



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:31 AM EDT

PDB ID : 3BNJ / pdb_00003bnj
Title : W. succinogenes NrfA Y218F Sulfite Complex
Authors : Lukat, P.; Einsle, O.
Deposited on : 2007-12-14
Resolution : 1.30 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

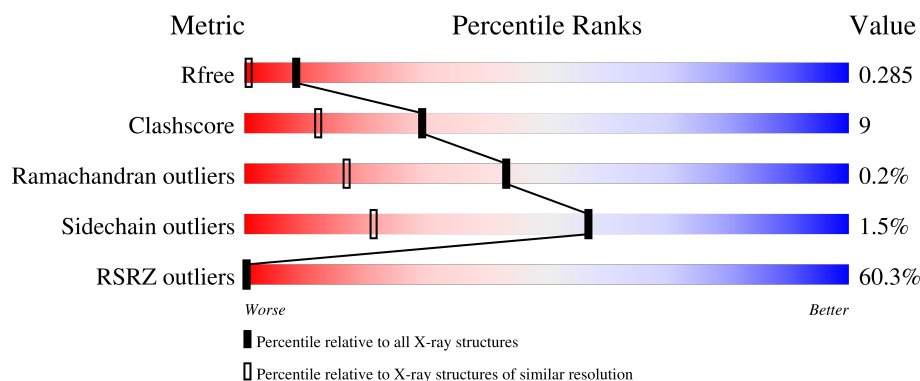
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	485	59% 85% 11% ..

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4756 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 c-552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	14	6	0
			3802	2410	651	720	21			

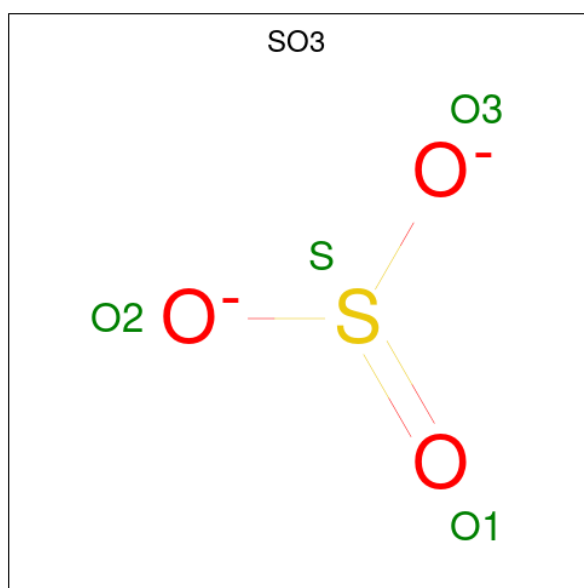
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	PHE	TYR	engineered mutation	UNP Q9S1E5

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			4	3	1		

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

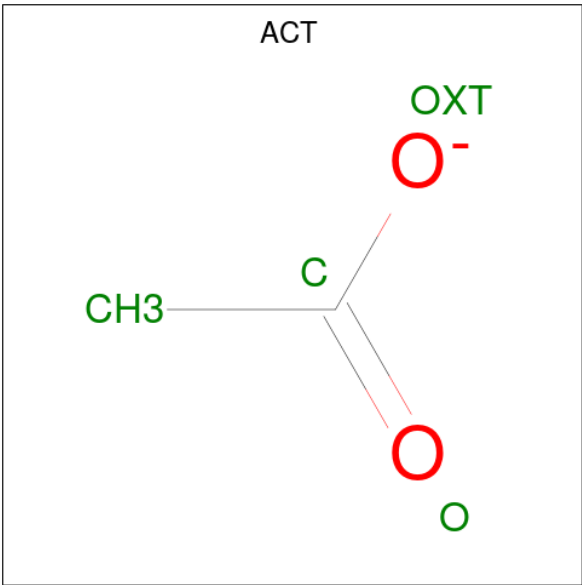


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is YTTRIUM ION (CCD ID: Y1) (formula: Y).

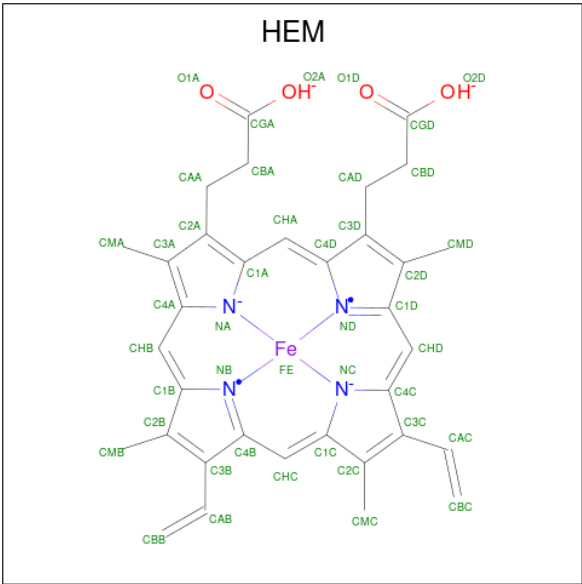
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Y	0	0
			3	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

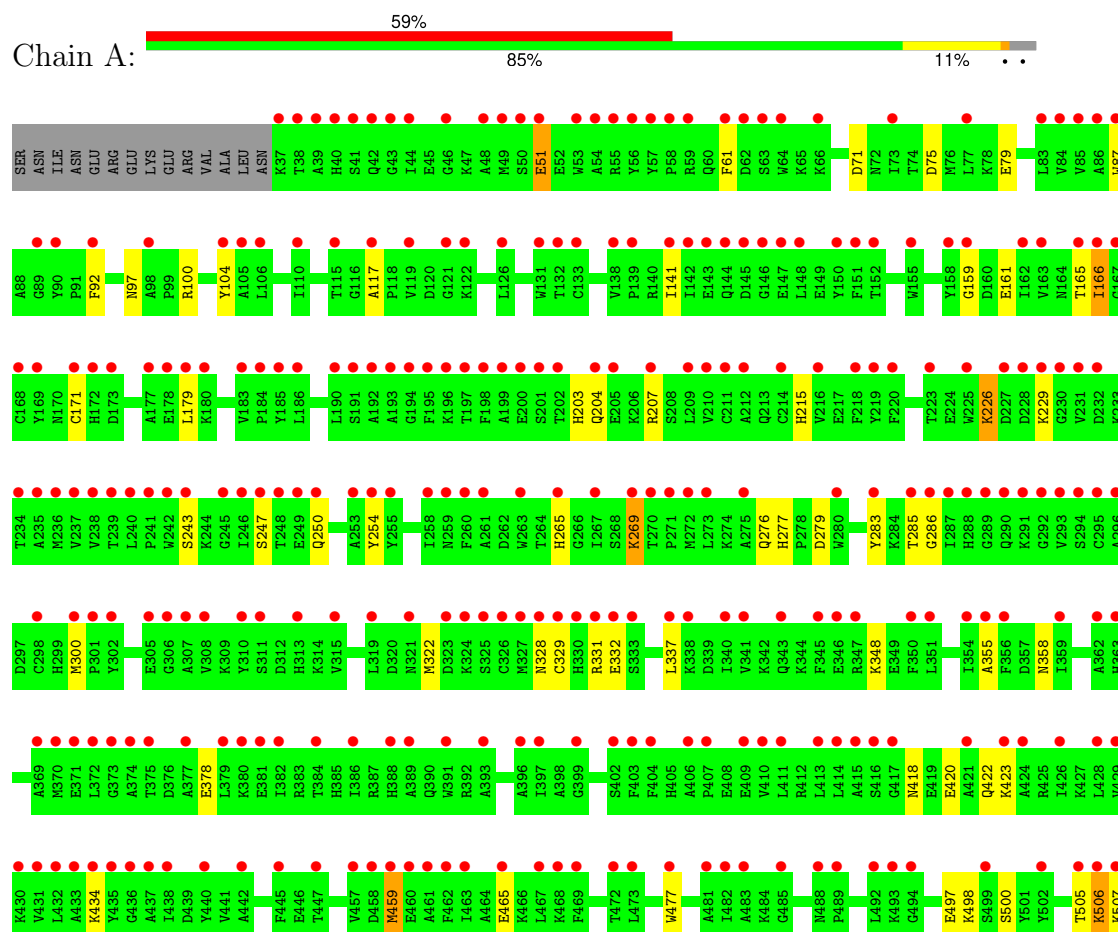
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	714	Total	O	0	0
			714	714		

3 Residue-property plots

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 c-552



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.40Å 119.40Å 184.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.39 – 1.30 40.39 – 1.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.39-1.30) 98.7 (40.39-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.181 , 0.208 0.270 , 0.285	Depositor DCC
R_{free} test set	8135 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4756	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Y1, CA, SO3, ACT, HEM, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/3911 (0.0%)	0.78	2/5265 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	LYS	CG-CD	-10.77	1.20	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	LYS	CB-CG-CD	6.13	125.40	111.30
1	A	226	LYS	N-CA-CB	-6.05	100.33	110.80

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	3802	0	3732	66	0
2	A	1	0	0	0	0
3	A	4	0	0	0	0
4	A	5	0	0	1	0
5	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	12	0	9	0	0
7	A	215	0	150	16	0
8	A	714	0	0	8	1
All	All	4756	0	3891	68	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 9.

