



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:46 AM UTC

PDB ID : 8U3N / pdb_00008u3n
Title : Structure of P450Blt from Micromonospora sp. MW-13
Authors : Hansen, M.H.; Cryle, M.J.; Zhao, Y.
Deposited on : 2023-09-08
Resolution : 2.15 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

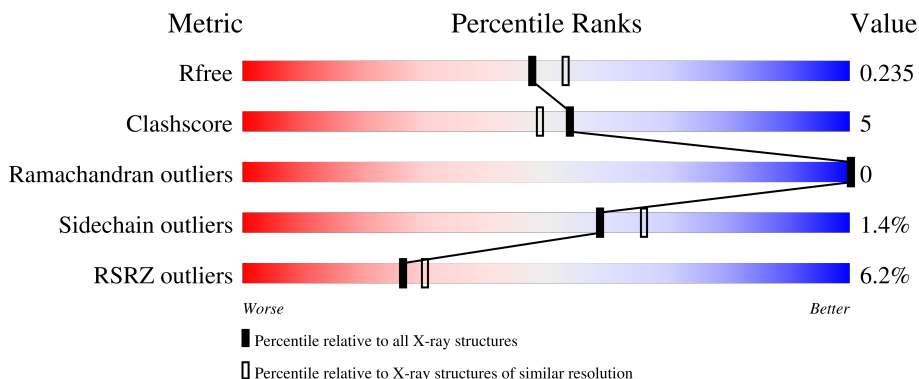
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

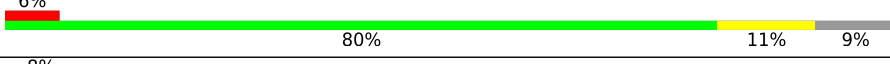
The reported resolution of this entry is 2.15 Å.

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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	420	
1	B	420	
1	C	420	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18078 atoms, of which 8857 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-SU1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	377	Total	C	H	N	O	S	0	4	0
			5757	1806	2885	542	520	4			
1	B	382	Total	C	H	N	O	S	0	6	0
			5882	1843	2947	556	532	4			
1	C	378	Total	C	H	N	O	S	0	3	0
			5790	1816	2899	547	524	4			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A3E2YLT4
A	-19	GLY	-	expression tag	UNP A0A3E2YLT4
A	-18	SER	-	expression tag	UNP A0A3E2YLT4
A	-17	SER	-	expression tag	UNP A0A3E2YLT4
A	-16	HIS	-	expression tag	UNP A0A3E2YLT4
A	-15	HIS	-	expression tag	UNP A0A3E2YLT4
A	-14	HIS	-	expression tag	UNP A0A3E2YLT4
A	-13	HIS	-	expression tag	UNP A0A3E2YLT4
A	-12	HIS	-	expression tag	UNP A0A3E2YLT4
A	-11	HIS	-	expression tag	UNP A0A3E2YLT4
A	-10	SER	-	expression tag	UNP A0A3E2YLT4
A	-9	SER	-	expression tag	UNP A0A3E2YLT4
A	-8	GLY	-	expression tag	UNP A0A3E2YLT4
A	-7	LEU	-	expression tag	UNP A0A3E2YLT4
A	-6	VAL	-	expression tag	UNP A0A3E2YLT4
A	-5	PRO	-	expression tag	UNP A0A3E2YLT4
A	-4	ARG	-	expression tag	UNP A0A3E2YLT4
A	-3	GLY	-	expression tag	UNP A0A3E2YLT4
A	-2	SER	-	expression tag	UNP A0A3E2YLT4
A	-1	HIS	-	expression tag	UNP A0A3E2YLT4
A	0	MET	-	expression tag	UNP A0A3E2YLT4
A	394	ALA	GLN	conflict	UNP A0A3E2YLT4
B	-20	MET	-	initiating methionine	UNP A0A3E2YLT4

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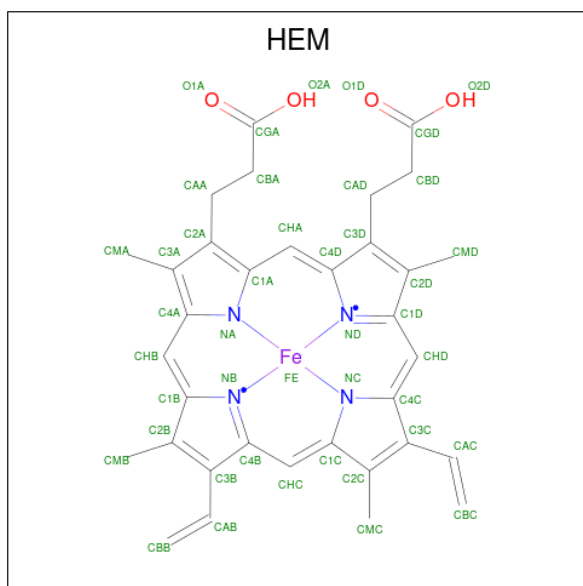
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	GLY	-	expression tag	UNP A0A3E2YLT4
B	-18	SER	-	expression tag	UNP A0A3E2YLT4
B	-17	SER	-	expression tag	UNP A0A3E2YLT4
B	-16	HIS	-	expression tag	UNP A0A3E2YLT4
B	-15	HIS	-	expression tag	UNP A0A3E2YLT4
B	-14	HIS	-	expression tag	UNP A0A3E2YLT4
B	-13	HIS	-	expression tag	UNP A0A3E2YLT4
B	-12	HIS	-	expression tag	UNP A0A3E2YLT4
B	-11	HIS	-	expression tag	UNP A0A3E2YLT4
B	-10	SER	-	expression tag	UNP A0A3E2YLT4
B	-9	SER	-	expression tag	UNP A0A3E2YLT4
B	-8	GLY	-	expression tag	UNP A0A3E2YLT4
B	-7	LEU	-	expression tag	UNP A0A3E2YLT4
B	-6	VAL	-	expression tag	UNP A0A3E2YLT4
B	-5	PRO	-	expression tag	UNP A0A3E2YLT4
B	-4	ARG	-	expression tag	UNP A0A3E2YLT4
B	-3	GLY	-	expression tag	UNP A0A3E2YLT4
B	-2	SER	-	expression tag	UNP A0A3E2YLT4
B	-1	HIS	-	expression tag	UNP A0A3E2YLT4
B	0	MET	-	expression tag	UNP A0A3E2YLT4
B	394	ALA	GLN	conflict	UNP A0A3E2YLT4
C	-20	MET	-	initiating methionine	UNP A0A3E2YLT4
C	-19	GLY	-	expression tag	UNP A0A3E2YLT4
C	-18	SER	-	expression tag	UNP A0A3E2YLT4
C	-17	SER	-	expression tag	UNP A0A3E2YLT4
C	-16	HIS	-	expression tag	UNP A0A3E2YLT4
C	-15	HIS	-	expression tag	UNP A0A3E2YLT4
C	-14	HIS	-	expression tag	UNP A0A3E2YLT4
C	-13	HIS	-	expression tag	UNP A0A3E2YLT4
C	-12	HIS	-	expression tag	UNP A0A3E2YLT4
C	-11	HIS	-	expression tag	UNP A0A3E2YLT4
C	-10	SER	-	expression tag	UNP A0A3E2YLT4
C	-9	SER	-	expression tag	UNP A0A3E2YLT4
C	-8	GLY	-	expression tag	UNP A0A3E2YLT4
C	-7	LEU	-	expression tag	UNP A0A3E2YLT4
C	-6	VAL	-	expression tag	UNP A0A3E2YLT4
C	-5	PRO	-	expression tag	UNP A0A3E2YLT4
C	-4	ARG	-	expression tag	UNP A0A3E2YLT4
C	-3	GLY	-	expression tag	UNP A0A3E2YLT4
C	-2	SER	-	expression tag	UNP A0A3E2YLT4
C	-1	HIS	-	expression tag	UNP A0A3E2YLT4
C	0	MET	-	expression tag	UNP A0A3E2YLT4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	394	ALA	GLN	conflict	UNP A0A3E2YLT4

