WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 01:46 AM EDT

PDB ID	:	6POT
Title	:	Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain in complex with 7-(3-(Aminomethyl)-4-(thiazol-5-ylmetho xy)phenyl)-4-methylquinolin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2019-07-05
Resolution	:	2.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

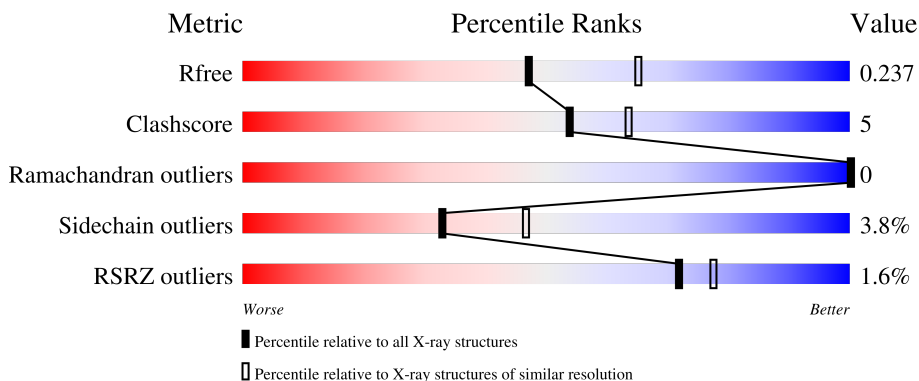|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.30 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	Percentile Ranks	Value
Rfree		0.237
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		3.8%
RSRZ outliers		1.6%

Worse ⟶ *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	421	88% ... 10% ··
1	B	421	81% ... 15% ··

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 7336 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	416	Total 3405	C 2180	N 580	O 622	S 23	0	4	0
1	B	412	Total 3370	C 2158	N 573	O 618	S 21	0	3	0

There are 4 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
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
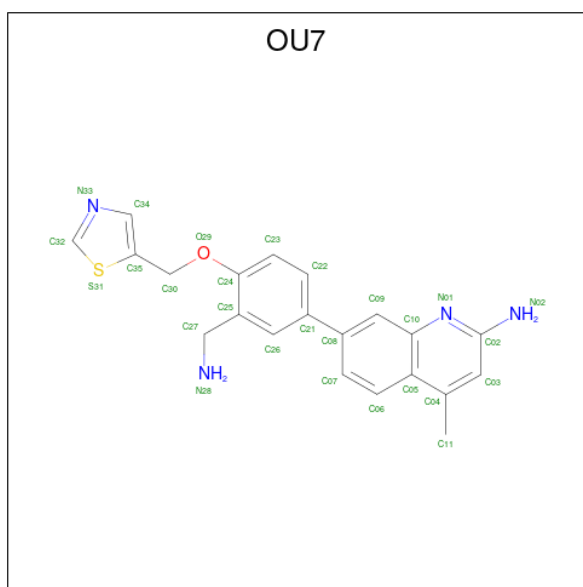
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).
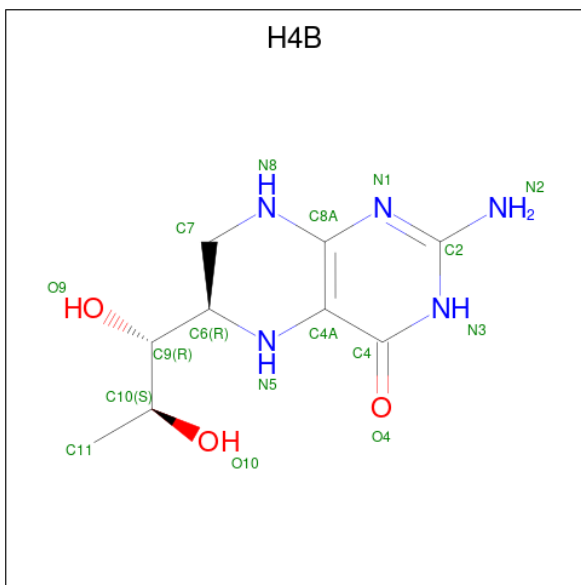
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 7-{3-(aminomethyl)-4-[(1,3-thiazol-5-yl)methoxy]phenyl}-4-methylquinolin-2-amine (three-letter code: OU7) (formula: $C_{21}H_{20}N_4OS$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	21	4	1	1		
4	B	1	Total	C	N	O	S	0	0
			27	21	4	1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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		

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

• Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

• Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	199	Total 199	O 199	0	0
7	B	169	Total 169	O 169	0	0

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: Nitric oxide synthase, brain

Chain A:

• Molecule 1: Nitric oxide synthase, brain

Chain B:
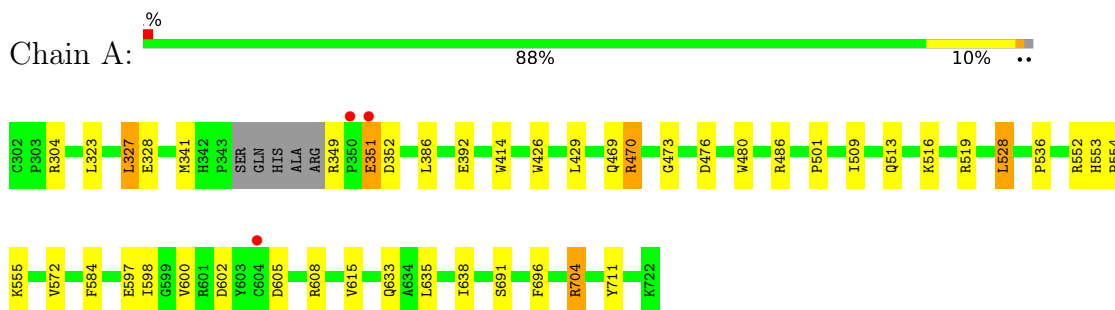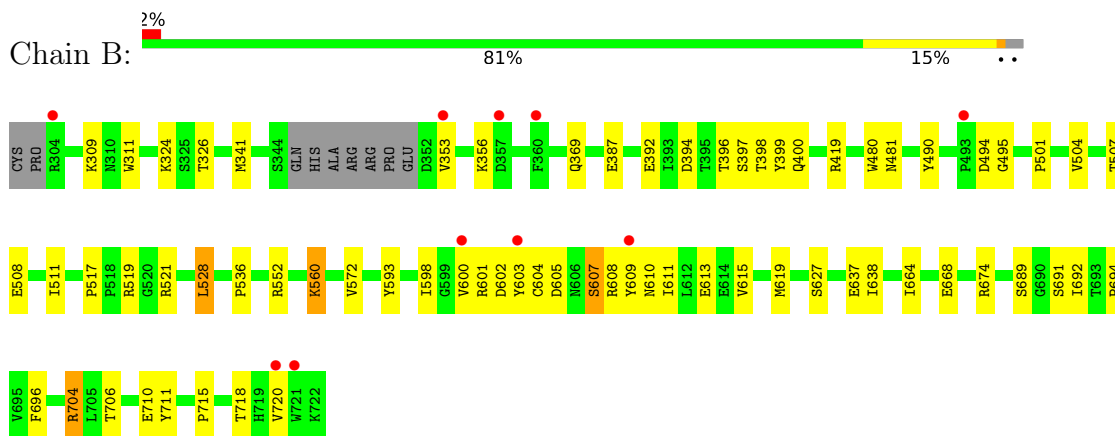
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.37Å 122.76Å 164.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.24 – 2.30 68.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.8 (68.24-2.30) 93.6 (68.24-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1496: ???)	Depositor
R, R_{free}	0.177 , 0.239 0.176 , 0.237	Depositor DCC
R_{free} test set	2185 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7336	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL, H4B, HEM, OU7

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	0.38	0/3514	0.55	1/4769 (0.0%)
1	B	0.36	0/3474	0.52	0/4712
All	All	0.37	0/6988	0.54	1/9481 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	LEU	CA-CB-CG	6.04	129.20	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3405	0	3320	29	0
1	B	3370	0	3281	39	0
2	A	43	0	30	1	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	2	0
4	A	27	0	0	3	0
4	B	27	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	16	1	0
5	B	6	0	8	1	0
6	B	1	0	0	0	0
7	A	199	0	0	7	1
7	B	169	0	0	5	1
All	All	7336	0	6715	72	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 5.