All (68) 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:A:171:CYS:SG	7:A:514:HEM:CAC	2.04	1.43
1:A:171:CYS:SG	7:A:514:HEM:HAC	1.69	1.22
1:A:329:CYS:SG	7:A:517:HEM:CAC	2.38	1.11
1:A:100:ARG:HH12	1:A:507:LYS:HD3	1.26	1.00
1:A:358:ASN:HD22	1:A:418:ASN:HD21	1.02	0.98
1:A:285:THR:HG21	8:A:907:HOH:O	1.66	0.95
1:A:497:GLU:OE1	1:A:507:LYS:HA	1.72	0.89
1:A:71:ASP:OD2	1:A:507:LYS:HB3	1.79	0.81
1:A:100:ARG:HH22	1:A:507:LYS:HZ3	1.29	0.80
1:A:100:ARG:NH1	1:A:507:LYS:HD3	2.01	0.75
1:A:117:ALA:CB	1:A:465:GLU:HG2	2.16	0.75
1:A:171:CYS:SG	7:A:514:HEM:C3C	2.80	0.75
1:A:497:GLU:H	1:A:507:LYS:HE3	1.54	0.72
1:A:329:CYS:HG	7:A:517:HEM:CAC	2.00	0.72
1:A:100:ARG:HH22	1:A:507:LYS:NZ	1.87	0.72
1:A:506:LYS:HE3	1:A:506:LYS:HA	1.72	0.72
1:A:117:ALA:HB3	1:A:465:GLU:HG2	1.71	0.72
1:A:286:GLY:HA2	4:A:509:SO4:O3	1.90	0.71
1:A:497:GLU:OE1	1:A:507:LYS:CA	2.39	0.69
1:A:329:CYS:SG	7:A:517:HEM:C3C	2.88	0.66
1:A:171:CYS:SG	7:A:514:HEM:CBC	2.79	0.66
7:A:514:HEM:HBC1	7:A:515:HEM:HHC	1.77	0.66
1:A:207:ARG:NH1	7:A:514:HEM:O1D	2.30	0.65
1:A:329:CYS:SG	7:A:517:HEM:HAC	2.35	0.64
1:A:497:GLU:OE1	1:A:507:LYS:N	2.31	0.64
1:A:285:THR:O	8:A:838:HOH:O	2.14	0.63
1:A:331:ARG:O	1:A:332:GLU:HG3	1.98	0.63
1:A:358:ASN:HD22	1:A:418:ASN:ND2	1.86	0.61
1:A:420:GLU:OE2	8:A:1124:HOH:O	2.16	0.61
7:A:517:HEM:HMC1	7:A:517:HEM:HBC2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:HH12	1:A:507:LYS:CD	2.09	0.59
1:A:79[B]:GLU:HG2	8:A:957:HOH:O	2.03	0.57
1:A:247:SER:H	1:A:250:GLN:HE21	1.52	0.57
1:A:422:GLN:HE21	1:A:422:GLN:HA	1.71	0.55
1:A:265:HIS:O	1:A:269:LYS:HD2	2.07	0.55
1:A:243:SER:HG	1:A:254:TYR:HD2	1.51	0.54
1:A:75:ASP:HA	1:A:97:ASN:HD22	1.73	0.54
1:A:506:LYS:HA	1:A:506:LYS:CE	2.38	0.54
1:A:322:MET:HE1	1:A:337:LEU:HB3	1.91	0.51
1:A:328:ASN:HB2	8:A:994:HOH:O	2.10	0.51
1:A:329:CYS:SG	7:A:517:HEM:CBC	2.96	0.51
1:A:104:TYR:CE1	1:A:507:LYS:HE2	2.47	0.49
1:A:505:THR:O	1:A:505:THR:HG22	2.13	0.48
1:A:61:PHE:HA	7:A:514:HEM:HBB2	1.95	0.47
1:A:300:MET:HE1	7:A:514:HEM:C1D	2.50	0.47
1:A:358:ASN:ND2	1:A:418:ASN:HD21	1.87	0.47
1:A:498:LYS:H	1:A:507:LYS:NZ	2.11	0.47
1:A:276:GLN:O	1:A:277:HIS:C	2.56	0.47
1:A:459:MET:HE3	1:A:459:MET:HB3	1.78	0.47
1:A:203:HIS:HE2	7:A:514:HEM:CGD	2.28	0.47
1:A:204:GLN:HE21	1:A:204:GLN:HA	1.80	0.46
1:A:159:GLY:HA3	1:A:477:TRP:CE2	2.51	0.46
1:A:247:SER:H	1:A:250:GLN:NE2	2.13	0.46
1:A:378:GLU:OE2	1:A:434:LYS:NZ	2.37	0.44
1:A:348:LYS:HD2	1:A:348:LYS:C	2.43	0.44
1:A:423:LYS:NZ	8:A:1036:HOH:O	2.51	0.44
1:A:165:THR:O	1:A:166:ILE:C	2.62	0.43
1:A:215:HIS:HB3	1:A:279:ASP:HB2	2.00	0.43
1:A:97:ASN:HD21	1:A:500:SER:HB3	1.81	0.43
1:A:179:LEU:HD11	7:A:514:HEM:HBD1	2.00	0.43
1:A:51:GLU:HG2	8:A:943:HOH:O	2.19	0.43
1:A:141[B]:ILE:HD11	1:A:161:GLU:HB3	2.01	0.43
1:A:51:GLU:CG	8:A:943:HOH:O	2.67	0.42
1:A:159:GLY:HA3	1:A:477:TRP:CD2	2.55	0.41
1:A:87:TRP:CE3	1:A:92:PHE:HB3	2.56	0.41
1:A:331:ARG:O	1:A:332:GLU:CG	2.68	0.41
1:A:355:ALA:HA	1:A:418:ASN:HD22	1.86	0.41
1:A:331:ARG:C	1:A:332:GLU:HG3	2.46	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)
8:A:646:HOH:O	8:A:1010:HOH:O[10_565]	2.15	0.05

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	475/485 (98%)	466 (98%)	8 (2%)	1 (0%)	43 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	ILE

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	403/410 (98%)	397 (98%)	6 (2%)	57 21

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	226	LYS
1	A	269	LYS
1	A	283	TYR
1	A	459	MET