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).

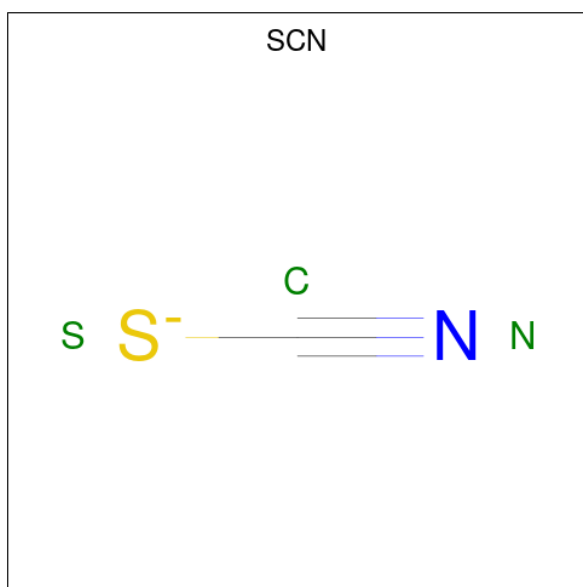


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			24	6	12	6		
3	B	1	Total	C	H	O	0	0
			24	6	12	6		
3	C	1	Total	C	H	O	0	0
			24	6	12	6		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	S	0	0
			3	1	1	1		
5	B	1	Total	C	N	S	0	0
			3	1	1	1		

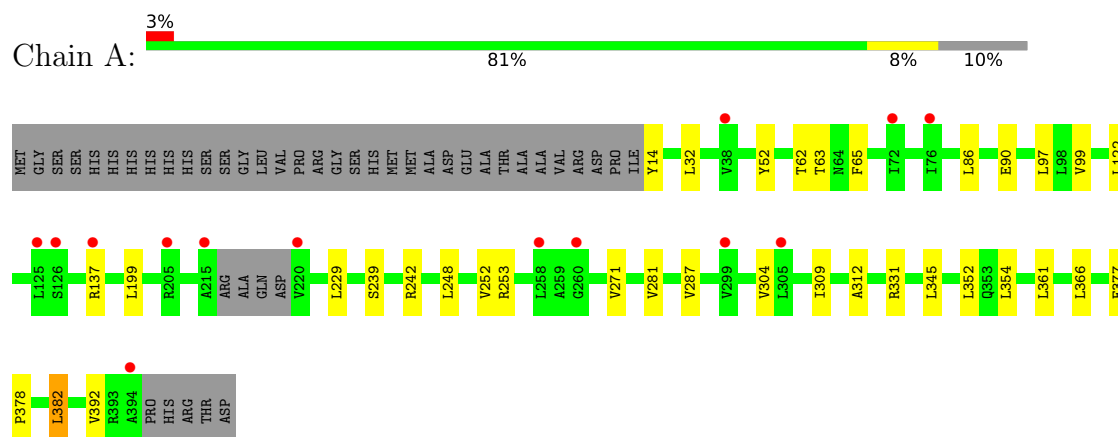
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	112	Total	O	0	0
			112	112		
6	B	150	Total	O	0	0
			150	150		
6	C	87	Total	O	0	0
			87	87		

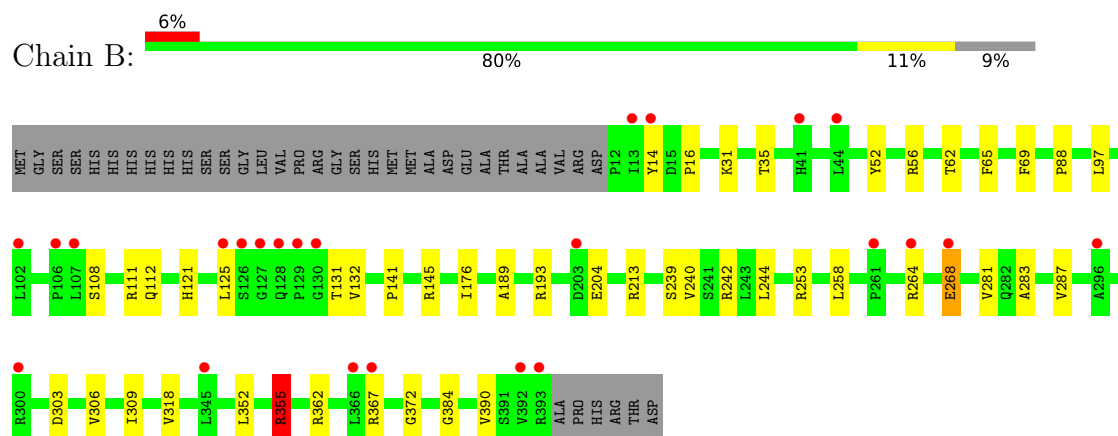
3 Residue-property plots [i](#)

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.

