



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 06:50 PM EST

PDB ID : 3TZO
Title : The role of I87 of CYP158A2 in oxidative coupling reaction
Authors : Zhao, B.; Waterman, M.R.
Deposited on : 2011-09-27
Resolution : 1.76 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

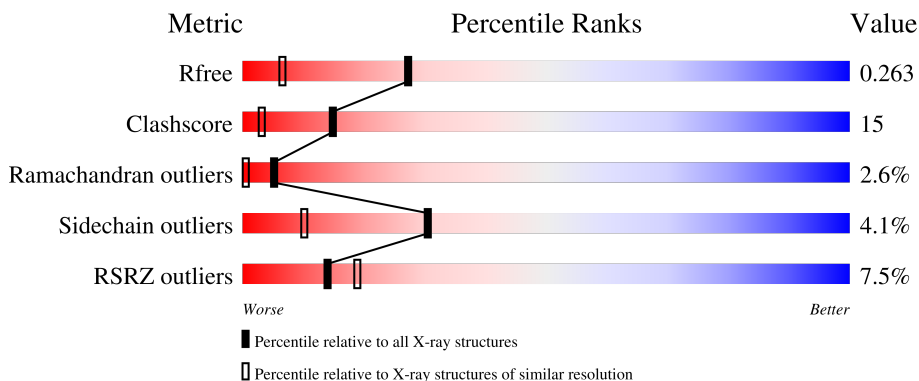
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	410	
1	B	410	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6954 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 Putative cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3110	1956	569	574	11	0	0	0
1	B	402	3110	1956	569	574	11	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

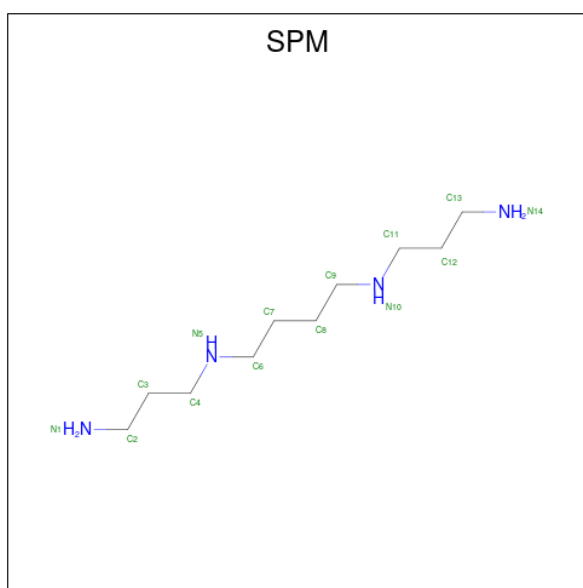
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	LYS	ILE	engineered mutation	UNP Q9FCA6
A	405	HIS	-	expression tag	UNP Q9FCA6
A	406	HIS	-	expression tag	UNP Q9FCA6
A	407	HIS	-	expression tag	UNP Q9FCA6
A	408	HIS	-	expression tag	UNP Q9FCA6
A	409	HIS	-	expression tag	UNP Q9FCA6
A	410	HIS	-	expression tag	UNP Q9FCA6
B	87	LYS	ILE	engineered mutation	UNP Q9FCA6
B	405	HIS	-	expression tag	UNP Q9FCA6
B	406	HIS	-	expression tag	UNP Q9FCA6
B	407	HIS	-	expression tag	UNP Q9FCA6
B	408	HIS	-	expression tag	UNP Q9FCA6
B	409	HIS	-	expression tag	UNP Q9FCA6
B	410	HIS	-	expression tag	UNP Q9FCA6

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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		

- Molecule 3 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			14	10	4		

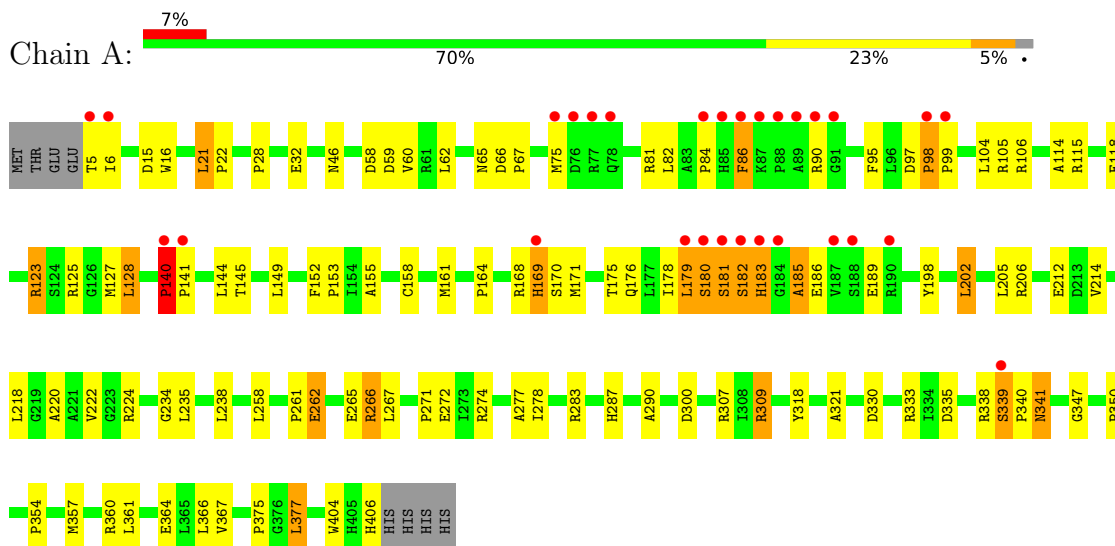
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	304	Total 304	O 304	0	0
4	B	330	Total 330	O 330	0	0