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Mol	Chain	Res	Type
1	A	506	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	144	GLN
1	A	204	GLN
1	A	250	GLN
1	A	352	GLN
1	A	418	ASN
1	A	422	GLN
1	A	480	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
4	SO4	A	509	-	4,4,4	0.27	0	6,6,6	0.41	0
7	HEM	A	515	5,1	50,50,50	1.40	5 (10%)	67,82,82	1.30	7 (10%)
7	HEM	A	513	3,1	50,50,50	1.41	4 (8%)	67,82,82	1.10	4 (5%)
7	HEM	A	517	5,1	50,50,50	1.67	7 (14%)	67,82,82	1.26	7 (10%)
7	HEM	A	516	5,1	50,50,50	1.56	7 (14%)	67,82,82	1.23	6 (8%)
7	HEM	A	514	1	50,50,50	1.51	6 (12%)	67,82,82	1.16	4 (5%)
6	ACT	A	4	-	3,3,3	0.81	0	3,3,3	1.26	0
6	ACT	A	512	-	3,3,3	0.86	0	3,3,3	1.20	0
3	SO3	A	508	7	1,3,3	0.48	0	0,3,3	-	-
6	ACT	A	511	-	3,3,3	0.82	0	3,3,3	1.33	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
7	HEM	A	515	5,1	-	4/14/54/54	-
7	HEM	A	513	3,1	-	4/14/54/54	-
7	HEM	A	516	5,1	-	6/14/54/54	-
7	HEM	A	517	5,1	-	7/14/54/54	-
7	HEM	A	514	1	-	6/14/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	517	HEM	C3D-C2D	7.58	1.53	1.36
7	A	516	HEM	C3D-C2D	6.99	1.51	1.36
7	A	514	HEM	C3D-C2D	6.35	1.50	1.36
7	A	513	HEM	C3D-C2D	5.65	1.48	1.36
7	A	515	HEM	C3D-C2D	5.55	1.48	1.36
7	A	517	HEM	CAC-C3C	3.38	1.56	1.47
7	A	516	HEM	CAC-C3C	2.90	1.55	1.47
7	A	513	HEM	CAC-C3C	2.88	1.55	1.47
7	A	517	HEM	FE-ND	2.82	2.03	1.94
7	A	517	HEM	CAB-C3B	2.70	1.54	1.47
7	A	514	HEM	CAC-C3C	2.69	1.54	1.47
7	A	515	HEM	CAC-C3C	2.66	1.54	1.47
7	A	514	HEM	CAB-C3B	2.55	1.54	1.47
7	A	515	HEM	CAB-C3B	2.51	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	517	HEM	FE-NA	2.46	2.03	1.95
7	A	515	HEM	FE-NB	2.29	2.02	1.94
7	A	514	HEM	FE-NC	2.29	2.02	1.95
7	A	514	HEM	CMB-C2B	2.26	1.55	1.50
7	A	513	HEM	CAB-C3B	2.15	1.53	1.47
7	A	515	HEM	CMB-C2B	2.13	1.55	1.50
7	A	513	HEM	FE-ND	2.08	2.01	1.94
7	A	516	HEM	FE-NA	2.07	2.02	1.95
7	A	516	HEM	CMC-C2C	2.05	1.55	1.50
7	A	514	HEM	CMC-C2C	2.04	1.54	1.50
7	A	517	HEM	CMC-C2C	2.03	1.54	1.50
7	A	516	HEM	C2A-C3A	-2.03	1.33	1.38
7	A	517	HEM	C2A-C3A	-2.02	1.33	1.38
7	A	516	HEM	CAB-C3B	2.01	1.52	1.47
7	A	516	HEM	C3C-C2C	-2.00	1.33	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	515	HEM	C4D-ND-C1D	4.47	110.50	105.21
7	A	517	HEM	C4D-ND-C1D	4.02	109.97	105.21
7	A	516	HEM	C4D-ND-C1D	3.39	109.22	105.21
7	A	513	HEM	C4D-ND-C1D	3.37	109.20	105.21
7	A	514	HEM	C4D-ND-C1D	3.34	109.16	105.21
7	A	515	HEM	C3B-C4B-NB	-3.30	107.10	109.47
7	A	515	HEM	CHD-C1D-ND	3.11	127.77	124.42
7	A	516	HEM	CBB-CAB-C3B	-2.99	112.60	127.53
7	A	515	HEM	C1B-NB-C4B	2.83	108.56	105.21
7	A	513	HEM	CAD-C3D-C4D	2.68	129.36	124.70
7	A	514	HEM	CMD-C2D-C1D	2.63	129.15	125.03
7	A	513	HEM	CBB-CAB-C3B	-2.63	114.38	127.53
7	A	517	HEM	CBA-CAA-C2A	-2.62	105.29	112.53
7	A	517	HEM	O2A-CGA-CBA	2.52	121.96	114.00
7	A	517	HEM	C1D-C2D-C3D	-2.51	104.34	106.98
7	A	517	HEM	C2A-C1A-NA	-2.45	107.43	110.15
7	A	517	HEM	O1A-CGA-CBA	-2.40	115.47	123.09
7	A	516	HEM	CHC-C4B-NB	2.35	126.95	124.42
7	A	515	HEM	CBA-CAA-C2A	-2.32	106.12	112.53
7	A	513	HEM	CHC-C4B-NB	2.17	126.76	124.42
7	A	516	HEM	C4C-C3C-C2C	2.15	108.68	106.81
7	A	514	HEM	CBD-CAD-C3D	-2.14	106.61	112.53
7	A	515	HEM	CBB-CAB-C3B	-2.14	116.84	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	514	HEM	CHA-C4D-ND	2.12	126.99	124.37
7	A	516	HEM	O2A-CGA-CBA	2.08	120.56	114.00
7	A	516	HEM	CMD-C2D-C1D	2.04	128.23	125.03
7	A	515	HEM	CAD-C3D-C4D	2.04	128.24	124.70
7	A	517	HEM	CAD-CBD-CGD	-2.03	108.28	113.67

There are no chirality outliers.

All (27) torsion outliers are listed below:

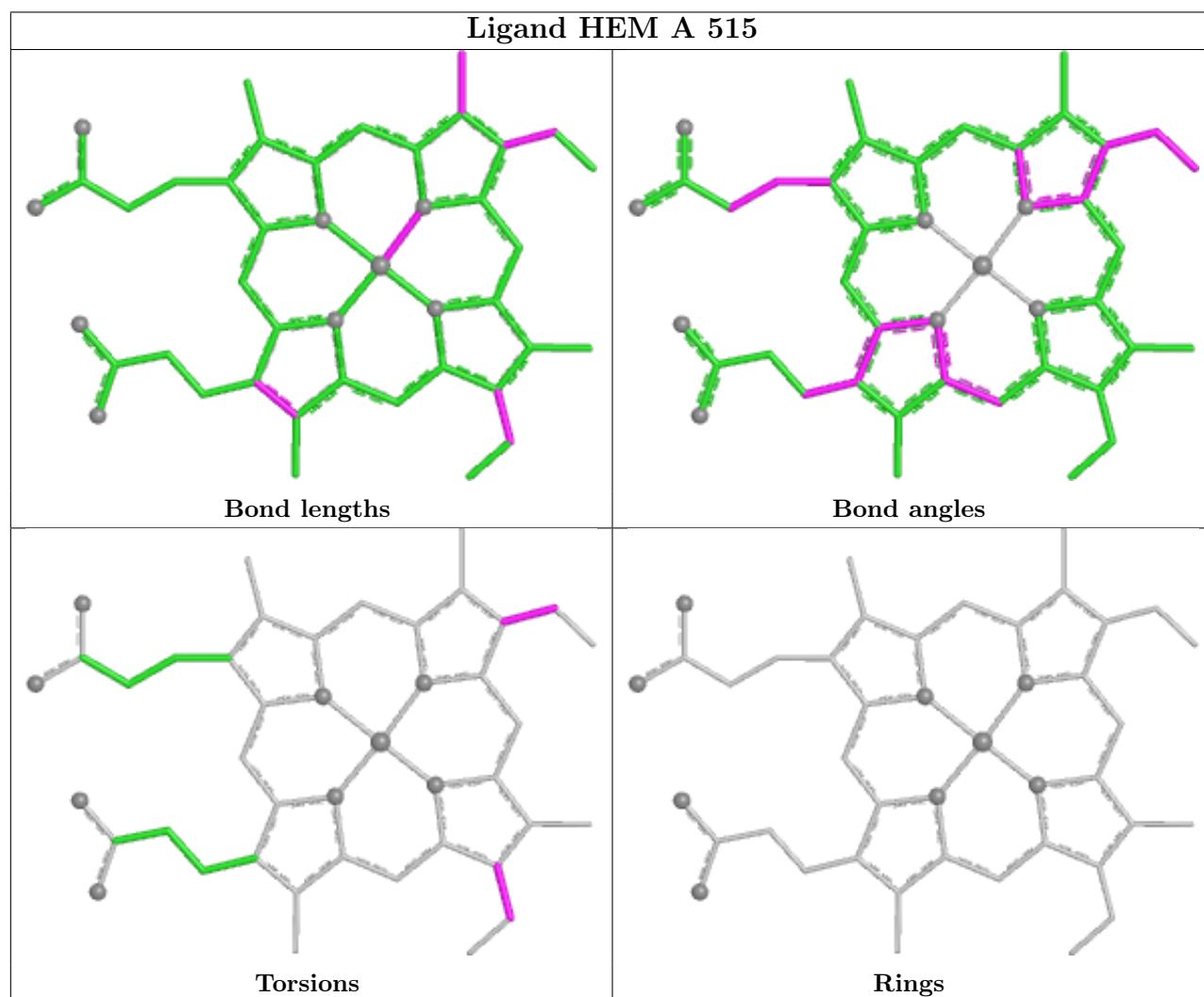
Mol	Chain	Res	Type	Atoms
7	A	513	HEM	C2B-C3B-CAB-CBB
7	A	513	HEM	C4B-C3B-CAB-CBB
7	A	517	HEM	C2A-CAA-CBA-CGA
7	A	515	HEM	C4B-C3B-CAB-CBB
7	A	514	HEM	C2B-C3B-CAB-CBB
7	A	514	HEM	C2C-C3C-CAC-CBC
7	A	515	HEM	C2B-C3B-CAB-CBB
7	A	516	HEM	C2B-C3B-CAB-CBB
7	A	517	HEM	C2B-C3B-CAB-CBB
7	A	517	HEM	C4B-C3B-CAB-CBB
7	A	514	HEM	C4B-C3B-CAB-CBB
7	A	513	HEM	CAA-CBA-CGA-O1A
7	A	513	HEM	CAA-CBA-CGA-O2A
7	A	514	HEM	CAA-CBA-CGA-O2A
7	A	517	HEM	CAA-CBA-CGA-O1A
7	A	514	HEM	CAA-CBA-CGA-O1A
7	A	517	HEM	CAA-CBA-CGA-O2A
7	A	516	HEM	CAD-CBD-CGD-O2D
7	A	517	HEM	CAD-CBD-CGD-O2D
7	A	517	HEM	CAD-CBD-CGD-O1D
7	A	514	HEM	C4C-C3C-CAC-CBC
7	A	515	HEM	C4C-C3C-CAC-CBC
7	A	516	HEM	C4B-C3B-CAB-CBB
7	A	516	HEM	C4C-C3C-CAC-CBC
7	A	516	HEM	CAD-CBD-CGD-O1D
7	A	515	HEM	C2C-C3C-CAC-CBC
7	A	516	HEM	C2C-C3C-CAC-CBC

