Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 10:35 pm BST

PDB ID	:	5OFQ
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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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.
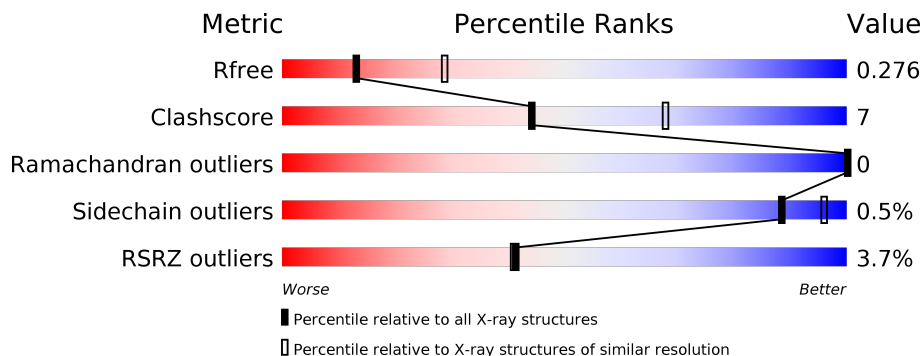
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
1	B	409	
1	C	409	
1	D	409	

2 Entry composition (i)

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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
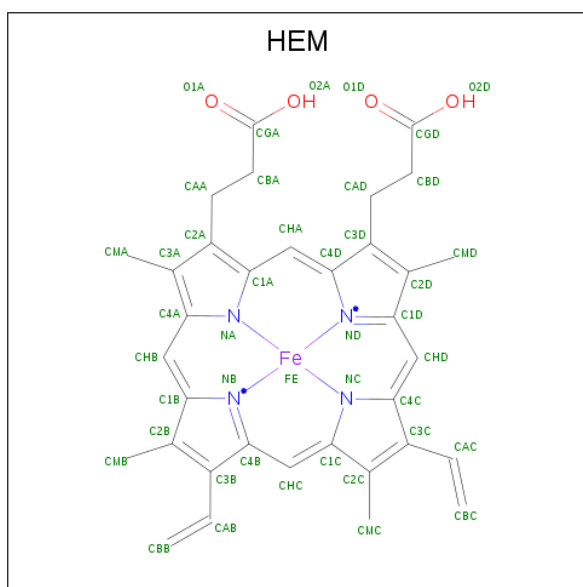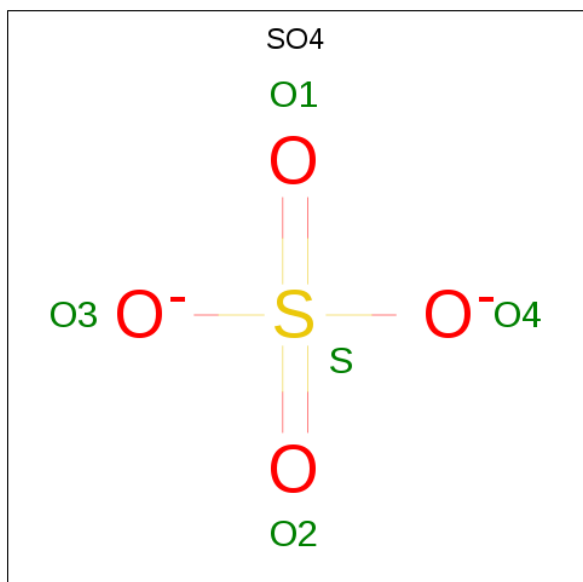

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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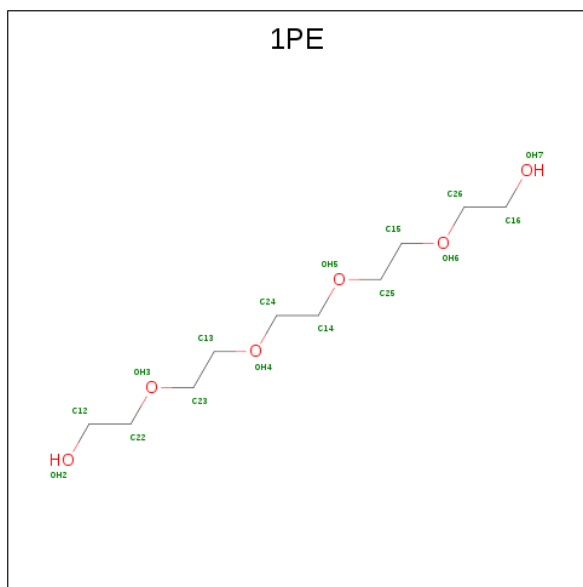
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 16	C 10	O 6	0	0
3	A	1	Total 16	C 10	O 6	0	0
3	B	1	Total 16	C 10	O 6	0	0
3	C	1	Total 16	C 10	O 6	0	0
3	C	1	Total 16	C 10	O 6	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 5 is water.

