



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 02:52 AM EDT

PDB ID : 3BDZ / pdb_00003bdz
Title : The Role of Asn 242 in P450cin
Authors : Mehareenna, Y.T.; Poulos, T.L.
Deposited on : 2007-11-15
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

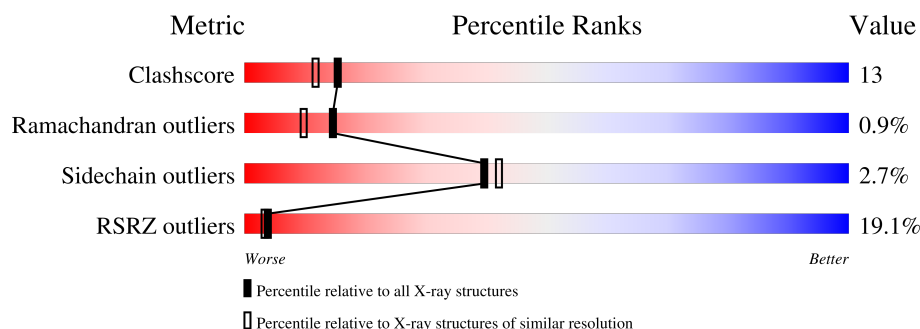
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 $\leq 5\%$. 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	397	<div> <div>18%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	B	397	<div> <div>20%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>

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	MLI	A	500[B]	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6933 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 P450cin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3146	2006	548	581	11			
1	B	397	Total	C	N	O	S	0	0	0
			3146	2006	548	581	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	ALA	ASN	engineered mutation	UNP Q8VQF6
B	242	ALA	ASN	engineered mutation	UNP Q8VQF6

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



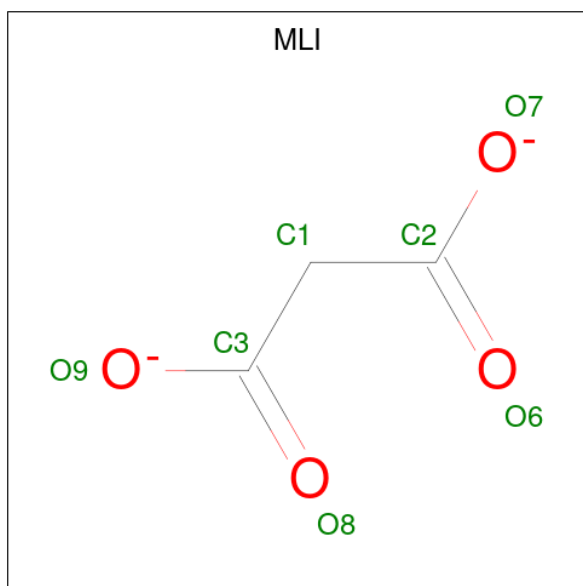
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			14	6	8		
3	B	1	Total	C	O	0	1
			14	6	8		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	289	Total	O	0	0
			289	289		
4	B	238	Total	O	0	0
			238	238		

- Molecule 1: P450cin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.33Å 68.23Å 103.56Å 90.00° 95.53° 90.00°	Depositor
Resolution (Å)	46.30 – 2.00 46.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.5 (46.30-2.00) 94.7 (46.30-2.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.181 , 0.227 0.244 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6933	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 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, MLI

