



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:03 PM UTC

PDB ID : 6HQW / pdb_00006hqw
Title : Cytochrome P450-153 from *Novosphingobium aromaticivorans*
Authors : Fiorentini, F.; Mattevi, A.
Deposited on : 2018-09-25
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 types of validation reports are described at

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

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

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

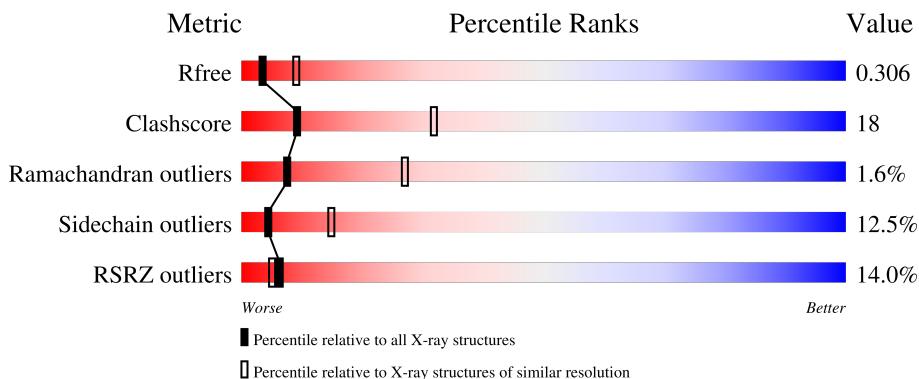
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	445	
1	B	445	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5668 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.

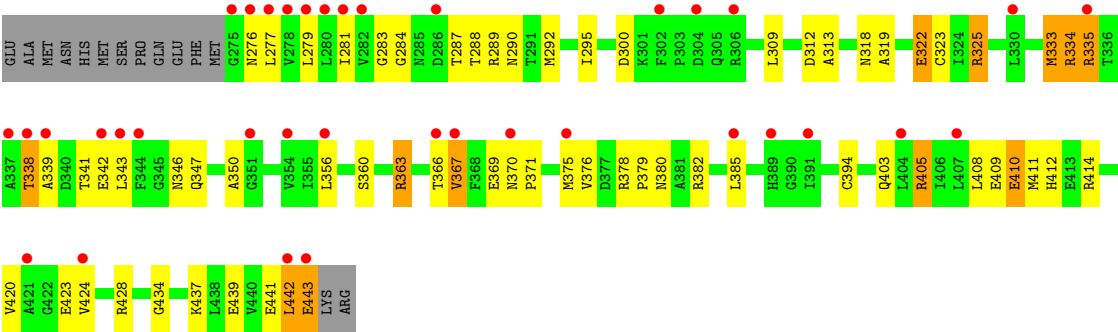
- Molecule 1 is a protein called Cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3146	1990	567	568	21			
1	B	307	Total	C	N	O	S	0	0	0
			2436	1535	447	440	14			

- 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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	113.13Å 113.13Å 72.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.98 – 2.90 97.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (97.98-2.90) 98.6 (97.98-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.248 , 0.299 0.255 , 0.306	Depositor DCC
R_{free} test set	1142 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l 0.030 for h,-h-k,-l 0.014 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5668	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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	0.81	0/3221	1.18	6/4365 (0.1%)
1	B	0.71	1/2488 (0.0%)	1.06	3/3371 (0.1%)
All	All	0.77	1/5709 (0.0%)	1.13	9/7736 (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	9
1	B	0	4
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	THR	N-CA	7.23	1.54	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	PRO	N-CA-C	8.85	121.49	110.70
1	A	410	GLU	CB-CG-CD	6.61	123.84	112.60
1	B	410	GLU	CB-CG-CD	6.54	123.72	112.60
1	B	166	SER	CA-C-N	5.55	127.77	120.60
1	B	166	SER	C-N-CA	5.55	127.77	120.60
1	A	129	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	149	THR	CB-CA-C	5.06	117.42	109.27
1	A	319	ALA	CA-C-N	5.01	126.87	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ALA	C-N-CA	5.01	126.87	120.56

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	PRO	Peptide
1	A	113	PRO	Peptide
1	A	141	ARG	Sidechain
1	A	176	ARG	Sidechain
1	A	325	ARG	Sidechain
1	A	363	ARG	Sidechain
1	A	393	ARG	Sidechain
1	A	417	ARG	Sidechain
1	A	436	ARG	Sidechain
1	B	333	MET	Peptide
1	B	363	ARG	Sidechain
1	B	382	ARG	Sidechain
1	B	405	ARG	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	3057	92	2
1	B	2436	0	2396	109	0
2	A	43	0	30	4	0
2	B	43	0	30	7	0
All	All	5668	0	5513	203	2

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 18.