All (72) 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:528:LEU:HD22	1:A:536:PRO:HB2	1.59	0.84
2:B:802:HEM:HHC	2:B:802:HEM:HBB2	1.66	0.78
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.69	0.75
1:A:470:ARG:HD3	1:A:476:ASP:OD1	1.92	0.70
1:B:605:ASP:HB2	1:B:608:ARG:HG2	1.74	0.69
1:B:610:ASN:O	7:B:901:HOH:O	2.11	0.68
1:B:664:ILE:O	1:B:668[B]:GLU:HG2	1.95	0.67
4:A:803:OU7:N33	7:A:904:HOH:O	2.29	0.65
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.81	0.63
1:A:486:ARG:NE	7:A:908:HOH:O	2.34	0.61
1:A:598:ILE:HA	1:A:602:ASP:HB2	1.83	0.60
1:A:572:VAL:HG21	4:A:803:OU7:C07	2.31	0.60
1:B:572:VAL:HG21	4:B:804:OU7:C07	2.33	0.58
1:A:711:TYR:OH	2:A:801:HEM:O2D	2.17	0.58
1:B:601:ARG:HH12	3:B:803:H4B:C4	2.17	0.57
1:A:349:ARG:HG2	1:A:351:GLU:H	1.68	0.57
1:A:516:LYS:NZ	7:A:911:HOH:O	2.38	0.56
1:B:605:ASP:HB2	1:B:608:ARG:CG	2.34	0.56
4:B:804:OU7:N28	7:B:909:HOH:O	2.33	0.55
1:B:711:TYR:OH	2:B:802:HEM:O2D	2.22	0.55
1:B:341:MET:HE2	3:B:803:H4B:H9	1.88	0.55
1:B:400:GLN:OE1	7:B:902:HOH:O	2.18	0.54
1:A:555:LYS:NZ	7:A:912:HOH:O	2.43	0.52
1:B:598:ILE:HA	1:B:602:ASP:HB2	1.91	0.52
1:A:304:ARG:HG3	1:A:323:LEU:HD11	1.92	0.51
1:B:674:ARG:HE	5:B:805:GOL:H31	1.74	0.51
1:B:398:THR:OG1	1:B:399:TYR:N	2.45	0.50
1:B:593:TYR:CD1	1:B:598:ILE:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLU:OE2	7:A:902:HOH:O	2.20	0.49
1:A:615:VAL:HG21	1:A:638:ILE:HD11	1.95	0.49
1:A:605:ASP:OD1	7:A:901:HOH:O	2.19	0.49
1:A:470:ARG:HD2	1:A:473:GLY:HA2	1.94	0.48
1:B:704:ARG:NH2	1:B:710:GLU:OE2	2.46	0.48
1:B:689:SER:HB3	1:B:692:ILE:HD11	1.95	0.48
1:A:328:GLU:O	1:A:704:ARG:NH1	2.46	0.47
1:B:603:TYR:HA	1:B:609:TYR:HB2	1.96	0.47
1:A:349:ARG:HB3	1:A:352:ASP:OD2	2.14	0.47
1:A:429:LEU:O	5:A:805:GOL:H12	2.15	0.47
1:B:419:ARG:NH1	1:B:711:TYR:OH	2.47	0.47
1:B:341:MET:HE1	7:B:993:HOH:O	2.14	0.47
1:A:341:MET:HE1	7:A:967:HOH:O	2.15	0.46
1:B:490:TYR:CE1	1:B:519:ARG:HA	2.51	0.46
1:B:507:THR:O	1:B:511:ILE:HG13	2.16	0.46
1:B:664:ILE:HG13	1:B:694:PRO:HB2	1.97	0.46
2:B:802:HEM:HHC	2:B:802:HEM:CBB	2.41	0.46
1:A:600:VAL:HG13	1:A:635:LEU:HD11	1.98	0.45
1:A:469:GLN:HB3	1:A:584:PHE:CE2	2.52	0.45
1:B:511:ILE:HG12	1:B:517:PRO:HG3	1.97	0.45
1:B:611:ILE:O	1:B:615:VAL:HG23	2.16	0.45
1:A:509:ILE:O	1:A:513:GLN:HG2	2.17	0.45
1:A:691:SER:HA	1:A:696:PHE:CG	2.52	0.45
1:B:495:GLY:O	7:B:903:HOH:O	2.21	0.45
1:A:501:PRO:HG2	1:A:608:ARG:O	2.17	0.44
1:A:553:HIS:CG	1:A:554:PRO:HD2	2.53	0.44
1:A:633:GLN:NE2	1:B:637:GLU:OE2	2.45	0.44
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.53	0.43
1:B:600:VAL:O	1:B:604:CYS:HB2	2.19	0.43
1:B:356:LYS:HG2	1:B:397:SER:HA	2.02	0.42
1:B:560:LYS:HB3	1:B:560:LYS:HE3	1.48	0.42
2:B:802:HEM:HBA2	4:B:804:OU7:C22	2.49	0.42
1:A:597:GLU:OE2	4:A:803:OU7:N02	2.53	0.42
1:A:528:LEU:HD23	1:A:528:LEU:HA	1.91	0.41
1:B:607:SER:O	1:B:608:ARG:HD2	2.21	0.41
1:B:601:ARG:O	1:B:608:ARG:HG3	2.21	0.41
1:B:615:VAL:O	1:B:619:MET:HG3	2.20	0.41
1:B:691:SER:HA	1:B:696:PHE:CG	2.56	0.41
1:B:615:VAL:HG21	1:B:638:ILE:HD11	2.03	0.41
1:B:309:LYS:HE2	1:B:311:TRP:CE3	2.56	0.40
1:B:480:TRP:CE2	1:B:715:PRO:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLU:O	1:B:396:THR:OG1	2.32	0.40
1:B:501:PRO:HA	1:B:504:VAL:HG23	2.03	0.40
1:B:704:ARG:HE	1:B:704:ARG:HB3	1.50	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)
7:A:949:HOH:O	7:B:987:HOH:O[4_499]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	416/421 (99%)	402 (97%)	14 (3%)	0	100	100
1	B	411/421 (98%)	396 (96%)	15 (4%)	0	100	100
All	All	827/842 (98%)	798 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	376/376 (100%)	368 (98%)	8 (2%)	53	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	371/376 (99%)	351 (95%)	20 (5%)	22	30
All	All	747/752 (99%)	719 (96%)	28 (4%)	33	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	LEU
1	A	351	GLU
1	A	386	LEU
1	A	470	ARG
1	A	519	ARG
1	A	528	LEU
1	A	552	ARG
1	A	704	ARG
1	B	324	LYS
1	B	326	THR
1	B	353	VAL
1	B	369	GLN
1	B	387	GLU
1	B	394	ASP
1	B	481	ASN
1	B	494	ASP
1	B	508	GLU
1	B	521	ARG
1	B	528	LEU
1	B	552	ARG
1	B	560	LYS
1	B	607	SER
1	B	613	GLU
1	B	627	SER
1	B	704	ARG
1	B	706	THR
1	B	718	THR
1	B	720	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	606	ASN
1	B	633	GLN
1	B	712	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	OU7	B	804	-	28,30,30	1.09	4 (14%)	35,42,42	3.04	14 (40%)
5	GOL	A	805	-	5,5,5	0.47	0	5,5,5	0.84	0
2	HEM	A	801	1	41,50,50	1.40	3 (7%)	45,82,82	1.49	8 (17%)
3	H4B	A	802	-	16,18,18	0.87	1 (6%)	11,26,26	2.54	7 (63%)
5	GOL	B	805	-	5,5,5	0.41	0	5,5,5	0.48	0
4	OU7	A	803	-	28,30,30	0.87	1 (3%)	35,42,42	1.83	5 (14%)
2	HEM	B	802	1	41,50,50	1.47	5 (12%)	45,82,82	1.64	9 (20%)
5	GOL	A	804	-	5,5,5	0.39	0	5,5,5	0.66	0
3	H4B	B	803	-	16,18,18	0.95	0	11,26,26	2.40	6 (54%)

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
4	OU7	B	804	-	-	3/9/20/20	0/4/4/4
5	GOL	A	805	-	-	4/4/4/4	-
2	HEM	A	801	1	-	0/12/54/54	-
3	H4B	A	802	-	-	3/8/17/17	0/2/2/2
5	GOL	B	805	-	-	3/4/4/4	-
4	OU7	A	803	-	-	3/9/20/20	0/4/4/4
2	HEM	B	802	1	-	5/12/54/54	-
5	GOL	A	804	-	-	4/4/4/4	-
3	H4B	B	803	-	-	3/8/17/17	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3C-CAC	3.80	1.55	1.47
2	B	802	HEM	C3C-C2C	-3.71	1.35	1.40
2	B	802	HEM	C3C-CAC	3.64	1.55	1.47
2	A	801	HEM	C3C-C2C	-3.60	1.35	1.40
2	A	801	HEM	CAB-C3B	2.95	1.55	1.47
2	B	802	HEM	CAB-C3B	2.89	1.55	1.47
4	B	804	OU7	C02-N01	2.71	1.36	1.33
4	B	804	OU7	C05-C10	-2.26	1.38	1.42
4	B	804	OU7	C04-C05	-2.18	1.38	1.42
4	B	804	OU7	C30-C35	2.14	1.53	1.50
3	A	802	H4B	C4A-C4	-2.07	1.38	1.41
2	B	802	HEM	CMC-C2C	2.07	1.56	1.51
2	B	802	HEM	CMD-C2D	2.06	1.55	1.50
4	A	803	OU7	C05-C10	-2.03	1.39	1.42

