:C:257:ARG:NH1	2.32	0.43
1:D:210:GLN:O	1:D:214:THR:HG23	2.18	0.43
1:D:326:LYS:HB2	1:D:351:TYR:CE2	2.53	0.43
1:D:418:ASN:HB3	1:D:420:LYS:H	1.81	0.43
1:C:97:GLU:O	1:C:374:VAL:HA	2.19	0.43
1:B:168:ILE:O	1:B:488:THR:HA	2.18	0.43
1:C:194:LYS:HA	1:C:194:LYS:HD3	1.82	0.43
1:C:418:ASN:HB2	1:C:422:GLN:H	1.82	0.43
1:B:253:GLU:HA	1:B:256:GLN:HG2	2.01	0.43
1:D:281:ASN:C	1:D:281:ASN:HD22	2.21	0.43
1:A:168:ILE:O	1:A:488:THR:HA	2.18	0.43
1:B:97:GLU:O	1:B:374:VAL:HA	2.18	0.43
1:B:213:SER:HA	1:B:479:GLY:HA3	2.01	0.43
1:D:157:ILE:HD11	1:D:455:THR:HG22	2.01	0.43
1:D:186:VAL:CG1	1:D:295:THR:HG23	2.44	0.43
1:C:480:PHE:CZ	3:C:501:8MO:H8	2.53	0.43
1:A:281:ASN:HD22	1:A:283:ASN:H	1.63	0.43
1:D:139:GLY:O	1:D:140:VAL:O	2.37	0.43
1:D:247:PHE:O	1:D:251:LYS:HG2	2.19	0.43
1:A:114:TYR:CG	1:A:289:LYS:HD3	2.54	0.43
1:A:416:PHE:O	1:A:417:LEU:HD13	2.18	0.43
1:B:176:ARG:HA	1:B:202:LEU:HD11	2.01	0.43
1:C:40:LEU:HD12	1:C:40:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:GLU:O	1:D:256:GLN:HB2	2.19	0.43
1:B:40:LEU:CD1	1:B:47:LEU:HD12	2.49	0.42
1:B:433:SER:HB3	2:B:500:HEM:HBA1	2.01	0.42
1:C:375:LYS:O	1:C:387:LYS:HG3	2.19	0.42
1:A:439:CYS:HB2	2:A:500:HEM:NA	2.33	0.42
1:B:276:GLN:O	1:B:279:GLU:HB2	2.19	0.42
1:C:176:ARG:HE	1:C:176:ARG:HB2	1.61	0.42
1:C:439:CYS:HB2	2:C:500:HEM:C1A	2.54	0.42
1:D:432:PHE:CE2	1:D:442:GLU:HG3	2.54	0.42
1:A:117:VAL:HG22	2:A:500:HEM:HAD1	2.01	0.42
1:B:418:ASN:HD22	1:B:418:ASN:HA	1.58	0.42
1:C:117:VAL:HG23	1:C:297:ASN:OD1	2.18	0.42
1:B:89:GLU:O	1:B:93:ASP:HB2	2.19	0.42
1:C:101:ARG:HD2	1:C:117:VAL:O	2.18	0.42
1:A:205:MET:CE	1:A:299:PHE:CE2	3.02	0.42
1:B:313:GLY:HA3	1:B:453:PHE:HZ	1.84	0.42
1:B:232:GLY:HA3	1:B:234:GLN:HE22	1.85	0.42
1:A:281:ASN:HD22	1:A:282:PRO:CD	2.33	0.42
1:B:172:PHE:HA	1:B:175:SER:OG	2.19	0.42
1:C:271:PHE:HB3	1:C:291:LEU:HD13	2.01	0.42
1:B:146:GLU:OE1	1:B:343:PHE:N	2.46	0.42
1:B:202:LEU:HD23	1:B:205:MET:CE	2.50	0.42
1:B:352:MET:HG2	1:B:454:THR:HG22	2.01	0.42
1:C:324:GLU:HG2	1:C:328:HIS:CD2	2.55	0.42
1:B:401:ASP:HA	1:B:402:PRO:HD2	1.86	0.42
1:C:376:LYS:HA	1:C:387:LYS:HG3	2.02	0.42
1:A:417:LEU:HD12	1:A:422:GLN:O	2.20	0.42
1:C:261:PRO:HA	1:C:273:ILE:HD11	2.01	0.42
1:B:100:GLY:O	1:B:372:ARG:HA	2.20	0.41
1:B:205:MET:CE	1:B:303:THR:HG21	2.50	0.41
1:C:148:ARG:HE	1:C:148:ARG:CA	2.33	0.41
1:D:50:ASN:HD22	1:D:52:GLU:N	2.11	0.41
1:D:433:SER:HB3	2:D:500:HEM:HBA1	2.02	0.41
1:B:62:SER:HB3	1:B:69:PHE:HE2	1.85	0.41
1:B:103:GLU:HB3	4:B:578:HOH:O	2.20	0.41
1:B:136:ARG:O	1:B:142:LYS:NZ	2.45	0.41
1:D:376:LYS:HA	1:D:387:LYS:HG3	2.02	0.41
1:A:117:VAL:CG2	3:A:501:8MO:H43	2.50	0.41
1:A:330:GLU:OE1	1:A:349:MET:HB3	2.21	0.41
1:B:413:PRO:O	1:B:417:LEU:CD2	2.69	0.41
1:A:467:SER:OG	1:A:469:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLY:HA3	1:B:453:PHE:CZ	2.55	0.41
1:A:99:SER:OG	1:A:375:LYS:HE3	2.20	0.41
1:B:331:ILE:O	1:B:335:ILE:HB	2.20	0.41
1:C:125:LYS:CE	1:C:129:ARG:NH2	2.79	0.41
1:D:331:ILE:HD11	1:D:352:MET:HE2	2.01	0.41
1:A:271:PHE:HB3	1:A:291:LEU:HD13	2.02	0.41
1:B:139:GLY:HA2	1:B:142:LYS:HD2	2.03	0.41
1:D:50:ASN:ND2	1:D:52:GLU:N	2.65	0.41
1:D:367:PRO:HD2	1:D:480:PHE:O	2.20	0.41
1:A:107:PHE:CZ	3:A:501:8MO:H7	2.55	0.41
1:B:101:ARG:HD3	1:B:117:VAL:O	2.21	0.41
1:C:446:ARG:HG2	1:C:446:ARG:NH1	2.34	0.41
1:B:208:ILE:HD11	1:B:237:ALA:O	2.20	0.41
1:B:302:GLY:HA2	2:B:500:HEM:CMC	2.51	0.41
1:B:432:PHE:HB3	1:B:439:CYS:HB3	2.03	0.41
1:C:302:GLY:HA2	2:C:500:HEM:CMC	2.51	0.41
1:D:199:LEU:HB2	4:D:550:HOH:O	2.21	0.41
1:D:323:VAL:HG13	1:D:351:TYR:OH	2.20	0.41
1:A:172:PHE:HA	1:A:175:SER:OG	2.20	0.41
1:A:385:LEU:HA	1:A:386:PRO:HD2	1.97	0.41
1:B:260:ASP:O	1:B:262:ASN:N	2.54	0.41
1:B:324:GLU:HG3	1:B:457:MET:HE1	2.01	0.41
1:C:186:VAL:HG13	1:C:295:THR:HG23	1.98	0.41
1:D:330:GLU:OE1	1:D:349:MET:HB3	2.21	0.41
1:D:478:VAL:HG12	4:D:560:HOH:O	2.21	0.41
1:B:297:ASN:O	3:B:501:8MO:H42	2.21	0.40
1:C:346:ARG:HD2	1:C:353:GLU:OE2	2.21	0.40
1:D:376:LYS:O	1:D:377:ASP:C	2.60	0.40
1:A:176:ARG:HG2	1:A:198:PHE:CE2	2.57	0.40
1:B:135:LEU:HD12	1:B:135:LEU:HA	1.89	0.40
1:B:160:LEU:HD13	1:B:491:PHE:CD2	2.57	0.40
1:D:327:VAL:O	1:D:331:ILE:HG13	2.21	0.40
1:A:152:GLU:HG3	1:A:177:THR:HG23	2.02	0.40
1:B:122:GLU:OE2	1:B:125:LYS:HD3	2.21	0.40
1:B:271:PHE:CE2	1:B:291:LEU:HB2	2.56	0.40
1:C:50:ASN:HD22	1:C:51:THR:N	2.20	0.40
1:C:317:LEU:HD13	1:C:457:MET:HE1	2.02	0.40
1:D:276:GLN:HA	1:D:279:GLU:HG3	2.03	0.40
1:D:476:LYS:HB2	1:D:485:ARG:HA	2.03	0.40
1:A:30:LYS:CD	1:A:32:LYS:HD2	2.40	0.40
1:C:352:MET:HG2	1:C:454:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HD23	1:D:43:ILE:HD11	2.04	0.40
1:D:358:GLU:HG3	1:D:411:PHE:CD1	2.57	0.40
1:A:346:ARG:HD2	1:A:353:GLU:OE1	2.22	0.40
1:A:418:ASN:HD21	1:A:422:GLN:NE2	2.20	0.40
1:C:135:LEU:HD12	1:C:135:LEU:HA	1.87	0.40
1:C:346:ARG:HE	1:C:346:ARG:HB3	1.78	0.40
1:D:142:LYS:HG3	1:D:144:GLY:H	1.86	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	465/476 (98%)	447 (96%)	18 (4%)	0	100 100
1	B	462/476 (97%)	434 (94%)	26 (6%)	2 (0%)	34 24
1	C	462/476 (97%)	437 (95%)	25 (5%)	0	100 100
1	D	462/476 (97%)	445 (96%)	13 (3%)	4 (1%)	17 8
All	All	1851/1904 (97%)	1763 (95%)	82 (4%)	6 (0%)	41 31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	140	VAL
1	D	288	LEU
1	B	263	SER
1	D	345	ASP
1	B	261	PRO
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	414/422 (98%)	404 (98%)	10 (2%)	49	42
1	B	412/422 (98%)	401 (97%)	11 (3%)	44	38
1	C	411/422 (97%)	394 (96%)	17 (4%)	30	23
1	D	411/422 (97%)	396 (96%)	15 (4%)	35	28
All	All	1648/1688 (98%)	1595 (97%)	53 (3%)	39	32

