



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 AM UTC

PDB ID : 5OFQ / pdb_00005ofq
Title : Crystal structure of substrate-free CYP109A2 from *Bacillus megaterium*
Authors : Jozwik, I.K.; Thunnissen, A.M.W.H.
Deposited on : 2017-07-11
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

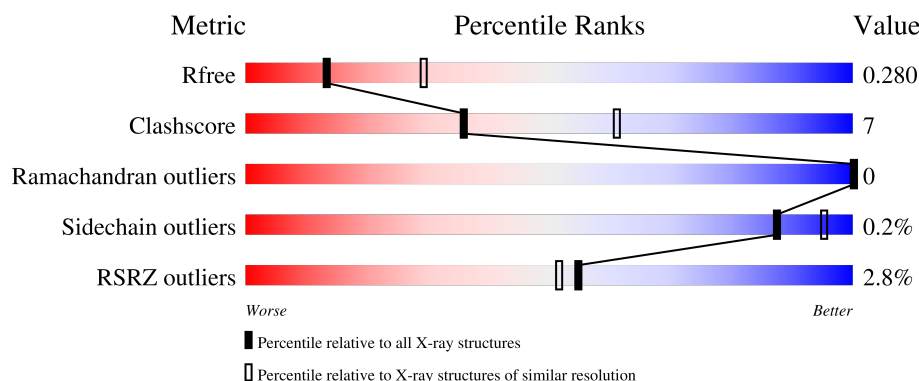
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	409	 2% 78% 16% 6%
1	B	409	 3% 81% 14% 6%
1	C	409	 2% 75% 19% 6%
1	D	409	 4% 75% 19% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12726 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	386	Total	C	N	O	S	0	0	0
			3109	1985	522	590	12			
1	B	386	Total	C	N	O	S	0	0	0
			3109	1985	522	590	12			
1	C	386	Total	C	N	O	S	0	0	0
			3109	1985	522	590	12			
1	D	387	Total	C	N	O	S	0	0	0
			3117	1991	523	591	12			

There are 24 discrepancies between the modelled and reference sequences:

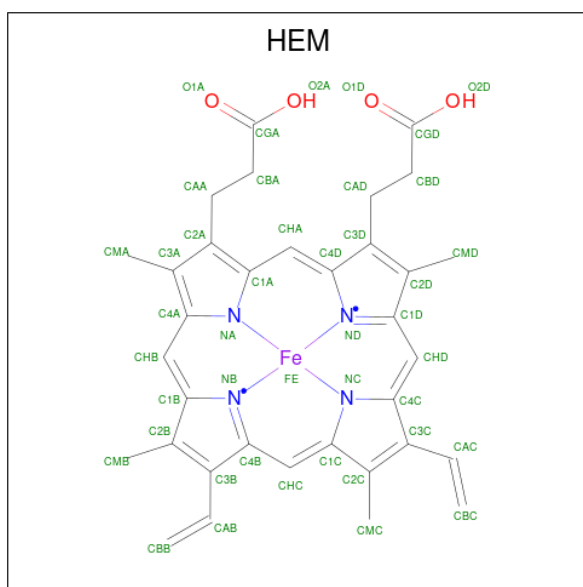
Chain	Residue	Modelled	Actual	Comment	Reference
A	404	HIS	-	expression tag	UNP D5DF88
A	405	HIS	-	expression tag	UNP D5DF88
A	406	HIS	-	expression tag	UNP D5DF88
A	407	HIS	-	expression tag	UNP D5DF88
A	408	HIS	-	expression tag	UNP D5DF88
A	409	HIS	-	expression tag	UNP D5DF88
B	404	HIS	-	expression tag	UNP D5DF88
B	405	HIS	-	expression tag	UNP D5DF88
B	406	HIS	-	expression tag	UNP D5DF88
B	407	HIS	-	expression tag	UNP D5DF88
B	408	HIS	-	expression tag	UNP D5DF88
B	409	HIS	-	expression tag	UNP D5DF88
C	404	HIS	-	expression tag	UNP D5DF88
C	405	HIS	-	expression tag	UNP D5DF88
C	406	HIS	-	expression tag	UNP D5DF88
C	407	HIS	-	expression tag	UNP D5DF88
C	408	HIS	-	expression tag	UNP D5DF88
C	409	HIS	-	expression tag	UNP D5DF88
D	404	HIS	-	expression tag	UNP D5DF88
D	405	HIS	-	expression tag	UNP D5DF88
D	406	HIS	-	expression tag	UNP D5DF88

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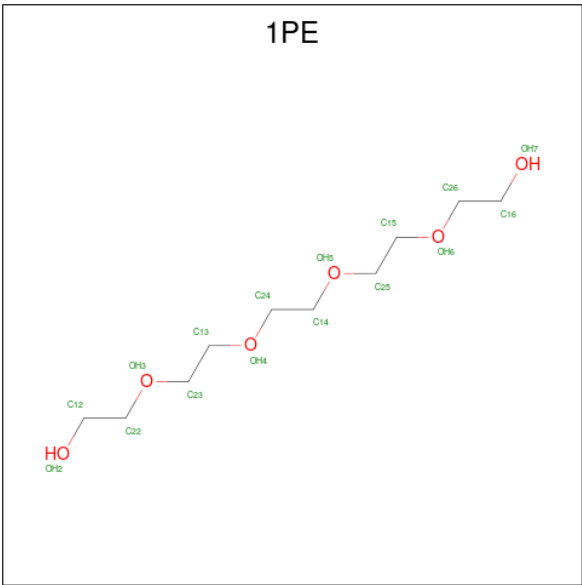
Chain	Residue	Modelled	Actual	Comment	Reference
D	407	HIS	-	expression tag	UNP D5DF88
D	408	HIS	-	expression tag	UNP D5DF88
D	409	HIS	-	expression tag	UNP D5DF88

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



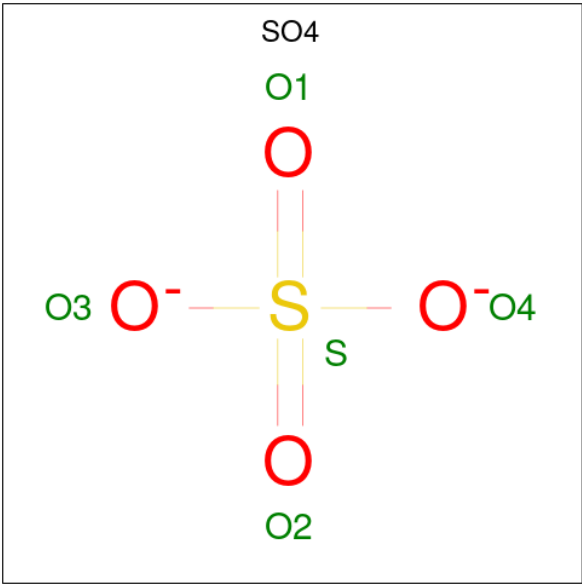
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

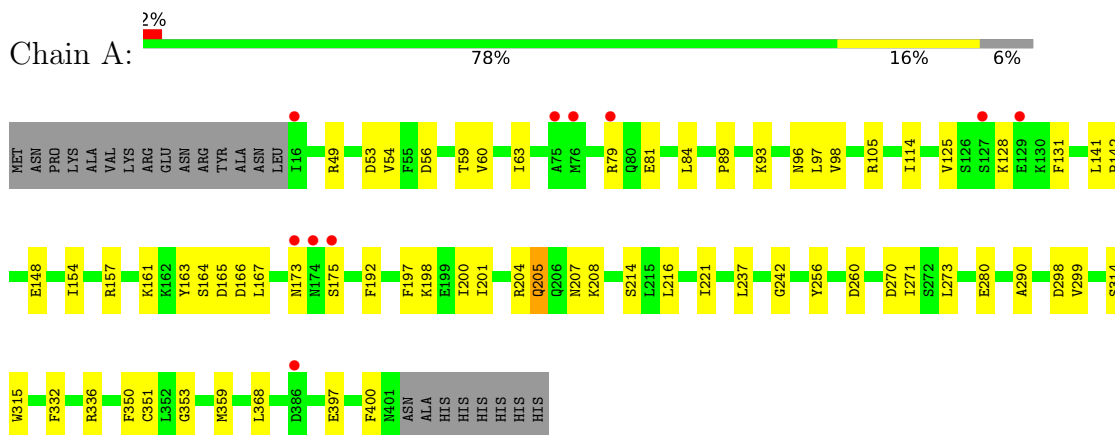
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	2	Total O 2 2	0	0
5	C	2	Total O 2 2	0	0
5	D	7	Total O 7 7	0	0