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	0.68	0/3226	0.75	2/4386 (0.0%)
1	B	0.69	0/3226	0.77	3/4386 (0.1%)
All	All	0.69	0/6452	0.76	5/8772 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	276	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	B	285	ALA	N-CA-C	5.76	126.56	111.00
1	A	285	ALA	N-CA-C	5.55	125.99	111.00
1	B	169	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	176	HIS	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	3146	0	3098	83	0
1	B	3146	0	3098	82	0
2	A	43	0	30	7	0
2	B	43	0	30	8	0
3	A	14	0	4	3	0
3	B	14	0	4	0	0
4	A	289	0	0	13	0
4	B	238	0	0	12	0
All	All	6933	0	6264	169	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 13.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TRP:CZ3	1:A:177:VAL:CG2	2.10	1.33
1:A:172:TRP:CZ3	1:A:177:VAL:HG22	1.71	1.24
1:A:172:TRP:CE3	4:A:778:HOH:O	1.96	1.14
1:A:172:TRP:HE3	4:A:778:HOH:O	1.27	1.13
1:A:172:TRP:CH2	1:A:177:VAL:HG22	1.90	1.05
1:B:172:TRP:CZ3	1:B:177:VAL:HG22	1.95	1.00
1:A:172:TRP:CE3	1:A:177:VAL:HG23	1.97	0.99
1:A:172:TRP:CZ3	1:A:177:VAL:HG23	2.03	0.94
1:A:172:TRP:CE3	1:A:177:VAL:CG2	2.54	0.87
1:B:172:TRP:CZ3	1:B:177:VAL:CG2	2.58	0.84
1:B:172:TRP:CH2	1:B:177:VAL:HG22	2.19	0.76
1:A:98:HIS:HE1	2:A:450:HEM:O1D	1.69	0.75
1:B:123:GLN:HG3	4:B:724:HOH:O	1.88	0.73
1:A:181:GLU:O	1:A:185:GLU:HB3	1.88	0.73
1:B:243:THR:HG22	1:B:353:ILE:HD13	1.70	0.73
1:B:345:HIS:O	1:B:346:ARG:O	2.09	0.70
3:A:500[B]:MLI:O6	4:A:685:HOH:O	2.10	0.69
1:B:347:CYS:HB2	2:B:450:HEM:NA	2.08	0.68
1:B:345:HIS:O	1:B:346:ARG:C	2.31	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:SER:O	1:A:404:GLU:HB3	1.95	0.66
1:A:293:GLN:HA	1:A:304:PRO:HG3	1.78	0.66
1:A:98:HIS:CE1	2:A:450:HEM:O1D	2.49	0.66
2:B:450:HEM:HBB2	2:B:450:HEM:HMB1	1.78	0.66
1:B:172:TRP:CE3	1:B:177:VAL:HG22	2.30	0.66
1:B:346:ARG:NH2	4:B:665:HOH:O	2.28	0.65
1:B:98:HIS:HE1	2:B:450:HEM:O1D	1.79	0.65
1:A:401:ARG:NH2	1:A:404:GLU:HG2	2.11	0.65
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.61	0.65
1:A:172:TRP:CZ3	1:A:177:VAL:HG21	2.27	0.64
1:A:172:TRP:CH2	1:A:177:VAL:CG2	2.65	0.64
1:A:120:GLN:HB3	4:A:771:HOH:O	1.96	0.64
1:B:177:VAL:HG11	1:B:182:GLU:CD	2.18	0.63
1:B:370:GLU:HB3	4:B:663:HOH:O	1.99	0.62
1:B:217:LYS:HE3	1:B:220:GLY:O	2.00	0.61
1:A:109:PHE:CD2	1:A:348:LEU:HD13	2.35	0.61
1:A:107:LYS:HB2	1:A:108:PRO:HD3	1.82	0.61
2:A:450:HEM:HMB1	2:A:450:HEM:HBB2	1.84	0.60
1:A:239:GLY:N	2:A:450:HEM:HAC	2.16	0.60
1:B:99:LYS:HE3	1:B:103:GLN:NE2	2.15	0.60
1:B:104:LEU:HD11	1:B:218:ILE:HD11	1.82	0.60
1:A:177:VAL:O	1:A:177:VAL:HG12	2.00	0.60
1:B:345:HIS:HD2	2:B:450:HEM:O2D	1.84	0.59
1:A:346:ARG:NH1	1:A:350:ALA:CB	2.66	0.59
1:B:347:CYS:HB2	2:B:450:HEM:C1A	2.38	0.59
1:A:177:VAL:HG11	1:A:183:GLY:N	2.17	0.59
1:B:178:GLU:HG3	4:B:728:HOH:O	2.03	0.58
1:B:108:PRO:HB2	1:B:209:ILE:CD1	2.34	0.57
1:A:190:LEU:C	1:A:190:LEU:HD23	2.25	0.57
1:B:108:PRO:CB	1:B:209:ILE:HD12	2.33	0.57
1:B:345:HIS:HE1	4:B:521:HOH:O	1.88	0.57
1:A:107:LYS:HG2	4:A:657:HOH:O	2.05	0.56
1:A:345:HIS:O	1:A:346:ARG:C	2.42	0.56
1:B:152:LEU:HD21	1:B:352:LEU:HD11	1.86	0.56
1:A:391:HIS:HE1	4:A:662:HOH:O	1.89	0.55
1:B:173:ALA:HA	1:B:177:VAL:HG23	1.88	0.55
1:A:162:GLU:H	1:A:162:GLU:CD	2.10	0.55
1:A:346:ARG:NH1	1:A:350:ALA:HB1	2.21	0.55
1:B:178:GLU:O	1:B:180:PRO:N	2.39	0.55
1:A:358:ARG:HD3	4:A:621:HOH:O	2.07	0.55
1:B:17:TYR:OH	1:B:176:HIS:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLU:HG3	4:B:721:HOH:O	2.07	0.54
1:B:172:TRP:CZ3	1:B:177:VAL:HG21	2.41	0.54
1:B:345:HIS:C	1:B:346:ARG:O	2.45	0.54
1:A:80:ARG:CZ	4:A:569:HOH:O	2.55	0.54
1:B:108:PRO:HB2	1:B:209:ILE:HD12	1.88	0.54
1:B:169:ARG:NH1	1:B:189:GLU:OE1	2.34	0.53
1:A:166:THR:HG21	4:A:774:HOH:O	2.07	0.52
1:A:345:HIS:O	1:A:346:ARG:O	2.27	0.52
1:B:175:THR:O	1:B:176:HIS:HB2	2.08	0.52
1:B:335:ASN:ND2	1:B:337:HIS:HD2	2.08	0.52
1:B:378:GLU:HA	1:B:378:GLU:OE1	2.08	0.52
1:A:203:THR:O	1:A:205:PRO:HD3	2.10	0.51
1:A:98:HIS:C	1:A:98:HIS:CD2	2.83	0.51
1:B:172:TRP:CE3	1:B:177:VAL:CG2	2.92	0.51
1:B:175:THR:O	1:B:176:HIS:CB	2.59	0.51
1:B:190:LEU:C	1:B:190:LEU:HD23	2.31	0.51
1:A:109:PHE:CG	1:A:348:LEU:HD13	2.47	0.50
1:A:234:ILE:HD11	3:A:500[B]:MLI:O8	2.12	0.50
1:A:253:ARG:HD3	1:A:282:TYR:OH	2.11	0.50
