Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 12:15 PM EDT

PDB ID	:	1PQ2
Title	:	Crystal Structure of Human Drug Metabolizing Cytochrome P450 2C8
Authors	:	Schoch, G.A.; Yano, J.K.; Wester, M.R.; Griffin, K.J.; Stout, C.D.; Johnson, E.F.
Deposited on	:	2003-06-17
Resolution	:	2.70 Å(reported)

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

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

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

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

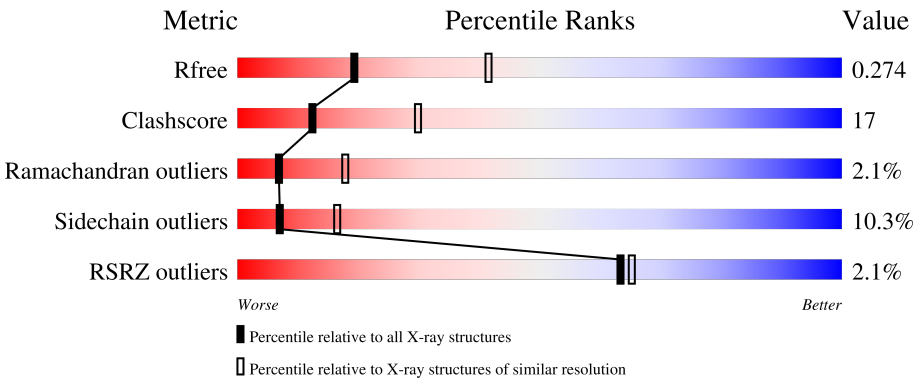
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	476	2% 61% 30% 6% • •
1	B	476	2% 63% 29% 5% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7550 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 2C8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	463	3693	2362	635	674	22	0	0	0
1	B	463	3693	2362	635	674	22	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	engineered mutation	UNP P10632
A	20	ALA	-	engineered mutation	UNP P10632
A	21	LYS	-	engineered mutation	UNP P10632
A	22	LYS	-	engineered mutation	UNP P10632
A	23	THR	-	engineered mutation	UNP P10632
A	24	SER	-	engineered mutation	UNP P10632
A	25	SER	-	engineered mutation	UNP P10632
A	26	LYS	-	engineered mutation	UNP P10632
A	27	GLY	-	engineered mutation	UNP P10632
A	491	HIS	-	expression tag	UNP P10632
A	492	HIS	-	expression tag	UNP P10632
A	493	HIS	-	expression tag	UNP P10632
A	494	HIS	-	expression tag	UNP P10632
B	19	MET	-	engineered mutation	UNP P10632
B	20	ALA	-	engineered mutation	UNP P10632
B	21	LYS	-	engineered mutation	UNP P10632
B	22	LYS	-	engineered mutation	UNP P10632
B	23	THR	-	engineered mutation	UNP P10632
B	24	SER	-	engineered mutation	UNP P10632
B	25	SER	-	engineered mutation	UNP P10632
B	26	LYS	-	engineered mutation	UNP P10632
B	27	GLY	-	engineered mutation	UNP P10632
B	491	HIS	-	expression tag	UNP P10632
B	492	HIS	-	expression tag	UNP P10632
B	493	HIS	-	expression tag	UNP P10632

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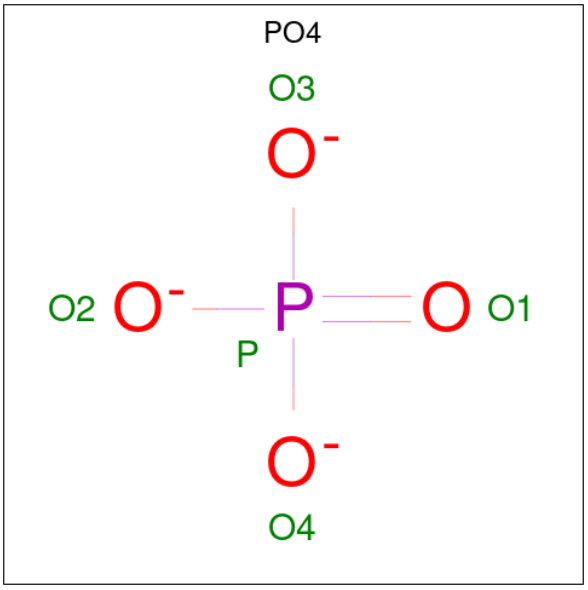
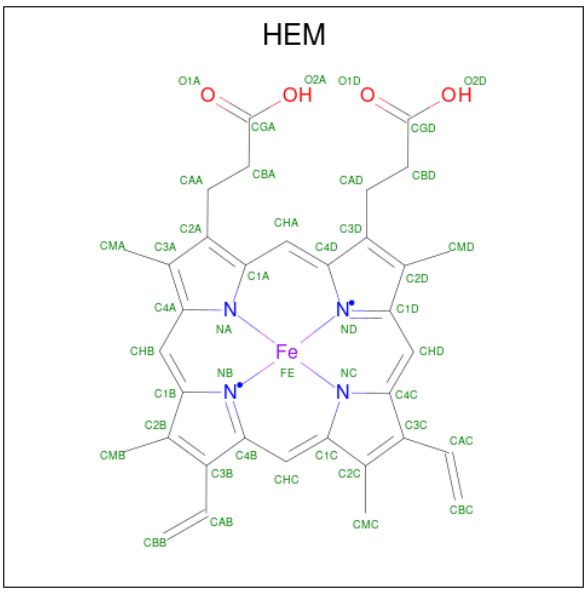
Chain	Residue	Modelled	Actual	Comment	Reference
B	494	HIS	-	expression tag	UNP P10632

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



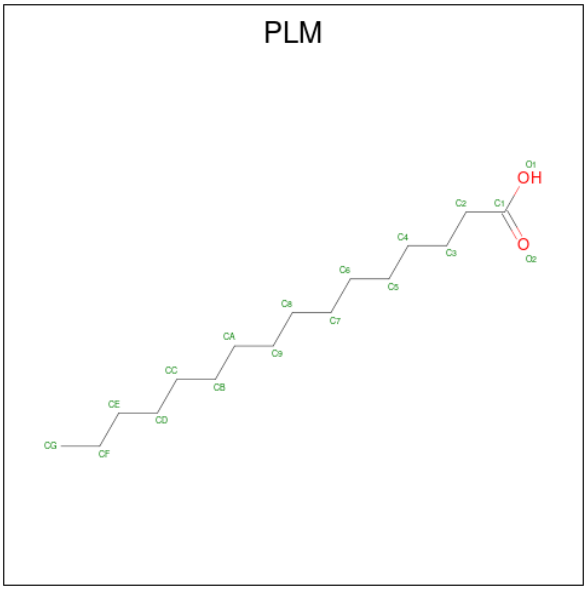
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

- Molecule 3 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		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	18	16	2	0	0
			Total	C	O		
4	B	1	18	16	2	0	0

- Molecule 5 is water.

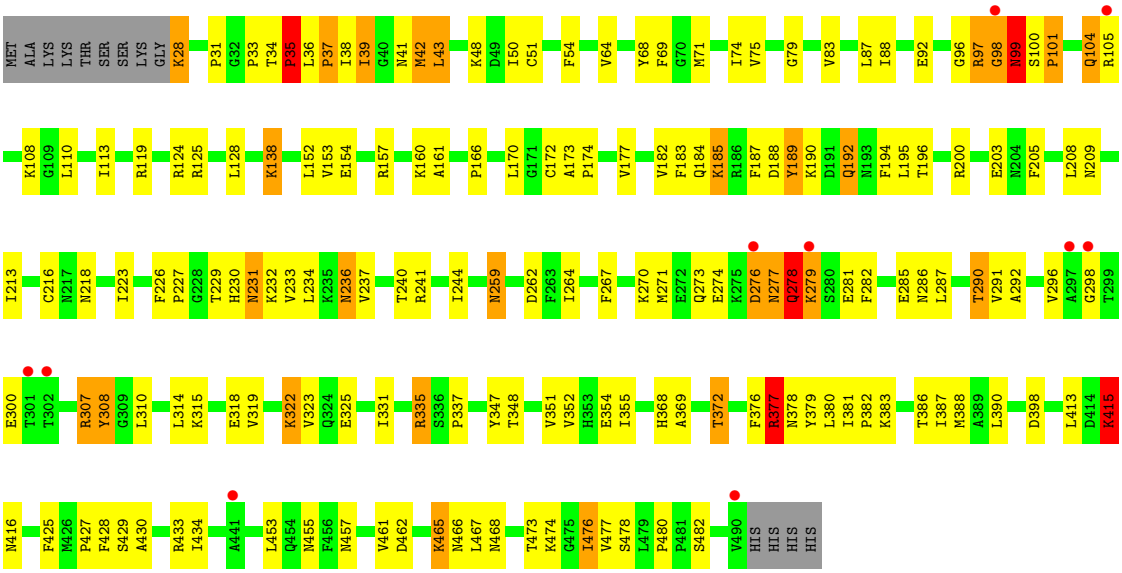
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	22	22	22	0	0
			Total	O		
5	B	15	15	15	0	0

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.