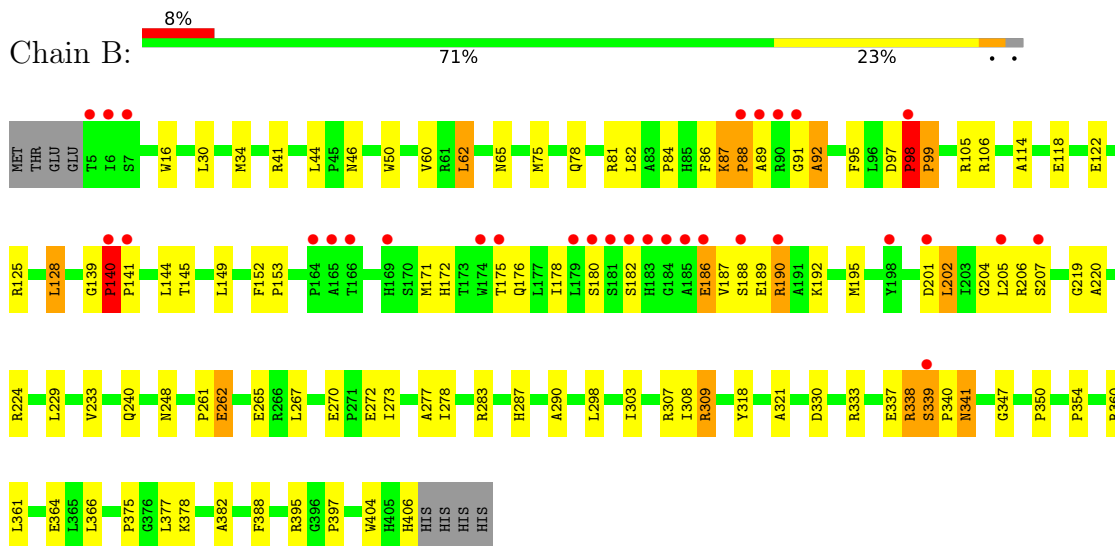
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Putative cytochrome P450



- Molecule 1: Putative cytochrome P450



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.61Å 79.31Å 87.66Å 90.00° 94.08° 90.00°	Depositor
Resolution (Å)	40.00 – 1.76 39.66 – 1.76	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.76) 93.5 (39.66-1.76)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.76Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.264 0.214 , 0.263	Depositor DCC
R_{free} test set	3798 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	10.3	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6954	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.40% 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, SPM

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	0.29	0/3183	0.58	0/4336
1	B	0.29	0/3183	0.58	0/4336
All	All	0.29	0/6366	0.58	0/8672

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	3110	0	3097	90	0
1	B	3110	0	3097	104	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	B	14	0	26	5	0
4	A	304	0	0	4	0
4	B	330	0	0	4	0
All	All	6954	0	6280	192	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 15.