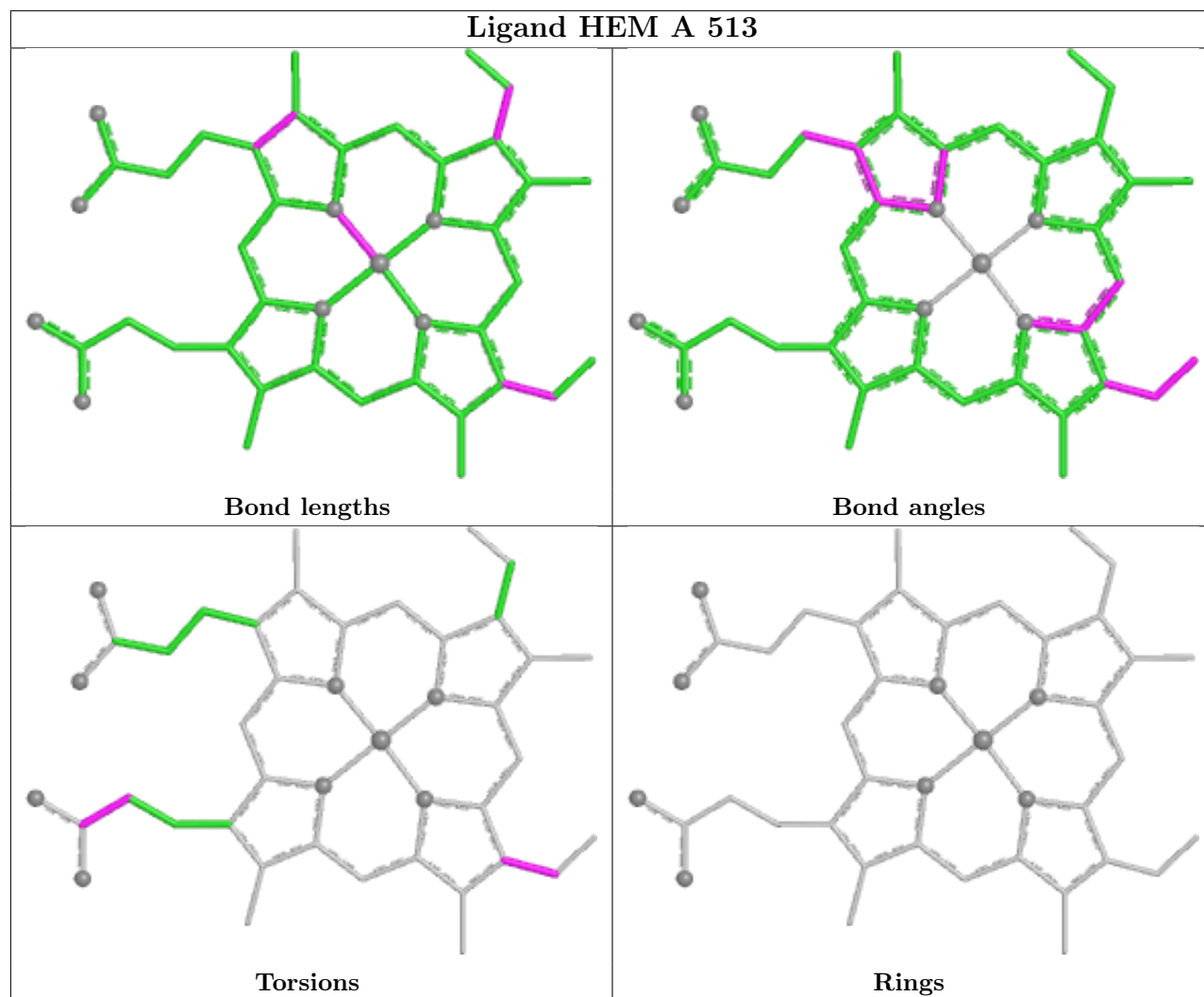
There are no ring outliers.