All (203) 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:108:THR:CA	1:B:334:ARG:HD3	1.61	1.31
1:A:410:GLU:OE2	1:B:410:GLU:OE1	1.72	1.06
1:A:410:GLU:CD	1:B:410:GLU:OE1	1.95	1.05
1:B:108:THR:HA	1:B:334:ARG:CD	1.89	1.02
1:B:108:THR:CA	1:B:334:ARG:CD	2.40	0.98
1:B:108:THR:HA	1:B:334:ARG:HD3	0.98	0.97
1:B:128:MET:HA	1:B:276:ASN:OD1	1.73	0.89
1:B:334:ARG:CZ	1:B:334:ARG:HB3	2.08	0.82
1:B:108:THR:C	1:B:334:ARG:NE	2.43	0.76
1:B:184:SER:O	1:B:188:THR:OG1	2.02	0.76
1:A:160:ILE:HG12	1:A:191:MET:CE	2.16	0.76
1:A:325:ARG:NH2	1:A:371:PRO:O	2.19	0.75
1:B:98:PHE:HB3	1:B:335:ARG:HG2	1.67	0.75
1:B:88:ILE:HD11	1:B:356:LEU:HB3	1.69	0.74
1:A:108:THR:HG23	1:A:110:GLY:H	1.52	0.74
1:B:88:ILE:HD11	1:B:356:LEU:CB	2.20	0.72
1:B:92:GLU:OE2	2:B:500:HEM:O1A	2.08	0.71
1:B:88:ILE:CG2	1:B:385:LEU:HD13	2.20	0.71
1:B:108:THR:N	1:B:334:ARG:HD3	2.06	0.71
1:B:88:ILE:CD1	1:B:356:LEU:HD22	2.23	0.69
1:B:40:HIS:N	1:B:41:PRO:HD2	2.08	0.69
1:B:107:ILE:HA	1:B:334:ARG:HB2	1.73	0.69
1:B:108:THR:N	1:B:334:ARG:HE	1.91	0.69
1:A:209:TRP:CD2	1:A:235:MET:HB3	2.28	0.68
1:A:92:GLU:OE2	2:A:500:HEM:O1A	2.11	0.67
1:A:334:ARG:HG3	1:A:335:ARG:N	2.10	0.66
1:B:86:LYS:NZ	1:B:366:THR:HG21	2.11	0.66
1:A:140:GLN:HE21	1:A:276:ASN:HD21	1.44	0.66
1:A:209:TRP:CE3	1:A:235:MET:HB3	2.31	0.66
1:A:189:THR:HG21	1:A:207:THR:HB	1.77	0.65
1:A:363:ARG:HG3	1:A:363:ARG:HH11	1.61	0.65
1:B:108:THR:N	1:B:334:ARG:CD	2.59	0.65
1:A:129:PHE:HB3	1:A:140:GLN:HG2	1.78	0.65
1:B:410:GLU:HB3	1:B:414:ARG:HH12	1.61	0.65
1:A:160:ILE:HG12	1:A:191:MET:HE1	1.77	0.65
1:B:108:THR:C	1:B:334:ARG:CD	2.70	0.63
1:A:343:LEU:O	1:A:344:PHE:CD1	2.52	0.63
1:B:339:ALA:HA	1:B:350:ALA:HB2	1.80	0.63
1:A:105:GLY:HA3	1:A:334:ARG:HH22	1.64	0.62
1:B:108:THR:N	1:B:334:ARG:NE	2.47	0.62
1:B:97:LEU:O	1:B:338:THR:HB	1.99	0.62
1:B:333:MET:O	1:B:356:LEU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:SER:O	1:A:131:ALA:HA	2.00	0.61
1:B:98:PHE:HB3	1:B:335:ARG:CG	2.30	0.61
1:B:107:ILE:C	1:B:334:ARG:HG3	2.26	0.61
1:A:143:THR:HG21	1:A:262:SER:OG	2.01	0.61
1:A:235:MET:HE1	1:A:277:LEU:HB3	1.83	0.61
1:A:334:ARG:NH1	1:A:336:THR:OG1	2.34	0.61
1:B:68:VAL:HA	1:B:81:ASN:O	2.01	0.60
1:A:62:MET:CE	1:A:83:ALA:HB2	2.32	0.60
1:B:107:ILE:HD12	1:B:107:ILE:O	2.02	0.59
1:B:107:ILE:O	1:B:334:ARG:HG3	2.01	0.59
1:B:318:ASN:ND2	1:B:376:VAL:O	2.34	0.59
1:A:343:LEU:HD13	1:A:344:PHE:HD1	1.67	0.59
1:B:423:GLU:HG2	1:B:439:GLU:OE2	2.03	0.58
1:A:88:ILE:HD13	1:A:356:LEU:HB3	1.86	0.58
1:A:134:ARG:HG2	1:A:138:THR:HG23	1.86	0.58
1:B:62:MET:CE	1:B:83:ALA:HB2	2.34	0.58
1:B:86:LYS:HZ1	1:B:366:THR:HG21	1.69	0.57
1:A:46:ARG:HD3	1:A:49:ILE:HG23	1.86	0.57
1:A:74:SER:C	1:A:76:TYR:H	2.12	0.57
1:B:334:ARG:O	1:B:335:ARG:NE	2.38	0.57
1:A:111:ASP:OD2	1:A:353:LYS:NZ	2.34	0.57
1:B:108:THR:CA	1:B:334:ARG:NE	2.67	0.57
1:B:188:THR:HA	1:B:191:MET:HE2	1.87	0.57
1:B:405:ARG:NH1	1:B:409:GLU:OE2	2.38	0.56
1:B:363:ARG:HG3	1:B:363:ARG:HH11	1.70	0.56
1:B:88:ILE:HG21	1:B:385:LEU:HD13	1.88	0.55
1:A:139:GLY:O	1:A:143:THR:HG23	2.06	0.55
1:A:324:ILE:HG22	1:A:384:HIS:CD2	2.42	0.55
1:B:185:ILE:HG12	1:B:289:ARG:HD2	1.88	0.55
1:A:295:ILE:CD1	1:A:404:LEU:HD22	2.37	0.55
1:A:263:GLU:HA	1:A:266:ASN:ND2	2.21	0.54
1:A:160:ILE:CG1	1:A:191:MET:HE1	2.38	0.54
2:B:500:HEM:HBB2	2:B:500:HEM:HMB2	1.88	0.54
1:A:140:GLN:NE2	1:A:276:ASN:HD21	2.05	0.54
1:B:85:HIS:O	1:B:88:ILE:HG22	2.07	0.54
1:B:88:ILE:HD11	1:B:356:LEU:CA	2.38	0.53
1:B:292:MET:HE3	1:B:403:GLN:HG3	1.90	0.53
1:A:48:ASP:OD1	1:A:48:ASP:N	2.39	0.53
1:A:192:LEU:HD21	1:A:281:ILE:HA	1.90	0.53
1:A:40:HIS:N	1:A:41:PRO:HD2	2.23	0.53
1:A:80:TRP:CE2	1:A:348:ILE:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ALA:O	1:B:69:ASN:ND2	2.40	0.53
1:A:327:VAL:O	1:A:433:HIS:CD2	2.61	0.53
1:B:313:ALA:HB2	1:B:412:HIS:CE1	2.44	0.53
1:B:62:MET:HE2	1:B:83:ALA:HB2	1.91	0.53
1:B:325:ARG:NH2	1:B:371:PRO:O	2.42	0.53
1:A:113:PRO:O	1:A:114:GLU:HG2	2.10	0.52
1:A:164:THR:O	1:A:168:LEU:HB2	2.10	0.52
1:B:107:ILE:C	1:B:334:ARG:CD	2.82	0.52
1:A:410:GLU:OE2	1:B:410:GLU:CD	2.44	0.51
1:A:239:PHE:HB3	1:A:277:LEU:HD21	1.92	0.51
1:B:405:ARG:HH11	1:B:409:GLU:CD	2.19	0.51
1:A:235:MET:HE3	1:A:239:PHE:CD2	2.45	0.51
1:B:80:TRP:HZ3	1:B:346:ASN:HD22	1.59	0.51
2:B:500:HEM:HBC2	2:B:500:HEM:HMC2	1.91	0.51
1:A:363:ARG:HH11	1:A:363:ARG:CG	2.25	0.50
1:B:168:LEU:HD21	1:B:411:MET:HG3	1.93	0.50
1:B:107:ILE:C	1:B:334:ARG:CG	2.84	0.50
1:A:105:GLY:HA3	1:A:334:ARG:NH2	2.27	0.50
1:A:123:GLU:HA	1:A:271:GLN:HE21	1.75	0.50
