



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 07:52 AM EDT

PDB ID : 4FVZ
Title : Structure of rat nNOS heme domain in complex with N(omega)-methyl- N(o
mega)-methoxy-L-arginine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2012-06-29
Resolution : 1.99 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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

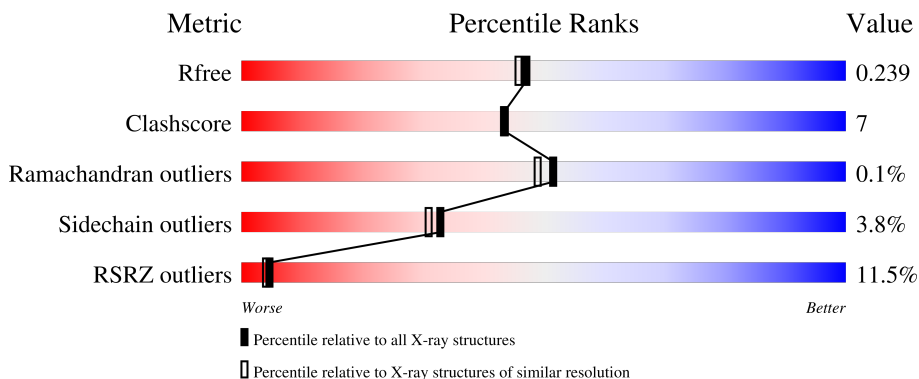
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

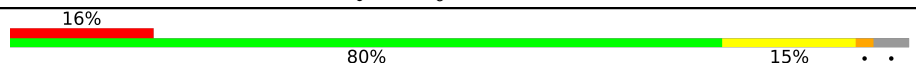
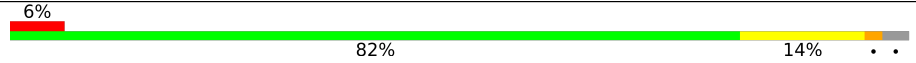
The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	422	
1	B	422	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7088 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
			Total	C	N	O	S			
1	A	407	Total 3318	C 2124	N 567	O 606	S 21	0	1	0
1	B	411	Total 3348	C 2142	N 574	O 610	S 22	0	1	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
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

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: C₉H₁₅N₅O₃).



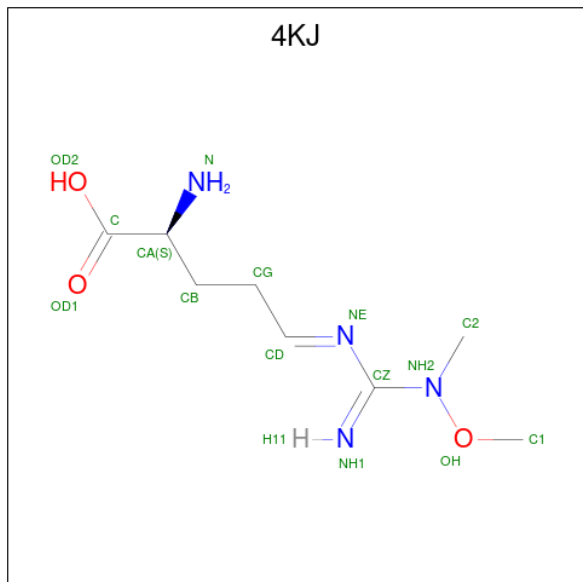
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
3	A	1	17	9	5	3	0	0
3	B	1	17	9	5	3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is (5E)-5-[(N-methoxy-N-methylcarbamimidoyl)imino]-L-norvaline (three-letter code: 4KJ) (formula: $C_8H_{16}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	8	4	3		
5	B	1	Total	C	N	O	0	0
			15	8	4	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

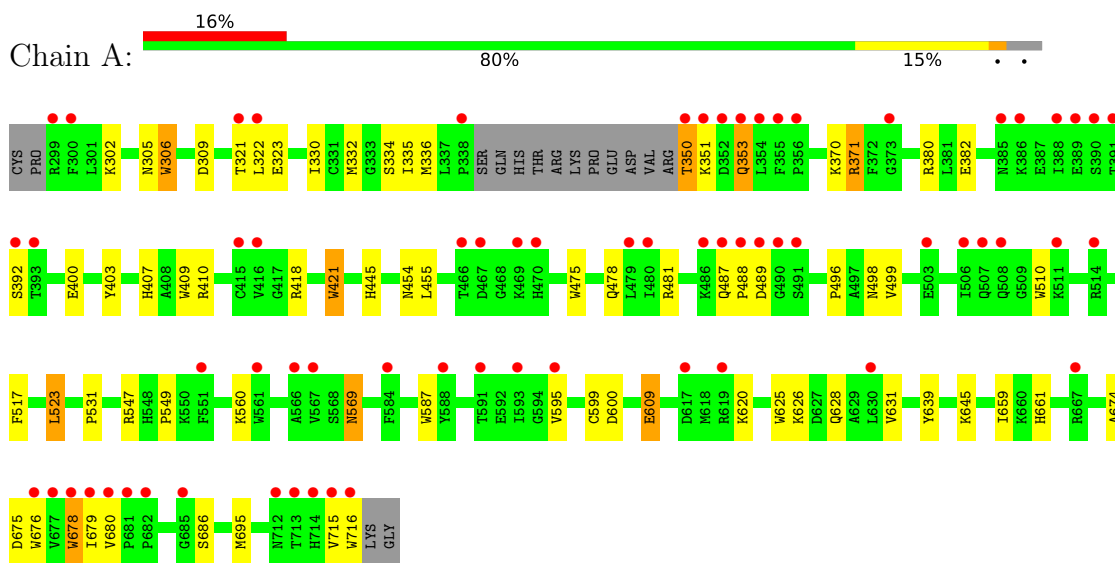
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	108	Total	O	0	0
			108	108		
7	B	155	Total	O	0	0
			155	155		