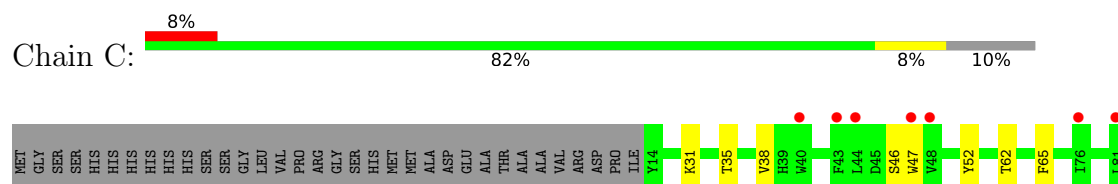
• Molecule 1: Cytochrome P450-SU1

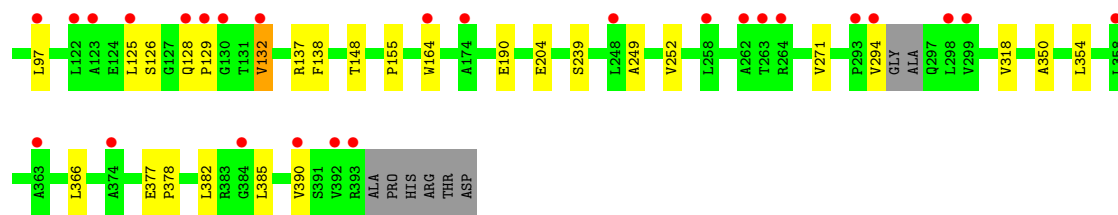


• Molecule 1: Cytochrome P450-SU1



• Molecule 1: Cytochrome P450-SU1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.08Å 95.75Å 105.22Å 90.00° 92.63° 90.00°	Depositor
Resolution (Å)	47.87 – 2.15 47.87 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.87-2.15) 96.8 (47.87-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.23 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.236 0.194 , 0.235	Depositor DCC
R_{free} test set	1994 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18078	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, HEM, K, BGC

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	0.37	0/2962	0.49	0/4042
1	B	0.45	3/3027 (0.1%)	0.56	3/4130 (0.1%)
1	C	0.36	0/2975	0.48	0/4059
All	All	0.40	3/8964 (0.0%)	0.51	3/12231 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	PRO	CA-C	6.54	1.55	1.51
1	B	355	ARG	CG-CD	-6.42	1.33	1.52
1	B	355	ARG	CZ-NH2	5.93	1.41	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	ARG	CB-CG-CD	-6.74	95.80	111.30
1	B	355	ARG	NH1-CZ-NH2	-5.33	112.37	119.30
1	B	88	PRO	O-C-N	5.08	123.65	121.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	ARG	Sidechain
1	B	355	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2872	2885	2859	21	0
1	B	2935	2947	2919	31	0
1	C	2891	2899	2880	25	0
2	A	43	30	30	2	0
2	B	43	30	30	5	0
2	C	43	30	30	6	0
3	A	12	12	12	0	0
3	B	12	12	11	2	0
3	C	12	12	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	6	0	0	0	0
6	A	112	0	0	1	0
6	B	150	0	0	0	0
6	C	87	0	0	0	0
All	All	9221	8857	8783	86	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (86) 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:C:125:LEU:HD23	1:C:132:VAL:HG11	1.60	0.81
1:B:303:ASP:OD2	3:B:404:BGC:O1	2.02	0.78
1:B:204:GLU:OE1	1:B:213:ARG:NH1	2.25	0.69
1:A:248:LEU:O	1:A:252:VAL:HG13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LYS:O	1:B:35:THR:HG23	1.97	0.63
1:C:271:VAL:HG13	1:C:354:LEU:HD23	1.82	0.60
1:B:264:ARG:NH1	1:B:355:ARG:HD3	2.17	0.59
1:A:352:LEU:C	1:A:352:LEU:HD23	2.28	0.59
1:C:125:LEU:HD11	1:C:138:PHE:HB2	1.85	0.58
1:C:128:GLN:HG3	1:C:129:PRO:HD2	1.87	0.57
1:B:352:LEU:O	1:B:352:LEU:HD23	2.05	0.56
2:C:401:HEM:HMB1	2:C:401:HEM:HBB2	1.88	0.55
1:C:164:TRP:CE2	1:C:190:GLU:HG2	2.41	0.55
1:B:52:TYR:CD2	1:B:318:VAL:HG21	2.43	0.54
1:C:125:LEU:HD23	1:C:132:VAL:CG1	2.35	0.53
1:C:126:SER:C	1:C:128:GLN:H	2.17	0.53
2:B:401:HEM:CMC	2:B:401:HEM:HBC2	2.39	0.52
1:B:352:LEU:HD23	1:B:352:LEU:C	2.34	0.52
2:C:401:HEM:HBB2	2:C:401:HEM:CMB	2.40	0.52
1:A:14:TYR:HE2	1:A:32:LEU:HD11	1.74	0.52
1:B:253:ARG:NH2	1:B:372:GLY:O	2.43	0.52
1:C:126:SER:HB3	1:C:366:LEU:HD11	1.92	0.52
2:B:401:HEM:HBC2	2:B:401:HEM:HMC1	1.92	0.50
1:A:281:VAL:HA	1:A:382:LEU:HD12	1.94	0.50
1:B:264:ARG:NH1	1:B:355:ARG:CD	2.75	0.50
1:C:126:SER:C	1:C:128:GLN:N	2.69	0.50
1:A:366:LEU:HD22	1:A:392:VAL:CG1	2.43	0.49
1:B:189:ALA:O	1:B:193:ARG:HG2	2.12	0.49
1:B:193:ARG:N	1:B:193:ARG:HD3	2.27	0.49
1:A:239:SER:HB3	2:A:401:HEM:C2C	2.49	0.48
1:B:108:SER:O	1:B:112:GLN:HG3	2.14	0.48
2:C:401:HEM:CMC	2:C:401:HEM:HBC2	2.44	0.48
1:B:131:THR:HA	1:B:390:VAL:O	2.14	0.47
1:A:86:LEU:HD13	1:A:90:GLU:HG2	1.96	0.47
1:A:122:LEU:HD21	1:A:361:LEU:HD23	1.96	0.47
1:B:16:PRO:HG2	1:B:176:ILE:HD11	1.96	0.47
1:C:97:LEU:C	1:C:97:LEU:HD23	2.39	0.47
1:B:264:ARG:HH11	1:B:355:ARG:HD3	1.79	0.47
1:C:125:LEU:HD21	1:C:137:ARG:CB	2.44	0.47
1:A:377:GLU:HG3	1:A:378:PRO:HD2	1.95	0.47
1:C:125:LEU:HD21	1:C:137:ARG:HB2	1.97	0.46
1:C:132:VAL:HG12	1:C:137:ARG:HG3	1.97	0.46
1:B:281:VAL:CG1	1:B:309:ILE:HD11	2.45	0.46
2:B:401:HEM:CMB	2:B:401:HEM:HBB2	2.46	0.46
1:B:258:LEU:O	1:B:362:ARG:HD3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLU:HB3	1:B:213:ARG:HH12	1.81	0.46
1:C:126:SER:O	1:C:128:GLN:N	2.49	0.46
2:B:401:HEM:HBB2	2:B:401:HEM:HMB1	1.98	0.45
1:A:253:ARG:HD3	6:A:539:HOH:O	2.17	0.45
2:C:401:HEM:HBC2	2:C:401:HEM:HMC1	1.98	0.45
1:A:52:TYR:HA	1:A:312:ALA:HB1	1.97	0.45
1:B:125:LEU:HD22	1:B:132:VAL:HG21	1.99	0.44
2:A:401:HEM:CMC	2:A:401:HEM:HBC2	2.47	0.44
1:A:97:LEU:C	1:A:97:LEU:HD23	2.43	0.44
1:C:31:LYS:O	1:C:35:THR:HG23	2.18	0.44
1:C:239:SER:HB3	2:C:401:HEM:C2C	2.53	0.44
1:A:62:THR:HA	1:A:65:PHE:O	2.18	0.44
1:C:38:VAL:HG21	1:C:294:VAL:O	2.17	0.44
1:C:62:THR:HA	1:C:65:PHE:O	2.18	0.44
1:C:249:ALA:HB2	1:C:385:LEU:HD11	2.00	0.44
1:A:281:VAL:CG1	1:A:309:ILE:HD11	2.48	0.43
1:B:240:VAL:O	1:B:244:LEU:HG	2.18	0.43
1:A:137:ARG:HA	1:A:137:ARG:HD2	1.83	0.43
1:A:287:VAL:HG12	1:A:304:VAL:HG22	2.01	0.43
1:B:62:THR:HA	1:B:65:PHE:O	2.18	0.43
1:A:99:VAL:HG22	1:A:345:LEU:HD12	1.99	0.43
1:B:121:HIS:CE1	1:B:141:PRO:HB2	2.54	0.43
1:C:350:ALA:HB1	2:C:401:HEM:HMC3	2.01	0.43
1:B:242:ARG:NH1	1:B:384:GLY:HA3	2.33	0.42
1:A:271:VAL:HG13	1:A:354:LEU:HD23	2.00	0.42
1:B:283:ALA:HB1	1:B:306:VAL:CG1	2.50	0.42
1:C:52:TYR:CD1	1:C:318:VAL:HG21	2.55	0.42
1:A:331:ARG:CZ	1:A:331:ARG:HB2	2.48	0.41
1:B:69:PHE:CZ	1:B:287:VAL:HG13	2.56	0.41
1:B:97:LEU:C	1:B:97:LEU:HD23	2.45	0.41
1:B:121:HIS:NE2	1:B:145:ARG:HD3	2.36	0.41
1:C:377:GLU:HG3	1:C:378:PRO:HD2	2.02	0.41
1:A:199:LEU:HD21	1:A:229:LEU:CD1	2.51	0.41
1:B:264:ARG:HD2	1:B:355:ARG:NH1	2.36	0.41
1:C:38:VAL:HG12	1:C:47:TRP:CE3	2.56	0.41
1:A:352:LEU:HD23	1:A:352:LEU:O	2.20	0.41
1:B:264:ARG:HD2	1:B:268[A]:GLU:OE2	2.22	0.40
1:C:252:VAL:HG11	1:C:390:VAL:HG11	2.02	0.40
1:B:239:SER:HB3	2:B:401:HEM:C2C	2.56	0.40
1:B:303:ASP:CG	3:B:404:BGC:HA	2.14	0.40
1:C:148:THR:HG21	1:C:155:PRO:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	377/420 (90%)	372 (99%)	5 (1%)	0	100	100
1	B	386/420 (92%)	381 (99%)	5 (1%)	0	100	100
1	C	377/420 (90%)	371 (98%)	6 (2%)	0	100	100
All	All	1140/1260 (90%)	1124 (99%)	16 (1%)	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	293/324 (90%)	291 (99%)	2 (1%)	76	82
1	B	300/324 (93%)	293 (98%)	7 (2%)	44	49
1	C	295/324 (91%)	291 (99%)	4 (1%)	59	66
All	All	888/972 (91%)	875 (98%)	13 (2%)	59	64