1:A:401:ARG:NH2	1:A:404:GLU:CG	2.74	0.50
1:A:346:ARG:HH11	1:A:350:ALA:CB	2.25	0.49
1:B:98:HIS:CE1	2:B:450:HEM:O1D	2.62	0.49
1:A:150:ALA:HA	1:A:240:ILE:HG12	1.94	0.49
1:B:172:TRP:CH2	1:B:177:VAL:HG13	2.47	0.49
1:A:62:GLN:HA	1:A:62:GLN:OE1	2.11	0.49
1:A:399:GLY:C	1:A:400:LYS:HD2	2.32	0.49
1:B:69:LYS:HG2	4:B:624:HOH:O	2.12	0.49
1:A:109:PHE:CD2	1:A:348:LEU:CD1	2.96	0.49
1:B:139:ASP:O	1:B:143:TRP:HB3	2.13	0.49
1:B:209:ILE:HD13	4:B:667:HOH:O	2.13	0.49
1:B:217:LYS:HE3	1:B:220:GLY:C	2.34	0.48
1:B:160:PRO:HD2	1:B:167:TYR:OH	2.14	0.48
1:A:346:ARG:HH12	1:A:350:ALA:HB1	1.78	0.48
1:A:56:ALA:HB1	1:A:314:ILE:HG21	1.94	0.48
1:A:166:THR:HG22	4:A:719:HOH:O	2.13	0.48
1:B:186:ILE:HD12	1:B:186:ILE:N	2.29	0.48
1:B:120:GLN:HG2	4:B:722:HOH:O	2.14	0.47
1:A:176:HIS:O	1:A:177:VAL:C	2.52	0.47
1:A:205:PRO:HG3	1:A:215:MET:CE	2.44	0.47
1:A:293:GLN:CA	1:A:304:PRO:HG3	2.43	0.47
1:B:150:ALA:HB1	4:B:708:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:C	1:A:205:PRO:HD3	2.34	0.47
1:B:181:GLU:O	1:B:185:GLU:HB2	2.13	0.47
1:A:345:HIS:O	2:A:450:HEM:HAA2	2.14	0.47
1:B:175:THR:O	1:B:176:HIS:CD2	2.68	0.47
1:B:179:ASN:O	1:B:182:GLU:HB3	2.15	0.47
1:A:61:ILE:HD12	1:A:315:ALA:HB2	1.97	0.46
1:B:335:ASN:HD22	1:B:335:ASN:C	2.18	0.46
1:B:88:LEU:HA	4:B:584:HOH:O	2.16	0.46
1:A:170:TRP:O	1:A:174:ILE:HG13	2.15	0.46
1:A:177:VAL:CG1	1:A:182:GLU:HB3	2.46	0.46
1:B:180:PRO:O	1:B:182:GLU:N	2.49	0.46
1:A:176:HIS:NE2	1:A:382:LEU:HD11	2.31	0.46
1:B:311:TRP:HB3	1:B:314:ILE:HG12	1.98	0.45
1:A:88:LEU:HA	4:A:595:HOH:O	2.16	0.45
1:B:38:ALA:HA	1:B:41:THR:O	2.16	0.45
1:B:70:ALA:HA	1:B:293:GLN:HG2	1.97	0.45
1:B:404:GLU:OE2	1:B:404:GLU:O	2.34	0.45
1:B:61:ILE:HD12	1:B:315:ALA:HB2	1.99	0.45
1:A:99:LYS:O	1:A:103:GLN:HG3	2.17	0.45
1:B:108:PRO:CB	1:B:209:ILE:CD1	2.95	0.45
1:A:172:TRP:CD2	1:A:177:VAL:HG23	2.50	0.44
1:B:171:VAL:HG21	1:B:240:ILE:HD11	1.98	0.44
1:B:367:ARG:CZ	1:B:402:LEU:HG	2.47	0.44
1:A:172:TRP:CZ3	4:A:778:HOH:O	2.40	0.44
1:B:245:ARG:NE	1:B:245:ARG:HA	2.32	0.44
1:B:189:GLU:O	1:B:193:HIS:HD2	2.00	0.44
1:A:62:GLN:NE2	1:A:338:LEU:HD21	2.32	0.44
1:B:54:VAL:HG13	1:B:311:TRP:CD1	2.53	0.44
1:A:207:ASN:HA	1:A:212:ARG:HH21	1.82	0.44
1:B:99:LYS:O	1:B:103:GLN:HG3	2.18	0.44
1:B:259:GLU:OE2	4:B:683:HOH:O	2.20	0.44
1:B:182:GLU:O	1:B:186:ILE:HD13	2.18	0.43
1:A:98:HIS:ND1	1:A:345:HIS:CE1	2.86	0.43
1:B:347:CYS:HB2	2:B:450:HEM:C4A	2.53	0.43
2:A:450:HEM:HBB2	2:A:450:HEM:CMB	2.48	0.43
1:A:139:ASP:O	1:A:143:TRP:HB3	2.19	0.43
1:A:177:VAL:HG11	1:A:182:GLU:HB3	2.00	0.43
1:A:400:LYS:HD2	1:A:400:LYS:N	2.34	0.43
1:B:56:ALA:HB1	1:B:314:ILE:HG21	2.00	0.43
1:B:211:SER:O	1:B:215:MET:HG3	2.19	0.42
1:A:141:ALA:HA	1:A:145:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:TYR:OH	1:B:176:HIS:CD2	2.71	0.42
1:A:181:GLU:OE2	1:A:181:GLU:CA	2.68	0.42
1:A:176:HIS:O	1:A:177:VAL:O	2.38	0.42
1:B:46:SER:O	1:B:51:GLY:HA2	2.19	0.42
1:B:76:VAL:HG23	1:B:287:VAL:CG2	2.49	0.42
1:B:98:HIS:CE1	1:B:345:HIS:CD2	3.07	0.42
1:A:118:THR:O	1:A:121:LEU:HB2	2.19	0.42
1:A:181:GLU:OE2	1:A:181:GLU:HA	2.19	0.42
1:B:169:ARG:HH12	1:B:189:GLU:CD	2.22	0.41
1:B:201:ARG:HB2	1:B:214:ILE:CD1	2.49	0.41
1:B:284:PRO:HD2	2:B:450:HEM:HMB3	2.02	0.41
1:B:180:PRO:C	1:B:182:GLU:N	2.73	0.41
1:A:163:ASP:HB3	1:A:166:THR:HG23	2.02	0.41
1:A:108:PRO:HB3	1:A:209:ILE:HG12	2.01	0.41
1:A:238:GLY:HA2	3:A:500[A]:MLI:O6	2.21	0.41
1:A:299:ASP:C	1:A:300:ILE:HD12	2.41	0.41
1:A:312:PHE:HB2	1:A:313:PRO:HD3	2.02	0.41
1:A:371:PHE:HB3	1:A:396:PHE:HB3	2.03	0.41
1:A:217:LYS:HD3	1:A:220:GLY:O	2.20	0.41
1:A:239:GLY:CA	2:A:450:HEM:HAC	2.51	0.41
1:A:273:ASN:HB2	4:A:582:HOH:O	2.21	0.41
1:B:80:ARG:HH11	1:B:80:ARG:CG	2.30	0.41
1:B:217:LYS:HB3	1:B:217:LYS:HE2	1.94	0.41
1:A:58:TYR:HA	1:A:315:ALA:HB1	2.03	0.40
1:A:208:ASP:O	1:A:212:ARG:HG2	2.22	0.40
1:A:345:HIS:C	1:A:346:ARG:O	2.58	0.40
1:B:108:PRO:HB2	1:B:209:ILE:HD11	2.02	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	395/397 (100%)	380 (96%)	12 (3%)	3 (1%)	16	12
1	B	395/397 (100%)	379 (96%)	12 (3%)	4 (1%)	13	8
All	All	790/794 (100%)	759 (96%)	24 (3%)	7 (1%)	14	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
1	A	346	ARG
1	B	176	HIS
1	B	181	GLU
1	B	346	ARG
1	B	180	PRO
1	A	180	PRO