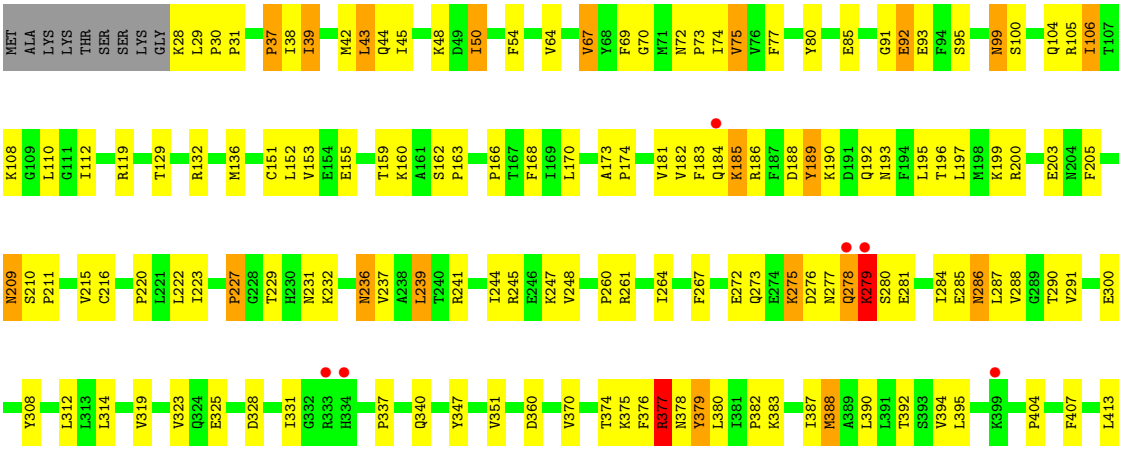
• Molecule 1: Cytochrome P450 2C8

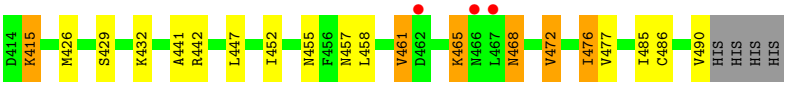
Chain A:



• Molecule 1: Cytochrome P450 2C8

Chain B:




D414
K415
M426
S429
K432
A441
R442
L447
I452
N455
F456
N457
L458
V461
D462
K465
N466
L467
N468
V472
I476
V477
I485
C486
V490
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.99Å 137.41Å 97.32Å 90.00° 112.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 32.20 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.70) 97.7 (32.20-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.288 0.232 , 0.274	Depositor DCC
R_{free} test set	1937 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7550	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: PO4, HEM, PLM

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	0.48	0/3778	0.79	9/5115 (0.2%)
1	B	0.44	0/3778	0.69	3/5115 (0.1%)
All	All	0.46	0/7556	0.74	12/10230 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	PRO	CA-N-CD	-14.62	91.03	111.50
1	A	101	PRO	CA-N-CD	-11.42	95.51	111.50
1	B	37	PRO	N-CA-C	7.59	131.83	112.10
1	B	37	PRO	CA-N-CD	-6.79	102.00	111.50
1	A	99	ASN	CA-C-N	-6.57	102.75	117.20
1	B	70	GLY	N-CA-C	-6.38	97.14	113.10
1	A	34	THR	C-N-CD	-5.65	108.18	120.60
1	A	278	GLN	CA-C-N	-5.48	105.14	117.20
1	A	37	PRO	N-CA-C	5.45	126.28	112.10
1	A	276	ASP	C-N-CA	5.38	135.15	121.70
1	A	277	ASN	N-CA-C	5.31	125.35	111.00
1	A	98	GLY	C-N-CA	-5.26	108.56	121.70

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	3693	0	3715	126	0
1	B	3693	0	3715	129	0
2	A	5	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	2	0
4	A	18	0	31	3	0
4	B	18	0	31	6	0
5	A	22	0	0	0	0
5	B	15	0	0	0	0
All	All	7550	0	7552	254	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 17.