All (192) 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:339:SER:HB2	1:B:340:PRO:HD3	1.39	1.05
1:A:178:ILE:HG22	1:A:179:LEU:HG	1.52	0.92
1:B:105:ARG:CZ	1:B:354:PRO:HG3	2.02	0.90
1:A:105:ARG:CZ	1:A:354:PRO:HG3	2.02	0.87
1:B:141:PRO:HA	4:B:563:HOH:O	1.76	0.86
1:B:378:LYS:HE3	3:B:432:SPM:HN5	1.42	0.84
1:B:378:LYS:CE	3:B:432:SPM:HN5	1.93	0.80
1:B:283:ARG:HD3	1:B:341:ASN:HD21	1.46	0.80
1:A:266:ARG:HG3	1:A:266:ARG:HH11	1.47	0.79
1:B:75:MET:HE2	1:B:89:ALA:HB2	1.65	0.78
1:A:283:ARG:HD3	1:A:341:ASN:HD21	1.50	0.77
1:A:140:PRO:HG2	1:A:406:HIS:HB2	1.67	0.77
1:A:278:ILE:HD11	1:A:367:VAL:HG21	1.68	0.76
1:B:87:LYS:H	1:B:88:PRO:CD	1.98	0.75
1:B:87:LYS:H	1:B:88:PRO:HD2	1.51	0.75
1:A:123:ARG:HA	1:A:123:ARG:HE	1.50	0.75
1:B:97:ASP:HB3	1:B:98:PRO:HD2	1.69	0.73
1:B:220:ALA:HB1	1:B:224:ARG:HH22	1.54	0.73
1:B:78:GLN:NE2	1:B:81:ARG:HH12	1.87	0.72
1:B:187:VAL:O	1:B:190:ARG:HG3	1.89	0.72
1:B:171:MET:HE1	1:B:240:GLN:HG2	1.71	0.72
1:A:140:PRO:CG	1:A:406:HIS:HB2	2.21	0.70
1:B:178:ILE:HD12	1:B:195:MET:HE3	1.73	0.70
1:B:144:LEU:HG	1:B:149:LEU:HD13	1.73	0.69
1:B:339:SER:HB2	1:B:340:PRO:CD	2.18	0.69
1:B:202:LEU:O	1:B:206:ARG:HG3	1.93	0.68
1:A:28:PRO:O	1:A:32:GLU:HG3	1.93	0.68
1:A:171:MET:O	1:A:175:THR:HG23	1.94	0.68
1:A:97:ASP:C	1:A:99:PRO:HD2	2.14	0.67
1:B:339:SER:CB	1:B:340:PRO:HD3	2.22	0.67
1:B:140:PRO:CG	1:B:406:HIS:HB2	2.25	0.67
1:A:339:SER:CB	1:A:340:PRO:HD3	2.25	0.66
1:B:171:MET:O	1:B:175:THR:HG23	1.96	0.66
1:B:140:PRO:HB2	1:B:141:PRO:HD3	1.78	0.66
1:A:169:HIS:HD2	1:A:170:SER:H	1.45	0.65
1:B:201:ASP:O	1:B:205:LEU:HD13	1.98	0.64
1:A:234:GLY:O	1:A:238:LEU:HD13	1.98	0.63
1:B:152:PHE:HB3	1:B:153:PRO:HD3	1.81	0.63
1:B:330:ASP:OD2	1:B:333:ARG:HD3	1.98	0.63
1:A:81:ARG:NE	1:A:86:PHE:HB2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:NH2	1:B:354:PRO:HG3	2.14	0.61
1:B:75:MET:CE	1:B:89:ALA:HB2	2.29	0.60
1:A:98:PRO:HG3	4:A:712:HOH:O	2.00	0.60
1:B:189:GLU:O	1:B:192:LYS:HG2	2.01	0.60
1:B:207:SER:HA	1:B:219:GLY:O	2.02	0.60
1:A:339:SER:HB2	1:A:340:PRO:HD3	1.82	0.60
1:A:274:ARG:O	1:A:278:ILE:HG12	2.02	0.59
1:B:145:THR:HA	1:B:149:LEU:HB2	1.85	0.59
1:A:144:LEU:HG	1:A:149:LEU:HD13	1.85	0.59
1:B:186:GLU:O	1:B:188:SER:N	2.32	0.59
1:B:86:PHE:CE1	1:B:95:PHE:HE2	2.21	0.58
1:B:261:PRO:O	1:B:265:GLU:HG3	2.03	0.58
1:B:303:ILE:HD12	1:B:308:ILE:HD12	1.84	0.58
1:A:114:ALA:O	1:A:118:GLU:HG2	2.04	0.58
1:B:140:PRO:CD	1:B:406:HIS:HB2	2.33	0.58
1:A:75:MET:HE1	1:A:90:ARG:HA	1.86	0.57
1:A:105:ARG:NH2	1:A:354:PRO:HG3	2.18	0.57
1:A:220:ALA:HB1	1:A:224:ARG:HH22	1.69	0.57
1:A:169:HIS:CD2	1:A:170:SER:H	2.21	0.57
1:A:46:ASN:ND2	1:A:84:PRO:HA	2.20	0.56
1:B:60:VAL:HG21	1:B:321:ALA:HB2	1.87	0.56
1:A:272:GLU:H	1:A:272:GLU:CD	2.08	0.56
1:B:65:ASN:HD22	1:B:350:PRO:HD3	1.71	0.56
1:B:176:GLN:O	1:B:180:SER:HB3	2.06	0.56
1:B:229:LEU:O	1:B:233:VAL:HG23	2.05	0.56
1:B:172:HIS:O	1:B:176:GLN:HG3	2.06	0.56
1:A:309:ARG:HD3	1:A:309:ARG:H	1.70	0.56
1:B:307:ARG:NH1	1:B:309:ARG:HG3	2.21	0.56
1:A:145:THR:HA	1:A:149:LEU:HB2	1.88	0.56
1:A:164:PRO:HD2	1:A:198:TYR:OH	2.06	0.56
1:B:318:TYR:CZ	1:B:347:GLY:HA2	2.41	0.56
1:A:262:GLU:H	1:A:262:GLU:CD	2.05	0.55
1:A:307:ARG:NH1	1:A:309:ARG:HG3	2.21	0.55
1:A:339:SER:OG	1:A:340:PRO:HD3	2.07	0.55
1:B:303:ILE:HD12	1:B:308:ILE:CD1	2.37	0.54
1:A:287:HIS:HE1	4:A:538:HOH:O	1.91	0.54
1:A:318:TYR:CZ	1:A:347:GLY:HA2	2.42	0.54
1:B:360:ARG:O	1:B:364:GLU:HG3	2.08	0.54
1:A:106:ARG:HH22	1:B:298:LEU:HB3	1.73	0.53
1:B:87:LYS:N	1:B:88:PRO:CD	2.66	0.53
1:B:382:ALA:N	3:B:432:SPM:H132	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ARG:HD3	1:B:309:ARG:H	1.74	0.53
1:A:158:CYS:HB3	1:A:168:ARG:HD3	1.91	0.53
1:B:86:PHE:HE1	1:B:95:PHE:HE2	1.55	0.52
1:A:115:ARG:HG2	4:A:551:HOH:O	2.08	0.52
1:A:182:SER:O	1:A:183:HIS:C	2.48	0.52
1:A:140:PRO:HA	1:A:404:TRP:CE2	2.44	0.52
1:B:287:HIS:HE1	4:B:536:HOH:O	1.92	0.52
1:B:378:LYS:NZ	3:B:432:SPM:HN5	2.08	0.51
1:A:169:HIS:CD2	1:A:170:SER:N	2.79	0.51
1:A:152:PHE:HB3	1:A:153:PRO:HD3	1.92	0.51
1:A:62:LEU:C	1:A:62:LEU:HD23	2.32	0.51
1:A:98:PRO:N	1:A:99:PRO:HD2	2.26	0.51
1:B:140:PRO:HA	1:B:404:TRP:CE2	2.46	0.51
1:A:205:LEU:C	1:A:205:LEU:HD13	2.32	0.50
1:A:360:ARG:O	1:A:364:GLU:HG3	2.11	0.50
1:A:339:SER:CB	1:A:340:PRO:CD	2.89	0.50
