



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:03 am BST

PDB ID : 2ZQJ
Title : Substrate-Free Form of Cytochrome P450BSbeta
Authors : Shoji, O.; Fujishiro, T.; Nagano, S.; Hirose, T.; Shiro, Y.; Watanabe, Y.
Deposited on : 2008-08-11
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

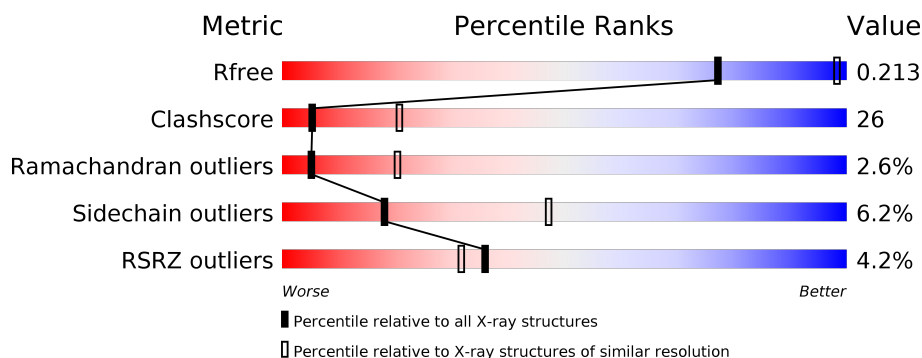
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	417	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>38%</div> <div>••</div> </div> </div>
1	B	417	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>40%</div> <div>5%</div> <div>•</div> </div> </div>
1	C	417	<div> <div>7%</div> <div> <div></div> <div>43%</div> <div>50%</div> <div>5%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

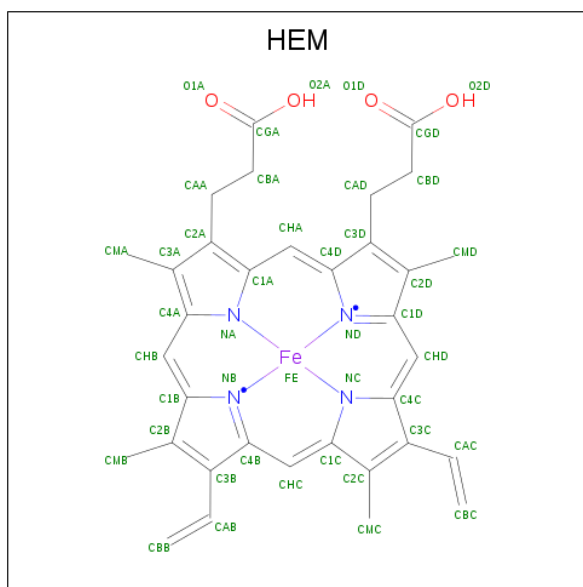
There are 3 unique types of molecules in this entry. The entry contains 10203 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 152A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3339	2125	594	601	19			
1	B	411	Total	C	N	O	S	0	0	0
			3339	2125	594	601	19			
1	C	411	Total	C	N	O	S	0	0	0
			3339	2125	594	601	19			

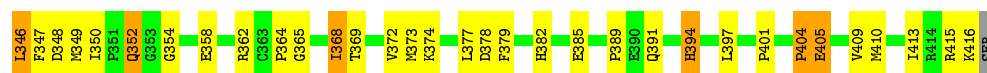
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



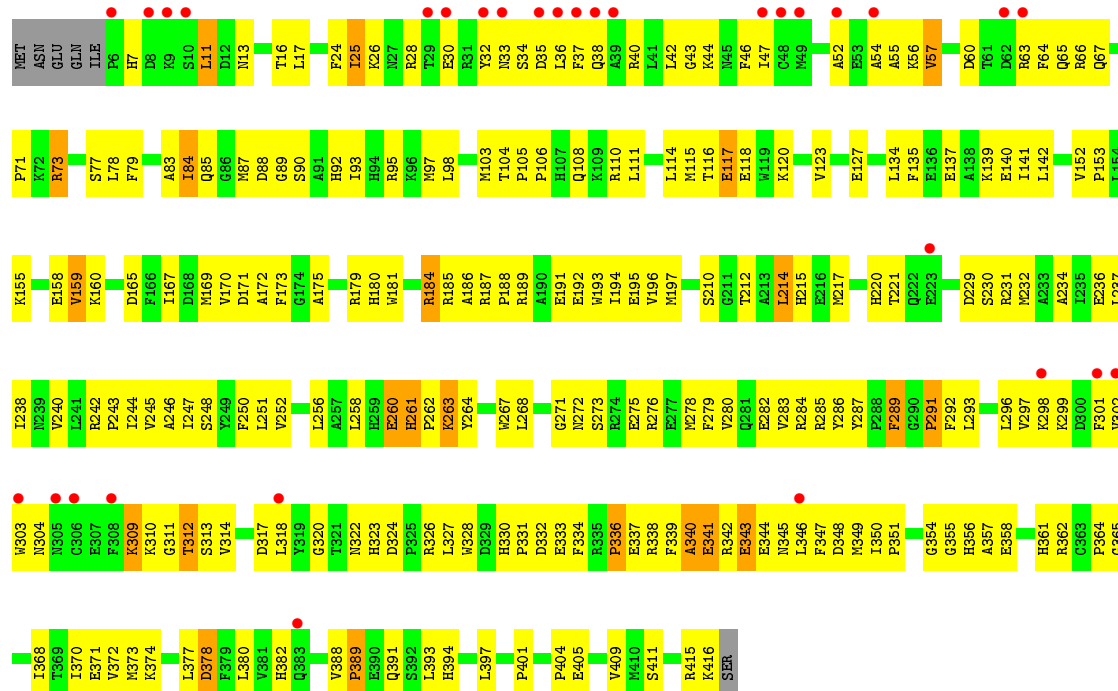
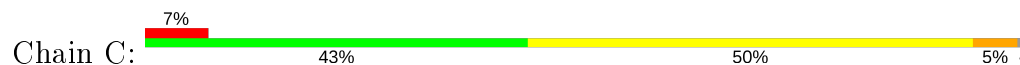
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	17	Total 17	O 17	0	0
3	C	12	Total 12	O 12	0	0



• Molecule 1: Cytochrome P450 152A1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	173.08Å 173.08Å 279.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 2.90 46.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (46.60-2.90) 95.0 (46.60-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.286 0.216 , 0.213	Depositor DCC
R_{free} test set	1704 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10203	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% 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

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	0.43	0/3422	0.62	0/4614
1	B	0.43	0/3422	0.63	0/4614
1	C	0.38	0/3422	0.57	0/4614
All	All	0.41	0/10266	0.61	0/13842

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3339	0	3290	133	0
1	B	3339	0	3290	158	0
1	C	3339	0	3290	240	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
2	C	43	0	30	6	0
3	A	28	0	0	2	0
3	B	17	0	0	2	0
3	C	12	0	0	0	0
All	All	10203	0	9960	531	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 26.