All (254) 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:B:85:GLU:HG2	1:B:376:PHE:CE1	1.93	1.03
1:A:35:PRO:HD3	1:A:41:ASN:HD21	1.22	1.00
1:B:278:GLN:HG2	1:B:279:LYS:H	1.34	0.93
1:A:105:ARG:HD2	4:B:501:PLM:HG3	1.51	0.92
1:A:209:ASN:HD22	1:A:476:ILE:HD13	1.35	0.90
1:A:35:PRO:HD3	1:A:41:ASN:ND2	1.89	0.88
1:B:209:ASN:HD22	1:B:476:ILE:HD13	1.41	0.85
1:B:43:LEU:HD12	1:B:43:LEU:H	1.41	0.85
1:B:415:LYS:HD3	1:B:415:LYS:H	1.40	0.85
1:A:307:ARG:HH21	1:A:307:ARG:HG3	1.43	0.81
1:A:98:GLY:O	1:A:99:ASN:ND2	2.13	0.81
1:B:468:ASN:H	1:B:468:ASN:HD22	1.25	0.81
1:B:151:CYS:SG	1:B:186:ARG:NH1	2.54	0.80
1:A:33:PRO:O	1:A:35:PRO:HD2	1.81	0.80
1:A:229:THR:HG21	4:B:501:PLM:H61	1.64	0.80
1:A:43:LEU:H	1:A:43:LEU:HD12	1.48	0.79
1:B:377:ARG:O	1:B:378:ASN:HB2	1.83	0.78
1:B:110:LEU:HD23	1:B:119:ARG:HH22	1.47	0.78
1:A:28:LYS:NZ	1:A:28:LYS:HA	2.01	0.76
1:B:119:ARG:HA	1:B:281:GLU:HG3	1.67	0.76
1:B:184:GLN:O	1:B:184:GLN:HG2	1.86	0.75
1:B:39:ILE:HG13	1:B:43:LEU:HD11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASN:O	1:B:290:THR:HG22	1.88	0.74
1:A:97:ARG:CD	1:A:113:ILE:O	2.37	0.73
1:B:85:GLU:HG2	1:B:376:PHE:HE1	1.50	0.73
1:A:209:ASN:HD21	1:A:477:VAL:H	1.38	0.72
1:B:110:LEU:HD23	1:B:119:ARG:NH2	2.04	0.72
1:B:465:LYS:HE3	1:B:465:LYS:HA	1.71	0.71
1:A:173:ALA:HB3	1:A:174:PRO:HD3	1.72	0.70
1:B:173:ALA:HB3	1:B:174:PRO:HD3	1.75	0.68
1:A:96:GLY:HA3	1:A:369:ALA:O	1.94	0.67
1:B:278:GLN:HG2	1:B:279:LYS:N	2.07	0.67
1:A:183:PHE:O	1:A:184:GLN:HG3	1.94	0.67
1:A:259:ASN:H	1:A:259:ASN:HD22	1.41	0.67
1:A:97:ARG:HD3	1:A:113:ILE:O	1.95	0.66
1:B:182:VAL:HG11	1:B:291:VAL:HG13	1.77	0.66
1:A:192:GLN:HE21	1:A:192:GLN:HA	1.61	0.66
1:A:35:PRO:HG2	1:A:68:TYR:CD1	2.32	0.65
1:A:192:GLN:HA	1:A:192:GLN:NE2	2.12	0.64
1:B:267:PHE:CE2	1:B:287:LEU:HB2	2.33	0.64
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.63	0.64
1:A:153:VAL:HG11	1:A:455:ASN:HD22	1.63	0.63
1:B:50:ILE:HD13	1:B:50:ILE:O	1.99	0.63
1:A:209:ASN:ND2	1:A:476:ILE:HD13	2.11	0.63
1:A:425:PHE:CZ	1:A:427:PRO:HG3	2.33	0.63
1:B:77:PHE:HE2	1:B:387:ILE:HD12	1.63	0.62
1:B:168:PHE:HZ	1:B:195:LEU:HD12	1.64	0.62
1:A:185:LYS:HD2	1:A:185:LYS:O	1.99	0.62
1:B:272:GLU:O	1:B:275:LYS:HG3	1.99	0.62
1:A:170:LEU:HD21	1:A:310:LEU:HD12	1.81	0.62
1:A:69:PHE:CD2	1:A:74:ILE:HD12	2.34	0.61
1:B:39:ILE:HD13	1:B:39:ILE:H	1.64	0.61
1:A:259:ASN:HD22	1:A:259:ASN:N	1.98	0.60
1:B:185:LYS:HD2	1:B:185:LYS:O	2.01	0.60
1:A:331:ILE:HG23	1:A:335:ARG:HE	1.66	0.60
1:B:267:PHE:CG	1:B:287:LEU:HD13	2.36	0.60
1:B:241:ARG:O	1:B:245:ARG:HG2	2.01	0.60
1:B:93:GLU:O	1:B:370:VAL:HA	2.01	0.60
1:A:205:PHE:CD1	1:A:300:GLU:HG2	2.37	0.59
1:B:209:ASN:HD22	1:B:476:ILE:CD1	2.13	0.59
1:B:39:ILE:O	1:B:42:MET:HB2	2.02	0.59
1:B:28:LYS:HA	1:B:28:LYS:NZ	2.17	0.59
1:B:29:LEU:HD21	1:B:382:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:PHE:CD1	1:B:300:GLU:HG2	2.38	0.58
1:A:64:VAL:HG21	1:A:376:PHE:CE2	2.39	0.58
1:B:216:CYS:HB3	1:B:223:ILE:HD13	1.86	0.58
1:A:39:ILE:HD13	1:A:39:ILE:H	1.69	0.57
1:A:119:ARG:HA	1:A:281:GLU:HG3	1.85	0.57
1:B:38:ILE:HG22	1:B:39:ILE:HG23	1.86	0.57
1:B:277:ASN:O	1:B:279:LYS:N	2.37	0.56
4:A:502:PLM:HG3	1:B:105:ARG:HD2	1.85	0.56
1:A:43:LEU:HD12	1:A:43:LEU:N	2.18	0.56
1:A:237:VAL:O	1:A:241:ARG:HG3	2.05	0.56
1:B:209:ASN:ND2	1:B:476:ILE:HD13	2.15	0.56
1:A:331:ILE:HD13	1:A:337:PRO:HB3	1.87	0.56
1:A:119:ARG:HD2	1:A:286:ASN:HD21	1.70	0.56
1:A:473:THR:HG23	1:A:478:SER:HB3	1.87	0.56
1:A:192:GLN:HE21	1:A:192:GLN:CA	2.18	0.56
1:B:248:VAL:HG22	1:B:264:ILE:HD12	1.87	0.56
1:A:192:GLN:O	1:A:196:THR:HG23	2.06	0.55
1:A:28:LYS:HA	1:A:28:LYS:HZ1	1.71	0.55
1:B:106:ILE:HG23	1:B:237:VAL:HG21	1.88	0.55
1:A:33:PRO:O	1:A:35:PRO:CD	2.54	0.55
1:A:182:VAL:HG11	1:A:291:VAL:HG13	1.88	0.55
1:A:75:VAL:CG1	1:A:387:ILE:HD13	2.36	0.55
1:A:415:LYS:H	1:A:415:LYS:HD3	1.71	0.55
1:A:287:LEU:O	1:A:290:THR:HG22	2.07	0.55
1:A:64:VAL:HG21	1:A:376:PHE:HE2	1.71	0.54
1:A:348:THR:O	1:A:352:VAL:HG23	2.07	0.54
1:A:229:THR:HG21	4:B:501:PLM:H81	1.88	0.54
1:B:360:ASP:OD2	1:B:392:THR:HG23	2.07	0.54
1:B:376:PHE:CD2	1:B:377:ARG:HG2	2.41	0.54
1:B:54:PHE:HB3	1:B:390:LEU:HD11	1.90	0.54
1:A:229:THR:CG2	4:B:501:PLM:H81	2.38	0.54
1:A:307:ARG:HE	1:A:480:PRO:HG2	1.73	0.54
1:B:277:ASN:O	1:B:278:GLN:HG2	2.07	0.54
1:A:189:TYR:O	1:A:195:LEU:HD21	2.08	0.54
1:A:229:THR:O	1:A:233:VAL:HG23	2.09	0.53
1:A:97:ARG:HB3	1:A:433:ARG:NH1	2.24	0.53
1:A:152:LEU:HD13	1:A:173:ALA:HB2	1.90	0.53
1:A:351:VAL:O	1:A:355:ILE:HG13	2.08	0.53
1:A:415:LYS:H	1:A:415:LYS:CD	2.21	0.53
1:B:216:CYS:HB3	1:B:223:ILE:CD1	2.38	0.53
1:A:307:ARG:HG3	1:A:307:ARG:NH2	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:HIS:HB2	1:A:387:ILE:HB	1.92	0.52
1:A:216:CYS:HB3	1:A:223:ILE:HD13	1.90	0.52
1:A:200:ARG:HG3	1:A:236:ASN:ND2	2.25	0.52
1:B:244:ILE:HB	1:B:288:VAL:HG13	1.92	0.52
1:A:184:GLN:HB3	1:A:262:ASP:HB3	1.92	0.52
1:A:33:PRO:HB2	1:A:41:ASN:ND2	2.25	0.52
1:B:284:ILE:O	1:B:288:VAL:HG23	2.09	0.52
1:B:200:ARG:NH1	1:B:239:LEU:HD12	2.25	0.52
1:B:319:VAL:HG13	1:B:347:TYR:OH	2.10	0.52
1:A:88:ILE:HD11	1:A:430:ALA:HB1	1.92	0.52
1:B:472:VAL:HG22	1:B:472:VAL:O	2.10	0.52
1:A:234:LEU:HG	4:B:501:PLM:HG2	1.93	0.51
1:B:182:VAL:HG11	1:B:291:VAL:CG1	2.39	0.51
1:A:298:GLY:HA2	3:A:500:HEM:C2C	2.45	0.51
1:A:461:VAL:HG12	1:A:461:VAL:O	2.10	0.51
1:A:227:PRO:O	1:A:231:ASN:HB2	2.11	0.51
1:A:216:CYS:HB3	1:A:223:ILE:CD1	2.41	0.50
1:B:184:GLN:O	1:B:184:GLN:CG	2.58	0.50
4:A:502:PLM:HA2	1:B:223:ILE:HD12	1.94	0.50
1:B:119:ARG:HD3	1:B:286:ASN:HD21	1.76	0.50
1:B:153:VAL:HG11	1:B:455:ASN:ND2	2.25	0.49
1:B:387:ILE:HG22	1:B:388:MET:N	2.27	0.49
1:B:370:VAL:HG23	1:B:383:LYS:HA	1.94	0.49
1:B:458:LEU:HD22	1:B:485:ILE:HD11	1.94	0.49