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	PRO
1	A	50	ASN
1	A	101	ARG
1	A	135	LEU
1	A	167	ASN
1	A	210	GLN
1	A	281	ASN
1	A	312	TYR
1	A	417	LEU
1	A	495	HIS
1	B	167	ASN
1	B	174	LEU
1	B	234	GLN
1	B	258	THR
1	B	260	ASP
1	B	281	ASN
1	B	312	TYR
1	B	316	LEU
1	B	418	ASN
1	B	419	GLU
1	B	463	LYS
1	C	40	LEU
1	C	50	ASN
1	C	61	ILE

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Mol	Chain	Res	Type
1	C	77	ARG
1	C	101	ARG
1	C	135	LEU
1	C	143	ARG
1	C	148	ARG
1	C	174	LEU
1	C	210	GLN
1	C	214	THR
1	C	234	GLN
1	C	281	ASN
1	C	312	TYR
1	C	376	LYS
1	C	417	LEU
1	C	436	LYS
1	D	40	LEU
1	D	50	ASN
1	D	101	ARG
1	D	108	ASP
1	D	174	LEU
1	D	209	PHE
1	D	210	GLN
1	D	234	GLN
1	D	263	SER
1	D	281	ASN
1	D	312	TYR
1	D	316	LEU
1	D	417	LEU
1	D	419	GLU
1	D	436	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	50	ASN
1	A	53	GLN
1	A	56	ASN
1	A	94	GLN
1	A	126	GLN
1	A	210	GLN
1	A	218	GLN
1	A	276	GLN

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Mol	Chain	Res	Type
1	A	281	ASN
1	A	407	ASN
1	A	414	GLN
1	A	422	GLN
1	B	56	ASN
1	B	218	GLN
1	B	234	GLN
1	B	236	GLN
1	B	256	GLN
1	B	281	ASN
1	B	340	GLN
1	B	414	GLN
1	B	418	ASN
1	C	45	ASN
1	C	50	ASN
1	C	53	GLN
1	C	56	ASN
1	C	94	GLN
1	C	218	GLN
1	C	234	GLN
1	C	256	GLN
1	C	281	ASN
1	C	418	ASN
1	C	422	GLN
1	D	50	ASN
1	D	53	GLN
1	D	56	ASN
1	D	94	GLN
1	D	218	GLN
1	D	234	GLN
1	D	239	GLN
1	D	262	ASN
1	D	281	ASN
1	D	407	ASN
1	D	409	GLN
1	D	412	ASN
1	D	414	GLN
1	D	415	HIS
1	D	418	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
3	8MO	B	501	-	11,18,18	1.67	3 (27%)	15,26,26	1.84	6 (40%)
3	8MO	C	501	-	11,18,18	1.66	1 (9%)	15,26,26	1.80	3 (20%)
2	HEM	B	500	1	41,50,50	2.14	14 (34%)	45,82,82	1.83	7 (15%)
2	HEM	C	500	1	41,50,50	2.18	16 (39%)	45,82,82	1.97	9 (20%)
3	8MO	A	501	-	11,18,18	1.57	2 (18%)	15,26,26	1.75	5 (33%)
2	HEM	A	500	1	41,50,50	2.11	13 (31%)	45,82,82	1.79	9 (20%)
3	8MO	D	501	-	11,18,18	1.69	2 (18%)	15,26,26	1.69	3 (20%)
2	HEM	D	500	1	41,50,50	2.13	16 (39%)	45,82,82	1.89	8 (17%)