5.3.2 Protein sidechains ⓘ

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	332/332 (100%)	324 (98%)	8 (2%)	44	47
1	B	332/332 (100%)	322 (97%)	10 (3%)	36	37
All	All	664/664 (100%)	646 (97%)	18 (3%)	40	42

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	65	ILE
1	A	120	GLN
1	A	166	THR
1	A	185	GLU
1	A	276	ASP
1	A	346	ARG
1	A	348	LEU
1	B	8	THR

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Mol	Chain	Res	Type
1	B	59	LYS
1	B	65	ILE
1	B	179	ASN
1	B	235	LEU
1	B	333	THR
1	B	335	ASN
1	B	346	ARG
1	B	347	CYS
1	B	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	204	ASN
1	A	391	HIS
1	B	66	GLN
1	B	98	HIS
1	B	103	GLN
1	B	176	HIS
1	B	179	ASN
1	B	193	HIS
1	B	335	ASN
1	B	345	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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	MLI	B	500[A]	2	6,6,6	2.10	3 (50%)	7,7,7	1.29	0
3	MLI	A	500[A]	2	6,6,6	2.36	5 (83%)	7,7,7	1.19	0
3	MLI	B	500[B]	-	6,6,6	2.23	3 (50%)	7,7,7	1.18	0
3	MLI	A	500[B]	-	6,6,6	2.09	3 (50%)	7,7,7	1.45	2 (28%)
2	HEM	B	450	3,1	42,50,50	1.82	11 (26%)	46,82,82	1.48	7 (15%)
2	HEM	A	450	3,1	42,50,50	1.75	9 (21%)	46,82,82	1.70	10 (21%)

