



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2025 – 02:41 PM EST

PDB ID : 9MYW / pdb_00009myw
Title : Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain bound 2-(2-amino-6-fluoro-4-methylquinolin-7-yl)-5-(2-aminoethyl)phenol
Authors : Li, H.; Poulos, T.L.
Deposited on : 2025-01-22
Resolution : 2.31 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	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

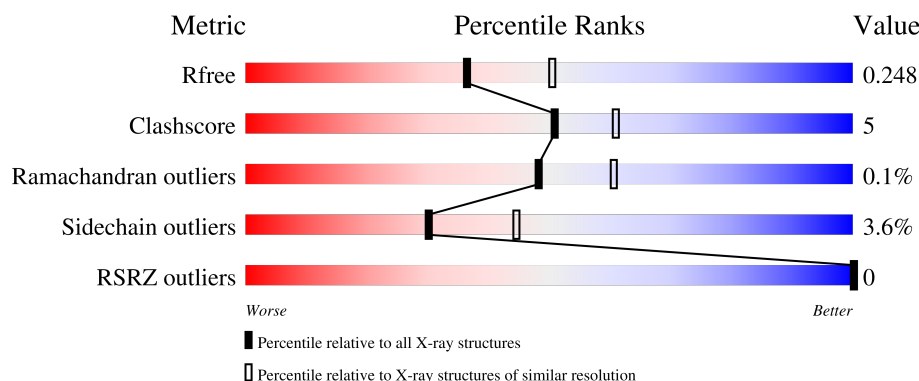
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.31 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	423	 83% 15% .
1	B	423	 84% 13% ..
1	C	423	 85% 12% ..
1	D	423	 84% 13% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14570 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 Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	4	0
			3421	2189	585	626	21			
1	B	414	Total	C	N	O	S	0	2	0
			3379	2165	575	618	21			
1	C	413	Total	C	N	O	S	0	6	0
			3388	2172	575	619	22			
1	D	418	Total	C	N	O	S	0	3	0
			3420	2188	585	626	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
A	723	LEU	-	expression tag	UNP P29475
A	724	VAL	-	expression tag	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475
B	723	LEU	-	expression tag	UNP P29475
B	724	VAL	-	expression tag	UNP P29475
C	354	ALA	ARG	engineered mutation	UNP P29475
C	357	ASP	GLY	engineered mutation	UNP P29475
C	723	LEU	-	expression tag	UNP P29475
C	724	VAL	-	expression tag	UNP P29475
D	354	ALA	ARG	engineered mutation	UNP P29475
D	357	ASP	GLY	engineered mutation	UNP P29475
D	723	LEU	-	expression tag	UNP P29475
D	724	VAL	-	expression tag	UNP P29475

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



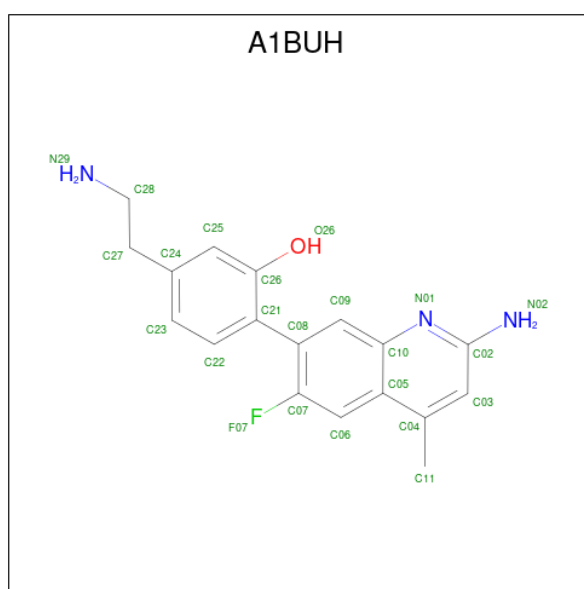
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C₉H₁₅N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is (2M)-5-(2-aminoethyl)-2-(2-amino-6-fluoro-4-methylquinolin-7-yl)phenol (CCD ID: A1BUH) (formula: C₁₈H₁₈FN₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 23	C 18	F 1	N 3	O 1	0	0
4	B	1	Total 23	C 18	F 1	N 3	O 1	0	0
4	C	1	Total 23	C 18	F 1	N 3	O 1	0	0
4	D	1	Total 23	C 18	F 1	N 3	O 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		

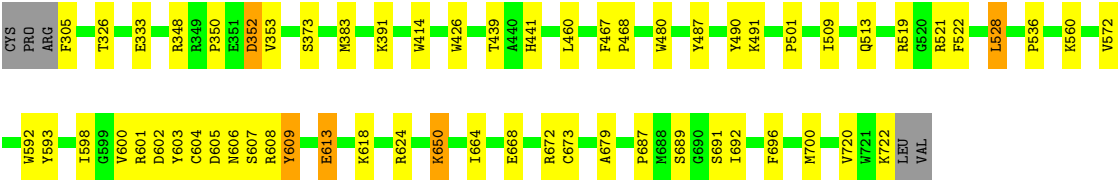
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	145	Total	O	0	0
			145	145		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	156	Total 156	O 156	0	0
7	C	147	Total 147	O 147	0	0
7	D	144	Total 144	O 144	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.28Å 118.37Å 164.85Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	39.18 – 2.31 39.18 – 2.31	Depositor EDS
% Data completeness (in resolution range)	90.5 (39.18-2.31) 97.7 (39.18-2.31)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.181 , 0.246 0.183 , 0.248	Depositor DCC
R_{free} test set	4287 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.450 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14570	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: H4B, ZN, HEM, A1BUH, GOL

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	0.30	0/3531	0.51	0/4794
1	B	0.32	0/3480	0.51	0/4721
1	C	0.33	0/3501	0.52	0/4751
1	D	0.30	0/3527	0.50	0/4787
All	All	0.31	0/14039	0.51	0/19053