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
3	8MO	B	501	-	-	2/2/2/2	0/3/3/3
3	8MO	C	501	-	-	0/2/2/2	0/3/3/3
2	HEM	B	500	1	-	3/12/54/54	-
2	HEM	C	500	1	-	4/12/54/54	-
3	8MO	A	501	-	-	0/2/2/2	0/3/3/3
2	HEM	A	500	1	-	4/12/54/54	-
3	8MO	D	501	-	-	0/2/2/2	0/3/3/3
2	HEM	D	500	1	-	2/12/54/54	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3C-CAC	-5.35	1.36	1.47
2	D	500	HEM	C3C-CAC	-4.92	1.37	1.47
2	B	500	HEM	C3C-CAC	-4.85	1.37	1.47
2	B	500	HEM	C4D-ND	-4.56	1.32	1.40
2	C	500	HEM	C3C-CAC	-4.24	1.39	1.47
3	C	501	8MO	C6-C5	4.21	1.45	1.37
2	C	500	HEM	C1D-ND	-4.20	1.30	1.38
2	D	500	HEM	C1D-ND	-4.13	1.30	1.38
2	C	500	HEM	C4D-ND	-3.97	1.33	1.40
2	A	500	HEM	CMA-C3A	3.88	1.59	1.51
2	A	500	HEM	CBB-CAB	3.87	1.49	1.30
2	B	500	HEM	CBB-CAB	3.85	1.49	1.30
2	B	500	HEM	C1D-ND	-3.77	1.31	1.38
3	B	501	8MO	C6-C5	3.76	1.45	1.37
2	C	500	HEM	C1B-NB	-3.73	1.33	1.40
2	B	500	HEM	C1B-NB	-3.72	1.33	1.40
2	D	500	HEM	C1B-NB	-3.65	1.34	1.40
3	D	501	8MO	C6-C5	3.63	1.44	1.37
2	C	500	HEM	CBB-CAB	3.60	1.48	1.30
2	A	500	HEM	C1D-ND	-3.56	1.31	1.38
2	A	500	HEM	C4D-ND	-3.55	1.34	1.40
2	D	500	HEM	CBB-CAB	3.51	1.47	1.30
2	C	500	HEM	CMA-C3A	3.46	1.58	1.51
2	D	500	HEM	CMA-C3A	3.43	1.58	1.51
2	D	500	HEM	C4D-ND	-3.35	1.34	1.40
3	A	501	8MO	C6-C5	3.30	1.44	1.37
2	B	500	HEM	CMA-C3A	3.11	1.58	1.51
2	B	500	HEM	C1D-C2D	-3.09	1.38	1.44
2	C	500	HEM	C3B-C2B	3.02	1.43	1.37
2	D	500	HEM	C4B-NB	-2.94	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	8MO	O1-C12	2.94	1.41	1.36
2	A	500	HEM	C1B-NB	-2.93	1.35	1.40
2	C	500	HEM	CMC-C2C	2.92	1.58	1.51
3	D	501	8MO	O1-C12	2.89	1.41	1.36
2	A	500	HEM	CMD-C2D	2.89	1.56	1.50
2	A	500	HEM	C4D-C3D	-2.89	1.40	1.45
2	C	500	HEM	C4B-NB	-2.82	1.33	1.38
2	A	500	HEM	C4B-NB	-2.82	1.33	1.38
2	D	500	HEM	C3B-C2B	2.82	1.43	1.37
2	B	500	HEM	O2A-CGA	-2.74	1.21	1.30
2	A	500	HEM	C3B-C2B	2.68	1.42	1.37
2	C	500	HEM	C4D-C3D	-2.66	1.40	1.45
2	B	500	HEM	CMD-C2D	2.65	1.56	1.50
2	D	500	HEM	C4D-C3D	-2.62	1.40	1.45
2	C	500	HEM	C1D-C2D	-2.57	1.39	1.44
2	C	500	HEM	CHD-C1D	-2.56	1.33	1.41
2	A	500	HEM	O2A-CGA	-2.56	1.22	1.30
2	B	500	HEM	C4D-C3D	-2.49	1.40	1.45
2	D	500	HEM	CMD-C2D	2.48	1.56	1.50
2	D	500	HEM	CAA-C2A	2.43	1.55	1.52
2	B	500	HEM	C4B-NB	-2.42	1.33	1.38
3	B	501	8MO	O1-C12	2.36	1.40	1.36
2	B	500	HEM	C3B-C2B	2.34	1.42	1.37
2	C	500	HEM	O2A-CGA	-2.34	1.22	1.30
2	C	500	HEM	CAA-C2A	2.31	1.55	1.52
2	D	500	HEM	C4A-NA	-2.31	1.31	1.36
3	B	501	8MO	C1-C12	2.22	1.44	1.41
2	D	500	HEM	O2A-CGA	-2.20	1.23	1.30
2	C	500	HEM	CMD-C2D	2.19	1.55	1.50
2	A	500	HEM	CMC-C2C	2.19	1.56	1.51
2	D	500	HEM	CMC-C2C	2.16	1.56	1.51
2	C	500	HEM	C4A-NA	-2.12	1.31	1.36
2	B	500	HEM	CBD-CAD	2.10	1.58	1.52
2	A	500	HEM	CHD-C1D	-2.09	1.35	1.41
2	D	500	HEM	C2C-C1C	-2.07	1.37	1.42
2	B	500	HEM	CHD-C1D	-2.05	1.35	1.41
2	D	500	HEM	CHD-C1D	-2.01	1.35	1.41