1:A:396:GLY:O	1:A:397:ALA:C	2.55	0.50
1:B:40:HIS:N	1:B:41:PRO:CD	2.75	0.50
1:B:319:ALA:HB2	1:B:376:VAL:HG13	1.93	0.50
1:A:145:ALA:N	1:A:146:PRO:CD	2.75	0.49
1:A:74:SER:C	1:A:76:TYR:N	2.70	0.49
1:A:179:TRP:CZ2	1:A:183:VAL:HG11	2.47	0.49
1:B:191:MET:HE1	1:B:288:THR:HG21	1.94	0.49
1:A:135:PRO:O	1:A:138:THR:OG1	2.31	0.49
1:A:140:GLN:HE21	1:A:276:ASN:ND2	2.10	0.49
1:A:191:MET:HG2	1:A:403:GLN:CD	2.38	0.49
1:A:375:MET:O	1:A:378:ARG:N	2.39	0.49
1:A:100:SER:HB2	1:A:107:ILE:HG22	1.95	0.48
1:B:145:ALA:N	1:B:146:PRO:CD	2.77	0.48
1:B:410:GLU:O	1:B:414:ARG:NH1	2.46	0.48
1:A:189:THR:HG21	1:A:207:THR:CG2	2.44	0.48
1:B:94:LEU:HD22	1:B:97:LEU:HD23	1.96	0.48
1:B:161:ARG:NH2	1:B:409:GLU:OE2	2.47	0.48
1:A:239:PHE:CE2	1:A:281:ILE:HD11	2.49	0.48
1:A:91:VAL:HG11	1:A:356:LEU:HD21	1.96	0.47
1:B:164:THR:O	1:B:168:LEU:HB2	2.15	0.47
1:B:322:GLU:HG3	1:B:375:MET:C	2.39	0.47
1:A:327:VAL:O	1:A:433:HIS:HD2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASN:O	1:A:381:ALA:C	2.57	0.47
1:B:410:GLU:HB3	1:B:414:ARG:NH1	2.29	0.47
1:B:97:LEU:C	1:B:97:LEU:HD12	2.39	0.47
1:A:143:THR:OG1	1:A:265:MET:CE	2.63	0.47
1:B:290:ASN:CG	1:B:434:GLY:HA3	2.40	0.46
1:A:163:ARG:HH12	1:A:191:MET:HE2	1.80	0.46
1:B:88:ILE:HD11	1:B:356:LEU:HA	1.96	0.46
1:B:441:GLU:C	1:B:442:LEU:HD13	2.41	0.46
1:B:51:VAL:CG2	1:B:428:ARG:HA	2.46	0.46
1:A:189:THR:HG21	1:A:207:THR:CB	2.44	0.46
2:A:500:HEM:HBB2	2:A:500:HEM:HMB2	1.98	0.46
1:B:284:GLY:HA2	2:B:500:HEM:C2C	2.51	0.46
1:B:369:GLU:C	1:B:370:ASN:HD22	2.24	0.46
1:B:312:ASP:OD1	1:B:312:ASP:O	2.35	0.45
1:A:121:LEU:HD23	1:A:121:LEU:O	2.16	0.45
1:B:107:ILE:C	1:B:334:ARG:HD3	2.39	0.45
1:B:375:MET:O	1:B:378:ARG:N	2.44	0.45
1:B:88:ILE:HD12	1:B:356:LEU:HD22	1.97	0.45
1:A:256:ILE:O	1:A:257:SER:C	2.59	0.45
1:A:392:HIS:O	2:A:500:HEM:HBA2	2.17	0.45
1:B:80:TRP:HZ3	1:B:346:ASN:ND2	2.15	0.45
1:A:114:GLU:HG3	1:A:115:ASP:N	2.31	0.45
1:B:39:SER:C	1:B:41:PRO:HD2	2.42	0.45
1:B:91:VAL:HG11	1:B:356:LEU:HD21	1.99	0.45
1:B:179:TRP:CZ2	1:B:183:VAL:HG11	2.52	0.45
1:B:312:ASP:OD1	1:B:312:ASP:C	2.58	0.45
1:A:88:ILE:O	1:A:92:GLU:HB2	2.17	0.44
1:A:98:PHE:O	1:A:335:ARG:HG2	2.17	0.44
1:A:255:LEU:O	1:A:259:MET:HG3	2.17	0.44
1:B:132:MET:HE1	1:B:140:GLN:NE2	2.32	0.44
1:A:74:SER:O	1:A:76:TYR:N	2.50	0.44
1:B:300:ASP:OD2	1:B:420:VAL:HG23	2.17	0.44
1:A:68:VAL:HG21	1:A:343:LEU:HD12	1.99	0.44
1:A:384:HIS:CD2	1:A:386:SER:H	2.35	0.44
1:A:193:ALA:O	1:A:194:ILE:C	2.60	0.44
1:B:283:GLY:O	2:B:500:HEM:C1C	2.71	0.44
1:B:442:LEU:O	1:B:443:GLU:C	2.59	0.44
1:A:123:GLU:HA	1:A:271:GLN:NE2	2.33	0.44
1:B:157:GLU:O	1:B:158:ALA:C	2.60	0.44
1:B:177:PHE:O	1:B:439:GLU:HA	2.18	0.44
1:A:192:LEU:HD13	1:A:284:GLY:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:O	1:B:107:ILE:CD1	2.66	0.43
1:A:123:GLU:CA	1:A:271:GLN:HE21	2.32	0.43
1:B:187:LEU:O	1:B:191:MET:N	2.46	0.43
1:B:295:ILE:HG12	1:B:323:CYS:SG	2.58	0.43
2:A:500:HEM:HMC1	2:A:500:HEM:HBC2	2.01	0.43
1:B:72:PRO:O	1:B:78:ALA:HB2	2.18	0.43
1:B:94:LEU:N	1:B:95:PRO:CD	2.82	0.43
1:B:109:ILE:N	1:B:334:ARG:CD	2.82	0.43
1:A:176:ARG:HA	1:A:440:VAL:O	2.18	0.43
1:A:322:GLU:OE2	1:A:378:ARG:HD2	2.19	0.43
1:A:143:THR:OG1	1:A:265:MET:HE2	2.19	0.42
1:B:56:GLN:HB2	1:B:57:PRO:HD3	2.01	0.42
1:B:101:SER:O	1:B:102:TRP:C	2.60	0.42
1:B:153:MET:HE2	1:B:156:MET:HE3	2.00	0.42
1:B:394:CYS:SG	2:B:500:HEM:C4B	3.10	0.42
1:A:402:LEU:O	1:A:403:GLN:C	2.61	0.42
1:B:423:GLU:CG	1:B:439:GLU:OE2	2.66	0.42
1:A:307:GLU:HA	1:A:310:GLU:HB2	2.01	0.42
1:B:66:ALA:O	1:B:67:PRO:C	2.63	0.42
1:B:88:ILE:HG21	1:B:385:LEU:CD1	2.49	0.42
1:A:192:LEU:HD13	1:A:284:GLY:C	2.45	0.42
1:B:88:ILE:HD12	1:B:88:ILE:HA	1.85	0.42
1:B:322:GLU:HG3	1:B:375:MET:O	2.19	0.42
1:A:153:MET:HA	1:A:153:MET:HE2	2.02	0.42
1:B:59:PHE:CD1	1:B:360:SER:HB2	2.55	0.42
1:A:149:THR:HG23	1:A:152:LYS:H	1.85	0.42
1:A:176:ARG:HD3	1:A:421:ALA:HB1	2.00	0.42
2:B:500:HEM:HBB2	2:B:500:HEM:CMB	2.50	0.41
1:A:140:GLN:NE2	1:A:276:ASN:ND2	2.67	0.41
1:B:378:ARG:HA	1:B:379:PRO:HD3	1.97	0.41
1:A:107:ILE:C	1:A:107:ILE:HD12	2.45	0.41
1:B:367:VAL:HG23	1:B:380:ASN:ND2	2.36	0.41
1:A:243:TRP:CD2	1:A:260:ILE:HD11	2.56	0.41
1:A:277:LEU:HD12	1:A:277:LEU:HA	1.89	0.41
1:A:291:THR:HG21	1:A:404:LEU:HD11	2.02	0.41
1:A:114:GLU:HG3	1:A:115:ASP:H	1.85	0.40
1:B:309:LEU:HD13	1:B:376:VAL:HG11	2.04	0.40
1:B:366:THR:O	1:B:366:THR:HG22	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:OE1	1:A:134:ARG:NH2[2_544]	2.16	0.04
1:A:103:GLN:OE1	1:A:343:LEU:O[2_544]	2.18	0.02