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	593	TYR	Peptide

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	3421	0	3334	37	0
1	B	3379	0	3295	33	0
1	C	3388	0	3313	33	0
1	D	3420	0	3328	34	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	4	0
2	D	43	0	30	1	0
3	A	17	0	15	3	0
3	B	17	0	15	1	0
3	C	17	0	15	1	0
3	D	17	0	15	1	0
4	A	23	0	0	1	0
4	B	23	0	0	2	0
4	C	23	0	0	2	0
4	D	23	0	0	1	0
5	A	12	0	16	1	0
5	B	6	0	8	0	0
5	C	12	0	16	0	0
5	D	6	0	8	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	145	0	0	2	0
7	B	156	0	0	1	0
7	C	147	0	0	0	0
7	D	144	0	0	4	0
All	All	14570	0	13498	139	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 (139) 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:598:ILE:HA	1:C:602:ASP:HB2	1.55	0.89
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.61	0.81
1:A:419:ARG:NH1	1:A:711:TYR:OH	2.15	0.80
1:D:624:ARG:NH2	7:D:901:HOH:O	2.15	0.79
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.63	0.78
1:B:598:ILE:HA	1:B:602:ASP:HB2	1.66	0.78
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.69	0.74
1:C:528:LEU:HD22	1:C:536:PRO:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:LEU:HD22	1:D:536:PRO:HB2	1.71	0.72
1:A:348:ARG:HD2	1:A:706[B]:THR:HG21	1.72	0.70
2:D:802:HEM:HBB2	2:D:802:HEM:HHC	1.76	0.68
1:C:557:GLU:OE1	1:C:560:LYS:NZ	2.26	0.66
1:C:711:TYR:OH	2:C:801:HEM:O1D	2.13	0.66
1:D:664:ILE:O	1:D:668[B]:GLU:HG2	1.95	0.66
1:C:723:LEU:HD23	1:C:724:VAL:HG22	1.78	0.65
2:B:802:HEM:HHC	2:B:802:HEM:HBB2	1.78	0.65
1:B:601:ARG:HH12	3:B:803:H4B:C4	2.10	0.64
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.80	0.64
2:C:801:HEM:HBC2	2:C:801:HEM:HMC2	1.79	0.63
2:C:801:HEM:HHC	2:C:801:HEM:HBB2	1.81	0.63
1:D:602:ASP:OD1	1:D:608:ARG:NH2	2.32	0.62
1:A:572:VAL:HG21	4:A:803:A1BUH:C07	2.30	0.61
1:C:600:VAL:HG22	1:C:639:ASN:HD21	1.64	0.61
1:B:480:TRP:HB2	1:B:528:LEU:HB3	1.83	0.60
1:D:668[A]:GLU:OE2	1:D:672:ARG:NH2	2.35	0.59
1:B:572:VAL:HG21	4:B:804:A1BUH:C07	2.32	0.59
1:A:601:ARG:HH12	3:A:802:H4B:C4	2.16	0.58
1:D:601:ARG:HH12	3:D:803:H4B:C4	2.14	0.58
1:A:600:VAL:HG22	1:A:635:LEU:HD11	1.86	0.58
1:A:407:ILE:HG21	5:A:804:GOL:H31	1.85	0.58
1:C:601:ARG:HH12	3:C:802:H4B:C4	2.16	0.57
1:D:572:VAL:HG21	4:D:804:A1BUH:C07	2.36	0.56
1:C:480:TRP:HB2	1:C:528:LEU:HB3	1.88	0.56
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.40	0.56
1:C:572:VAL:HG21	4:C:803:A1BUH:C07	2.37	0.55
1:D:689:SER:HB3	1:D:692:ILE:HD11	1.88	0.55
1:D:490:TYR:CE1	1:D:519:ARG:HA	2.42	0.55
1:A:337:MET:HE2	1:A:340:ILE:HG13	1.88	0.55
1:D:600:VAL:O	1:D:604:CYS:HB2	2.07	0.54
1:A:598:ILE:O	1:A:602:ASP:HB2	2.06	0.54
1:C:679:ALA:HB3	1:C:700:MET:HB3	1.91	0.53
1:C:691:SER:HB3	1:D:687:PRO:HB2	1.91	0.53
1:A:518:PRO:HG2	1:A:523:ASP:CG	2.34	0.53
1:C:598:ILE:CA	1:C:602:ASP:HB2	2.34	0.53
1:C:414:TRP:CE3	1:C:426:TRP:HA	2.43	0.53
1:C:691:SER:HA	1:C:696:PHE:CG	2.45	0.52
1:B:603:TYR:HA	1:B:609:TYR:HB2	1.92	0.51
1:A:357:ASP:HB3	1:D:673:CYS:O	2.10	0.51
1:D:691:SER:HA	1:D:696:PHE:CG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:598:ILE:HA	1:D:602:ASP:HB2	1.91	0.51
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.47	0.50
1:B:601:ARG:O	1:B:608:ARG:HG3	2.11	0.50
1:A:506:PHE:HD2	1:A:525:LEU:HD13	1.77	0.50
1:A:305:PHE:HE1	1:A:307:LYS:HE2	1.77	0.50
1:B:706:THR:HA	1:B:707:PRO:C	2.36	0.50
1:C:485:ILE:HD13	1:C:546:VAL:HG13	1.93	0.50
1:C:430:GLN:HG2	1:C:453:TYR:CZ	2.47	0.49
1:D:414:TRP:CE3	1:D:426:TRP:HA	2.48	0.49
1:B:353:VAL:HG12	1:B:470:ARG:HD3	1.94	0.49
1:D:603:TYR:HA	1:D:609:TYR:HB2	1.94	0.49
2:C:801:HEM:HBA2	4:C:803:A1BUH:C26	2.43	0.49
1:A:364:LYS:NZ	1:A:368:ASP:OD2	2.45	0.49
1:A:454:ALA:HB1	7:A:907:HOH:O	2.13	0.48
1:B:679:ALA:HB3	1:B:700:MET:HB3	1.94	0.48
1:A:340:ILE:HD13	1:B:699:GLU:HB3	1.95	0.48
1:A:691:SER:HA	1:A:696:PHE:CG	2.48	0.48
1:A:387:GLU:O	1:A:391:LYS:HG2	2.15	0.47
1:C:328:GLU:HA	1:D:333:GLU:O	2.13	0.47
1:B:576:LEU:HD11	1:B:583:GLU:HB3	1.96	0.47
1:A:624:ARG:NH2	7:A:906:HOH:O	2.46	0.47
1:A:308:VAL:HG22	1:A:317:LEU:HB2	1.96	0.47
1:C:327:LEU:HG	1:C:328:GLU:H	1.80	0.47
1:A:603:TYR:HA	1:A:609:TYR:HB2	1.96	0.47
1:B:530:GLN:HG3	1:B:534:ASN:O	2.14	0.47
1:B:598:ILE:CA	1:B:602:ASP:HB2	2.42	0.47
1:B:602:ASP:OD1	1:B:608:ARG:NH2	2.48	0.46
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.98	0.46
1:A:501:PRO:HG2	1:A:608:ARG:O	2.15	0.46
1:A:501:PRO:HD2	1:A:608:ARG:HA	1.97	0.46
1:B:691:SER:HA	1:B:696:PHE:CG	2.51	0.46
1:C:600:VAL:HA	1:C:635:LEU:HD11	1.96	0.46
1:C:327:LEU:HG	1:C:328:GLU:N	2.31	0.46
1:A:341:MET:HE2	1:A:341:MET:HB2	1.76	0.45
1:D:509:ILE:O	1:D:513:GLN:HG2	2.16	0.45
1:D:487:TYR:CE2	1:D:522:PHE:HB3	2.51	0.45
1:A:467:PHE:HB3	1:A:468:PRO:HD2	1.98	0.45
1:A:636:VAL:HG11	1:B:633:GLN:HG3	1.99	0.45
1:D:348:ARG:NH2	7:D:902:HOH:O	2.25	0.45
1:D:501:PRO:HG2	1:D:608:ARG:O	2.16	0.45
1:A:600:VAL:O	1:A:604:CYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LEU:HD12	1:A:592:TRP:HB3	1.97	0.45
2:A:801:HEM:CGA	3:A:802:H4B:HN3	2.30	0.45
1:D:613:GLU:H	1:D:613:GLU:HG3	1.61	0.45
3:A:802:H4B:O10	3:A:802:H4B:H71	2.17	0.44
1:C:600:VAL:HG13	1:C:635:LEU:HD11	1.99	0.44
1:A:690:GLY:O	1:A:696:PHE:HB2	2.18	0.44
1:D:480:TRP:HB2	1:D:528:LEU:HB3	2.00	0.44
1:B:605:ASP:HB3	1:B:608:ARG:HG2	1.99	0.44
1:C:480:TRP:CE2	1:C:715:PRO:HB2	2.53	0.44
1:D:679:ALA:HB3	1:D:700:MET:HB3	1.99	0.44
1:C:556:PHE:HB3	1:C:558:TRP:CE2	2.53	0.44
1:D:460:LEU:HD12	1:D:592:TRP:HB3	2.00	0.43
1:A:333:GLU:HA	1:B:331:CYS:O	2.18	0.43
1:B:501:PRO:HB2	1:B:607:SER:O	2.18	0.43
1:C:415:ARG:CZ	1:C:674:ARG:HD2	2.48	0.43
1:D:605:ASP:HB2	1:D:608:ARG:CG	2.49	0.43
1:D:668[B]:GLU:HG2	1:D:668[B]:GLU:H	1.66	0.43
1:D:352:ASP:HB3	1:D:353:VAL:H	1.50	0.43
1:B:557:GLU:OE1	1:B:557:GLU:N	2.42	0.43
1:A:354:ALA:HB1	1:A:358:GLN:HB2	2.01	0.43
1:C:553:HIS:CG	1:C:554:PRO:HD2	2.53	0.43
1:C:636:VAL:HG22	1:C:688:MET:HE1	2.01	0.43
1:B:414:TRP:CZ3	1:B:426:TRP:HA	2.54	0.43
1:A:507:THR:O	1:A:511:ILE:HG13	2.18	0.42
1:A:623:MET:HE3	1:A:630:TRP:CZ3	2.54	0.42
1:D:598:ILE:O	1:D:602:ASP:HB2	2.20	0.42
1:D:650:LYS:HB2	1:D:650:LYS:HE3	1.76	0.42
1:A:553:HIS:CE1	1:A:555:LYS:HB3	2.55	0.42
1:B:364:LYS:NZ	7:B:912:HOH:O	2.51	0.42
1:A:335:ILE:HD11	1:B:701:LEU:HD22	2.01	0.42
1:B:507:THR:O	1:B:511:ILE:HG13	2.20	0.41
1:C:460:LEU:HD12	1:C:592:TRP:HB3	2.01	0.41
1:D:467:PHE:HB3	1:D:468:PRO:HD2	2.02	0.41
1:B:594:MET:HA	1:B:654:VAL:O	2.21	0.41
1:B:612:LEU:HD23	1:B:612:LEU:HA	1.85	0.41
1:C:312:GLU:OE2	1:D:606:ASN:ND2	2.54	0.41
1:C:542:PRO:HA	1:C:543:PRO:HD3	1.95	0.41
1:C:600:VAL:CG2	1:C:639:ASN:HD21	2.31	0.41
1:B:600:VAL:HA	1:B:635:LEU:HD11	2.03	0.41
1:B:469:GLN:HB3	1:B:584:PHE:CE2	2.55	0.41
1:B:327:LEU:HD12	1:B:704:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:TYR:CE1	1:B:412:HIS:CE1	3.09	0.41
1:B:602:ASP:O	1:B:603:TYR:CG	2.74	0.41
1:C:551:ILE:HG12	1:C:565:LYS:HA	2.01	0.41
1:C:460:LEU:HD12	1:C:592:TRP:CB	2.51	0.41
2:B:802:HEM:HBA2	4:B:804:A1BUH:C26	2.51	0.40
1:D:441:HIS:HD2	7:D:1010:HOH:O	2.04	0.40
1:C:577:LEU:HB3	1:C:584:PHE:HB2	2.04	0.40
1:D:439:THR:HB	7:D:1010:HOH:O	2.22	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	420/423 (99%)	406 (97%)	14 (3%)	0	100	100
1	B	412/423 (97%)	400 (97%)	11 (3%)	1 (0%)	44	55
1	C	415/423 (98%)	405 (98%)	10 (2%)	0	100	100
1	D	419/423 (99%)	404 (96%)	14 (3%)	1 (0%)	44	55
All	All	1666/1692 (98%)	1615 (97%)	49 (3%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	603	TYR
1	D	350	PRO

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	377/378 (100%)	366 (97%)	11 (3%)	37	54
1	B	372/378 (98%)	358 (96%)	14 (4%)	28	42
1	C	375/378 (99%)	364 (97%)	11 (3%)	37	54
1	D	376/378 (100%)	359 (96%)	17 (4%)	23	34
All	All	1500/1512 (99%)	1447 (96%)	53 (4%)	30	46

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	LYS
1	A	326	THR
1	A	349	ARG
1	A	491	LYS
1	A	528	LEU
1	A	607	SER
1	A	609	TYR
1	A	611	ILE
1	A	613	GLU
1	A	617	LYS
1	A	720	VAL
1	B	314	GLU
1	B	324	LYS
1	B	326	THR
1	B	341	MET
1	B	365	GLU
1	B	376	ARG
1	B	380	LYS
1	B	516	LYS
1	B	528	LEU
1	B	578	GLU
1	B	605	ASP
1	B	613	GLU
1	B	720	VAL
1	B	724	VAL
1	C	324	LYS
1	C	428	LYS
1	C	457	LYS

