Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:59 AM EDT

PDB ID	:	2YOO
Title	:	Cholest-4-en-3-one bound structure of CYP142 from Mycobacterium smegmatis
Authors	:	Garcia-Fernandez, E.; Frank, D.J.; Galan, B.; Kells, P.M.; Podust, L.M.; Garcia, J.L.; Ortiz de Montellano, P.R.
Deposited on	:	2012-10-25
Resolution	:	1.69 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

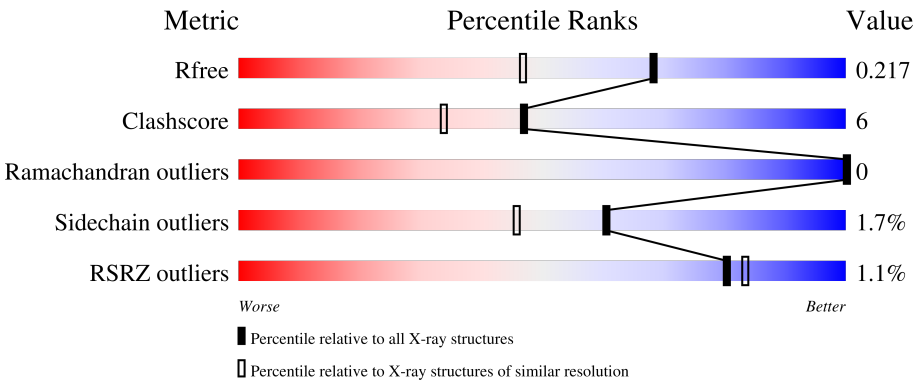
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.69 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	407	% 89% 8% •
1	B	407	% 85% 11% • •
1	C	407	% 85% 11% • •
1	D	407	85% 11% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14507 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 P450 HEME-THIOLATE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3084	1934	544	583	23	0	2	0
1	B	395	3146	1964	563	595	24	0	8	0
1	C	395	3092	1937	548	584	23	0	1	0
1	D	394	3107	1943	551	590	23	0	2	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A0R4Q6
A	2	THR	-	expression tag	UNP A0R4Q6
A	3	GLN	-	expression tag	UNP A0R4Q6
A	402	HIS	-	expression tag	UNP A0R4Q6
A	403	HIS	-	expression tag	UNP A0R4Q6
A	404	HIS	-	expression tag	UNP A0R4Q6
A	405	HIS	-	expression tag	UNP A0R4Q6
A	406	HIS	-	expression tag	UNP A0R4Q6
A	407	HIS	-	expression tag	UNP A0R4Q6
B	1	MET	-	expression tag	UNP A0R4Q6
B	2	THR	-	expression tag	UNP A0R4Q6
B	3	GLN	-	expression tag	UNP A0R4Q6
B	402	HIS	-	expression tag	UNP A0R4Q6
B	403	HIS	-	expression tag	UNP A0R4Q6
B	404	HIS	-	expression tag	UNP A0R4Q6
B	405	HIS	-	expression tag	UNP A0R4Q6
B	406	HIS	-	expression tag	UNP A0R4Q6
B	407	HIS	-	expression tag	UNP A0R4Q6
C	1	MET	-	expression tag	UNP A0R4Q6
C	2	THR	-	expression tag	UNP A0R4Q6
C	3	GLN	-	expression tag	UNP A0R4Q6

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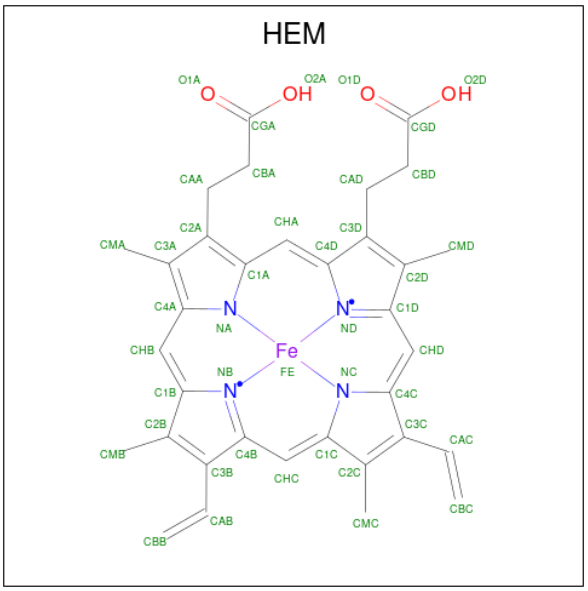
Chain	Residue	Modelled	Actual	Comment	Reference
C	402	HIS	-	expression tag	UNP A0R4Q6
C	403	HIS	-	expression tag	UNP A0R4Q6
C	404	HIS	-	expression tag	UNP A0R4Q6
C	405	HIS	-	expression tag	UNP A0R4Q6
C	406	HIS	-	expression tag	UNP A0R4Q6
C	407	HIS	-	expression tag	UNP A0R4Q6
D	1	MET	-	expression tag	UNP A0R4Q6
D	2	THR	-	expression tag	UNP A0R4Q6
D	3	GLN	-	expression tag	UNP A0R4Q6
D	402	HIS	-	expression tag	UNP A0R4Q6
D	403	HIS	-	expression tag	UNP A0R4Q6
D	404	HIS	-	expression tag	UNP A0R4Q6
D	405	HIS	-	expression tag	UNP A0R4Q6
D	406	HIS	-	expression tag	UNP A0R4Q6
D	407	HIS	-	expression tag	UNP A0R4Q6

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

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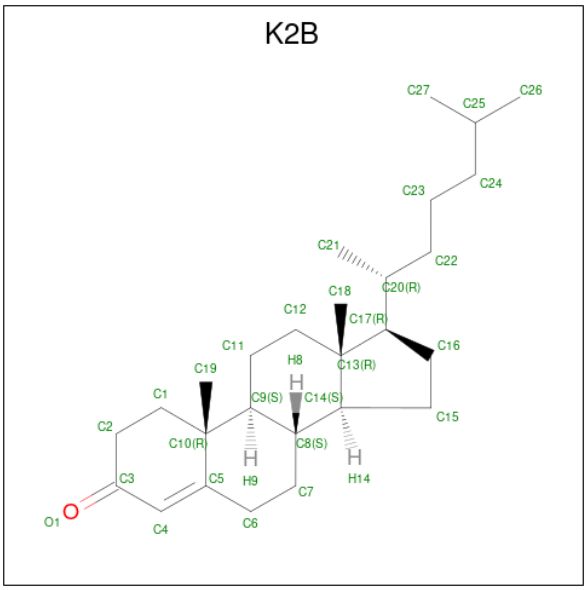
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is (8ALPHA,9BETA)-CHOLEST-4-EN-3-ONE (three-letter code: K2B) (formula: $C_{27}H_{44}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	28	27	1	0	0
3	B	1	28	27	1	0	0
3	C	1	28	27	1	0	0
3	D	1	28	27	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	B	1	1	1	0	0

- Molecule 5 is water.

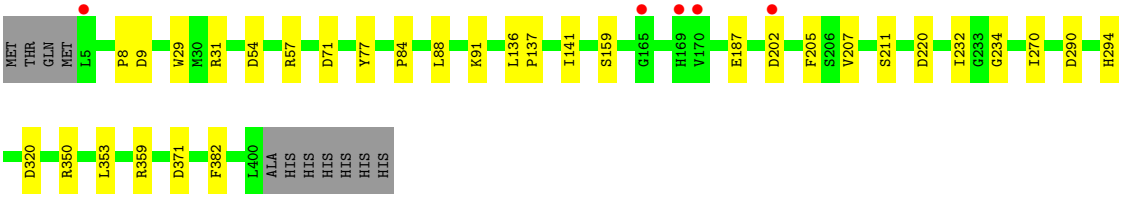
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	417	417	417	0	0
			Total	O		
5	B	459	459	459	0	0
			Total	O		
5	C	495	495	495	0	0
			Total	O		
5	D	422	422	422	0	0

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.

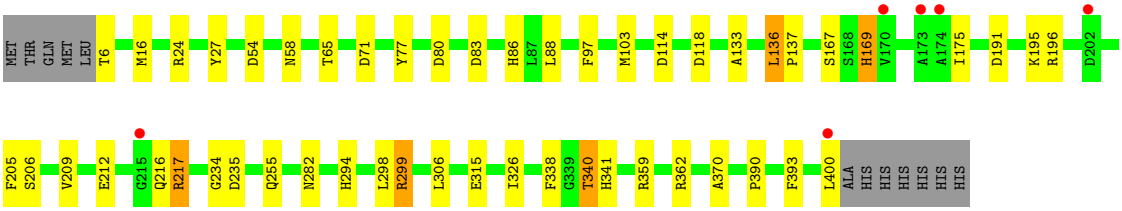
• Molecule 1: P450 HEME-THIOLATE PROTEIN

Chain A:



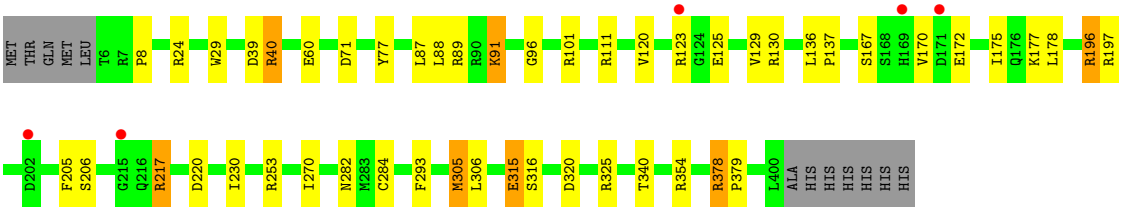
• Molecule 1: P450 HEME-THIOLATE PROTEIN

Chain B:



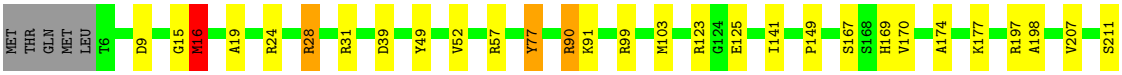
• Molecule 1: P450 HEME-THIOLATE PROTEIN

Chain C:



• Molecule 1: P450 HEME-THIOLATE PROTEIN

Chain D:



G215
Q216
R217
G234
D235
E236
R239
D262
I270
N282
D290
L306
D322
D327
R350
R354
R359
R362
R363
L364
F382
E387
S388
M389
V399
LEU
ALA
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.68Å 106.21Å 126.54Å 90.00° 90.67° 90.00°	Depositor
Resolution (Å)	126.53 – 1.69 81.35 – 1.69	Depositor EDS
% Data completeness (in resolution range)	93.3 (126.53-1.69) 93.3 (81.35-1.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.219 0.164 , 0.217	Depositor DCC
R_{free} test set	7821 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	14.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.087 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14507	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: K2B, MG, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.10	2/3144 (0.1%)	1.01	8/4267 (0.2%)
1	B	1.21	3/3207 (0.1%)	1.05	8/4347 (0.2%)
1	C	1.12	3/3153 (0.1%)	1.03	15/4277 (0.4%)
1	D	1.13	6/3168 (0.2%)	1.04	16/4295 (0.4%)
All	All	1.14	14/12672 (0.1%)	1.04	47/17186 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	315	GLU	CG-CD	8.25	1.64	1.51
1	B	27	TYR	CD1-CE1	7.20	1.50	1.39
1	D	198	ALA	CA-CB	6.53	1.66	1.52
1	C	293	PHE	CD2-CE2	6.11	1.51	1.39
1	D	77	TYR	CD1-CE1	5.99	1.48	1.39
1	B	133	ALA	CA-CB	5.73	1.64	1.52
1	D	49	TYR	CD2-CE2	5.71	1.48	1.39
1	B	393	PHE	CE1-CZ	5.43	1.47	1.37
1	D	52	VAL	CB-CG1	5.40	1.64	1.52
1	D	382	PHE	CE2-CZ	5.37	1.47	1.37
1	D	387	GLU	CG-CD	5.35	1.59	1.51
1	A	31	ARG	CG-CD	5.23	1.65	1.51
1	A	382	PHE	CE2-CZ	5.20	1.47	1.37
1	C	60	GLU	CG-CD	5.09	1.59	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	71	ASP	CB-CG-OD1	10.99	128.19	118.30
1	A	71[A]	ASP	CB-CG-OD1	9.44	126.80	118.30
1	A	71[B]	ASP	CB-CG-OD1	9.44	126.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	16	MET	CG-SD-CE	8.69	114.10	100.20
1	B	359	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	D	31	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	B	24	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	C	24	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	C	40	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	C	71	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	290	ASP	CB-CG-OD1	6.75	124.37	118.30
1	D	24	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	197	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	C	320	ASP	CB-CG-OD1	6.59	124.23	118.30
1	C	39	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	118	ASP	CB-CG-OD1	6.35	124.02	118.30
1	C	320	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	C	91	LYS	CD-CE-NZ	-6.29	97.23	111.70
1	D	31	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	C	89	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	220	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	320	ASP	CB-CG-OD1	5.98	123.68	118.30
1	D	39	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	197	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	235	ASP	CB-CG-OD1	5.85	123.56	118.30
1	C	40	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	D	90	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	118	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	D	9	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	327	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	71	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	C	315	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	C	220	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	D	90	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	C	220	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	325	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	196	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	D	350	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	71[A]	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	71[B]	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	D	262	ASP	CB-CG-OD1	5.13	122.92	118.30
1	D	290	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	359	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	197	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	389	MET	CG-SD-CE	5.03	108.24	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	LEU	CB-CG-CD2	5.02	119.53	111.00
1	A	350	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	3084	0	3011	21	0
1	B	3146	0	3071	52	1
1	C	3092	0	3035	48	0
1	D	3107	0	3051	31	0
2	A	43	0	30	7	0
2	B	43	0	30	7	0
2	C	43	0	30	4	0
2	D	43	0	30	8	0
3	A	28	0	44	0	0
3	B	28	0	44	0	0
3	C	28	0	44	0	0
3	D	28	0	44	0	0
4	B	1	0	0	0	0
5	A	417	0	0	4	0
5	B	459	0	0	19	2
5	C	495	0	0	14	0
5	D	422	0	0	7	0
All	All	14507	0	12464	155	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (155) 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:6:THR:HA	5:B:2001:HOH:O	1.40	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:MET:SD	5:C:2022:HOH:O	2.01	1.14
1:B:299[A]:ARG:N	1:B:299[A]:ARG:HD2	1.75	0.99
1:C:217:ARG:HH11	1:C:217:ARG:HG3	1.21	0.99
1:C:123[B]:ARG:CB	1:C:123[B]:ARG:HH11	1.81	0.92
1:B:196[B]:ARG:HA	1:B:196[B]:ARG:HE	1.36	0.89
1:A:141:ILE:CD1	2:A:1402:HEM:HBC1	2.04	0.88
1:D:362:ARG:NH2	5:D:2197:HOH:O	2.05	0.88
1:C:123[B]:ARG:HH11	1:C:123[B]:ARG:HB3	1.41	0.86
1:D:28:ARG:NH2	5:D:2054:HOH:O	2.08	0.86
1:B:196[B]:ARG:HE	1:B:196[B]:ARG:CA	1.91	0.83
1:C:282:ASN:HB2	1:C:305:MET:HE2	1.59	0.83
1:B:212:GLU:O	5:B:2315:HOH:O	1.98	0.82
1:C:123[A]:ARG:HH11	1:C:123[A]:ARG:HG3	1.43	0.82
1:B:340:THR:HB	5:B:2154:HOH:O	1.80	0.80
1:D:167:SER:OG	1:D:169:HIS:HD2	1.64	0.80
1:B:167:SER:OG	1:B:169:HIS:HD2	1.65	0.79
1:A:141:ILE:HD13	2:A:1402:HEM:HBC1	1.62	0.79
1:D:91:LYS:HD3	5:D:2164:HOH:O	1.82	0.79
1:B:86:HIS:HE1	2:B:1402:HEM:O2D	1.68	0.77
1:B:196[B]:ARG:HA	1:B:196[B]:ARG:NE	1.99	0.76
1:D:16:MET:HE3	1:D:19:ALA:HB3	1.67	0.76
1:D:141:ILE:HD13	2:D:1402:HEM:HBC1	1.68	0.75
1:C:217:ARG:HG3	1:C:217:ARG:NH1	1.93	0.75
1:C:217:ARG:HH11	1:C:217:ARG:CG	1.99	0.74
1:C:315:GLU:HG2	5:C:2056:HOH:O	1.87	0.74
5:A:2359:HOH:O	1:B:103:MET:HG3	1.85	0.74
1:A:54:ASP:OD1	1:A:57[A]:ARG:NH2	2.20	0.74
1:A:141:ILE:HD13	2:A:1402:HEM:CBC	2.19	0.73
2:C:1402:HEM:HBC2	2:C:1402:HEM:HHD	1.71	0.73
1:B:341:HIS:HD2	2:B:1402:HEM:O1D	1.72	0.72
1:B:114:ASP:OD1	5:B:2202:HOH:O	2.06	0.72
1:B:97:PHE:CE1	2:B:1402:HEM:CBC	2.72	0.71
1:B:167:SER:OG	1:B:169:HIS:CD2	2.42	0.71
1:C:111:ARG:HB3	5:C:2238:HOH:O	1.92	0.70
1:D:141:ILE:CD1	2:D:1402:HEM:HBC1	2.21	0.70
1:A:141:ILE:HD11	2:A:1402:HEM:HBC1	1.75	0.67
1:B:175:ILE:HG23	5:B:2277:HOH:O	1.94	0.67
1:D:141:ILE:HD13	2:D:1402:HEM:CBC	2.25	0.66
1:B:400:LEU:CB	5:B:2212:HOH:O	2.43	0.66
1:D:167:SER:OG	1:D:169:HIS:CD2	2.48	0.66
1:B:6:THR:N	5:B:2003:HOH:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ILE:HD11	1:D:354:ARG:HA	1.80	0.64
1:D:217:ARG:CG	1:D:217:ARG:HH11	2.11	0.63
1:B:340:THR:HG21	5:B:2155:HOH:O	1.97	0.62
1:A:187:GLU:CG	5:A:2269:HOH:O	2.47	0.62
1:B:97:PHE:CE1	2:B:1402:HEM:HBC2	2.35	0.61
1:C:123[A]:ARG:HG3	1:C:123[A]:ARG:NH1	2.14	0.61
1:A:84:PRO:O	1:A:88:LEU:HD13	2.00	0.61
1:C:340:THR:HG22	5:C:2450:HOH:O	2.01	0.61
5:C:2449:HOH:O	1:D:57:ARG:HD2	2.00	0.60
1:C:378:ARG:HD3	1:C:379:PRO:HD2	1.83	0.60
1:C:378:ARG:CG	1:C:378:ARG:HH11	2.14	0.60
1:B:299[A]:ARG:N	1:B:299[A]:ARG:CD	2.52	0.60
1:C:96:GLY:HA2	1:C:101:ARG:HG2	1.84	0.59
1:B:83:ASP:OD1	1:B:86:HIS:HD2	1.85	0.59
1:B:196[A]:ARG:HD2	1:B:206:SER:HB2	1.84	0.59
1:C:136:LEU:HB3	1:C:137:PRO:HD3	1.85	0.59
1:B:299[A]:ARG:HD2	1:B:299[A]:ARG:H	1.65	0.57
1:D:177:LYS:HE2	5:D:2261:HOH:O	2.04	0.57
1:B:97:PHE:HE1	2:B:1402:HEM:CBC	2.16	0.57
1:C:284:CYS:SG	1:C:305:MET:CE	2.92	0.57
1:B:136:LEU:HB3	1:B:137:PRO:HD3	1.88	0.56
1:B:298:LEU:C	1:B:299[A]:ARG:HD2	2.26	0.56
1:C:270:ILE:HD11	1:C:354:ARG:HA	1.87	0.56
1:D:28:ARG:CZ	5:D:2054:HOH:O	2.50	0.56
1:B:340:THR:HG23	5:B:2107:HOH:O	2.05	0.56
1:B:54:ASP:OD2	1:B:294:HIS:HE1	1.88	0.56
1:B:338:PHE:HZ	5:B:2111:HOH:O	1.89	0.56
1:A:234:GLY:HA2	2:A:1402:HEM:HMC3	1.88	0.55
1:C:378:ARG:HH11	1:C:378:ARG:HG2	1.71	0.55
2:C:1402:HEM:HMB2	2:C:1402:HEM:HBB2	1.88	0.55
1:B:299[A]:ARG:NH1	5:B:2382:HOH:O	2.38	0.54
1:B:196[B]:ARG:HE	1:B:196[B]:ARG:N	2.05	0.54
1:B:6:THR:HA	5:B:2003:HOH:O	2.06	0.54
1:C:123[B]:ARG:HB3	1:C:123[B]:ARG:NH1	2.18	0.54
1:C:378:ARG:HD3	1:C:379:PRO:CD	2.38	0.54
1:A:207:VAL:O	1:A:211:SER:HB3	2.07	0.53
1:B:282:ASN:HA	1:B:306:LEU:O	2.08	0.53
1:C:284:CYS:SG	1:C:305:MET:HE3	2.49	0.53
1:B:255:GLN:HE21	1:B:326:ILE:HG23	1.74	0.52
1:B:362:ARG:CZ	5:B:2425:HOH:O	2.58	0.52
1:A:9:ASP:CG	1:C:130:ARG:HD2	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:C	1:C:178:LEU:HD23	2.31	0.51
1:A:234:GLY:HA2	2:A:1402:HEM:HBC2	1.93	0.51
1:C:88:LEU:HD23	5:C:2072:HOH:O	2.10	0.51
1:A:234:GLY:CA	2:A:1402:HEM:HBC2	2.41	0.51
1:B:255:GLN:NE2	1:B:326:ILE:H	2.08	0.51
1:C:378:ARG:HD3	1:C:379:PRO:N	2.26	0.51
1:C:123[B]:ARG:HH11	1:C:123[B]:ARG:CG	2.24	0.50
1:A:136:LEU:HB3	1:A:137:PRO:HD3	1.93	0.50
1:B:196[A]:ARG:HD2	1:B:206:SER:CB	2.41	0.50
1:B:315:GLU:HG3	5:B:2061:HOH:O	2.12	0.49
1:B:97:PHE:CE1	2:B:1402:HEM:HBC1	2.45	0.49
1:C:340:THR:HB	5:C:2450:HOH:O	2.12	0.49
1:C:172:GLU:HA	1:C:175:ILE:HG22	1.95	0.49
2:C:1402:HEM:HBB2	2:C:1402:HEM:CMB	2.43	0.49
1:B:6:THR:CA	5:B:2003:HOH:O	2.61	0.48
1:B:341:HIS:HE1	5:B:2149:HOH:O	1.94	0.48
1:C:120:VAL:O	1:C:123[A]:ARG:HB3	2.14	0.48
1:C:123[A]:ARG:NH1	1:C:123[A]:ARG:CG	2.76	0.48
1:C:340:THR:CB	5:C:2450:HOH:O	2.61	0.48
1:A:54:ASP:OD2	1:A:294:HIS:HE1	1.97	0.48
1:C:172:GLU:O	1:C:175:ILE:HG22	2.14	0.48
1:C:196:ARG:HD2	1:C:206:SER:HB2	1.95	0.48
1:C:167:SER:HB3	1:C:170:VAL:HG13	1.96	0.47
1:A:57[B]:ARG:NH1	5:A:2104:HOH:O	2.34	0.47
1:C:123[A]:ARG:NH2	1:C:125:GLU:OE2	2.47	0.47
1:A:270:ILE:HD12	1:A:353:LEU:HB3	1.95	0.47
1:D:90:ARG:NH2	5:D:2159:HOH:O	2.47	0.47
1:A:91:LYS:NZ	1:B:58:ASN:ND2	2.63	0.47
1:B:65:THR:HA	1:B:80:ASP:O	2.15	0.47
1:C:378:ARG:HH11	1:C:378:ARG:HB2	1.80	0.47
1:C:87:LEU:O	1:C:91:LYS:HG2	2.16	0.46
1:D:28:ARG:NE	5:D:2054:HOH:O	2.48	0.46
1:C:230:ILE:HG23	2:C:1402:HEM:HBC1	1.97	0.46
1:B:205:PHE:O	1:B:209:VAL:HG23	2.15	0.45
1:D:234:GLY:HA2	2:D:1402:HEM:HMC2	1.98	0.45
2:D:1402:HEM:HMB2	2:D:1402:HEM:HBB2	1.98	0.45
1:B:83:ASP:OD1	1:B:86:HIS:CD2	2.67	0.45
1:C:40:ARG:HD2	5:C:2099:HOH:O	2.15	0.45
1:B:338:PHE:CZ	5:B:2111:HOH:O	2.56	0.45
1:D:207:VAL:O	1:D:211:SER:HB3	2.15	0.45
1:B:370:ALA:HB3	1:B:390:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ARG:HH11	1:D:217:ARG:HG3	1.82	0.45
1:C:340:THR:CG2	5:C:2450:HOH:O	2.60	0.44
1:C:217:ARG:HD2	5:C:2166:HOH:O	2.17	0.44
1:D:236:GLU:HA	1:D:239:ARG:HD3	1.99	0.44
1:C:316:SER:O	1:D:99:ARG:HD3	2.16	0.44
1:D:28:ARG:NH1	1:D:322:ASP:OD2	2.41	0.43
1:A:159:SER:HB3	1:A:232:ILE:HD13	2.00	0.43
1:B:299[B]:ARG:NH1	5:B:2383:HOH:O	2.39	0.43
1:C:282:ASN:HA	1:C:306:LEU:O	2.18	0.43
1:D:217:ARG:CG	1:D:217:ARG:NH1	2.76	0.43
1:D:282:ASN:HA	1:D:306:LEU:O	2.19	0.43
1:C:378:ARG:HH11	1:C:378:ARG:CB	2.32	0.42
1:A:202:ASP:OD1	1:A:202:ASP:C	2.58	0.42
1:B:234:GLY:HA2	2:B:1402:HEM:HMC2	2.01	0.42
1:C:8:PRO:HD3	1:C:29:TRP:CD2	2.54	0.42
1:A:8:PRO:HD3	1:A:29:TRP:CD2	2.55	0.42
1:D:141:ILE:HD11	2:D:1402:HEM:HBC1	1.99	0.41
2:D:1402:HEM:HMC2	2:D:1402:HEM:HBC2	2.02	0.41
1:B:212:GLU:HB2	1:B:216[B]:GLN:O	2.20	0.41
1:B:217:ARG:HD3	5:B:2130:HOH:O	2.21	0.41
5:C:2211:HOH:O	1:D:57:ARG:NH1	2.53	0.41
1:D:170:VAL:HB	1:D:174:ALA:HB3	2.02	0.41
1:D:15:GLY:H	1:D:167:SER:HG	1.69	0.41
1:D:363:ARG:O	1:D:364:LEU:HD23	2.21	0.41
2:D:1402:HEM:HBB2	2:D:1402:HEM:CMB	2.51	0.41
1:A:359:ARG:NH2	5:A:2190:HOH:O	2.47	0.40
1:D:123[A]:ARG:HG3	1:D:125:GLU:HG2	2.02	0.40
1:C:129:VAL:HG13	5:C:2349:HOH:O	2.21	0.40
5:C:2419:HOH:O	1:D:103:MET:HG3	2.21	0.40
1:B:191:ASP:O	1:B:195:LYS:HG3	2.21	0.40
1:C:305:MET:HE3	1:C:305:MET:HA	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2373:HOH:O	5:B:2454:HOH:O[2_645]	1.91	0.29
1:B:362:ARG:NH1	5:B:2375:HOH:O[2_655]	2.17	0.03