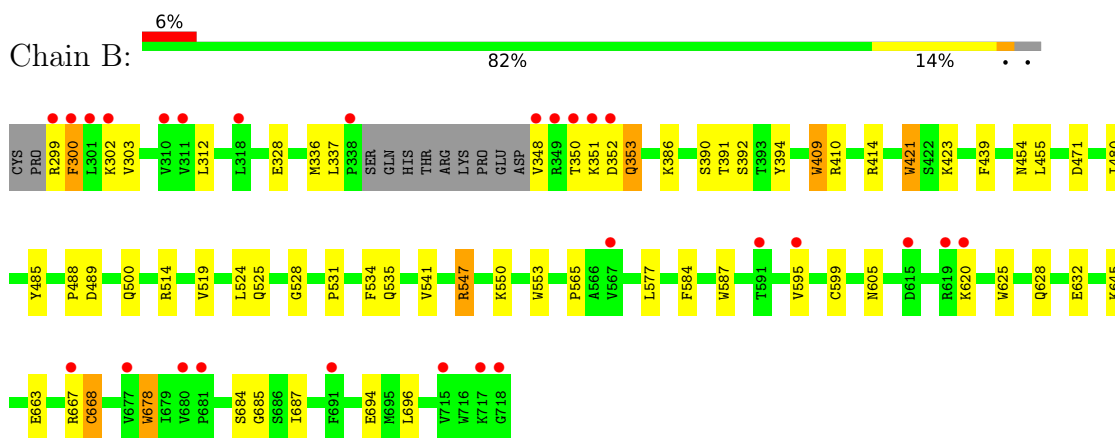
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, brain



- Molecule 1: Nitric oxide synthase, brain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.90Å 110.84Å 164.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.56 – 1.99 38.56 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.56-1.99) 98.4 (38.56-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.98Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.245 0.199 , 0.239	Depositor DCC
R_{free} test set	3217 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtrriage
Anisotropy	0.780	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7088	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: HEM, H4B, 4KJ, ACT, ZN