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	382	LEU

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Mol	Chain	Res	Type
1	B	14	TYR
1	B	56	ARG
1	B	111	ARG
1	B	268[A]	GLU
1	B	268[B]	GLU
1	B	355	ARG
1	B	367	ARG
1	C	46	SER
1	C	132	VAL
1	C	204	GLU
1	C	382	LEU

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	292	GLN
1	C	41	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are 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	BGC	A	402	-	12,12,12	1.09	1 (8%)	17,17,17	3.73	6 (35%)
3	BGC	B	404	-	12,12,12	1.09	1 (8%)	17,17,17	3.36	5 (29%)
3	BGC	C	402	-	12,12,12	1.39	2 (16%)	17,17,17	2.80	5 (29%)
2	HEM	A	401	1,6	50,50,50	1.50	8 (16%)	67,82,82	1.20	7 (10%)
2	HEM	B	401	1	50,50,50	1.51	8 (16%)	67,82,82	1.42	12 (17%)
5	SCN	B	403	-	1,2,2	0.99	0	0,1,1	-	-
2	HEM	C	401	1	50,50,50	1.66	9 (18%)	67,82,82	1.34	9 (13%)
5	SCN	B	402	-	1,2,2	0.52	0	0,1,1	-	-

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	BGC	A	402	-	-	0/2/22/22	0/1/1/1
3	BGC	B	404	-	-	1/2/22/22	0/1/1/1
3	BGC	C	402	-	-	2/2/22/22	0/1/1/1
2	HEM	A	401	1,6	-	2/14/54/54	-
2	HEM	B	401	1	-	2/14/54/54	-
2	HEM	C	401	1	-	2/14/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	FE-NB	6.44	2.14	1.94
2	B	401	HEM	FE-NB	5.04	2.10	1.94
2	B	401	HEM	FE-NC	4.29	2.09	1.95
2	C	401	HEM	FE-NA	3.76	2.07	1.95
2	A	401	HEM	FE-ND	3.71	2.06	1.94
2	A	401	HEM	FE-NC	3.66	2.07	1.95
2	A	401	HEM	CAC-C3C	3.37	1.56	1.47
2	A	401	HEM	CAB-C3B	3.31	1.56	1.47
3	B	404	BGC	O5-C1	3.27	1.50	1.42
2	C	401	HEM	FE-ND	3.22	2.04	1.94
2	A	401	HEM	FE-NB	3.15	2.04	1.94
2	B	401	HEM	FE-NA	3.14	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	CAC-C3C	3.07	1.55	1.47
3	A	402	BGC	O1-C1	2.89	1.48	1.39
2	C	401	HEM	CAB-C3B	2.88	1.55	1.47
2	A	401	HEM	FE-NA	2.83	2.04	1.95
3	C	402	BGC	O1-C1	2.79	1.48	1.39
3	C	402	BGC	O5-C1	2.54	1.49	1.42
2	B	401	HEM	CMC-C2C	2.51	1.55	1.50
2	A	401	HEM	CMC-C2C	2.48	1.55	1.50
2	C	401	HEM	C4D-ND	-2.38	1.36	1.40
2	B	401	HEM	CMA-C3A	2.36	1.55	1.50
2	B	401	HEM	CAC-C3C	2.28	1.53	1.47
2	B	401	HEM	CAB-C3B	2.15	1.53	1.47
2	C	401	HEM	CMC-C2C	2.12	1.55	1.50
2	B	401	HEM	FE-ND	2.06	2.01	1.94
2	C	401	HEM	C1B-NB	-2.06	1.36	1.40
2	C	401	HEM	CMA-C3A	2.05	1.55	1.50
2	A	401	HEM	CMA-C3A	2.04	1.54	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	BGC	O1-C1-C2	10.35	139.02	108.98