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	HEM	C4B-CHC-C1C	6.80	131.54	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	HEM	C4C-CHD-C1D	6.50	131.14	122.56
2	C	500	HEM	C4B-CHC-C1C	6.44	131.05	122.56
2	B	500	HEM	C4C-CHD-C1D	6.21	130.76	122.56
2	B	500	HEM	C4B-CHC-C1C	5.91	130.35	122.56
2	A	500	HEM	C4B-CHC-C1C	5.90	130.35	122.56
2	A	500	HEM	C4C-CHD-C1D	5.51	129.84	122.56
2	D	500	HEM	C4C-CHD-C1D	5.12	129.31	122.56
3	C	501	8MO	C11-C12-C1	4.80	122.83	118.63
3	D	501	8MO	C11-C12-C1	4.03	122.15	118.63
3	A	501	8MO	C11-C12-C1	3.82	121.97	118.63
3	B	501	8MO	C11-C12-C1	3.73	121.89	118.63
2	D	500	HEM	C2C-C3C-C4C	-3.58	104.40	106.90
2	C	500	HEM	C2C-C3C-C4C	-3.50	104.46	106.90
2	A	500	HEM	O2A-CGA-CBA	2.96	123.55	114.03
2	C	500	HEM	C1B-NB-C4B	2.95	108.12	105.07
2	B	500	HEM	C4B-C3B-C2B	-2.86	104.85	107.11
2	D	500	HEM	C1B-NB-C4B	2.82	107.98	105.07
3	C	501	8MO	C9-C8-C1	-2.80	117.87	121.92
2	D	500	HEM	O2A-CGA-CBA	2.78	122.95	114.03
3	B	501	8MO	O1-C12-C11	2.76	119.31	116.03
3	C	501	8MO	O3-C11-C10	2.76	124.69	120.23
2	C	500	HEM	O2A-CGA-CBA	2.73	122.80	114.03
2	C	500	HEM	C4D-ND-C1D	2.71	107.88	105.07
3	B	501	8MO	C4-O3-C11	2.68	119.94	113.89
2	B	500	HEM	C2C-C3C-C4C	-2.68	105.03	106.90
2	B	500	HEM	O2A-CGA-CBA	2.63	122.48	114.03
2	D	500	HEM	C4B-C3B-C2B	-2.61	105.04	107.11
2	D	500	HEM	C4D-ND-C1D	2.60	107.76	105.07
2	A	500	HEM	C4B-C3B-C2B	-2.57	105.07	107.11
2	B	500	HEM	C4D-ND-C1D	2.57	107.72	105.07
2	C	500	HEM	C4B-C3B-C2B	-2.50	105.13	107.11
2	C	500	HEM	C3B-C2B-C1B	-2.49	104.64	106.49
3	A	501	8MO	C9-C8-C1	-2.47	118.34	121.92
3	D	501	8MO	C9-C8-C1	-2.42	118.42	121.92
2	D	500	HEM	C3B-C2B-C1B	-2.40	104.71	106.49
3	A	501	8MO	O1-C12-C11	2.38	118.85	116.03
2	A	500	HEM	C3B-C2B-C1B	-2.32	104.76	106.49
3	B	501	8MO	C9-C8-C1	-2.29	118.61	121.92
3	B	501	8MO	O1-C12-C1	-2.26	118.81	121.10
2	A	500	HEM	C2C-C3C-C4C	-2.25	105.33	106.90
2	B	500	HEM	C3B-C2B-C1B	-2.23	104.83	106.49
2	A	500	HEM	CMA-C3A-C4A	-2.15	125.15	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	8MO	C7-C6-C5	2.14	121.12	118.45
2	A	500	HEM	CMA-C3A-C2A	2.13	128.96	124.94
3	B	501	8MO	O3-C11-C12	2.12	123.65	120.23
3	A	501	8MO	C4-O3-C11	2.09	118.60	113.89
2	C	500	HEM	O2D-CGD-CBD	2.08	120.70	114.03
2	A	500	HEM	C4D-ND-C1D	2.01	107.15	105.07
3	D	501	8MO	O1-C12-C11	2.01	118.41	116.03

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	8MO	C10-C11-O3-C4
3	B	501	8MO	C12-C11-O3-C4
2	B	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAD-CBD-CGD-O2D
2	C	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAD-CBD-CGD-O2D
2	A	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAD-CBD-CGD-O1D
2	D	500	HEM	CAD-CBD-CGD-O2D

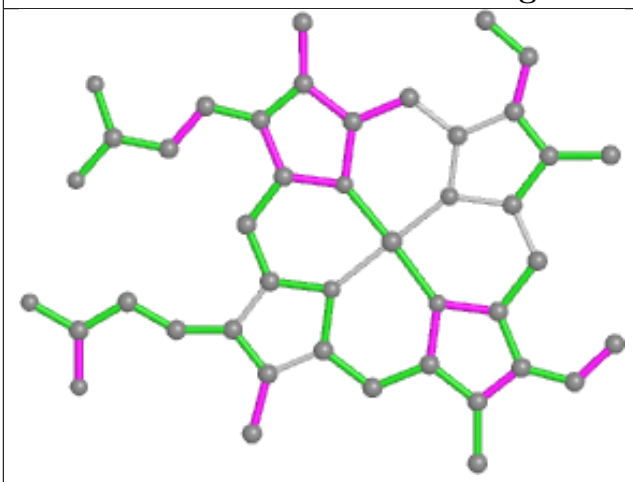
There are no ring outliers.

8 monomers are involved in 47 short contacts:

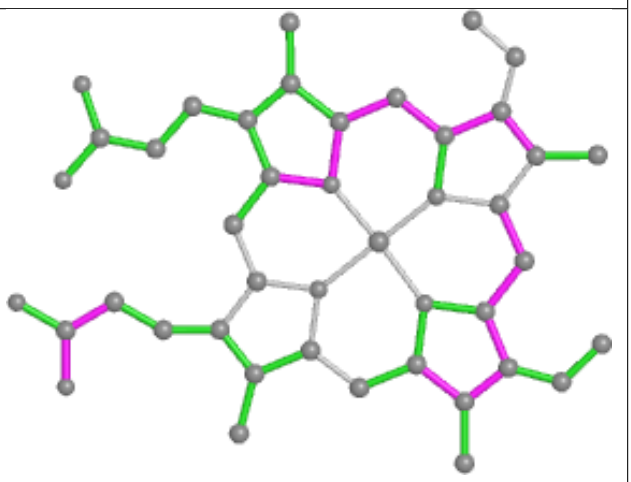
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	8MO	9	0
3	C	501	8MO	6	0
2	B	500	HEM	4	0
2	C	500	HEM	5	0
3	A	501	8MO	9	0
2	A	500	HEM	5	0
3	D	501	8MO	7	0
2	D	500	HEM	2	0

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.