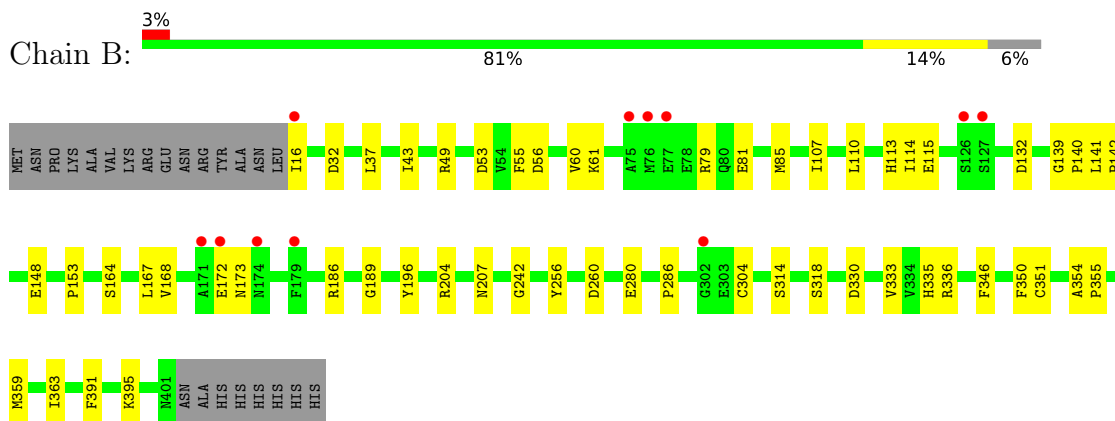
3 Residue-property plots [i](#)

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

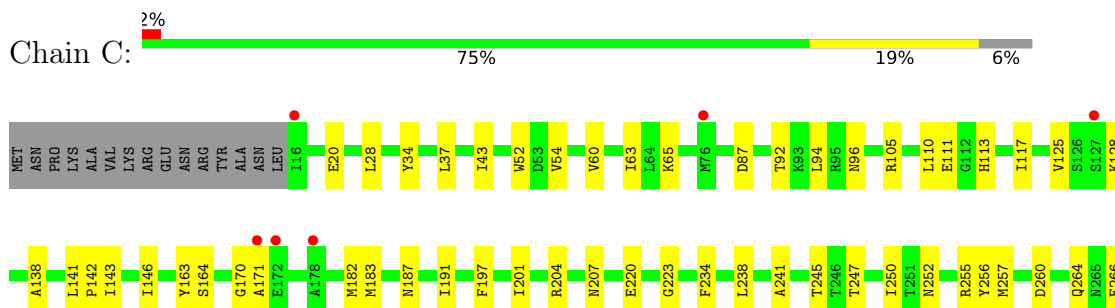
• Molecule 1: Cytochrome P450

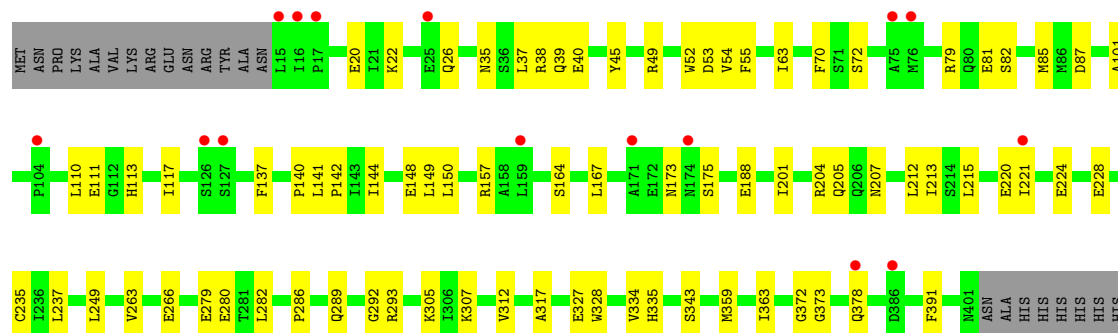


• Molecule 1: Cytochrome P450



• Molecule 1: Cytochrome P450





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.12Å 155.53Å 158.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 2.70 49.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.93-2.70) 96.7 (49.93-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.224 , 0.275 0.233 , 0.280	Depositor DCC
R_{free} test set	2610 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 19.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.033 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12726	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.87% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 1PE, SO4

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	0.78	1/3172 (0.0%)	0.80	0/4286
1	B	0.74	0/3172	0.77	0/4286
1	C	0.75	0/3172	0.81	3/4286 (0.1%)
1	D	0.72	0/3180	0.81	2/4297 (0.0%)
All	All	0.75	1/12696 (0.0%)	0.80	5/17155 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLN	CD-OE1	5.64	1.34	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	87	ASP	CA-C-N	-7.48	112.67	120.38
1	D	87	ASP	C-N-CA	-7.48	112.67	120.38
1	C	171	ALA	N-CA-C	-5.60	100.97	108.86
1	C	87	ASP	CA-C-N	-5.04	115.98	119.66
1	C	87	ASP	C-N-CA	-5.04	115.98	119.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3109	0	3092	46	0
1	B	3109	0	3092	36	0
1	C	3109	0	3092	46	1
1	D	3117	0	3103	60	1
2	A	43	0	30	3	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	32	0	44	2	0
3	B	16	0	22	0	0
3	C	32	0	44	4	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	7	0	0	0	0
All	All	12726	0	12609	184	1

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 7.