3	A	402	BGC	O5-C1-C2	9.37	126.77	110.30
3	A	402	BGC	C1-O5-C5	-8.57	97.08	113.65
3	C	402	BGC	C1-O5-C5	6.68	126.57	113.65
3	A	402	BGC	O2-C2-C1	-6.38	94.51	109.25
3	C	402	BGC	C1-C2-C3	-4.75	100.66	110.36
3	B	404	BGC	C1-C2-C3	-4.62	100.92	110.36
3	B	404	BGC	C1-O5-C5	4.48	122.32	113.65
3	B	404	BGC	O2-C2-C1	-4.38	99.13	109.25
3	C	402	BGC	C4-C3-C2	-4.37	103.16	110.83
3	B	404	BGC	C4-C3-C2	-4.20	103.45	110.83
3	C	402	BGC	O1-C1-C2	4.19	121.15	108.98
3	C	402	BGC	O2-C2-C1	-3.53	101.10	109.25
2	C	401	HEM	C1B-NB-C4B	3.38	109.21	105.21
2	C	401	HEM	C4D-ND-C1D	3.10	108.88	105.21
2	A	401	HEM	C3B-C2B-C1B	3.06	108.71	106.41
2	B	401	HEM	C4D-ND-C1D	3.02	108.79	105.21
2	B	401	HEM	C2A-C1A-NA	-3.00	106.83	110.15
2	A	401	HEM	C2A-C1A-NA	-2.96	106.87	110.15
2	B	401	HEM	C1B-NB-C4B	2.90	108.64	105.21
3	A	402	BGC	O5-C5-C6	2.87	113.55	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	BGC	C4-C3-C2	2.86	115.85	110.83
2	B	401	HEM	C2B-C1B-NB	-2.82	106.60	109.84
2	C	401	HEM	C3B-C2B-C1B	2.71	108.45	106.41
2	B	401	HEM	C3B-C2B-C1B	2.63	108.38	106.41
2	A	401	HEM	CAD-CBD-CGD	-2.61	106.75	113.67
2	C	401	HEM	C2D-C1D-ND	-2.57	106.93	109.90
2	B	401	HEM	C4C-C3C-C2C	2.57	109.04	106.81
2	B	401	HEM	C2D-C1D-ND	-2.57	106.94	109.90
2	C	401	HEM	CHD-C4C-NC	2.50	127.18	124.45
2	C	401	HEM	C2B-C1B-NB	-2.49	106.98	109.84
2	B	401	HEM	CHC-C4B-NB	2.48	127.10	124.42
2	A	401	HEM	C4C-C3C-C2C	2.44	108.93	106.81
2	A	401	HEM	CHC-C4B-NB	2.40	127.01	124.42
2	B	401	HEM	CHD-C1D-ND	2.34	126.94	124.42
2	B	401	HEM	C3B-C4B-NB	-2.31	107.81	109.47
2	C	401	HEM	CAD-CBD-CGD	-2.28	107.61	113.67
3	A	402	BGC	O6-C6-C5	-2.21	103.81	111.33
2	B	401	HEM	C3D-C4D-ND	-2.20	107.75	110.17
2	A	401	HEM	C4A-NA-C1A	2.15	109.32	105.82
2	A	401	HEM	C3A-C4A-NA	-2.14	106.71	110.14
2	C	401	HEM	C3D-C4D-ND	-2.10	107.87	110.17
2	B	401	HEM	C1D-C2D-C3D	2.04	109.13	106.98
2	C	401	HEM	CHD-C1D-ND	2.01	126.58	124.42

There are no chirality outliers.

All (9) torsion outliers are listed below:

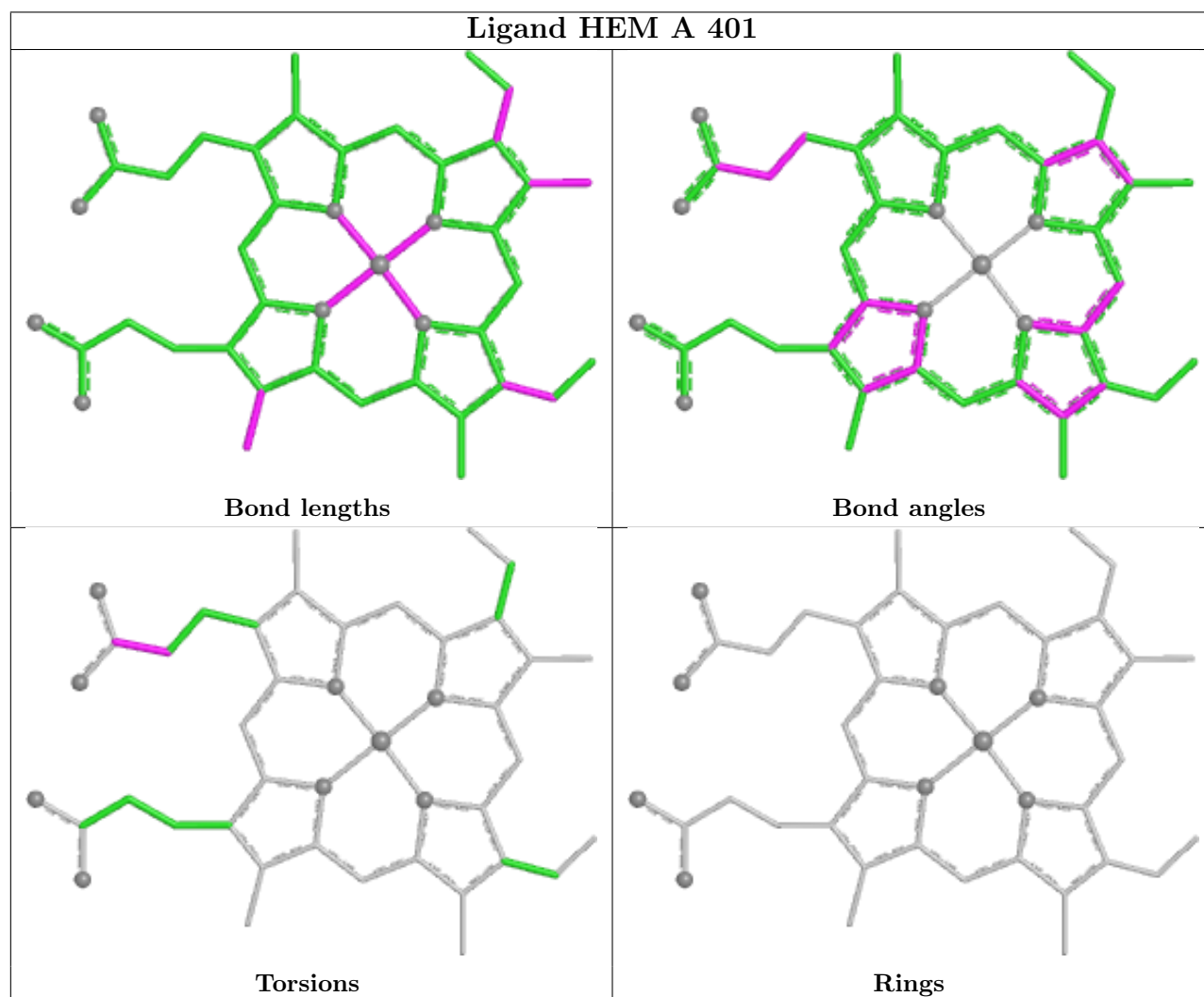
Mol	Chain	Res	Type	Atoms
3	C	402	BGC	O5-C5-C6-O6
3	C	402	BGC	C4-C5-C6-O6
2	A	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	CAD-CBD-CGD-O2D
3	B	404	BGC	O5-C5-C6-O6
2	C	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	CAD-CBD-CGD-O1D