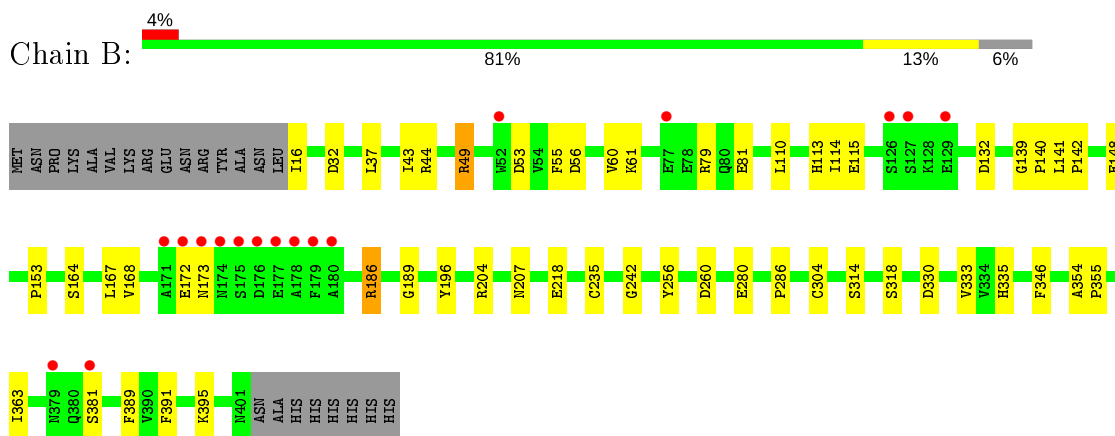| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	O 4	0	0
5	B	2	Total 2	O 2	0	0
5	C	2	Total 2	O 2	0	0
5	D	7	Total 7	O 7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.
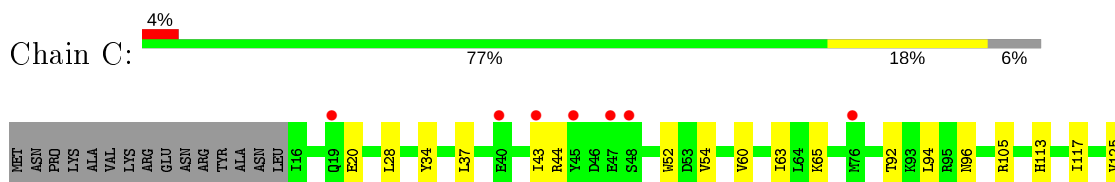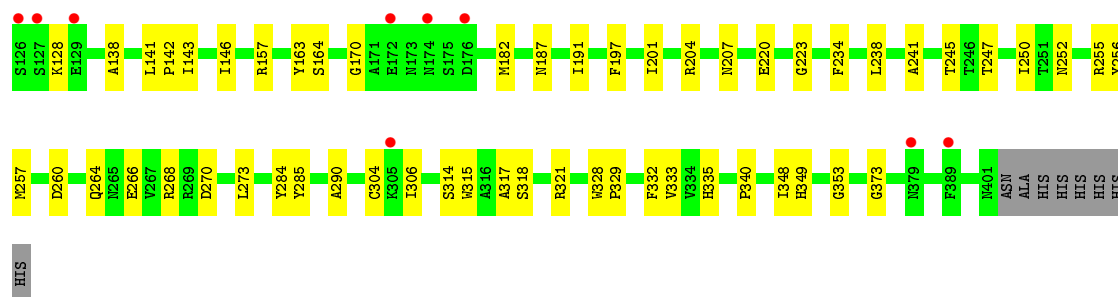
- Molecule 1: Cytochrome P450
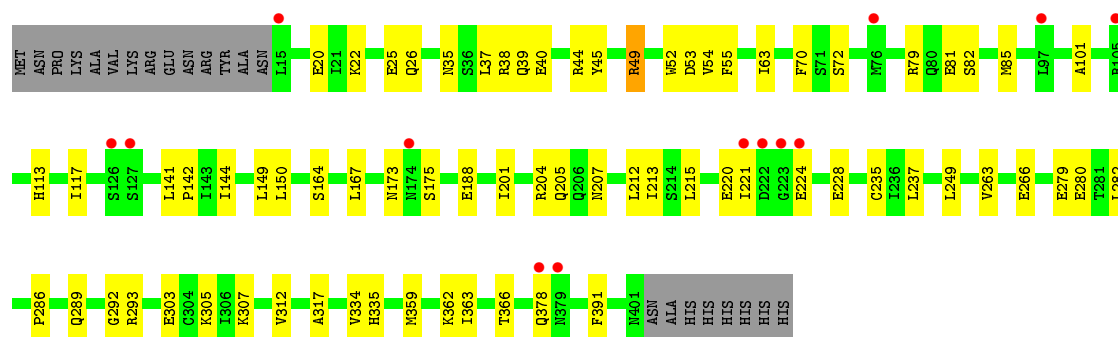

- Molecule 1: Cytochrome P450

- Molecule 1: Cytochrome P450

S126 S127 K128 E129 A138 L141 P142 I143 I146 R157 Y163 S164 G170 A171 E172 N173 N174 S175 D176 M182 N187 I191 F197 I201 R204 N207 E220 G223 F234 L238 A241 T245 T246 T247 I250 T251 N252 R255 Y256

M257 D260 Q264 N265 E266 V267 R268 R269 D270 L273 Y284 Y285 A290 C304 K305 I306 S314 W315 A316 A317 S318 R321 W328 P329 F332 V333 H335 P340 I348 H349 G353 G373 N379 F389 N401 ASN ALA HIS HIS HIS HIS HIS

HIS

• Molecule 1: Cytochrome P450

Chain D:

3%

77%   17%   5%

MET ASN PRO LYS ALA VAL LYS ARG GLU ASN ARG TYR ALA ASN L15 E20 I21 K22 E25 Q26 N35 S36 L37 R38 Q39 E40 R44 Y45 R49 W52 D53 V54 F55 I63 F70 S71 S72 M76 R79 Q80 E81 S82 M85 L97 A101 R105

H113 I117 S126 S127 L141 P142 I143 I144 L149 L150 S164 L167 N173 N174 S175 E188 I201 R204 Q205 Q206 N207 L212 I213 S214 L215 E220 I221 D222 G223 E224 E228 C235 I236 L237 L249 V263 E266 E279 E280 T281 L282

P286 Q289 G292 R293 E303 C304 K305 I306 K307 V312 A317 V334 H335 M359 K362 I363 T366 Q378 N379 F391 N401 ASN ALA HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [1]	3.41 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.224　,　0.275 0.227　,　0.276	Depositor DCC
R_{free} test set	2610 reflections (5.08%)	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)	0.35 , 20.8	EDS
L-test for twinning [2]	$<|L|> = 0.45$, $<L^2> = 0.27$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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, SO4, 1PE.