All (184) 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:D:305:LYS:HE2	1:D:307:LYS:NZ	1.54	1.21
1:D:305:LYS:CE	1:D:307:LYS:NZ	2.04	1.19
1:D:305:LYS:CE	1:D:307:LYS:HZ2	1.66	1.02
1:D:305:LYS:HE3	1:D:307:LYS:NZ	1.82	0.90
1:D:305:LYS:HE3	1:D:307:LYS:HZ2	1.40	0.84
1:D:305:LYS:CE	1:D:307:LYS:HZ1	1.87	0.81
1:D:204:ARG:HA	1:D:207:ASN:O	1.89	0.73
1:D:305:LYS:HE2	1:D:307:LYS:HZ3	1.51	0.72
1:C:266:GLU:OE2	1:C:335:HIS:NE2	2.23	0.71
1:B:79:ARG:NH2	1:B:81:GLU:OE2	2.24	0.70
1:D:305:LYS:HE2	1:D:307:LYS:HZ2	1.30	0.68
1:A:49:ARG:NH2	1:A:53:ASP:OD2	2.28	0.67
1:D:79:ARG:NH2	1:D:81:GLU:OE2	2.29	0.66
1:A:173:ASN:OD1	1:A:175:SER:OG	2.06	0.65
1:B:204:ARG:HA	1:B:207:ASN:O	1.97	0.65
1:B:55:PHE:O	1:B:318:SER:OG	2.18	0.61
1:D:279:GLU:HA	1:D:282:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:TYR:O	1:C:321:ARG:NH2	2.33	0.61
1:D:266:GLU:OE2	1:D:335:HIS:NE2	2.29	0.60
1:A:164:SER:O	1:A:167:LEU:HB2	2.01	0.60
1:A:60:VAL:HG22	1:A:314:SER:HB3	1.84	0.58
1:A:81:GLU:HB3	1:A:237:LEU:HD13	1.86	0.58
1:C:241:ALA:O	1:C:245:THR:OG1	2.17	0.58
1:D:49:ARG:NH2	1:D:53:ASP:OD2	2.36	0.58
1:A:204:ARG:HA	1:A:207:ASN:O	2.03	0.57
1:B:61:LYS:HE2	1:B:346:PHE:CZ	2.39	0.57
1:B:132:ASP:OD2	1:B:395:LYS:HG3	2.04	0.57
1:C:28:LEU:O	1:C:255:ARG:NH2	2.34	0.57
1:D:49:ARG:HH22	1:D:53:ASP:CG	2.12	0.57
1:D:213:ILE:CD1	1:D:235:CYS:SG	2.93	0.57
1:C:353:GLY:HA3	2:C:503:HEM:C3C	2.39	0.56
1:C:333:VAL:HG12	1:C:335:HIS:H	1.70	0.56
1:B:43:ILE:HG23	1:B:304:CYS:SG	2.46	0.56
3:A:503:1PE:H161	1:C:105:ARG:HH12	1.70	0.55
1:B:256:TYR:CE2	1:B:260:ASP:HB3	2.41	0.55
1:D:101:ALA:HB2	1:D:215:LEU:HD22	1.89	0.55
1:D:150:LEU:O	1:D:213:ILE:HG12	2.05	0.55
1:C:268:ARG:NH2	1:C:373:GLY:HA2	2.22	0.54
1:A:79:ARG:NH1	1:A:81:GLU:HG3	2.23	0.53
1:C:328:TRP:N	1:C:329:PRO:CD	2.72	0.53
1:D:22:LYS:N	1:D:26:GLN:OE1	2.38	0.53
1:C:65:LYS:HE2	3:C:501:1PE:OH6	2.09	0.53
1:C:43:ILE:HG23	1:C:304:CYS:SG	2.49	0.53
1:B:333:VAL:HG12	1:B:335:HIS:H	1.74	0.53
1:A:350:PHE:O	1:A:351:CYS:C	2.53	0.52
1:B:49:ARG:NH2	1:B:53:ASP:OD1	2.41	0.52
1:B:60:VAL:HG13	1:B:314:SER:HB3	1.92	0.52
1:C:257:MET:O	1:C:264:GLN:NE2	2.39	0.52
1:D:359:MET:O	1:D:363:ILE:HG12	2.10	0.51
1:D:101:ALA:HB2	1:D:215:LEU:CD2	2.40	0.51
1:C:197:PHE:O	1:C:201:ILE:HG12	2.10	0.51
1:C:43:ILE:HD11	1:C:306:ILE:HD11	1.92	0.51
1:B:286:PRO:O	1:B:391:PHE:HB3	2.10	0.51
1:A:89:PRO:HB2	1:D:40:GLU:OE2	2.11	0.50
1:C:65:LYS:CE	3:C:501:1PE:H161	2.41	0.50
1:C:92:THR:HG22	1:C:96:ASN:ND2	2.26	0.50
1:B:164:SER:O	1:B:167:LEU:HB2	2.12	0.50
1:A:49:ARG:HH22	1:A:53:ASP:CG	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:VAL:HG21	1:C:63:ILE:HD11	1.92	0.50
1:C:65:LYS:HE2	3:C:501:1PE:H161	1.92	0.50
1:C:125:VAL:HG12	1:C:128:LYS:HD2	1.94	0.49
1:A:163:TYR:CD2	1:A:192:PHE:CD2	3.01	0.49
1:B:107:ILE:HD12	1:B:359:MET:HE2	1.93	0.49
1:B:280:GLU:OE1	1:B:280:GLU:HA	2.12	0.49
1:D:82:SER:HB3	1:D:237:LEU:HD22	1.93	0.49
1:C:20:GLU:OE2	1:C:37:LEU:HD21	2.13	0.49
1:B:56:ASP:O	1:B:60:VAL:HG23	2.12	0.49
1:B:115:GLU:CG	1:B:363:ILE:HD12	2.43	0.49
1:A:131:PHE:O	1:A:397:GLU:HA	2.13	0.48
1:D:63:ILE:HD13	1:D:312:VAL:CG1	2.43	0.48
1:A:141:LEU:HB3	1:A:142:PRO:HD3	1.95	0.48
1:C:187:ASN:O	1:C:191:ILE:HG12	2.13	0.48
1:B:16:ILE:HG22	1:B:16:ILE:O	2.12	0.48
1:A:105:ARG:HG2	1:B:330:ASP:HB3	1.96	0.48
1:B:113:HIS:NE2	1:B:148:GLU:HG3	2.29	0.48
1:C:141:LEU:HB3	1:C:142:PRO:HD3	1.95	0.48
1:A:198:LYS:HE2	3:A:503:1PE:OH7	2.12	0.48
1:C:204:ARG:HA	1:C:207:ASN:O	2.14	0.47
1:C:256:TYR:CE2	1:C:260:ASP:HB3	2.49	0.47
1:D:72:SER:O	1:D:85:MET:HA	2.15	0.47
1:A:256:TYR:CZ	1:A:332:PHE:HB3	2.49	0.47
1:A:353:GLY:HA3	2:A:501:HEM:C3C	2.50	0.47
1:C:170:GLY:O	1:C:182:MET:HG3	2.13	0.47
1:C:220:GLU:CD	1:C:223:GLY:HA2	2.39	0.47
1:D:35:ASN:HA	1:D:38:ARG:NH1	2.31	0.46
1:A:161:LYS:NZ	1:A:165:ASP:OD2	2.49	0.46
1:D:293:ARG:HH22	2:D:501:HEM:CGA	2.27	0.46
1:B:168:VAL:HG23	1:B:168:VAL:O	2.14	0.46
1:A:97:LEU:HD23	1:A:221:ILE:HD12	1.98	0.46
1:C:340:PRO:HA	3:C:502:1PE:H262	1.97	0.46
1:C:348:ILE:HG13	1:C:349:HIS:CD2	2.51	0.46
1:C:290:ALA:HB2	1:C:315:TRP:CE3	2.51	0.46
1:A:54:VAL:HG21	1:A:63:ILE:HD11	1.98	0.46
1:D:54:VAL:HG21	1:D:63:ILE:HD11	1.97	0.46
1:D:205:GLN:HG2	1:D:228:GLU:OE2	2.16	0.46
1:A:197:PHE:O	1:A:201:ILE:HG12	2.16	0.46
1:C:34:TYR:HB3	1:C:318:SER:HB2	1.98	0.45
1:A:84:LEU:HA	2:A:501:HEM:O2D	2.16	0.45
1:D:282:LEU:O	1:D:343:SER:OG	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PHE:O	1:A:200:ILE:N	2.49	0.45
1:A:256:TYR:CZ	1:A:332:PHE:CB	3.00	0.45
1:B:172:GLU:O	1:B:173:ASN:HB3	2.16	0.45
1:D:164:SER:O	1:D:167:LEU:HB2	2.17	0.45
1:C:146:ILE:HD11	1:C:238:LEU:HB3	1.98	0.45
1:D:141:LEU:HB3	1:D:142:PRO:HD3	1.99	0.45
1:D:221:ILE:O	1:D:221:ILE:HG13	2.18	0.44
1:A:242:GLY:HA2	2:A:501:HEM:C2C	2.53	0.44
1:A:270:ASP:HB3	1:A:273:LEU:HD12	2.00	0.44
1:A:96:ASN:HB3	1:A:221:ILE:HD13	1.99	0.44
1:C:143:ILE:HD12	1:C:164:SER:CB	2.48	0.44
1:A:125:VAL:HG12	1:A:128:LYS:HD2	1.99	0.44
1:D:148:GLU:CD	1:D:157:ARG:HH22	2.24	0.44
1:D:286:PRO:O	1:D:391:PHE:HB3	2.17	0.44
1:A:98:VAL:HG12	1:A:216:LEU:HD22	2.00	0.44
1:C:113:HIS:NE2	1:C:117:ILE:HD11	2.33	0.44
1:C:317:ALA:O	1:C:321:ARG:HG3	2.18	0.44
1:D:149:LEU:HG	1:D:212:LEU:HB2	2.00	0.44
1:B:280:GLU:CD	1:B:336:ARG:HE	2.26	0.43
1:A:208:LYS:HD2	1:A:214:SER:HB3	2.00	0.43
1:C:350:PHE:O	1:C:351:CYS:C	2.61	0.43
1:D:263:VAL:HG13	1:D:334:VAL:HG11	2.00	0.43
1:B:37:LEU:HD13	1:B:55:PHE:CZ	2.53	0.43
1:C:252:ASN:HB3	1:C:285:TYR:HB3	1.99	0.43
1:D:220:GLU:HA	1:D:224:GLU:O	2.17	0.43
1:B:81:GLU:OE1	1:B:85:MET:HE3	2.18	0.43
1:D:63:ILE:HD13	1:D:312:VAL:HG12	2.00	0.43
1:D:378:GLN:OE1	1:D:378:GLN:N	2.51	0.43
1:A:298:ASP:O	1:A:299:VAL:CG2	2.67	0.43
1:C:182:MET:HE3	1:C:183:MET:SD	2.59	0.43
1:A:93:LYS:HZ1	1:D:40:GLU:HA	1.84	0.43
1:A:163:TYR:HA	1:A:166:ASP:HB2	1.99	0.43
1:A:201:ILE:O	1:A:205:GLN:N	2.50	0.43
1:A:271:ILE:HD12	1:A:271:ILE:HA	1.90	0.43
1:A:290:ALA:HB2	1:A:315:TRP:CE3	2.54	0.43
1:B:153:PRO:HD2	1:B:196:TYR:OH	2.19	0.43
1:C:138:ALA:HB2	1:C:250:ILE:CG2	2.49	0.43
1:C:270:ASP:HB3	1:C:273:LEU:HD12	2.00	0.43
1:C:110:LEU:O	1:C:111:GLU:C	2.62	0.42
1:D:173:ASN:OD1	1:D:175:SER:OG	2.18	0.42
1:A:280:GLU:CD	1:A:336:ARG:HE	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:LEU:HB2	2:D:501:HEM:HBB1	2.01	0.42
1:B:139:GLY:N	1:B:140:PRO:CD	2.83	0.42
1:B:242:GLY:HA2	2:B:501:HEM:C2C	2.54	0.42
1:B:110:LEU:O	1:B:114:ILE:HG13	2.20	0.42
1:D:150:LEU:HA	1:D:212:LEU:HB3	2.00	0.42
1:A:54:VAL:HG21	1:A:63:ILE:CD1	2.49	0.42
1:A:197:PHE:O	1:A:198:LYS:C	2.62	0.42
1:D:292:GLY:O	1:D:293:ARG:NH1	2.50	0.42
1:A:56:ASP:OD1	1:A:59:THR:HB	2.20	0.42
1:A:154:ILE:O	1:A:157:ARG:HG2	2.20	0.42
1:B:60:VAL:HG22	1:B:314:SER:HB3	2.02	0.42
1:D:20:GLU:HG2	1:D:37:LEU:HD21	2.02	0.42
1:B:354:ALA:HB3	1:B:355:PRO:HD3	2.01	0.41
1:C:234:PHE:O	1:C:238:LEU:HG	2.21	0.41
1:D:22:LYS:HB2	1:D:26:GLN:OE1	2.20	0.41
1:D:63:ILE:HG23	1:D:70:PHE:CG	2.56	0.41
1:D:280:GLU:HA	1:D:280:GLU:OE1	2.19	0.41
1:C:52:TRP:CZ3	1:C:304:CYS:HB3	2.55	0.41
1:D:110:LEU:O	1:D:111:GLU:C	2.64	0.41
1:D:137:PHE:C	1:D:140:PRO:HD2	2.45	0.41
1:A:256:TYR:CE2	1:A:260:ASP:HB3	2.56	0.41
1:A:368:LEU:HD23	1:A:400:PHE:HZ	1.85	0.41
1:C:142:PRO:HG2	1:C:247:THR:OG1	2.21	0.41
1:A:54:VAL:HG11	1:A:59:THR:HG22	2.03	0.41
1:C:60:VAL:HG22	1:C:314:SER:HB3	2.02	0.41
1:D:372:GLY:O	1:D:373:GLY:C	2.63	0.41
1:A:114:ILE:HD12	1:A:359:MET:HE3	2.02	0.41
1:D:117:ILE:CD1	1:D:144:ILE:HG22	2.50	0.41
1:C:256:TYR:CZ	1:C:332:PHE:CB	3.04	0.41
1:D:201:ILE:O	1:D:205:GLN:N	2.52	0.41
1:B:115:GLU:HG2	1:B:363:ILE:HD12	2.03	0.41
1:D:305:LYS:HE3	1:D:307:LYS:HZ1	1.59	0.40
1:A:105:ARG:NH1	1:B:32:ASP:OD2	2.53	0.40
1:D:45:TYR:HD1	1:D:52:TRP:NE1	2.19	0.40
1:D:117:ILE:HD13	1:D:144:ILE:HG22	2.02	0.40
1:B:115:GLU:HG3	1:B:363:ILE:HD12	2.03	0.40
1:B:186:ARG:O	1:B:189:GLY:N	2.54	0.40
1:D:38:ARG:HB2	1:D:55:PHE:HB3	2.03	0.40
1:B:350:PHE:O	1:B:351:CYS:C	2.64	0.40
1:C:94:LEU:N	1:C:94:LEU:HD12	2.37	0.40
1:D:289:GLN:HB2	1:D:317:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:GLU:O	1:D:328:TRP:C	2.63	0.40
1:B:141:LEU:HB3	1:B:142:PRO:HD3	2.04	0.40
1:D:81:GLU:HB3	1:D:237:LEU:HD13	2.03	0.40