1:A:128:LEU:HD11	1:A:366:LEU:HA	1.94	0.49
1:B:46:ASN:ND2	1:B:84:PRO:HA	2.27	0.49
1:A:205:LEU:HD13	1:A:205:LEU:O	2.13	0.49
1:B:78:GLN:HE22	1:B:81:ARG:HH12	1.60	0.49
1:A:178:ILE:CG2	1:A:179:LEU:HG	2.33	0.49
1:A:16:TRP:CZ2	1:A:290:ALA:HA	2.48	0.49
1:A:86:PHE:HE2	1:A:95:PHE:HZ	1.61	0.49
1:B:205:LEU:C	1:B:206:ARG:HG2	2.34	0.48
1:B:267:LEU:HD21	1:B:277:ALA:CB	2.43	0.48
1:A:81:ARG:HD3	1:A:86:PHE:CD1	2.48	0.48
1:A:123:ARG:HE	1:A:123:ARG:CA	2.24	0.48
1:B:375:PRO:O	1:B:404:TRP:HB2	2.13	0.48
1:A:206:ARG:HH21	1:A:206:ARG:HG3	1.77	0.48
1:B:30:LEU:O	1:B:34:MET:HG3	2.13	0.48
1:A:375:PRO:O	1:A:404:TRP:HB2	2.12	0.48
1:B:140:PRO:HG2	1:B:406:HIS:HB2	1.94	0.47
1:B:139:GLY:HA2	1:B:406:HIS:HD2	1.80	0.47
1:A:140:PRO:HB2	1:A:141:PRO:HD3	1.96	0.47
1:B:262:GLU:CD	1:B:262:GLU:H	2.11	0.47
1:A:97:ASP:HB3	1:A:98:PRO:HD2	1.95	0.47
1:B:99:PRO:HG2	4:B:575:HOH:O	2.15	0.47
1:A:161:MET:HA	1:A:214:VAL:HB	1.97	0.47
1:A:185:ALA:O	1:A:189:GLU:HG3	2.15	0.46
1:A:198:TYR:HE2	1:A:202:LEU:HD12	1.80	0.46
1:A:333:ARG:NH1	1:A:335:ASP:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ALA:HB1	1:B:224:ARG:NH2	2.27	0.46
1:A:300:ASP:OD2	1:A:307:ARG:NH2	2.48	0.46
1:B:62:LEU:C	1:B:62:LEU:HD23	2.36	0.46
1:B:278:ILE:HD12	1:B:364:GLU:HG2	1.97	0.46
1:B:361:LEU:C	1:B:361:LEU:HD23	2.36	0.45
1:B:87:LYS:HG2	1:B:88:PRO:HD3	1.98	0.45
1:B:140:PRO:O	1:B:404:TRP:CZ3	2.70	0.45
1:B:144:LEU:HG	1:B:149:LEU:CD1	2.45	0.45
1:B:128:LEU:HD11	1:B:366:LEU:HA	1.98	0.45
1:A:104:LEU:HG	1:A:235:LEU:HD22	1.97	0.45
1:A:180:SER:O	1:A:181:SER:HB3	2.15	0.45
1:B:171:MET:CE	1:B:240:GLN:HG2	2.43	0.45
1:B:171:MET:HE3	1:B:171:MET:HA	1.97	0.45
1:A:202:LEU:O	1:A:206:ARG:HG2	2.17	0.45
1:A:330:ASP:OD1	1:A:333:ARG:HD3	2.17	0.45
1:A:99:PRO:HB3	1:B:99:PRO:HB3	1.99	0.45
1:B:62:LEU:C	1:B:62:LEU:CD2	2.85	0.45
1:B:114:ALA:O	1:B:118:GLU:HG2	2.17	0.45
1:A:114:ALA:HA	1:A:357:MET:HG2	1.99	0.44
1:A:123:ARG:HA	1:A:123:ARG:NE	2.26	0.44
1:B:140:PRO:HD3	1:B:406:HIS:HB2	2.00	0.44
1:B:378:LYS:HE3	3:B:432:SPM:N5	2.21	0.44
1:B:283:ARG:HD3	1:B:341:ASN:ND2	2.24	0.44
1:A:140:PRO:CD	1:A:406:HIS:HB2	2.47	0.43
1:B:41:ARG:HD2	1:B:50:TRP:CE3	2.52	0.43
1:A:266:ARG:HG3	1:A:266:ARG:NH1	2.22	0.43
1:B:204:GLY:C	1:B:206:ARG:H	2.21	0.43
1:B:140:PRO:HD3	1:B:406:HIS:CD2	2.54	0.43
1:B:278:ILE:CD1	1:B:364:GLU:HG2	2.49	0.43
1:A:218:LEU:O	1:A:222:VAL:HG23	2.19	0.43
1:B:88:PRO:HB2	1:B:95:PHE:CE1	2.54	0.43
1:A:82:LEU:HD22	1:A:290:ALA:HB3	2.01	0.43
1:B:272:GLU:H	1:B:272:GLU:CD	2.22	0.43
1:B:82:LEU:HD22	1:B:290:ALA:HB3	2.01	0.42
1:A:65:ASN:HD22	1:A:350:PRO:HD3	1.84	0.42
1:A:66:ASP:HA	1:A:67:PRO:HD3	1.83	0.42
1:A:220:ALA:HB1	1:A:224:ARG:NH2	2.33	0.42
1:B:278:ILE:CD1	1:B:364:GLU:HA	2.49	0.42
1:B:16:TRP:HB3	1:B:44:LEU:HD23	2.01	0.42
1:A:5:THR:HG23	1:A:6:ILE:N	2.34	0.42
1:A:176:GLN:HG2	4:A:585:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:CE1	1:B:95:PHE:CE2	3.06	0.42
1:B:388:PHE:HA	1:B:397:PRO:HA	2.02	0.42
1:B:270:GLU:O	1:B:273:ILE:HG22	2.20	0.42
1:B:339:SER:CB	1:B:340:PRO:CD	2.89	0.42
1:B:91:GLY:O	1:B:92:ALA:O	2.37	0.42
1:A:164:PRO:HD3	1:A:202:LEU:HD11	2.02	0.41
1:A:361:LEU:C	1:A:361:LEU:HD23	2.40	0.41
1:A:198:TYR:CE2	1:A:202:LEU:HD12	2.55	0.41
1:A:271:PRO:HD2	1:A:272:GLU:OE2	2.21	0.41
1:A:267:LEU:HD21	1:A:277:ALA:CB	2.50	0.41
1:B:16:TRP:CZ2	1:B:290:ALA:HA	2.55	0.41
1:B:106:ARG:NH1	4:B:570:HOH:O	2.53	0.41
1:B:309:ARG:HD3	1:B:309:ARG:N	2.35	0.41
1:B:189:GLU:HA	1:B:192:LYS:CD	2.51	0.41
1:B:337:GLU:O	1:B:338:ARG:C	2.59	0.41
1:B:46:ASN:CG	1:B:84:PRO:HA	2.41	0.41
1:A:60:VAL:HG21	1:A:321:ALA:HB2	2.03	0.41
1:A:21:LEU:HA	1:A:22:PRO:HD3	1.87	0.41
1:A:58:ASP:OD1	1:A:59:ASP:N	2.54	0.41
1:B:149:LEU:CD1	1:B:149:LEU:N	2.84	0.41
1:B:62:LEU:HD23	1:B:62:LEU:O	2.21	0.41
1:A:127:MET:CE	1:A:155:ALA:HB1	2.51	0.40
1:A:258:LEU:HD21	1:A:377:LEU:HD13	2.03	0.40
1:A:261:PRO:O	1:A:265:GLU:HG3	2.22	0.40
1:B:97:ASP:C	1:B:99:PRO:HD2	2.42	0.40
1:B:171:MET:CE	1:B:171:MET:HA	2.52	0.40
1:B:176:GLN:O	1:B:180:SER:CB	2.70	0.40
1:A:114:ALA:HA	1:A:357:MET:CG	2.51	0.40
1:B:248:ASN:HB3	1:B:395:ARG:O	2.22	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	400/410 (98%)	377 (94%)	12 (3%)	11 (3%)	5	0
1	B	400/410 (98%)	375 (94%)	15 (4%)	10 (2%)	5	0
All	All	800/820 (98%)	752 (94%)	27 (3%)	21 (3%)	5	0