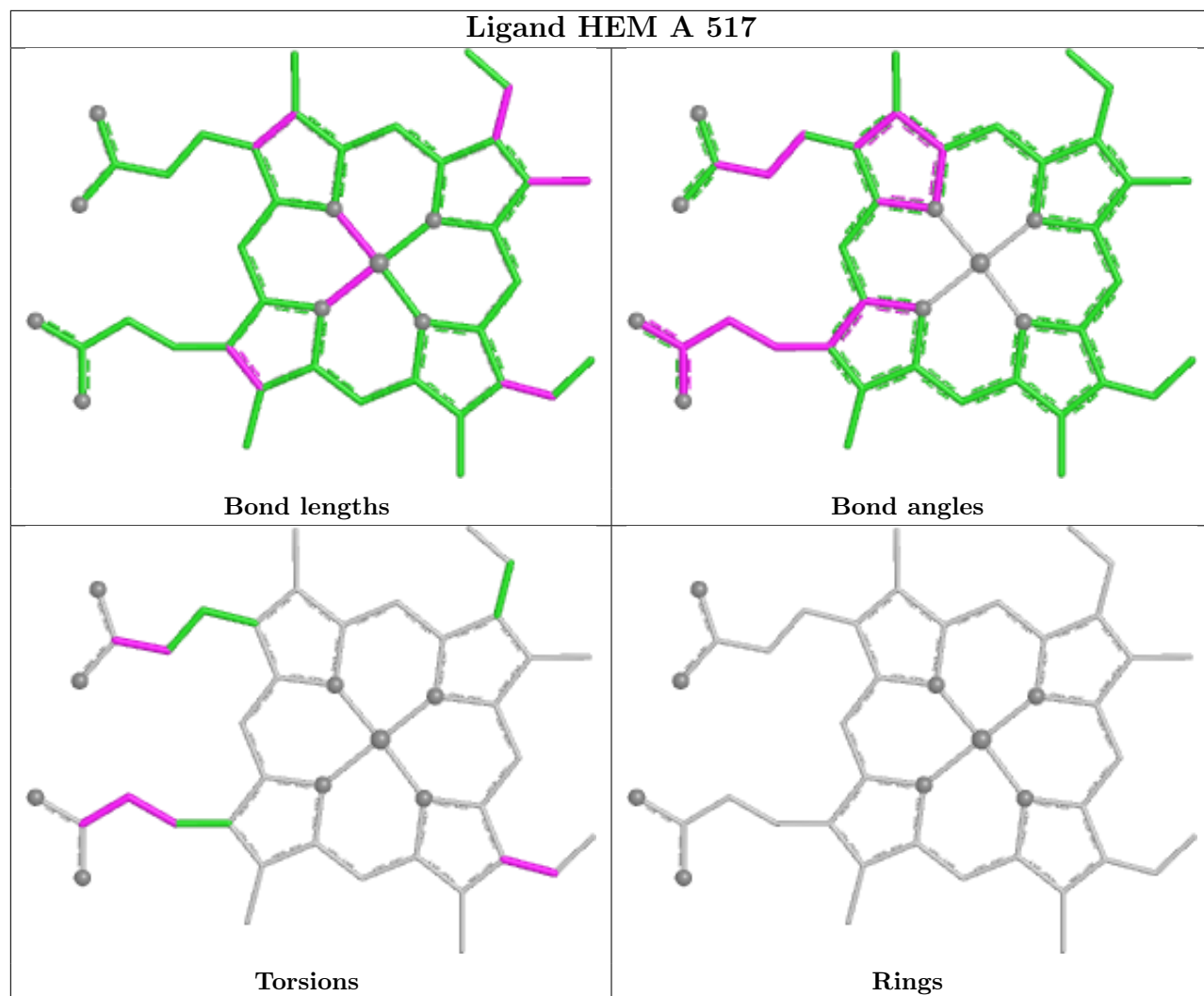
4 monomers are involved in 17 short contacts:

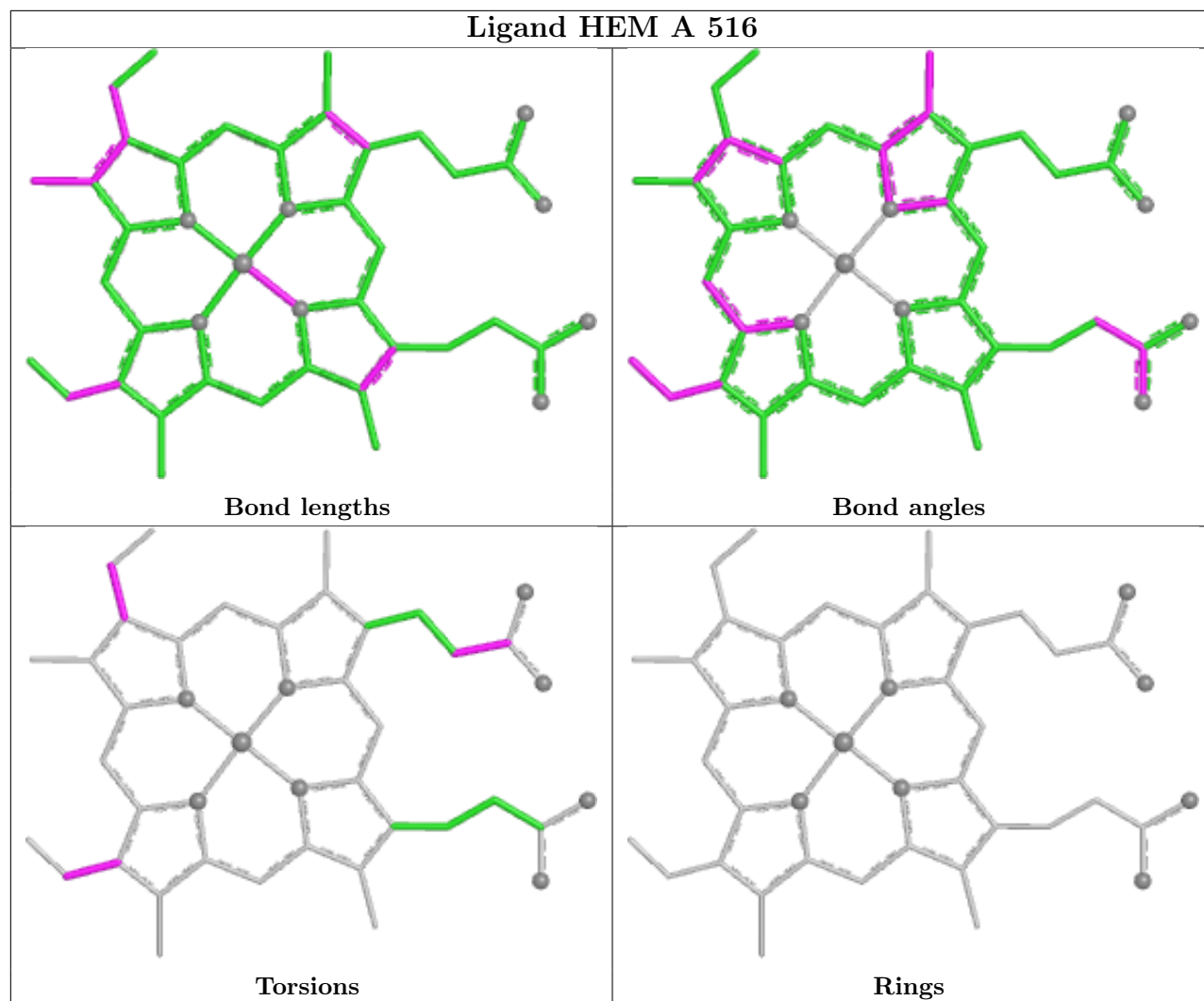
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	509	SO4	1	0
7	A	515	HEM	1	0
7	A	517	HEM	6	0
7	A	514	HEM	10	0