All (531) 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:284:ARG:HH11	1:C:370:ILE:HD11	1.19	1.05
1:A:109:LYS:HE3	1:A:109:LYS:HA	1.43	0.99
1:B:391:GLN:HE22	1:B:409:VAL:H	1.09	0.96
1:C:25:ILE:HD12	1:C:26:LYS:H	1.30	0.95
1:B:44:LYS:HE2	1:B:45:ASN:H	1.31	0.94
1:C:345:ASN:HD22	1:C:348:ASP:HB3	1.32	0.94
1:B:153:PRO:HD2	1:B:197:MET:SD	2.11	0.90
1:A:160:LYS:HD3	1:A:161:GLU:H	1.37	0.89
1:A:391:GLN:HE22	1:A:409:VAL:H	1.16	0.87
1:C:84:ILE:HD13	1:C:95:ARG:HB3	1.57	0.86
1:C:65:GLN:NE2	1:C:67:GLN:HB2	1.91	0.86
1:B:280:VAL:HG21	1:B:374:LYS:HG2	1.56	0.85
1:B:328:TRP:O	1:B:331:PRO:HD3	1.77	0.85
1:C:11:LEU:HD22	1:C:40:ARG:HG2	1.59	0.82
1:B:342:ARG:HH11	1:B:342:ARG:HG3	1.44	0.82
1:C:391:GLN:HE21	1:C:393:LEU:HD21	1.44	0.82
1:A:391:GLN:NE2	1:A:409:VAL:H	1.77	0.81
1:A:160:LYS:HE3	1:A:161:GLU:HG3	1.62	0.80
1:B:272:ASN:CG	1:B:273:SER:H	1.85	0.79
1:C:73:ARG:HB2	1:C:73:ARG:NH1	1.97	0.79
1:B:391:GLN:HE22	1:B:409:VAL:N	1.81	0.78
1:C:114:LEU:O	1:C:117:GLU:HG3	1.82	0.78
1:A:292:PHE:HA	1:A:318:LEU:HD13	1.64	0.78
1:A:403:LEU:HD12	1:A:404:PRO:HD2	1.66	0.78
1:A:391:GLN:HE22	1:A:409:VAL:N	1.81	0.77
1:C:127:GLU:CD	1:C:415:ARG:HG2	2.05	0.77
1:C:268:LEU:HD23	1:C:275:GLU:HB3	1.66	0.77
1:C:272:ASN:CG	1:C:273:SER:H	1.85	0.77
1:B:150:ALA:HB1	1:B:213:ALA:HB3	1.66	0.76
1:A:160:LYS:CE	1:A:161:GLU:HG3	2.17	0.75
1:C:260:GLU:O	1:C:262:PRO:HD3	1.87	0.75
1:C:54:ALA:O	1:C:57:VAL:HG23	1.87	0.75
1:C:264:TYR:CZ	1:C:336:PRO:HD2	2.22	0.74
1:C:73:ARG:HH11	1:C:73:ARG:CB	2.00	0.74
1:B:242:ARG:HB3	1:B:243:PRO:HD3	1.69	0.74
1:C:328:TRP:O	1:C:331:PRO:HD3	1.88	0.74
1:B:26:LYS:O	1:B:30:GLU:HG3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:TRP:HB3	1:C:185:ARG:NH1	2.03	0.73
1:C:343:GLU:HG3	1:C:344:GLU:H	1.53	0.73
1:C:187:ARG:HB3	1:C:188:PRO:HD3	1.69	0.73
1:C:247:ILE:HA	2:C:501:HEM:HBB1	1.71	0.73
1:A:385:GLU:HB2	1:A:414:ARG:NH1	2.03	0.73
1:A:52:ALA:O	1:A:56:LYS:HG3	1.88	0.72
1:C:279:PHE:O	1:C:283:VAL:HG23	1.89	0.72
1:B:264:TYR:CZ	1:B:336:PRO:HD2	2.25	0.72
1:A:213:ALA:O	1:A:217:MET:HG2	1.88	0.72
1:B:104:THR:O	1:B:108:GLN:HG3	1.89	0.72
1:B:139:LYS:HE2	1:B:167:ILE:HG13	1.71	0.71
1:A:280:VAL:HG21	1:A:374:LYS:HG2	1.72	0.71
1:B:243:PRO:O	1:B:246:ALA:HB3	1.91	0.71
1:C:95:ARG:HG2	1:C:95:ARG:HH11	1.56	0.71
1:B:210:SER:HA	1:B:215:HIS:CD2	2.26	0.71
1:B:217:MET:HE2	1:B:237:LEU:HA	1.73	0.71
1:B:44:LYS:CE	1:B:45:ASN:H	2.01	0.70
1:A:26:LYS:O	1:A:30:GLU:HG3	1.91	0.70
1:B:44:LYS:HE2	1:B:45:ASN:N	2.05	0.70
1:C:210:SER:HA	1:C:215:HIS:CD2	2.27	0.69
1:C:191:GLU:HB3	1:C:231:ARG:HH11	1.57	0.69
1:A:187:ARG:HB3	1:A:188:PRO:HD3	1.75	0.69
1:B:279:PHE:O	1:B:283:VAL:HG23	1.92	0.69
1:B:385:GLU:HG2	1:B:416:LYS:HD3	1.74	0.69
1:A:382:HIS:O	1:A:416:LYS:HD3	1.93	0.69
1:A:264:TYR:CE1	1:A:336:PRO:HD2	2.27	0.68
1:B:385:GLU:OE2	1:B:416:LYS:HD3	1.93	0.68
1:C:67:GLN:NE2	1:C:298:LYS:NZ	2.42	0.68
1:B:150:ALA:CB	1:B:213:ALA:HB3	2.22	0.68
1:C:25:ILE:CD1	1:C:26:LYS:H	2.04	0.68
1:C:391:GLN:NE2	1:C:393:LEU:HD21	2.08	0.68
1:C:191:GLU:HB3	1:C:231:ARG:NH1	2.09	0.68
1:C:275:GLU:HA	1:C:278:MET:HE3	1.74	0.68
1:A:70:LEU:HD22	1:A:71:PRO:HD2	1.77	0.67
1:C:345:ASN:HB3	1:C:348:ASP:OD1	1.94	0.67
1:A:242:ARG:HB3	1:A:243:PRO:HD3	1.77	0.67
1:C:317:ASP:OD2	1:C:320:GLY:HA3	1.94	0.67
1:B:144:ARG:NH1	1:B:156:GLU:OE2	2.28	0.66
1:B:17:LEU:HD12	1:B:17:LEU:O	1.95	0.66
1:C:139:LYS:HE3	1:C:167:ILE:HG13	1.77	0.66
1:A:127:GLU:OE1	1:A:415:ARG:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:THR:O	1:A:212:THR:HG23	1.96	0.66
1:B:25:ILE:O	1:B:29:THR:HG23	1.96	0.66
1:C:293:LEU:HD21	2:C:501:HEM:HAA2	1.78	0.65
1:B:269:ARG:HA	1:B:382:HIS:HE1	1.62	0.65
1:C:397:LEU:HD12	1:C:397:LEU:N	2.12	0.64
1:B:391:GLN:NE2	1:B:409:VAL:H	1.88	0.64
1:C:240:VAL:O	1:C:243:PRO:HD2	1.97	0.64
1:C:250:PHE:HB3	1:C:373:MET:CE	2.27	0.64
1:B:78:LEU:CD1	1:B:170:VAL:HA	2.29	0.63
1:A:380:LEU:HA	1:A:384:ILE:HD11	1.79	0.63
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.63	0.63
1:C:7:HIS:HA	1:C:38:GLN:HB2	1.81	0.63
1:A:349:MET:HG2	1:A:351:PRO:HD3	1.80	0.63
1:A:277:GLU:HG2	1:A:374:LYS:HD3	1.80	0.62
1:A:109:LYS:CE	1:A:109:LYS:HA	2.24	0.62
1:B:28:ARG:NH1	1:B:28:ARG:HG3	2.15	0.62
1:B:138:ALA:O	1:B:142:LEU:HB2	1.99	0.62
1:B:175:ALA:HB2	1:B:179:ARG:NH1	2.15	0.62
1:A:328:TRP:O	1:A:331:PRO:HD3	2.00	0.62
1:C:180:HIS:NE2	1:C:184:ARG:NH1	2.47	0.62
1:C:79:PHE:HB3	1:C:85:GLN:OE1	2.00	0.61
1:A:385:GLU:HB2	1:A:414:ARG:HH12	1.64	0.61
1:A:64:PHE:CE1	1:A:314:VAL:HG21	2.36	0.61
1:C:236:GLU:HA	1:C:236:GLU:OE2	1.99	0.61
1:C:25:ILE:HD12	1:C:26:LYS:N	2.11	0.61
1:C:256:LEU:HD12	1:C:287:TYR:OH	1.99	0.61
1:A:279:PHE:O	1:A:283:VAL:HG23	2.01	0.61
1:C:397:LEU:HD12	1:C:397:LEU:H	1.66	0.61
1:C:370:ILE:HG22	1:C:374:LYS:HE2	1.82	0.61
1:B:250:PHE:HB3	1:B:373:MET:CE	2.30	0.61
1:C:284:ARG:NH1	1:C:370:ILE:HD11	2.03	0.61
1:C:73:ARG:HB2	1:C:73:ARG:HH11	1.62	0.61
1:C:30:GLU:N	1:C:30:GLU:OE2	2.34	0.61
1:B:76:LYS:O	1:B:187:ARG:HD2	2.00	0.60
1:C:17:LEU:C	1:C:17:LEU:HD23	2.21	0.60
1:C:324:ASP:HB3	1:C:327:LEU:HD12	1.84	0.60
1:B:119:TRP:HB3	1:B:379:PHE:CD1	2.36	0.60
1:A:293:LEU:HG	1:A:318:LEU:HD11	1.83	0.60
1:C:17:LEU:O	1:C:17:LEU:HD23	2.02	0.60
1:B:277:GLU:HA	1:B:374:LYS:HD3	1.83	0.60
1:B:31:ARG:O	1:B:31:ARG:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLN:O	1:A:68:ASN:HB2	2.01	0.60
1:B:63:ARG:HG2	1:B:301:PHE:CD1	2.37	0.59
1:C:104:THR:HB	1:C:105:PRO:CD	2.33	0.59
1:C:63:ARG:HD3	1:C:301:PHE:CE2	2.38	0.59
1:C:64:PHE:HA	1:C:296:LEU:O	2.02	0.59
1:B:239:ASN:HD22	1:B:242:ARG:HH12	1.50	0.59
1:A:17:LEU:HD12	1:A:17:LEU:O	2.03	0.59
1:C:110:ARG:NH1	1:C:114:LEU:HD21	2.18	0.59
1:C:104:THR:HB	1:C:105:PRO:HD2	1.84	0.58
1:B:272:ASN:HB3	1:B:275:GLU:OE2	2.02	0.58
1:C:52:ALA:O	1:C:55:ALA:HB3	2.03	0.58
1:C:191:GLU:HA	1:C:238:ILE:HD11	1.84	0.58
1:C:83:ALA:HA	1:C:232:MET:HE1	1.85	0.58
1:C:73:ARG:NH1	1:C:73:ARG:CB	2.62	0.58
