



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:20 am BST

PDB ID : 3NLO
Title : Structure of neuronal nitric oxide synthase R349A mutant heme domain in complex with 6-{{(3'S,4'R)-3'-[2''-(3'''-fluorophenethylamino)ethoxy]pyrrolidin-4'-yl}methyl}-4-methylpyridin-2-amine
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Deposited on : 2010-06-21
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 ⓘ symbol.

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 : 2.11
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) : 2.11

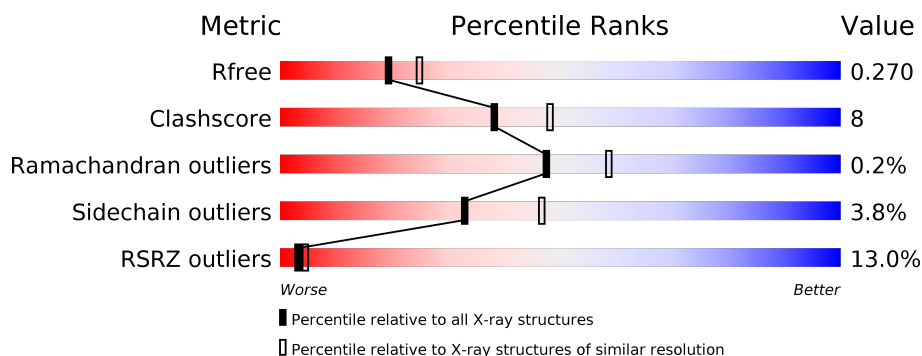
1 Overall quality at a glance

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	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 on 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	JSR	A	800	-	-	-	X
6	EDO	A	890	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6948 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.

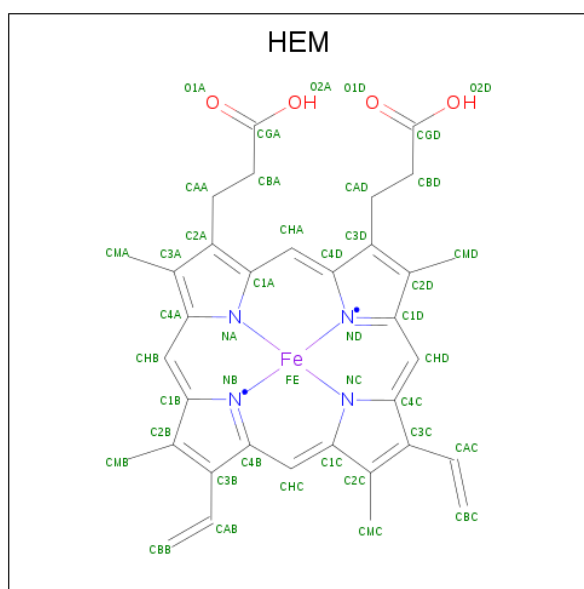
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3313	2121	566	605	21			
1	B	411	Total	C	N	O	S	0	0	0
			3339	2137	571	610	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	ALA	ARG	ENGINEERED MUTATION	UNP P29476
B	349	ALA	ARG	ENGINEERED MUTATION	UNP P29476

- 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		

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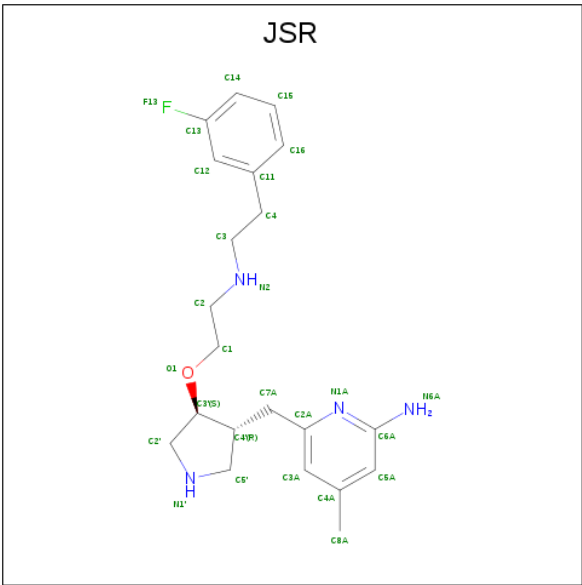
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



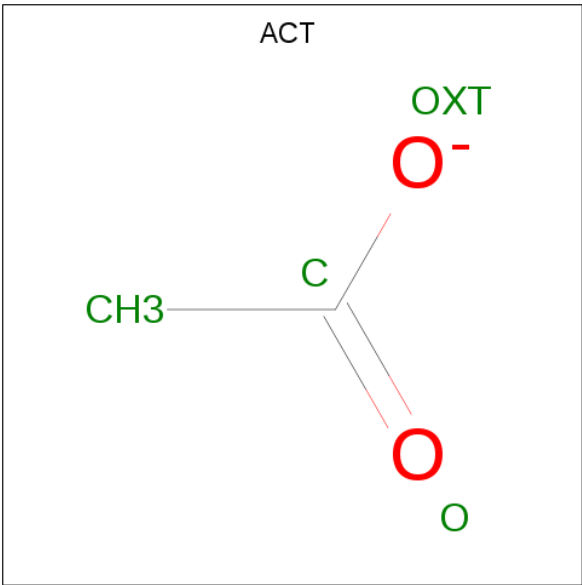
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-[(3R,4S)-4-(2-{[2-(3-fluorophenyl)ethyl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: JSR) (formula: $C_{21}H_{29}FN_4O$).