All (1) 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:C:163:TYR:OH	1:D:188:GLU:OE2[2_555]	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	384/409 (94%)	371 (97%)	13 (3%)	0	100	100
1	B	384/409 (94%)	367 (96%)	17 (4%)	0	100	100
1	C	384/409 (94%)	363 (94%)	21 (6%)	0	100	100
1	D	385/409 (94%)	368 (96%)	17 (4%)	0	100	100
All	All	1537/1636 (94%)	1469 (96%)	68 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	341/361 (94%)	340 (100%)	1 (0%)	86	94
1	B	341/361 (94%)	341 (100%)	0	100	100
1	C	341/361 (94%)	341 (100%)	0	100	100
1	D	342/361 (95%)	340 (99%)	2 (1%)	78	91
All	All	1365/1444 (94%)	1362 (100%)	3 (0%)	87	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	GLU
1	D	39	GLN
1	D	113	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	265	ASN
1	C	205	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	1PE	C	501	-	15,15,15	0.74	0	14,14,14	1.14	1 (7%)
3	1PE	B	502	-	15,15,15	0.70	0	14,14,14	0.72	0
2	HEM	C	503	1	50,50,50	1.61	6 (12%)	67,82,82	1.12	8 (11%)
2	HEM	A	501	1	50,50,50	1.73	14 (28%)	67,82,82	0.96	4 (5%)
2	HEM	B	501	1	50,50,50	1.48	9 (18%)	67,82,82	0.98	2 (2%)
3	1PE	A	503	-	15,15,15	0.56	0	14,14,14	0.73	0
2	HEM	D	501	1	50,50,50	1.74	8 (16%)	67,82,82	0.98	2 (2%)
4	SO4	A	504	-	4,4,4	0.28	0	6,6,6	0.77	0
3	1PE	A	502	-	15,15,15	0.61	0	14,14,14	0.71	0
3	1PE	C	502	-	15,15,15	0.66	0	14,14,14	0.74	0
4	SO4	A	505	-	4,4,4	0.25	0	6,6,6	0.47	0
4	SO4	B	503	-	4,4,4	0.16	0	6,6,6	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	C	501	-	-	7/13/13/13	-
3	1PE	B	502	-	-	8/13/13/13	-
2	HEM	C	503	1	-	0/14/54/54	-
2	HEM	A	501	1	-	0/14/54/54	-
2	HEM	B	501	1	-	1/14/54/54	-
3	1PE	A	503	-	-	11/13/13/13	-
2	HEM	D	501	1	-	0/14/54/54	-
3	1PE	A	502	-	-	6/13/13/13	-
3	1PE	C	502	-	-	4/13/13/13	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-NC	7.28	2.19	1.95
2	C	503	HEM	FE-NC	6.03	2.15	1.95
2	A	501	HEM	FE-NC	5.01	2.11	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-ND	4.20	2.07	1.94
2	C	503	HEM	FE-NB	4.07	2.07	1.94
2	A	501	HEM	C2A-C3A	-3.38	1.30	1.38
2	B	501	HEM	FE-NC	3.24	2.05	1.95
2	C	503	HEM	CAC-C3C	3.23	1.56	1.47
2	A	501	HEM	FE-NB	-2.91	1.85	1.94
2	A	501	HEM	CAC-C3C	2.87	1.55	1.47
2	C	503	HEM	CAB-C3B	2.84	1.55	1.47
2	A	501	HEM	C3C-C2C	-2.84	1.31	1.37
2	B	501	HEM	C2A-C3A	-2.81	1.31	1.38
2	A	501	HEM	CAB-C3B	2.69	1.54	1.47
2	D	501	HEM	FE-NA	-2.68	1.86	1.95
2	A	501	HEM	C3D-C2D	-2.63	1.31	1.36
2	B	501	HEM	FE-ND	2.63	2.03	1.94
2	B	501	HEM	C3C-C2C	-2.60	1.31	1.37
2	D	501	HEM	CAB-C3B	2.59	1.54	1.47
2	B	501	HEM	C3D-C2D	-2.57	1.31	1.36
2	D	501	HEM	CAC-C3C	2.55	1.54	1.47
2	A	501	HEM	FE-NA	-2.39	1.87	1.95
2	A	501	HEM	C4D-ND	-2.37	1.36	1.40
2	C	503	HEM	FE-ND	2.30	2.02	1.94
2	B	501	HEM	CAC-C3C	2.28	1.53	1.47
2	D	501	HEM	CMA-C3A	2.25	1.55	1.50
2	B	501	HEM	C4D-ND	-2.17	1.36	1.40
2	D	501	HEM	CMD-C2D	2.17	1.55	1.50
2	A	501	HEM	C1C-NC	-2.14	1.35	1.39
2	D	501	HEM	C3D-C2D	-2.12	1.32	1.36
2	B	501	HEM	CMB-C2B	2.10	1.55	1.50
2	A	501	HEM	C3B-C2B	-2.10	1.32	1.37
2	A	501	HEM	FE-ND	2.09	2.01	1.94
2	C	503	HEM	CMB-C2B	2.09	1.55	1.50
2	B	501	HEM	O2D-CGD	-2.08	1.23	1.30
2	A	501	HEM	CHC-C1C	-2.05	1.34	1.38
2	A	501	HEM	CMB-C2B	2.05	1.55	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CHC-C4B-NB	3.19	127.86	124.42
2	C	503	HEM	C1B-NB-C4B	2.41	108.06	105.21
2	B	501	HEM	CHD-C4C-NC	2.40	127.06	124.45
2	C	503	HEM	C4D-ND-C1D	2.37	108.01	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	O1A-CGA-CBA	-2.30	115.79	123.09
2	D	501	HEM	O1D-CGD-CBD	-2.30	115.79	123.09
2	C	503	HEM	C3B-C2B-C1B	2.27	108.12	106.41
2	D	501	HEM	CBD-CAD-C3D	-2.27	106.25	112.53
2	C	503	HEM	C4A-C3A-C2A	2.22	109.36	106.82
2	C	503	HEM	C2D-C1D-ND	-2.19	107.38	109.90
2	C	503	HEM	C3A-C4A-NA	-2.16	106.68	110.14
2	C	503	HEM	O2A-CGA-CBA	2.14	120.75	114.00
2	C	503	HEM	C2B-C1B-NB	-2.07	107.46	109.84
2	B	501	HEM	C1C-CHC-C4B	-2.07	121.62	126.02
2	A	501	HEM	CAD-CBD-CGD	-2.03	108.27	113.67
3	C	501	1PE	C25-OH5-C14	2.02	122.08	113.26
2	A	501	HEM	O2A-CGA-CBA	2.01	120.34	114.00