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	0.83	1/3172 (0.0%)	0.81	3/4286 (0.1%)
1	B	0.83	4/3172 (0.1%)	0.77	2/4286 (0.0%)
1	C	0.82	0/3172	0.77	1/4286 (0.0%)
1	D	0.78	2/3180 (0.1%)	0.76	2/4297 (0.0%)
All	All	0.82	7/12696 (0.1%)	0.78	8/17155 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	25	GLU	CG-CD	6.38	1.61	1.51
1	B	381	SER	CA-CB	5.68	1.61	1.52
1	B	235	CYS	CB-SG	-5.62	1.72	1.81
1	A	327	GLU	CG-CD	5.49	1.60	1.51
1	D	303	GLU	CG-CD	5.25	1.59	1.51
1	B	218	GLU	CG-CD	-5.10	1.44	1.51
1	B	389	PHE	CE2-CZ	5.08	1.47	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	49	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	C	157	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	D	49	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	A	136	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	49	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	B	186	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	46	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	32	ASP	CB-CG-OD1	5.37	123.13	118.30

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	43	0
1	B	3109	0	3092	32	0
1	C	3109	0	3092	43	1
1	D	3117	0	3103	54	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	168	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 (168) 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:HE3	1:D:307:LYS:HZ1	1.32	0.94
1:D:305:LYS:CE	1:D:307:LYS:HZ1	1.72	0.92
1:D:305:LYS:HE2	1:D:307:LYS:HZ2	1.26	0.92
1:D:305:LYS:HE3	1:D:307:LYS:NZ	1.82	0.90
1:D:305:LYS:CE	1:D:307:LYS:HZ2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ARG:HA	1:D:207:ASN:O	1.89	0.73
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: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:D:279:GLU:HA	1:D:282:LEU:HD12	1.83	0.61
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:D:305:LYS:HE2	1:D:307:LYS:HZ3	1.59	0.59
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: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:B:55:PHE:O	1:B:318:SER:OG	2.18	0.55
1:D:150:LEU:O	1:D:213:ILE:HG12	2.05	0.55
1:D:101:ALA:HB2	1:D:215:LEU:HD22	1.89	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:D:49:ARG:HH22	1:D:53:ASP:CG	2.12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:362:LYS:O	1:D:366:THR:OG1	2.21	0.49
1:B:280:GLU:HA	1:B:280:GLU:OE1	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:115:GLU:CG	1:B:363:ILE:HD12	2.43	0.49
1:B:56:ASP:O	1:B:60:VAL:HG23	2.12	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:350:PHE:O	1:A:351:CYS:C	2.53	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: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:O	1:B:168:VAL:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:205:GLN:HG2	1:D:228:GLU:OE2	2.16	0.46
1:D:54:VAL:HG21	1:D:63:ILE:HD11	1.97	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:D:173:ASN:OD1	1:D:175:SER:OG	2.18	0.45
1:A:84:LEU:HA	2:A:501:HEM:O2D	2.16	0.45
1:A:49:ARG:HH22	1:A:53:ASP:CG	2.19	0.45
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:HG13	1:D:221:ILE:O	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: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:A:208:LYS:HD2	1:A:214:SER:HB3	2.00	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:D:63:ILE:HD13	1:D:312:VAL:HG12	2.00	0.43
1:D:378:GLN:N	1:D:378:GLN:OE1	2.51	0.43
1:A:298:ASP:O	1:A:299:VAL:CG2	2.67	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:HA	1:A:271:ILE:HD12	1.90	0.43
1:A:290:ALA:HB2	1:A:315:TRP:CE3	2.54	0.43
1:A:93:LYS:HZ1	1:D:40:GLU:HA	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ASP:HB3	1:C:273:LEU:HD12	2.00	0.43
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:C:220:GLU:CD	1:C:223:GLY:HA2	2.39	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:D:292:GLY:O	1:D:293:ARG:NH1	2.50	0.42
1:A:154:ILE:O	1:A:157:ARG:HG2	2.20	0.42
1:A:56:ASP:OD1	1:A:59:THR:HB	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:280:GLU:OE1	1:D:280:GLU:HA	2.19	0.41
1:D:63:ILE:HG23	1:D:70:PHE:CG	2.56	0.41
1:C:52:TRP:CZ3	1:C:304:CYS:HB3	2.55	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:117:ILE:CD1	1:D:144:ILE:HG22	2.50	0.41
1:D:201:ILE:O	1:D:205:GLN:N	2.52	0.41
1:C:256:TYR:CZ	1:C:332:PHE:CB	3.04	0.41
1:B:115:GLU:HG2	1:B:363:ILE:HD12	2.03	0.41
1:A:105:ARG:NH1	1:B:32:ASP:OD2	2.53	0.40
1:D:117:ILE:HD13	1:D:144:ILE:HG22	2.02	0.40
1:D:45:TYR:HD1	1:D:52:TRP:NE1	2.19	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: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
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%)	339 (99%)	2 (1%)	86	95
1	B	341/361 (94%)	340 (100%)	1 (0%)	92	98
1	C	341/361 (94%)	340 (100%)	1 (0%)	92	98
1	D	342/361 (95%)	339 (99%)	3 (1%)	78	92
All	All	1365/1444 (94%)	1358 (100%)	7 (0%)	88	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	148	GLU
1	B	44	ARG
1	C	44	ARG
1	D	39	GLN
1	D	44	ARG
1	D	113	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	502	-	15,15,15	0.65	0	14,14,14	0.74	0
3	1PE	A	503	-	15,15,15	0.55	0	14,14,14	0.74	0
2	HEM	D	501	1	27,50,50	2.00	5 (18%)	17,82,82	1.78	3 (17%)
2	HEM	B	501	1	27,50,50	1.98	6 (22%)	17,82,82	1.41	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	HEM	C	503	1	27,50,50	1.89	5 (18%)	17,82,82	1.58	4 (23%)
4	SO4	B	503	-	4,4,4	0.06	0	6,6,6	0.28	0
3	1PE	C	501	-	15,15,15	0.72	0	14,14,14	1.15	1 (7%)
4	SO4	A	505	-	4,4,4	0.21	0	6,6,6	0.46	0
4	SO4	A	504	-	4,4,4	0.25	0	6,6,6	0.81	0
2	HEM	A	501	1	27,50,50	2.19	6 (22%)	17,82,82	1.28	3 (17%)
3	1PE	A	502	-	15,15,15	0.60	0	14,14,14	0.71	0
3	1PE	B	502	-	15,15,15	0.68	0	14,14,14	0.73	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	502	-	-	4/13/13/13	-
3	1PE	A	503	-	-	11/13/13/13	-
2	HEM	D	501	1	-	0/6/54/54	-
2	HEM	B	501	1	-	0/6/54/54	-
2	HEM	C	503	1	-	0/6/54/54	-
3	1PE	C	501	-	-	6/13/13/13	-
2	HEM	A	501	1	-	0/6/54/54	-
3	1PE	A	502	-	-	6/13/13/13	-
3	1PE	B	502	-	-	8/13/13/13	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	-6.47	1.31	1.40
2	B	501	HEM	C3C-C2C	-6.12	1.31	1.40
2	A	501	HEM	C3B-C2B	-5.39	1.32	1.40
2	D	501	HEM	C3C-C2C	-5.20	1.33	1.40
2	D	501	HEM	C3B-C2B	-5.11	1.33	1.40
2	B	501	HEM	C3B-C2B	-5.10	1.33	1.40
2	C	503	HEM	C3C-C2C	-4.81	1.33	1.40
2	C	503	HEM	C3C-CAC	4.00	1.56	1.47
2	C	503	HEM	C3B-C2B	-3.90	1.35	1.40
2	A	501	HEM	C3C-CAC	3.53	1.55	1.47
2	C	503	HEM	C3B-CAB	3.46	1.55	1.47
2	A	501	HEM	C3B-CAB	3.25	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3B-CAB	3.12	1.54	1.47
2	D	501	HEM	C3C-CAC	3.11	1.54	1.47
2	B	501	HEM	C3C-CAC	2.76	1.53	1.47
2	C	503	HEM	CAA-C2A	2.68	1.56	1.52
2	D	501	HEM	CAA-C2A	2.61	1.55	1.52
2	A	501	HEM	C2A-C3A	-2.55	1.30	1.37
2	A	501	HEM	C3D-C2D	-2.22	1.31	1.37
2	B	501	HEM	C3B-CAB	2.19	1.52	1.47
2	B	501	HEM	C3D-C2D	-2.17	1.31	1.37
2	B	501	HEM	C2A-C3A	-2.05	1.31	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CMA-C3A-C4A	-3.53	123.04	128.46
2	C	503	HEM	C4A-C3A-C2A	3.40	109.36	107.00
2	D	501	HEM	CBD-CAD-C3D	-3.38	106.25	112.48
2	C	503	HEM	C1D-C2D-C3D	2.69	108.87	107.00
2	A	501	HEM	CAD-CBD-CGD	-2.62	108.27	112.67
2	A	501	HEM	CMC-C2C-C3C	2.58	129.51	124.68
2	C	503	HEM	CMB-C2B-C3B	2.52	129.40	124.68
2	B	501	HEM	CAA-CBA-CGA	-2.45	108.56	112.67
2	B	501	HEM	C4A-C3A-C2A	2.40	108.67	107.00
2	B	501	HEM	CMB-C2B-C3B	2.40	129.16	124.68
2	A	501	HEM	C4A-C3A-C2A	2.33	108.61	107.00
2	D	501	HEM	C4A-C3A-C2A	2.23	108.55	107.00
2	C	503	HEM	CMA-C3A-C4A	-2.22	125.05	128.46
3	C	501	1PE	C25-OH5-C14	2.03	122.08	113.29