1:C:192:GLU:O	1:C:196:VAL:HG23	2.04	0.58
1:B:342:ARG:HH11	1:B:342:ARG:CG	2.14	0.58
1:C:194:ILE:CG2	1:C:237:LEU:HD23	2.34	0.58
1:A:345:ASN:HB3	1:A:348:ASP:OD1	2.04	0.57
1:B:152:VAL:HG13	1:B:197:MET:SD	2.44	0.57
1:B:272:ASN:ND2	1:B:273:SER:H	2.02	0.57
1:C:127:GLU:OE1	1:C:415:ARG:HG2	2.03	0.57
1:C:272:ASN:CG	1:C:273:SER:N	2.57	0.57
1:C:11:LEU:CD2	1:C:40:ARG:HG2	2.30	0.57
1:C:123:VAL:CG1	1:C:415:ARG:HB3	2.33	0.57
1:C:280:VAL:HG21	1:C:374:LYS:HG2	1.86	0.57
1:B:166:PHE:HE1	1:B:238:ILE:HG23	1.68	0.57
1:C:309:LYS:HG2	1:C:310:LYS:H	1.69	0.57
1:C:391:GLN:OE1	1:C:409:VAL:HB	2.04	0.57
1:C:95:ARG:HG2	1:C:95:ARG:NH1	2.19	0.57
1:C:93:ILE:O	1:C:97:MET:HG2	2.05	0.57
1:B:232:MET:HE3	1:B:235:ILE:HB	1.85	0.57
1:B:272:ASN:CG	1:B:273:SER:N	2.56	0.57
1:B:317:ASP:OD1	1:B:320:GLY:N	2.37	0.57
1:B:385:GLU:CG	1:B:416:LYS:HD3	2.34	0.57
1:A:300:ASP:OD2	1:A:309:LYS:HD3	2.05	0.57
1:B:7:HIS:CD2	1:B:38:GLN:HG3	2.39	0.57
1:C:67:GLN:HE22	1:C:298:LYS:NZ	2.01	0.57
1:C:240:VAL:C	1:C:243:PRO:HD2	2.25	0.56
1:C:78:LEU:O	1:C:78:LEU:HG	2.04	0.56
1:B:368:ILE:O	1:B:372:VAL:HG23	2.04	0.56
1:C:110:ARG:O	1:C:114:LEU:HG	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ASP:HB3	1:C:63:ARG:HB2	1.86	0.56
1:C:155:LYS:O	1:C:159:VAL:HG23	2.06	0.56
1:C:260:GLU:C	1:C:262:PRO:HD3	2.25	0.56
1:B:272:ASN:ND2	1:B:273:SER:N	2.53	0.56
1:A:208:THR:HG22	1:A:215:HIS:HB2	1.88	0.56
1:B:345:ASN:ND2	1:B:346:LEU:H	2.04	0.56
1:B:73:ARG:NH2	1:B:175:ALA:O	2.39	0.55
1:B:369:THR:O	1:B:373:MET:HG3	2.05	0.55
1:C:186:ALA:O	1:C:189:ARG:HB2	2.06	0.55
1:B:56:LYS:HD3	1:B:347:PHE:CD2	2.41	0.55
1:C:194:ILE:HG23	1:C:237:LEU:HD23	1.87	0.55
1:B:274:ARG:HH12	1:B:278:MET:HG3	1.72	0.55
1:B:415:ARG:HG2	1:B:416:LYS:H	1.72	0.55
1:C:302:VAL:HG12	1:C:303:TRP:N	2.21	0.55
1:C:46:PHE:HA	1:C:313:SER:O	2.06	0.55
1:A:66:ARG:HG3	1:A:361:HIS:CD2	2.42	0.55
1:B:274:ARG:NH1	1:B:274:ARG:O	2.40	0.55
1:B:258:LEU:HD11	1:B:268:LEU:HD12	1.89	0.55
1:C:250:PHE:HB3	1:C:373:MET:HE1	1.89	0.55
1:C:309:LYS:HG2	1:C:310:LYS:N	2.22	0.55
1:C:114:LEU:HA	1:C:117:GLU:CG	2.37	0.55
1:B:284:ARG:HH12	1:B:352:GLN:HG3	1.72	0.54
1:C:118:GLU:HG3	1:C:141:ILE:HG23	1.89	0.54
1:C:92:HIS:CD2	1:C:361:HIS:CE1	2.95	0.54
1:C:272:ASN:HB3	1:C:275:GLU:OE1	2.07	0.54
1:C:282:GLU:O	1:C:286:TYR:HB3	2.07	0.54
1:A:109:LYS:O	1:A:113:GLU:HG3	2.08	0.54
1:B:29:THR:HG21	1:B:50:THR:CG2	2.38	0.54
1:C:272:ASN:ND2	1:C:273:SER:H	2.04	0.54
1:A:165:ASP:O	1:A:169:MET:HG3	2.07	0.54
1:A:384:ILE:H	1:A:384:ILE:HD13	1.73	0.54
1:C:330:HIS:N	1:C:331:PRO:CD	2.71	0.54
1:C:16:THR:HG21	1:C:28:ARG:NH2	2.22	0.54
1:A:109:LYS:CA	1:A:109:LYS:HE3	2.26	0.54
1:B:16:THR:HA	1:B:19:LYS:HG2	1.89	0.54
1:B:276:ARG:HH11	1:B:276:ARG:CB	2.21	0.54
1:A:139:LYS:HD2	1:A:167:ILE:HG13	1.90	0.54
1:A:385:GLU:HA	3:A:518:HOH:O	2.08	0.54
1:B:98:LEU:HD22	1:B:220:HIS:CG	2.43	0.54
1:B:24:PHE:HE2	1:B:41:LEU:HD11	1.73	0.54
1:C:105:PRO:HB2	1:C:106:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:THR:CG2	1:C:120:LYS:HE3	2.38	0.54
1:C:328:TRP:HB2	1:C:331:PRO:HB3	1.90	0.54
1:B:394:HIS:HB3	1:B:405:GLU:OE1	2.08	0.54
1:C:181:TRP:HE3	1:C:185:ARG:HD3	1.72	0.54
1:C:229:ASP:O	1:C:232:MET:N	2.40	0.54
1:C:263:LYS:H	1:C:263:LYS:HD3	1.73	0.54
1:C:89:GLY:O	1:C:93:ILE:HG12	2.08	0.54
1:C:111:LEU:HD12	1:C:368:ILE:HD12	1.89	0.53
1:A:160:LYS:HD3	1:A:161:GLU:N	2.15	0.53
1:B:269:ARG:HA	1:B:382:HIS:CE1	2.43	0.53
1:C:282:GLU:HG3	1:C:334:PHE:CE1	2.42	0.53
1:C:343:GLU:HG3	1:C:344:GLU:N	2.22	0.53
1:A:293:LEU:HD13	2:A:501:HEM:CGA	2.37	0.53
1:B:23:LEU:HD21	1:B:397:LEU:HD13	1.90	0.53
1:B:24:PHE:CE2	1:B:41:LEU:HD11	2.43	0.53
1:C:389:PRO:HD3	1:C:411:SER:HB3	1.89	0.53
1:B:16:THR:HG22	1:B:19:LYS:HZ3	1.73	0.53
1:B:281:GLN:OE1	1:B:281:GLN:HA	2.07	0.53
1:C:11:LEU:HD13	1:C:40:ARG:HG2	1.89	0.53
1:C:282:GLU:HG3	1:C:334:PHE:CD1	2.43	0.53
1:C:123:VAL:CG1	1:C:415:ARG:NH1	2.72	0.53
1:C:36:LEU:HD22	1:C:303:TRP:HZ3	1.74	0.53
1:B:285:ARG:HB2	1:B:349:MET:SD	2.48	0.53
1:C:371:GLU:OE2	1:C:371:GLU:HA	2.08	0.53
1:C:283:VAL:HG13	1:C:287:TYR:CD2	2.44	0.53
1:A:191:GLU:HB3	1:A:231:ARG:NH2	2.24	0.52
1:A:352:GLN:HE22	1:A:366:GLU:HA	1.73	0.52
1:A:247:ILE:HA	2:A:501:HEM:HBB1	1.90	0.52
1:B:158:GLU:O	1:B:162:ARG:HG2	2.09	0.52
1:B:239:ASN:ND2	1:B:242:ARG:HH12	2.07	0.52
1:C:63:ARG:HD3	1:C:301:PHE:CD2	2.45	0.52
1:B:155:LYS:HB2	1:B:158:GLU:HG2	1.91	0.52
1:B:155:LYS:O	1:B:159:VAL:HG23	2.09	0.52
1:C:191:GLU:O	1:C:195:GLU:HB2	2.10	0.52
1:C:283:VAL:HG13	1:C:287:TYR:HD2	1.74	0.52
1:C:416:LYS:NZ	1:C:416:LYS:HB3	2.25	0.52
1:A:335:ARG:HB3	1:A:337:GLU:OE1	2.09	0.51
1:B:264:TYR:CE1	1:B:336:PRO:HD2	2.44	0.51
1:C:338:ARG:O	1:C:342:ARG:NH1	2.43	0.51
1:B:247:ILE:HA	2:B:501:HEM:HBB1	1.91	0.51
1:A:71:PRO:HG2	1:A:74:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HD3	1:A:416:LYS:HZ1	1.75	0.51
1:B:187:ARG:HB3	1:B:188:PRO:HD3	1.92	0.51
1:C:355:GLY:O	1:C:362:ARG:HD3	2.10	0.51
1:C:73:ARG:HB3	1:C:73:ARG:HH11	1.75	0.51
1:A:261:HIS:HB3	1:A:264:TYR:HD2	1.75	0.51
1:B:244:ILE:HG13	2:B:501:HEM:HBC2	1.93	0.51
1:C:181:TRP:HE3	1:C:185:ARG:CD	2.23	0.51
1:C:394:HIS:O	1:C:404:PRO:HA	2.11	0.51
1:B:259:HIS:O	1:B:262:PRO:HD3	2.10	0.50
1:B:57:VAL:HG12	1:B:64:PHE:HE2	1.75	0.50
1:C:283:VAL:O	1:C:287:TYR:HB2	2.11	0.50
1:C:327:LEU:HB2	1:C:328:TRP:CD1	2.46	0.50
1:C:173:PHE:CE2	1:C:401:PRO:HD3	2.45	0.50
1:C:28:ARG:HB2	1:C:37:PHE:CE2	2.47	0.50
1:C:79:PHE:CG	1:C:85:GLN:HG2	2.46	0.50
1:A:103:MET:SD	1:A:364:PRO:HG2	2.51	0.50
1:A:274:ARG:NE	1:A:278:MET:HE2	2.27	0.50
1:B:293:LEU:O	1:B:315:LEU:HA	2.12	0.50
1:C:285:ARG:HB2	1:C:349:MET:SD	2.51	0.50
1:B:268:LEU:HD22	1:B:276:ARG:HG2	1.93	0.50
1:C:65:GLN:HB3	1:C:298:LYS:HD3	1.92	0.50
1:A:198:ILE:HG21	1:A:230:SER:HA	1.92	0.50
1:A:277:GLU:HG2	1:A:374:LYS:CD	2.40	0.50
1:C:272:ASN:ND2	1:C:273:SER:N	2.59	0.50
1:C:337:GLU:CD	1:C:337:GLU:H	2.14	0.50