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	PRO
1	A	339	SER
1	B	87	LYS
1	B	98	PRO
1	A	179	LEU
1	A	183	HIS
1	B	92	ALA
1	B	99	PRO
1	B	140	PRO
1	A	180	SER
1	A	181	SER
1	A	186	GLU
1	B	88	PRO
1	B	338	ARG
1	A	185	ALA
1	A	338	ARG
1	B	186	GLU
1	B	339	SER
1	A	98	PRO
1	A	182	SER
1	B	182	SER

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	332/340 (98%)	317 (96%)	15 (4%)	27	8
1	B	332/340 (98%)	320 (96%)	12 (4%)	35	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	664/680 (98%)	637 (96%)	27 (4%)	30 10

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	21	LEU
1	A	86	PHE
1	A	123	ARG
1	A	125	ARG
1	A	128	LEU
1	A	140	PRO
1	A	169	HIS
1	A	202	LEU
1	A	212	GLU
1	A	262	GLU
1	A	266	ARG
1	A	309	ARG
1	A	341	ASN
1	A	377	LEU
1	B	62	LEU
1	B	98	PRO
1	B	122	GLU
1	B	125	ARG
1	B	128	LEU
1	B	140	PRO
1	B	190	ARG
1	B	202	LEU
1	B	262	GLU
1	B	309	ARG
1	B	341	ASN
1	B	377	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	46	ASN
1	A	65	ASN
1	A	169	HIS
1	A	193	ASN

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Mol	Chain	Res	Type
1	A	240	GLN
1	A	249	ASN
1	A	287	HIS
1	A	341	ASN
1	B	65	ASN
1	B	78	GLN
1	B	193	ASN
1	B	240	GLN
1	B	249	ASN
1	B	287	HIS
1	B	341	ASN
1	B	406	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 monosaccharides 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	B	430	1,4	41,50,50	1.73	8 (19%)	45,82,82	1.39	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	430	1,4	41,50,50	1.80	9 (21%)	45,82,82	1.36	7 (15%)
3	SPM	B	432	-	13,13,13	0.29	0	12,12,12	1.30	1 (8%)

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	B	430	1,4	-	6/12/54/54	-
2	HEM	A	430	1,4	-	4/12/54/54	-
3	SPM	B	432	-	-	0/11/11/11	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	430	HEM	CBB-CAB	5.05	1.55	1.30
2	B	430	HEM	CBB-CAB	4.50	1.52	1.30
2	A	430	HEM	CBC-CAC	3.80	1.54	1.29
2	B	430	HEM	CBC-CAC	3.77	1.54	1.29
2	B	430	HEM	C3C-C2C	-3.69	1.35	1.40
2	A	430	HEM	C3C-CAC	3.55	1.55	1.47
2	A	430	HEM	C3C-C2C	-3.54	1.35	1.40
2	B	430	HEM	C3C-CAC	3.52	1.55	1.47
2	A	430	HEM	CAB-C3B	3.00	1.55	1.47
2	A	430	HEM	CMB-C2B	2.31	1.55	1.50
2	A	430	HEM	CAA-C2A	2.30	1.55	1.52
2	A	430	HEM	O2A-CGA	-2.23	1.23	1.30
2	B	430	HEM	O2A-CGA	-2.19	1.23	1.30
2	B	430	HEM	CAB-C3B	2.17	1.53	1.47
2	B	430	HEM	CAA-C2A	2.12	1.55	1.52
2	A	430	HEM	C2C-C1C	2.10	1.47	1.42
2	B	430	HEM	C2C-C1C	2.01	1.47	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	HEM	C4C-CHD-C1D	3.97	127.80	122.56
2	A	430	HEM	C4C-CHD-C1D	3.90	127.70	122.56
2	A	430	HEM	CBA-CAA-C2A	3.28	118.22	112.62
2	B	430	HEM	CBA-CAA-C2A	3.27	118.20	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	HEM	CBB-CAB-C3B	-2.94	112.97	127.62
2	A	430	HEM	C4B-CHC-C1C	2.91	126.39	122.56
2	B	430	HEM	CMA-C3A-C4A	-2.89	124.03	128.46
2	A	430	HEM	CMA-C3A-C4A	-2.81	124.14	128.46
2	B	430	HEM	C4B-CHC-C1C	2.63	126.03	122.56
2	B	430	HEM	CMC-C2C-C3C	2.56	129.47	124.68
2	B	430	HEM	O1A-CGA-CBA	-2.55	114.89	123.08
2	A	430	HEM	CMC-C2C-C3C	2.39	129.15	124.68
2	A	430	HEM	O1A-CGA-CBA	-2.24	115.89	123.08
3	B	432	SPM	C7-C6-N5	-2.13	106.38	112.14
2	A	430	HEM	CBB-CAB-C3B	-2.02	117.58	127.62