There are no chirality outliers.

All (35) torsion outliers are listed below:

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

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

There are no ring outliers.

7 monomers are involved in 13 short contacts:

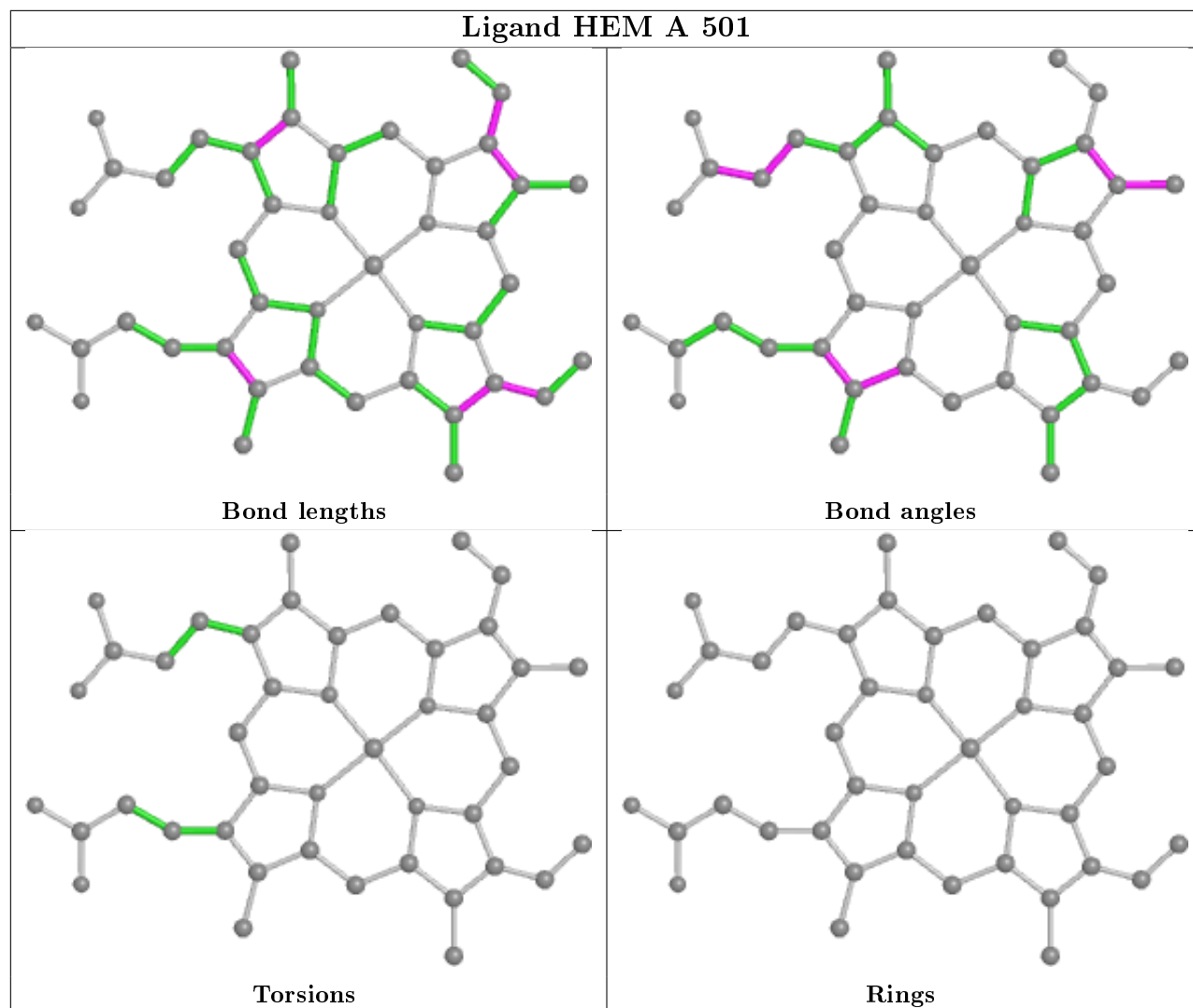| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	1PE	1	0
3	A	503	1PE	2	0
2	D	501	HEM	2	0
2	B	501	HEM	1	0
2	C	503	HEM	1	0
3	C	501	1PE	3	0
2	A	501	HEM	3	0

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 then 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.