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	0.74	7/3414 (0.2%)	0.75	2/4632 (0.0%)
1	B	0.82	6/3444 (0.2%)	0.79	3/4669 (0.1%)
All	All	0.78	13/6858 (0.2%)	0.77	5/9301 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	TRP	CD2-CE2	5.86	1.48	1.41
1	A	678	TRP	CD2-CE2	5.85	1.48	1.41
1	B	678	TRP	CD2-CE2	5.79	1.48	1.41
1	B	421	TRP	CD2-CE2	5.75	1.48	1.41
1	B	625	TRP	CD2-CE2	5.35	1.47	1.41
1	A	421	TRP	CD2-CE2	5.34	1.47	1.41
1	B	488	PRO	C-O	-5.34	1.12	1.23
1	A	306	TRP	CD2-CE2	5.31	1.47	1.41
1	A	510	TRP	CD2-CE2	5.23	1.47	1.41
1	A	475	TRP	CD2-CE2	5.18	1.47	1.41
1	A	716	TRP	CD2-CE2	5.16	1.47	1.41
1	B	553	TRP	CD2-CE2	5.08	1.47	1.41
1	A	625	TRP	CD2-CE2	5.04	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	A	418	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	410	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	B	471	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	489	ASP	CB-CG-OD2	5.25	123.02	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3227	53	0
1	B	3348	0	3264	43	0
2	A	43	0	30	4	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	15	0	14	2	0
5	B	15	0	14	2	0
6	A	1	0	0	0	0
7	A	108	0	0	2	0
7	B	155	0	0	4	0
All	All	7088	0	6615	90	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 7.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668[B]:CYS:SG	7:B:1054:HOH:O	2.31	0.87
1:A:332:MET:CE	1:A:335:ILE:HG13	2.12	0.80
1:A:371:ARG:CG	1:A:371:ARG:HH21	1.96	0.78
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.69	0.73
1:B:595:VAL:O	1:B:599:CYS:HB2	1.90	0.72
1:B:353:GLN:HE21	1:B:353:GLN:H	1.36	0.72
1:B:663:GLU:O	1:B:667:ARG:HD2	1.89	0.72
1:A:332:MET:HE3	1:A:335:ILE:HG13	1.73	0.71
1:A:350:THR:N	1:A:353:GLN:NE2	2.39	0.71
1:B:353:GLN:H	1:B:353:GLN:NE2	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:PRO:HG2	5:B:803:4KJ:H13	1.76	0.66
1:B:391:THR:O	1:B:392:SER:HB2	1.94	0.66
1:A:332:MET:HE2	1:A:335:ILE:HG13	1.77	0.65
1:A:481:ARG:HD3	1:A:498:ASN:HD21	1.60	0.65
5:A:804:4KJ:OH	5:A:804:4KJ:H10	1.98	0.62
1:A:371:ARG:HH21	1:A:371:ARG:HG2	1.63	0.61
1:A:321:THR:HG23	1:A:322:LEU:HG	1.85	0.58
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.62	0.58
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.85	0.58
1:A:371:ARG:HG2	1:A:371:ARG:NH2	2.19	0.57
1:A:661:HIS:ND1	7:A:1008:HOH:O	2.33	0.57
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.88	0.55
1:A:321:THR:HG23	1:A:322:LEU:H	1.71	0.55
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.07	0.54
1:B:300:PHE:N	1:B:300:PHE:CD1	2.74	0.54
1:B:300:PHE:H	1:B:300:PHE:HD1	1.55	0.54
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.72	0.53
1:A:631:VAL:HG11	1:B:628:GLN:CG	2.38	0.53
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.91	0.53
1:A:323:GLU:HG2	1:B:328:GLU:HB3	1.90	0.52
1:A:517:PHE:HB2	1:A:560:LYS:HE3	1.90	0.52
2:A:801:HEM:C4B	5:A:804:4KJ:H14	2.44	0.52
2:A:801:HEM:HMC1	2:A:801:HEM:HBC2	1.93	0.51
1:A:569:ASN:HD22	1:A:569:ASN:H	1.58	0.50
1:B:525:GLN:HE21	1:B:528:GLY:HA2	1.76	0.50
2:A:801:HEM:HBC2	2:A:801:HEM:CMC	2.42	0.49
1:B:348:VAL:HG13	1:B:348:VAL:O	2.12	0.49
1:A:321:THR:HA	7:A:938:HOH:O	2.14	0.48
1:A:332:MET:HE1	7:B:1046:HOH:O	2.12	0.48
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.96	0.48
1:B:584:PHE:CD1	2:B:801:HEM:HAC	2.48	0.48
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.95	0.48
1:B:587:TRP:H	2:B:801:HEM:HAB	1.79	0.48
1:A:336:MET:CE	1:A:678:TRP:HZ2	2.26	0.47
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.97	0.46
1:B:480:ILE:HA	7:B:906:HOH:O	2.15	0.46
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.51	0.45
1:A:675:ASP:O	1:A:679:ILE:HG12	2.16	0.45
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.98	0.45
1:A:481:ARG:HD3	1:A:498:ASN:ND2	2.29	0.45
1:B:605:ASN:ND2	7:B:904:HOH:O	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LYS:HE2	1:A:392:SER:HB3	2.00	0.44
1:A:569:ASN:H	1:A:569:ASN:ND2	2.15	0.44
1:A:306:TRP:CG	1:B:336:MET:HE1	2.53	0.44
1:A:332:MET:O	1:A:335:ILE:HG12	2.18	0.43
1:A:445:HIS:CD2	1:A:445:HIS:C	2.91	0.43
1:B:684:SER:O	1:B:685:GLY:C	2.56	0.43
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.06	0.43
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.54	0.43
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.00	0.43
1:B:584:PHE:CD1	2:B:801:HEM:CAC	3.02	0.43
5:B:803:4KJ:H16	5:B:803:4KJ:H10	2.00	0.43
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.99	0.43
1:B:302:LYS:HE3	1:B:302:LYS:HB2	1.70	0.43
1:B:350:THR:HG22	1:B:351:LYS:H	1.83	0.43
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.53	0.43
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.53	0.43
1:A:334:SER:O	1:B:694:GLU:HG2	2.19	0.42
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.54	0.42
1:B:684:SER:HB3	1:B:687:ILE:HG12	2.01	0.42
1:B:352:ASP:HB3	1:B:353:GLN:NE2	2.35	0.42
1:B:439:PHE:CD2	1:B:534:PHE:HB3	2.54	0.42
1:A:659:ILE:HD13	1:A:659:ILE:HA	1.94	0.42
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.53	0.42
1:A:595:VAL:O	1:A:599:CYS:HB2	2.20	0.41
1:B:524:LEU:O	1:B:531:PRO:HA	2.20	0.41
1:A:609:GLU:H	1:A:609:GLU:HG3	1.60	0.41
1:B:519:VAL:HG21	1:B:541:VAL:HG11	2.03	0.41
1:A:686:SER:OG	1:B:595:VAL:HG12	2.20	0.41
1:B:394:TYR:CE2	1:B:577:LEU:HD21	2.55	0.41
1:A:631:VAL:CG1	1:B:628:GLN:HG3	2.51	0.41
1:A:306:TRP:CD2	1:B:336:MET:CE	3.04	0.41
1:A:306:TRP:CD2	1:B:336:MET:HE1	2.56	0.40
1:A:599:CYS:O	1:A:600:ASP:C	2.60	0.40
1:B:547:ARG:H	1:B:547:ARG:HD3	1.86	0.40
1:A:305:ASN:O	1:A:309:ASP:N	2.54	0.40
1:B:303:VAL:HG23	1:B:312:LEU:HB2	2.03	0.40
1:B:386:LYS:HE2	1:B:386:LYS:HB3	1.90	0.40
1:A:382:GLU:OE1	1:A:382:GLU:HA	2.21	0.40
1:A:549:PRO:HB3	1:A:639:TYR:CE1	2.57	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	404/422 (96%)	387 (96%)	16 (4%)	1 (0%)	47	44
1	B	408/422 (97%)	395 (97%)	13 (3%)	0	100	100
All	All	812/844 (96%)	782 (96%)	29 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP

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	364/377 (97%)	351 (96%)	13 (4%)	35	34
1	B	367/377 (97%)	351 (96%)	16 (4%)	28	25
All	All	731/754 (97%)	702 (96%)	29 (4%)	33	29

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	LYS
1	A	350	THR
1	A	353	GLN
1	A	370	LYS
1	A	371	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	454	ASN
1	A	523	LEU
1	A	547	ARG
1	A	569	ASN
1	A	609	GLU
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	299	ARG
1	B	300	PHE
1	B	337	LEU
1	B	353	GLN
1	B	390	SER
1	B	423	LYS
1	B	454	ASN
1	B	455	LEU
1	B	500	GLN
1	B	535	GLN
1	B	547	ARG
1	B	550	LYS
1	B	620	LYS
1	B	645	LYS
1	B	668[A]	CYS
1	B	668[B]	CYS

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	353	GLN
1	A	454	ASN
1	A	507	GLN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	B	353	GLN
1	B	385	ASN
1	B	454	ASN
1	B	601	ASN
1	B	642	GLN
1	B	697	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	801	1	41,50,50	2.43	20 (48%)	45,82,82	3.46	22 (48%)
3	H4B	B	802	-	16,18,18	0.91	0	11,26,26	2.61	4 (36%)
4	ACT	A	803	-	3,3,3	0.82	0	3,3,3	0.56	0
3	H4B	A	802	-	16,18,18	0.93	0	11,26,26	3.02	7 (63%)
5	4KJ	B	803	-	11,14,14	2.47	3 (27%)	9,17,17	1.39	1 (11%)
4	ACT	B	804	-	3,3,3	0.83	0	3,3,3	0.38	0
2	HEM	A	801	1	41,50,50	2.43	19 (46%)	45,82,82	3.28	23 (51%)
5	4KJ	A	804	-	11,14,14	2.27	3 (27%)	9,17,17	1.40	2 (22%)