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	1PE	OH5-C14-C24-OH4
3	C	502	1PE	OH6-C15-C25-OH5
3	C	501	1PE	OH4-C13-C23-OH3
3	A	502	1PE	OH5-C14-C24-OH4
3	A	503	1PE	OH5-C14-C24-OH4
3	C	501	1PE	OH7-C16-C26-OH6
3	A	503	1PE	OH7-C16-C26-OH6
3	A	503	1PE	C13-C23-OH3-C22
3	C	501	1PE	OH2-C12-C22-OH3
3	B	502	1PE	OH2-C12-C22-OH3
3	A	503	1PE	OH6-C15-C25-OH5
3	A	503	1PE	OH2-C12-C22-OH3
3	A	502	1PE	OH4-C13-C23-OH3
3	C	502	1PE	OH5-C14-C24-OH4
3	B	502	1PE	C16-C26-OH6-C15
3	A	502	1PE	OH2-C12-C22-OH3
3	A	502	1PE	C24-C14-OH5-C25
3	A	503	1PE	C15-C25-OH5-C14
3	B	502	1PE	C25-C15-OH6-C26
3	C	501	1PE	C13-C23-OH3-C22
3	A	503	1PE	C23-C13-OH4-C24
3	C	501	1PE	C12-C22-OH3-C23
3	A	503	1PE	C12-C22-OH3-C23
3	A	503	1PE	C25-C15-OH6-C26

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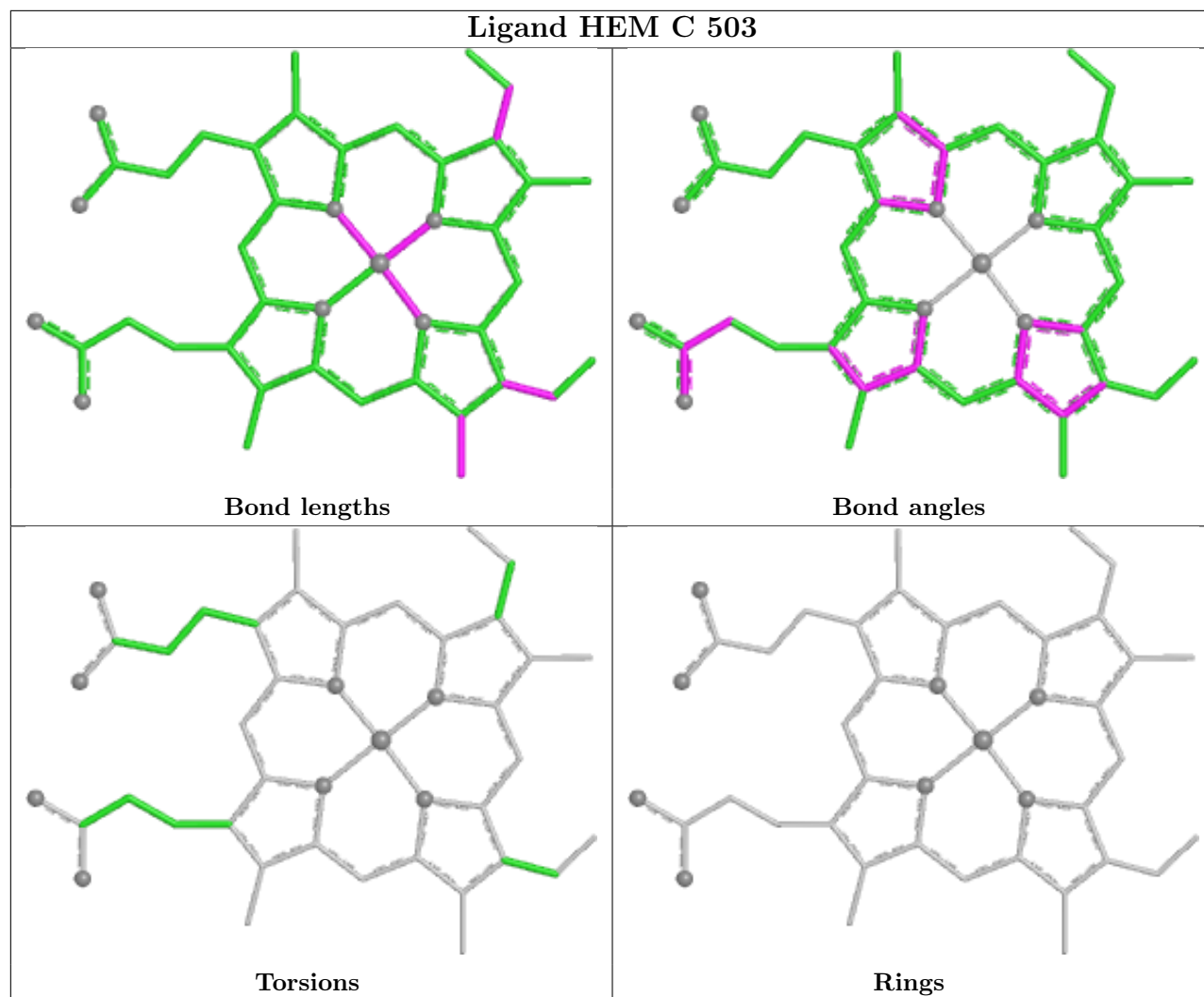
Mol	Chain	Res	Type	Atoms
3	B	502	1PE	C14-C24-OH4-C13
3	B	502	1PE	OH4-C13-C23-OH3
3	C	501	1PE	C25-C15-OH6-C26
3	A	503	1PE	C16-C26-OH6-C15
3	B	502	1PE	OH6-C15-C25-OH5
3	C	502	1PE	C15-C25-OH5-C14
3	A	502	1PE	C12-C22-OH3-C23
3	C	502	1PE	C24-C14-OH5-C25
3	B	502	1PE	C23-C13-OH4-C24
3	A	503	1PE	C24-C14-OH5-C25
3	C	501	1PE	C14-C24-OH4-C13
3	A	502	1PE	C25-C15-OH6-C26
2	B	501	HEM	CAD-CBD-CGD-O2D