Ligand HEM D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 503

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 501

Bond lengths

Bond angles

Torsions

Rings
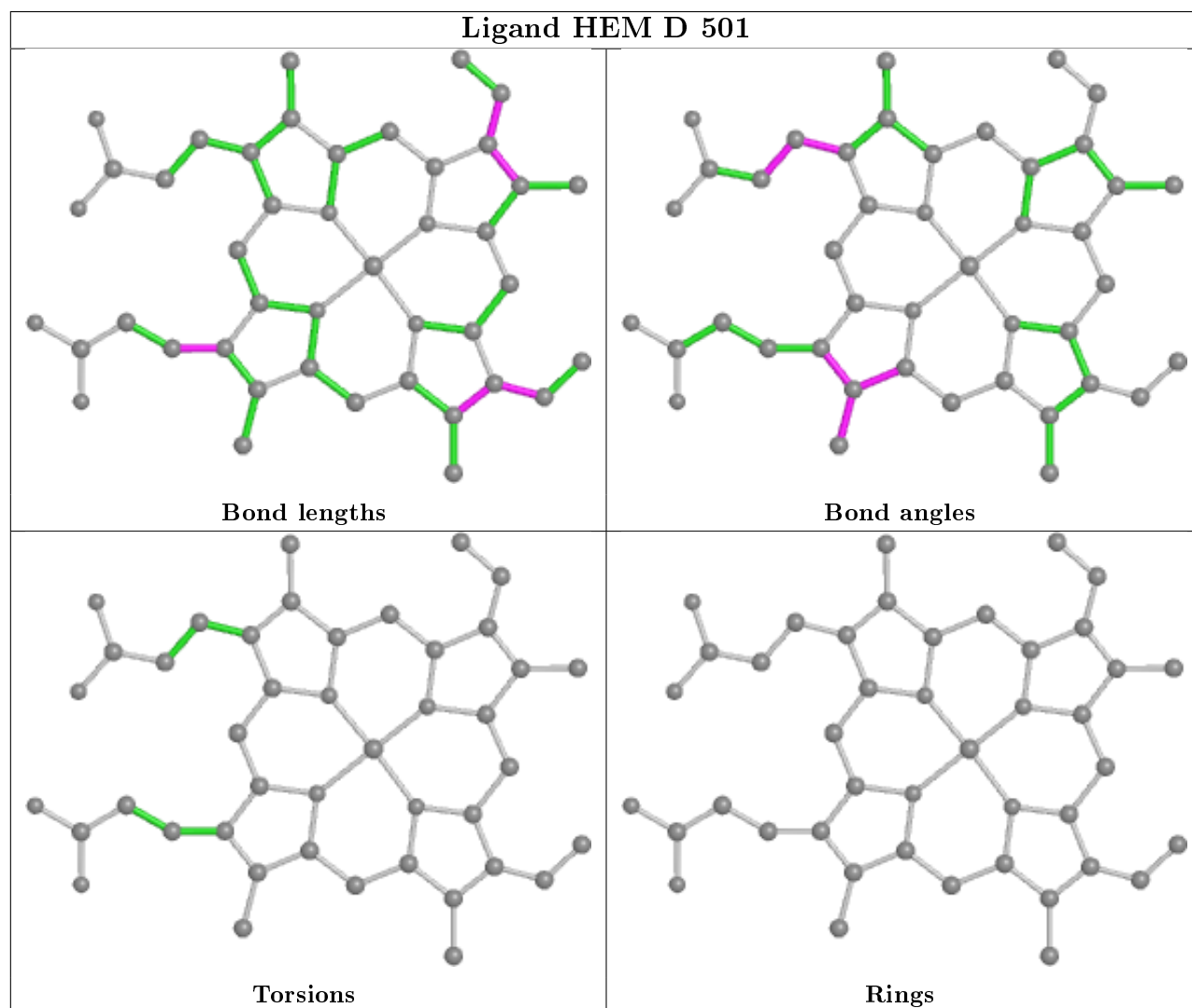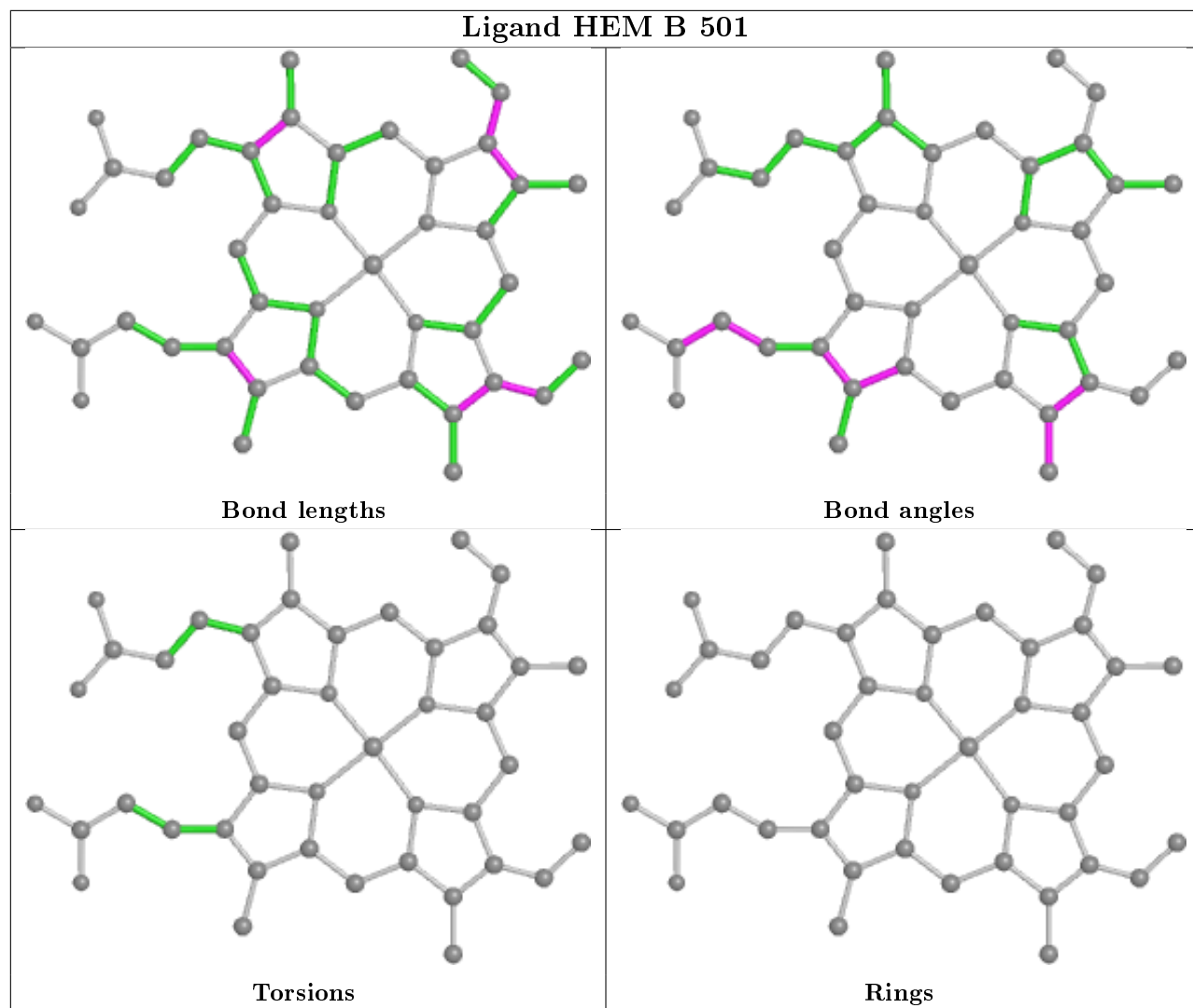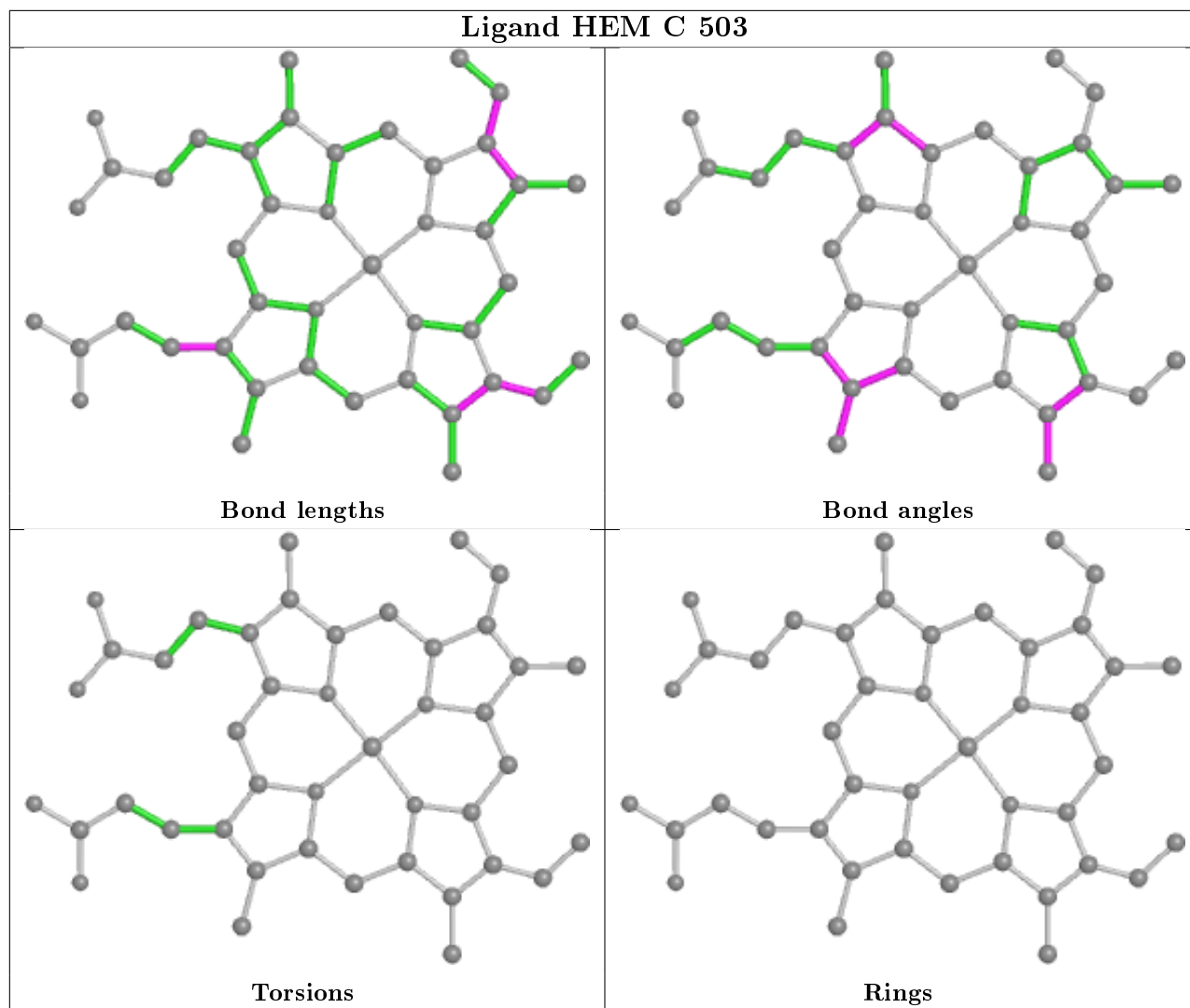
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	386/409 (94%)	0.18	11 (2%)	53	54	31, 39, 58, 82	0
1	B	386/409 (94%)	0.15	17 (4%)	34	33	32, 42, 64, 90	0
1	C	386/409 (94%)	0.20	16 (4%)	37	36	40, 45, 62, 89	0
1	D	387/409 (94%)	0.23	13 (3%)	45	45	36, 48, 66, 98	0
All	All	1545/1636 (94%)	0.19	57 (3%)	41	41	31, 44, 64, 98	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ASN	5.7
1	B	174	ASN	5.6
1	B	179	PHE	5.0
1	B	127	SER	4.9
1	D	221	ILE	4.2
1	C	172	GLU	4.1
1	B	177	GLU	4.0