1:B:183:PHE:CE1	1:B:247:LYS:HG2	2.47	0.49
1:B:331:ILE:HD13	1:B:337:PRO:HB3	1.95	0.49
1:B:278:GLN:O	1:B:280:SER:N	2.46	0.49
1:A:292:ALA:O	1:A:296:VAL:HG23	2.13	0.48
1:B:319:VAL:O	1:B:323:VAL:HG23	2.12	0.48
1:A:476:ILE:HG12	1:A:477:VAL:HG23	1.95	0.48
1:B:129:THR:HA	1:B:132:ARG:HD3	1.96	0.48
1:B:188:ASP:C	1:B:190:LYS:H	2.16	0.48
1:A:271:MET:HG2	1:A:282:PHE:O	2.12	0.48
1:A:183:PHE:HB3	1:A:185:LYS:HE3	1.95	0.48
1:A:315:LYS:HB2	1:A:467:LEU:HD23	1.95	0.48
1:B:395:LEU:HD21	1:B:426:MET:H	1.78	0.48
1:B:43:LEU:HD12	1:B:43:LEU:N	2.20	0.48
1:B:168:PHE:HZ	1:B:195:LEU:CD1	2.26	0.48
1:A:428:PHE:O	1:A:429:SER:HB3	2.14	0.48
1:B:99:ASN:C	1:B:99:ASN:HD22	2.17	0.47
1:A:174:PRO:O	1:A:177:VAL:HB	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:N	1:A:36:LEU:HD12	2.29	0.47
1:B:184:GLN:OE1	1:B:261:ARG:HB3	2.15	0.47
1:B:415:LYS:H	1:B:415:LYS:CD	2.11	0.47
1:B:159:THR:O	1:B:162:SER:HB3	2.14	0.47
1:A:354:GLU:O	1:A:354:GLU:HG3	2.15	0.46
1:B:199:LYS:O	1:B:203:GLU:HG3	2.15	0.46
1:B:136:MET:O	1:B:260:PRO:HB2	2.16	0.46
1:A:153:VAL:HG11	1:A:455:ASN:ND2	2.29	0.46
1:B:468:ASN:H	1:B:468:ASN:ND2	2.02	0.46
1:A:188:ASP:O	1:A:190:LYS:N	2.49	0.46
1:B:476:ILE:HG12	1:B:477:VAL:HG23	1.98	0.46
1:A:240:THR:O	1:A:244:ILE:HG13	2.16	0.46
1:A:31:PRO:HD3	1:A:379:TYR:CE2	2.51	0.46
1:A:97:ARG:HD2	1:A:113:ILE:O	2.13	0.46
1:A:28:LYS:HA	1:A:28:LYS:HZ2	1.77	0.46
1:B:92:GLU:HG2	1:B:432:LYS:HE2	1.98	0.46
1:B:429:SER:CB	3:B:500:HEM:HBA1	2.47	0.45
1:B:75:VAL:HG22	1:B:77:PHE:CE2	2.52	0.45
1:B:220:PRO:O	1:B:223:ILE:HG12	2.17	0.45
1:A:377:ARG:O	1:A:378:ASN:HB2	2.16	0.45
1:A:322:LYS:HE3	1:A:322:LYS:HB2	1.77	0.45
1:A:226:PHE:N	1:A:227:PRO:HD3	2.32	0.45
1:A:267:PHE:CG	1:A:287:LEU:HD13	2.50	0.45
1:A:278:GLN:OE1	1:A:278:GLN:O	2.35	0.45
1:B:108:LYS:HG3	1:B:241:ARG:HH22	1.82	0.45
1:A:205:PHE:CG	1:A:300:GLU:HG2	2.53	0.44
1:A:54:PHE:HD2	1:A:390:LEU:HD11	1.83	0.44
1:B:195:LEU:HD22	1:B:195:LEU:H	1.82	0.44
1:B:192:GLN:O	1:B:196:THR:HG22	2.17	0.44
1:A:74:ILE:HG12	1:A:386:THR:CG2	2.46	0.44
1:B:91:GLY:O	1:B:95:SER:HB3	2.17	0.44
1:A:318:GLU:HG2	1:A:319:VAL:N	2.32	0.44
1:A:465:LYS:HE3	1:A:465:LYS:HA	2.00	0.44
1:B:45:ILE:HD11	1:B:67:VAL:HG21	2.00	0.44
1:A:187:PHE:HB3	1:A:194:PHE:HB2	2.00	0.44
4:A:502:PLM:H61	1:B:229:THR:HG21	2.00	0.44
1:A:79:GLY:O	1:A:83:VAL:HG23	2.17	0.44
1:B:347:TYR:O	1:B:351:VAL:HG23	2.17	0.44
1:A:308:TYR:CD1	1:A:480:PRO:HB3	2.52	0.44
1:B:387:ILE:CG2	1:B:388:MET:N	2.79	0.44
1:A:166:PRO:O	1:A:170:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ASN:HD21	1:B:477:VAL:H	1.65	0.44
1:A:138:LYS:N	1:A:138:LYS:HD2	2.33	0.43
1:A:203:GLU:OE2	1:A:232:LYS:HE2	2.18	0.43
1:A:157:ARG:HG3	1:A:157:ARG:NH1	2.33	0.43
1:B:69:PHE:CD2	1:B:74:ILE:HD12	2.53	0.43
1:B:159:THR:O	1:B:160:LYS:HB2	2.18	0.43
1:B:196:THR:HG23	1:B:197:LEU:N	2.33	0.43
1:B:490:VAL:HG12	1:B:490:VAL:O	2.19	0.43
1:A:208:LEU:HA	1:A:213:ILE:HG21	2.01	0.43
1:B:181:VAL:O	1:B:181:VAL:CG1	2.66	0.43
1:A:183:PHE:O	1:A:185:LYS:HG3	2.18	0.43
1:B:236:ASN:HD22	1:B:236:ASN:N	2.17	0.43
1:B:186:ARG:NH2	1:B:188:ASP:HA	2.34	0.43
1:B:28:LYS:O	1:B:379:TYR:HB3	2.19	0.43
1:B:287:LEU:O	1:B:291:VAL:HG23	2.19	0.43
1:B:110:LEU:CD1	1:B:285:GLU:HG3	2.48	0.42
1:B:54:PHE:HE1	1:B:67:VAL:HG11	1.85	0.42
1:B:312:LEU:HD13	1:B:407:PHE:CE1	2.54	0.42
1:A:172:CYS:HB3	1:A:189:TYR:CE2	2.54	0.42
1:B:163:PRO:HB3	1:B:486:CYS:SG	2.59	0.42
1:A:259:ASN:N	1:A:259:ASN:ND2	2.67	0.42
1:B:166:PRO:O	1:B:170:LEU:HB2	2.18	0.42
1:B:28:LYS:HA	1:B:28:LYS:HZ2	1.84	0.42
1:B:72:ASN:HA	1:B:73:PRO:HD2	1.93	0.42
1:B:375:LYS:HZ3	1:B:380:LEU:HD12	1.83	0.42
1:B:152:LEU:HD21	1:B:452:ILE:HD11	2.02	0.42
1:B:387:ILE:HD13	1:B:387:ILE:HA	1.88	0.42
1:A:71:MET:HE2	1:A:71:MET:HB2	1.84	0.42
1:A:372:THR:HA	1:A:383:LYS:HB2	2.00	0.42
1:B:110:LEU:HD13	1:B:285:GLU:HG3	2.02	0.41
1:B:31:PRO:HD3	1:B:379:TYR:CE2	2.55	0.41
1:B:69:PHE:CE2	1:B:74:ILE:HD12	2.55	0.41
1:B:441:ALA:HB1	3:B:500:HEM:HAB	2.02	0.41
1:B:468:ASN:HD22	1:B:468:ASN:N	2.02	0.41
1:A:474:LYS:HE2	1:B:227:PRO:HG2	2.01	0.41
1:B:155:GLU:HG3	1:B:189:TYR:CD1	2.54	0.41
1:B:457:ASN:OD1	1:B:490:VAL:HG21	2.20	0.41
1:A:347:TYR:O	1:A:351:VAL:HG23	2.20	0.41
1:A:110:LEU:HD11	1:A:285:GLU:HG3	2.02	0.41
1:A:154:GLU:O	1:A:157:ARG:HB2	2.20	0.41
1:B:415:LYS:HD3	1:B:415:LYS:N	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:CB	1:A:433:ARG:CZ	2.99	0.41
1:A:87:LEU:HD23	1:A:430:ALA:O	2.21	0.41
1:A:230:HIS:HD2	4:B:501:PLM:HC1	1.86	0.41
1:B:205:PHE:CE1	1:B:300:GLU:HG2	2.56	0.41
1:A:264:ILE:HD11	1:A:291:VAL:HG21	2.01	0.41
1:A:270:LYS:O	1:A:274:GLU:HG2	2.20	0.41
1:A:381:ILE:HA	1:A:382:PRO:HD2	1.89	0.41
1:A:415:LYS:C	1:A:416:ASN:HD22	2.24	0.41
1:A:429:SER:O	1:A:434:ILE:HG13	2.21	0.41
1:B:182:VAL:O	1:B:264:ILE:HG12	2.20	0.41
1:B:376:PHE:O	1:B:377:ARG:C	2.59	0.41
1:B:447:LEU:HA	1:B:447:LEU:HD23	1.88	0.41
1:A:97:ARG:NH2	3:A:500:HEM:O2A	2.51	0.41
1:A:236:ASN:HD22	1:A:236:ASN:HA	1.56	0.41
1:B:30:PRO:HA	1:B:31:PRO:HD3	1.91	0.41
1:B:64:VAL:HG21	1:B:376:PHE:HE2	1.86	0.41
1:B:210:SER:HA	1:B:211:PRO:HD3	1.82	0.41
1:A:124:ARG:HE	1:A:128:LEU:HD11	1.86	0.40
1:A:160:LYS:O	1:A:161:ALA:HB3	2.21	0.40
1:B:28:LYS:HA	1:B:28:LYS:HZ3	1.85	0.40
1:B:80:TYR:HA	1:B:394:VAL:HG22	2.04	0.40
1:A:69:PHE:HB3	1:A:218:ASN:CG	2.42	0.40
1:A:104:GLN:O	1:A:108:LYS:HA	2.22	0.40
1:B:99:ASN:HD22	1:B:100:SER:N	2.19	0.40
1:B:375:LYS:NZ	1:B:380:LEU:CD1	2.84	0.40
1:A:323:VAL:HG11	1:A:453:LEU:HD12	2.02	0.40
1:B:232:LYS:HD2	1:B:232:LYS:HA	1.85	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	461/476 (97%)	429 (93%)	23 (5%)	9 (2%)	7 19
1	B	461/476 (97%)	408 (88%)	43 (9%)	10 (2%)	6 17
All	All	922/952 (97%)	837 (91%)	66 (7%)	19 (2%)	7 18