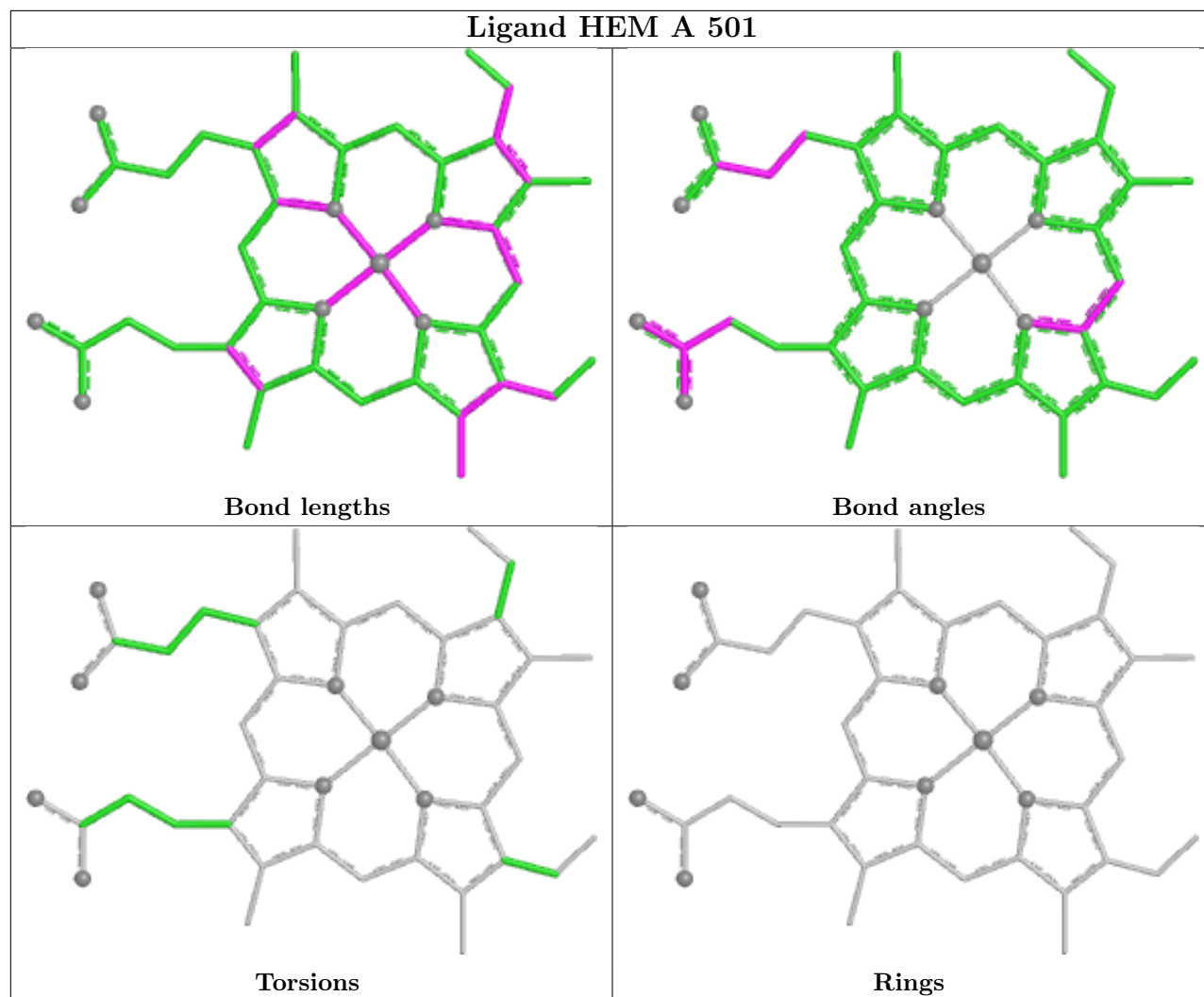
There are no ring outliers.

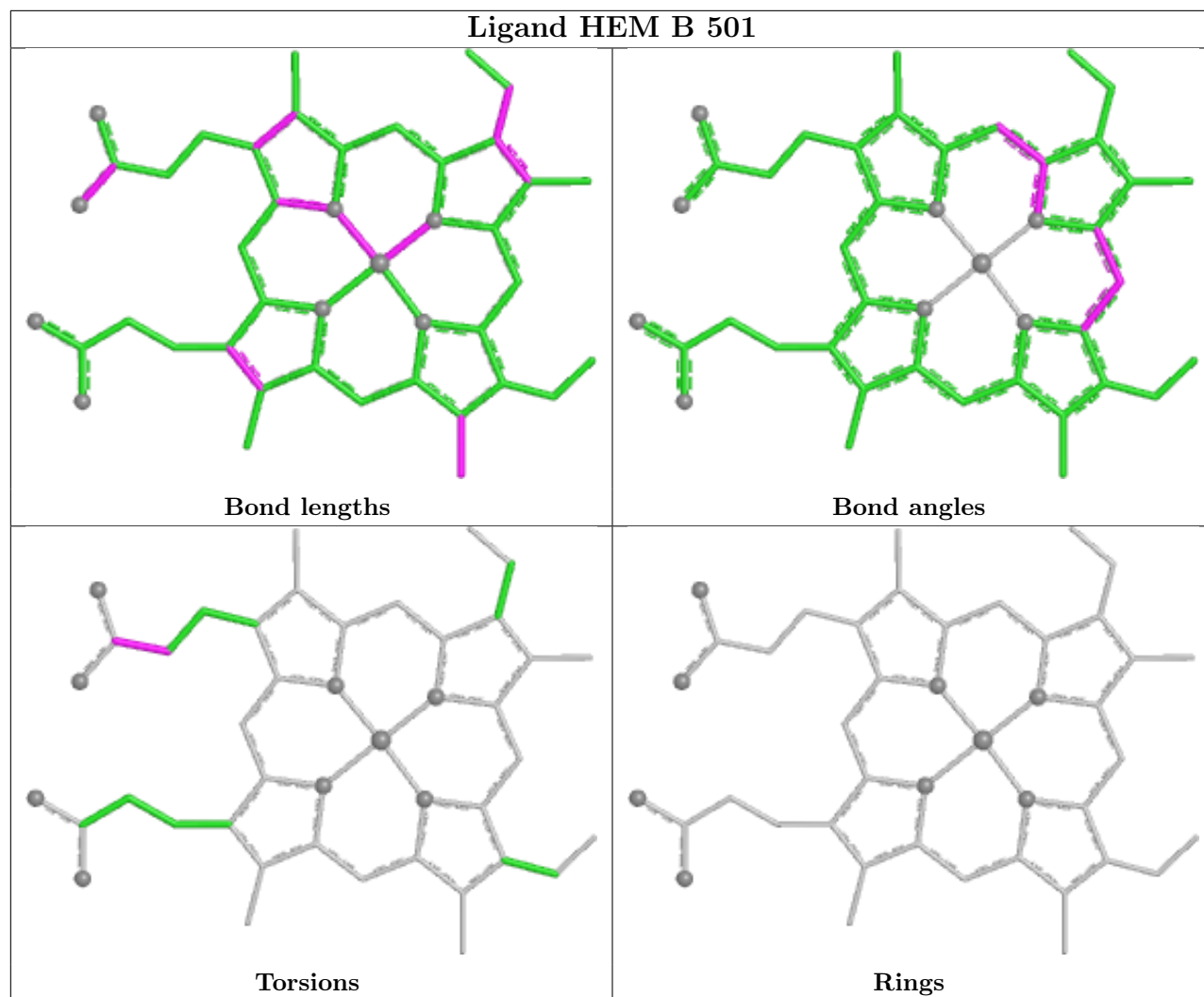
7 monomers are involved in 13 short contacts:

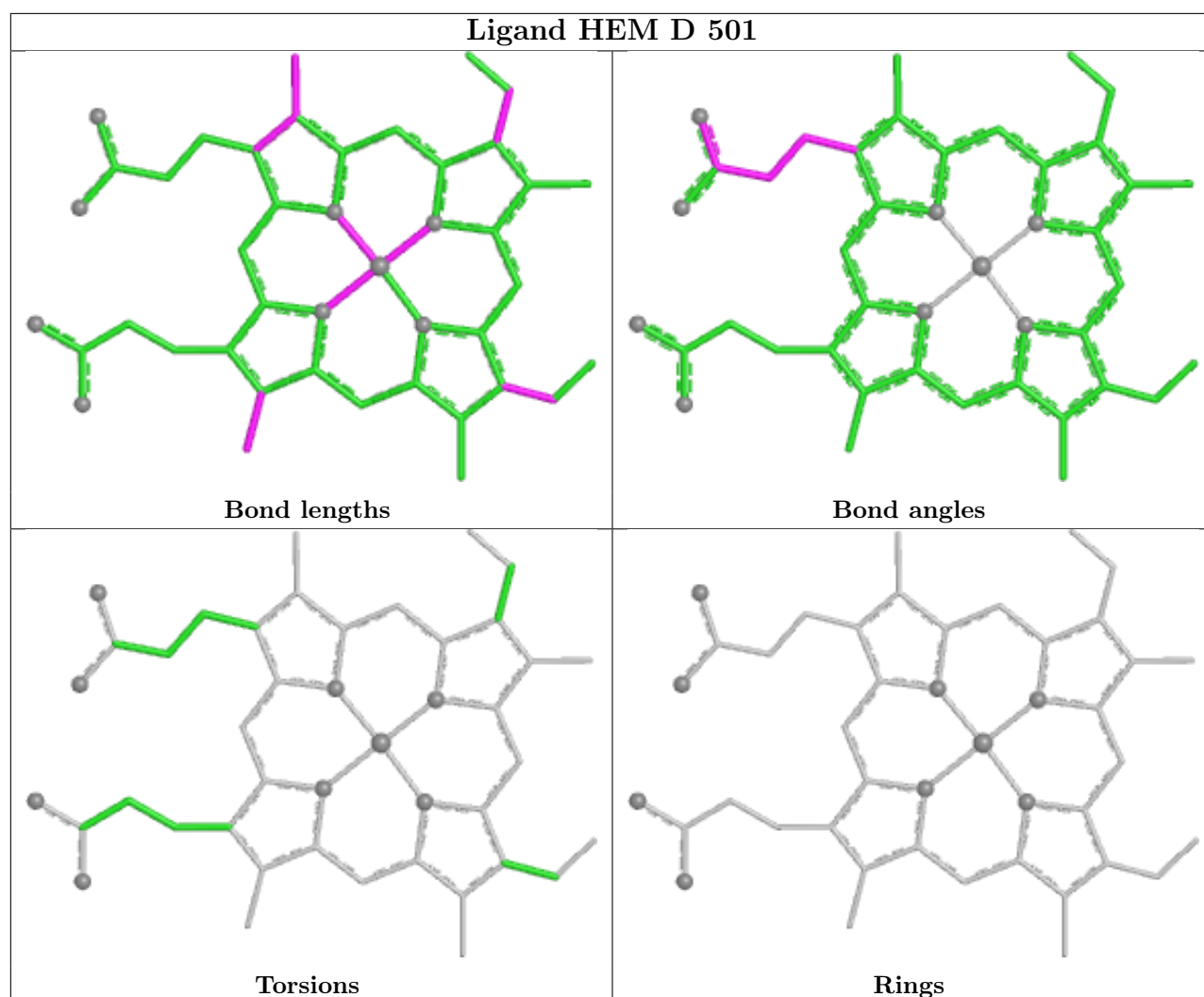
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	1PE	3	0
2	C	503	HEM	1	0
2	A	501	HEM	3	0
2	B	501	HEM	1	0
3	A	503	1PE	2	0
2	D	501	HEM	2	0
3	C	502	1PE	1	0

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	386/409 (94%)	0.09	10 (2%) 57 54	31, 39, 58, 82	0
1	B	386/409 (94%)	0.16	11 (2%) 55 51	32, 42, 64, 90	0
1	C	386/409 (94%)	0.28	8 (2%) 63 61	40, 45, 62, 89	0
1	D	387/409 (94%)	0.32	15 (3%) 43 39	36, 48, 66, 98	0
All	All	1545/1636 (94%)	0.21	44 (2%) 55 51	31, 44, 64, 98	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	15	LEU	5.3
1	C	16	ILE	4.3
1	D	75	ALA	3.8
1	D	16	ILE	3.8
1	C	172	GLU	3.6
1	D	159	LEU	3.6
1	B	16	ILE	3.5
1	A	175	SER	3.3
1	A	16	ILE	3.3
1	A	174	ASN	3.3
1	D	76	MET	3.1
1	D	386	ASP	3.1
1	B	179	PHE	3.1
1	C	171	ALA	3.0
1	C	76	MET	2.9
1	B	171	ALA	2.8
1	D	25	GLU	2.8
1	D	127	SER	2.8
1	D	174	ASN	2.6
1	D	17	PRO	2.6
1	A	75	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	75	ALA	2.4
1	B	127	SER	2.4
1	C	323	SER	2.4
1	A	79	ARG	2.4
1	C	127	SER	2.4
1	B	126	SER	2.4
1	B	76	MET	2.4
1	C	305	LYS	2.3
1	A	76	MET	2.3
1	B	174	ASN	2.3
1	A	386	ASP	2.3
1	D	171	ALA	2.2
1	C	178	ALA	2.2
1	A	173	ASN	2.2
1	D	126	SER	2.2
1	A	129	GLU	2.1
1	B	77	GLU	2.1
1	A	127	SER	2.1
1	D	378	GLN	2.1
1	D	221	ILE	2.1
1	B	172	GLU	2.0
1	D	104	PRO	2.0
1	B	302	GLY	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 [i](#)