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Mol	Chain	Res	Type
1	C	521	ARG
1	C	528	LEU
1	C	557	GLU
1	C	608	ARG
1	C	612	LEU
1	C	672	ARG
1	C	704	ARG
1	C	724	VAL
1	D	305	PHE
1	D	326	THR
1	D	352	ASP
1	D	373	SER
1	D	383	MET
1	D	391	LYS
1	D	491	LYS
1	D	521	ARG
1	D	528	LEU
1	D	560	LYS
1	D	607	SER
1	D	609	TYR
1	D	613	GLU
1	D	618	LYS
1	D	650	LYS
1	D	720	VAL
1	D	722	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	GLN
1	A	430	GLN
1	A	534	ASN
1	A	633	GLN
1	B	412	HIS
1	B	503	ASN
1	B	610	ASN
1	B	633	GLN
1	C	322	HIS
1	C	647	GLN
1	D	369	GLN
1	D	606	ASN
1	D	719	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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\# Z > 2$
5	GOL	B	805	-	5,5,5	0.33	0	5,5,5	0.31	0
5	GOL	C	805	-	5,5,5	0.36	0	5,5,5	0.19	0
2	HEM	A	801	1	42,50,50	1.46	5 (11%)	46,82,82	1.81	14 (30%)
3	H4B	B	803	-	16,18,18	0.80	0	14,26,26	2.47	7 (50%)
2	HEM	B	802	1	42,50,50	1.52	6 (14%)	46,82,82	1.61	10 (21%)
4	A1BUH	A	803	-	25,25,25	1.08	2 (8%)	35,36,36	1.22	5 (14%)
5	GOL	C	804	-	5,5,5	0.40	0	5,5,5	0.20	0
4	A1BUH	B	804	-	25,25,25	1.08	2 (8%)	35,36,36	1.04	4 (11%)
4	A1BUH	C	803	-	25,25,25	1.07	2 (8%)	35,36,36	1.12	3 (8%)
5	GOL	A	805	-	5,5,5	0.46	0	5,5,5	0.19	0
5	GOL	D	805	-	5,5,5	0.40	0	5,5,5	0.41	0
2	HEM	C	801	1	42,50,50	1.46	6 (14%)	46,82,82	1.66	12 (26%)
2	HEM	D	802	1	42,50,50	1.42	6 (14%)	46,82,82	1.88	13 (28%)
3	H4B	D	803	-	16,18,18	0.86	0	14,26,26	2.35	7 (50%)
3	H4B	C	802	-	16,18,18	0.82	0	14,26,26	2.42	7 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H4B	A	802	-	16,18,18	0.91	1 (6%)	14,26,26	2.48	7 (50%)
4	A1BUH	D	804	-	25,25,25	1.02	2 (8%)	35,36,36	1.66	7 (20%)
5	GOL	A	804	-	5,5,5	0.30	0	5,5,5	0.56	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
5	GOL	B	805	-	-	1/4/4/4	-
5	GOL	C	805	-	-	0/4/4/4	-
2	HEM	A	801	1	-	5/12/54/54	-
3	H4B	B	803	-	-	4/8/17/17	0/2/2/2
2	HEM	B	802	1	-	5/12/54/54	-
4	A1BUH	A	803	-	-	0/7/7/7	0/3/3/3
5	GOL	C	804	-	-	4/4/4/4	-
4	A1BUH	B	804	-	-	0/7/7/7	0/3/3/3
4	A1BUH	C	803	-	-	2/7/7/7	0/3/3/3
5	GOL	A	805	-	-	4/4/4/4	-
5	GOL	D	805	-	-	3/4/4/4	-
2	HEM	C	801	1	-	5/12/54/54	-
2	HEM	D	802	1	-	7/12/54/54	-
3	H4B	D	803	-	-	4/8/17/17	0/2/2/2
3	H4B	C	802	-	-	4/8/17/17	0/2/2/2
3	H4B	A	802	-	-	4/8/17/17	0/2/2/2
4	A1BUH	D	804	-	-	2/7/7/7	0/3/3/3
5	GOL	A	804	-	-	4/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	HEM	C3C-C2C	-4.55	1.34	1.40
2	C	801	HEM	C3C-C2C	-4.03	1.34	1.40
2	A	801	HEM	C3C-C2C	-3.95	1.35	1.40
2	D	802	HEM	C3C-C2C	-3.93	1.35	1.40
2	B	802	HEM	C3C-C4C	3.70	1.46	1.41
2	D	802	HEM	C3C-CAC	3.28	1.55	1.47
2	A	801	HEM	C3C-CAC	3.25	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	HEM	CAB-C3B	3.22	1.56	1.47
2	C	801	HEM	C3C-C4C	3.22	1.46	1.41
2	B	802	HEM	C3C-CAC	3.07	1.54	1.47
2	C	801	HEM	C3C-CAC	3.07	1.54	1.47
2	B	802	HEM	CAB-C3B	2.83	1.54	1.47
2	A	801	HEM	CAB-C3B	2.78	1.54	1.47
4	B	804	A1BUH	C06-C07	2.72	1.40	1.35
4	C	803	A1BUH	C06-C07	2.67	1.40	1.35
4	A	803	A1BUH	C05-C10	-2.62	1.38	1.42
2	D	802	HEM	CAB-C3B	2.57	1.54	1.47
2	A	801	HEM	C3C-C4C	2.54	1.45	1.41
2	A	801	HEM	FE-NB	2.48	2.11	1.98
4	A	803	A1BUH	C06-C07	2.44	1.39	1.35
3	A	802	H4B	C4-N3	2.23	1.36	1.33
2	C	801	HEM	CMB-C2B	2.22	1.55	1.50
4	C	803	A1BUH	C05-C10	-2.20	1.39	1.42
2	B	802	HEM	CMD-C2D	2.17	1.55	1.50
4	B	804	A1BUH	C05-C10	-2.16	1.39	1.42
2	D	802	HEM	CMB-C2B	2.15	1.55	1.50
4	D	804	A1BUH	C05-C10	-2.15	1.39	1.42
2	C	801	HEM	CMD-C2D	2.10	1.55	1.50
4	D	804	A1BUH	C06-C07	2.06	1.39	1.35
2	B	802	HEM	CHA-C4D	2.06	1.39	1.34
2	D	802	HEM	CMD-C2D	2.02	1.54	1.50
2	D	802	HEM	CHA-C4D	2.02	1.39	1.34

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	H4B	C8A-C4A-C4	4.94	118.99	114.50
4	D	804	A1BUH	C21-C08-C07	-4.88	118.03	122.45
3	A	802	H4B	C8A-C4A-C4	4.82	118.89	114.50
3	D	803	H4B	C8A-C4A-C4	4.75	118.82	114.50
2	D	802	HEM	C3B-C4B-NB	-4.56	106.19	109.47
2	A	801	HEM	C4B-CHC-C1C	4.51	128.51	122.56
3	C	802	H4B	C8A-C4A-C4	4.43	118.53	114.50
2	D	802	HEM	CBA-CAA-C2A	-4.11	105.64	112.54
2	A	801	HEM	CBA-CAA-C2A	-3.89	105.99	112.54
3	C	802	H4B	C2-N3-C4	3.84	121.30	115.96
3	A	802	H4B	C2-N3-C4	3.79	121.23	115.96
2	D	802	HEM	C4C-CHD-C1D	3.68	127.42	122.56
3	A	802	H4B	N1-C2-N3	-3.68	119.84	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	H4B	N1-C2-N3	-3.66	119.87	125.48
2	C	801	HEM	C4B-CHC-C1C	3.63	127.35	122.56
3	B	803	H4B	C2-N3-C4	3.60	120.97	115.96
3	D	803	H4B	N1-C2-N3	-3.55	120.04	125.48
2	C	801	HEM	CMA-C3A-C4A	-3.53	123.28	128.46
3	B	803	H4B	N1-C2-N3	-3.48	120.15	125.48
3	D	803	H4B	C2-N3-C4	3.47	120.78	115.96
4	D	804	A1BUH	C04-C05-C10	3.36	120.05	118.00
2	A	801	HEM	C4D-ND-C1D	3.20	109.00	105.21
4	C	803	A1BUH	C09-C08-C07	3.19	119.75	116.03
4	D	804	A1BUH	C09-C08-C07	3.18	119.72	116.03
2	A	801	HEM	CMA-C3A-C4A	-3.13	123.87	128.46
4	D	804	A1BUH	C05-C10-N01	-3.09	119.53	122.80
2	D	802	HEM	C4B-CHC-C1C	3.07	126.61	122.56
2	B	802	HEM	CBA-CAA-C2A	-3.06	107.39	112.54
2	B	802	HEM	C4D-ND-C1D	3.04	108.81	105.21
2	C	801	HEM	CAD-CBD-CGD	-2.99	105.74	113.67
2	D	802	HEM	C1B-NB-C4B	2.96	108.71	105.21
4	A	803	A1BUH	C05-C10-N01	-2.92	119.71	122.80
2	A	801	HEM	C3B-C4B-NB	-2.90	107.38	109.47
4	B	804	A1BUH	C09-C08-C07	2.89	119.39	116.03
2	D	802	HEM	CHC-C4B-C3B	2.75	128.78	124.57
2	B	802	HEM	C4C-CHD-C1D	2.72	126.15	122.56
2	B	802	HEM	CMA-C3A-C4A	-2.69	124.51	128.46
3	C	802	H4B	N2-C2-N3	2.68	121.24	117.22
2	D	802	HEM	CMA-C3A-C4A	-2.68	124.54	128.46
3	A	802	H4B	N2-C2-N3	2.66	121.21	117.22
2	A	801	HEM	C3D-C4D-ND	-2.65	107.27	110.17
2	A	801	HEM	CHD-C1D-ND	2.62	127.25	124.44
2	D	802	HEM	C2C-C3C-C4C	2.61	108.72	106.90
2	B	802	HEM	C3D-C4D-ND	-2.60	107.32	110.17
2	D	802	HEM	C3B-C2B-C1B	2.60	108.36	106.41
2	C	801	HEM	CMC-C2C-C3C	2.59	129.85	124.68
4	D	804	A1BUH	C22-C21-C08	-2.58	113.53	118.74
2	D	802	HEM	C4D-ND-C1D	2.53	108.21	105.21
4	A	803	A1BUH	C09-C08-C07	2.53	118.97	116.03
3	B	803	H4B	C2-N1-C8A	2.53	120.59	114.59
2	A	801	HEM	C4C-CHD-C1D	2.53	125.89	122.56
3	A	802	H4B	C2-N1-C8A	2.51	120.56	114.59
2	A	801	HEM	C2D-C1D-ND	-2.51	107.00	109.90
2	C	801	HEM	CHA-C4D-ND	2.51	127.48	124.37
2	C	801	HEM	C4D-ND-C1D	2.50	108.17	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	803	H4B	C2-N1-C8A	2.50	120.53	114.59
2	B	802	HEM	CAD-CBD-CGD	-2.49	107.05	113.67
2	B	802	HEM	C3B-C2B-C1B	2.48	108.28	106.41
2	D	802	HEM	CHD-C1D-ND	2.47	127.09	124.44
3	B	803	H4B	N2-C2-N3	2.46	120.91	117.22
3	B	803	H4B	C4A-N5-C6	-2.45	114.49	121.16
3	C	802	H4B	C2-N1-C8A	2.45	120.41	114.59
3	D	803	H4B	N2-C2-N3	2.44	120.89	117.22
2	B	802	HEM	CMC-C2C-C3C	2.44	129.55	124.68
4	A	803	A1BUH	C06-C07-C08	-2.42	119.74	123.59
3	C	802	H4B	C4A-N5-C6	-2.40	114.62	121.16
3	A	802	H4B	C4A-N5-C6	-2.37	114.70	121.16
2	A	801	HEM	C3B-C2B-C1B	2.37	108.19	106.41
4	C	803	A1BUH	C05-C10-N01	-2.37	120.29	122.80
3	B	803	H4B	C4-C4A-N5	2.32	121.88	118.57
2	B	802	HEM	C2C-C3C-C4C	2.32	108.52	106.90
2	C	801	HEM	C2D-C1D-ND	-2.32	107.23	109.90
3	C	802	H4B	C4-C4A-N5	2.31	121.86	118.57
2	D	802	HEM	CHB-C1B-NB	2.29	127.22	124.37
4	C	803	A1BUH	C21-C08-C07	-2.25	120.42	122.45
4	A	803	A1BUH	C03-C04-C05	2.19	120.05	117.84
2	C	801	HEM	C3D-C4D-ND	-2.19	107.77	110.17
2	B	802	HEM	C2D-C1D-ND	-2.19	107.37	109.90
2	A	801	HEM	C1B-NB-C4B	2.18	107.79	105.21
2	A	801	HEM	CHC-C4B-C3B	2.18	127.90	124.57
2	A	801	HEM	C2C-C3C-C4C	2.17	108.41	106.90
2	C	801	HEM	CBA-CAA-C2A	-2.16	108.91	112.54
4	B	804	A1BUH	C21-C08-C07	-2.16	120.50	122.45
4	B	804	A1BUH	C06-C07-C08	-2.15	120.17	123.59
3	D	803	H4B	C4A-N5-C6	-2.15	115.30	121.16
3	D	803	H4B	C4-C4A-N5	2.12	121.59	118.57
2	A	801	HEM	CHA-C4D-ND	2.11	126.99	124.37
2	C	801	HEM	C2C-C3C-C4C	2.09	108.36	106.90
2	D	802	HEM	C3D-C4D-ND	-2.08	107.89	110.17
4	A	803	A1BUH	C04-C05-C10	2.08	119.27	118.00
4	D	804	A1BUH	C06-C07-C08	-2.04	120.34	123.59
2	C	801	HEM	O2A-CGA-CBA	2.03	120.42	114.00
2	C	801	HEM	CMA-C3A-C2A	2.03	128.76	124.94
3	A	802	H4B	O10-C10-C9	2.02	113.11	109.77
4	D	804	A1BUH	C09-C08-C21	2.02	122.08	117.47
4	B	804	A1BUH	C05-C10-N01	-2.00	120.68	122.80