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	430	HEM	C2B-C3B-CAB-CBB
2	B	430	HEM	C4B-C3B-CAB-CBB
2	A	430	HEM	CAA-CBA-CGA-O1A
2	A	430	HEM	CAA-CBA-CGA-O2A
2	B	430	HEM	CAA-CBA-CGA-O2A
2	B	430	HEM	CAD-CBD-CGD-O1D
2	B	430	HEM	CAA-CBA-CGA-O1A
2	B	430	HEM	CAD-CBD-CGD-O2D
2	A	430	HEM	CAD-CBD-CGD-O1D
2	A	430	HEM	CAD-CBD-CGD-O2D

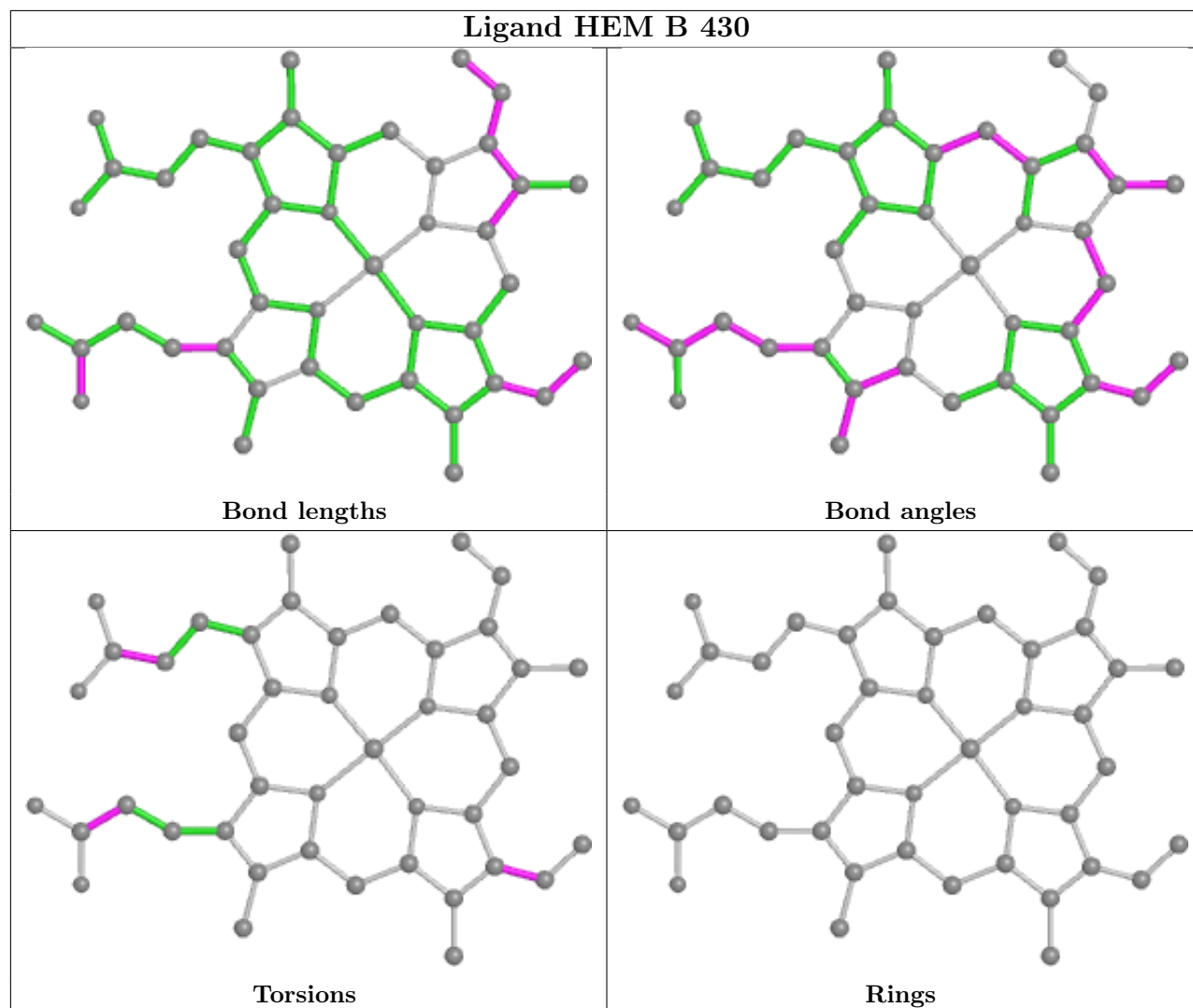
There are no ring outliers.