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	396/407 (97%)	386 (98%)	10 (2%)	0	100	100
1	B	401/407 (98%)	392 (98%)	9 (2%)	0	100	100
1	C	394/407 (97%)	380 (96%)	14 (4%)	0	100	100
1	D	394/407 (97%)	385 (98%)	9 (2%)	0	100	100
All	All	1585/1628 (97%)	1543 (97%)	42 (3%)	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	329/349 (94%)	326 (99%)	3 (1%)	78	70
1	B	339/349 (97%)	330 (97%)	9 (3%)	44	26
1	C	334/349 (96%)	327 (98%)	7 (2%)	53	36
1	D	338/349 (97%)	332 (98%)	6 (2%)	59	43
All	All	1340/1396 (96%)	1315 (98%)	25 (2%)	60	41

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	TYR
1	A	205	PHE

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Mol	Chain	Res	Type
1	A	371	ASP
1	B	16[A]	MET
1	B	16[B]	MET
1	B	77	TYR
1	B	88	LEU
1	B	169	HIS
1	B	217	ARG
1	B	299[A]	ARG
1	B	299[B]	ARG
1	B	340	THR
1	C	77	TYR
1	C	177	LYS
1	C	205	PHE
1	C	217	ARG
1	C	253	ARG
1	C	305	MET
1	C	378	ARG
1	D	16	MET
1	D	28	ARG
1	D	77	TYR
1	D	149	PRO
1	D	217	ARG
1	D	399	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	294	HIS
1	A	323	ASN
1	B	58	ASN
1	B	86	HIS
1	B	169	HIS
1	B	210	ASN
1	B	255	GLN
1	B	294	HIS
1	B	341	HIS
1	C	210	ASN
1	C	323	ASN
1	D	169	HIS
1	D	210	ASN
1	D	323	ASN

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Mol	Chain	Res	Type
1	D	347	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	K2B	A	1404	-	31,31,31	0.94	0	48,48,48	1.65	10 (20%)
2	HEM	D	1402	1	42,50,50	1.96	9 (21%)	46,82,82	1.84	12 (26%)
3	K2B	B	1404	-	31,31,31	1.12	3 (9%)	48,48,48	1.54	9 (18%)
2	HEM	B	1402	1	42,50,50	1.88	12 (28%)	46,82,82	1.81	12 (26%)
2	HEM	C	1402	1	42,50,50	1.89	11 (26%)	46,82,82	1.89	12 (26%)
3	K2B	C	1404	-	31,31,31	1.13	2 (6%)	48,48,48	1.58	13 (27%)
3	K2B	D	1404	-	31,31,31	0.90	0	48,48,48	1.43	5 (10%)
2	HEM	A	1402	1	42,50,50	1.93	12 (28%)	46,82,82	2.07	14 (30%)