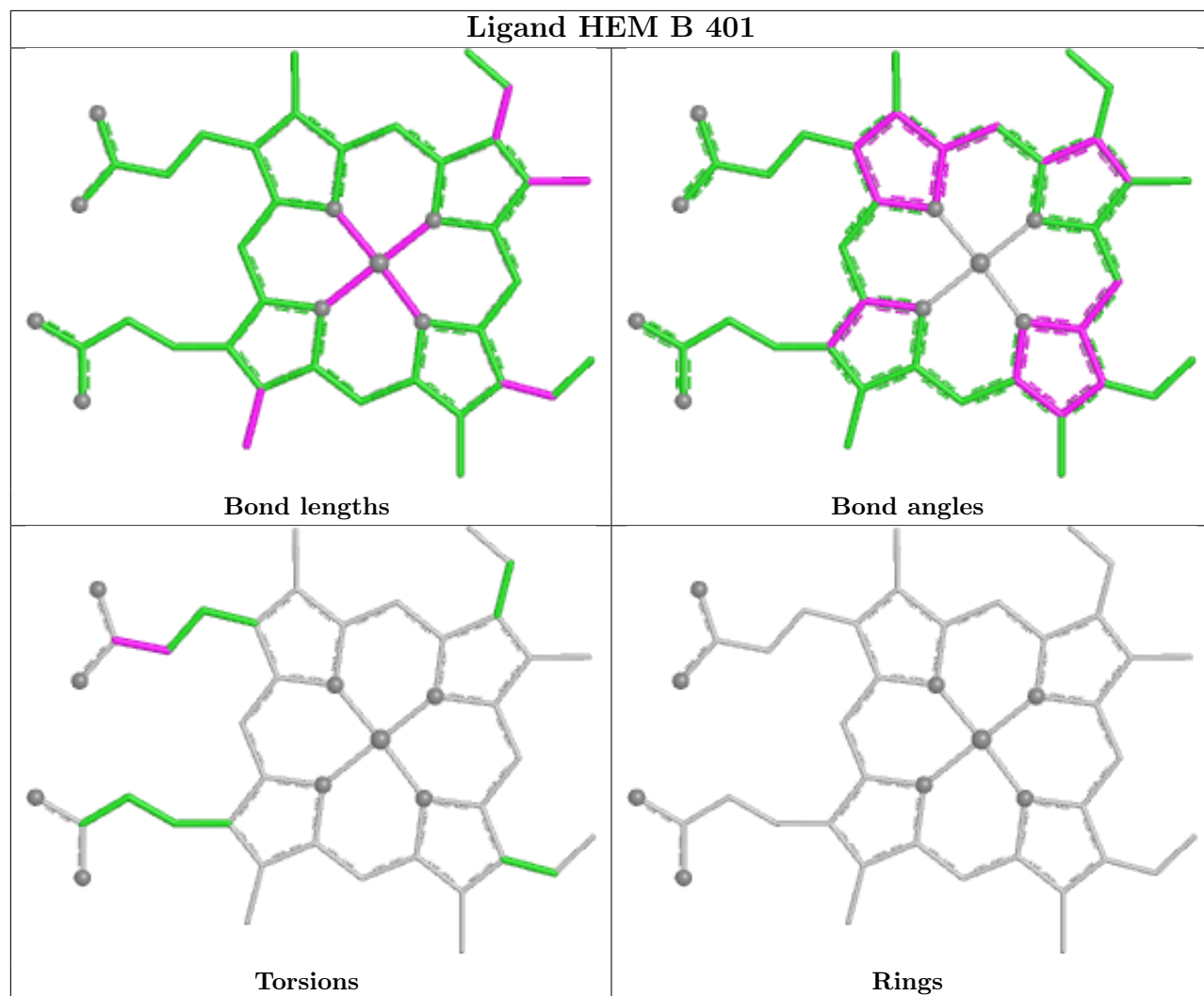
There are no ring outliers.