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	H4B	N5-C6-C9-O9
3	A	802	H4B	C7-C6-C9-O9
3	A	802	H4B	C7-C6-C9-C10
3	B	803	H4B	N5-C6-C9-O9
3	B	803	H4B	C7-C6-C9-O9
3	B	803	H4B	C7-C6-C9-C10
3	C	802	H4B	N5-C6-C9-O9
3	C	802	H4B	C7-C6-C9-O9
3	C	802	H4B	C7-C6-C9-C10
3	D	803	H4B	N5-C6-C9-O9
3	D	803	H4B	N5-C6-C9-C10
3	D	803	H4B	C7-C6-C9-O9
3	D	803	H4B	C7-C6-C9-C10
5	A	805	GOL	O1-C1-C2-C3
5	C	804	GOL	C1-C2-C3-O3
5	A	804	GOL	O1-C1-C2-O2
5	A	805	GOL	O2-C2-C3-O3
5	A	804	GOL	O1-C1-C2-C3
5	A	804	GOL	C1-C2-C3-O3
5	A	805	GOL	C1-C2-C3-O3
5	C	804	GOL	O1-C1-C2-C3
5	D	805	GOL	O1-C1-C2-C3
5	D	805	GOL	C1-C2-C3-O3
5	C	804	GOL	O1-C1-C2-O2
5	A	805	GOL	O1-C1-C2-O2
5	C	804	GOL	O2-C2-C3-O3
3	A	802	H4B	N5-C6-C9-C10
3	B	803	H4B	N5-C6-C9-C10
3	C	802	H4B	N5-C6-C9-C10
2	B	802	HEM	C4D-C3D-CAD-CBD
2	D	802	HEM	C4D-C3D-CAD-CBD
5	B	805	GOL	O1-C1-C2-O2
5	D	805	GOL	O2-C2-C3-O3
2	D	802	HEM	C2D-C3D-CAD-CBD
2	B	802	HEM	C2D-C3D-CAD-CBD
5	A	804	GOL	O2-C2-C3-O3
2	B	802	HEM	C4B-C3B-CAB-CBB
2	C	801	HEM	C4B-C3B-CAB-CBB
2	D	802	HEM	C4B-C3B-CAB-CBB
2	C	801	HEM	C4D-C3D-CAD-CBD
2	C	801	HEM	C2D-C3D-CAD-CBD
2	D	802	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	C	801	HEM	CAD-CBD-CGD-O2D
2	A	801	HEM	CAD-CBD-CGD-O2D
2	C	801	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	CAD-CBD-CGD-O1D
2	D	802	HEM	CAD-CBD-CGD-O1D
4	C	803	A1BUH	C23-C24-C27-C28
2	A	801	HEM	CAA-CBA-CGA-O2A
4	D	804	A1BUH	C23-C24-C27-C28
4	C	803	A1BUH	C25-C24-C27-C28
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	802	HEM	CAD-CBD-CGD-O1D
2	B	802	HEM	CAD-CBD-CGD-O2D
2	A	801	HEM	C2D-C3D-CAD-CBD
4	D	804	A1BUH	C25-C24-C27-C28
2	D	802	HEM	CAA-CBA-CGA-O2A
2	D	802	HEM	CAA-CBA-CGA-O1A

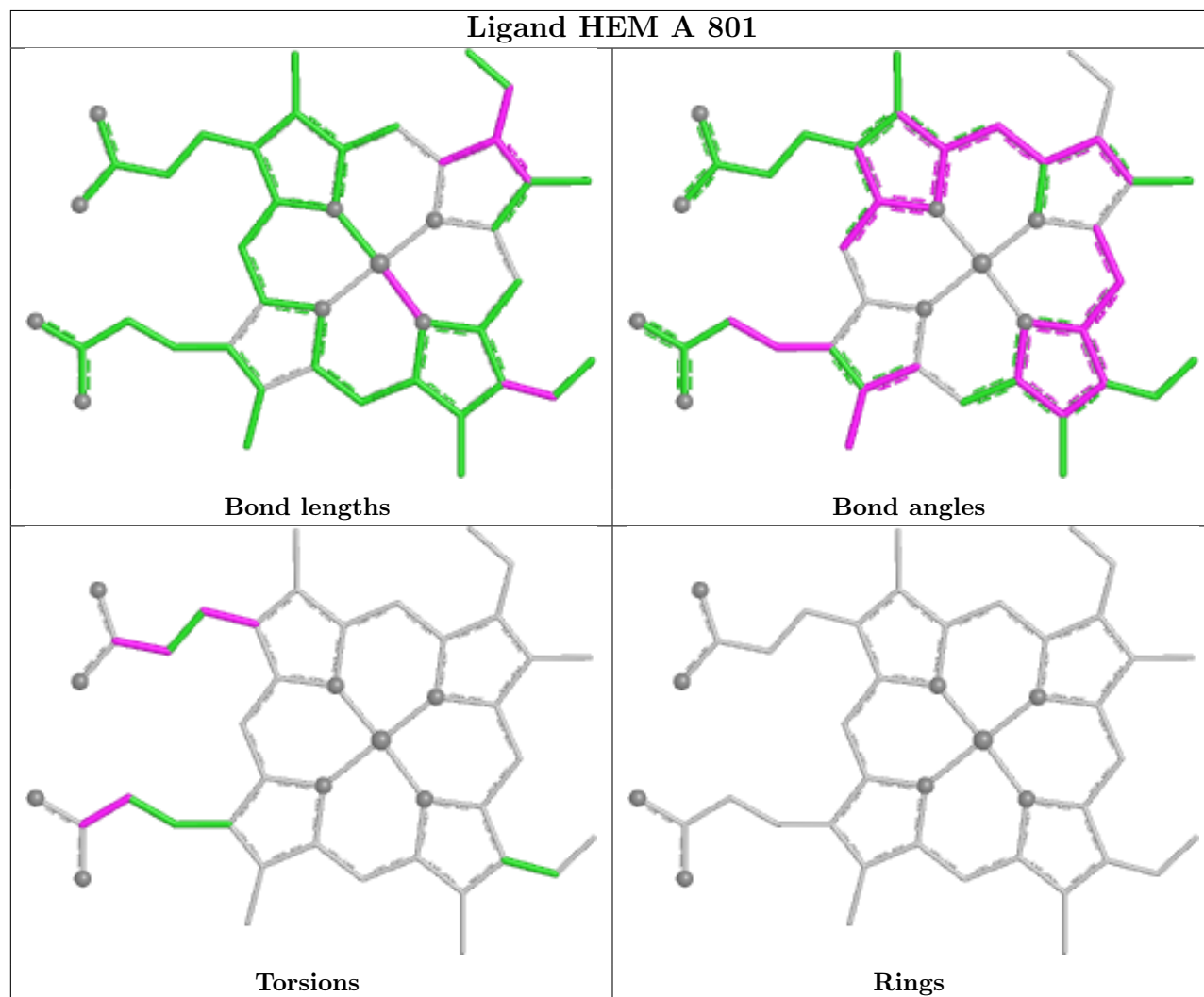
There are no ring outliers.