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	K2B	A	1404	-	-	0/10/68/68	0/4/4/4
2	HEM	D	1402	1	-	0/12/54/54	-
3	K2B	B	1404	-	-	0/10/68/68	0/4/4/4
2	HEM	B	1402	1	-	0/12/54/54	-
2	HEM	C	1402	1	-	0/12/54/54	-
3	K2B	C	1404	-	-	0/10/68/68	0/4/4/4
3	K2B	D	1404	-	-	0/10/68/68	0/4/4/4
2	HEM	A	1402	1	-	0/12/54/54	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1402	HEM	C3D-C2D	6.75	1.51	1.36
2	A	1402	HEM	C3D-C2D	5.71	1.49	1.36
2	C	1402	HEM	C3C-C2C	-5.53	1.32	1.40
2	C	1402	HEM	C3D-C2D	5.39	1.48	1.36
2	B	1402	HEM	C3D-C2D	5.31	1.48	1.36
2	A	1402	HEM	CMB-C2B	5.29	1.61	1.50
2	D	1402	HEM	C3C-CAC	4.79	1.58	1.47
2	D	1402	HEM	CMB-C2B	4.05	1.59	1.50
2	C	1402	HEM	C3C-C4C	3.86	1.47	1.41
2	B	1402	HEM	C3C-C4C	3.59	1.46	1.41
2	D	1402	HEM	CHB-C1B	3.30	1.42	1.34
2	B	1402	HEM	C3C-CAC	3.29	1.55	1.47
2	A	1402	HEM	C3C-CAC	3.25	1.54	1.47
2	C	1402	HEM	C3C-CAC	3.24	1.54	1.47
2	B	1402	HEM	C4A-CHB	-2.92	1.32	1.41
2	A	1402	HEM	FE-ND	2.90	2.14	1.98
2	B	1402	HEM	CAB-C3B	2.88	1.55	1.47
2	A	1402	HEM	CAB-C3B	2.76	1.54	1.47
2	A	1402	HEM	C3C-C2C	-2.74	1.36	1.40
2	B	1402	HEM	CMD-C2D	2.69	1.56	1.50
2	B	1402	HEM	CAA-C2A	2.67	1.58	1.52
2	B	1402	HEM	CMC-C2C	2.67	1.58	1.51
3	B	1404	K2B	C11-C9	2.66	1.58	1.53
3	C	1404	K2B	C16-C17	2.65	1.59	1.54
2	D	1402	HEM	C3C-C4C	2.61	1.45	1.41
2	B	1402	HEM	C3C-C2C	-2.60	1.36	1.40
2	C	1402	HEM	CMB-C2B	2.51	1.55	1.50
2	B	1402	HEM	CMB-C2B	2.49	1.55	1.50
2	C	1402	HEM	CMD-C2D	2.44	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1402	HEM	CHB-C1B	2.40	1.40	1.34
2	D	1402	HEM	C3C-C2C	-2.40	1.37	1.40
2	D	1402	HEM	FE-NB	2.40	2.11	1.98
2	B	1402	HEM	CHB-C1B	2.37	1.40	1.34
3	B	1404	K2B	C16-C17	2.35	1.59	1.54
2	A	1402	HEM	C2C-C1C	2.35	1.47	1.42
2	C	1402	HEM	CAB-C3B	2.33	1.53	1.47
3	C	1404	K2B	C21-C20	2.30	1.58	1.53
2	C	1402	HEM	C4B-NB	2.29	1.43	1.38
2	C	1402	HEM	CHB-C1B	2.27	1.40	1.34
2	A	1402	HEM	CMD-C2D	2.27	1.55	1.50
2	A	1402	HEM	C1B-NB	-2.24	1.36	1.40
2	C	1402	HEM	CAA-C2A	2.24	1.57	1.52
2	D	1402	HEM	CAB-C3B	2.20	1.53	1.47
2	A	1402	HEM	O1D-CGD	2.14	1.29	1.22
2	C	1402	HEM	C2C-C1C	2.11	1.47	1.42
2	B	1402	HEM	C2C-C1C	2.10	1.47	1.42
2	A	1402	HEM	FE-NB	2.08	2.09	1.98
3	B	1404	K2B	C13-C14	-2.05	1.51	1.55
2	D	1402	HEM	FE-ND	2.05	2.09	1.98

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1402	HEM	C3B-C4B-NB	-6.16	105.05	109.47
2	B	1402	HEM	CMA-C3A-C4A	-5.54	120.34	128.46
2	D	1402	HEM	C4C-CHD-C1D	4.96	129.11	122.56
2	C	1402	HEM	CMA-C3A-C4A	-4.75	121.49	128.46
2	C	1402	HEM	C4B-CHC-C1C	4.54	128.55	122.56
3	D	1404	K2B	C18-C13-C12	4.47	117.19	110.61
2	A	1402	HEM	C4B-CHC-C1C	4.44	128.42	122.56
2	A	1402	HEM	C2C-C3C-C4C	4.26	109.87	106.90
2	B	1402	HEM	CMA-C3A-C2A	4.07	132.62	124.94
3	B	1404	K2B	C2-C3-C4	3.97	122.77	116.73
2	C	1402	HEM	CBA-CAA-C2A	-3.92	105.95	112.54
2	C	1402	HEM	C4C-CHD-C1D	3.90	127.70	122.56
2	B	1402	HEM	C4B-CHC-C1C	3.86	127.66	122.56
2	D	1402	HEM	C4D-ND-C1D	3.85	109.76	105.21
2	C	1402	HEM	C4D-ND-C1D	3.73	109.62	105.21
3	B	1404	K2B	C7-C8-C9	-3.68	106.11	110.52
2	B	1402	HEM	CBA-CAA-C2A	-3.65	106.40	112.54
2	D	1402	HEM	CBA-CAA-C2A	-3.63	106.44	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1404	K2B	C1-C10-C9	-3.53	104.07	108.74
3	A	1404	K2B	C19-C10-C9	3.50	115.58	111.66
2	A	1402	HEM	C1B-NB-C4B	3.48	109.33	105.21
3	A	1404	K2B	C16-C17-C13	-3.46	99.77	103.84
2	D	1402	HEM	CMA-C3A-C4A	-3.44	123.42	128.46
2	A	1402	HEM	CBA-CAA-C2A	-3.39	106.83	112.54
2	C	1402	HEM	C3B-C2B-C1B	3.37	108.94	106.41
3	C	1404	K2B	C10-C9-C8	3.34	117.60	112.71
2	A	1402	HEM	CBD-CAD-C3D	-3.29	103.44	112.53
2	A	1402	HEM	C4D-ND-C1D	3.23	109.03	105.21
3	C	1404	K2B	C19-C10-C5	-3.14	103.58	108.38
2	D	1402	HEM	C3B-C4B-NB	-3.14	107.21	109.47
2	A	1402	HEM	C4B-C3B-C2B	3.14	110.16	107.28
3	D	1404	K2B	C19-C10-C1	3.13	114.19	109.43
3	C	1404	K2B	C19-C10-C1	3.11	114.16	109.43
2	D	1402	HEM	CMC-C2C-C3C	3.10	130.88	124.68
3	A	1404	K2B	C16-C15-C14	-3.09	99.10	105.14
3	A	1404	K2B	C15-C16-C17	3.07	111.15	105.14
3	D	1404	K2B	C6-C5-C4	-3.03	116.01	120.86
2	D	1402	HEM	CBD-CAD-C3D	-2.98	104.28	112.53
2	B	1402	HEM	CMC-C2C-C3C	2.95	130.58	124.68
3	B	1404	K2B	O1-C3-C4	-2.92	116.39	121.65
2	B	1402	HEM	CMD-C2D-C1D	2.86	129.51	125.03
2	A	1402	HEM	CHA-C4D-ND	2.82	127.87	124.37
2	C	1402	HEM	C3C-C4C-NC	-2.81	105.64	110.94
3	A	1404	K2B	C15-C14-C8	-2.81	114.62	119.10
3	A	1404	K2B	C18-C13-C12	2.78	114.71	110.61
3	D	1404	K2B	C6-C7-C8	2.78	116.51	111.64
3	B	1404	K2B	C16-C17-C13	-2.77	100.58	103.84
3	B	1404	K2B	C5-C4-C3	-2.75	119.42	123.67
3	C	1404	K2B	C7-C6-C5	-2.73	106.92	111.93
3	A	1404	K2B	C12-C13-C14	-2.72	103.17	107.25
2	C	1402	HEM	C2C-C3C-C4C	2.68	108.77	106.90
3	A	1404	K2B	C12-C13-C17	-2.66	112.68	116.60
2	A	1402	HEM	C3C-C4C-NC	-2.66	105.92	110.94
2	B	1402	HEM	CHA-C4D-ND	2.66	127.67	124.37
2	D	1402	HEM	C1B-NB-C4B	2.64	108.34	105.21
2	C	1402	HEM	C4A-C3A-C2A	2.61	108.81	107.00
2	B	1402	HEM	C3B-C4B-NB	-2.61	107.60	109.47
2	A	1402	HEM	CMC-C2C-C3C	2.59	129.87	124.68
2	D	1402	HEM	CMD-C2D-C1D	2.54	129.01	125.03
2	A	1402	HEM	C4C-CHD-C1D	2.52	125.88	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1404	K2B	C16-C15-C14	-2.49	100.27	105.14
2	B	1402	HEM	C1B-NB-C4B	2.49	108.16	105.21
2	C	1402	HEM	CMA-C3A-C2A	2.48	129.62	124.94
3	C	1404	K2B	C15-C14-C13	2.46	106.74	103.84
3	D	1404	K2B	C12-C13-C14	-2.45	103.58	107.25
2	D	1402	HEM	CHC-C4B-NB	2.44	127.06	124.44
2	C	1402	HEM	CHA-C4D-ND	2.44	127.39	124.37
2	B	1402	HEM	C2C-C3C-C4C	2.38	108.56	106.90
3	B	1404	K2B	C16-C17-C20	-2.38	108.58	112.18
2	A	1402	HEM	C3B-C2B-C1B	-2.37	104.63	106.41
2	D	1402	HEM	C1D-C2D-C3D	-2.35	104.51	106.98
3	C	1404	K2B	C1-C2-C3	-2.34	106.83	111.60
2	B	1402	HEM	C3C-C4C-NC	-2.34	106.53	110.94
3	C	1404	K2B	C15-C16-C17	2.33	109.71	105.14
3	B	1404	K2B	C15-C14-C13	2.26	106.50	103.84
3	C	1404	K2B	C2-C3-C4	2.25	120.16	116.73
2	B	1402	HEM	C4D-ND-C1D	2.25	107.87	105.21
3	C	1404	K2B	C17-C13-C14	2.23	102.66	100.10
2	D	1402	HEM	C3C-C4C-NC	-2.23	106.74	110.94
3	C	1404	K2B	C12-C13-C17	-2.14	113.44	116.60
2	C	1402	HEM	CAD-C3D-C4D	2.14	128.43	124.70
3	C	1404	K2B	C7-C8-C9	-2.13	107.96	110.52
3	B	1404	K2B	C19-C10-C1	2.12	112.65	109.43
2	A	1402	HEM	CHC-C4B-C3B	2.10	127.78	124.57
3	A	1404	K2B	C2-C3-C4	2.09	119.90	116.73
3	B	1404	K2B	C11-C12-C13	-2.06	109.27	112.74
3	C	1404	K2B	C12-C11-C9	-2.03	109.68	113.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