1:A:297:VAL:HG12	1:A:310:LYS:HA	1.94	0.50
1:C:114:LEU:HA	1:C:117:GLU:HG2	1.94	0.50
1:C:87:MET:HB3	1:C:92:HIS:HB2	1.94	0.49
1:C:391:GLN:HE21	1:C:393:LEU:CD2	2.20	0.49
1:B:298:LYS:O	1:B:310:LYS:HG3	2.13	0.49
1:B:49:MET:HE3	1:B:314:VAL:HG21	1.93	0.49
1:B:96:LYS:HE3	1:B:364:PRO:HD3	1.94	0.49
1:C:312:THR:O	1:C:314:VAL:HG13	2.13	0.49
1:B:276:ARG:HB2	1:B:276:ARG:NH1	2.28	0.49
1:C:232:MET:HE3	1:C:236:GLU:HG2	1.94	0.49
1:A:95:ARG:NH1	1:A:236:GLU:OE2	2.46	0.49
1:A:25:ILE:HG21	1:A:317:ASP:HB2	1.93	0.49
1:C:118:GLU:CG	1:C:141:ILE:HG23	2.42	0.49
1:C:244:ILE:HA	2:C:501:HEM:HMC3	1.94	0.49
1:B:162:ARG:HD2	1:B:193:TRP:CZ3	2.48	0.49
1:C:416:LYS:HZ2	1:C:416:LYS:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:CYS:SG	1:A:154:LEU:HD22	2.53	0.48
1:B:342:ARG:HD3	1:B:343:GLU:O	2.13	0.48
1:C:246:ALA:C	1:C:248:SER:H	2.15	0.48
1:A:185:ARG:C	1:A:188:PRO:HD2	2.32	0.48
1:A:317:ASP:OD2	1:A:320:GLY:HA3	2.13	0.48
1:A:368:ILE:HD12	2:A:501:HEM:HBC2	1.94	0.48
1:C:242:ARG:HB3	1:C:243:PRO:HD3	1.94	0.48
1:A:381:VAL:HG12	1:A:382:HIS:ND1	2.28	0.48
1:C:67:GLN:NE2	1:C:298:LYS:HZ3	2.09	0.48
1:C:221:THR:O	1:C:221:THR:HG23	2.13	0.48
1:C:56:LYS:HG2	1:C:347:PHE:CD2	2.48	0.48
1:A:244:ILE:HG12	2:A:501:HEM:HMC2	1.95	0.48
1:A:328:TRP:CE3	1:A:342:ARG:NH1	2.82	0.48
1:B:73:ARG:HD2	3:B:503:HOH:O	2.14	0.48
1:B:250:PHE:HE2	1:B:352:GLN:NE2	2.12	0.48
1:C:77:SER:O	1:C:169:MET:HB3	2.14	0.48
1:A:327:LEU:HB2	1:A:328:TRP:CD1	2.48	0.48
1:A:36:LEU:C	1:A:36:LEU:HD12	2.34	0.48
1:B:247:ILE:HG22	1:B:247:ILE:O	2.14	0.48
1:B:409:VAL:HG12	1:B:410:MET:N	2.28	0.48
1:C:165:ASP:HB3	1:C:186:ALA:HB1	1.95	0.48
1:C:43:GLY:O	1:C:44:LYS:HG2	2.14	0.48
1:C:135:PHE:HD1	1:C:252:VAL:HG21	1.78	0.48
1:C:25:ILE:CD1	1:C:26:LYS:N	2.73	0.48
1:C:95:ARG:NH1	1:C:236:GLU:OE1	2.47	0.48
1:B:46:PHE:HA	1:B:313:SER:O	2.14	0.48
1:B:126:TRP:HB3	1:B:413:ILE:HD12	1.95	0.48
1:C:246:ALA:C	1:C:248:SER:N	2.65	0.48
1:A:354:GLY:HA2	1:A:362:ARG:NH1	2.29	0.48
1:A:282:GLU:HG3	1:A:334:PHE:CE1	2.49	0.47
1:C:127:GLU:OE2	1:C:415:ARG:HG2	2.13	0.47
1:A:63:ARG:CZ	1:A:301:PHE:CD2	2.96	0.47
1:A:385:GLU:CB	1:A:414:ARG:HH12	2.26	0.47
1:B:93:ILE:HD12	1:B:358:GLU:O	2.14	0.47
1:B:261:HIS:CE1	1:B:334:PHE:HB3	2.50	0.47
1:C:170:VAL:C	1:C:172:ALA:H	2.17	0.47
1:B:162:ARG:HD2	1:B:193:TRP:CH2	2.49	0.47
1:B:221:THR:HA	1:B:227:GLN:HA	1.96	0.47
1:C:339:PHE:O	1:C:341:GLU:N	2.48	0.47
1:C:345:ASN:O	1:C:348:ASP:OD1	2.33	0.47
1:A:104:THR:HB	1:A:105:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:HG2	1:A:377:LEU:HD23	1.95	0.47
1:B:244:ILE:CG1	2:B:501:HEM:HBC2	2.45	0.47
1:C:65:GLN:HE21	1:C:67:GLN:HB2	1.77	0.47
1:C:67:GLN:HG3	1:C:88:ASP:OD2	2.14	0.47
1:A:185:ARG:O	1:A:188:PRO:HD2	2.14	0.47
1:B:240:VAL:O	1:B:244:ILE:HG13	2.15	0.47
1:B:232:MET:HA	1:B:232:MET:HE3	1.97	0.47
1:B:274:ARG:O	1:B:278:MET:HE2	2.15	0.47
1:B:250:PHE:HE2	1:B:352:GLN:HE22	1.63	0.47
1:B:154:LEU:HD12	1:B:158:GLU:HG3	1.96	0.47
1:C:247:ILE:HG22	1:C:251:LEU:HD13	1.97	0.47
1:C:268:LEU:HD13	1:C:377:LEU:HD21	1.95	0.47
1:C:47:ILE:HB	1:C:314:VAL:HG12	1.95	0.47
1:C:64:PHE:CE1	1:C:314:VAL:HG21	2.50	0.47
1:B:6:PRO:HD2	1:B:36:LEU:O	2.15	0.46
1:C:32:TYR:O	1:C:34:SER:N	2.48	0.46
1:C:247:ILE:HD11	2:C:501:HEM:HMC2	1.98	0.46
1:C:98:LEU:HB2	1:C:220:HIS:CE1	2.51	0.46
1:C:123:VAL:HG11	1:C:415:ARG:NH1	2.31	0.46
1:A:394:HIS:O	1:A:405:GLU:HG3	2.16	0.46
1:B:187:ARG:NH1	1:B:191:GLU:OE2	2.48	0.46
1:B:345:ASN:HB3	1:B:348:ASP:OD1	2.15	0.46
1:C:214:LEU:O	1:C:214:LEU:HD22	2.16	0.46
1:C:297:VAL:HG23	1:C:312:THR:O	2.16	0.46
1:A:264:TYR:CZ	1:A:336:PRO:HD2	2.51	0.46
1:A:99:PHE:CZ	1:A:236:GLU:HG3	2.50	0.46
1:B:330:HIS:HB3	1:B:333:GLU:HB2	1.97	0.46
1:C:247:ILE:HG22	1:C:247:ILE:O	2.15	0.46
1:C:267:TRP:CZ2	1:C:275:GLU:HG3	2.51	0.46
1:A:152:VAL:HG13	1:A:197:MET:SD	2.56	0.46
1:B:234:ALA:O	1:B:238:ILE:HG12	2.16	0.46
1:B:250:PHE:HB3	1:B:373:MET:HE1	1.97	0.46
1:B:282:GLU:HG3	1:B:334:PHE:CE1	2.51	0.46
1:C:374:LYS:O	1:C:377:LEU:HB3	2.16	0.46
1:A:13:ASN:OD1	1:A:39:ALA:HB1	2.16	0.45
1:B:276:ARG:HH11	1:B:276:ARG:HB2	1.81	0.45
1:C:167:ILE:HD11	1:C:245:VAL:HG12	1.97	0.45
1:A:54:ALA:O	1:A:57:VAL:N	2.48	0.45
1:B:103:MET:CE	2:B:501:HEM:HAC	2.47	0.45
1:B:111:LEU:HD12	1:B:368:ILE:HD13	1.97	0.45
1:C:158:GLU:O	1:C:159:VAL:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASP:O	1:C:231:ARG:N	2.50	0.45
1:A:46:PHE:CZ	1:A:313:SER:HB3	2.52	0.45
1:B:342:ARG:NH1	1:B:342:ARG:HG3	2.21	0.45
1:B:365:GLY:HA3	2:B:501:HEM:C3C	2.51	0.45
1:C:280:VAL:HG21	1:C:374:LYS:CG	2.45	0.45
1:A:330:HIS:HB3	1:A:333:GLU:HG3	1.98	0.45
1:A:47:ILE:HB	1:A:314:VAL:HG12	1.99	0.45
1:B:160:LYS:CD	1:B:160:LYS:H	2.30	0.45
1:B:96:LYS:HE3	1:B:364:PRO:HB3	1.99	0.45
1:B:277:GLU:HG2	1:B:374:LYS:HE2	1.99	0.45
1:B:354:GLY:HA2	1:B:362:ARG:NH1	2.32	0.45
1:C:365:GLY:O	1:C:368:ILE:HB	2.16	0.45
1:C:111:LEU:CD1	1:C:368:ILE:HD12	2.47	0.45
1:C:71:PRO:HB2	1:C:73:ARG:HG2	1.98	0.45
1:A:229:ASP:OD2	1:A:229:ASP:N	2.45	0.44
1:A:337:GLU:C	1:A:339:PHE:N	2.70	0.44
1:A:93:ILE:O	1:A:97:MET:HG2	2.17	0.44
1:C:175:ALA:HB2	1:C:179:ARG:NH1	2.32	0.44
1:A:403:LEU:CD1	1:A:404:PRO:HD2	2.43	0.44
1:A:324:ASP:OD2	1:A:326:ARG:HB2	2.17	0.44
1:C:152:VAL:HG13	1:C:197:MET:SD	2.58	0.44
1:B:404:PRO:O	1:B:405:GLU:C	2.55	0.44
1:C:210:SER:C	1:C:212:THR:H	2.21	0.44
1:C:195:GLU:HA	1:C:234:ALA:HB2	1.99	0.44
1:A:269:ARG:HE	1:A:269:ARG:HB2	1.61	0.44
1:A:282:GLU:HG3	1:A:334:PHE:CD1	2.53	0.44
1:A:406:SER:C	1:A:408:PHE:H	2.20	0.44
1:B:264:TYR:HA	1:B:267:TRP:HB3	1.99	0.44
1:A:84:ILE:HG23	1:A:85:GLN:N	2.33	0.44
1:C:115:MET:HG3	1:C:372:VAL:HG13	2.00	0.44
1:A:269:ARG:NH1	1:A:416:LYS:NZ	2.66	0.43
1:B:115:MET:HG3	1:B:372:VAL:HG13	2.00	0.43
1:B:16:THR:HG22	1:B:19:LYS:NZ	2.33	0.43
1:B:36:LEU:HD22	1:B:303:TRP:HZ3	1.81	0.43
1:B:173:PHE:CD1	1:B:174:GLY:N	2.87	0.43
1:C:296:LEU:HG	1:C:311:GLY:HA2	2.00	0.43