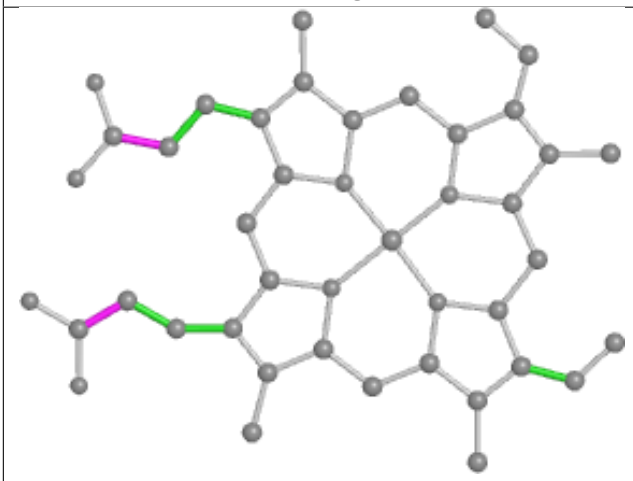
Ligand HEM B 500



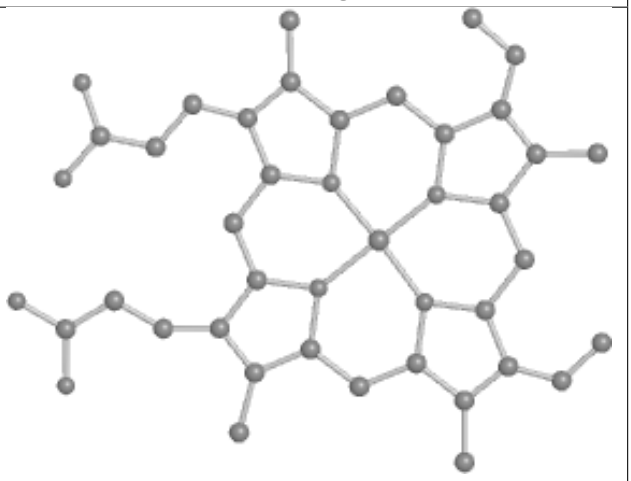
Bond lengths



Bond angles

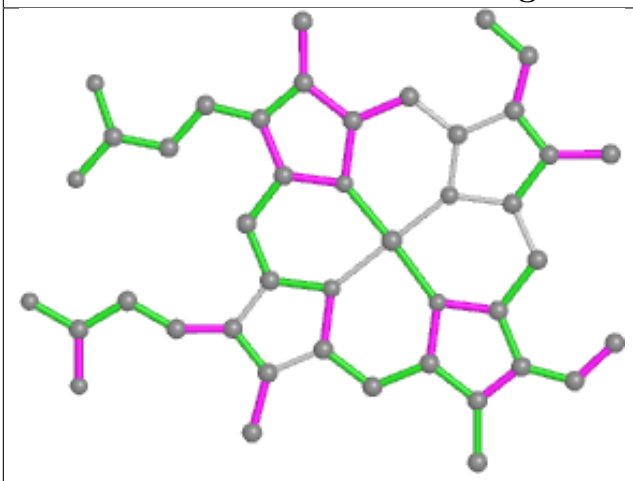


Torsions

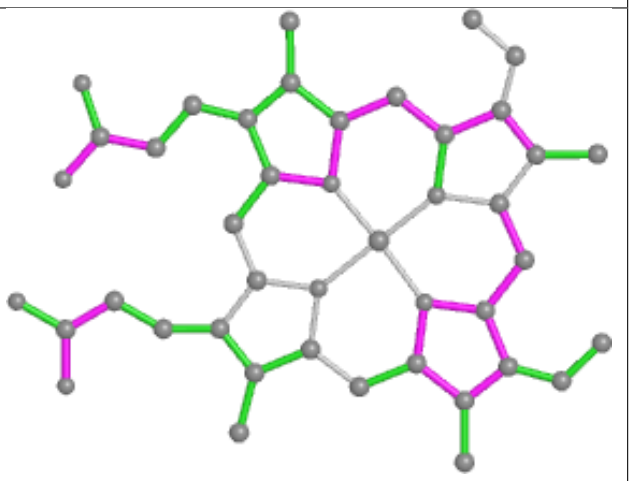


Rings

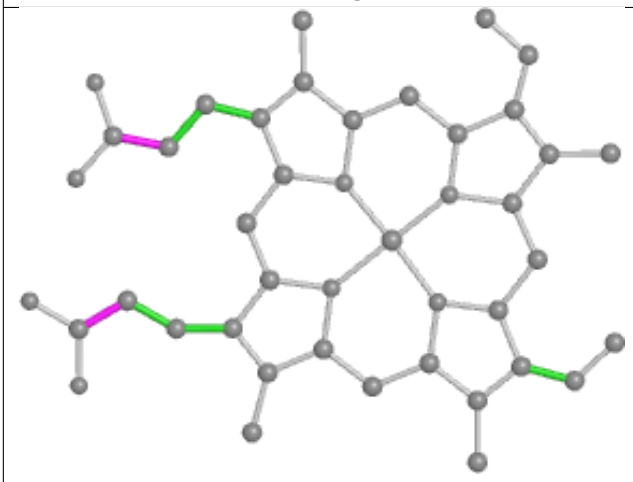
Ligand HEM C 500



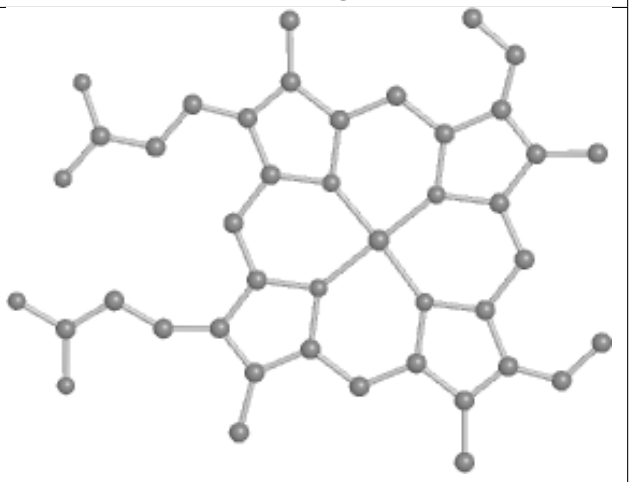
Bond lengths



Bond angles

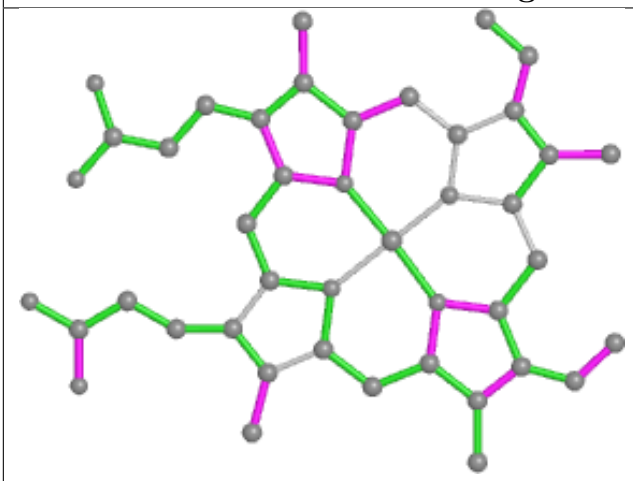


Torsions

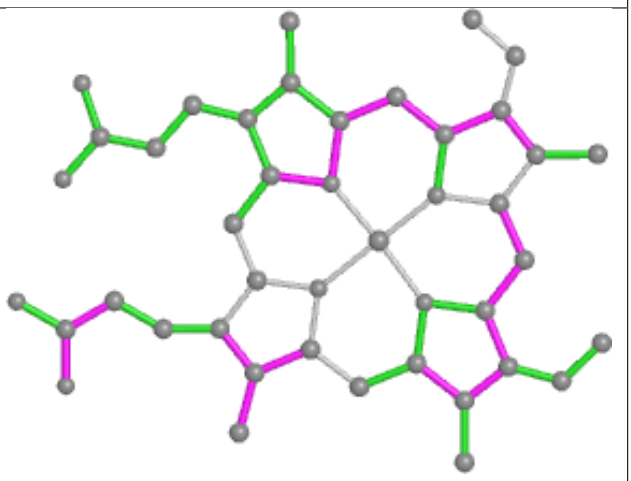


Rings

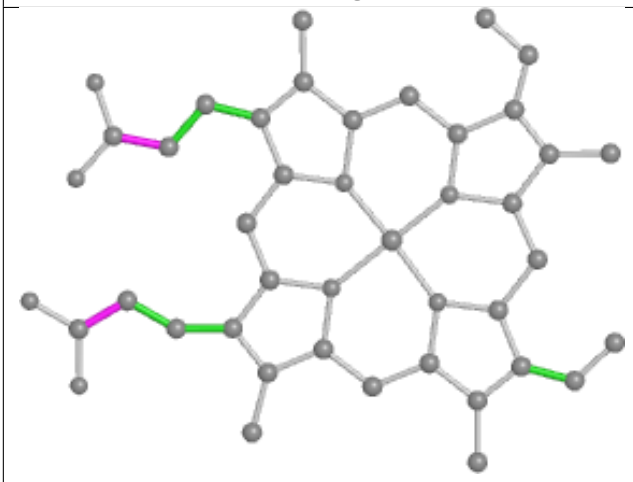
Ligand HEM A 500



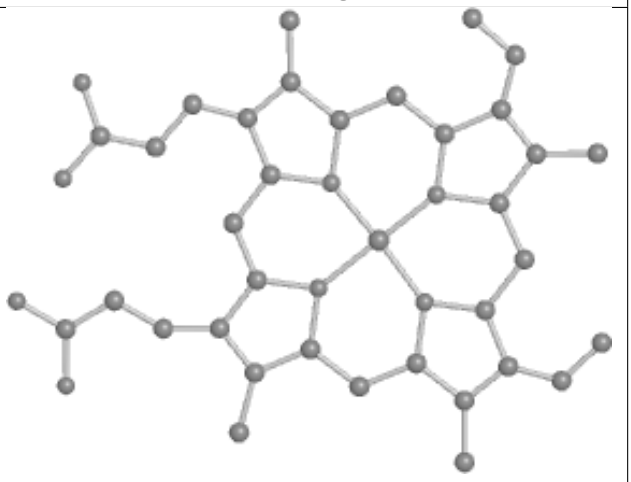
Bond lengths



Bond angles

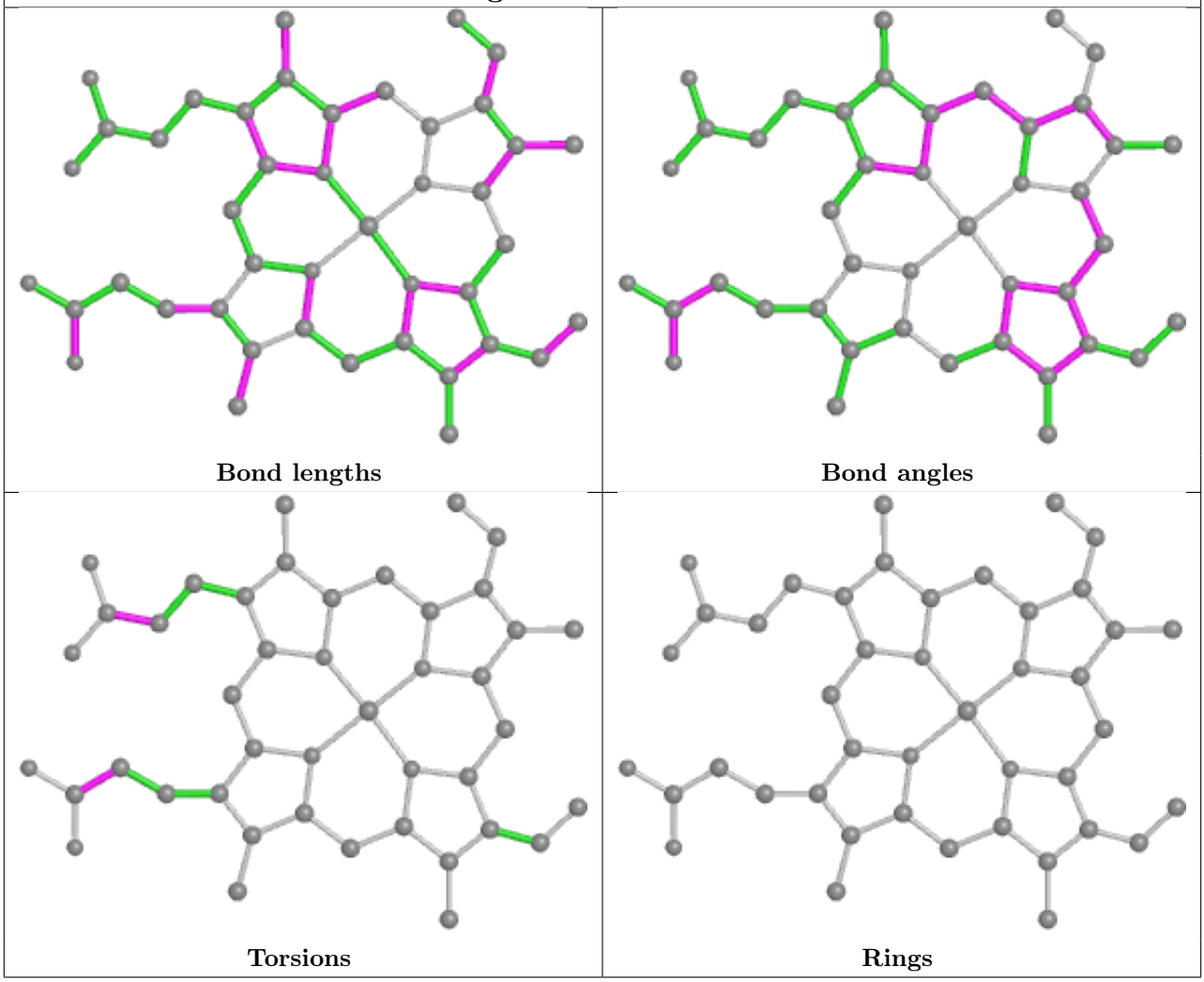


Torsions



Rings

Ligand HEM D 500



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	467/476 (98%)	0.28	18 (3%)	39	42	28, 47, 71, 97	1 (0%)
1	B	464/476 (97%)	0.48	25 (5%)	25	28	32, 54, 80, 90	0
1	C	464/476 (97%)	-0.01	8 (1%)	70	73	30, 51, 80, 93	0
1	D	464/476 (97%)	0.12	15 (3%)	47	52	31, 52, 81, 94	0