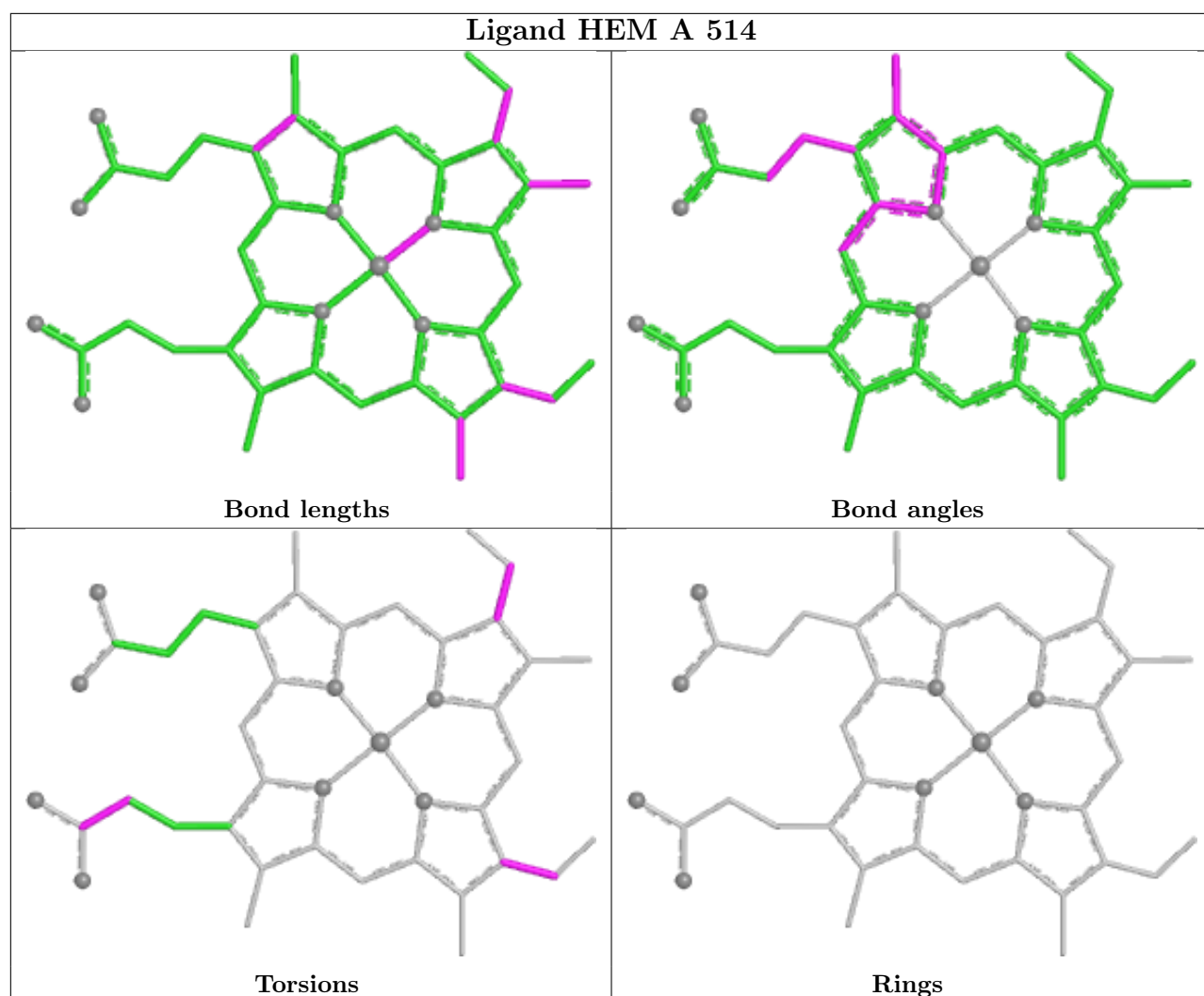
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	471/485 (97%)	2.36	284 (60%) 0 0	12, 20, 34, 45	10 (2%)

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	505	THR	6.8
1	A	507	LYS	6.6
1	A	231	VAL	6.5
1	A	307	ALA	6.4
1	A	308	VAL	5.8
1	A	506	LYS	5.6
1	A	230	GLY	5.6
1	A	332	GLU	5.3
1	A	287	ILE	5.2
1	A	254	TYR	5.0
1	A	285	THR	4.9
1	A	142	ILE	4.7
1	A	195	PHE	4.6
1	A	141[A]	ILE	4.6
1	A	38	THR	4.5
1	A	220	PHE	4.5
1	A	327	MET	4.4
1	A	437	ALA	4.3
1	A	225	TRP	4.3
1	A	37	LYS	4.3
1	A	375	THR	4.3
1	A	310	TYR	4.3
1	A	198	PHE	4.2
1	A	269	LYS	4.2
1	A	283	TYR	4.1
1	A	199	ALA	4.1
1	A	218	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	152	THR	4.0
1	A	169	TYR	4.0
1	A	280	TRP	4.0
1	A	302	TYR	3.9
1	A	201	SER	3.9
1	A	291	LYS	3.9
1	A	197	THR	3.8
1	A	329	CYS	3.8
1	A	56	TYR	3.8
1	A	460	GLU	3.8
1	A	57	TYR	3.7
1	A	145	ASP	3.7
1	A	48	ALA	3.7
1	A	219	TYR	3.7
1	A	210	VAL	3.7
1	A	410	VAL	3.7
1	A	431	VAL	3.7
1	A	194	GLY	3.7
1	A	248	THR	3.6
1	A	163	VAL	3.6
1	A	212	ALA	3.6
1	A	424	ALA	3.6
1	A	294	SER	3.6
1	A	148	LEU	3.5
1	A	379	LEU	3.5
1	A	44	ILE	3.5
1	A	295	CYS	3.5
1	A	321	ASN	3.5
1	A	333	SER	3.5
1	A	331	ARG	3.4
1	A	177	ALA	3.4
1	A	211	CYS	3.4
1	A	62	ASP	3.4
1	A	90	TYR	3.4
1	A	246	ILE	3.4
1	A	138	VAL	3.4
1	A	258	ILE	3.4
1	A	373	GLY	3.4
1	A	438	ILE	3.4
1	A	263	TRP	3.4
1	A	229	LYS	3.4
1	A	330	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	293	VAL	3.3
1	A	380	LYS	3.3
1	A	41	SER	3.3
1	A	286	GLY	3.3
1	A	404	PHE	3.3
1	A	227	ASP	3.3
1	A	289	GLY	3.3
1	A	323	ASP	3.3
1	A	214	CYS	3.3
1	A	235	ALA	3.2
1	A	296	ALA	3.2
1	A	377	ALA	3.2
1	A	162	ILE	3.2
1	A	243	SER	3.2
1	A	242	TRP	3.2
1	A	143	GLU	3.2
1	A	461	ALA	3.2
1	A	435	TYR	3.2
1	A	200	GLU	3.2
1	A	337	LEU	3.2
1	A	372	LEU	3.2
1	A	328	ASN	3.1
1	A	384	THR	3.1
1	A	502	TYR	3.1
1	A	469	PHE	3.1
1	A	178	GLU	3.1
1	A	261	ALA	3.1
1	A	150	TYR	3.1
1	A	59	ARG	3.1
1	A	271	PRO	3.1
1	A	399	GLY	3.1
1	A	462	PHE	3.1
1	A	110	ILE	3.1
1	A	43	GLY	3.1
1	A	440	TYR	3.1
1	A	183	VAL	3.1
1	A	397	ILE	3.0
1	A	406	ALA	3.0
1	A	179	LEU	3.0
1	A	216	VAL	3.0
1	A	171	CYS	3.0
1	A	355	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	382	ILE	3.0
1	A	396	ALA	3.0
1	A	132	THR	3.0
1	A	228	ASP	3.0
1	A	245	GLY	3.0
1	A	192	ALA	3.0
1	A	436	GLY	2.9
1	A	247	SER	2.9
1	A	255	TYR	2.9
1	A	369	ALA	2.9
1	A	421	ALA	2.9
1	A	209	LEU	2.9
1	A	319	LEU	2.9
1	A	288	HIS	2.9
1	A	433	ALA	2.9
1	A	290	GLN	2.9
1	A	83	LEU	2.9
1	A	428	LEU	2.9
1	A	386	ILE	2.9
1	A	301	PRO	2.9
1	A	196	LYS	2.9
1	A	53	TRP	2.8
1	A	391	TRP	2.8
1	A	232	ASP	2.8
1	A	259	ASN	2.8
1	A	54	ALA	2.8
1	A	133	CYS	2.8
1	A	205	GLU	2.8
1	A	191	SER	2.8
1	A	300	MET	2.8
1	A	184	PRO	2.8
1	A	64	TRP	2.8
1	A	166	ILE	2.8
1	A	463	ILE	2.8
1	A	223	THR	2.7
1	A	119	VAL	2.7
1	A	403	PHE	2.7
1	A	42[A]	GLN	2.7
1	A	155	TRP	2.7
1	A	477	TRP	2.7
1	A	326	CYS	2.7
1	A	315	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	457	VAL	2.7
1	A	493	LYS	2.7
1	A	173	ASP	2.7
1	A	275	ALA	2.7
1	A	354	ILE	2.7
1	A	115	THR	2.7
1	A	122	LYS	2.7
1	A	158	TYR	2.7
1	A	236	MET	2.7
1	A	85	VAL	2.7
1	A	350	PHE	2.6
1	A	374	ALA	2.6
1	A	423	LYS	2.6
1	A	239	THR	2.6
1	A	40	HIS	2.6
1	A	73	ILE	2.6
1	A	159	GLY	2.6
1	A	139	PRO	2.6
1	A	325	SER	2.6
1	A	238	VAL	2.6
1	A	492	LEU	2.6
1	A	146	GLY	2.6
1	A	260	PHE	2.6
1	A	416	SER	2.6
1	A	58	PRO	2.6
1	A	482	ILE	2.6
1	A	84	VAL	2.6
1	A	186	LEU	2.6
1	A	273	LEU	2.6
1	A	414	LEU	2.6
1	A	202	THR	2.6
1	A	167	GLY	2.6
1	A	92	PHE	2.6
1	A	371	GLU	2.6
1	A	144	GLN	2.5
1	A	270	THR	2.5
1	A	190	LEU	2.5
1	A	180	LYS	2.5
1	A	298	CYS	2.5
1	A	193	ALA	2.5
1	A	338	LYS	2.5
1	A	393	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	483	ALA	2.5
1	A	489	PRO	2.5
1	A	250	GLN	2.5
1	A	267	ILE	2.5
1	A	359	ILE	2.5
1	A	63	SER	2.5
1	A	89	GLY	2.5
1	A	104	TYR	2.5
1	A	253	ALA	2.5
1	A	343	GLN	2.5
1	A	292	GLY	2.5
1	A	265	HIS	2.5
1	A	313	HIS	2.5
1	A	305	GLU	2.5
1	A	66	LYS	2.4
1	A	117	ALA	2.4
1	A	311	SER	2.4
1	A	77	LEU	2.4
1	A	185	TYR	2.4
1	A	467	LEU	2.4
1	A	429	VAL	2.4
1	A	131	TRP	2.4
1	A	49	MET	2.4
1	A	168	CYS	2.4
1	A	426	ILE	2.4
1	A	306	GLY	2.4
1	A	485	GLY	2.4
1	A	106	LEU	2.4
1	A	432	LEU	2.4
1	A	55	ARG	2.4
1	A	341	VAL	2.4
1	A	61	PHE	2.4
1	A	98	ALA	2.4
1	A	151	PHE	2.4
1	A	389	ALA	2.4
1	A	340	ILE	2.3
1	A	126	LEU	2.3
1	A	473	LEU	2.3
1	A	172	HIS	2.3
1	A	234	THR	2.3
1	A	472	THR	2.3
1	A	407	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	459	MET	2.3
1	A	445	PHE	2.3
1	A	240	LEU	2.3
1	A	468	LYS	2.3
1	A	121	GLY	2.3
1	A	381	GLU	2.3
1	A	388	HIS	2.3
1	A	87	TRP	2.3
1	A	362	ALA	2.3
1	A	411	LEU	2.3
1	A	465	GLU	2.3
1	A	494	GLY	2.3
1	A	237	VAL	2.3
1	A	207	ARG	2.2
1	A	415	ALA	2.2
1	A	346	GLU	2.2
1	A	241	PRO	2.2
1	A	499	SER	2.2
1	A	51	GLU	2.2
1	A	488	ASN	2.2
1	A	434	LYS	2.2
1	A	105	ALA	2.2
1	A	447	THR	2.2
1	A	147	GLU	2.2
1	A	356	PHE	2.2
1	A	413	LEU	2.2
1	A	409	GLU	2.2
1	A	204	GLN	2.1
1	A	46	GLY	2.1
1	A	417	GLY	2.1
1	A	86	ALA	2.1
1	A	442	ALA	2.1
1	A	50	SER	2.1
1	A	402	SER	2.1
1	A	249	GLU	2.1
1	A	272	MET	2.1
1	A	370	MET	2.1
1	A	324	LYS	2.1
1	A	430	LYS	2.1
1	A	347	ARG	2.1
1	A	351	LEU	2.1
1	A	363	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	39	ALA	2.1
1	A	345	PHE	2.1
1	A	481	ALA	2.1
1	A	458	ASP	2.0
1	A	165	THR	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](#)