1:C:304:ASN:O	1:C:304:ASN:OD1	2.36	0.43
1:C:349:MET:HG3	1:C:351:PRO:HD3	2.00	0.43
1:A:340:ALA:O	1:A:341:GLU:HB2	2.18	0.43
1:A:78:LEU:HD23	1:A:79:PHE:CE1	2.53	0.43
1:C:191:GLU:HA	1:C:238:ILE:CD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ARG:CZ	1:C:378:ASP:OD1	2.66	0.43
1:C:247:ILE:HD11	2:C:501:HEM:CMC	2.48	0.43
1:A:261:HIS:N	1:A:262:PRO:HD3	2.34	0.43
1:C:83:ALA:O	1:C:85:GLN:N	2.51	0.43
1:B:78:LEU:HD13	1:B:170:VAL:HA	2.00	0.43
1:B:209:THR:O	1:B:212:THR:HG23	2.18	0.43
1:B:62:ASP:O	1:B:299:LYS:HE3	2.19	0.43
1:C:11:LEU:HD22	1:C:40:ARG:CG	2.40	0.43
1:A:104:THR:HB	1:A:105:PRO:CD	2.48	0.43
1:C:13:ASN:HB2	1:C:40:ARG:O	2.18	0.43
1:C:56:LYS:HG2	1:C:347:PHE:CE2	2.54	0.43
1:A:345:ASN:ND2	1:A:346:LEU:H	2.17	0.43
1:B:58:PHE:HA	1:B:64:PHE:CD2	2.54	0.43
1:C:104:THR:OG1	1:C:106:PRO:HD2	2.19	0.43
1:C:330:HIS:HD2	1:C:333:GLU:HG3	1.83	0.43
1:A:292:PHE:O	1:A:293:LEU:HD23	2.19	0.43
1:A:36:LEU:O	1:A:36:LEU:HD12	2.19	0.43
1:B:119:TRP:HA	1:B:119:TRP:CE3	2.54	0.43
1:C:324:ASP:OD2	1:C:326:ARG:HB2	2.19	0.43
1:A:170:VAL:O	1:A:173:PHE:CD2	2.72	0.43
1:A:214:LEU:O	1:A:214:LEU:HD23	2.18	0.43
1:A:261:HIS:HB3	1:A:264:TYR:CD2	2.54	0.43
1:C:262:PRO:O	1:C:263:LYS:C	2.57	0.43
1:A:102:LEU:HD21	1:A:216:GLU:HG3	2.00	0.43
1:A:406:SER:C	1:A:408:PHE:N	2.72	0.43
1:B:296:LEU:HD12	1:B:296:LEU:HA	1.75	0.43
1:B:318:LEU:HG	1:B:350:ILE:O	2.19	0.43
1:C:322:ASN:O	1:C:323:HIS:HD2	2.02	0.43
1:C:357:ALA:HA	1:C:362:ARG:HB3	2.01	0.43
1:C:330:HIS:HB3	1:C:333:GLU:HB2	2.01	0.42
1:C:140:GLU:OE2	1:C:160:LYS:HG3	2.19	0.42
1:A:261:HIS:CD2	1:A:334:PHE:CD2	3.06	0.42
1:B:269:ARG:C	1:B:271:GLY:H	2.22	0.42
1:B:33:ASN:OD1	3:B:504:HOH:O	2.21	0.42
1:B:7:HIS:CG	1:B:38:GLN:HG3	2.53	0.42
1:C:361:HIS:HA	2:C:501:HEM:O1D	2.19	0.42
1:A:155:LYS:O	1:A:158:GLU:HB3	2.19	0.42
1:A:337:GLU:O	1:A:339:PHE:N	2.52	0.42
1:A:386:TYR:CD2	1:A:386:TYR:N	2.87	0.42
1:A:70:LEU:CD2	1:A:71:PRO:HD2	2.48	0.42
1:B:377:LEU:O	1:B:378:ASP:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:MET:O	1:C:236:GLU:HG2	2.19	0.42
1:C:309:LYS:CG	1:C:310:LYS:H	2.28	0.42
1:C:84:ILE:HD13	1:C:95:ARG:CB	2.40	0.42
1:A:107:HIS:O	1:A:108:GLN:C	2.56	0.42
1:A:399:ARG:NH1	1:A:401:PRO:O	2.53	0.42
1:B:269:ARG:C	1:B:271:GLY:N	2.73	0.42
1:C:88:ASP:N	1:C:92:HIS:HB2	2.35	0.42
1:A:12:ASP:N	3:A:520:HOH:O	2.52	0.42
1:B:123:VAL:O	1:B:127:GLU:HG3	2.19	0.42
1:C:261:HIS:HA	1:C:263:LYS:HE3	2.02	0.42
1:C:311:GLY:O	1:C:312:THR:C	2.58	0.42
1:C:354:GLY:HA2	1:C:362:ARG:HH11	1.84	0.42
1:C:36:LEU:N	1:C:36:LEU:HD23	2.35	0.42
1:A:337:GLU:C	1:A:339:PHE:H	2.23	0.42
1:A:42:LEU:O	1:A:44:LYS:N	2.53	0.42
1:B:280:VAL:O	1:B:284:ARG:HG3	2.20	0.42
1:B:49:MET:CE	1:B:314:VAL:HG21	2.50	0.42
1:C:152:VAL:HA	1:C:153:PRO:HD3	1.83	0.42
1:C:356:HIS:C	1:C:358:GLU:N	2.71	0.42
1:C:92:HIS:NE2	1:C:361:HIS:CE1	2.87	0.42
1:A:236:GLU:OE1	1:A:236:GLU:HA	2.19	0.42
1:B:53:GLU:O	1:B:57:VAL:HG23	2.20	0.42
1:C:26:LYS:O	1:C:26:LYS:HG2	2.20	0.42
1:A:105:PRO:HB2	1:A:106:PRO:HD3	2.02	0.42
1:A:352:GLN:NE2	1:A:366:GLU:HA	2.34	0.42
1:B:29:THR:HG21	1:B:50:THR:HG21	2.01	0.42
1:C:187:ARG:NH1	1:C:187:ARG:HG3	2.34	0.42
1:C:282:GLU:O	1:C:282:GLU:HG3	2.20	0.42
1:A:124:THR:O	1:A:128:LYS:HE3	2.19	0.41
1:A:337:GLU:CD	1:A:337:GLU:H	2.22	0.41
1:A:364:PRO:HD2	2:A:501:HEM:C1D	2.55	0.41
1:A:40:ARG:NH2	1:A:45:ASN:OD1	2.53	0.41
1:A:46:PHE:CE1	1:A:313:SER:HB3	2.55	0.41
1:C:302:VAL:CG1	1:C:303:TRP:N	2.83	0.41
1:C:328:TRP:CZ3	1:C:342:ARG:NH1	2.88	0.41
1:A:66:ARG:NH1	1:A:66:ARG:HG3	2.35	0.41
1:C:139:LYS:HE3	1:C:167:ILE:CG1	2.49	0.41
1:C:291:PRO:O	1:C:318:LEU:HB2	2.20	0.41
1:B:284:ARG:NH1	1:B:352:GLN:HG3	2.33	0.41
1:C:280:VAL:HG13	1:C:373:MET:SD	2.60	0.41
1:A:36:LEU:HA	1:A:48:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ARG:NH1	1:B:342:ARG:CG	2.74	0.41
1:C:339:PHE:HE2	1:C:349:MET:CE	2.34	0.41
1:C:388:VAL:O	1:C:389:PRO:O	2.38	0.41
1:A:35:ASP:O	1:A:49:MET:HA	2.20	0.41
1:B:385:GLU:HG2	1:B:416:LYS:CD	2.47	0.41
1:C:24:PHE:CE1	1:C:28:ARG:CZ	3.03	0.41
1:C:345:ASN:C	1:C:347:PHE:H	2.23	0.41
1:B:36:LEU:HD22	1:B:303:TRP:CZ3	2.55	0.41
1:B:280:VAL:CG2	1:B:374:LYS:HG2	2.40	0.41
1:C:232:MET:CE	1:C:236:GLU:HG2	2.50	0.41
1:A:160:LYS:HE3	1:A:161:GLU:CG	2.44	0.41
1:B:236:GLU:OE1	1:B:236:GLU:HA	2.21	0.41
1:C:137:GLU:O	1:C:141:ILE:HG13	2.21	0.41
1:C:350:ILE:N	1:C:351:PRO:CD	2.84	0.41
1:A:103:MET:HG2	1:A:368:ILE:HD12	2.03	0.41
1:A:328:TRP:CZ3	1:A:342:ARG:NH1	2.89	0.40
1:B:191:GLU:OE2	1:B:235:ILE:HG12	2.21	0.40
1:C:108:GLN:HB3	1:C:371:GLU:HG3	2.03	0.40
1:C:297:VAL:HG12	1:C:299:LYS:O	2.21	0.40
1:C:296:LEU:HG	1:C:311:GLY:O	2.21	0.40
1:C:380:LEU:HA	1:C:380:LEU:HD23	1.80	0.40
1:A:280:VAL:HG21	1:A:374:LYS:CG	2.46	0.40
1:B:120:LYS:O	1:B:123:VAL:HG23	2.21	0.40
1:B:29:THR:HG21	1:B:50:THR:HG22	2.03	0.40
1:C:250:PHE:HB3	1:C:373:MET:HE3	2.00	0.40
1:C:32:TYR:C	1:C:34:SER:N	2.73	0.40
1:C:34:SER:OG	1:C:35:ASP:N	2.53	0.40
1:C:103:MET:SD	1:C:364:PRO:O	2.80	0.40
1:B:335:ARG:O	1:B:336:PRO:C	2.57	0.40
1:C:340:ALA:O	1:C:341:GLU:C	2.59	0.40
1:C:36:LEU:HG	1:C:36:LEU:O	2.21	0.40
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.90	0.40
1:B:185:ARG:O	1:B:188:PRO:HD2	2.21	0.40
1:C:279:PHE:CE2	1:C:334:PHE:HE2	2.39	0.40
1:C:296:LEU:HD12	1:C:313:SER:HA	2.04	0.40
1:C:388:VAL:HA	1:C:389:PRO:HD2	1.87	0.40
1:C:11:LEU:CD1	1:C:40:ARG:HG2	2.51	0.40
1:A:211:GLY:N	1:A:216:GLU:OE2	2.47	0.40
1:A:293:LEU:O	1:A:315:LEU:HA	2.22	0.40
1:B:171:ASP:HA	1:B:401:PRO:HD2	2.04	0.40
1:C:349:MET:HG2	1:C:351:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ILE:O	1:C:372:VAL:HG23	2.21	0.40
1:C:66:ARG:HA	1:C:66:ARG:HD3	1.81	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	409/417 (98%)	372 (91%)	33 (8%)	4 (1%)	15	45
1	B	409/417 (98%)	375 (92%)	24 (6%)	10 (2%)	6	22
1	C	409/417 (98%)	349 (85%)	42 (10%)	18 (4%)	2	10
All	All	1227/1251 (98%)	1096 (89%)	99 (8%)	32 (3%)	5	20