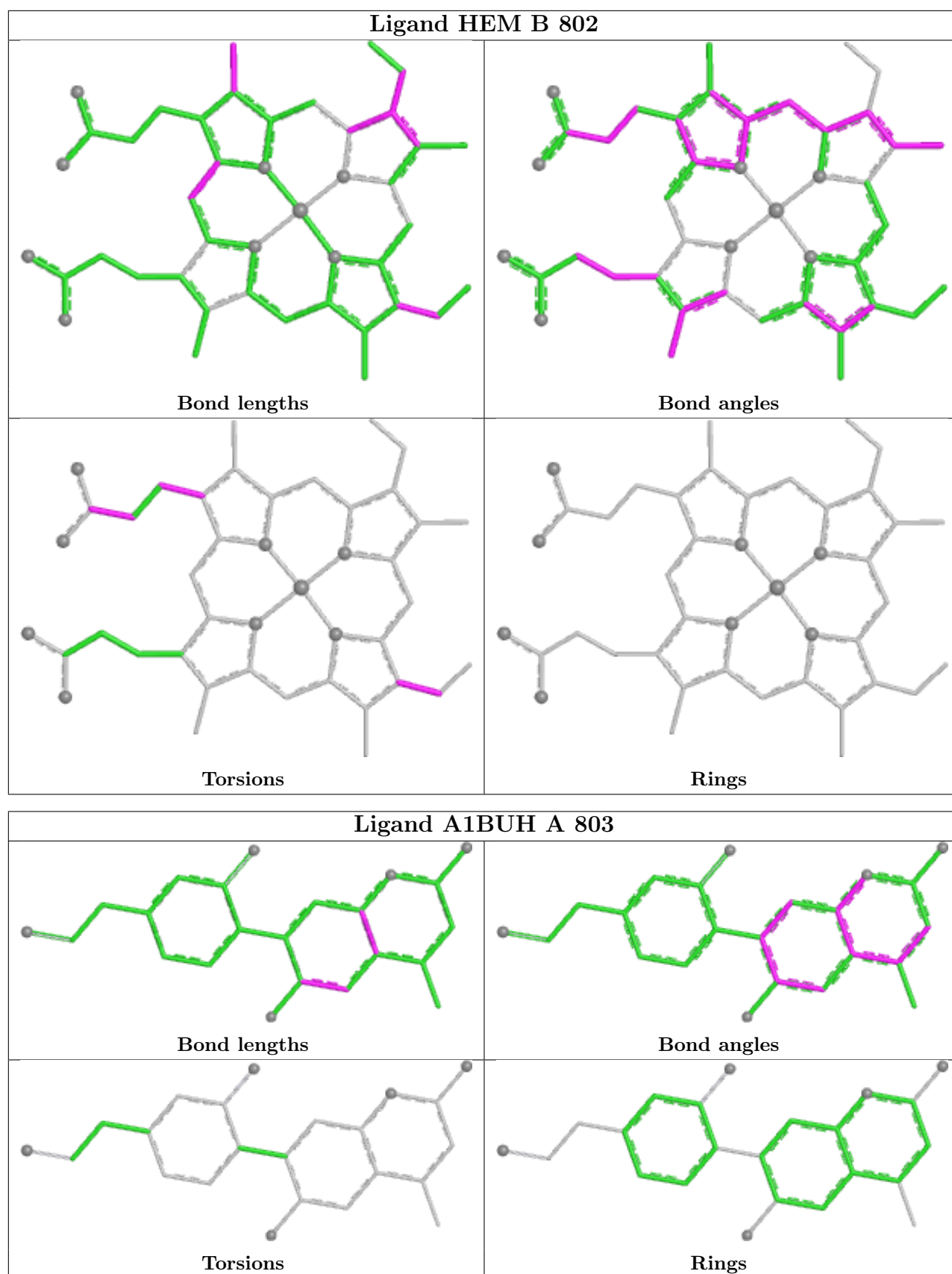
13 monomers are involved in 20 short contacts:

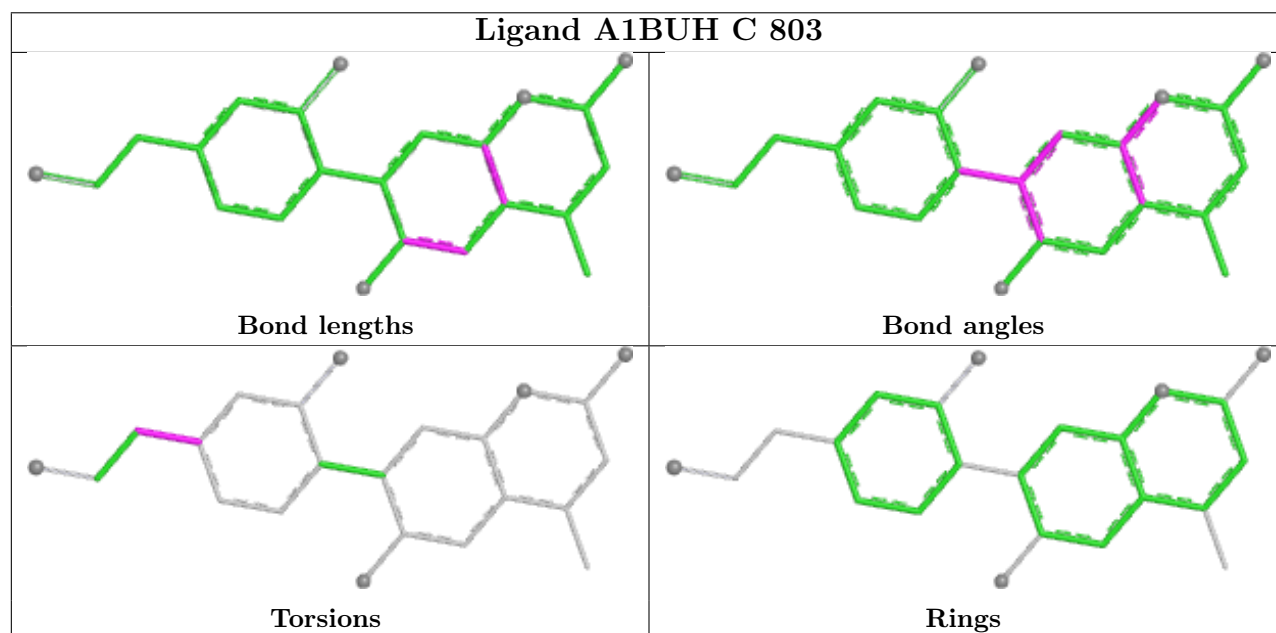
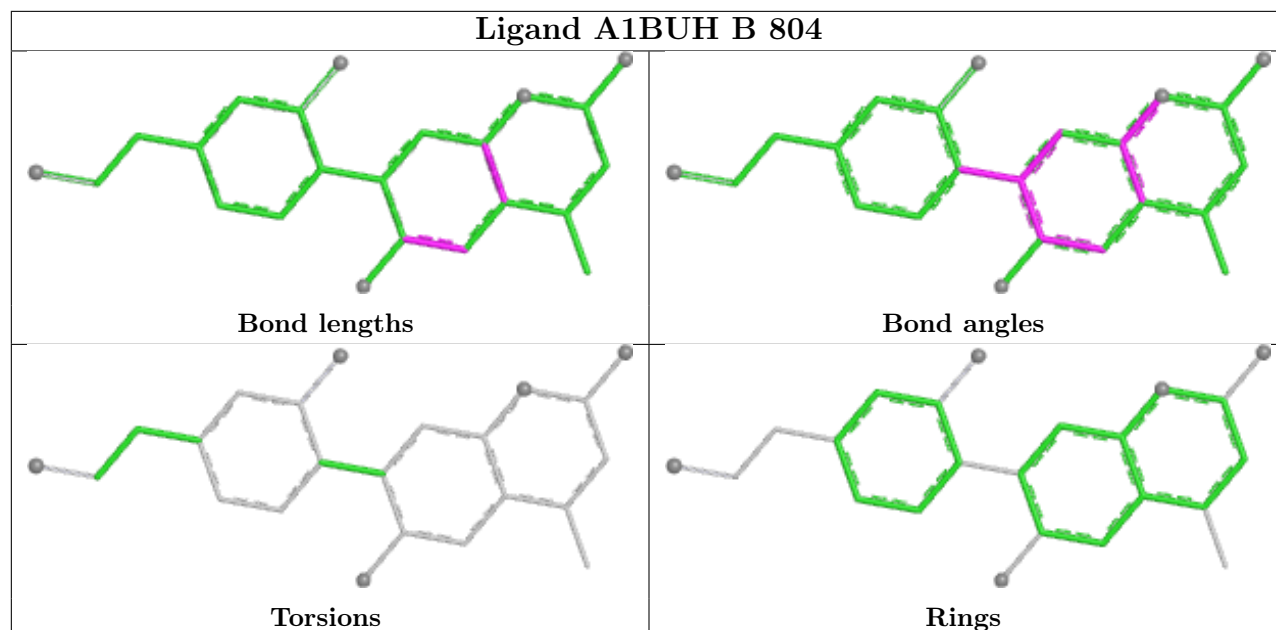
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	3	0
3	B	803	H4B	1	0
2	B	802	HEM	2	0
4	A	803	A1BUH	1	0
4	B	804	A1BUH	2	0
4	C	803	A1BUH	2	0
2	C	801	HEM	4	0
2	D	802	HEM	1	0
3	D	803	H4B	1	0
3	C	802	H4B	1	0
3	A	802	H4B	3	0
4	D	804	A1BUH	1	0
5	A	804	GOL	1	0