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	804	OU7	O29-C24-C25	9.21	127.82	115.78
4	B	804	OU7	C30-O29-C24	7.66	132.85	117.76
4	B	804	OU7	C34-N33-C32	7.09	116.85	105.78
4	A	803	OU7	C34-N33-C32	6.71	116.25	105.78
2	A	801	HEM	CBA-CAA-C2A	-5.57	103.11	112.62
3	A	802	H4B	C8A-C4A-C4	4.67	118.72	114.57
2	B	802	HEM	C4B-CHC-C1C	4.51	128.51	122.56
4	A	803	OU7	O29-C24-C25	4.40	121.53	115.78
4	B	804	OU7	C04-C05-C10	4.34	120.36	118.01
4	A	803	OU7	C04-C05-C10	4.30	120.34	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	804	OU7	O29-C24-C23	-4.25	114.77	123.97
3	B	803	H4B	C8A-C4A-C4	4.23	118.32	114.57
4	B	804	OU7	C05-C10-N01	-4.19	118.36	122.81
2	B	802	HEM	CBA-CAA-C2A	-3.82	106.11	112.62
3	B	803	H4B	N1-C2-N3	-3.43	120.04	125.42
3	A	802	H4B	N1-C2-N3	-3.36	120.14	125.42
3	A	802	H4B	C2-N3-C4	3.28	121.14	115.93
4	A	803	OU7	C05-C10-N01	-3.25	119.36	122.81
2	B	802	HEM	C4D-ND-C1D	3.21	108.39	105.07
4	B	804	OU7	C03-C04-C05	2.94	120.68	117.78
3	B	803	H4B	C2-N3-C4	2.91	120.55	115.93
4	B	804	OU7	N02-C02-N01	2.84	120.61	118.26
2	A	801	HEM	CAD-CBD-CGD	-2.72	107.74	113.60
2	B	802	HEM	C3D-C4D-ND	-2.67	107.20	110.17
3	B	803	H4B	C2-N1-C8A	2.65	120.49	114.54
3	A	802	H4B	C4-C4A-N5	2.63	121.33	119.12
3	B	803	H4B	N2-C2-N3	2.59	121.28	117.25
3	A	802	H4B	N2-C2-N3	2.53	121.18	117.25
4	B	804	OU7	C27-C25-C24	2.49	124.99	120.12
3	B	803	H4B	C4-C4A-N5	2.49	121.21	119.12
2	B	802	HEM	CHA-C4D-ND	2.47	127.43	124.38
3	A	802	H4B	C2-N1-C8A	2.45	120.04	114.54
4	B	804	OU7	C06-C05-C04	-2.43	119.02	123.66
2	B	802	HEM	CAD-CBD-CGD	-2.42	108.39	113.60
2	A	801	HEM	CMC-C2C-C3C	2.41	129.18	124.68
2	B	802	HEM	CMA-C3A-C4A	-2.39	124.79	128.46
4	B	804	OU7	C07-C08-C21	-2.32	117.33	121.36
4	B	804	OU7	C27-C25-C26	-2.29	116.31	120.38
2	A	801	HEM	CHD-C1D-ND	2.12	126.74	124.43
4	B	804	OU7	C09-C10-N01	2.12	121.94	118.72
4	A	803	OU7	O29-C24-C23	-2.12	119.39	123.97
3	A	802	H4B	C4A-N5-C6	-2.09	115.48	121.16
2	B	802	HEM	C2D-C1D-ND	-2.08	107.39	109.88
2	A	801	HEM	C4B-CHC-C1C	2.07	125.29	122.56
2	A	801	HEM	C3B-C2B-C1B	2.07	108.02	106.49
2	B	802	HEM	C3B-C2B-C1B	2.06	108.02	106.49
4	B	804	OU7	C06-C05-C10	2.04	120.61	118.33
2	A	801	HEM	CHA-C4D-ND	2.04	126.90	124.38
2	A	801	HEM	CMA-C3A-C4A	-2.01	125.37	128.46

There are no chirality outliers.

All (28) torsion outliers are listed below:

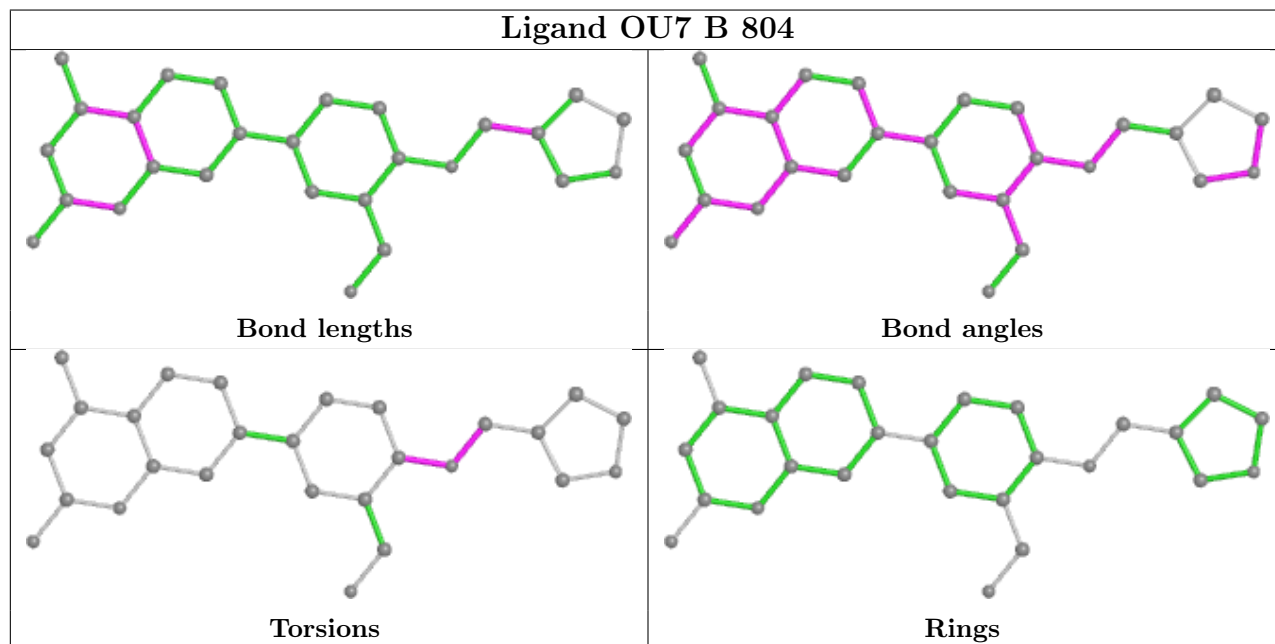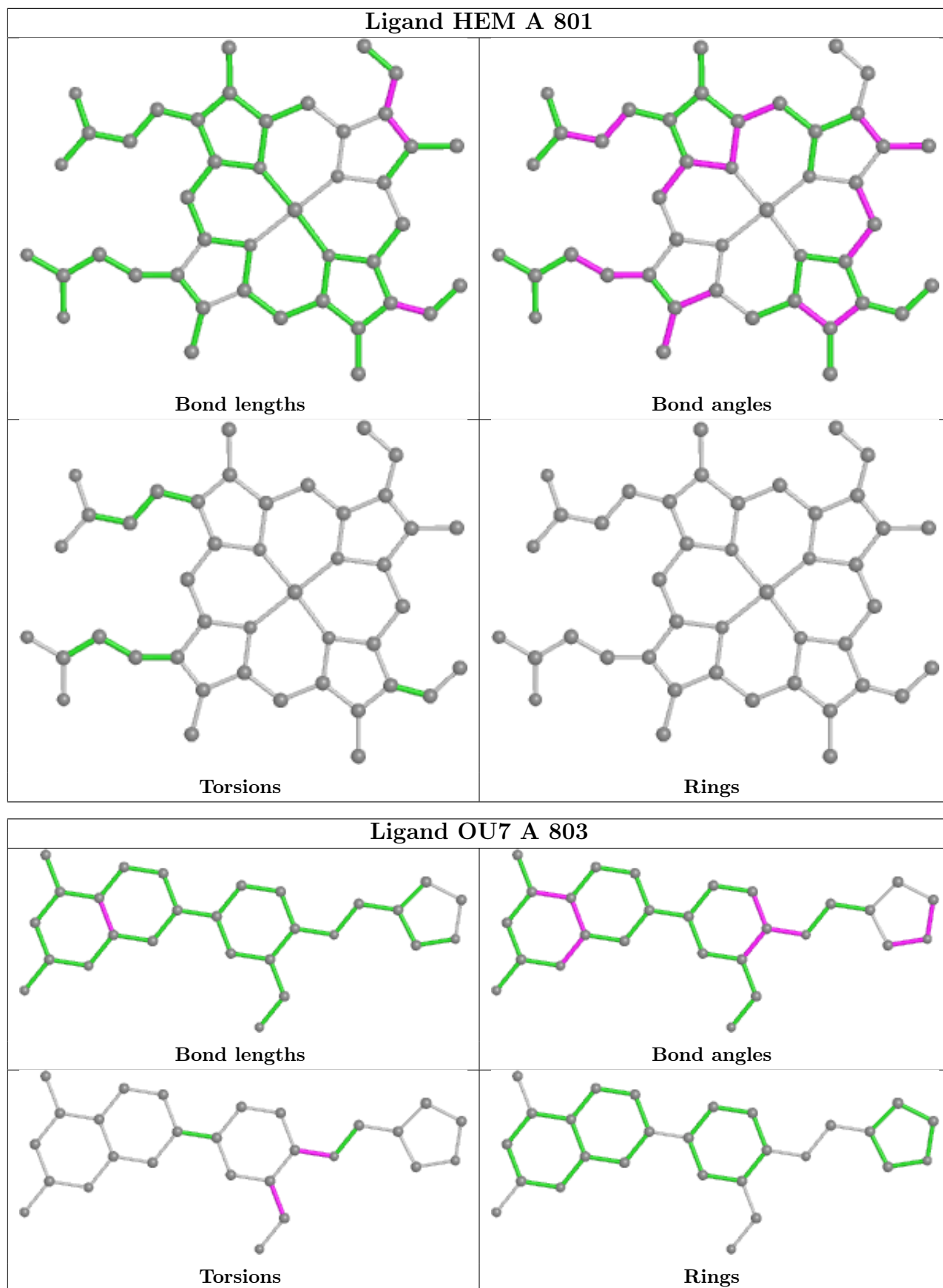| Mol	Chain	Res	Type	Atoms
5	A	804	GOL	O1-C1-C2-O2
5	A	804	GOL	O1-C1-C2-C3
5	A	804	GOL	C1-C2-C3-O3
5	A	805	GOL	O1-C1-C2-C3
5	B	805	GOL	O1-C1-C2-C3
4	B	804	OU7	C25-C24-O29-C30
4	B	804	OU7	C23-C24-O29-C30
5	A	805	GOL	O1-C1-C2-O2
5	A	805	GOL	O2-C2-C3-O3
5	A	805	GOL	C1-C2-C3-O3
5	B	805	GOL	O1-C1-C2-O2
3	A	802	H4B	C7-C6-C9-O9
3	B	803	H4B	C7-C6-C9-O9
5	A	804	GOL	O2-C2-C3-O3
3	B	803	H4B	C7-C6-C9-C10
4	A	803	OU7	C23-C24-O29-C30
4	B	804	OU7	C35-C30-O29-C24
3	A	802	H4B	C7-C6-C9-C10
4	A	803	OU7	C25-C24-O29-C30
4	A	803	OU7	C24-C25-C27-N28
2	B	802	HEM	CAD-CBD-CGD-O2D
2	B	802	HEM	CAA-CBA-CGA-O2A
2	B	802	HEM	C4B-C3B-CAB-CBB
2	B	802	HEM	CAA-CBA-CGA-O1A
2	B	802	HEM	CAD-CBD-CGD-O1D
3	A	802	H4B	N5-C6-C9-O9
3	B	803	H4B	N5-C6-C9-O9
5	B	805	GOL	O2-C2-C3-O3