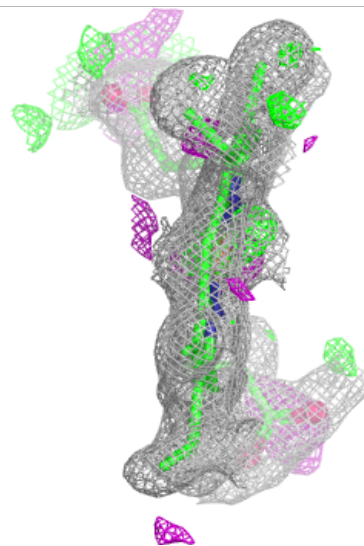
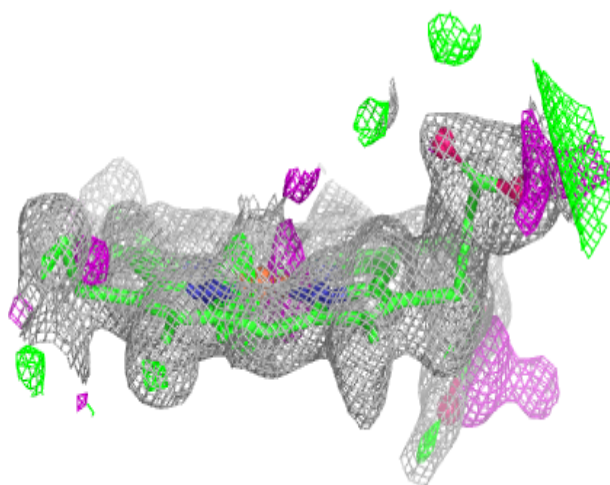
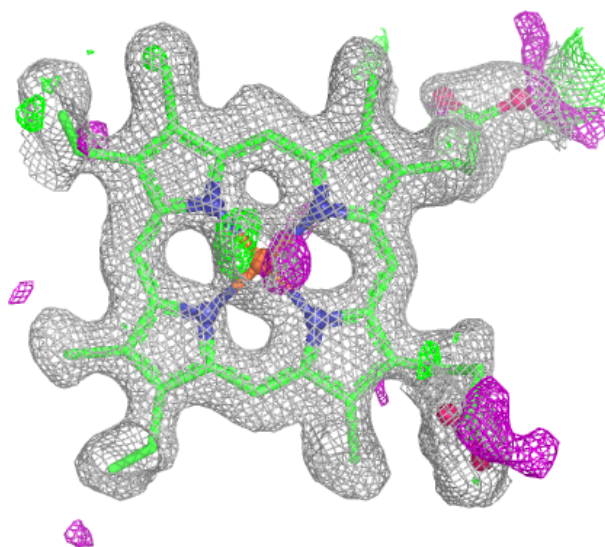
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	ACT	A	511	4/4	0.62	0.21	60,60,61,61	0
6	ACT	A	4	4/4	0.71	0.20	39,40,40,40	0
4	SO4	A	509	5/5	0.76	0.23	15,19,21,22	5
5	Y1	A	3	1/1	0.78	0.33	54,54,54,54	1
5	Y1	A	510	1/1	0.85	0.14	16,16,16,16	1
6	ACT	A	512	4/4	0.87	0.13	24,26,26,27	0
5	Y1	A	2	1/1	0.87	0.17	29,29,29,29	1
7	HEM	A	517	43/43	0.89	0.15	21,24,33,37	0
7	HEM	A	516	43/43	0.90	0.15	15,18,27,29	0
7	HEM	A	515	43/43	0.91	0.14	13,15,17,26	0
2	CA	A	1	1/1	0.91	0.16	12,12,12,12	1
7	HEM	A	514	43/43	0.91	0.14	17,19,26,34	0
3	SO3	A	508	4/4	0.93	0.15	16,21,21,22	0
7	HEM	A	513	43/43	0.93	0.12	12,14,16,17	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.