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	A	278	GLN
1	B	275	LYS
1	A	42	MET
1	A	189	TYR
1	A	279	LYS
1	A	377	ARG
1	B	48	LYS
1	B	278	GLN
1	B	279	LYS
1	B	377	ARG
1	A	415	LYS
1	A	48	LYS
1	A	462	ASP
1	B	189	TYR
1	B	404	PRO
1	B	461	VAL
1	B	227	PRO
1	B	106	ILE

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	419/430 (97%)	373 (89%)	46 (11%)	6 14
1	B	419/430 (97%)	379 (90%)	40 (10%)	8 20
All	All	838/860 (97%)	752 (90%)	86 (10%)	7 16

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	35	PRO
1	A	37	PRO
1	A	38	ILE
1	A	39	ILE
1	A	42	MET
1	A	43	LEU
1	A	50	ILE
1	A	51	CYS
1	A	92	GLU
1	A	97	ARG
1	A	99	ASN
1	A	100	SER
1	A	101	PRO
1	A	104	GLN
1	A	125	ARG
1	A	138	LYS
1	A	185	LYS
1	A	192	GLN
1	A	231	ASN
1	A	236	ASN
1	A	259	ASN
1	A	273	GLN
1	A	276	ASP
1	A	278	GLN
1	A	279	LYS
1	A	290	THR
1	A	307	ARG
1	A	308	TYR
1	A	314	LEU
1	A	322	LYS
1	A	325	GLU
1	A	335	ARG
1	A	372	THR
1	A	377	ARG
1	A	380	LEU
1	A	388	MET
1	A	398	ASP
1	A	413	LEU
1	A	415	LYS
1	A	457	ASN
1	A	465	LYS

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Mol	Chain	Res	Type
1	A	466	ASN
1	A	468	ASN
1	A	476	ILE
1	A	482	SER
1	B	37	PRO
1	B	39	ILE
1	B	43	LEU
1	B	44	GLN
1	B	50	ILE
1	B	67	VAL
1	B	75	VAL
1	B	92	GLU
1	B	99	ASN
1	B	104	GLN
1	B	112	ILE
1	B	185	LYS
1	B	193	ASN
1	B	209	ASN
1	B	215	VAL
1	B	222	LEU
1	B	231	ASN
1	B	236	ASN
1	B	239	LEU
1	B	273	GLN
1	B	276	ASP
1	B	279	LYS
1	B	286	ASN
1	B	308	TYR
1	B	314	LEU
1	B	325	GLU
1	B	328	ASP
1	B	340	GLN
1	B	374	THR
1	B	377	ARG
1	B	379	TYR
1	B	388	MET
1	B	413	LEU
1	B	415	LYS
1	B	442	ARG
1	B	461	VAL
1	B	465	LYS
1	B	468	ASN

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Mol	Chain	Res	Type
1	B	472	VAL
1	B	476	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	99	ASN
1	A	192	GLN
1	A	193	ASN
1	A	209	ASN
1	A	214	GLN
1	A	230	HIS
1	A	236	ASN
1	A	259	ASN
1	A	286	ASN
1	A	378	ASN
1	A	405	ASN
1	A	416	ASN
1	A	457	ASN
1	A	468	ASN
1	B	56	ASN
1	B	72	ASN
1	B	99	ASN
1	B	104	GLN
1	B	192	GLN
1	B	193	ASN
1	B	209	ASN
1	B	218	ASN
1	B	236	ASN
1	B	286	ASN
1	B	324	GLN
1	B	378	ASN
1	B	396	HIS
1	B	405	ASN
1	B	457	ASN
1	B	468	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	PLM	B	501	-	17,17,17	0.48	0	17,17,17	0.82	0
2	PO4	A	504	-	4,4,4	2.34	2 (50%)	6,6,6	0.84	0
4	PLM	A	502	-	17,17,17	0.49	0	17,17,17	0.94	0
3	HEM	A	500	1	41,50,50	2.28	17 (41%)	45,82,82	1.91	9 (20%)
3	HEM	B	500	1	41,50,50	2.15	16 (39%)	45,82,82	1.85	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
4	PLM	B	501	-	-	1/15/15/15	-
3	HEM	A	500	1	-	2/12/54/54	-
3	HEM	B	500	1	-	4/12/54/54	-
4	PLM	A	502	-	-	3/15/15/15	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C3C-CAC	-5.28	1.37	1.47
3	B	500	HEM	C3C-CAC	-5.19	1.37	1.47
3	A	500	HEM	C1D-ND	-4.87	1.28	1.38
3	A	500	HEM	C1B-NB	-4.36	1.32	1.40
3	B	500	HEM	C1D-ND	-4.19	1.30	1.38
3	B	500	HEM	C4D-ND	-4.15	1.33	1.40
2	A	504	PO4	P-O1	4.02	1.60	1.50
3	A	500	HEM	C4D-ND	-3.99	1.33	1.40
3	B	500	HEM	C4B-NB	-3.98	1.30	1.38
3	A	500	HEM	CBB-CAB	3.68	1.48	1.30
3	B	500	HEM	C1B-NB	-3.60	1.34	1.40
3	A	500	HEM	C1D-C2D	-3.45	1.37	1.44
3	B	500	HEM	CBB-CAB	3.34	1.46	1.30
3	B	500	HEM	CMA-C3A	3.17	1.58	1.51
3	A	500	HEM	C4D-C3D	-3.14	1.39	1.45
3	A	500	HEM	C4B-NB	-3.05	1.32	1.38
3	A	500	HEM	C4A-NA	-2.86	1.30	1.36
3	B	500	HEM	CAB-C3B	-2.84	1.39	1.47
3	A	500	HEM	CBD-CGD	2.40	1.56	1.50
3	B	500	HEM	O2A-CGA	-2.38	1.22	1.30
3	B	500	HEM	C4D-C3D	-2.35	1.41	1.45
3	A	500	HEM	C3B-C2B	2.29	1.41	1.37
3	B	500	HEM	C1D-C2D	-2.25	1.40	1.44
3	A	500	HEM	FE-ND	2.23	2.07	1.96
3	B	500	HEM	CAD-C3D	2.23	1.57	1.51
2	A	504	PO4	P-O3	2.15	1.61	1.54
3	A	500	HEM	CHD-C1D	-2.14	1.34	1.41
3	A	500	HEM	O2A-CGA	-2.14	1.23	1.30
3	A	500	HEM	C2C-C1C	-2.12	1.37	1.42
3	B	500	HEM	FE-ND	2.08	2.07	1.96
3	B	500	HEM	CMC-C2C	2.08	1.56	1.51
3	A	500	HEM	CAB-C3B	-2.05	1.41	1.47
3	A	500	HEM	CMA-C3A	2.03	1.55	1.51
3	B	500	HEM	C4A-NA	-2.02	1.32	1.36
3	B	500	HEM	CBD-CGD	2.01	1.55	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	500	HEM	C4B-CHC-C1C	6.75	131.47	122.56
3	A	500	HEM	C4B-CHC-C1C	6.33	130.91	122.56
3	A	500	HEM	C4C-CHD-C1D	5.91	130.35	122.56
3	B	500	HEM	C4C-CHD-C1D	5.67	130.04	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	HEM	C2C-C3C-C4C	-3.45	104.49	106.90
3	B	500	HEM	C2C-C3C-C4C	-2.94	104.84	106.90
3	A	500	HEM	C1B-NB-C4B	2.87	108.04	105.07
3	B	500	HEM	C1B-NB-C4B	2.65	107.81	105.07
3	A	500	HEM	C4D-ND-C1D	2.65	107.81	105.07
3	B	500	HEM	C4D-ND-C1D	2.60	107.75	105.07
3	A	500	HEM	C4B-C3B-C2B	-2.54	105.09	107.11
3	A	500	HEM	C3B-C2B-C1B	-2.53	104.61	106.49
3	B	500	HEM	C3B-C2B-C1B	-2.48	104.64	106.49
3	A	500	HEM	CAD-CBD-CGD	2.28	118.50	113.60
3	A	500	HEM	O2A-CGA-CBA	2.24	121.24	114.03
3	B	500	HEM	C4B-C3B-C2B	-2.21	105.36	107.11
3	B	500	HEM	O2A-CGA-CBA	2.17	121.01	114.03