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
2	HEM	B	801	1	-	2/12/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	B	802	-	-	1/8/17/17	0/2/2/2
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
5	4KJ	B	803	-	-	2/10/17/17	-
2	HEM	A	801	1	-	0/12/54/54	-
5	4KJ	A	804	-	-	3/10/17/17	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3C-C2C	6.66	1.49	1.40
5	B	803	4KJ	OH-NH2	6.39	1.49	1.40
5	A	804	4KJ	OH-NH2	5.62	1.48	1.40
2	B	801	HEM	C3D-C2D	5.13	1.47	1.36
2	B	801	HEM	C3C-C2C	4.94	1.47	1.40
2	A	801	HEM	C3D-C2D	4.57	1.46	1.36
2	A	801	HEM	C1A-NA	4.34	1.45	1.36
2	B	801	HEM	C4A-NA	4.33	1.45	1.36
2	B	801	HEM	CHA-C4D	4.25	1.45	1.35
2	B	801	HEM	CHB-C1B	4.13	1.45	1.35
2	A	801	HEM	CHA-C4D	4.10	1.45	1.35
2	B	801	HEM	C3B-C2B	4.09	1.45	1.37
2	A	801	HEM	C4A-NA	3.96	1.44	1.36
2	B	801	HEM	C4D-ND	-3.79	1.33	1.40
2	A	801	HEM	C4D-ND	-3.77	1.33	1.40
2	A	801	HEM	CHB-C1B	3.52	1.44	1.35
5	B	803	4KJ	CG-CD	3.35	1.52	1.49
2	A	801	HEM	C3B-C2B	3.31	1.44	1.37
5	A	804	4KJ	CD-NE	3.28	1.38	1.26
2	B	801	HEM	C2A-C3A	3.19	1.47	1.37
2	B	801	HEM	C1A-NA	3.11	1.42	1.36
2	A	801	HEM	C2C-C1C	3.01	1.49	1.42
2	B	801	HEM	C3B-C4B	2.99	1.50	1.44
2	B	801	HEM	C1B-C2B	2.91	1.50	1.44
5	B	803	4KJ	CD-NE	2.88	1.37	1.26
2	A	801	HEM	FE-NB	2.87	2.11	1.96
2	B	801	HEM	FE-NB	2.83	2.10	1.96
2	B	801	HEM	FE-ND	2.72	2.10	1.96
2	A	801	HEM	C2A-C3A	2.66	1.45	1.37
2	A	801	HEM	O2D-CGD	-2.63	1.21	1.30
2	A	801	HEM	C4A-CHB	2.60	1.48	1.41
5	A	804	4KJ	CG-CD	2.58	1.51	1.49
2	A	801	HEM	C1B-C2B	2.48	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1A-CHA	2.45	1.47	1.41
2	B	801	HEM	C4D-C3D	2.42	1.49	1.45
2	B	801	HEM	C2C-C1C	2.38	1.48	1.42
2	A	801	HEM	C1B-NB	-2.35	1.36	1.40
2	A	801	HEM	C3B-C4B	2.35	1.49	1.44
2	B	801	HEM	O2A-CGA	-2.30	1.23	1.30
2	B	801	HEM	C1B-NB	-2.25	1.36	1.40
2	A	801	HEM	CHC-C4B	2.19	1.47	1.41
2	A	801	HEM	C1D-ND	-2.13	1.34	1.38
2	B	801	HEM	C1D-ND	-2.10	1.34	1.38
2	A	801	HEM	FE-ND	2.08	2.07	1.96
2	B	801	HEM	CHC-C4B	2.08	1.47	1.41