1	B	77	GLU	3.9
1	C	127	SER	3.8
1	D	127	SER	3.7
1	B	172	GLU	3.6
1	D	378	GLN	3.5
1	B	173	ASN	3.4
1	A	176	ASP	3.4
1	B	176	ASP	3.2
1	D	126	SER	3.1
1	D	174	ASN	3.0
1	A	175	SER	3.0
1	A	127	SER	2.9
1	D	15	LEU	2.9
1	B	180	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	76	MET	2.8
1	A	77	GLU	2.8
1	D	379	ASN	2.8
1	C	305	LYS	2.7
1	C	48	SER	2.7
1	C	47	GLU	2.7
1	D	222	ASP	2.6
1	A	47	GLU	2.6
1	A	179	PHE	2.5
1	A	177	GLU	2.5
1	B	126	SER	2.5
1	B	178	ALA	2.5
1	C	43	ILE	2.5
1	C	176	ASP	2.5
1	C	129	GLU	2.4
1	D	223	GLY	2.4
1	B	175	SER	2.4
1	C	379	ASN	2.4
1	D	224	GLU	2.4
1	C	45	TYR	2.3
1	B	171	ALA	2.3
1	B	129	GLU	2.3
1	C	126	SER	2.3
1	B	381	SER	2.2
1	B	379	ASN	2.2
1	D	97	LEU	2.2
1	A	48	SER	2.2
1	C	174	ASN	2.2
1	C	389	PHE	2.1
1	D	76	MET	2.1
1	A	173	ASN	2.1
1	B	52	TRP	2.1