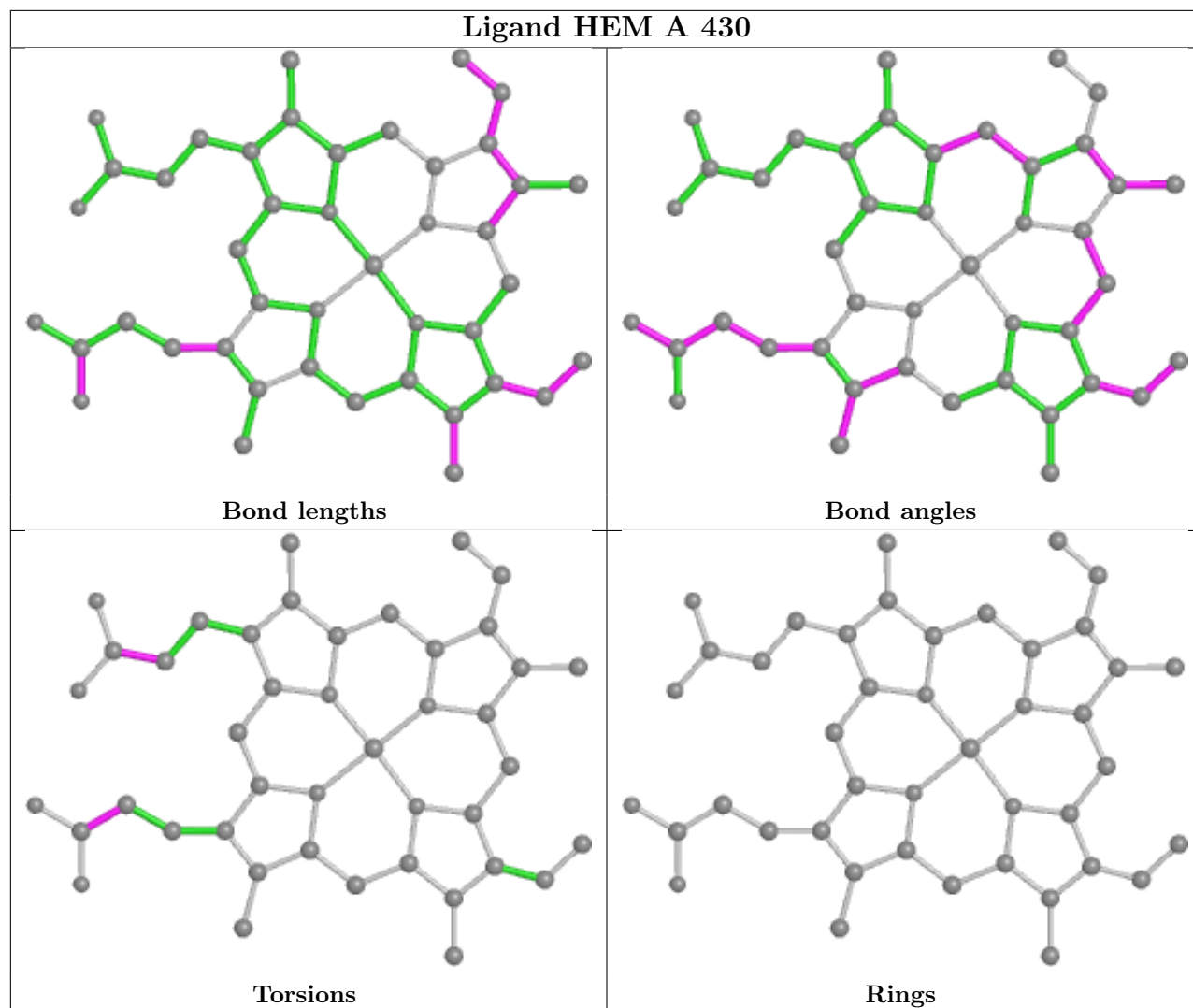
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	432	SPM	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	402/410 (98%)	0.44	29 (7%) 15 20	4, 14, 49, 92	0
1	B	402/410 (98%)	0.50	31 (7%) 13 18	3, 13, 49, 109	0
All	All	804/820 (98%)	0.47	60 (7%) 14 19	3, 14, 49, 109	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	ALA	13.7
1	B	184	GLY	12.8
1	B	182	SER	11.4
1	B	88	PRO	11.3
1	A	179	LEU	11.3
1	B	183	HIS	10.7
1	A	86	PHE	10.7
1	B	179	LEU	10.2
1	B	181	SER	9.1
1	A	88	PRO	8.6
1	B	89	ALA	6.9
1	A	339	SER	6.7
1	A	87	LYS	6.6
1	A	90	ARG	6.5
1	B	339	SER	6.1
1	A	89	ALA	6.1
1	B	166	THR	5.9
1	B	164	PRO	5.3
1	B	6	ILE	5.1
1	B	98	PRO	4.7
1	A	181	SER	4.6
1	A	91	GLY	4.5
1	A	183	HIS	4.4
1	A	180	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	188	SER	4.2
1	A	99	PRO	4.2
1	B	140	PRO	4.1
1	A	75	MET	4.1
1	A	5	THR	4.0
1	A	184	GLY	3.9
1	B	91	GLY	3.9
1	A	190	ARG	3.9
1	B	205	LEU	3.9
1	A	169	HIS	3.8
1	A	85	HIS	3.7
1	A	187	VAL	3.6
1	A	140	PRO	3.6
1	A	182	SER	3.5
1	B	90	ARG	3.5
1	A	6	ILE	3.5
1	B	190	ARG	3.4
1	A	84	PRO	3.2
1	B	180	SER	3.1
1	B	141	PRO	3.1
1	B	5	THR	2.9
1	B	186	GLU	2.9
1	A	141	PRO	2.8
1	B	165	ALA	2.7
1	A	98	PRO	2.5
1	B	198	TYR	2.5
1	B	175	THR	2.4
1	B	7	SER	2.4
1	B	188	SER	2.3
1	A	76	ASP	2.3
1	B	207	SER	2.2
1	B	201	ASP	2.2
1	A	78	GLN	2.2
1	A	77	ARG	2.1
1	B	174	TRP	2.1
1	B	169	HIS	2.1

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 monosaccharides in this entry.