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C3B-C2B-C1B	-9.23	99.64	106.49
2	B	801	HEM	C2B-C1B-NB	8.67	120.11	109.84
2	A	801	HEM	C3B-C2B-C1B	-8.65	100.07	106.49
2	B	801	HEM	C2D-C1D-ND	8.11	119.60	109.88
2	A	801	HEM	C2B-C1B-NB	7.72	118.99	109.84
2	B	801	HEM	C1D-C2D-C3D	-6.83	99.78	106.96
3	B	802	H4B	C8A-C4A-C4	6.76	120.58	114.57
2	A	801	HEM	CBA-CAA-C2A	-6.18	102.08	112.62
2	A	801	HEM	C2D-C1D-ND	5.94	117.00	109.88
2	A	801	HEM	C1D-C2D-C3D	-5.79	100.87	106.96
2	A	801	HEM	C3D-C4D-ND	5.76	116.58	110.17
2	B	801	HEM	CBA-CAA-C2A	-5.56	103.14	112.62
2	A	801	HEM	CMB-C2B-C1B	5.54	133.48	125.04
2	B	801	HEM	C3D-C4D-ND	5.54	116.33	110.17
2	B	801	HEM	C1B-NB-C4B	-5.35	99.55	105.07
2	B	801	HEM	C4A-C3A-C2A	-5.18	103.39	107.00
3	A	802	H4B	C8A-C4A-C4	4.75	118.79	114.57
2	A	801	HEM	CAD-CBD-CGD	-4.70	103.49	113.60
2	A	801	HEM	C1B-NB-C4B	-4.33	100.60	105.07
2	B	801	HEM	CHD-C1D-C2D	-4.23	118.36	124.98
2	A	801	HEM	CHA-C4D-C3D	-4.22	117.41	125.33
3	A	802	H4B	C2-N3-C4	4.19	122.59	115.93
3	A	802	H4B	N2-C2-N3	4.04	123.54	117.25
3	A	802	H4B	N1-C2-N3	-4.02	119.12	125.42
2	B	801	HEM	C4D-ND-C1D	-3.96	100.98	105.07
3	A	802	H4B	C4-C4A-N5	3.65	122.18	119.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CMD-C2D-C1D	3.61	130.53	125.04
2	A	801	HEM	CHB-C1B-NB	-3.37	120.22	124.38
2	A	801	HEM	CMC-C2C-C3C	3.34	130.93	124.68
2	B	801	HEM	CMB-C2B-C1B	3.09	129.75	125.04
2	B	801	HEM	C4B-C3B-C2B	-3.07	104.68	107.11
2	A	801	HEM	C4D-ND-C1D	-2.99	101.98	105.07
3	B	802	H4B	C4-C4A-N5	2.94	121.59	119.12
2	B	801	HEM	CHB-C1B-NB	-2.89	120.81	124.38
3	B	802	H4B	C2-N3-C4	2.89	120.51	115.93
2	B	801	HEM	CHB-C1B-C2B	-2.78	119.02	126.72
3	A	802	H4B	C2-N1-C8A	2.76	120.71	114.54
2	B	801	HEM	CMD-C2D-C1D	2.72	129.18	125.04
2	B	801	HEM	CHC-C4B-C3B	-2.72	120.41	124.57
5	A	804	4KJ	C1-OH-NH2	2.72	113.54	109.88
2	A	801	HEM	CAD-C3D-C2D	2.66	132.84	127.88
2	A	801	HEM	C4C-CHD-C1D	2.63	126.03	122.56
2	A	801	HEM	CHD-C1D-C2D	-2.60	120.91	124.98
2	B	801	HEM	CHA-C4D-ND	-2.60	121.17	124.38
2	A	801	HEM	CHC-C4B-C3B	-2.54	120.68	124.57
2	B	801	HEM	C4D-C3D-C2D	-2.50	103.25	106.90
2	B	801	HEM	CAD-CBD-CGD	-2.47	108.29	113.60
2	A	801	HEM	CBD-CAD-C3D	-2.39	105.99	112.63
5	A	804	4KJ	OD2-C-OD1	-2.37	118.71	124.09
2	A	801	HEM	CHD-C1D-ND	-2.35	121.88	124.43
2	A	801	HEM	C4D-C3D-C2D	-2.32	103.51	106.90
2	B	801	HEM	CBD-CAD-C3D	-2.32	106.19	112.63
2	B	801	HEM	CHD-C1D-ND	-2.24	121.99	124.43
2	A	801	HEM	CHB-C1B-C2B	-2.15	120.77	126.72
5	B	803	4KJ	OD2-C-CA	2.12	120.59	113.38
3	B	802	H4B	C4A-C4-N3	-2.08	118.11	124.01
3	A	802	H4B	C4A-C4-N3	-2.08	118.11	124.01
2	A	801	HEM	CAB-C3B-C2B	-2.04	121.90	128.60
2	B	801	HEM	CAD-C3D-C4D	2.02	128.19	124.66

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	804	4KJ	NE-CD-CG-CB
5	A	804	4KJ	C2-NH2-OH-C1
5	B	803	4KJ	NE-CD-CG-CB
5	B	803	4KJ	C2-NH2-OH-C1

Continued on next page...

Continued from previous page...

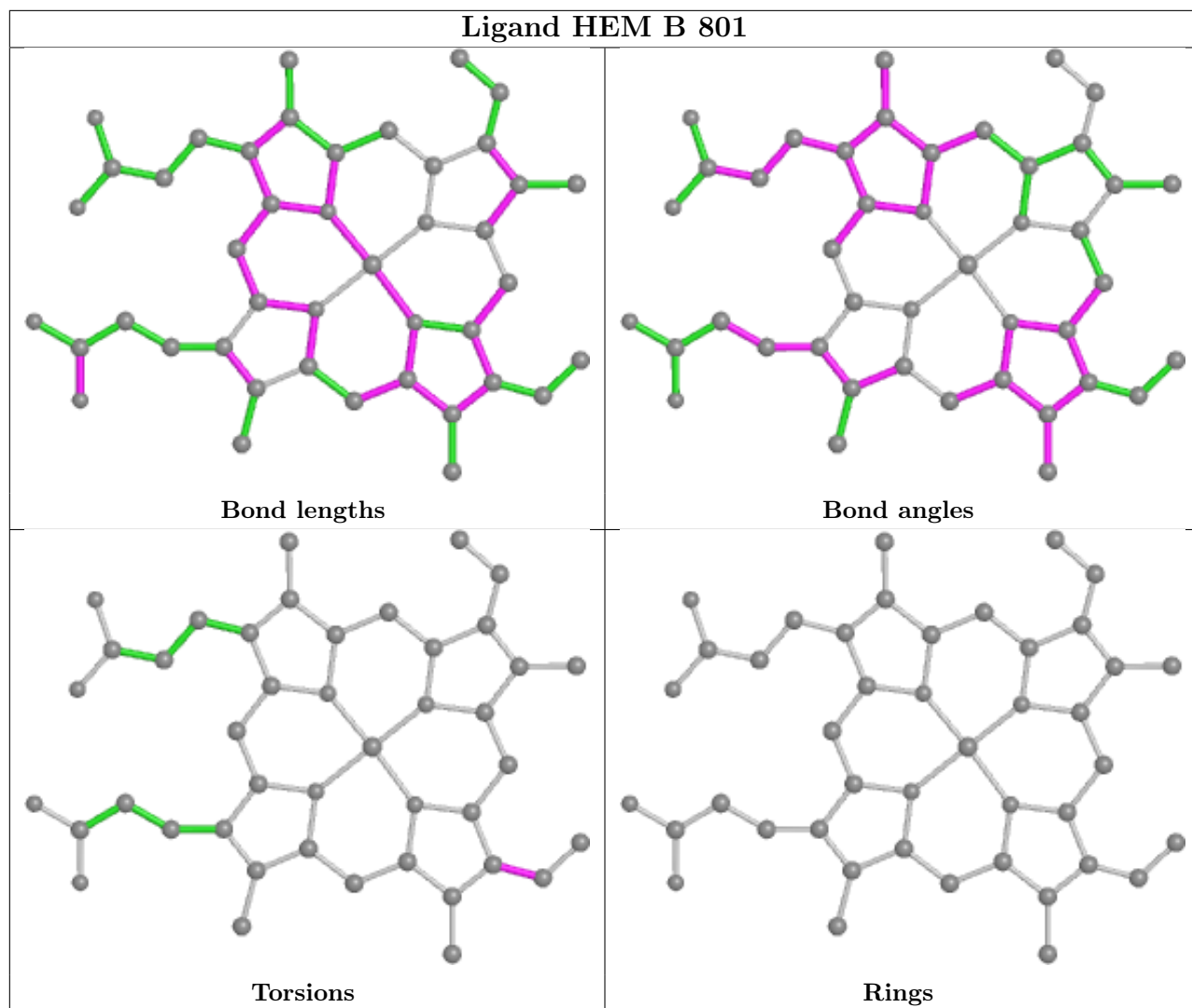
Mol	Chain	Res	Type	Atoms
2	B	801	HEM	C2B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
5	A	804	4KJ	CA-CB-CG-CD
3	B	802	H4B	N5-C6-C9-O9