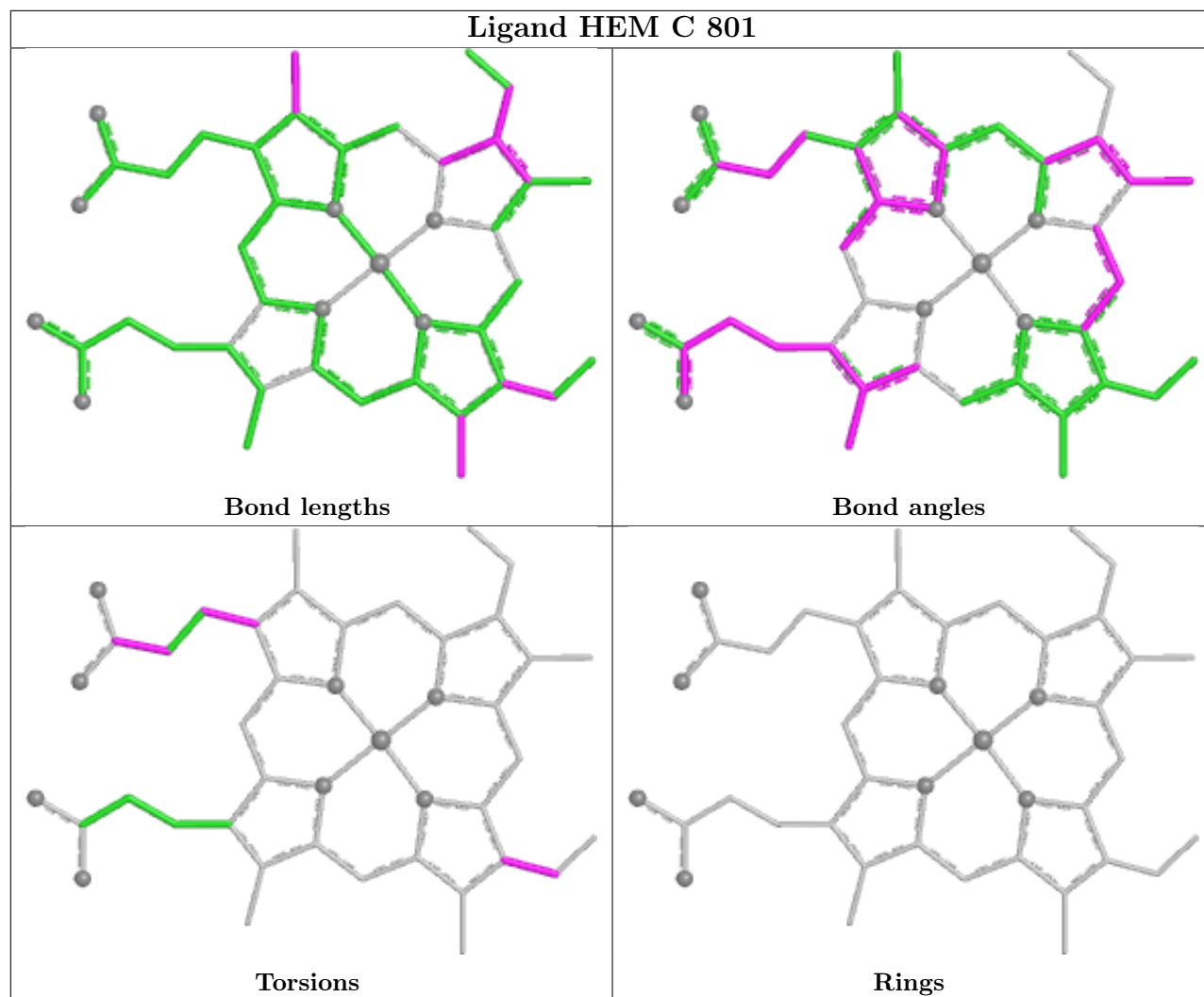
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

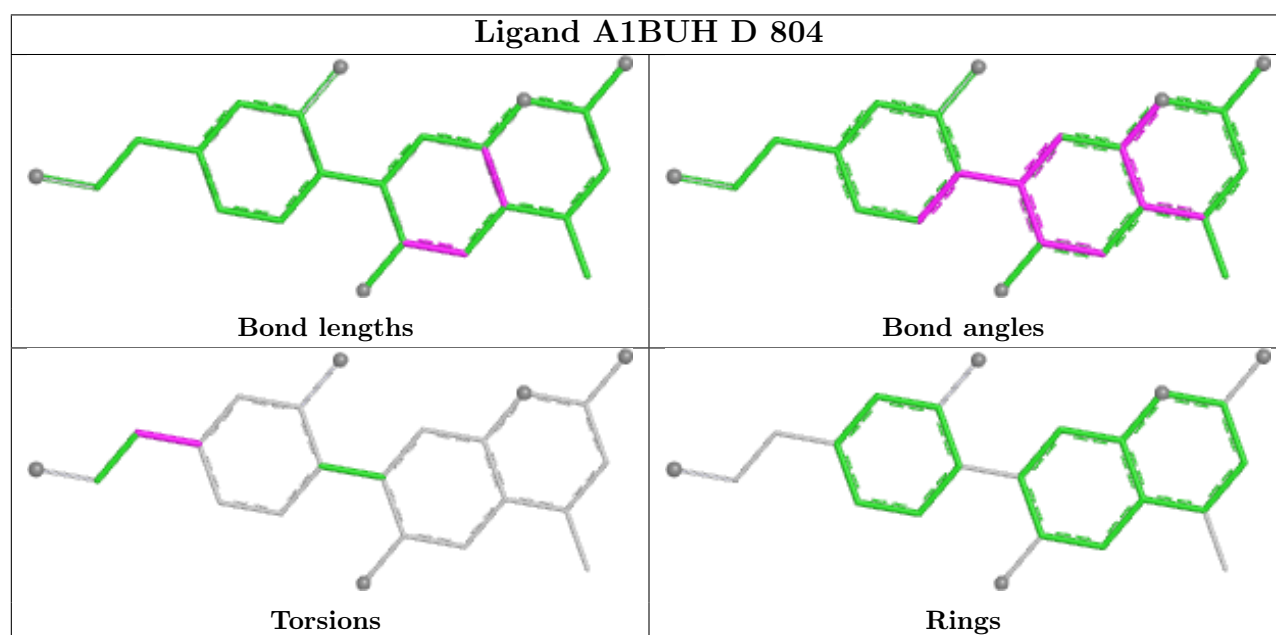
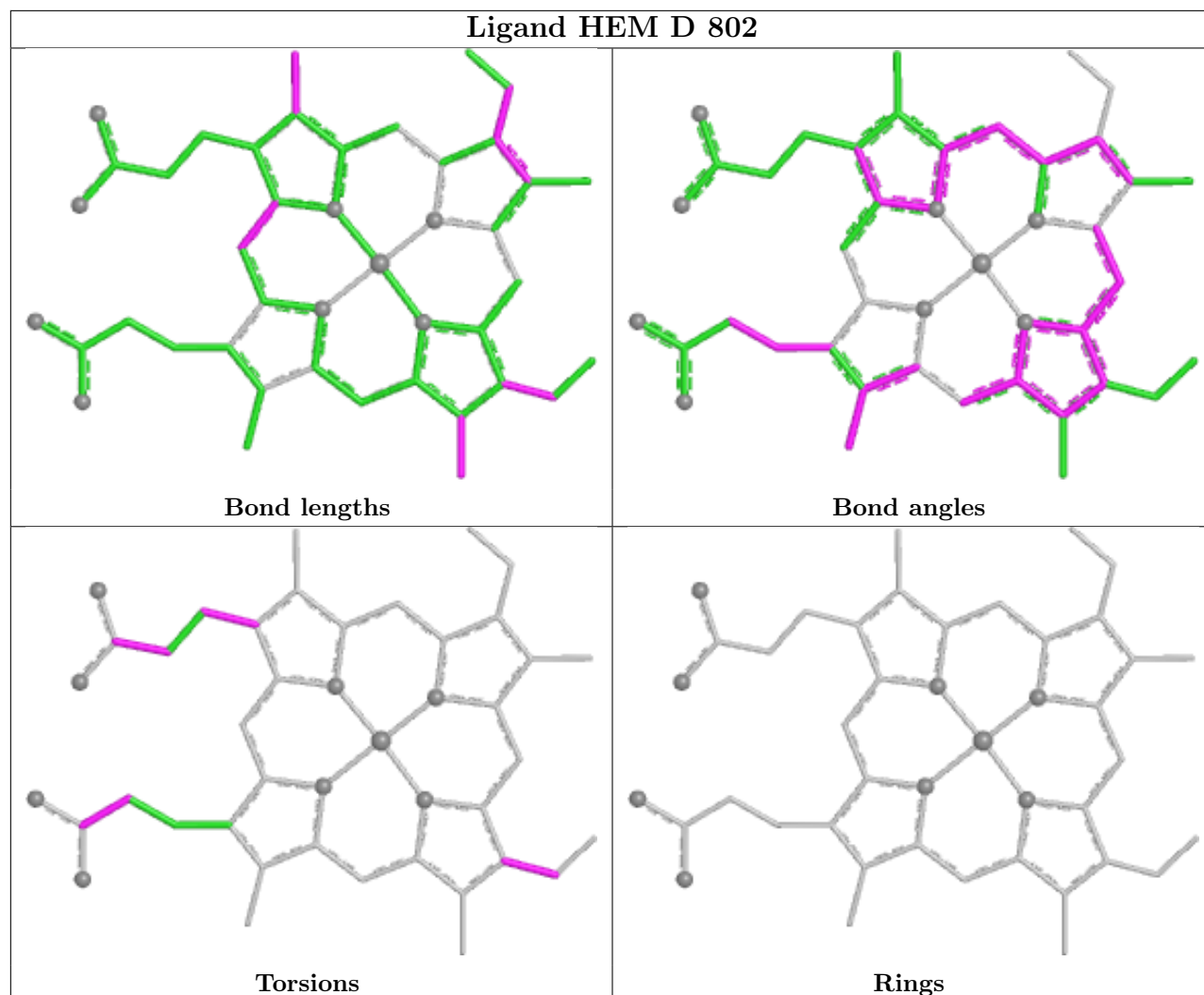
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	418/423 (98%)	-1.54	0 100 100	23, 48, 94, 133	4 (0%)
1	B	414/423 (97%)	-1.56	0 100 100	25, 45, 85, 139	2 (0%)
1	C	413/423 (97%)	-1.56	0 100 100	22, 43, 83, 127	6 (1%)
1	D	418/423 (98%)	-1.55	0 100 100	24, 49, 91, 121	3 (0%)
All	All	1663/1692 (98%)	-1.55	0 100 100	22, 46, 90, 139	15 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
5	GOL	A	805	6/6	0.98	0.05	58,67,67,73	0
5	GOL	C	804	6/6	0.98	0.06	62,65,68,76	0
3	H4B	C	802	17/17	0.99	0.04	52,78,87,89	0
3	H4B	D	803	17/17	0.99	0.04	67,81,97,100	0