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	C	159	VAL
1	C	289	PHE
1	C	309	LYS
1	C	340	ALA
1	C	389	PRO
1	B	343	GLU
1	C	33	ASN
1	C	84	ILE
1	C	230	SER
1	B	257	ALA
1	B	260	GLU
1	B	405	GLU
1	C	171	ASP
1	C	271	GLY

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Mol	Chain	Res	Type
1	C	291	PRO
1	C	346	LEU
1	B	289	PHE
1	C	193	TRP
1	C	258	LEU
1	C	343	GLU
1	C	405	GLU
1	A	43	GLY
1	B	291	PRO
1	B	389	PRO
1	C	312	THR
1	A	289	PHE
1	A	291	PRO
1	B	178	PRO
1	B	262	PRO
1	B	404	PRO
1	C	261	HIS

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	352/358 (98%)	332 (94%)	20 (6%)	20	51
1	B	352/358 (98%)	328 (93%)	24 (7%)	16	42
1	C	352/358 (98%)	331 (94%)	21 (6%)	19	49
All	All	1056/1074 (98%)	991 (94%)	65 (6%)	18	47

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	23	LEU
1	A	82	ASN
1	A	109	LYS
1	A	160	LYS

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Mol	Chain	Res	Type
1	A	192	GLU
1	A	208	THR
1	A	221	THR
1	A	229	ASP
1	A	231	ARG
1	A	236	GLU
1	A	237	LEU
1	A	251	LEU
1	A	289	PHE
1	A	292	PHE
1	A	305	ASN
1	A	310	LYS
1	A	336	PRO
1	A	384	ILE
1	A	414	ARG
1	B	17	LEU
1	B	31	ARG
1	B	36	LEU
1	B	44	LYS
1	B	82	ASN
1	B	134	LEU
1	B	142	LEU
1	B	160	LYS
1	B	214	LEU
1	B	217	MET
1	B	237	LEU
1	B	251	LEU
1	B	277	GLU
1	B	289	PHE
1	B	292	PHE
1	B	296	LEU
1	B	305	ASN
1	B	307	GLU
1	B	333	GLU
1	B	342	ARG
1	B	346	LEU
1	B	352	GLN
1	B	368	ILE
1	B	394	HIS
1	C	11	LEU
1	C	25	ILE
1	C	42	LEU

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Mol	Chain	Res	Type
1	C	57	VAL
1	C	73	ARG
1	C	90	SER
1	C	117	GLU
1	C	134	LEU
1	C	142	LEU
1	C	184	ARG
1	C	214	LEU
1	C	217	MET
1	C	260	GLU
1	C	263	LYS
1	C	289	PHE
1	C	292	PHE
1	C	332	ASP
1	C	336	PRO
1	C	341	GLU
1	C	378	ASP
1	C	382	HIS

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

Mol	Chain	Res	Type
1	A	7	HIS
1	A	38	GLN
1	A	107	HIS
1	A	305	ASN
1	A	352	GLN
1	A	391	GLN
1	B	227	GLN
1	B	239	ASN
1	B	261	HIS
1	B	272	ASN
1	B	304	ASN
1	B	305	ASN
1	B	345	ASN
1	B	352	GLN
1	B	382	HIS
1	B	391	GLN
1	C	67	GLN
1	C	107	HIS
1	C	108	GLN
1	C	215	HIS

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Mol	Chain	Res	Type
1	C	272	ASN
1	C	304	ASN
1	C	345	ASN
1	C	391	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	C	501	1	27,50,50	1.98	7 (25%)	17,82,82	1.88	5 (29%)
2	HEM	A	501	1	27,50,50	1.64	5 (18%)	17,82,82	2.33	8 (47%)
2	HEM	B	501	1	27,50,50	1.92	4 (14%)	17,82,82	2.28	8 (47%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	501	1	-	0/6/54/54	-
2	HEM	A	501	1	-	0/6/54/54	-
2	HEM	B	501	1	-	0/6/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-CAC	-5.68	1.36	1.47
2	C	501	HEM	C3C-CAC	-5.34	1.36	1.47
2	A	501	HEM	C3C-CAC	-5.21	1.37	1.47
2	B	501	HEM	C3B-CAB	-4.50	1.38	1.47
2	B	501	HEM	C4B-NB	4.21	1.44	1.36
2	C	501	HEM	C3B-CAB	-3.76	1.40	1.47
2	C	501	HEM	C1D-ND	3.65	1.43	1.36
2	C	501	HEM	C1D-CHD	3.28	1.50	1.41
2	C	501	HEM	C4B-NB	3.13	1.42	1.36
2	A	501	HEM	C4B-NB	2.99	1.42	1.36
2	B	501	HEM	C1D-ND	2.87	1.42	1.36
2	A	501	HEM	C1D-ND	2.81	1.42	1.36
2	A	501	HEM	C4A-NA	2.78	1.41	1.36
2	C	501	HEM	C1A-NA	2.54	1.41	1.36
2	A	501	HEM	C3B-CAB	-2.53	1.42	1.47
2	C	501	HEM	C3B-C2B	-2.28	1.37	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CBA-CAA-C2A	5.57	122.76	112.49
2	C	501	HEM	C1D-C2D-C3D	4.77	110.32	107.00
2	B	501	HEM	CBD-CAD-C3D	3.64	119.18	112.48
2	B	501	HEM	C3C-C4C-NC	-3.56	104.23	110.94
2	B	501	HEM	C1D-C2D-C3D	3.44	109.39	107.00
2	B	501	HEM	CMC-C2C-C3C	3.26	130.77	124.68
2	A	501	HEM	CMA-C3A-C4A	-3.14	123.64	128.46
2	C	501	HEM	C3C-C4C-NC	-3.03	105.23	110.94
2	A	501	HEM	C3C-C4C-NC	-3.03	105.23	110.94
2	B	501	HEM	C4C-C3C-C2C	2.93	108.94	106.90
2	A	501	HEM	C1D-C2D-C3D	2.79	108.94	107.00
2	A	501	HEM	CMC-C2C-C3C	2.77	129.85	124.68
2	A	501	HEM	CMA-C3A-C2A	2.68	130.00	124.94
2	B	501	HEM	CMD-C2D-C3D	-2.51	120.21	124.94
2	C	501	HEM	CBD-CAD-C3D	-2.51	107.86	112.48
2	B	501	HEM	CBA-CAA-C2A	2.46	117.01	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CMB-C2B-C3B	2.43	129.22	124.68
2	B	501	HEM	CMB-C2B-C3B	2.37	129.12	124.68
2	C	501	HEM	CMD-C2D-C3D	-2.23	120.73	124.94
2	C	501	HEM	CMA-C3A-C4A	-2.19	125.10	128.46
2	A	501	HEM	C4C-C3C-C2C	2.10	108.36	106.90

There are no chirality outliers.

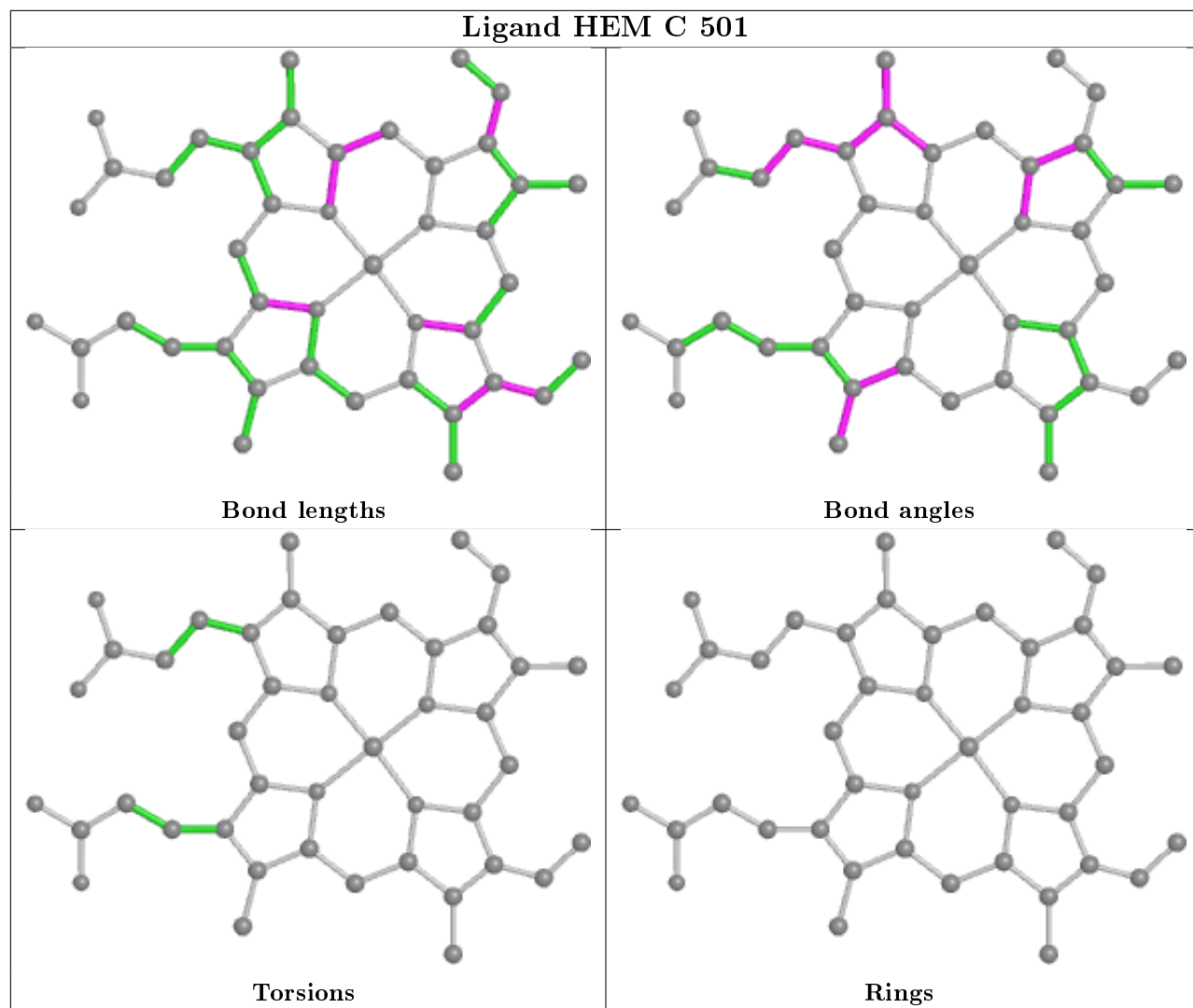
There are no torsion outliers.