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	MLI	B	500[A]	2	-	0/4/4/4	-
3	MLI	A	500[A]	2	-	0/4/4/4	-
3	MLI	B	500[B]	-	-	0/4/4/4	-
3	MLI	A	500[B]	-	-	0/4/4/4	-
2	HEM	B	450	3,1	-	0/12/54/54	-
2	HEM	A	450	3,1	-	0/12/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	HEM	C3C-C2C	-4.34	1.34	1.40
2	A	450	HEM	C1B-NB	-4.18	1.33	1.40
2	B	450	HEM	CMB-C2B	4.14	1.59	1.50
2	A	450	HEM	C3C-CAC	-4.12	1.37	1.47
2	B	450	HEM	C3C-C2C	-4.06	1.34	1.40
2	B	450	HEM	C3C-CAC	-3.85	1.38	1.47
2	A	450	HEM	C2C-C1C	3.33	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500[B]	MLI	O7-C2	-3.26	1.20	1.30
2	B	450	HEM	C4D-C3D	3.16	1.50	1.45
2	B	450	HEM	CMD-C2D	3.12	1.57	1.50
2	A	450	HEM	CMB-C2B	3.09	1.57	1.50
3	B	500[A]	MLI	O7-C2	-3.07	1.20	1.30
2	A	450	HEM	C3C-C4C	3.05	1.45	1.41
2	A	450	HEM	C1B-C2B	3.02	1.50	1.44
3	A	500[A]	MLI	O6-C2	2.97	1.31	1.22
3	A	500[A]	MLI	C1-C3	2.76	1.55	1.51
2	B	450	HEM	CAB-C3B	-2.61	1.40	1.47
3	A	500[B]	MLI	C1-C2	2.57	1.55	1.51
2	B	450	HEM	C1B-NB	-2.54	1.35	1.40
3	A	500[B]	MLI	O7-C2	-2.54	1.22	1.30
2	A	450	HEM	O2A-CGA	-2.53	1.22	1.30
3	A	500[A]	MLI	O9-C3	-2.51	1.22	1.30
3	B	500[B]	MLI	O9-C3	-2.49	1.22	1.30
3	A	500[A]	MLI	O7-C2	-2.48	1.22	1.30
3	A	500[B]	MLI	O9-C3	-2.47	1.22	1.30
2	B	450	HEM	C1A-NA	2.41	1.41	1.36
3	B	500[B]	MLI	C1-C3	2.40	1.54	1.51
2	B	450	HEM	CHA-C4D	2.30	1.40	1.34
3	B	500[A]	MLI	C1-C2	2.27	1.54	1.51
3	B	500[A]	MLI	O8-C3	2.25	1.29	1.22
3	A	500[A]	MLI	O8-C3	2.12	1.29	1.22
2	B	450	HEM	O2A-CGA	-2.09	1.23	1.30
2	B	450	HEM	C4D-ND	-2.03	1.36	1.40
2	A	450	HEM	O2D-CGD	-2.01	1.24	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	450	HEM	C3B-C4B-NB	5.27	113.25	109.47
2	A	450	HEM	C4B-C3B-C2B	-4.24	103.39	107.28
2	B	450	HEM	CBA-CAA-C2A	-3.81	106.14	112.54
2	B	450	HEM	C1D-C2D-C3D	-3.66	103.13	106.98
2	A	450	HEM	CMC-C2C-C3C	3.39	131.45	124.68
2	A	450	HEM	C2C-C3C-C4C	3.12	109.07	106.90
2	B	450	HEM	C2D-C1D-ND	2.99	113.36	109.90
2	A	450	HEM	CHC-C4B-C3B	-2.74	120.37	124.57
2	B	450	HEM	CMD-C2D-C3D	2.70	133.45	126.15
2	B	450	HEM	CMA-C3A-C4A	-2.42	124.92	128.46
2	A	450	HEM	C4B-CHC-C1C	2.41	125.74	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	450	HEM	C4C-CHD-C1D	2.31	125.61	122.56
2	A	450	HEM	CBD-CAD-C3D	-2.31	106.14	112.53
2	A	450	HEM	CMA-C3A-C4A	-2.27	125.13	128.46
2	B	450	HEM	C4C-CHD-C1D	2.19	125.45	122.56
3	A	500[B]	MLI	O7-C2-C1	2.16	121.20	114.51
3	A	500[B]	MLI	O7-C2-O6	-2.11	117.89	123.33
2	A	450	HEM	CMD-C2D-C1D	-2.11	121.73	125.03
2	B	450	HEM	CHD-C1D-C2D	-2.10	121.72	125.03

There are no chirality outliers.

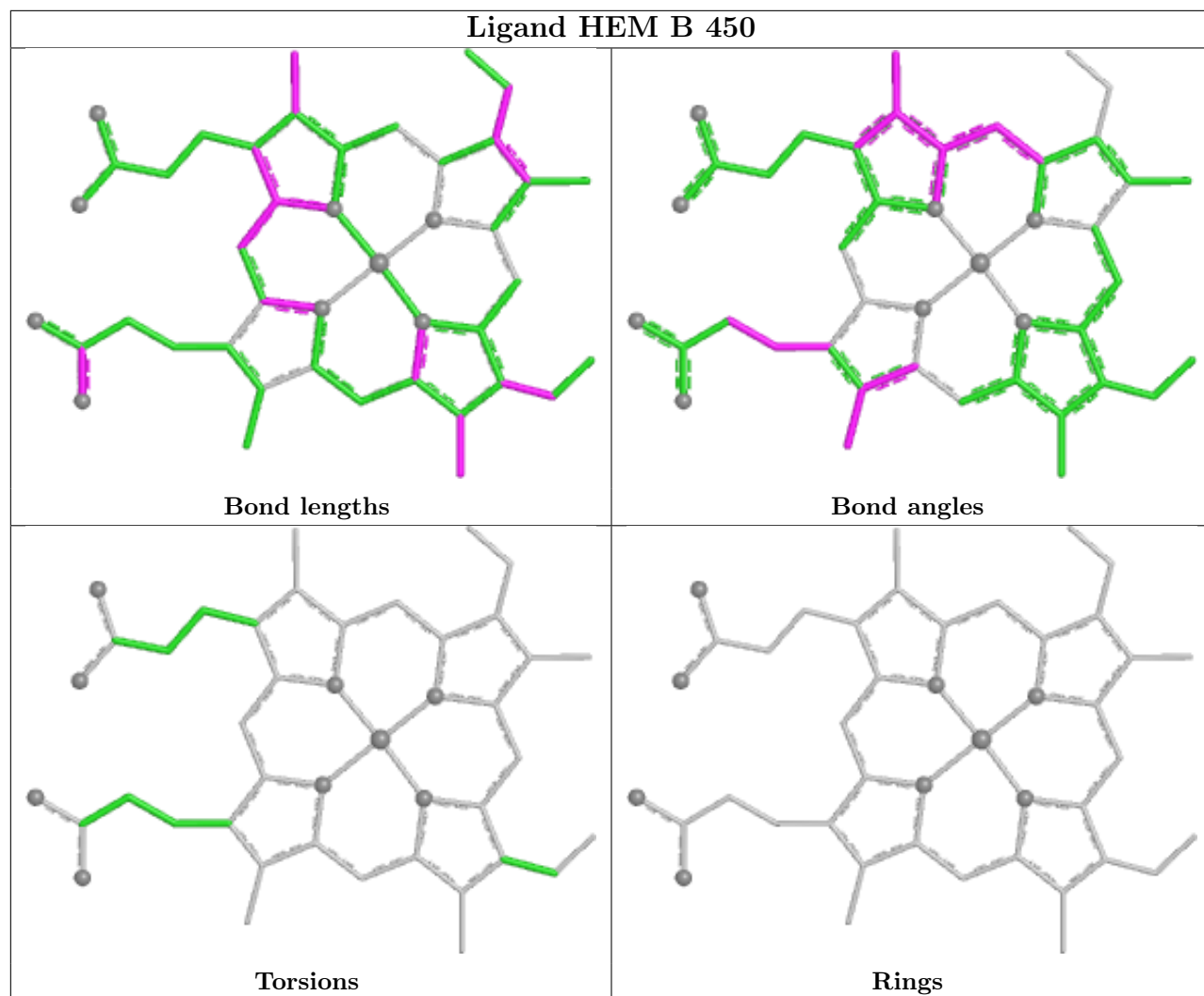
There are no torsion outliers.