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	PLM	CC-CD-CE-CF
4	B	501	PLM	C8-C9-CA-CB
3	B	500	HEM	C2B-C3B-CAB-CBB
3	B	500	HEM	C4B-C3B-CAB-CBB
3	B	500	HEM	CAA-CBA-CGA-O1A
3	A	500	HEM	CAA-CBA-CGA-O2A
3	A	500	HEM	CAA-CBA-CGA-O1A
3	B	500	HEM	CAA-CBA-CGA-O2A
4	A	502	PLM	O1-C1-C2-C3
4	A	502	PLM	O2-C1-C2-C3

There are no ring outliers.

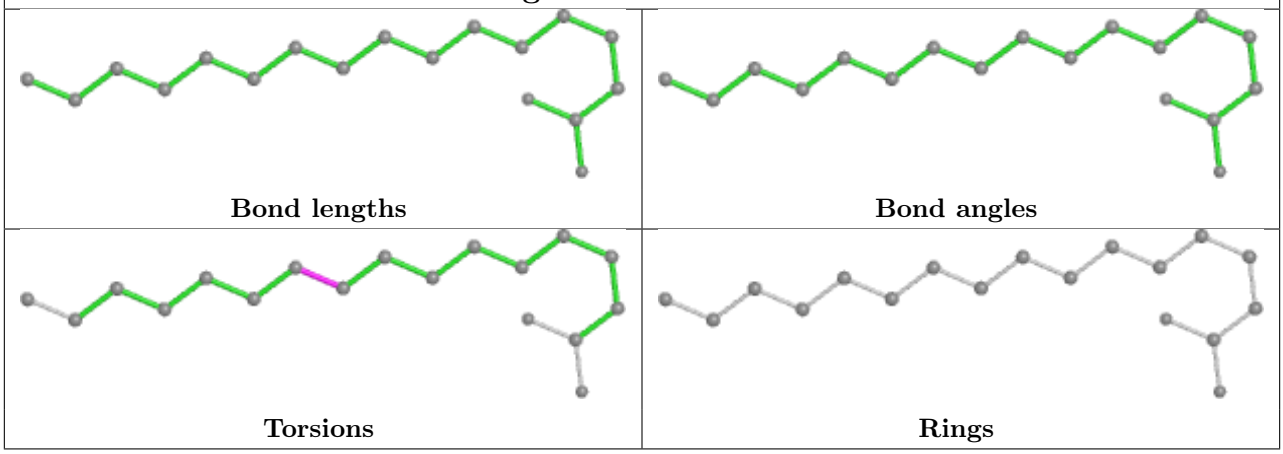
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	PLM	6	0
4	A	502	PLM	3	0
3	A	500	HEM	2	0
3	B	500	HEM	2	0

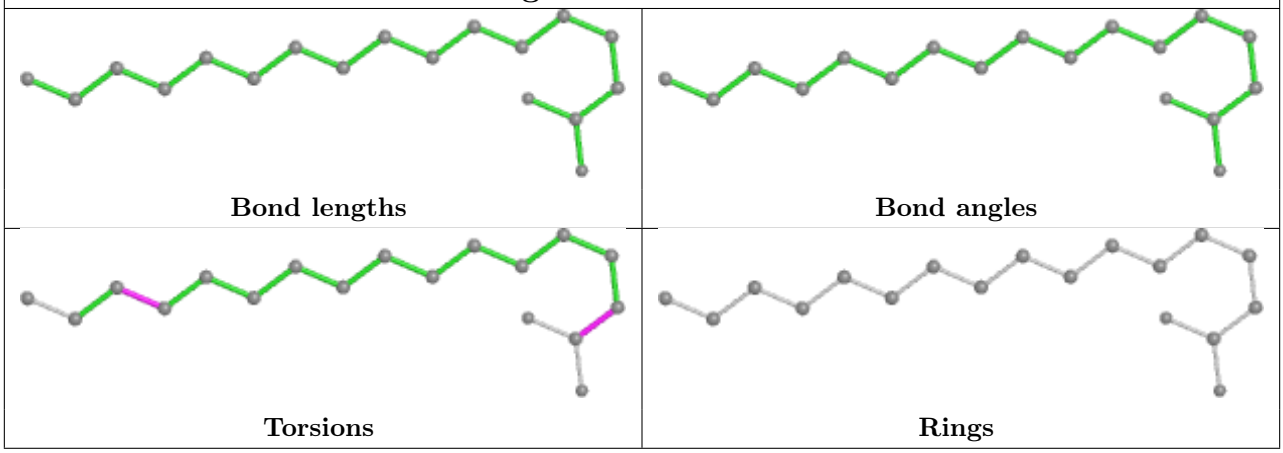
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