All	All	1859/1904 (97%)	0.22	66 (3%)	42	46	28, 51, 79, 97	1 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	HIS	7.7
1	A	370	LEU	6.3
1	C	31	GLY	6.0
1	A	495	HIS	5.1
1	D	31	GLY	4.9
1	B	382	ASP	4.1
1	D	143	ARG	4.1
1	A	30	LYS	3.9
1	A	31	GLY	3.9
1	B	495	HIS	3.8
1	B	337	LYS	3.4
1	B	257	ARG	3.4
1	C	282	PRO	3.3
1	A	208	ILE	3.3
1	C	338	ASN	3.2
1	A	209	PHE	3.1
1	D	421	GLY	3.1
1	B	417	LEU	3.1
1	D	325	ALA	2.8
1	B	140	VAL	2.7
1	D	331	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	278	GLU	2.7
1	A	207	GLY	2.7
1	C	276	GLN	2.7
1	C	280	LYS	2.7
1	D	327	VAL	2.7
1	C	339	ARG	2.7
1	A	483	ILE	2.7
1	B	216	THR	2.6
1	D	419	GLU	2.6
1	B	300	ILE	2.6
1	A	106	THR	2.6
1	A	468	PRO	2.5
1	A	206	LEU	2.5
1	C	335	ILE	2.5
1	B	414	GLN	2.4
1	D	138	PHE	2.4
1	B	211	PHE	2.4
1	D	423	PHE	2.4
1	B	210	GLN	2.4
1	B	69	PHE	2.3
1	B	385	LEU	2.3
1	B	250	LYS	2.3
1	B	276	GLN	2.3
1	D	280	LYS	2.3
1	B	256	GLN	2.3
1	B	259	LEU	2.3
1	C	286	PHE	2.3
1	B	106	THR	2.3