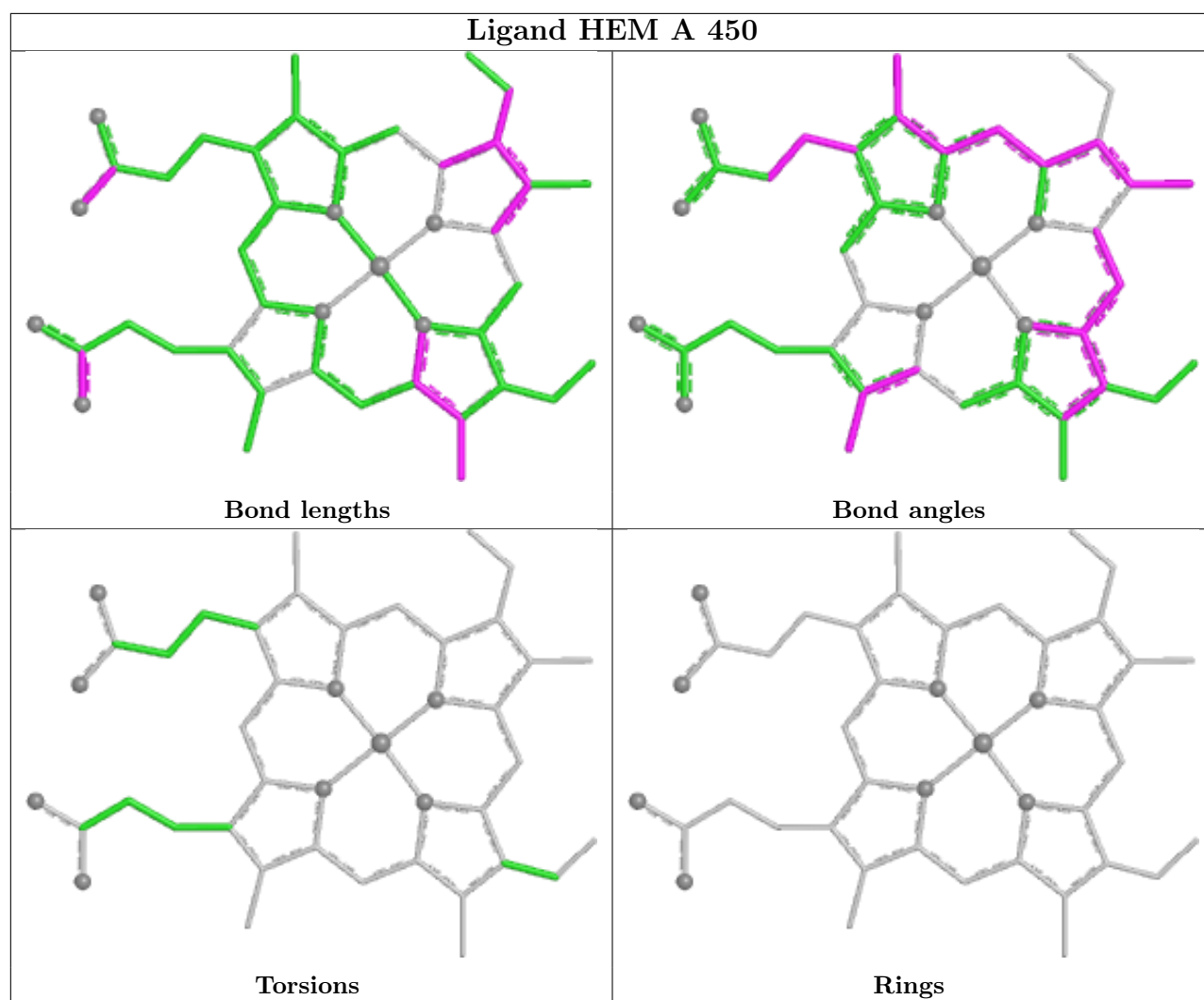
There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500[A]	MLI	1	0
3	A	500[B]	MLI	2	0
2	B	450	HEM	8	0
2	A	450	HEM	7	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	397/397 (100%)	1.52	73 (18%) 4 3	42, 52, 74, 89	0
1	B	397/397 (100%)	1.57	79 (19%) 3 3	43, 54, 73, 89	0
All	All	794/794 (100%)	1.55	152 (19%) 4 3	42, 53, 74, 89	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	TRP	7.4
1	A	172	TRP	7.1
1	B	177	VAL	6.1
1	A	177	VAL	6.1
1	B	180	PRO	5.2
1	A	220	GLY	4.6
1	A	180	PRO	4.4
1	A	218	ILE	4.4
1	A	181	GLU	4.3
1	B	346	ARG	4.3
1	A	179	ASN	4.1
1	B	402	LEU	4.0
1	B	8	THR	4.0
1	B	178	GLU	3.8
1	A	346	ARG	3.8
1	A	176	HIS	3.8
1	B	181	GLU	3.7
1	B	209	ILE	3.6
1	B	223	LEU	3.5
1	B	398	LYS	3.5
1	A	207	ASN	3.5
1	A	404	GLU	3.5
1	A	370	GLU	3.4
1	A	215	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	402	LEU	3.3
1	B	179	ASN	3.3
1	B	207	ASN	3.3
1	A	178	GLU	3.2
1	B	62	GLN	3.2
1	B	297	VAL	3.2
1	B	403	SER	3.2
1	B	215	MET	3.2
1	A	297	VAL	3.1
1	B	404	GLU	3.1
1	A	116	LEU	3.1
1	B	220	GLY	3.1
1	A	219	ASP	3.1
1	A	403	SER	3.1
1	B	176	HIS	3.0
1	B	399	GLY	3.0
1	B	185	GLU	3.0
1	A	333	THR	3.0
1	A	133	ILE	2.9
1	A	111	PRO	2.9
1	A	213	VAL	2.9
1	B	103	GLN	2.8
1	A	217	LYS	2.8
1	B	218	ILE	2.8
1	A	100	LYS	2.8
1	B	217	LYS	2.8
1	A	197	LEU	2.8
1	A	135	LEU	2.7
1	B	66	GLN	2.7
1	B	133	ILE	2.7
1	B	69	LYS	2.7
1	B	267	HIS	2.6
1	B	68	THR	2.6
1	A	376	ASN	2.6
1	A	216	SER	2.6
1	A	223	LEU	2.6
1	B	378	GLU	2.6
1	A	400	LYS	2.5
1	B	202	ARG	2.5
1	A	107	LYS	2.5
1	B	214	ILE	2.5
1	B	392	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	401	ARG	2.5
1	B	109	PHE	2.5
1	B	206	GLY	2.5
1	A	401	ARG	2.5
1	B	97	VAL	2.5
1	B	216	SER	2.4
1	B	116	LEU	2.4
1	A	295	VAL	2.4
1	B	205	PRO	2.4
1	B	173	ALA	2.4
1	A	183	GLY	2.4
1	B	135	LEU	2.4
1	A	212	ARG	2.3
1	B	160	PRO	2.3
1	A	299	ASP	2.3
1	B	221	GLU	2.3
1	B	271	ILE	2.3
1	A	204	ASN	2.3
1	B	144	LEU	2.3
1	B	391	HIS	2.3
1	A	29	ALA	2.3
1	A	203	THR	2.3
1	A	108	PRO	2.3
1	B	393	PRO	2.3
1	B	213	VAL	2.3
1	A	378	GLU	2.3
1	B	137	GLU	2.3
1	B	237	LEU	2.3
1	B	141	ALA	2.3
1	A	222	SER	2.3
1	B	96	PRO	2.3
1	B	295	VAL	2.3
1	A	206	GLY	2.3
1	B	335	ASN	2.3
1	B	88	LEU	2.3
1	B	199	ALA	2.3
1	A	227	ASP	2.2
1	B	98	HIS	2.2
1	A	209	ILE	2.2
1	A	214	ILE	2.2
1	B	175	THR	2.2
1	A	321	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	70	ALA	2.2
1	A	334	PRO	2.2
1	B	59	LYS	2.2
1	B	400	LYS	2.2
1	A	298	GLY	2.2
1	A	120	GLN	2.2
1	A	109	PHE	2.2
1	A	185	GLU	2.2
1	B	174	ILE	2.2
1	A	156	LEU	2.2
1	B	197	LEU	2.2
1	B	143	TRP	2.2
1	A	199	ALA	2.2
1	A	304	PRO	2.2
1	A	232	PHE	2.1
1	A	237	LEU	2.1
1	B	219	ASP	2.1
1	A	76	VAL	2.1
1	A	137	GLU	2.1
1	A	366	LYS	2.1
1	A	175	THR	2.1
1	A	173	ALA	2.1
1	B	63	ALA	2.1
1	B	188	ALA	2.1
1	A	273	ASN	2.1
1	A	240	ILE	2.1
1	A	251	PHE	2.1
1	A	103	GLN	2.1
1	B	355	VAL	2.1
1	A	336	ARG	2.1
1	B	83	THR	2.1
1	B	186	ILE	2.1
1	B	322	PHE	2.1
1	A	56	ALA	2.0
1	B	45	TRP	2.0
1	A	226	ASP	2.0
1	B	222	SER	2.0
1	A	88	LEU	2.0
1	A	144	LEU	2.0
1	A	296	THR	2.0
1	B	123	GLN	2.0
1	B	85	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	288	GLY	2.0
1	B	191	VAL	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](#)