There are no ring outliers.

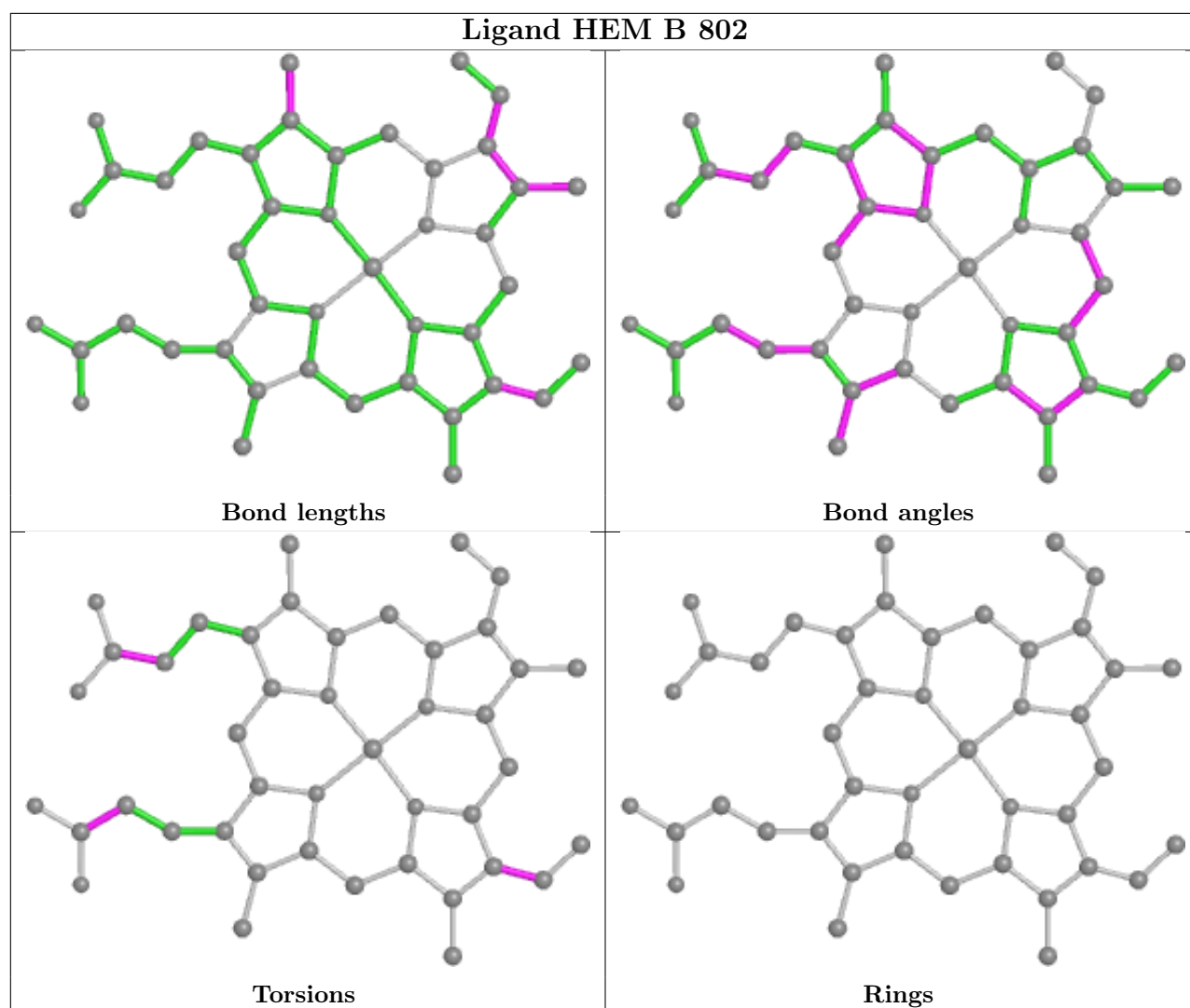7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	804	OU7	3	0
5	A	805	GOL	1	0
2	A	801	HEM	1	0
5	B	805	GOL	1	0
4	A	803	OU7	3	0
2	B	802	HEM	4	0
3	B	803	H4B	2	0