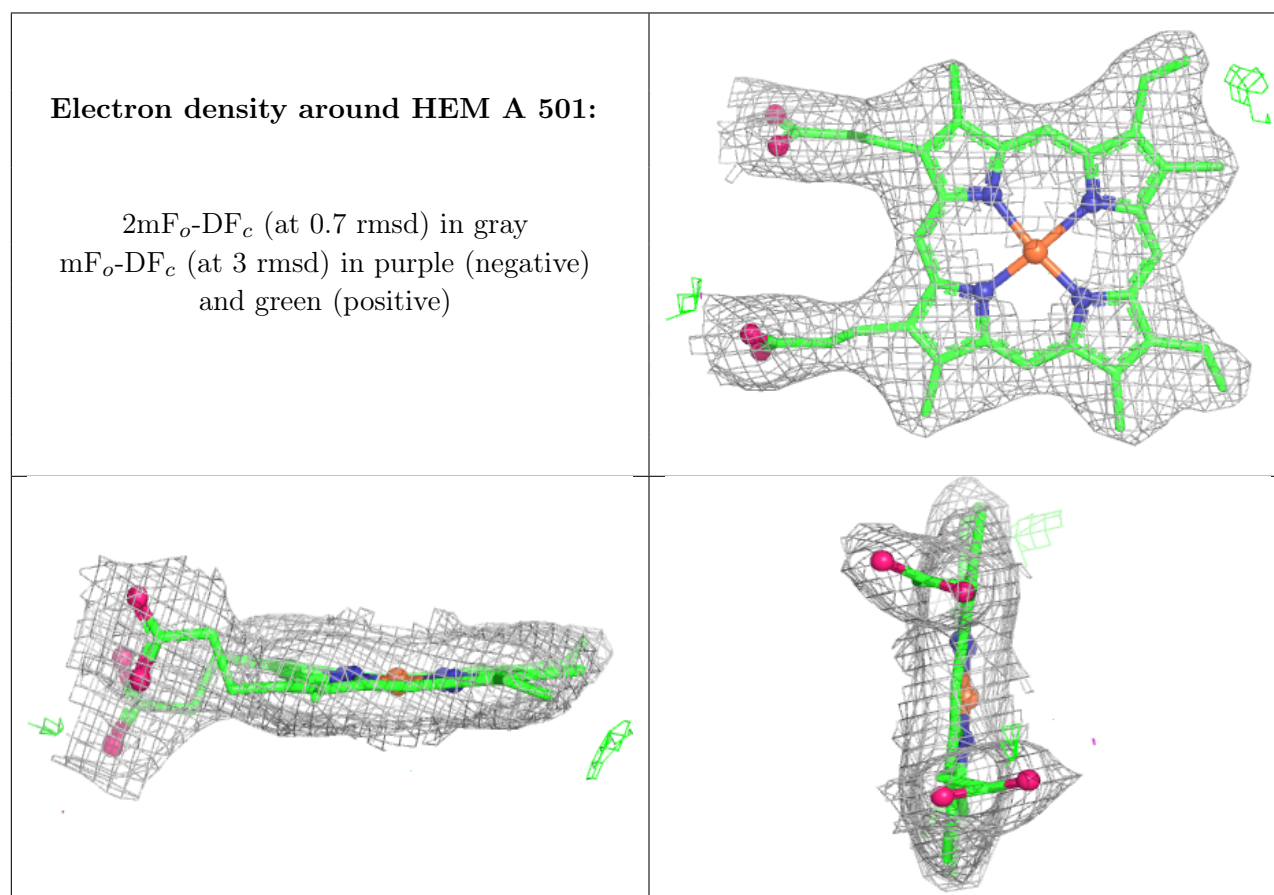
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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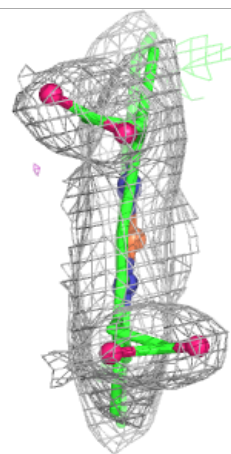
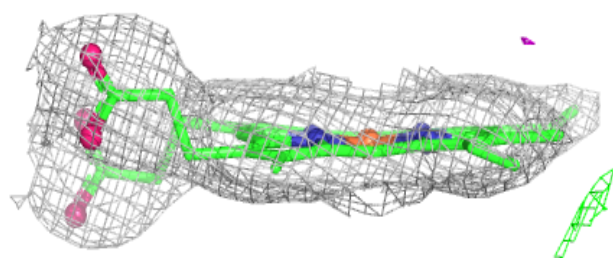
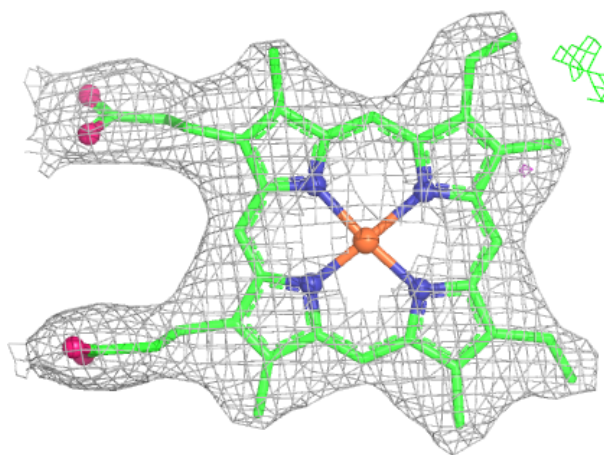
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	1PE	B	502	16/16	0.83	0.17	44,48,58,59	0
4	SO4	A	504	5/5	0.85	0.11	67,67,72,102	0
3	1PE	A	503	16/16	0.87	0.15	57,66,75,77	0
3	1PE	C	501	16/16	0.89	0.13	41,47,54,57	0
3	1PE	A	502	16/16	0.89	0.12	36,39,52,53	0
3	1PE	C	502	16/16	0.90	0.12	41,44,46,47	0
4	SO4	A	505	5/5	0.94	0.11	52,57,58,60	0
4	SO4	B	503	5/5	0.94	0.12	42,44,48,50	0
2	HEM	A	501	43/43	0.97	0.10	38,42,45,46	0
2	HEM	B	501	43/43	0.97	0.10	41,44,45,49	0
2	HEM	C	503	43/43	0.97	0.09	42,48,50,51	0
2	HEM	D	501	43/43	0.97	0.10	42,50,53,54	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.



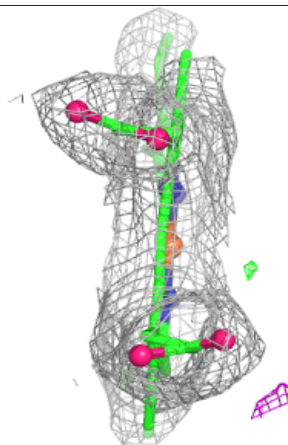
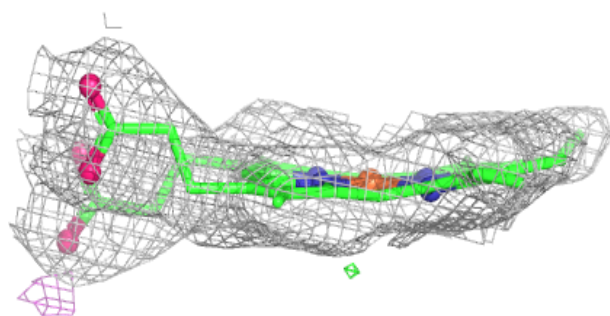
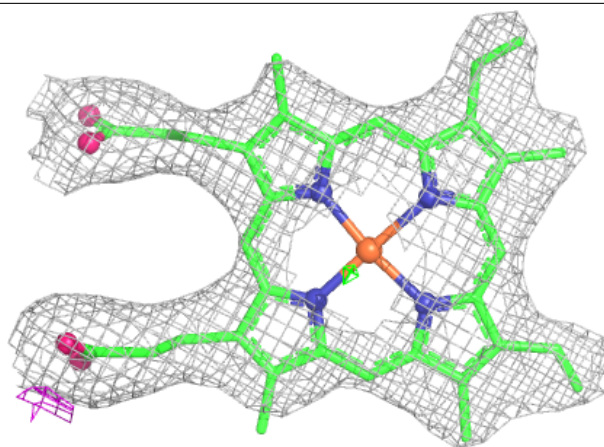
Electron density around HEM B 501:

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

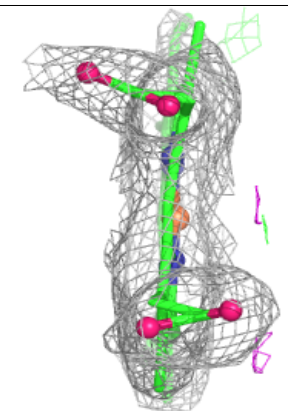
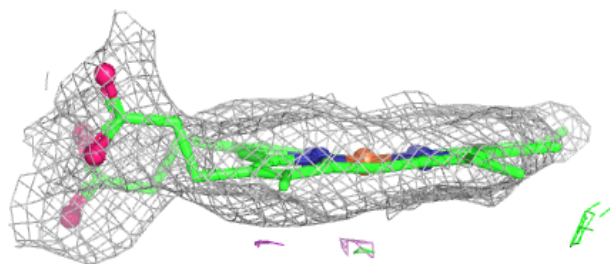
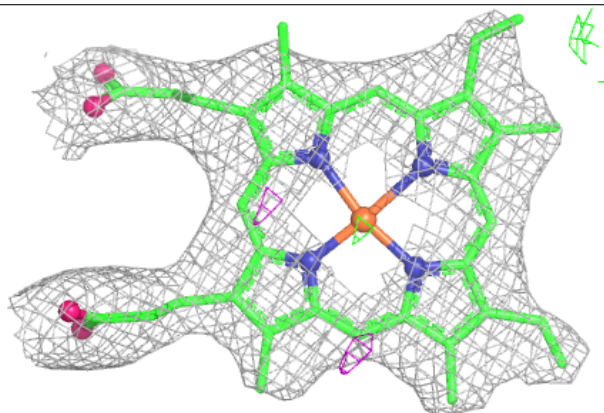


Electron density around HEM C 503:

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

**Electron density around HEM D 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.