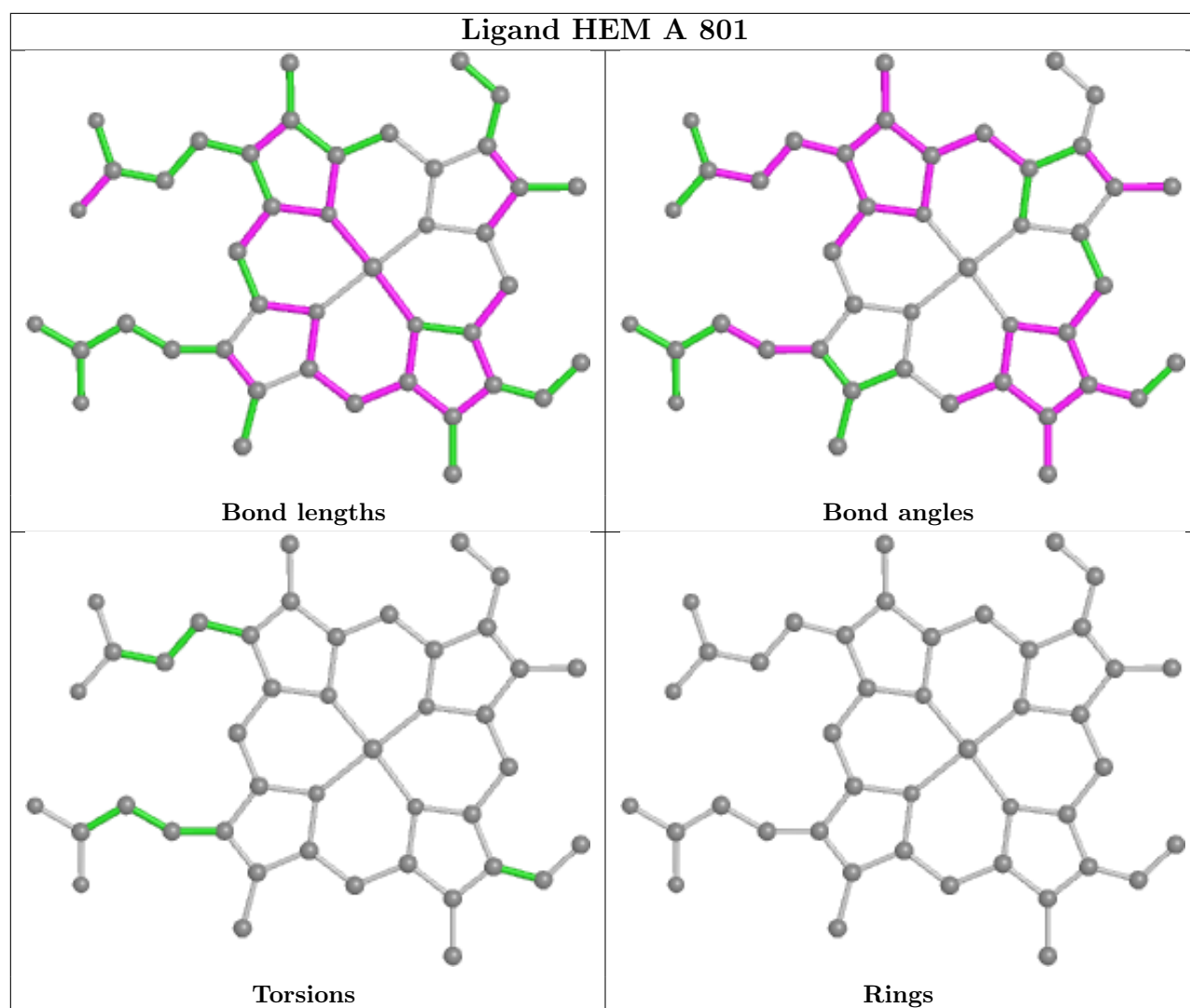
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	3	0
5	B	803	4KJ	2	0
2	A	801	HEM	4	0
5	A	804	4KJ	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 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	407/422 (96%)	0.89	67 (16%) 1 1	32, 58, 98, 128	0
1	B	411/422 (97%)	0.43	27 (6%) 18 17	32, 47, 77, 110	0
All	All	818/844 (96%)	0.66	94 (11%) 4 4	32, 52, 94, 128	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	9.2
1	B	350	THR	7.9
1	A	715	VAL	6.9
1	A	299	ARG	6.5
1	B	718	GLY	6.3
1	B	348	VAL	5.9
1	A	350	THR	5.3
1	A	355	PHE	5.0
1	B	619	ARG	4.8
1	A	716	TRP	4.8
1	A	352	ASP	4.6
1	A	351	LYS	4.5
1	B	299	ARG	4.3
1	A	488	PRO	4.3
1	A	506	ILE	4.2
1	A	300	PHE	4.2
1	B	352	ASP	4.1
1	B	351	LYS	4.0
1	A	712	ASN	3.9
1	A	567	VAL	3.7
1	A	713	THR	3.7
1	A	388	ILE	3.7
1	A	392	SER	3.6
1	B	620	LYS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	490	GLY	3.6
1	A	491	SER	3.5
1	B	715	VAL	3.5
1	B	301	LEU	3.5
1	A	391	THR	3.5
1	A	389	GLU	3.3
1	A	678	TRP	3.3
1	A	619	ARG	3.3
1	B	567	VAL	3.2
1	A	588	TYR	3.2
1	B	310	VAL	3.2
1	A	385	ASN	3.2
1	A	566	ALA	3.1
1	A	354	LEU	3.1
1	A	386	LYS	3.0
1	A	507	GLN	3.0
1	A	390	SER	3.0
1	A	682	PRO	3.0
1	A	470	HIS	3.0
1	A	486	LYS	3.0
1	A	591	THR	3.0
1	A	322	LEU	2.9
1	A	393	THR	2.9
1	A	667	ARG	2.9
1	A	489	ASP	2.9
1	B	349	ARG	2.9
1	B	677	VAL	2.9
1	A	503	GLU	2.9
1	A	415	CYS	2.9
1	A	584	PHE	2.9
1	A	487	GLN	2.8
1	A	679	ILE	2.8
1	B	615	ASP	2.7
1	A	681	PRO	2.7
1	A	676	TRP	2.6
1	A	321	THR	2.6
1	A	416	VAL	2.6
1	A	353	GLN	2.6
1	A	680	VAL	2.6
1	A	561	TRP	2.5
1	A	593	ILE	2.5
1	A	508	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	338	PRO	2.5
1	A	480	ILE	2.5
1	A	714	HIS	2.4
1	A	373	GLY	2.4
1	B	681	PRO	2.4
1	A	514	ARG	2.3
1	A	469	LYS	2.3
1	A	338	PRO	2.3
1	A	617	ASP	2.3
1	B	680	VAL	2.3
1	A	511	LYS	2.3
1	B	302	LYS	2.3
1	A	595	VAL	2.3
1	A	479	LEU	2.3
1	B	691	PHE	2.3
1	B	595	VAL	2.2
1	A	630	LEU	2.2
1	A	551	PHE	2.2
1	A	685	GLY	2.2
1	A	356	PRO	2.2
1	B	318	LEU	2.1
1	B	667	ARG	2.1
1	B	591	THR	2.1
1	A	467	ASP	2.1
1	B	717	LYS	2.1
1	A	466	THR	2.0
1	A	677	VAL	2.0
1	B	311	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