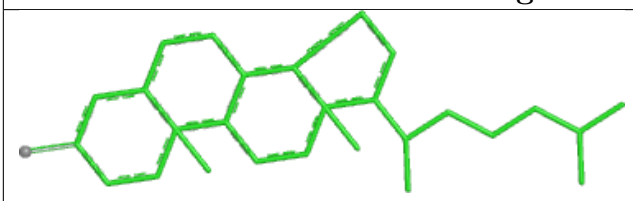
4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1402	HEM	8	0
2	B	1402	HEM	7	0
2	C	1402	HEM	4	0
2	A	1402	HEM	7	0

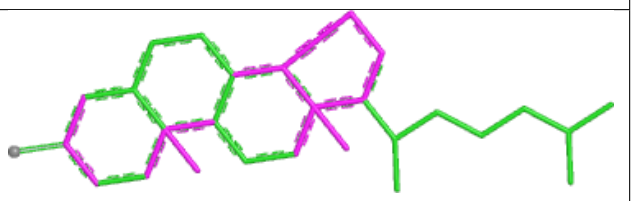
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

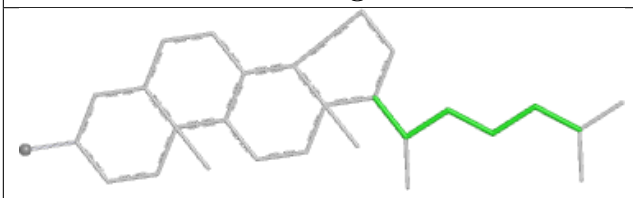
Ligand K2B A 1404



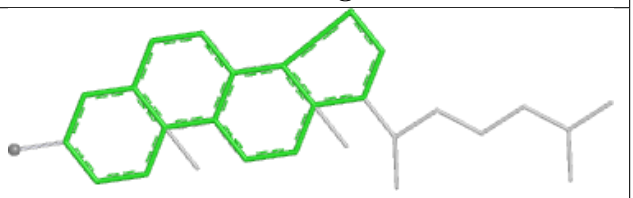
Bond lengths



Bond angles

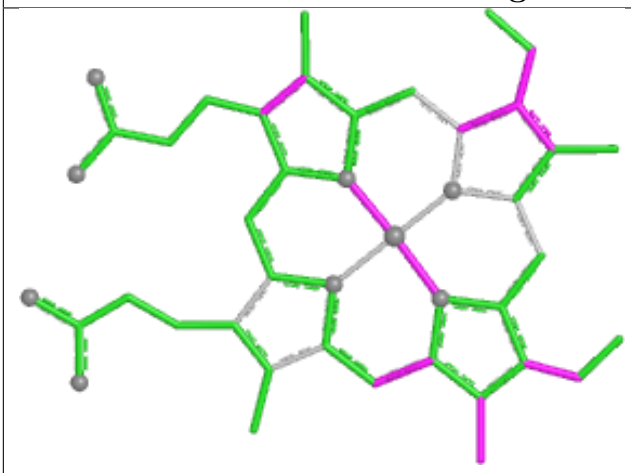


Torsions

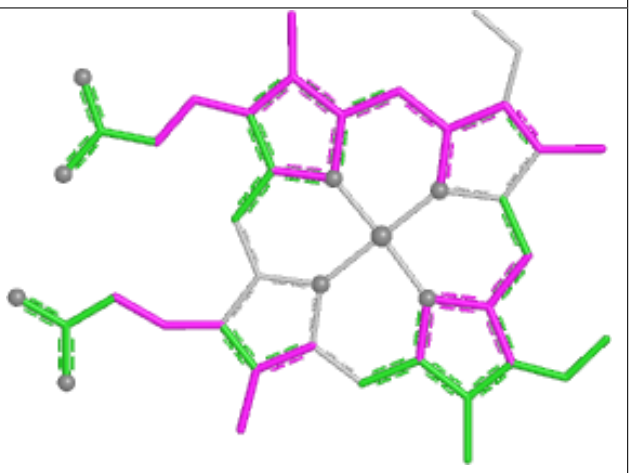


Rings

Ligand HEM D 1402



Bond lengths



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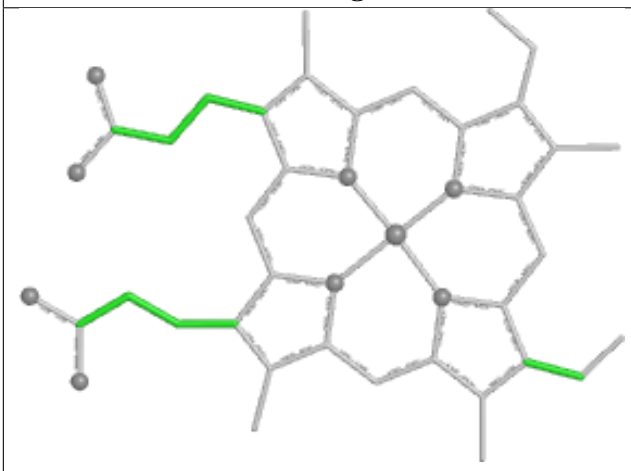

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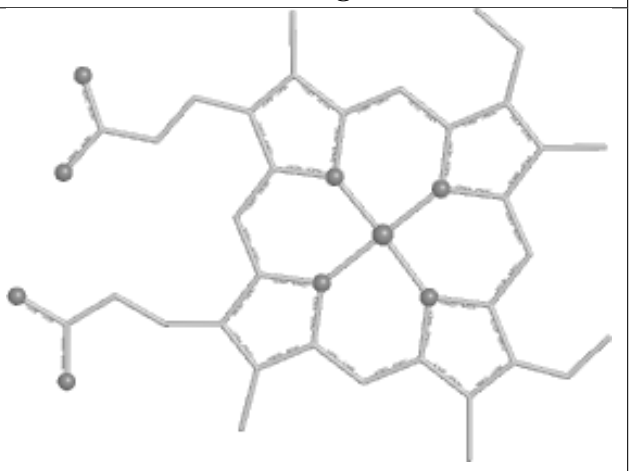
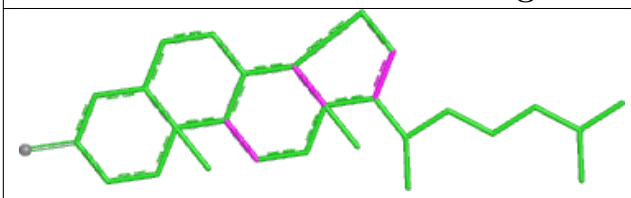


Rings

Ligand K2B B 1404



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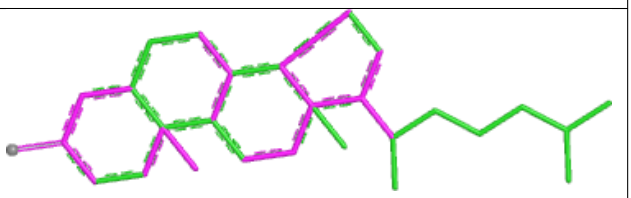
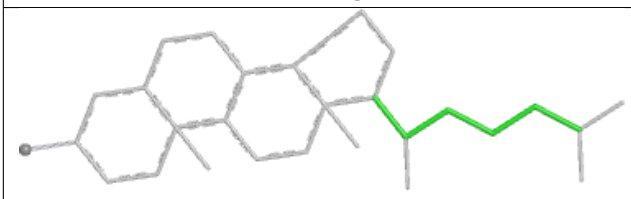
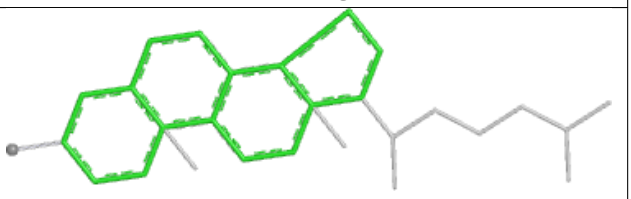