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	387/445 (87%)	345 (89%)	34 (9%)	8 (2%)	5	21
1	B	299/445 (67%)	262 (88%)	34 (11%)	3 (1%)	12	39
All	All	686/890 (77%)	607 (88%)	68 (10%)	11 (2%)	7	27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PRO
1	A	114	GLU
1	A	116	VAL
1	A	119	GLN
1	B	75	PRO
1	A	56	GLN
1	A	381	ALA
1	A	402	LEU
1	B	53	ASP
1	B	172	PRO
1	A	75	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/378 (87%)	293 (89%)	36 (11%)	6	20
1	B	257/378 (68%)	220 (86%)	37 (14%)	3	11
All	All	586/756 (78%)	513 (88%)	73 (12%)	4	15

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	88	ILE
1	A	108	THR
1	A	115	ASP
1	A	116	VAL
1	A	117	ASP
1	A	120	LYS
1	A	140	GLN
1	A	152	LYS
1	A	163	ARG
1	A	166	SER
1	A	200	TRP
1	A	206	LEU
1	A	207	THR
1	A	210	SER
1	A	218	LEU
1	A	220	LEU
1	A	222	ARG
1	A	242	LEU
1	A	243	TRP
1	A	265	MET
1	A	271	GLN
1	A	277	LEU
1	A	279	LEU
1	A	322	GLU
1	A	334	ARG
1	A	335	ARG
1	A	338	THR
1	A	341	THR
1	A	343	LEU
1	A	347	GLN
1	A	367	VAL
1	A	408	LEU
1	A	419	ARG