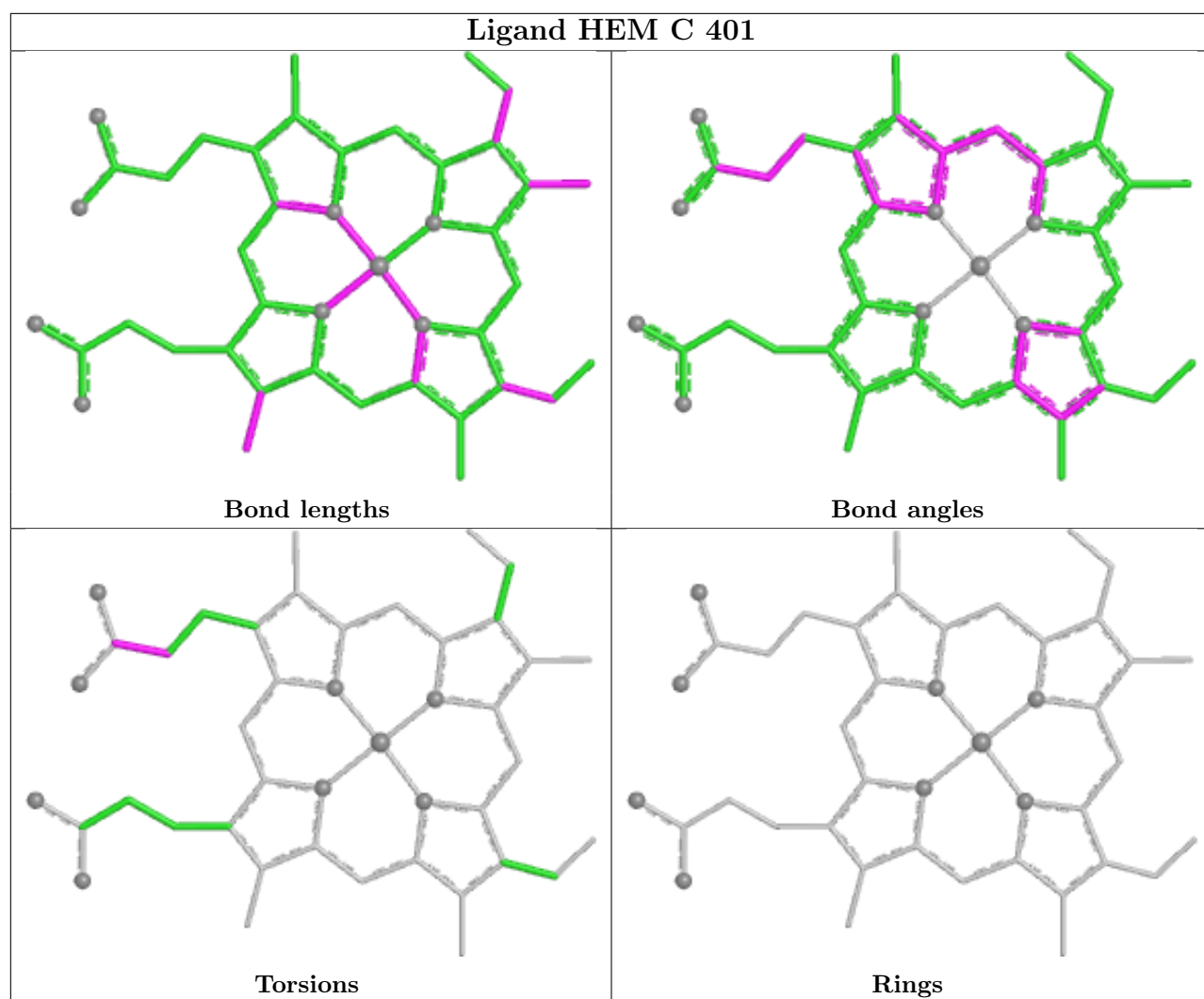
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	BGC	2	0
2	A	401	HEM	2	0
2	B	401	HEM	5	0
2	C	401	HEM	6	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	377/420 (89%)	0.57	14 (3%)	45 49	22, 49, 79, 98	1 (0%)
1	B	382/420 (90%)	0.52	24 (6%)	26 29	19, 44, 77, 113	3 (0%)
1	C	378/420 (90%)	0.82	33 (8%)	16 17	21, 58, 94, 119	1 (0%)
All	All	1137/1260 (90%)	0.64	71 (6%)	26 30	19, 50, 87, 119	5 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	PRO	4.9
1	A	394	ALA	4.4
1	A	215	ALA	4.4
1	B	13	ILE	4.1
1	A	125	LEU	4.0
1	C	125	LEU	4.0
1	C	132	VAL	3.6
1	C	294	VAL	3.4
1	A	137	ARG	3.2
1	B	392	VAL	3.2
1	B	366	LEU	3.1
1	C	262	ALA	3.1
1	C	44	LEU	3.1
1	B	14	TYR	3.0
1	C	43	PHE	3.0
1	A	38	VAL	3.0
1	B	102	LEU	3.0
1	C	392	VAL	3.0
1	B	264	ARG	3.0
1	B	345	LEU	3.0
1	C	390	VAL	3.0
1	B	44	LEU	2.9
1	B	107	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	384	GLY	2.9
1	A	220	VAL	2.9
1	B	106	PRO	2.9
1	C	299	VAL	2.8
1	A	205	ARG	2.8
1	B	393	ARG	2.8
1	B	127	GLY	2.8
1	C	298	LEU	2.7
1	B	126	SER	2.7
1	C	97	LEU	2.7
1	C	40[A]	TRP	2.7
1	B	128	GLN	2.6
1	B	125	LEU	2.6
1	C	263	THR	2.6
1	B	261	PRO	2.6
1	C	258	LEU	2.6
1	C	248	LEU	2.5
1	A	305	LEU	2.5
1	B	41	HIS	2.5
1	C	264	ARG	2.5
1	B	268[A]	GLU	2.4
1	C	164	TRP	2.4
1	C	122	LEU	2.4
1	A	260	GLY	2.4
1	B	130	GLY	2.4
1	C	128	GLN	2.4
1	C	48	VAL	2.3
1	C	374	ALA	2.3
1	A	126	SER	2.3
1	C	47	TRP	2.3
1	B	300	ARG	2.2
1	C	393	ARG	2.2
1	A	72	ILE	2.2
1	C	129	PRO	2.2
1	B	367	ARG	2.2
1	C	76	ILE	2.2
1	B	296	ALA	2.2
1	C	130	GLY	2.1
1	A	258	LEU	2.1
1	C	358	LEU	2.1
1	C	123	ALA	2.1
1	C	174	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	363	ALA	2.1
1	C	293	PRO	2.1
1	A	299	VAL	2.1
1	C	81	LEU	2.0
1	A	76	ILE	2.0
1	B	203	ASP	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](#)

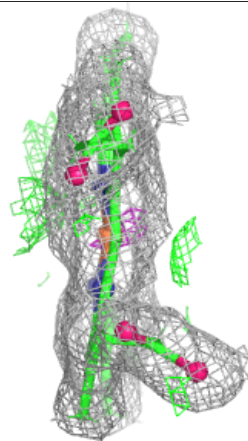
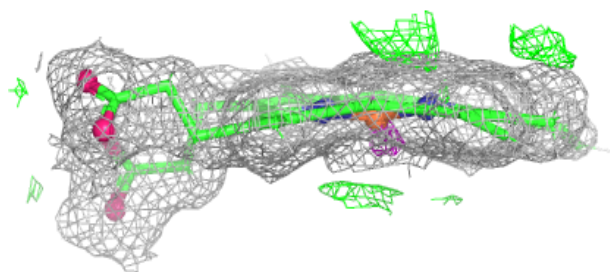
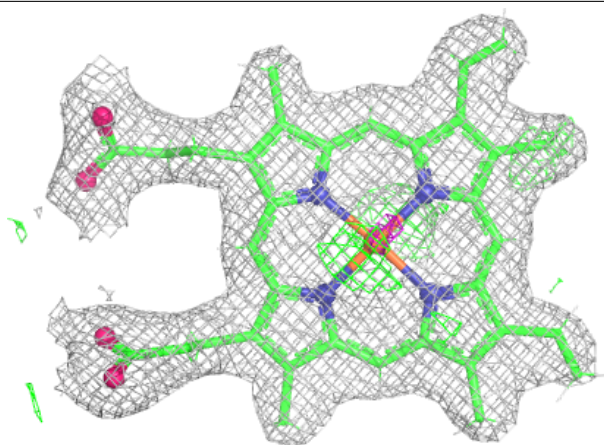
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	A	403	1/1	0.57	0.18	103,103,103,103	0
4	K	C	403	1/1	0.73	0.21	78,78,78,78	0
3	BGC	C	402	12/12	0.78	0.20	57,88,119,127	0
3	BGC	B	404	12/12	0.81	0.22	69,113,136,143	0
3	BGC	A	402	12/12	0.83	0.17	50,99,129,139	0
5	SCN	B	402	3/3	0.86	0.18	38,38,47,55	0
5	SCN	B	403	3/3	0.89	0.14	39,39,47,52	0
4	K	B	405	1/1	0.93	0.11	58,58,58,58	0
2	HEM	C	401	43/43	0.97	0.08	26,36,45,56	0
2	HEM	A	401	43/43	0.97	0.08	22,34,42,51	0
2	HEM	B	401	43/43	0.97	0.07	23,29,45,47	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.