Bond angles

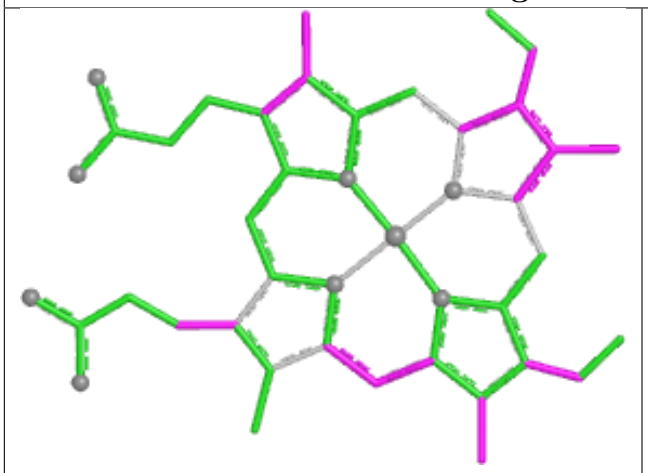


Torsions



Rings

Ligand HEM B 1402



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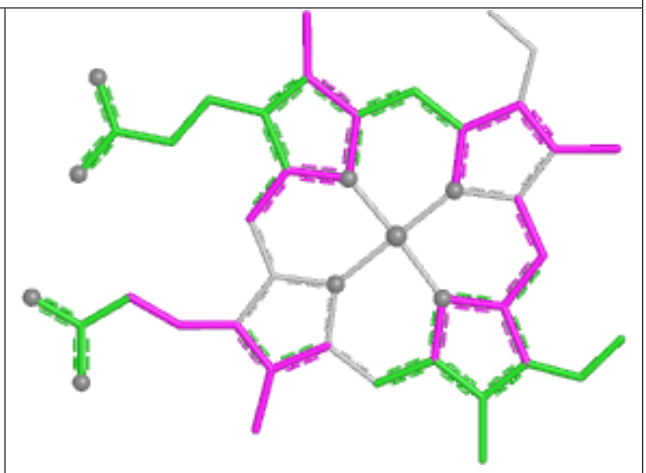
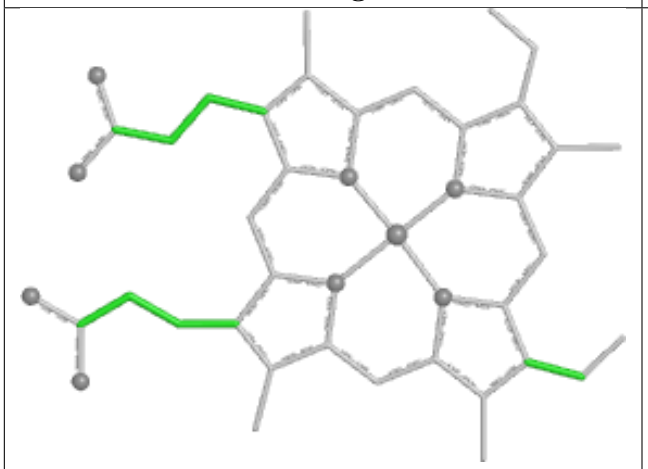
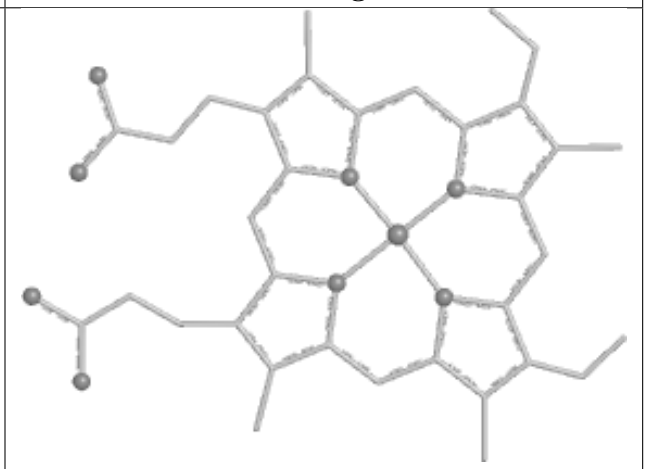


Bond angles

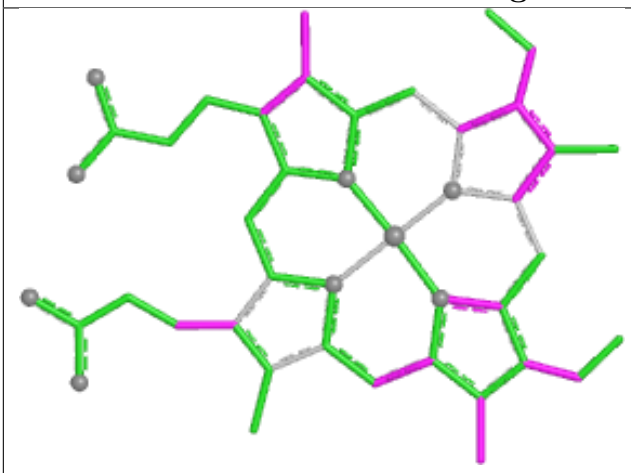


Torsions

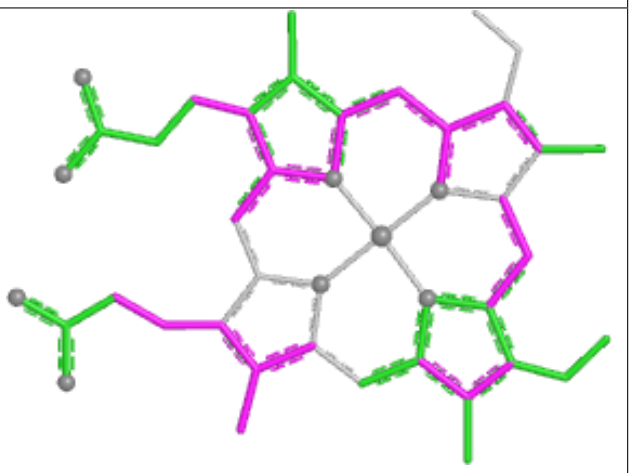


Rings

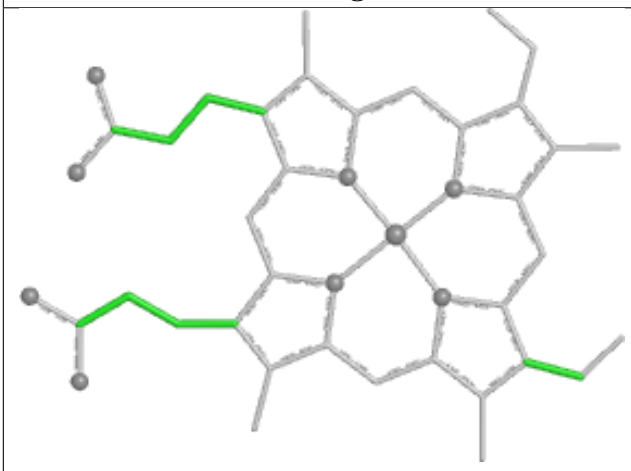
Ligand HEM C 1402



Bond lengths



Bond angles



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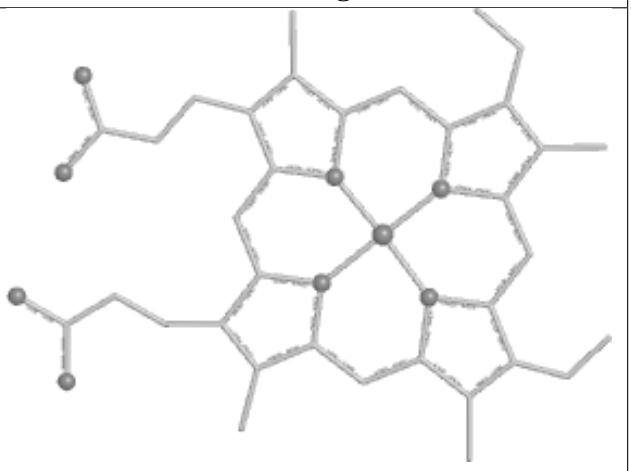
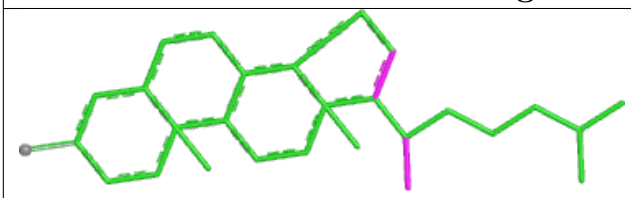
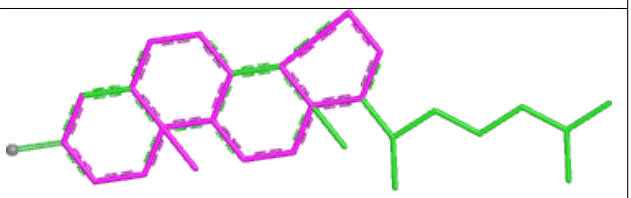