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Mol	Chain	Res	Type
1	A	437	LYS
1	A	442	LEU
1	B	44	VAL
1	B	48	ASP
1	B	86	LYS
1	B	88	ILE
1	B	92	GLU
1	B	94	LEU
1	B	96	GLU
1	B	97	LEU
1	B	100	SER
1	B	108	THR
1	B	135	PRO
1	B	140	GLN
1	B	152	LYS
1	B	175	GLU
1	B	184	SER
1	B	188	THR
1	B	192	LEU
1	B	195	LEU
1	B	277	LEU
1	B	279	LEU
1	B	281	ILE
1	B	287	THR
1	B	322	GLU
1	B	325	ARG
1	B	334	ARG
1	B	335	ARG
1	B	338	THR
1	B	341	THR
1	B	342	GLU
1	B	343	LEU
1	B	347	GLN
1	B	367	VAL
1	B	408	LEU
1	B	424	VAL
1	B	437	LYS
1	B	442	LEU
1	B	443	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	85	HIS
1	A	140	GLN
1	A	271	GLN
1	A	305	GLN
1	A	346	ASN
1	A	384	HIS
1	A	433	HIS
1	B	40	HIS
1	B	140	GLN
1	B	370	ASN
1	B	433	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	A	500	1	50,50,50	1.75	12 (24%)	67,82,82	1.84	11 (16%)
2	HEM	B	500	1	50,50,50	1.63	10 (20%)	67,82,82	1.66	13 (19%)

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	A	500	1	-	2/14/54/54	-
2	HEM	B	500	1	-	2/14/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	FE-NB	5.06	2.10	1.94
2	B	500	HEM	FE-NC	4.29	2.09	1.95
2	A	500	HEM	FE-NC	4.21	2.09	1.95
2	A	500	HEM	C1B-NB	-4.21	1.33	1.40
2	A	500	HEM	FE-NB	3.86	2.06	1.94
2	A	500	HEM	C4D-ND	-3.46	1.34	1.40
2	B	500	HEM	C1B-NB	-3.43	1.34	1.40
2	B	500	HEM	C4D-ND	-3.15	1.34	1.40
2	A	500	HEM	C4B-NB	-2.79	1.33	1.38
2	A	500	HEM	C3C-C4C	-2.76	1.41	1.46
2	A	500	HEM	C1D-ND	-2.64	1.33	1.38
2	A	500	HEM	C1C-NC	-2.63	1.34	1.39
2	B	500	HEM	C1D-ND	-2.63	1.33	1.38
2	A	500	HEM	C1A-C2A	-2.59	1.39	1.44
2	B	500	HEM	C3B-C4B	2.42	1.49	1.44
2	A	500	HEM	C1A-NA	-2.41	1.35	1.39
2	A	500	HEM	FE-ND	-2.37	1.87	1.94
2	B	500	HEM	C3C-C4C	-2.14	1.42	1.46
2	A	500	HEM	C4A-NA	-2.13	1.35	1.39
2	B	500	HEM	C1C-C2C	-2.07	1.41	1.45
2	B	500	HEM	FE-ND	-2.05	1.88	1.94
2	B	500	HEM	C1C-NC	-2.04	1.35	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	CHC-C4B-NB	5.85	130.72	124.42
2	A	500	HEM	C1B-NB-C4B	4.95	111.07	105.21
2	B	500	HEM	CHC-C4B-NB	4.61	129.38	124.42
2	A	500	HEM	CHD-C1D-ND	4.58	129.35	124.42
2	B	500	HEM	C1B-NB-C4B	4.23	110.21	105.21
2	B	500	HEM	O2A-CGA-CBA	3.83	126.09	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CHA-C4D-ND	3.72	128.96	124.37
2	A	500	HEM	CBD-CAD-C3D	-3.62	102.53	112.53
2	A	500	HEM	CHD-C1D-C2D	-3.58	119.37	125.03
2	A	500	HEM	CHB-C1B-NB	3.57	128.79	124.37
2	A	500	HEM	C3B-C4B-NB	-3.35	107.06	109.47
2	B	500	HEM	CHD-C1D-ND	3.29	127.97	124.42
2	B	500	HEM	O2A-CGA-O1A	-3.12	115.30	123.33
2	B	500	HEM	C3B-C4B-NB	-2.94	107.36	109.47
2	B	500	HEM	CHA-C4D-C3D	-2.85	119.98	125.23
2	A	500	HEM	O2A-CGA-CBA	2.68	122.46	114.00
2	A	500	HEM	C4B-C3B-C2B	-2.50	104.98	107.28
2	B	500	HEM	CHD-C4C-NC	2.45	127.12	124.45
2	B	500	HEM	CHB-C1B-NB	2.24	127.14	124.37
2	A	500	HEM	CHA-C4D-ND	2.18	127.06	124.37
2	A	500	HEM	O2D-CGD-CBD	2.16	120.83	114.00
2	B	500	HEM	C1A-CHA-C4D	-2.09	121.33	126.25
2	B	500	HEM	C4A-C3A-C2A	2.07	109.19	106.82
2	B	500	HEM	CHD-C1D-C2D	-2.07	121.76	125.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAD-CBD-CGD-O2D
2	A	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A