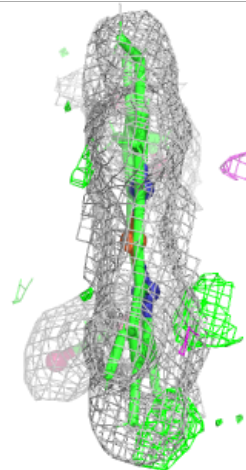
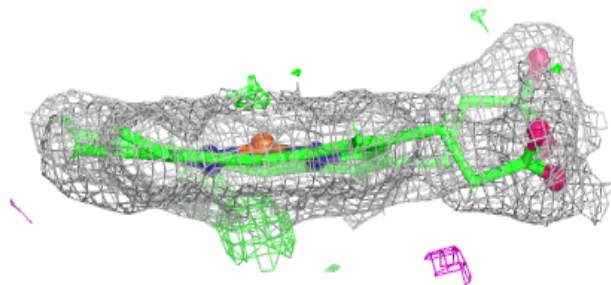
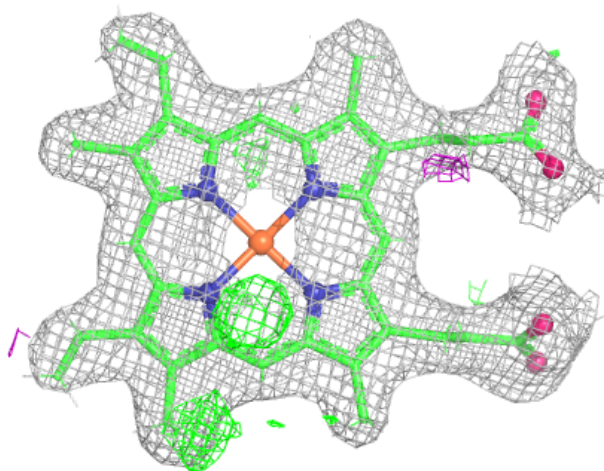
Electron density around HEM C 401:

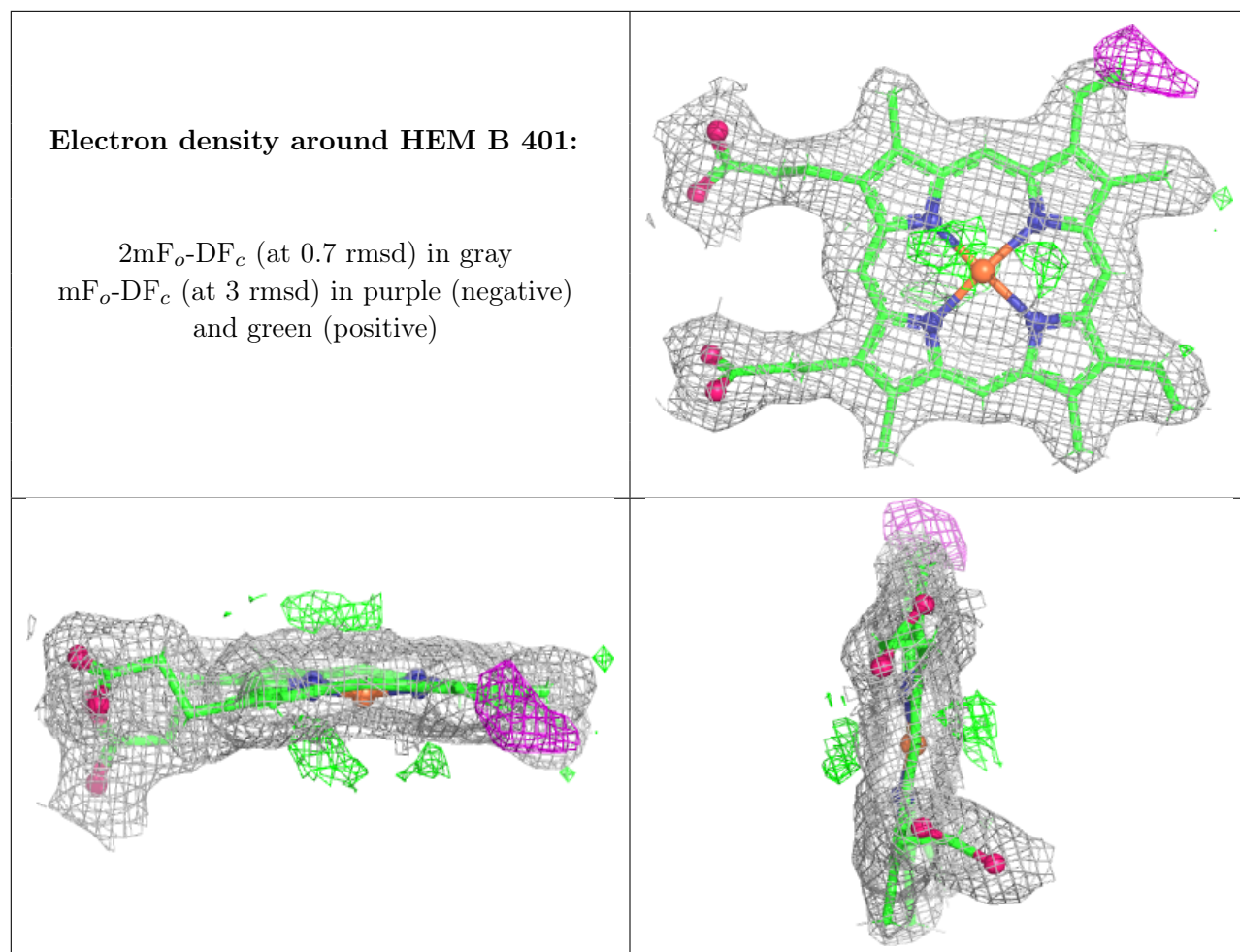
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 401:

$2mF_o-DF_c$ (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.