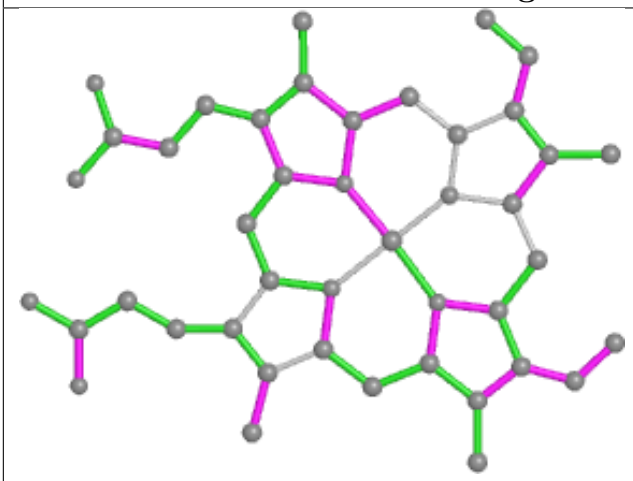
Ligand PLM B 501



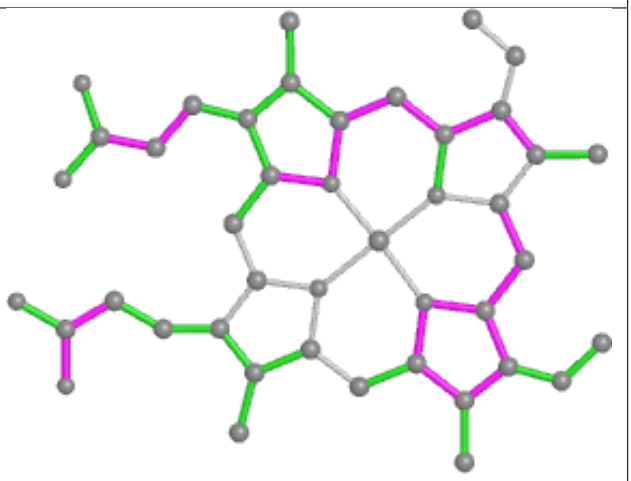
Ligand PLM A 502



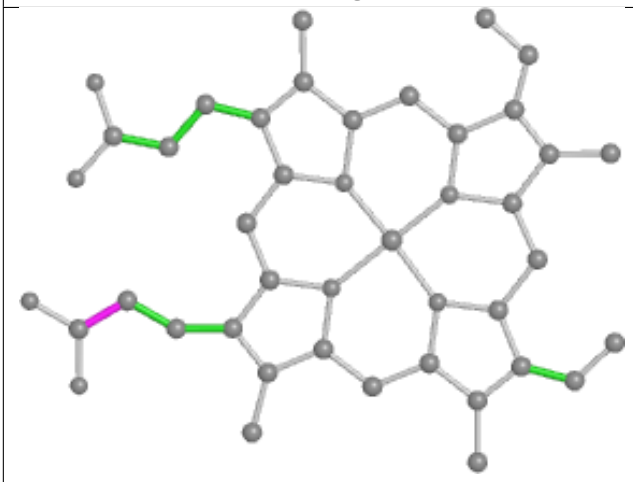
Ligand HEM A 500



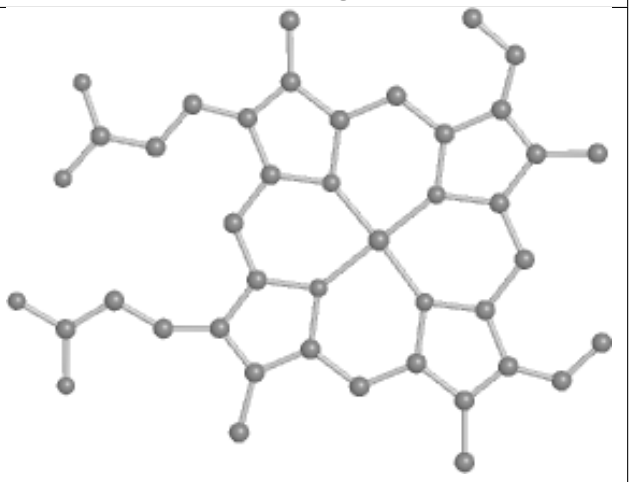
Bond lengths



Bond angles

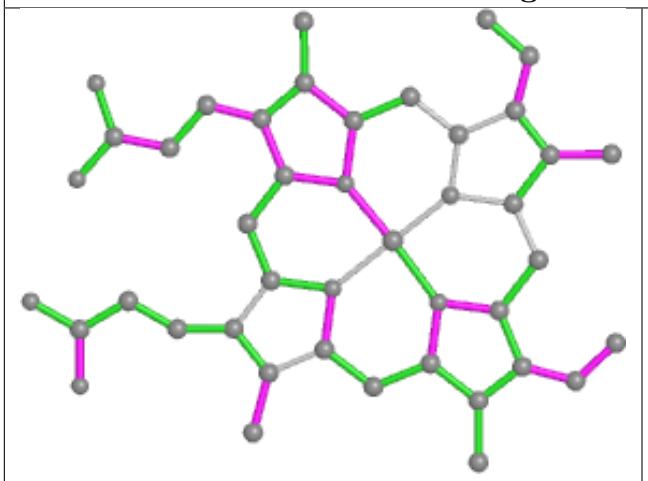


Torsions

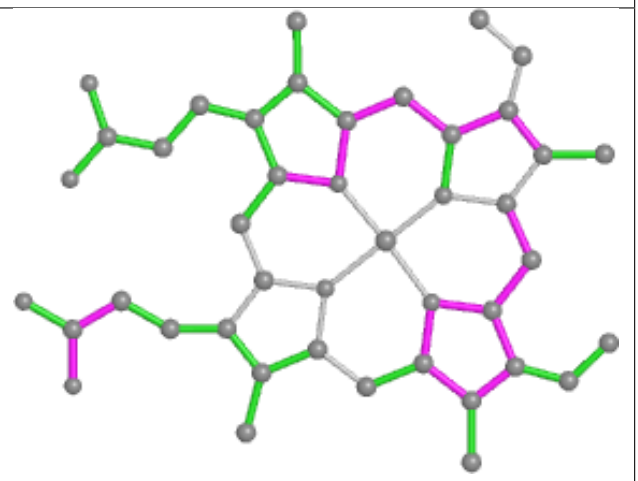


Rings

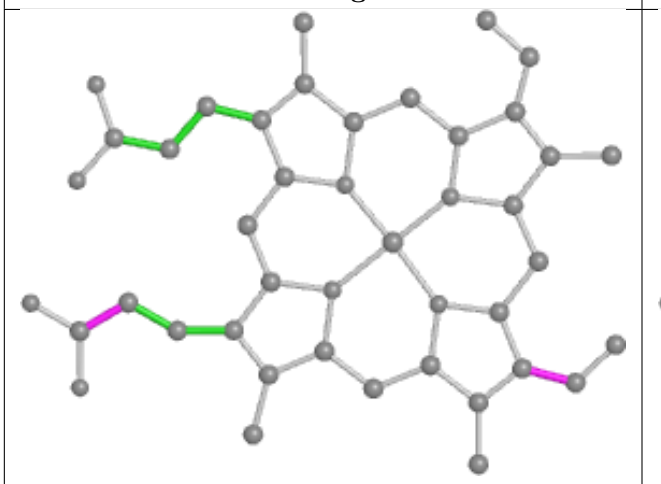
Ligand HEM B 500



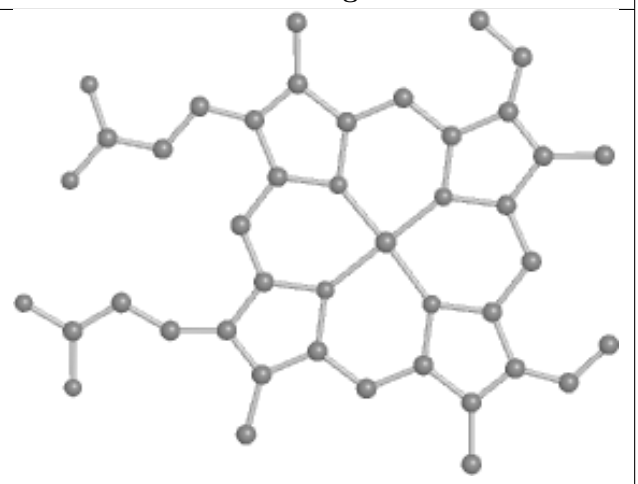
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	463/476 (97%)	-0.01	10 (2%)	62	63	28, 58, 84, 112	0
1	B	463/476 (97%)	-0.03	9 (1%)	66	69	34, 65, 96, 109	0
All	All	926/952 (97%)	-0.02	19 (2%)	63	65	28, 61, 92, 112	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	333	ARG	4.4
1	B	278	GLN	3.4
1	A	490	VAL	3.3
1	B	334	HIS	3.2
1	A	276	ASP	3.2
1	B	466	ASN	3.1
1	B	279	LYS	3.1
1	A	279	LYS	3.0
1	A	301	THR	2.8
1	A	98	GLY	2.6
1	A	105	ARG	2.5
1	B	467	LEU	2.5
1	A	298	GLY	2.3
1	B	399	LYS	2.3
1	A	302	THR	2.2
1	A	441	ALA	2.2
1	B	184	GLN	2.1
1	B	462	ASP	2.1
1	A	297	ALA	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)