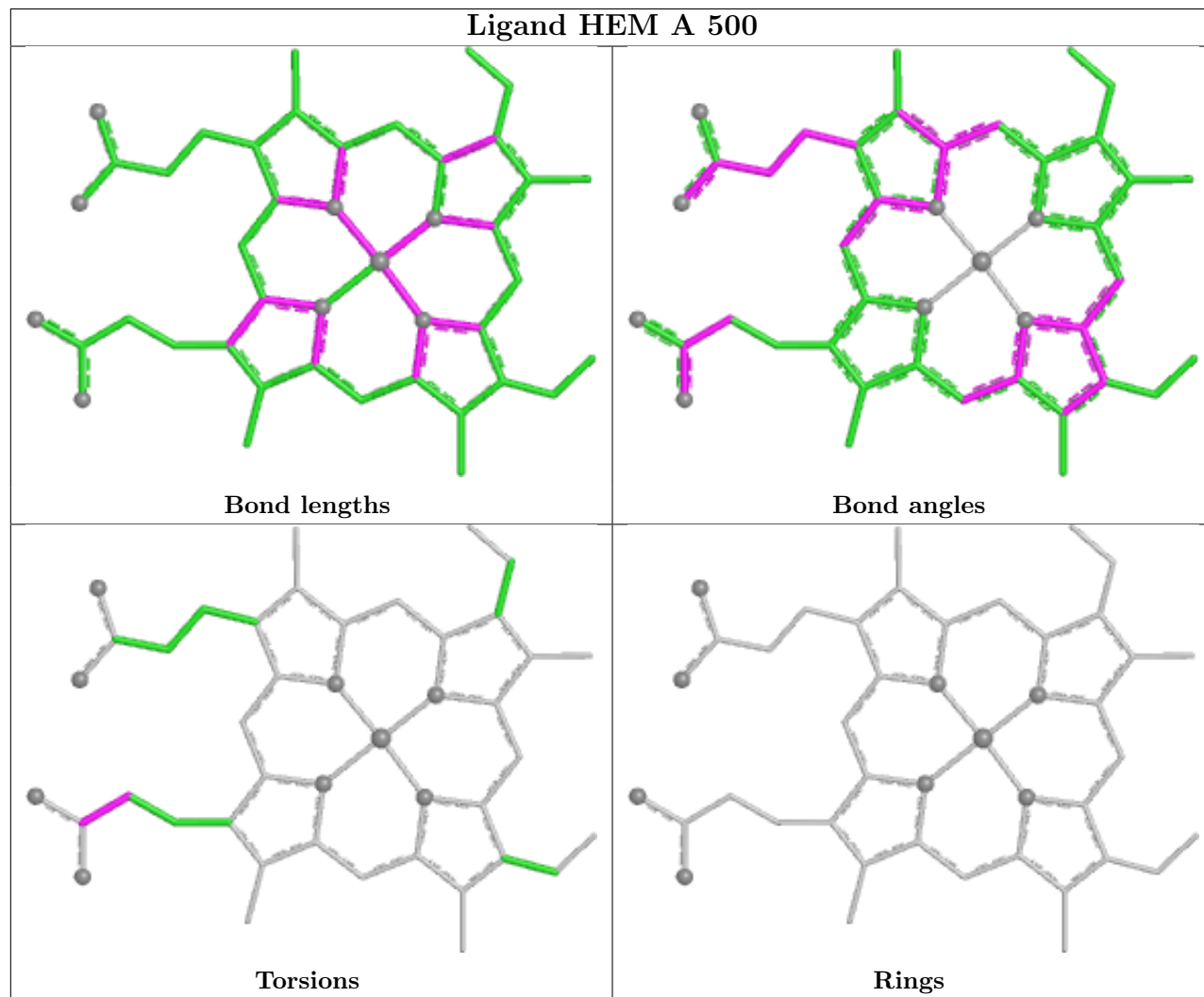
There are no ring outliers.