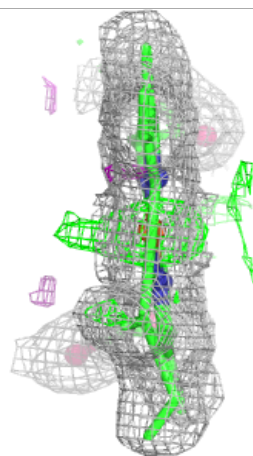
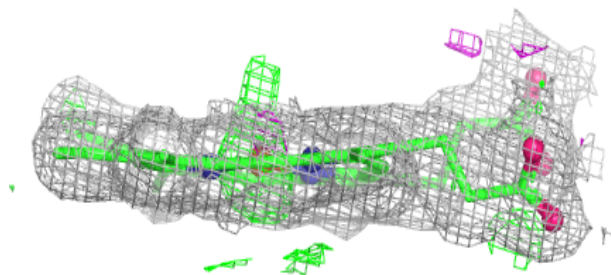
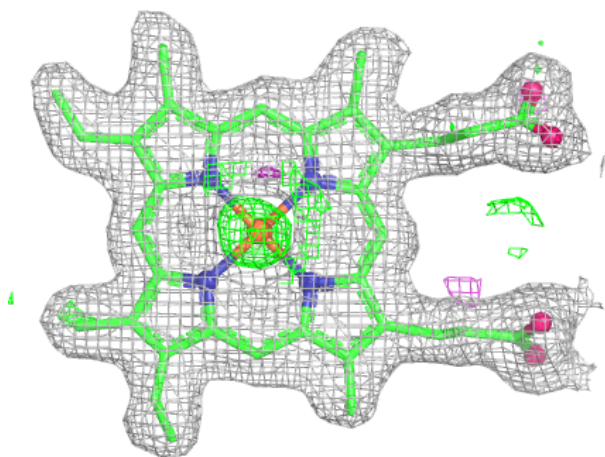
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