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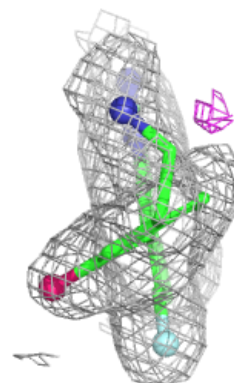
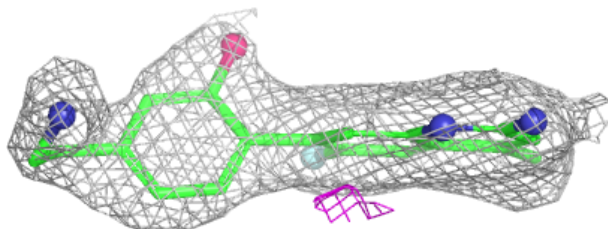
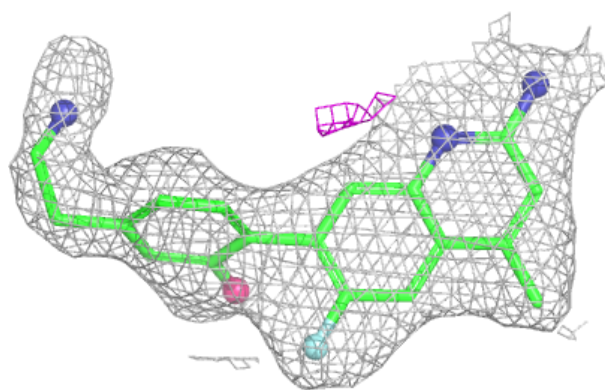
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	A1BUH	A	803	23/23	0.99	0.03	37,47,77,78	0
4	A1BUH	B	804	23/23	0.99	0.04	36,52,68,73	0
4	A1BUH	C	803	23/23	0.99	0.04	42,53,75,81	0
4	A1BUH	D	804	23/23	0.99	0.04	37,51,82,89	0
5	GOL	A	804	6/6	0.99	0.04	58,61,65,66	0
3	H4B	A	802	17/17	0.99	0.04	59,79,96,98	0
5	GOL	B	805	6/6	0.99	0.05	73,76,80,81	0
3	H4B	B	803	17/17	0.99	0.04	71,89,103,103	0
5	GOL	C	805	6/6	0.99	0.03	46,53,56,60	0
5	GOL	D	805	6/6	0.99	0.04	48,59,60,61	0
2	HEM	C	801	43/43	1.00	0.02	25,36,56,63	0
2	HEM	D	802	43/43	1.00	0.03	25,39,52,71	0
2	HEM	A	801	43/43	1.00	0.03	26,40,53,63	0
2	HEM	B	802	43/43	1.00	0.03	28,39,52,59	0
6	ZN	B	801	1/1	1.00	0.01	45,45,45,45	0
6	ZN	D	801	1/1	1.00	0.01	37,37,37,37	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.

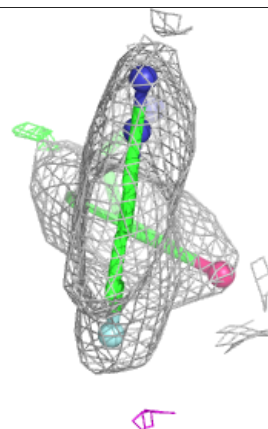
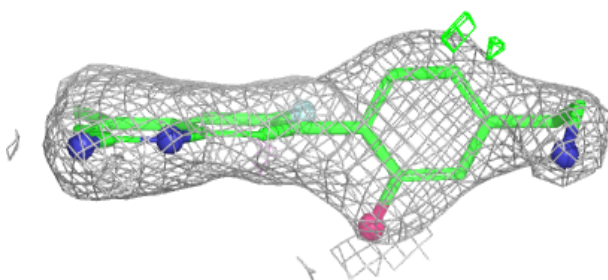
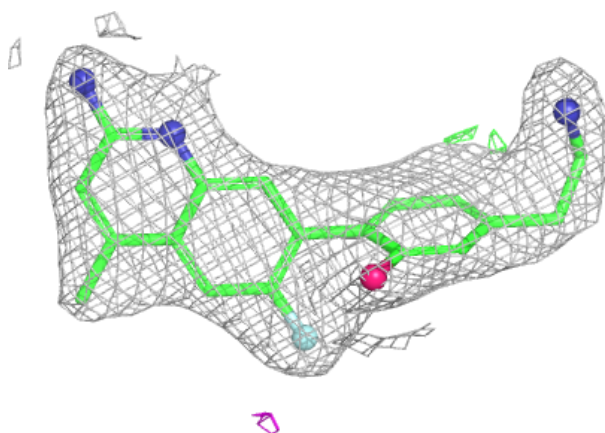
Electron density around A1BUH A 803:

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

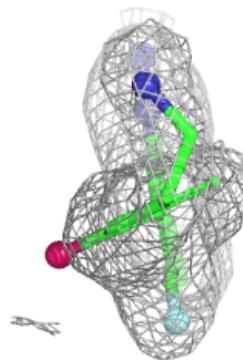
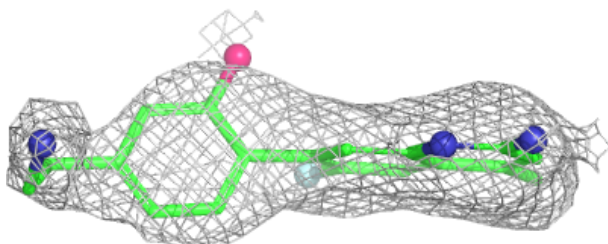
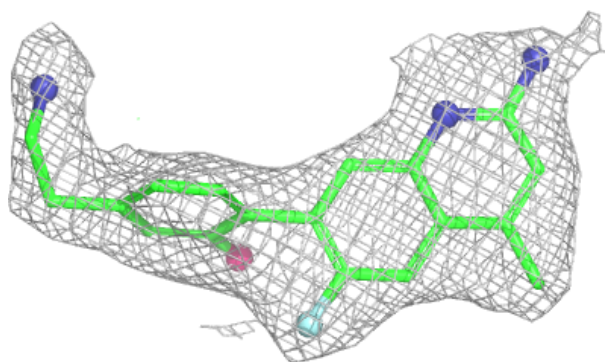


Electron density around A1BUH B 804:

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

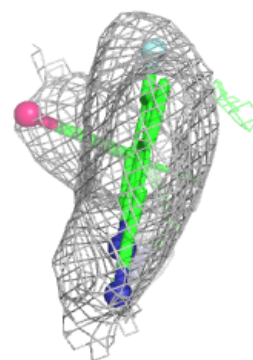
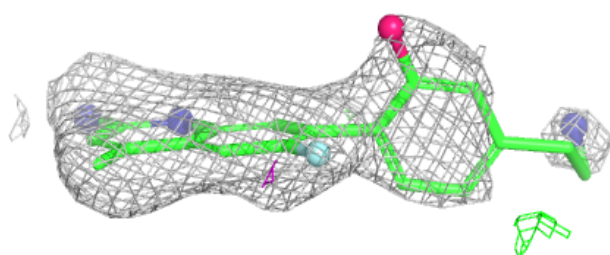
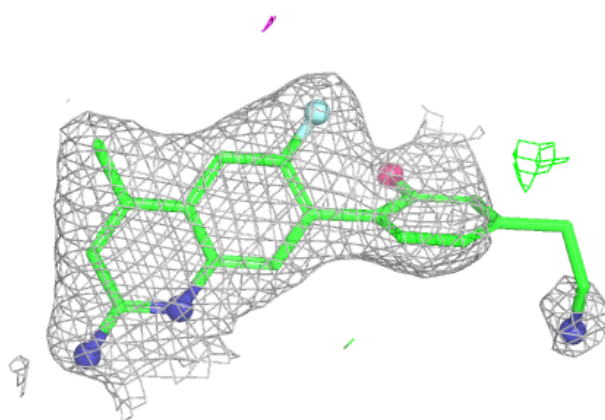
**Electron density around A1BUH C 803:**