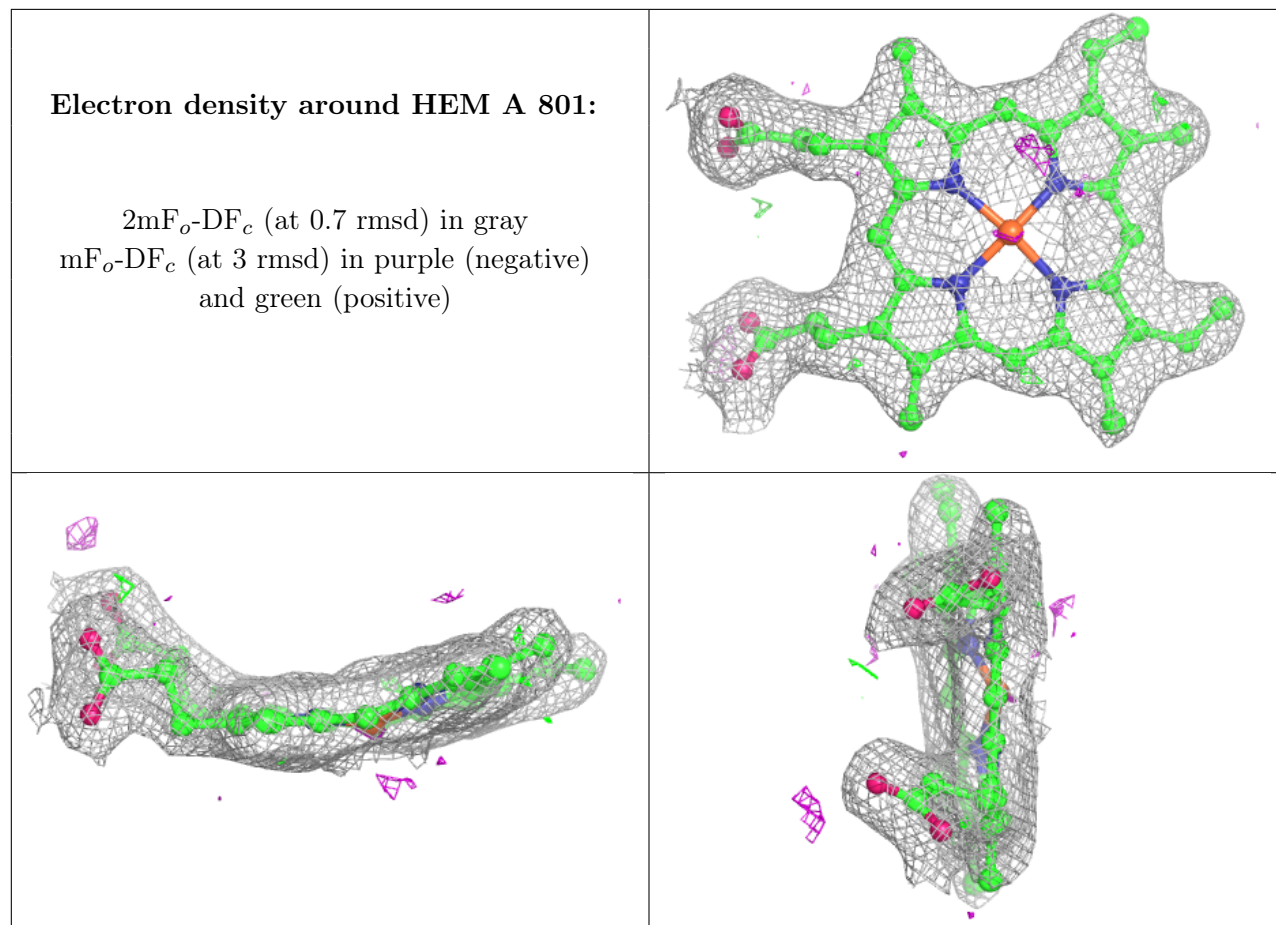
6.4 Ligands [i](#)