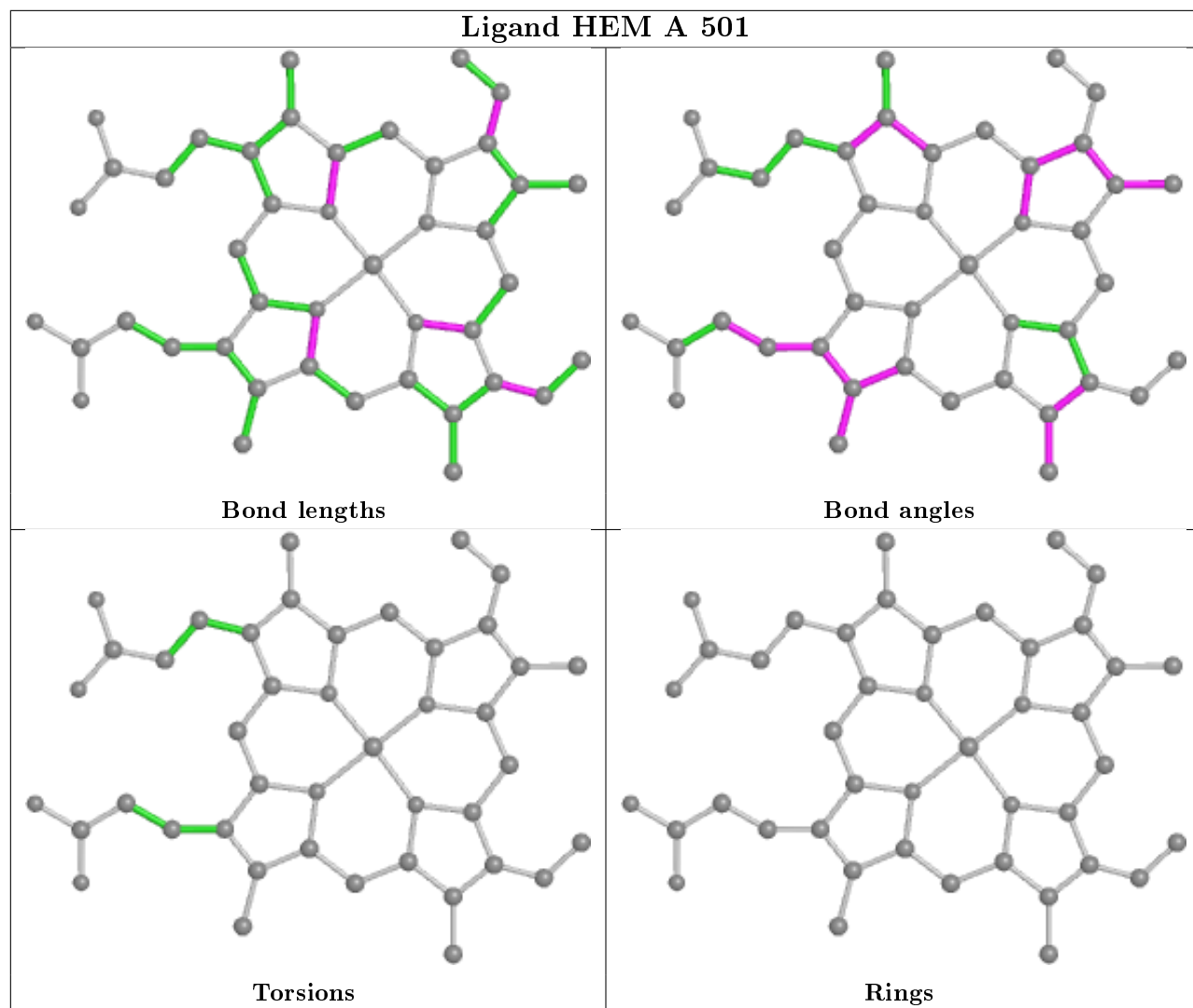
There are no ring outliers.

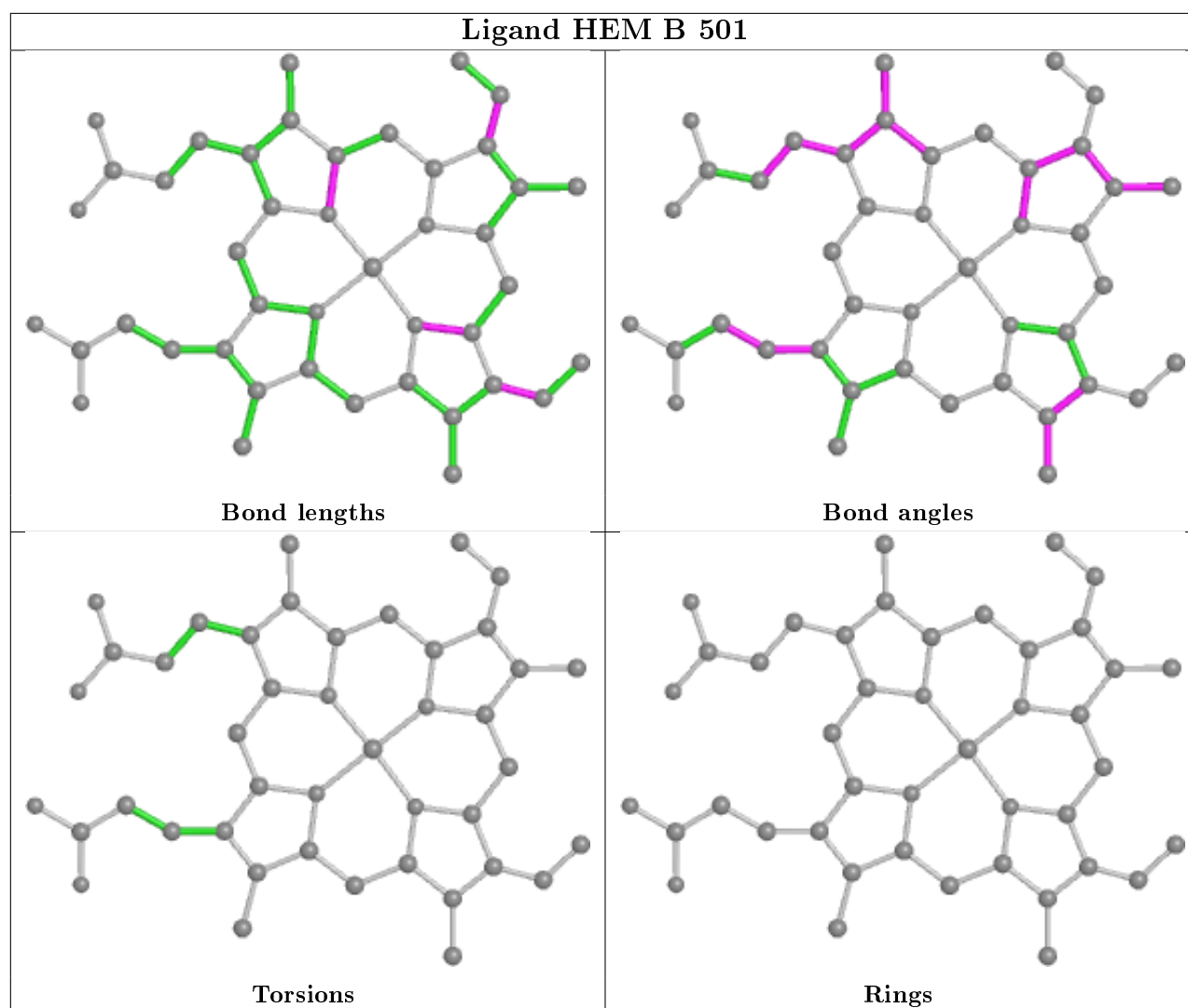
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	6	0
2	A	501	HEM	5	0
2	B	501	HEM	5	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	411/417 (98%)	-0.01	13 (3%) 47 43	20, 36, 58, 72	0
1	B	411/417 (98%)	0.02	8 (1%) 66 65	16, 37, 62, 74	0
1	C	411/417 (98%)	0.39	31 (7%) 14 11	33, 56, 72, 80	0
All	All	1233/1251 (98%)	0.13	52 (4%) 36 32	16, 43, 68, 80	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	10	SER	4.9
1	C	36	LEU	4.6
1	C	47	ILE	4.0
1	C	301	PHE	3.9
1	B	341	GLU	3.6
1	A	343	GLU	3.6
1	C	306	CYS	3.6
1	C	48	CYS	3.5
1	C	8	ASP	3.4
1	A	11	LEU	3.4
1	C	38	GLN	3.2
1	B	258	LEU	3.1
1	B	270	SER	3.0
1	C	49	MET	3.0
1	C	223	GLU	2.9
1	C	346	LEU	2.9
1	B	340	ALA	2.8
1	C	9	LYS	2.8
1	C	29	THR	2.7
1	A	341	GLU	2.6
1	C	303	TRP	2.6
1	A	267	TRP	2.6
1	C	308	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	298	LYS	2.5
1	C	32	TYR	2.5
1	C	302	VAL	2.5
1	C	305	ASN	2.5
1	C	63	ARG	2.4
1	C	37	PHE	2.4
1	A	336	PRO	2.4
1	B	181	TRP	2.4
1	C	6	PRO	2.4
1	A	344	GLU	2.4
1	B	10	SER	2.3
1	C	39	ALA	2.3
1	B	342	ARG	2.3
1	A	10	SER	2.3
1	C	318	LEU	2.3
1	A	9	LYS	2.2
1	B	343	GLU	2.2
1	C	35	ASP	2.2
1	C	30	GLU	2.2
1	C	33	ASN	2.2
1	A	8	ASP	2.2
1	A	7	HIS	2.2
1	A	328	TRP	2.1
1	A	335	ARG	2.1
1	C	383	GLN	2.1
1	C	52	ALA	2.1
1	C	62	ASP	2.0
1	C	54	ALA	2.0
1	A	6	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