Rings

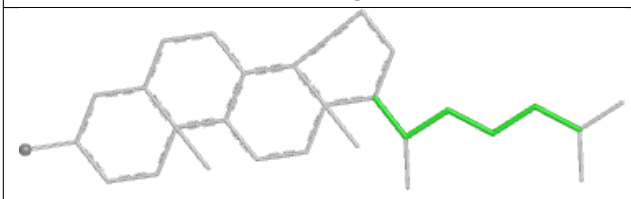
Ligand K2B C 1404



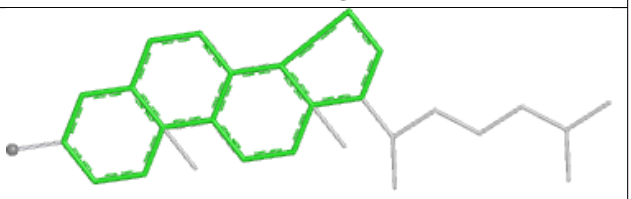
Bond lengths



Bond angles

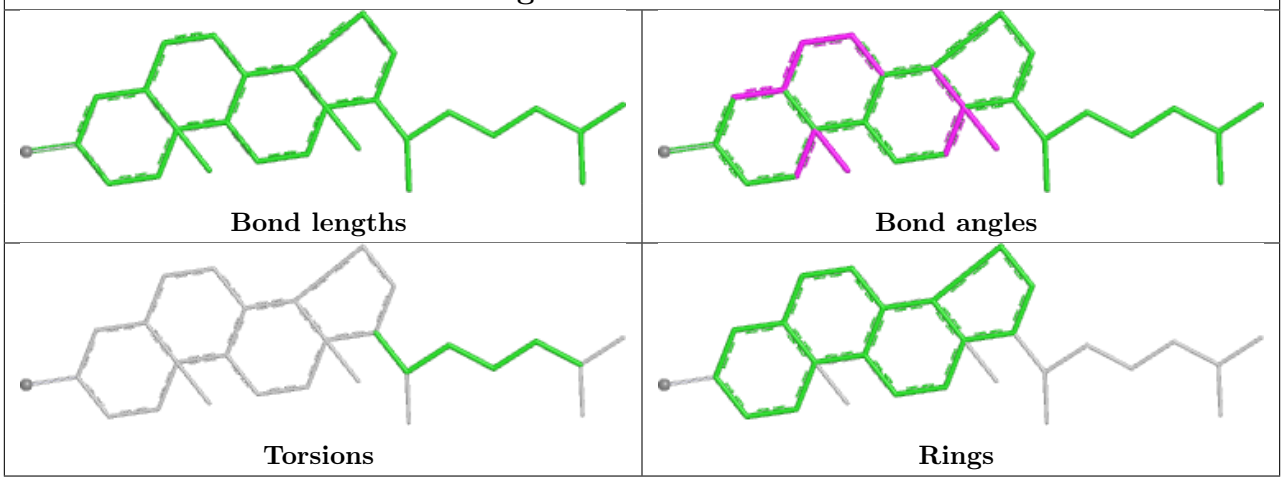


Torsions

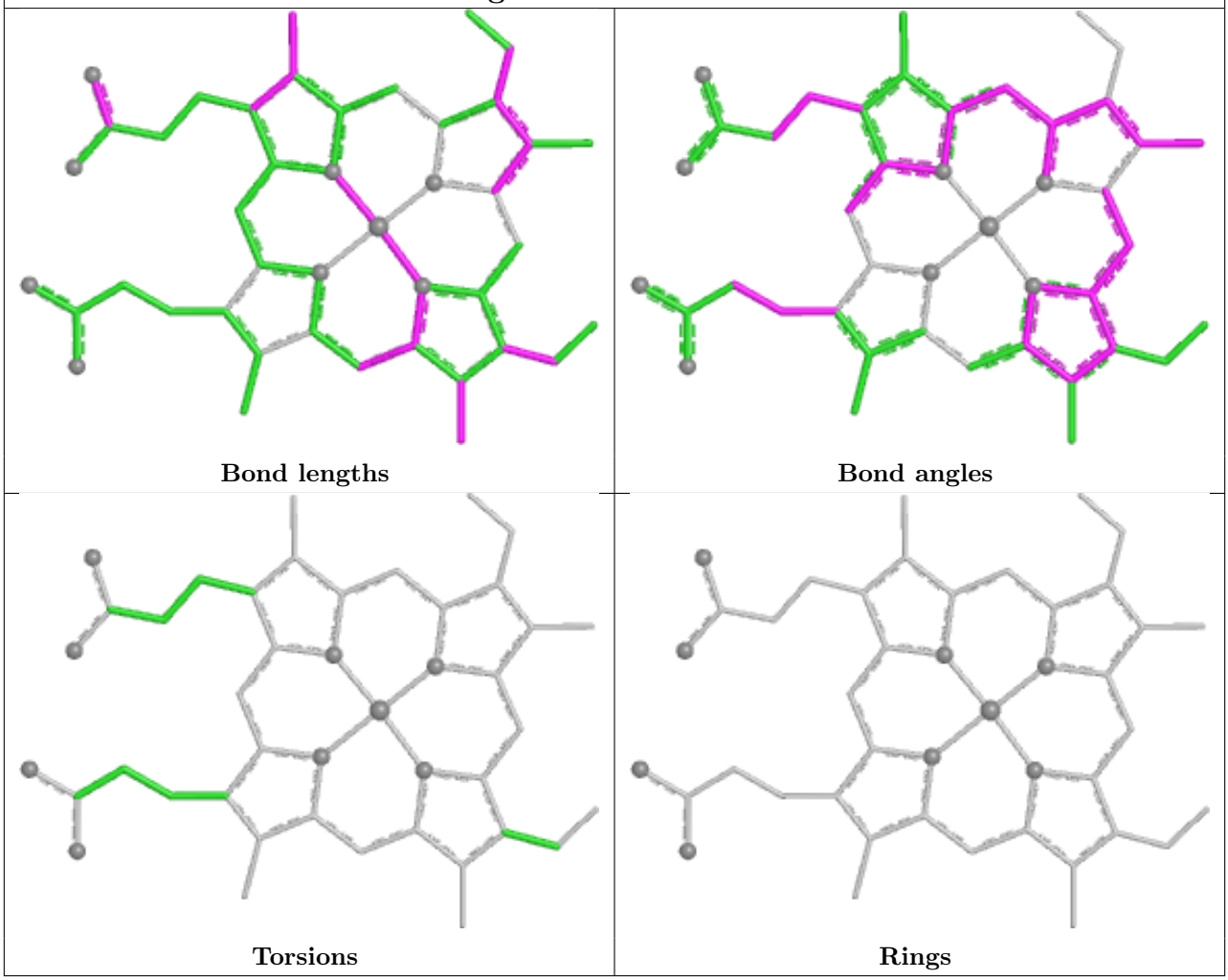


Rings

Ligand K2B D 1404



Ligand HEM A 1402



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(Å^2)	Q<0.9
1	A	396/407 (97%)	-0.35	5 (1%)	77	81	7, 14, 29, 49	0
1	B	395/407 (97%)	-0.42	6 (1%)	73	77	5, 11, 28, 40	0
1	C	395/407 (97%)	-0.34	5 (1%)	77	81	6, 13, 28, 45	0
1	D	394/407 (96%)	-0.42	1 (0%)	94	94	6, 12, 28, 40	0
All	All	1580/1628 (97%)	-0.38	17 (1%)	80	83	5, 13, 28, 49	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	LEU	4.7
1	B	173	ALA	4.0
1	B	174	ALA	3.6
1	A	202	ASP	3.2
1	A	169	HIS	3.0
1	C	202	ASP	3.0
1	A	170	VAL	3.0
1	D	215	GLY	2.8
1	B	215	GLY	2.8
1	B	202	ASP	2.8
1	C	171	ASP	2.8
1	B	400	LEU	2.6
1	C	215	GLY	2.5
1	A	165	GLY	2.3
1	C	169	HIS	2.3
1	C	123[A]	ARG	2.3
1	B	170	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

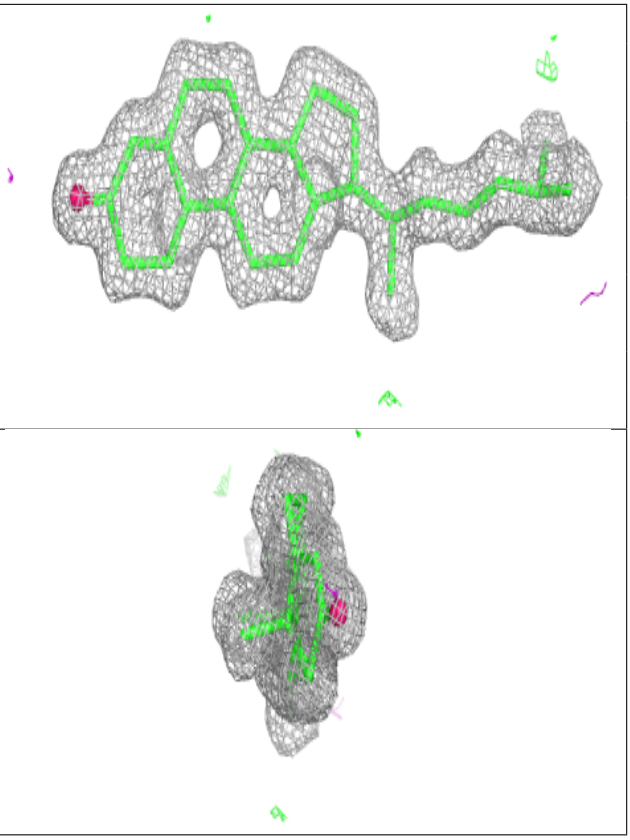
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	K2B	A	1404	28/28	0.94	0.07	8,11,16,19	0
3	K2B	B	1404	28/28	0.94	0.08	4,9,20,23	0
3	K2B	C	1404	28/28	0.94	0.09	5,10,18,18	0
3	K2B	D	1404	28/28	0.95	0.07	5,9,13,16	0
4	MG	B	1405	1/1	0.96	0.06	21,21,21,21	0
2	HEM	B	1402	43/43	0.98	0.08	4,7,10,22	0
2	HEM	A	1402	43/43	0.98	0.08	4,8,10,24	0
2	HEM	D	1402	43/43	0.99	0.07	2,7,9,25	0
2	HEM	C	1402	43/43	0.99	0.07	5,8,11,19	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.

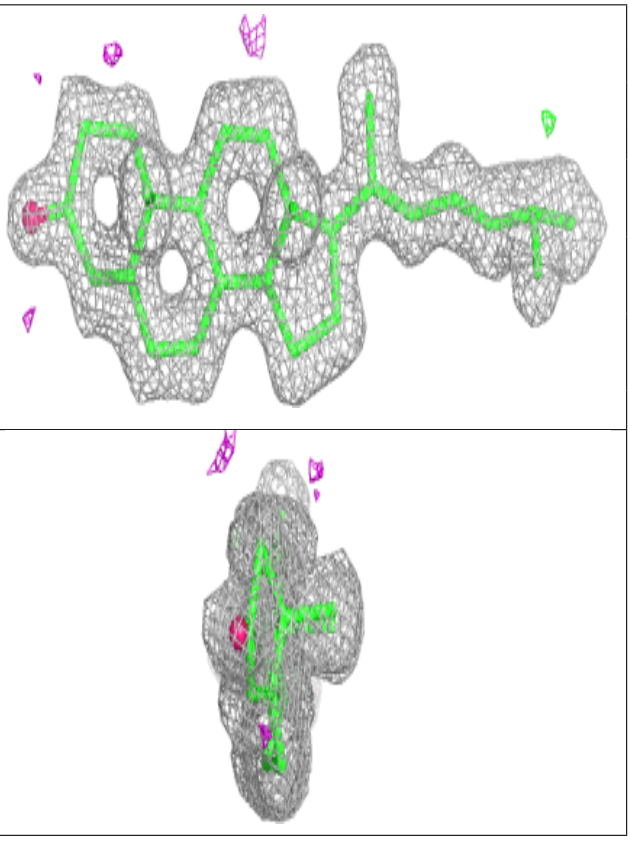
Electron density around K2B A 1404:

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



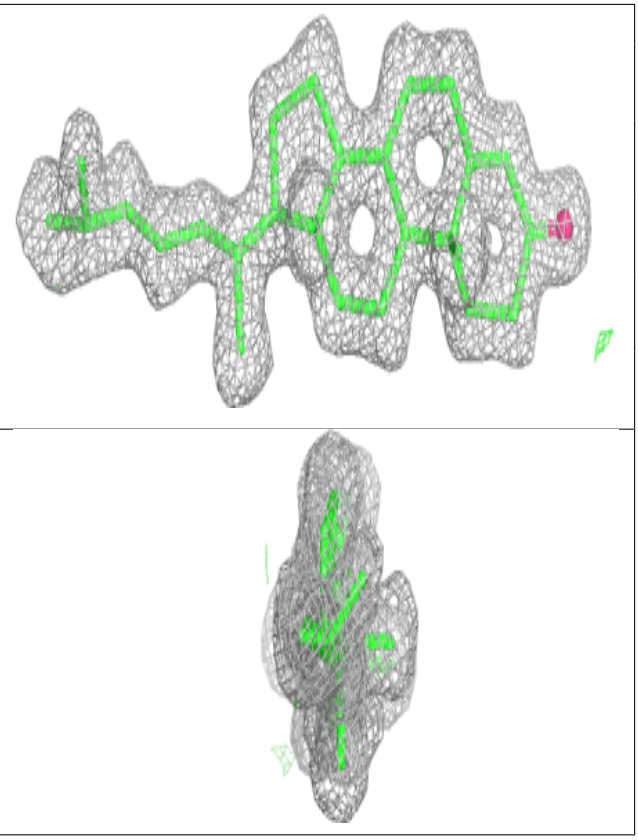
Electron density around K2B B 1404:

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



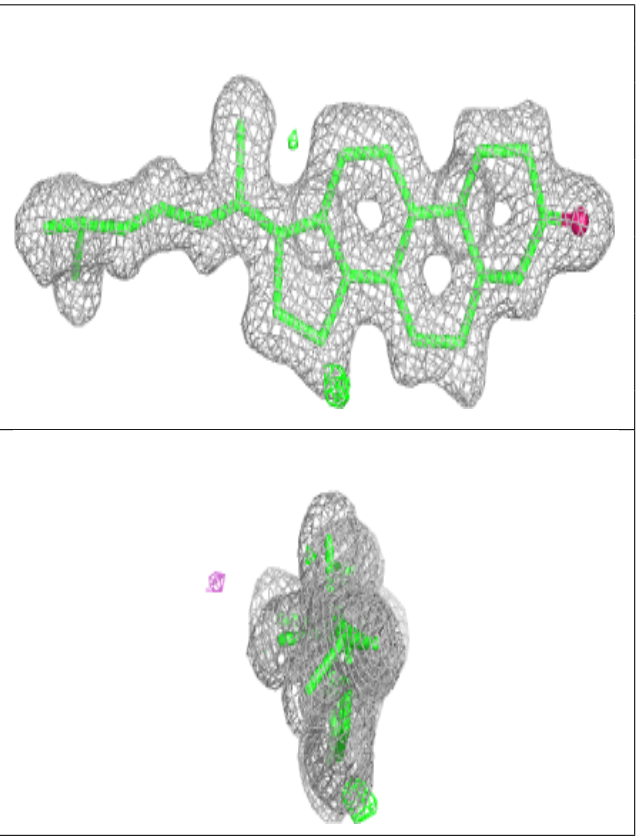
Electron density around K2B C 1404:

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



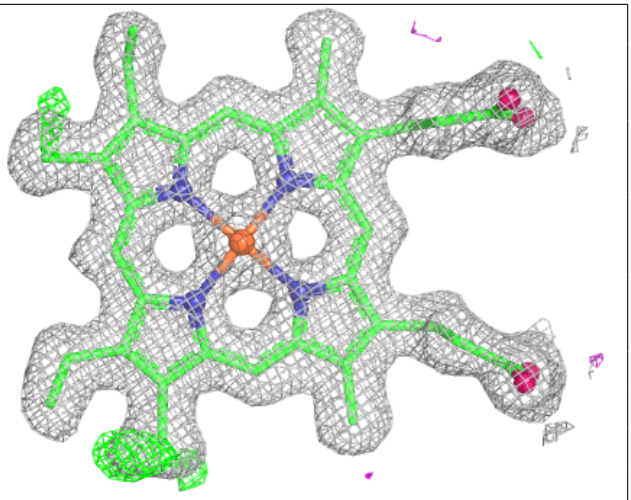
Electron density around K2B D 1404:

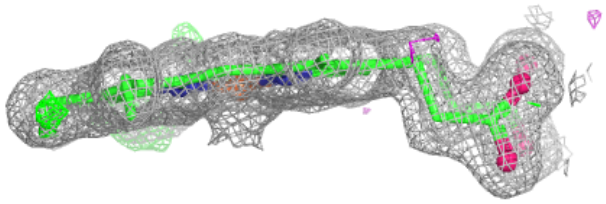
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

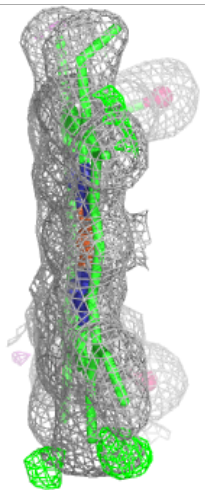


Electron density around HEM B 1402:

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

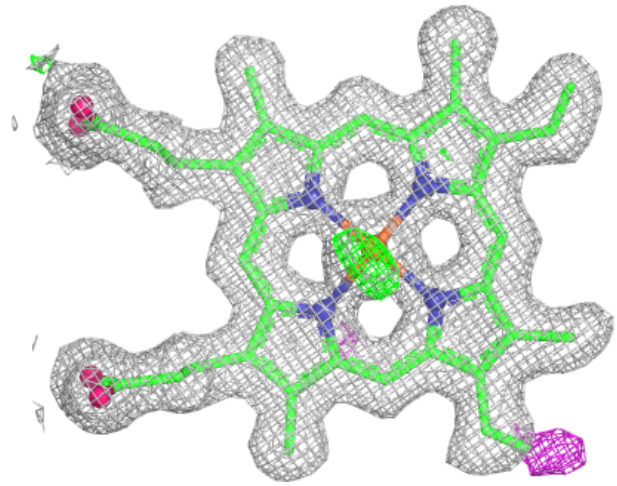


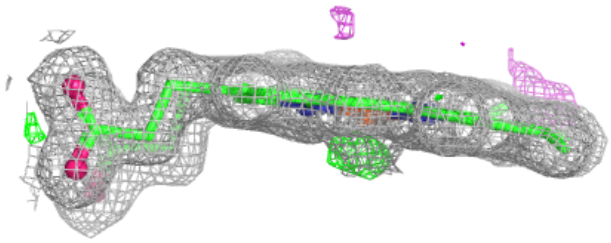


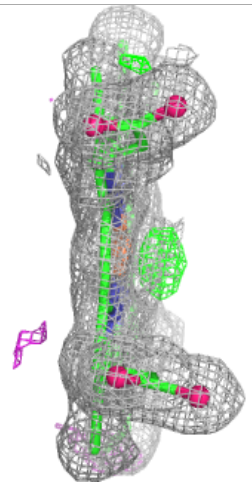


Electron density around HEM A 1402:

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

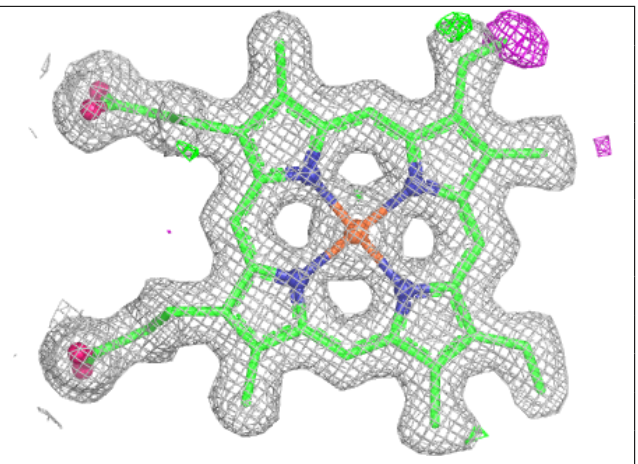


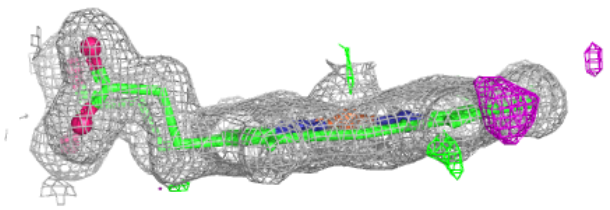


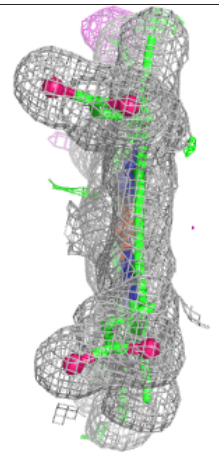


Electron density around HEM D 1402:

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

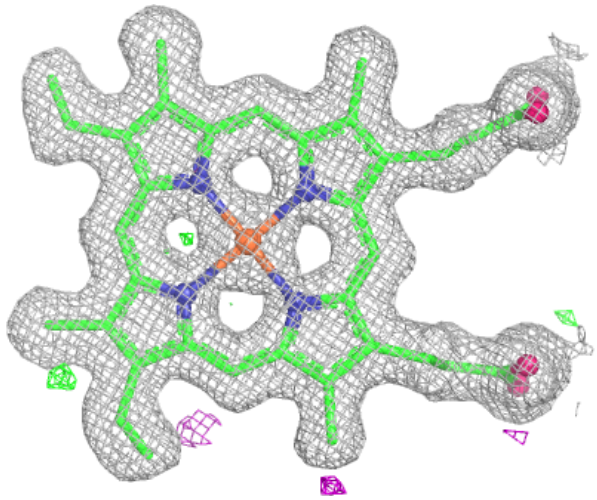


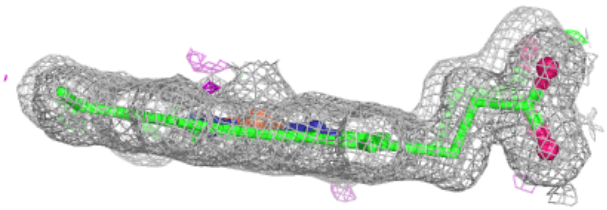


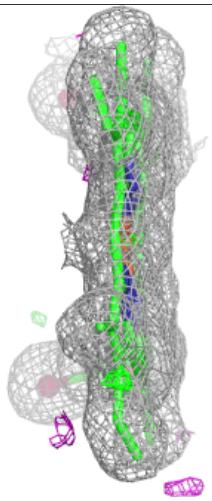


Electron density around HEM C 1402:

$2mF_o$-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.