1	C	19	GLN	2.1
1	D	105	ARG	2.0
1	C	40	GLU	2.0
1	A	294	ILE	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	1PE	A	503	16/16	0.87	0.23	57,66,75,77	0
4	SO4	A	504	5/5	0.89	0.13	67,67,72,102	0
3	1PE	B	502	16/16	0.89	0.26	44,48,58,59	0
3	1PE	C	502	16/16	0.92	0.23	41,44,46,47	0
3	1PE	C	501	16/16	0.92	0.26	41,47,54,57	0
3	1PE	A	502	16/16	0.93	0.16	36,39,52,53	0
2	HEM	B	501	43/43	0.97	0.19	41,44,45,49	0
2	HEM	A	501	43/43	0.97	0.21	38,42,45,46	0
4	SO4	B	503	5/5	0.97	0.11	42,44,48,50	0
2	HEM	D	501	43/43	0.97	0.20	42,50,53,54	0
2	HEM	C	503	43/43	0.98	0.17	42,48,50,51	0
4	SO4	A	505	5/5	0.98	0.11	52,57,58,60	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.
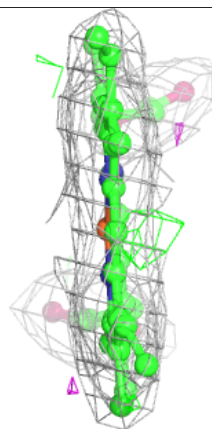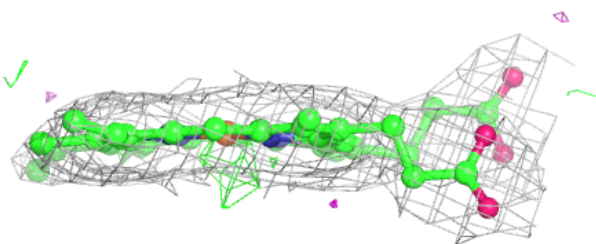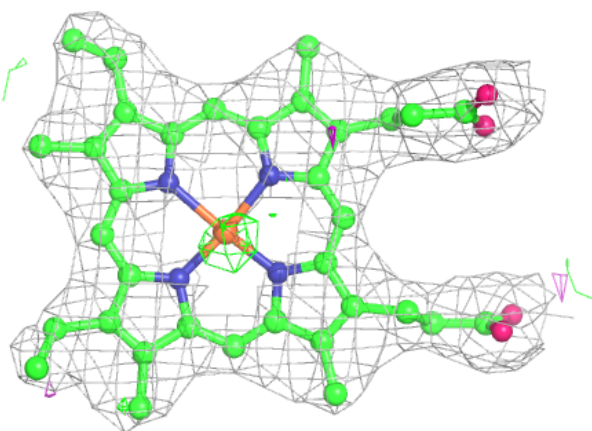