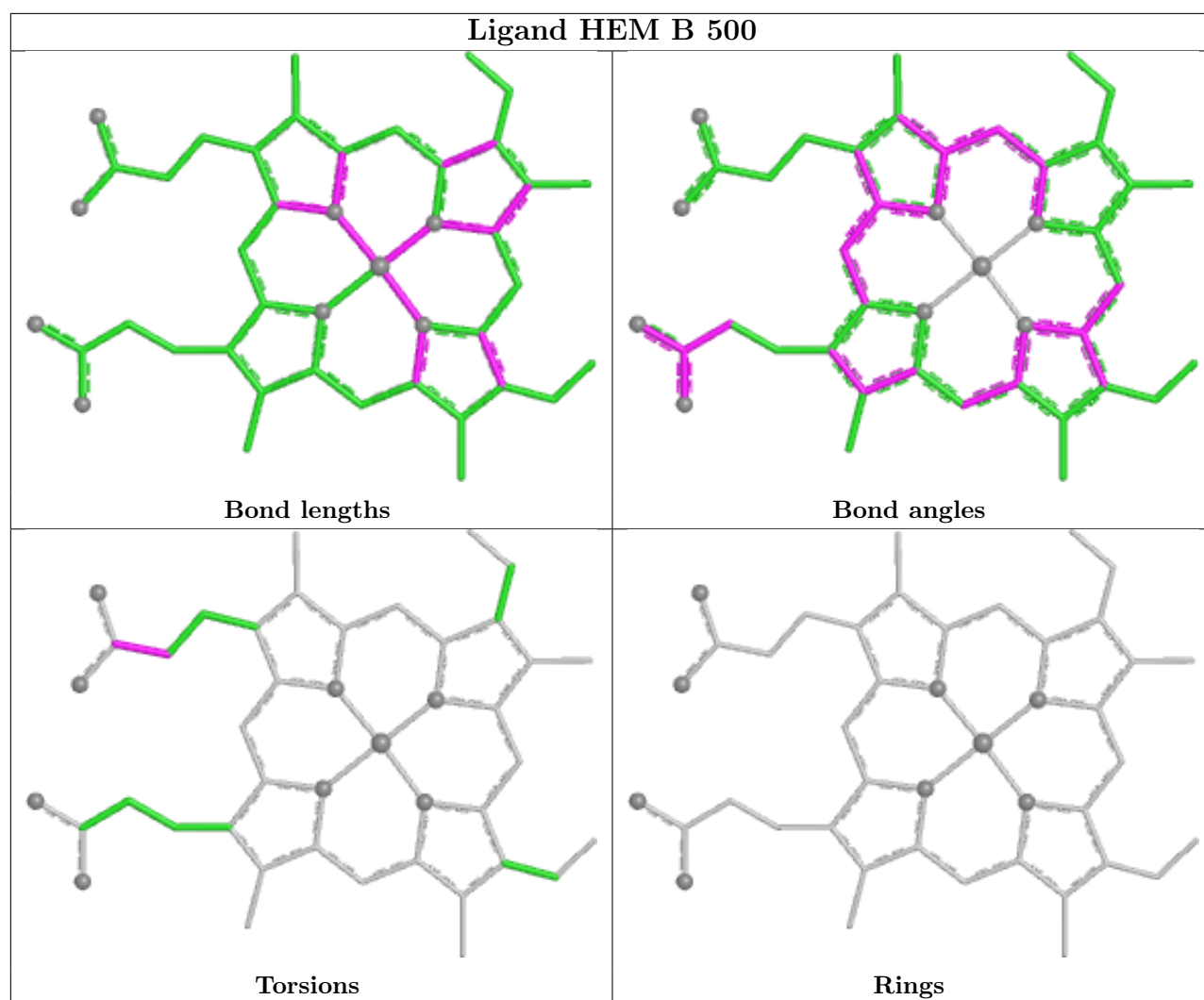
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	4	0
2	B	500	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	395/445 (88%)	0.52	25 (6%) 26 20	28, 55, 93, 134	0
1	B	307/445 (68%)	1.39	73 (23%) 2 2	43, 85, 132, 175	0
All	All	702/890 (78%)	0.90	98 (13%) 6 5	28, 69, 120, 175	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	HIS	5.1
1	B	277	LEU	5.0
1	B	278	VAL	4.6
1	B	282	VAL	4.6
1	B	280	LEU	4.3
1	B	275	GLY	4.3
1	B	276	ASN	4.1
1	A	124	ARG	4.0
1	B	91	VAL	4.0
1	B	335	ARG	4.0
1	B	343	LEU	3.8
1	B	338	THR	3.8
1	A	120	LYS	3.7
1	A	119	GLN	3.7
1	B	342	GLU	3.6
1	A	205	LEU	3.6
1	B	110	GLY	3.5
1	B	85	HIS	3.5
1	B	41	PRO	3.4
1	B	281	ILE	3.4
1	B	39	SER	3.4
1	B	108	THR	3.4
1	A	204	ARG	3.3
1	A	200	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	84	SER	3.3
1	B	149	THR	3.3
1	A	121	LEU	3.2
1	A	209	TRP	3.2
1	A	118	PRO	3.2
1	B	337	ALA	3.1
1	B	109	ILE	3.1
1	B	106	GLY	3.1
1	B	105	GLY	3.1
1	A	122	ALA	3.0
1	B	88	ILE	3.0
1	B	107	ILE	3.0
1	B	102	TRP	2.9
1	A	126	LEU	2.9
1	B	173	TRP	2.9
1	B	132	MET	2.9
1	B	370	ASN	2.9
1	B	40	HIS	2.8
1	A	113	PRO	2.8
1	B	279	LEU	2.8
1	B	61	GLU	2.7
1	A	323	CYS	2.7
1	B	286	ASP	2.7
1	A	410	GLU	2.7
1	B	391	ILE	2.7
1	B	98	PHE	2.6
1	A	173	TRP	2.6
1	B	64	ALA	2.6
1	A	243	TRP	2.6
1	B	330	LEU	2.6
1	B	304	ASP	2.6
1	B	354	VAL	2.6
1	A	125	GLN	2.6
1	B	145	ALA	2.6
1	B	133	ASP	2.6
1	A	231	PHE	2.5
1	B	65	LYS	2.5
1	B	138	THR	2.5
1	A	206	LEU	2.5
1	B	367	VAL	2.5
1	A	248	GLN	2.5
1	B	356	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	407	LEU	2.5
1	B	146	PRO	2.4
1	B	135	PRO	2.4
1	B	148	PHE	2.4
1	A	226	ASP	2.4
1	B	443	GLU	2.4
1	B	375	MET	2.4
1	B	344	PHE	2.3
1	B	128	MET	2.3
1	B	97	LEU	2.3
1	B	75	PRO	2.3
1	B	151	ALA	2.3
1	B	366	THR	2.3
1	B	389	HIS	2.3
1	A	123	GLU	2.3
1	B	134	ARG	2.3
1	B	92	GLU	2.2
1	B	339	ALA	2.2
1	B	404	LEU	2.2
1	B	421	ALA	2.2
1	B	71	VAL	2.1
1	A	73	ASP	2.1
1	B	306	ARG	2.1
1	A	117	ASP	2.1
1	B	385	LEU	2.1
1	B	424	VAL	2.1
1	A	218	LEU	2.1
1	B	192	LEU	2.1
1	B	442	LEU	2.0
1	B	351	GLY	2.0
1	B	87	ALA	2.0
1	B	302	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