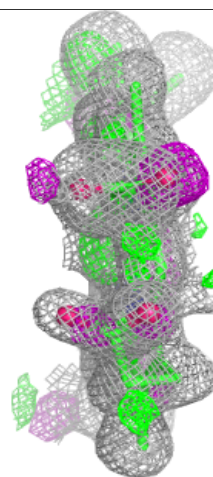
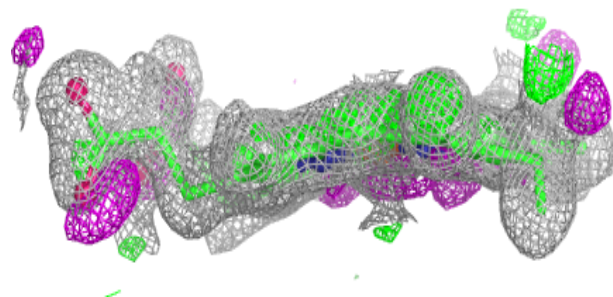
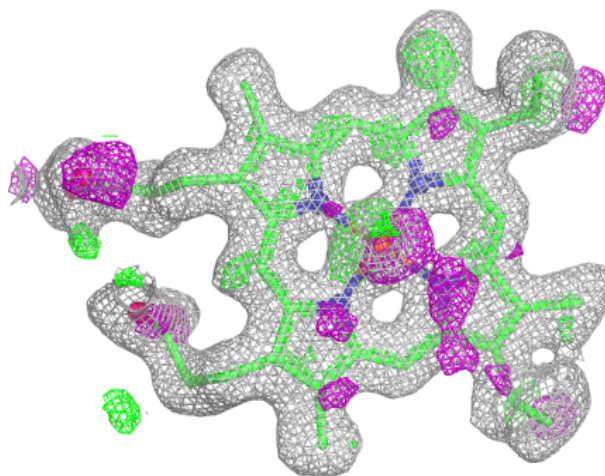
Electron density around HEM A 517:

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



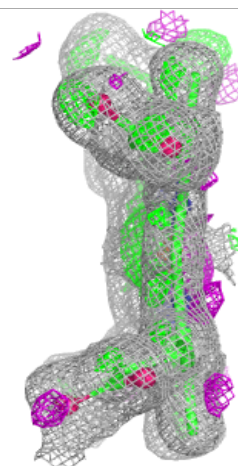
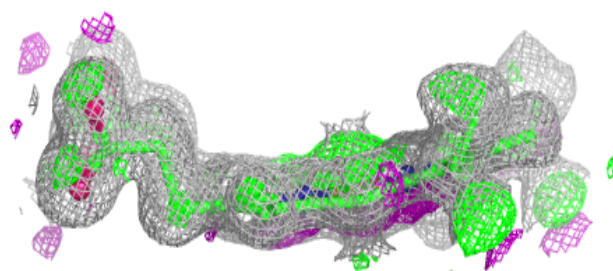
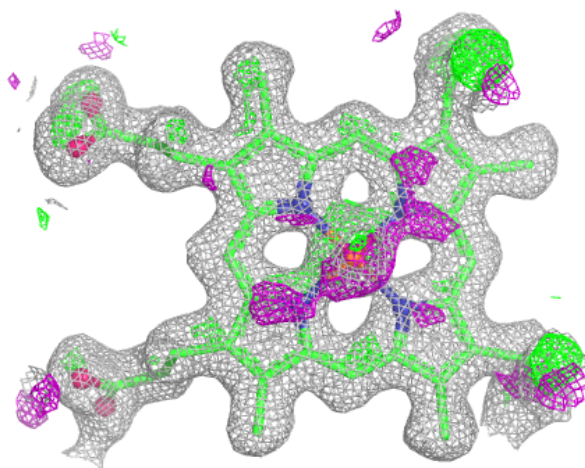
Electron density around HEM A 516:

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



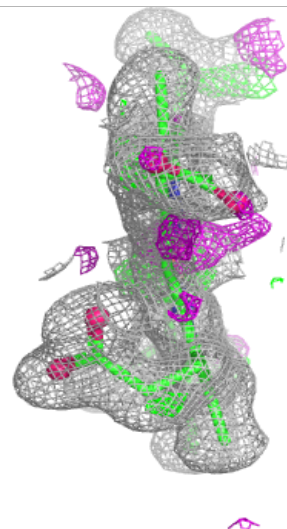
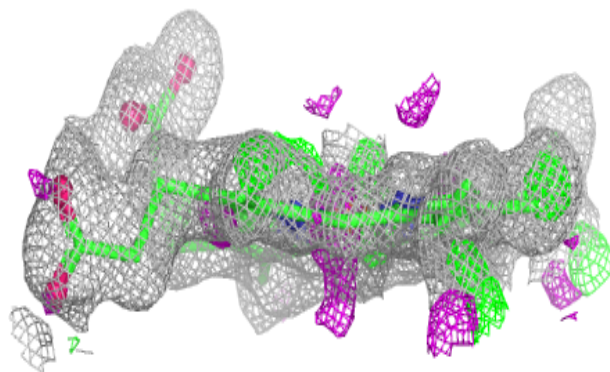
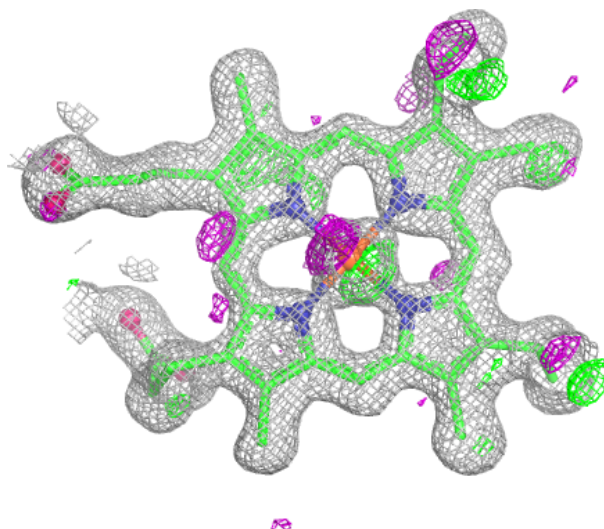
Electron density around HEM A 515:

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



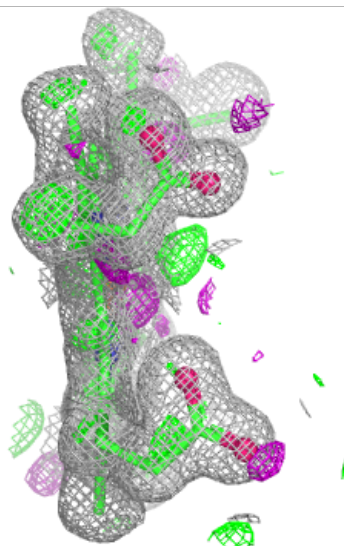
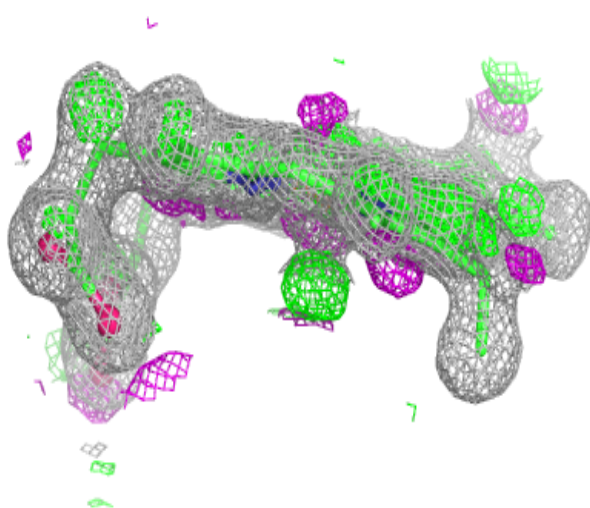
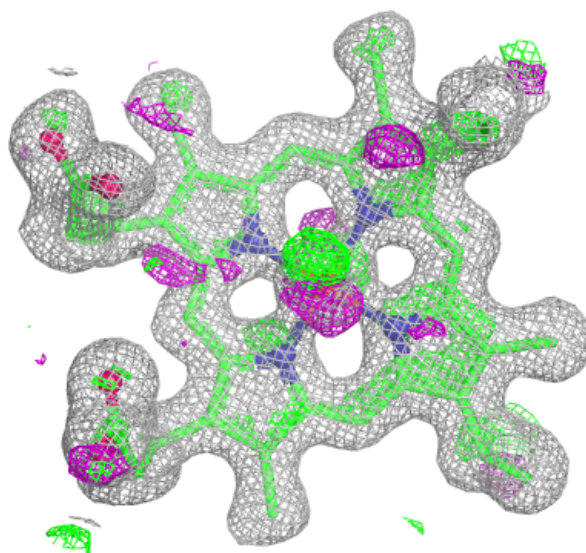
Electron density around HEM A 514:

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



Electron density around HEM A 513:

$2mF_o-DF_c$ (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.