Electron density around HEM B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
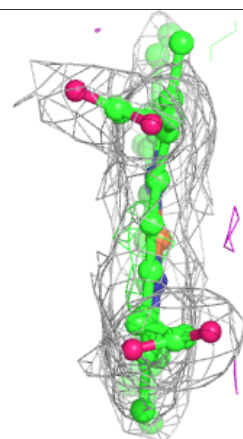mF_o-DF_c (at 3 rmsd) in purple (negative)
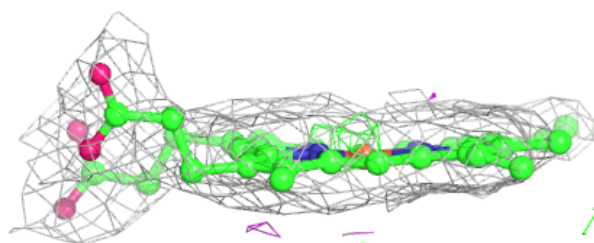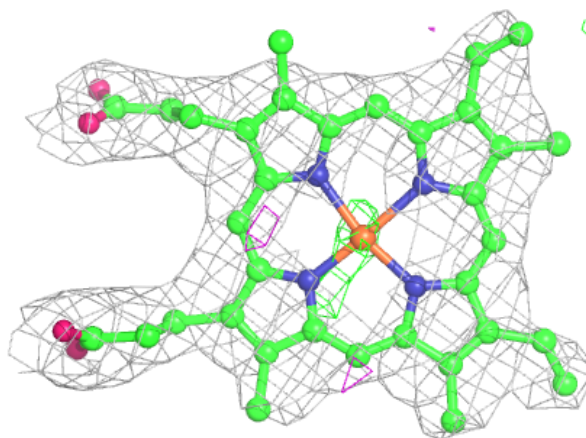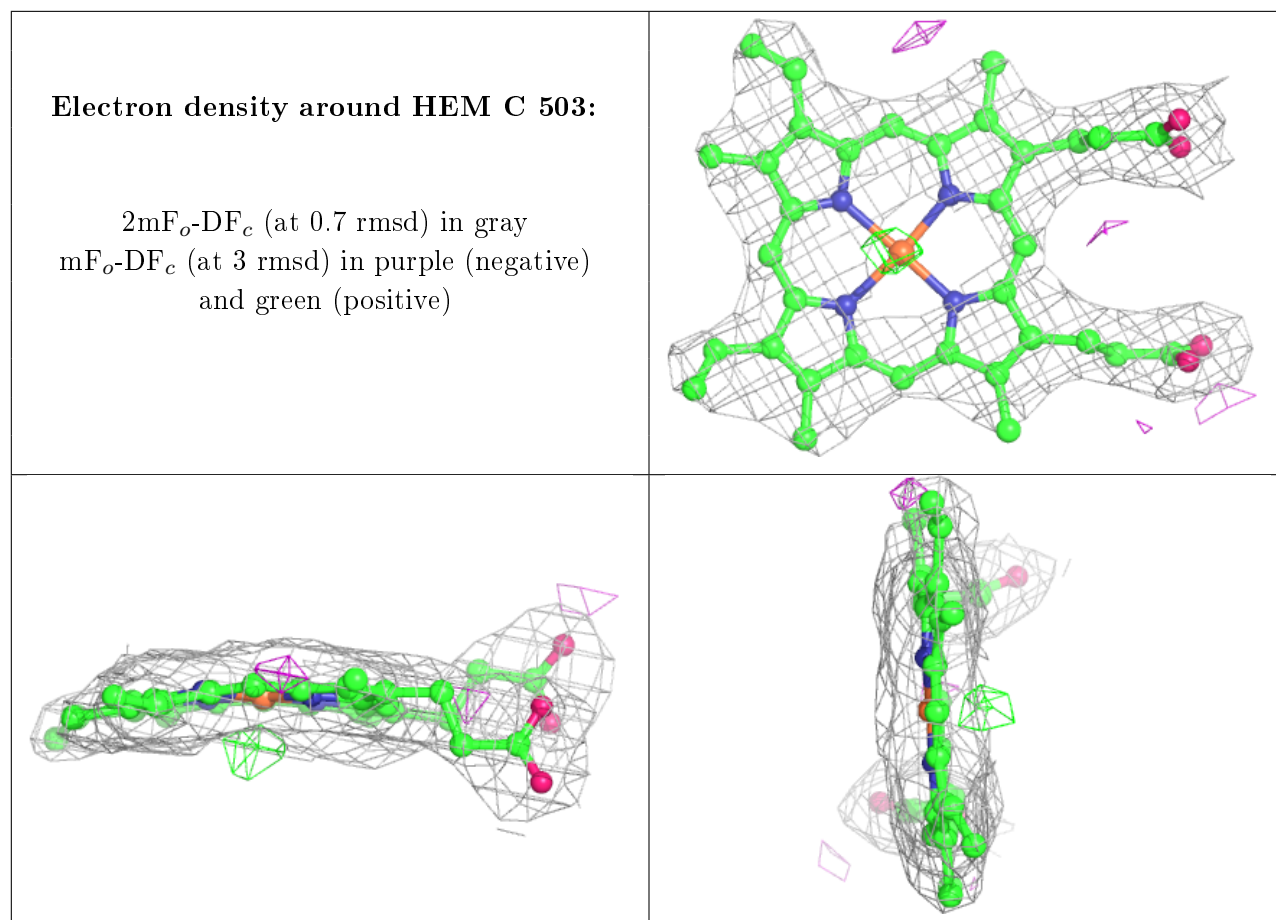and green (positive)
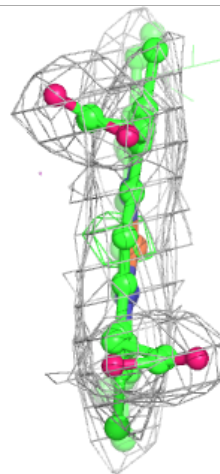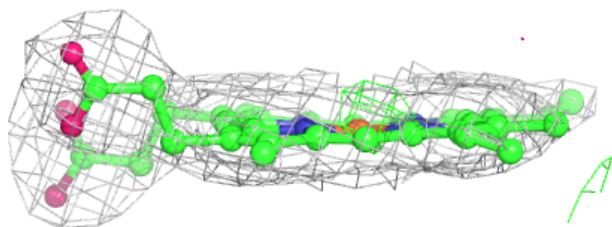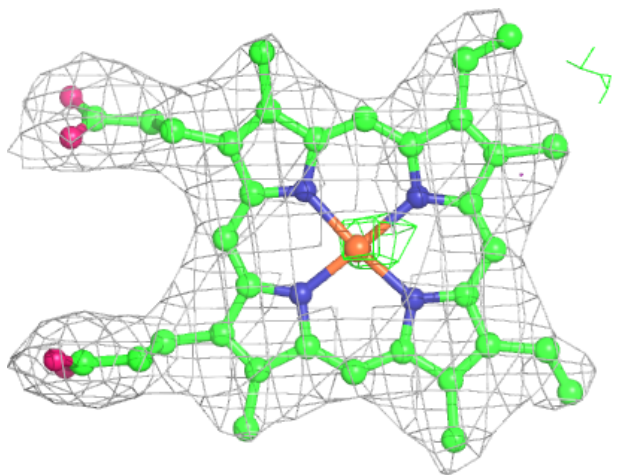
Electron density around HEM A 501:

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

Electron density around HEM D 501:

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

Electron density around HEM C 503:

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

6.5 Other polymers (i)

There are no such residues in this entry.