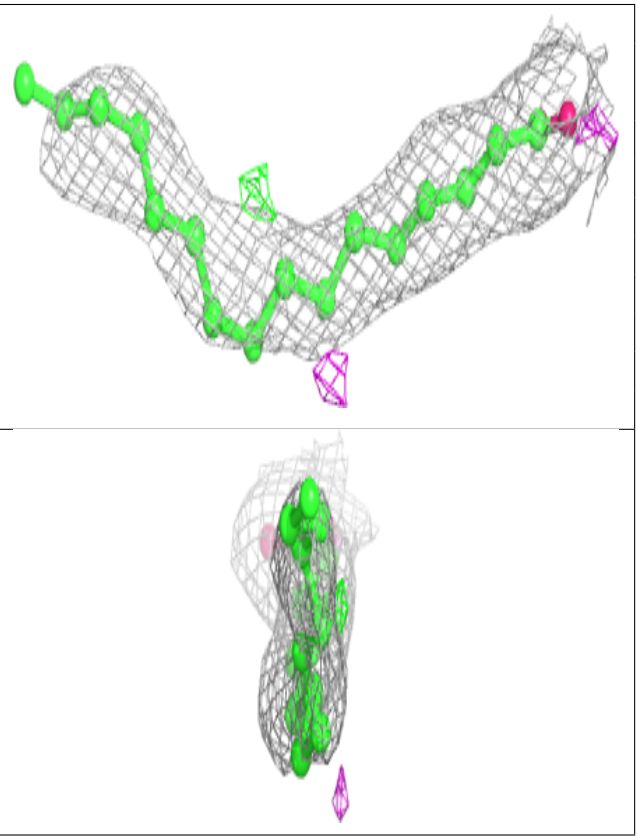
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PLM	A	502	18/18	0.86	0.31	53,58,70,72	0
2	PO4	A	504	5/5	0.90	0.20	91,92,93,93	0
4	PLM	B	501	18/18	0.91	0.28	56,59,62,64	0
3	HEM	A	500	43/43	0.96	0.22	37,42,49,53	0
3	HEM	B	500	43/43	0.97	0.21	39,44,45,49	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.

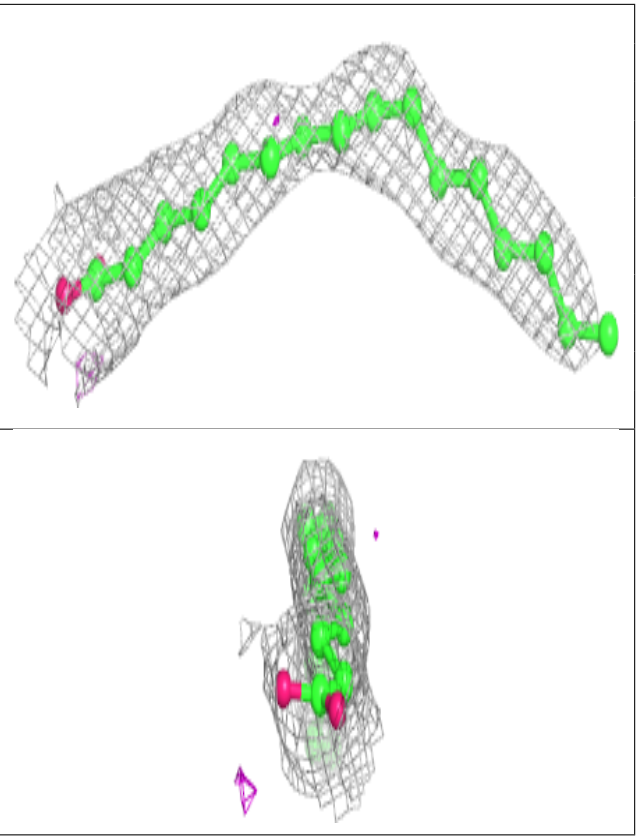
Electron density around PLM A 502:

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



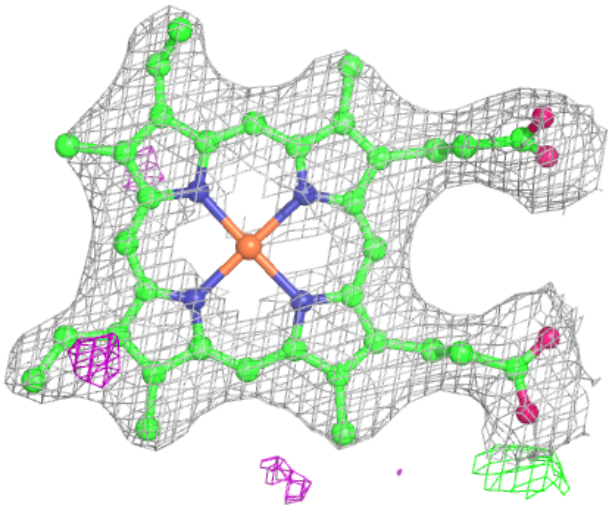
Electron density around PLM B 501:

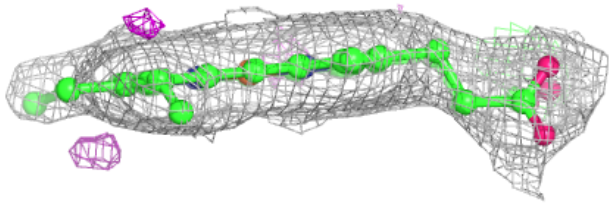
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

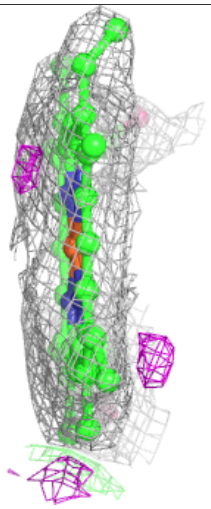


Electron density around HEM A 500:

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

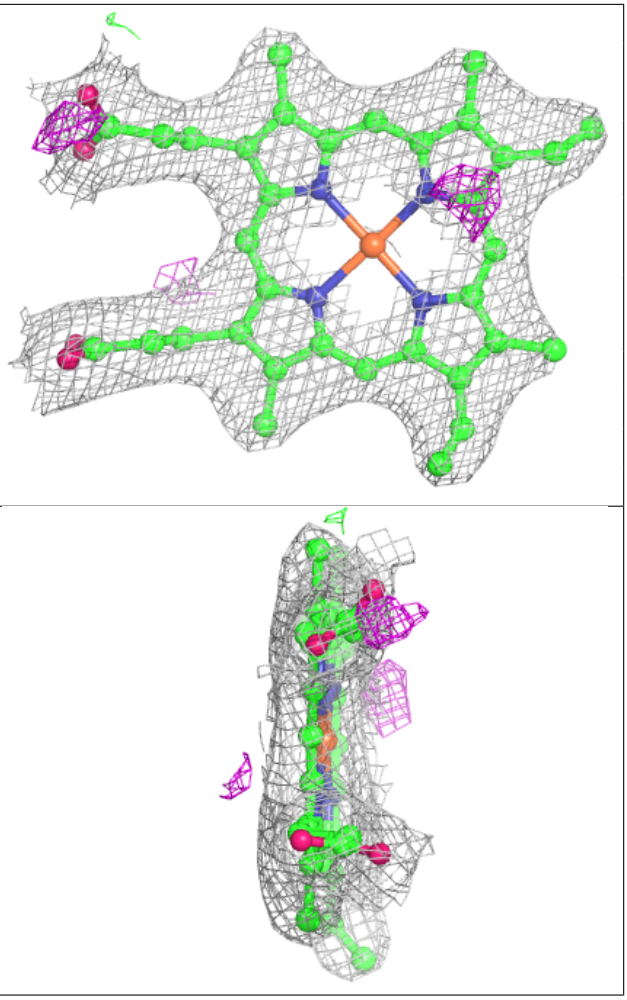






Electron density around HEM B 500:

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



6.5 Other polymers (i)

There are no such residues in this entry.