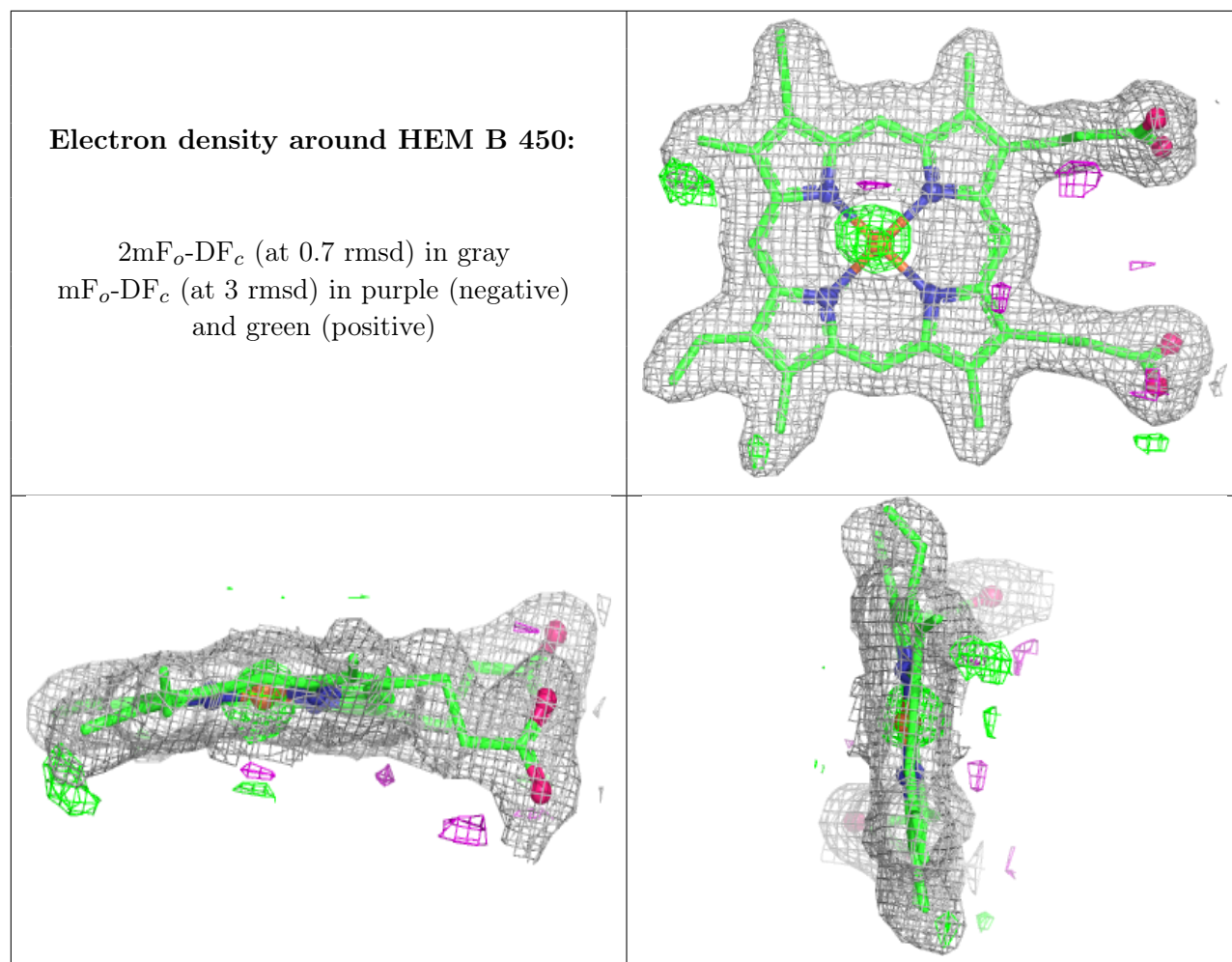
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MLI	A	500[A]	7/7	0.67	0.19	21,27,30,31	7
3	MLI	A	500[B]	7/7	0.67	0.19	9,13,20,23	7
3	MLI	B	500[A]	7/7	0.77	0.16	26,29,30,31	7
3	MLI	B	500[B]	7/7	0.77	0.16	24,27,28,28	7
2	HEM	A	450	43/43	0.95	0.13	42,45,47,55	0
2	HEM	B	450	43/43	0.96	0.12	45,47,52,55	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 450:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.