6.4 Ligands

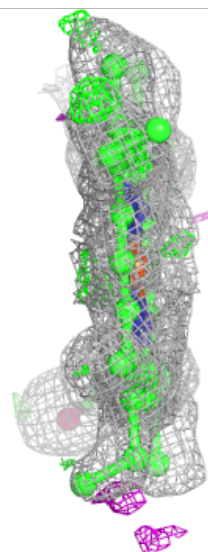
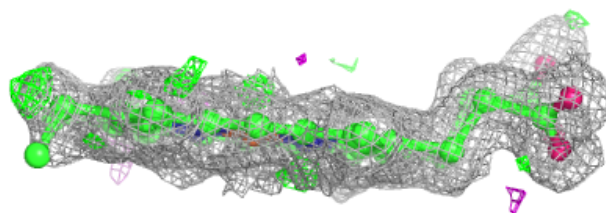
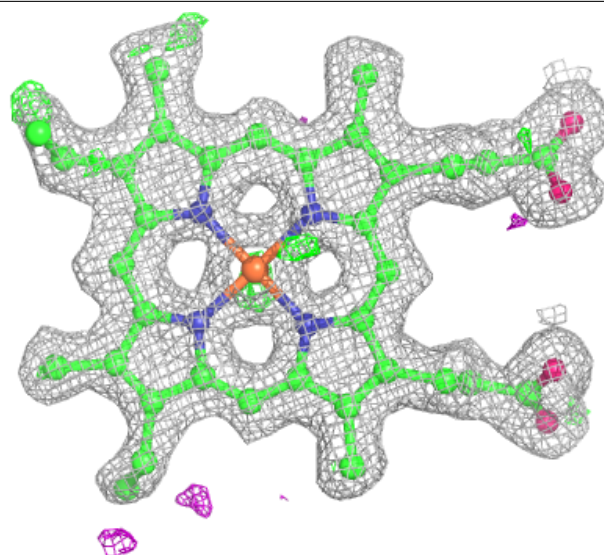
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

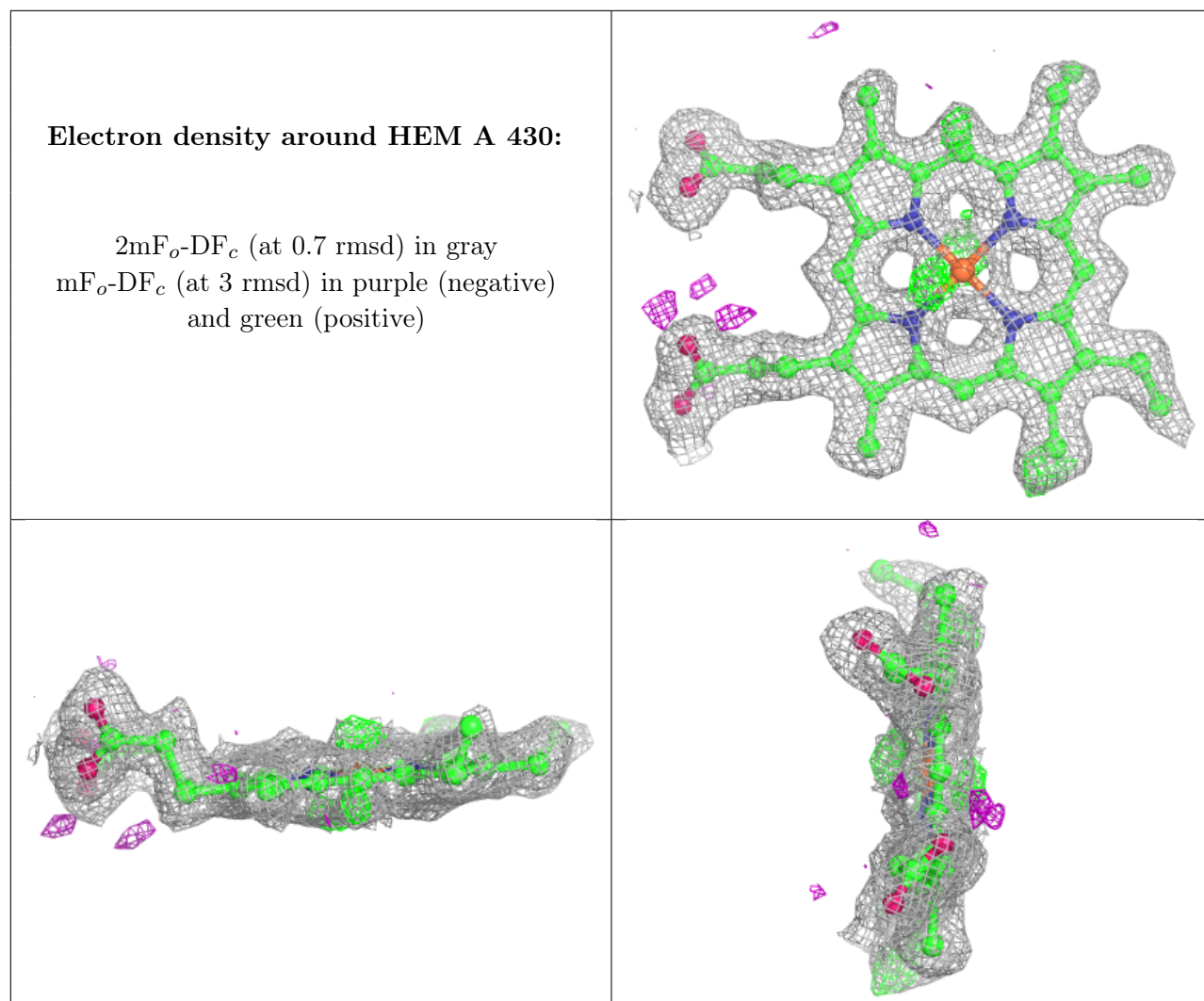
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SPM	B	432	14/14	0.81	0.33	15,46,99,101	0
2	HEM	B	430	43/43	0.97	0.12	1,6,14,41	0
2	HEM	A	430	43/43	0.97	0.12	1,7,12,31	0

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 B 430:

$2mF_o-DF_c$ (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.