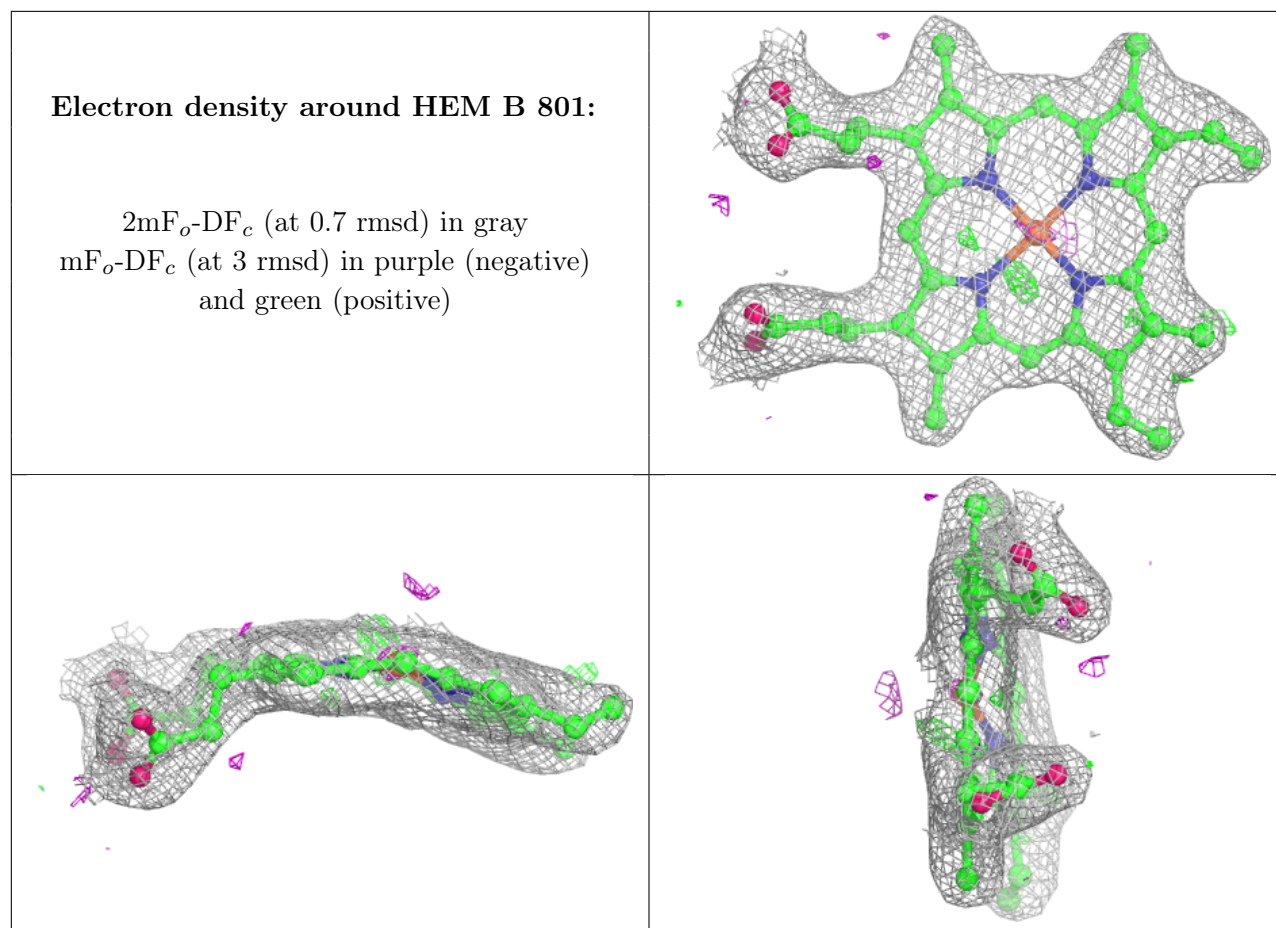
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACT	A	803	4/4	0.91	0.23	71,71,74,75	0
4	ACT	B	804	4/4	0.95	0.18	48,54,58,58	0
3	H4B	A	802	17/17	0.96	0.18	35,39,43,44	0
3	H4B	B	802	17/17	0.96	0.17	33,38,42,44	0
5	4KJ	A	804	15/15	0.96	0.25	38,41,46,59	0
2	HEM	A	801	43/43	0.97	0.21	36,38,41,45	0
5	4KJ	B	803	15/15	0.97	0.18	32,38,61,65	0
2	HEM	B	801	43/43	0.98	0.17	29,37,42,46	0
6	ZN	A	805	1/1	0.99	0.06	48,48,48,48	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.