1	A	240	LEU	2.2
1	B	323	VAL	2.2
1	B	61	ILE	2.1
1	B	469	LYS	2.1
1	A	300	ILE	2.1
1	A	67	PRO	2.1
1	D	264	PRO	2.1
1	B	208	ILE	2.1
1	A	323	VAL	2.1
1	A	210	GLN	2.1
1	A	216	THR	2.0
1	B	59	MET	2.0
1	B	321	PRO	2.0
1	B	214	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	334	VAL	2.0
1	D	142	LYS	2.0
1	D	348	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 monosaccharides in this entry.

6.4 Ligands (i)

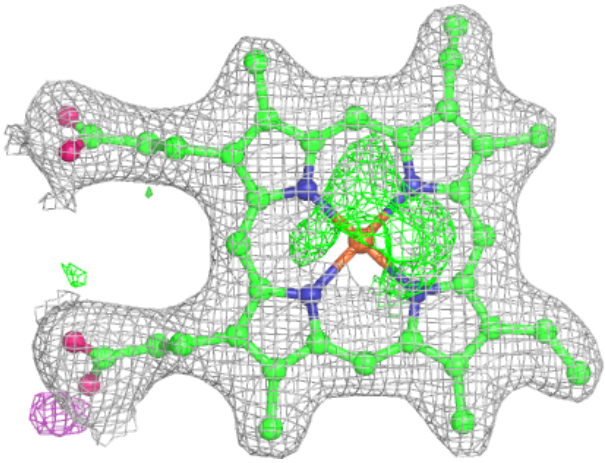
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

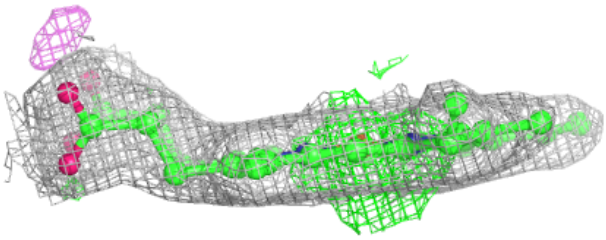
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	8MO	D	501	16/16	0.86	0.30	91,92,94,94	0
3	8MO	C	501	16/16	0.88	0.28	82,82,84,85	0
3	8MO	B	501	16/16	0.89	0.30	80,82,85,86	0
3	8MO	A	501	16/16	0.90	0.27	79,79,82,82	0
2	HEM	A	500	43/43	0.98	0.17	29,34,40,45	0
2	HEM	B	500	43/43	0.98	0.17	32,37,45,49	0
2	HEM	C	500	43/43	0.98	0.13	38,42,45,48	0
2	HEM	D	500	43/43	0.98	0.14	33,42,45,48	0