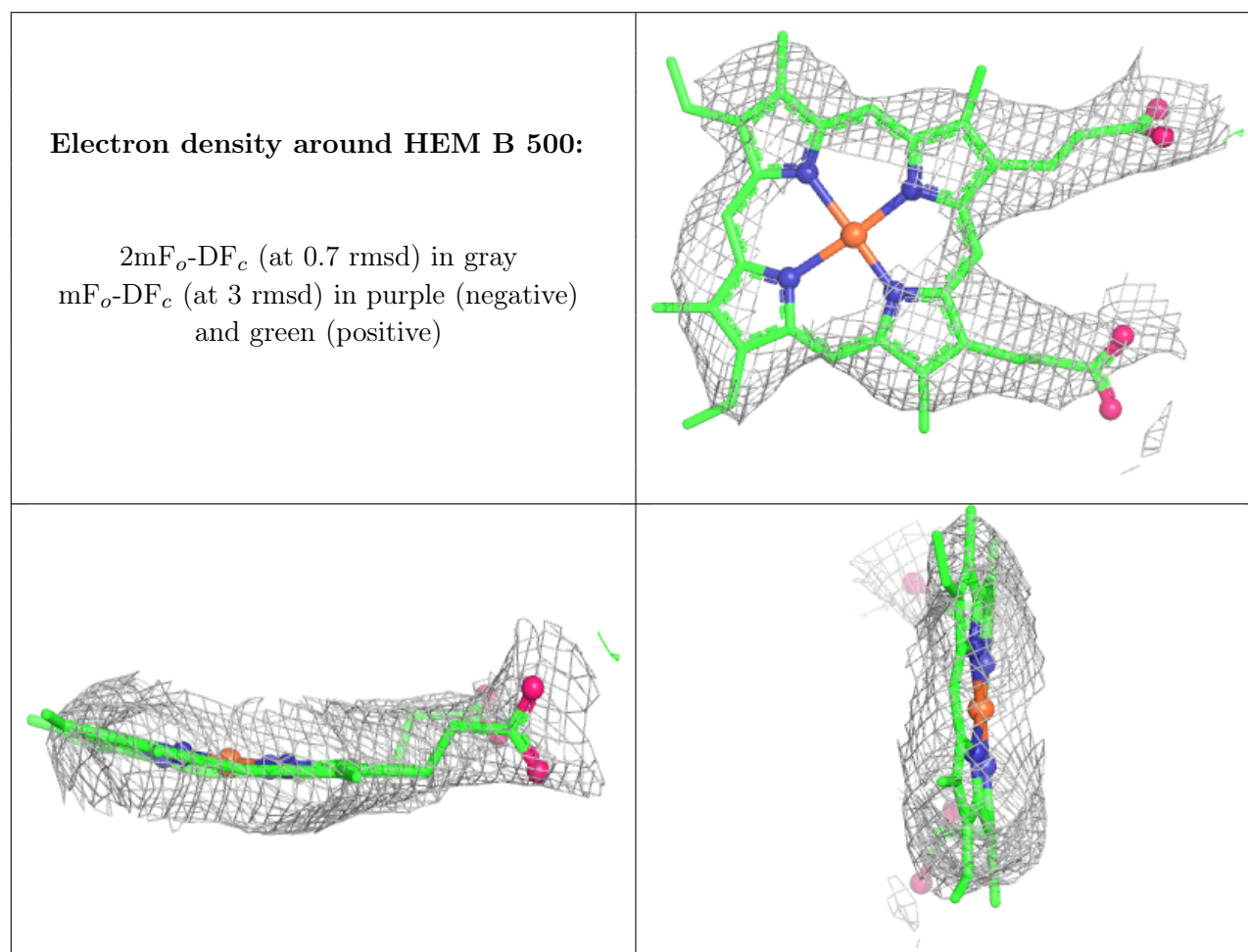
There are no oligosaccharides in this entry.

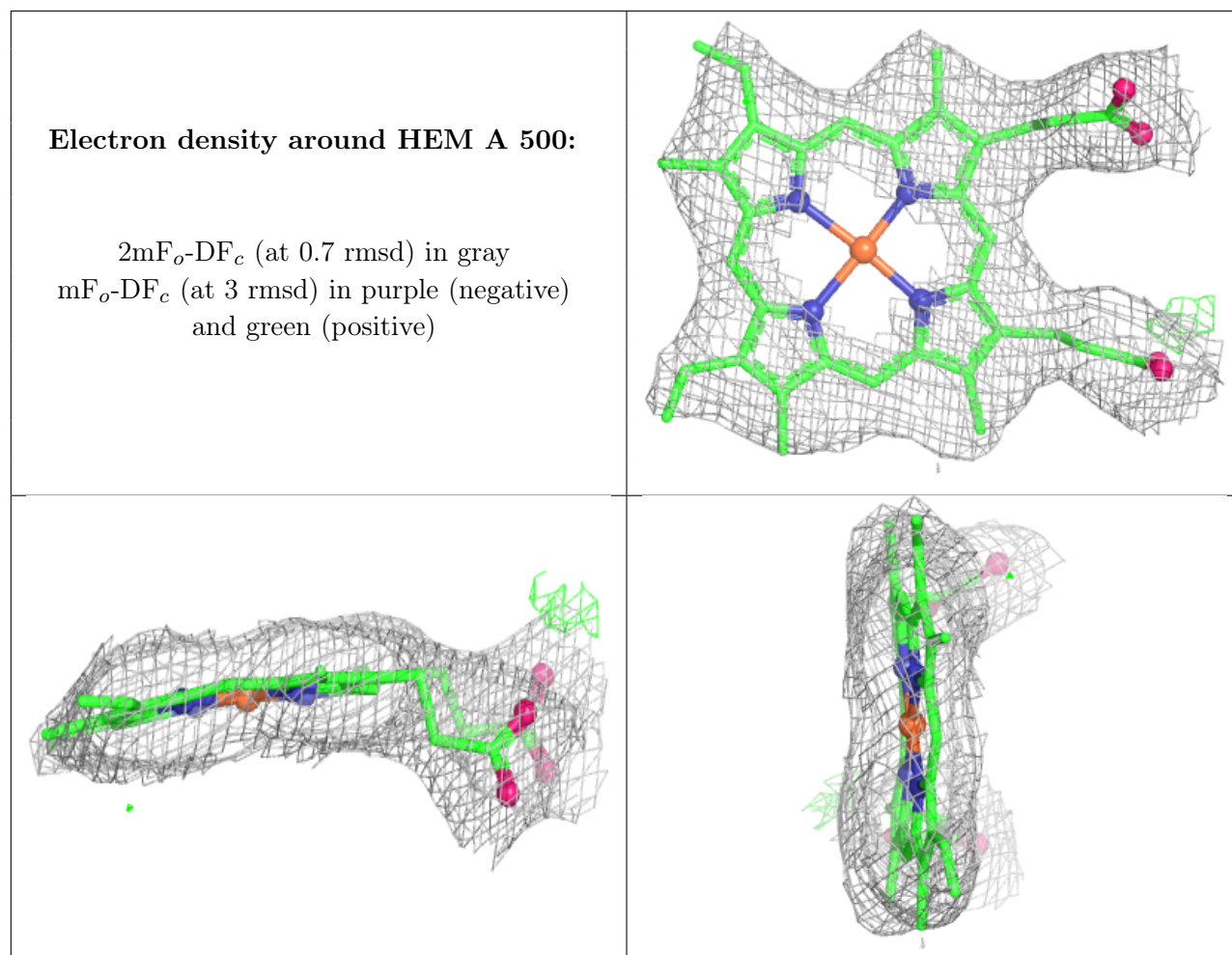
6.4 Ligands ⓘ

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	B	500	43/43	0.94	0.14	62,93,102,122	0
2	HEM	A	500	43/43	0.97	0.08	31,44,49,56	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.