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

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand OU7 B 804

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 801

Bond lengths

Bond angles

Torsions

Rings

Ligand OU7 A 803

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 802

Bond lengths

Bond angles

Torsions

Rings

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 ⓘ

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	416/421 (98%)	-0.19	3 (0%)	87	91	31, 49, 85, 146	0
1	B	412/421 (97%)	-0.06	10 (2%)	59	66	35, 59, 108, 140	0
All	All	828/842 (98%)	-0.13	13 (1%)	72	77	31, 53, 101, 146	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	GLU	5.2
1	A	350	PRO	5.2
1	B	721	TRP	3.9
1	B	360	PHE	3.8
1	B	357	ASP	3.2
1	B	603	TYR	3.2
1	A	604	CYS	2.8
1	B	720	VAL	2.8
1	B	304	ARG	2.7
1	B	600	VAL	2.7
1	B	493	PRO	2.5
1	B	353	VAL	2.2
1	B	609	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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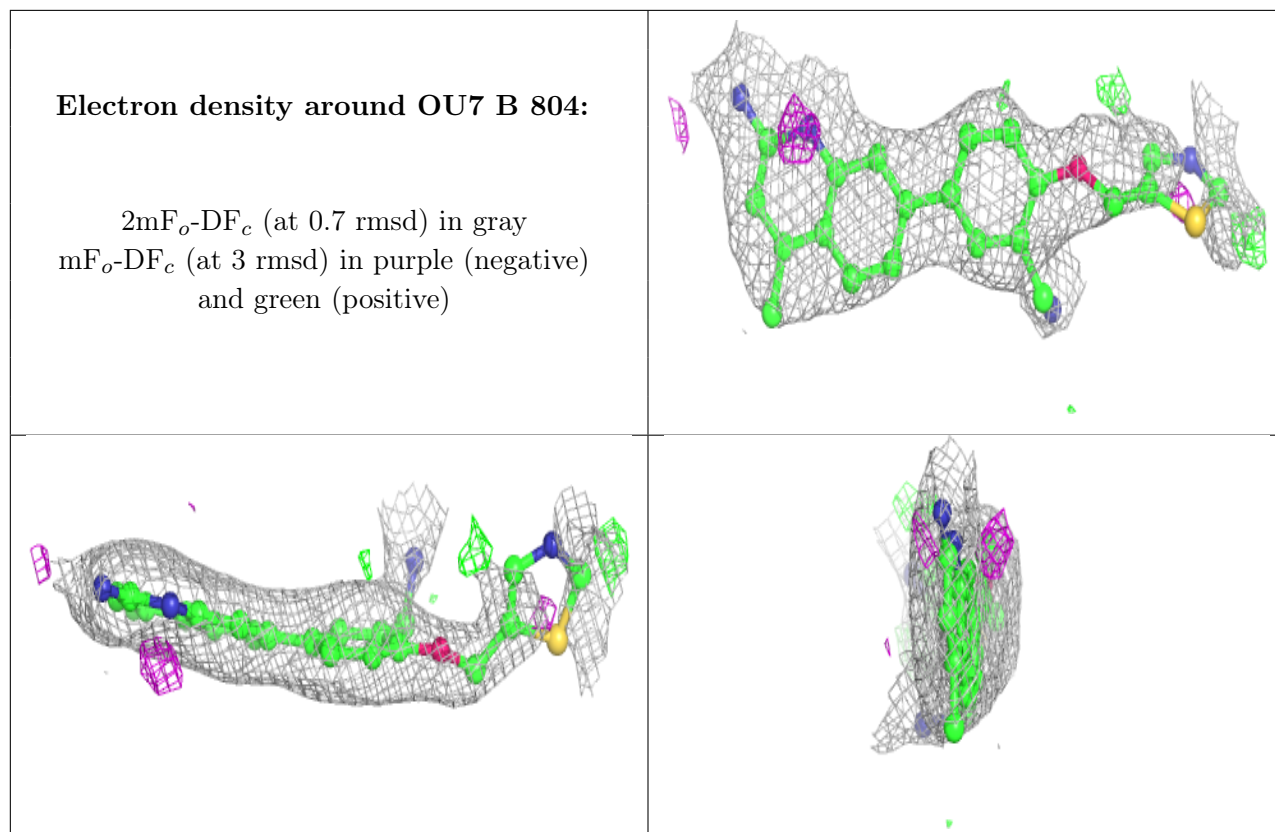
6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	804	6/6	0.80	0.27	61,66,73,78	0
5	GOL	B	805	6/6	0.82	0.15	72,75,77,78	0
5	GOL	A	805	6/6	0.87	0.19	50,60,65,71	0
3	H4B	B	803	17/17	0.90	0.24	60,78,100,103	0
4	OU7	B	804	27/27	0.92	0.18	30,66,138,142	0
3	H4B	A	802	17/17	0.92	0.15	39,62,73,75	0
4	OU7	A	803	27/27	0.93	0.16	44,66,117,121	0
2	HEM	B	802	43/43	0.98	0.13	30,43,59,75	0
2	HEM	A	801	43/43	0.98	0.12	26,38,60,75	0
6	ZN	B	801	1/1	0.99	0.14	51,51,51,51	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.
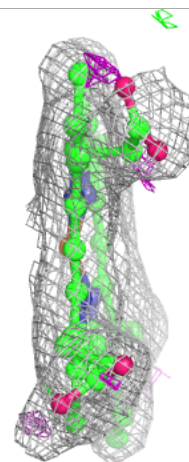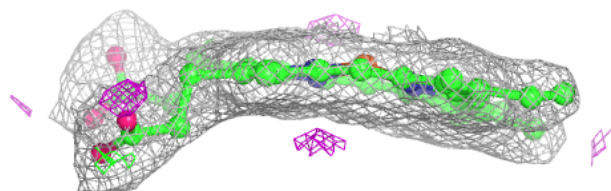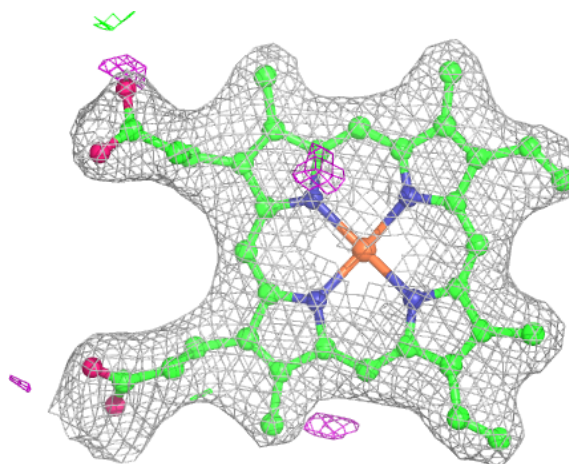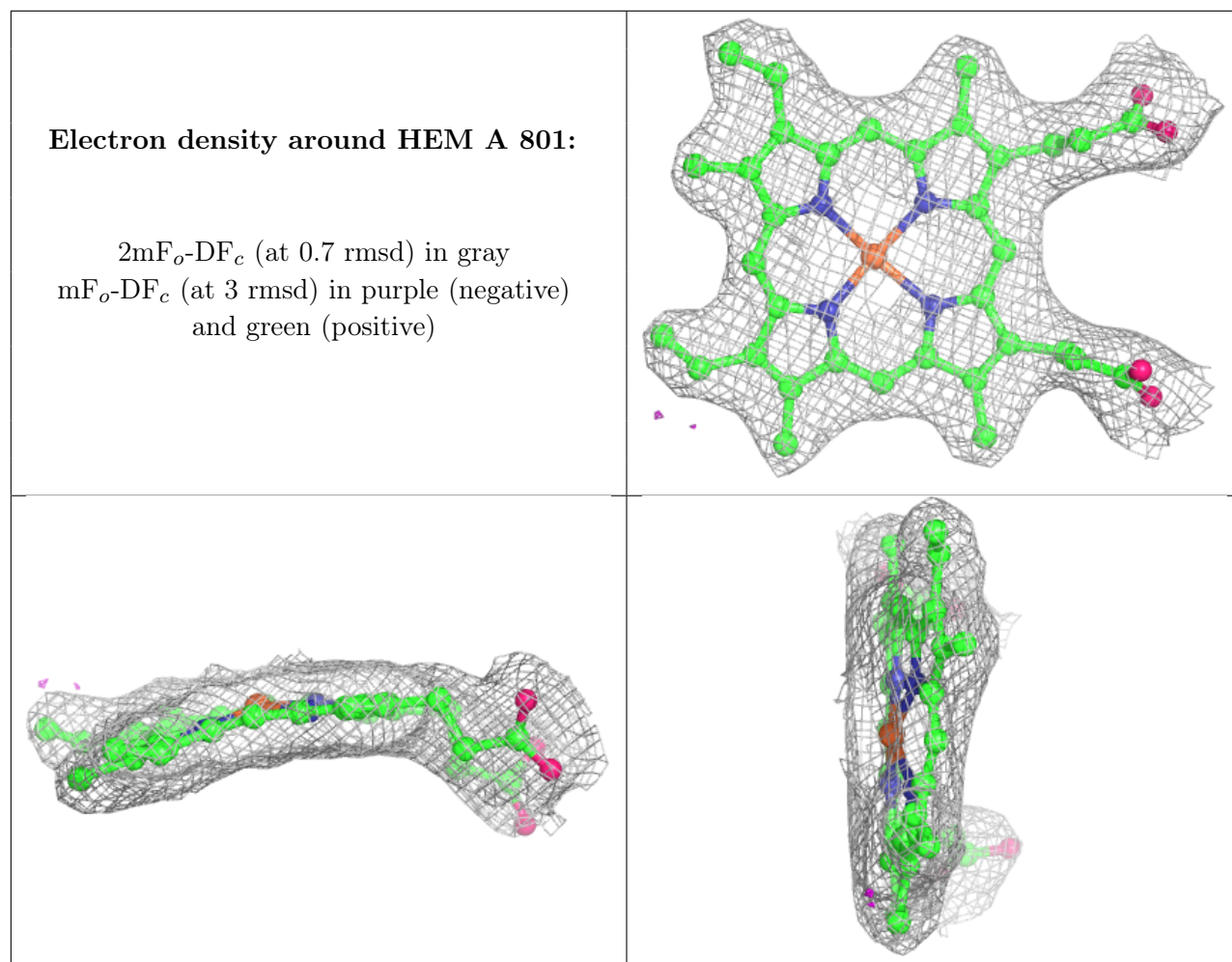
Electron density around OU7 B 804:

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

Electron density around OU7 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)
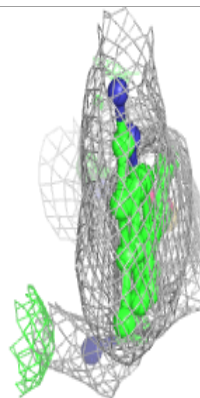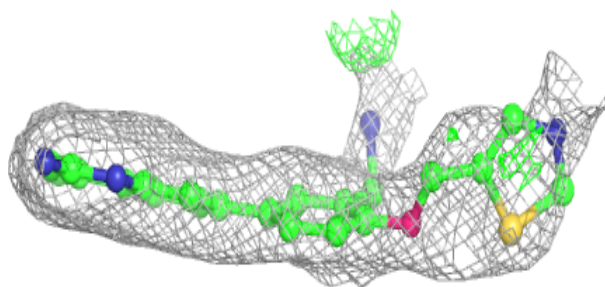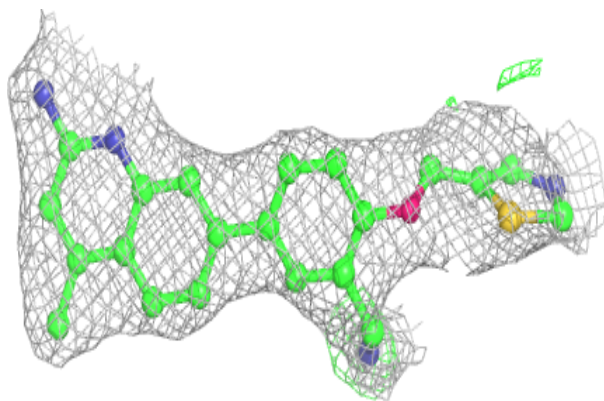
Electron density around HEM B 802:

$2mF_o$-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 ⓘ

There are no such residues in this entry.