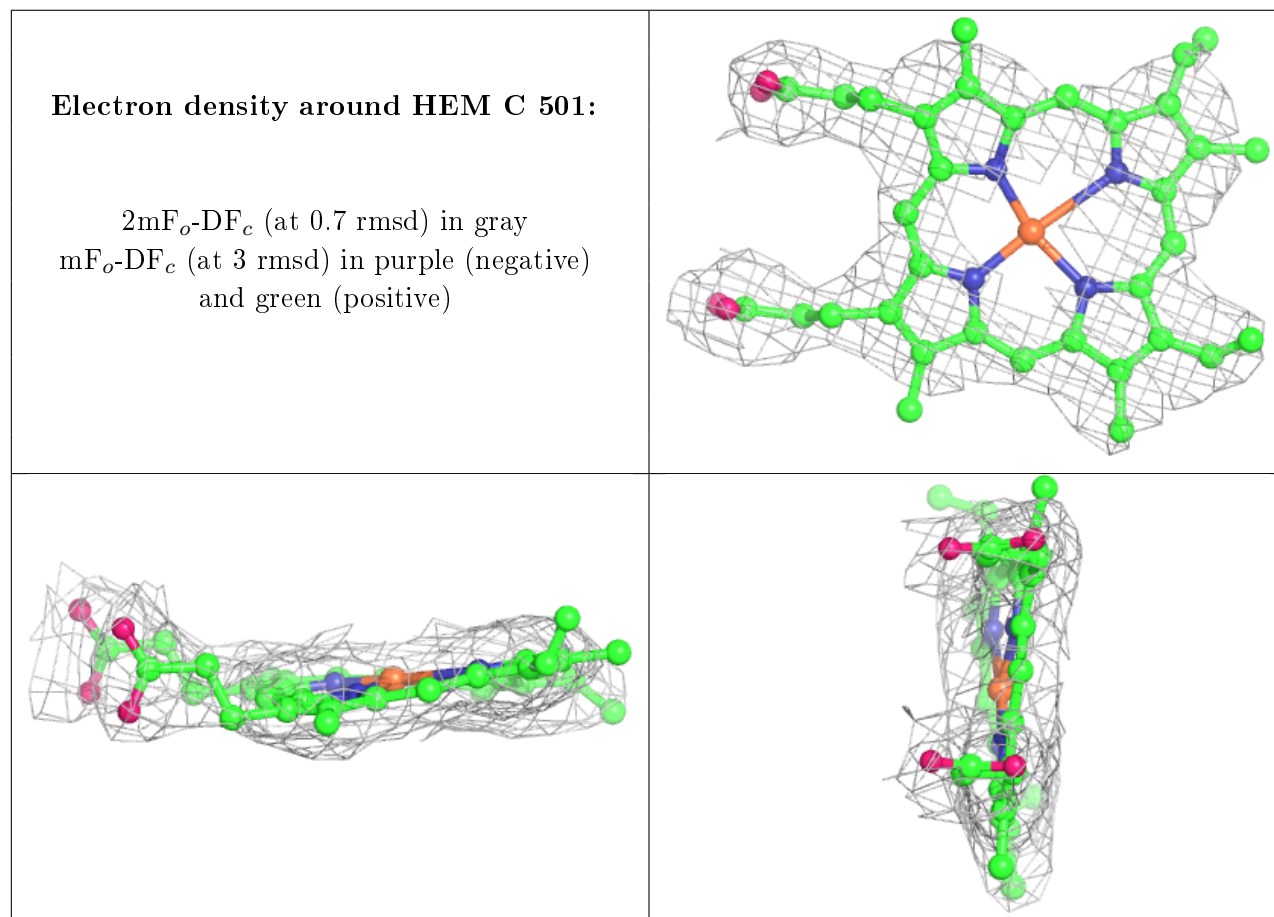
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

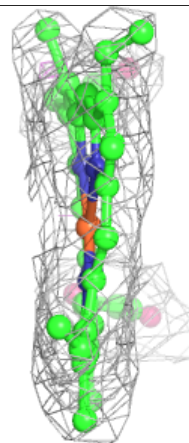
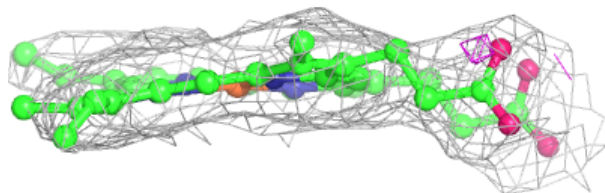
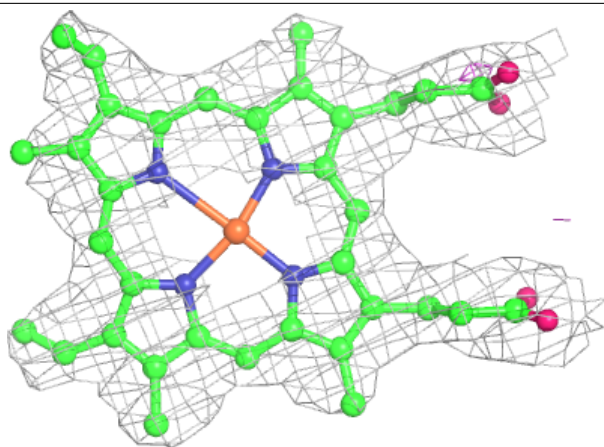
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	C	501	43/43	0.97	0.20	35,41,47,50	0
2	HEM	A	501	43/43	0.97	0.19	15,21,26,31	0
2	HEM	B	501	43/43	0.97	0.20	20,24,27,29	0

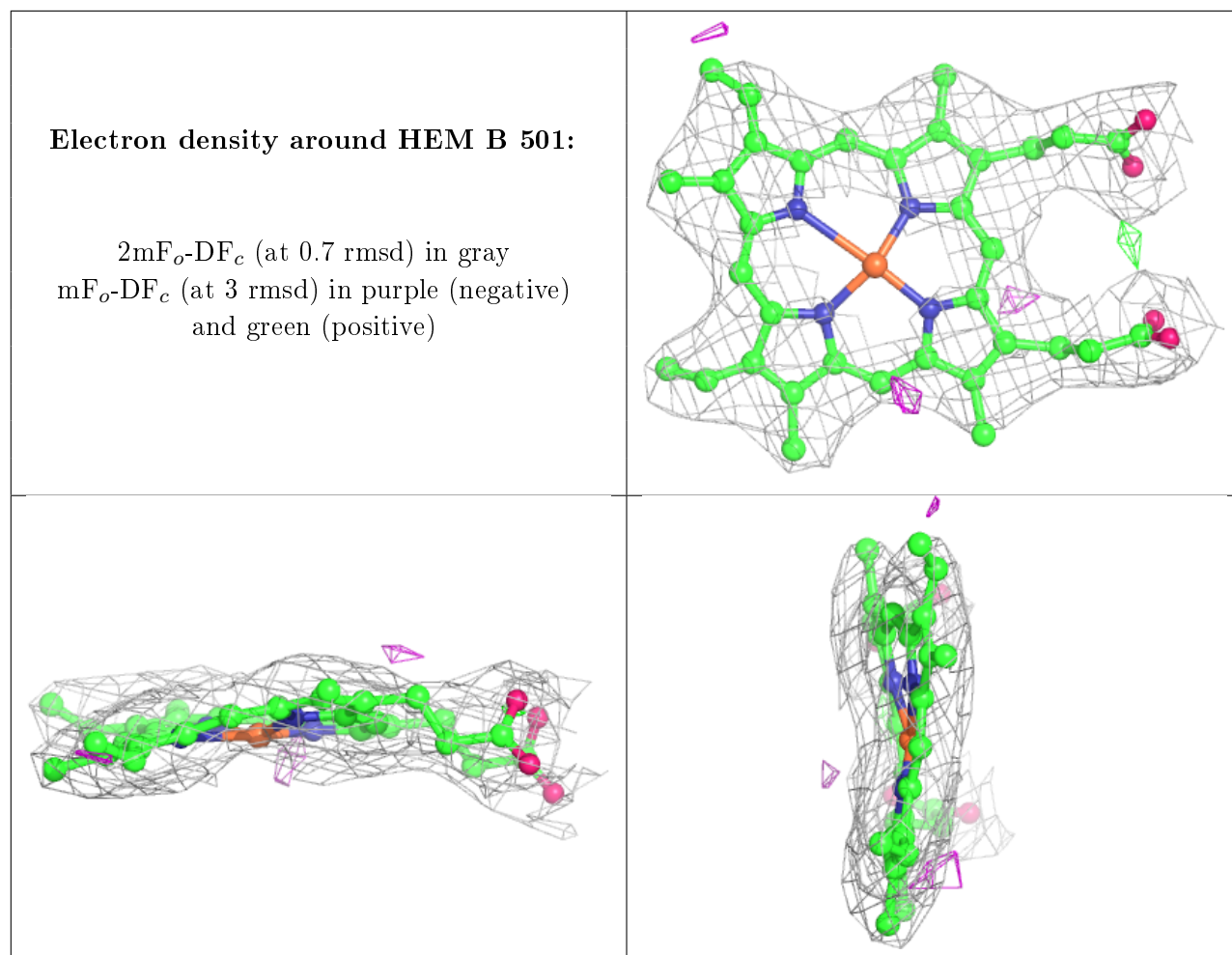
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around HEM A 501:

$2mF_o-DF_c$ (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.