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



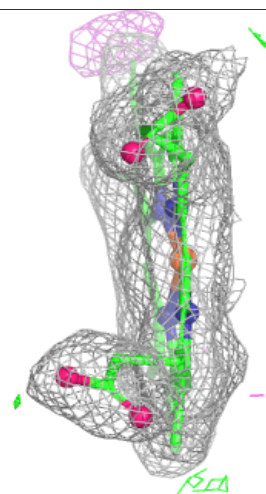
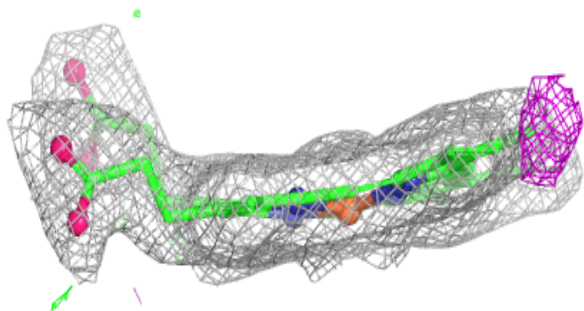
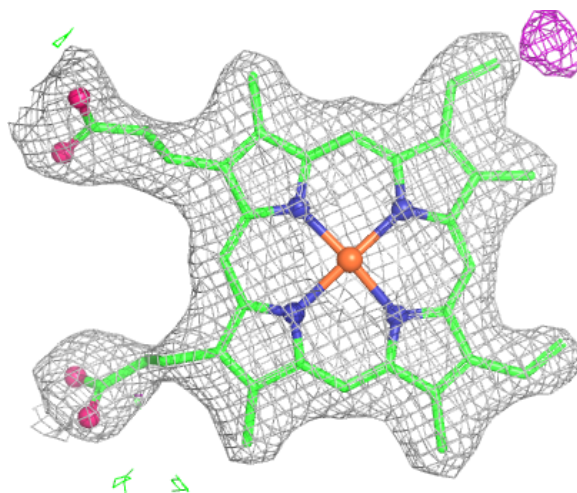
Electron density around A1BUH D 804:

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



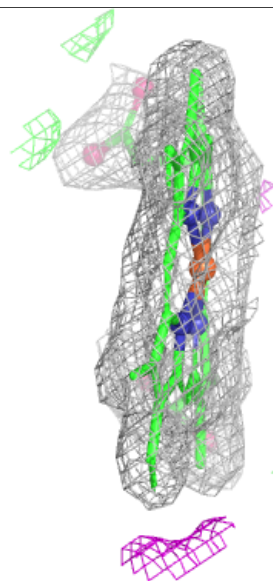
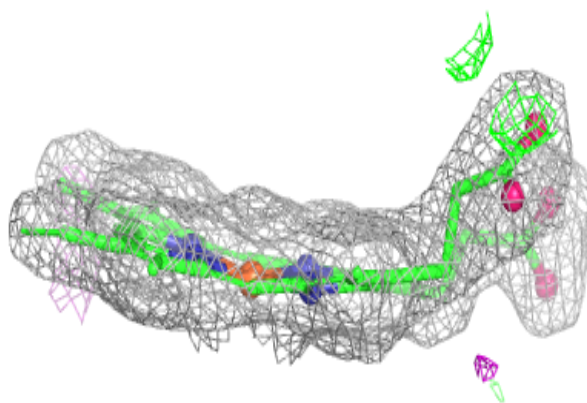
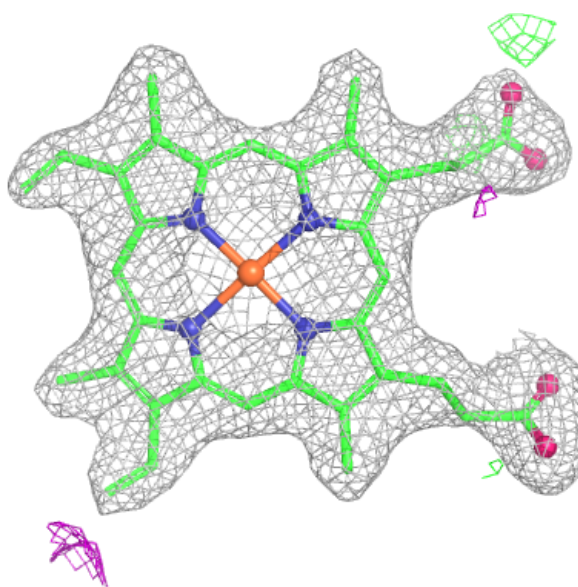
Electron density around HEM C 801:

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



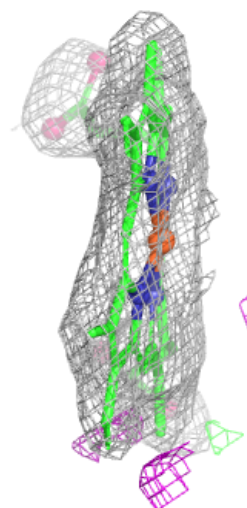
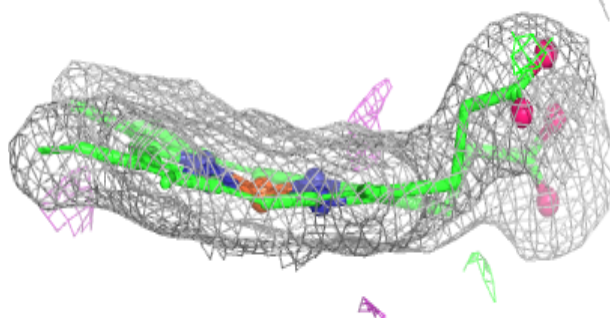
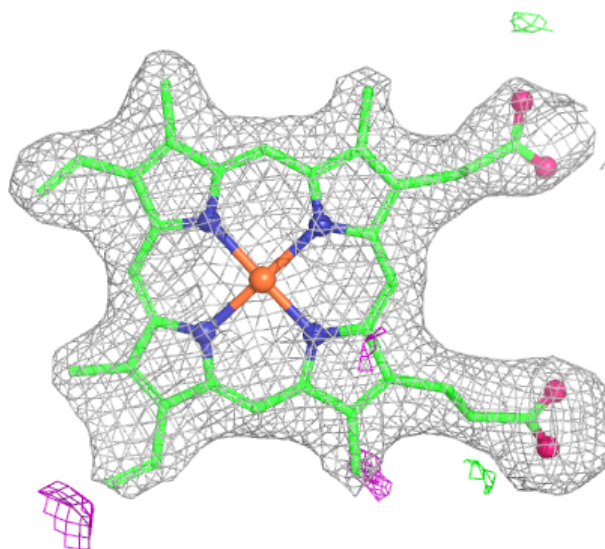
Electron density around HEM D 802:

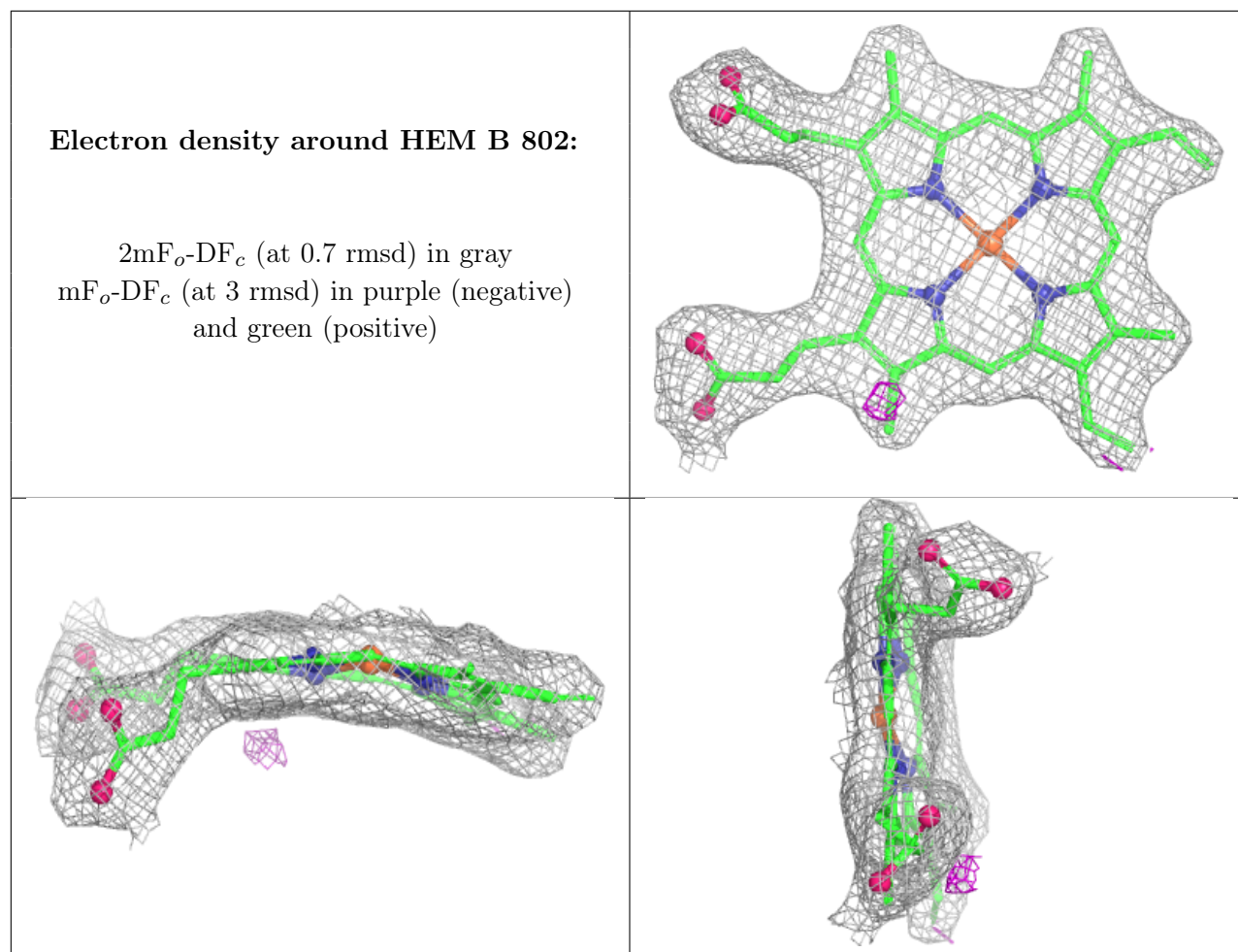
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 801:

$2mF_o-DF_c$ (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.