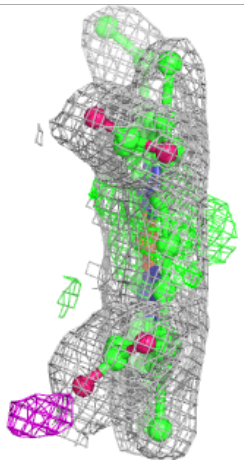
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM 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)

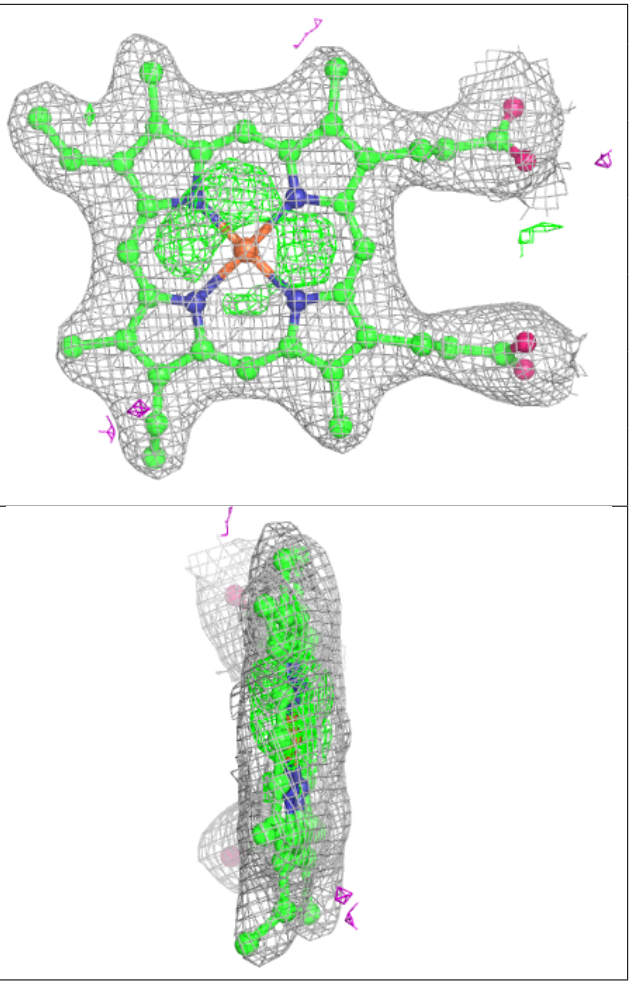






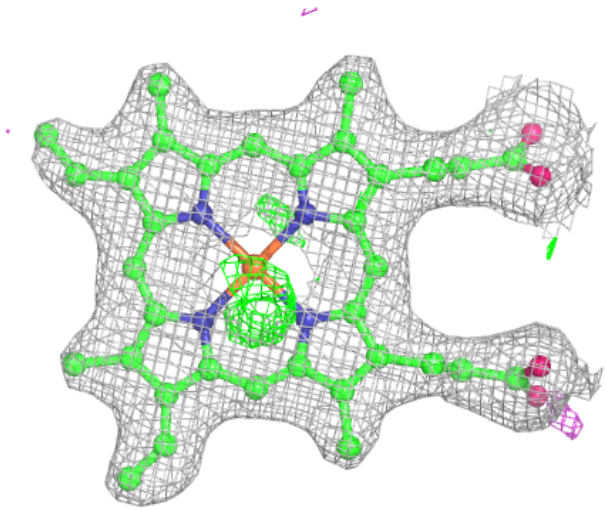
Electron density around HEM B 500:

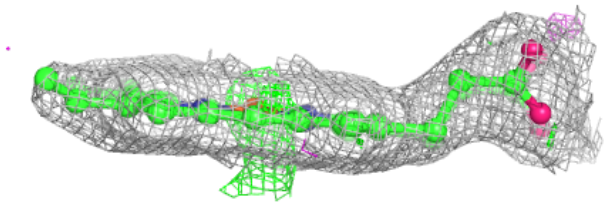
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

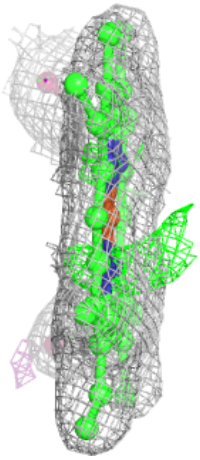


Electron density around HEM C 500:

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

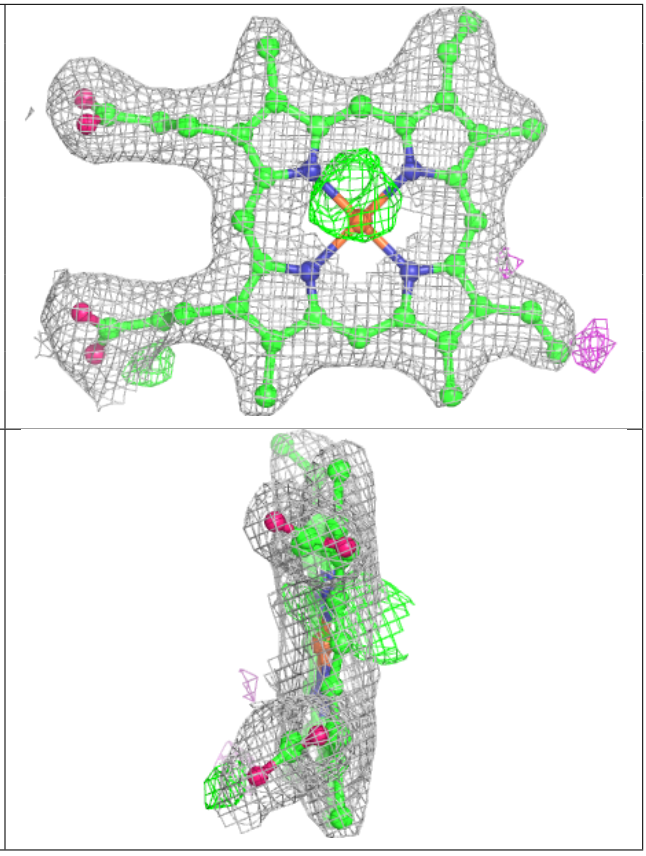






Electron density around HEM D 500:

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



6.5 Other polymers (i)

There are no such residues in this entry.