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	43	Total	O	0	0
			43	43		
8	B	62	Total	O	0	0
			62	62		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.41Å 112.00Å 164.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.62 – 2.30 39.15 – 2.29	Depositor EDS
% Data completeness (in resolution range)	96.6 (40.62-2.30) 96.6 (39.15-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, R_{free}	0.197 , 0.262 0.208 , 0.270	Depositor DCC
R_{free} test set	2103 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6948	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.84	0/3406	0.78	2/4621 (0.0%)
1	B	0.86	1/3432 (0.0%)	0.80	3/4654 (0.1%)
All	All	0.85	1/6838 (0.0%)	0.79	5/9275 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	582	CYS	CB-SG	6.54	1.93	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	B	675	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	570	MET	CA-CB-CG	-5.42	104.09	113.30
1	B	428	ASP	CB-CG-OD2	5.22	122.99	118.30
1	B	675	ASP	CB-CG-OD2	-5.19	113.63	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	3313	0	3221	58	0
1	B	3339	0	3251	42	0
2	A	43	0	30	2	0
2	B	43	0	30	7	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	29	5	0
4	B	27	0	29	6	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	8	0	12	0	0
7	A	1	0	0	0	0
8	A	43	0	0	1	0
8	B	62	0	0	3	0
All	All	6948	0	6638	103	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 8.

All (103) 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:371:ARG:HH21	1:A:371:ARG:HG2	1.04	1.11
1:B:567:VAL:CG2	4:B:800:JSR:H5'A	1.86	1.06
1:B:567:VAL:HG21	4:B:800:JSR:H5'A	1.45	0.97
1:A:567:VAL:CG2	4:A:800:JSR:H5'A	1.96	0.95
1:B:706:TYR:OH	2:B:750:HEM:O1D	1.86	0.94
1:A:371:ARG:HG2	1:A:371:ARG:NH2	1.82	0.93
1:A:567:VAL:HG22	4:A:800:JSR:H5'A	1.57	0.84
1:B:567:VAL:HG22	4:B:800:JSR:H5'A	1.63	0.78
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.68	0.76
1:A:350:THR:N	8:A:1008:HOH:O	2.20	0.75
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.72	0.70
1:A:567:VAL:HG21	4:A:800:JSR:H5'A	1.74	0.67
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.31	0.65
1:B:494:GLY:O	1:B:496:PRO:HD3	1.98	0.64
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.80	0.63
1:A:507:GLN:O	1:A:507:GLN:HG2	1.97	0.63
1:A:300:PHE:HD2	1:A:315:THR:HG22	1.64	0.62
1:B:525:GLN:HG3	1:B:529:ASN:O	2.01	0.61
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.16	0.60
1:A:371:ARG:CG	1:A:371:ARG:HH21	1.94	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.84	0.60
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.84	0.59
4:B:800:JSR:H2'	4:B:800:JSR:C2	2.31	0.59
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.33	0.59
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.03	0.59
1:B:473:ARG:HD3	1:B:580:SER:HB2	1.85	0.58
2:B:750:HEM:CMC	2:B:750:HEM:HBC2	2.34	0.57
1:B:317:HIS:O	1:B:320:SER:HB3	2.06	0.56
1:B:300:PHE:HD2	1:B:315:THR:HG22	1.70	0.55
1:A:485:TYR:CZ	1:A:514:ARG:HA	2.42	0.55
1:B:567:VAL:HG21	4:B:800:JSR:C5'	2.29	0.55
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.60	0.53
1:B:600:ASP:OD2	8:B:1055:HOH:O	2.19	0.51
1:A:354:LEU:HD21	1:A:393:THR:HA	1.91	0.51
1:B:386:LYS:O	1:B:389:GLU:HG3	2.11	0.51
1:B:332:MET:CE	1:B:338:PRO:HB3	2.41	0.50
1:A:686:SER:HA	1:A:691:PHE:CG	2.47	0.49
1:A:675:ASP:O	1:A:679:ILE:HG12	2.12	0.49
1:A:567:VAL:HG21	4:A:800:JSR:C5'	2.40	0.49
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.48	0.49
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.95	0.49
1:B:299:ARG:CB	1:B:299:ARG:CZ	2.90	0.48
1:A:524:LEU:O	1:A:531:PRO:HA	2.14	0.48
1:B:299:ARG:CZ	1:B:299:ARG:HB3	2.44	0.48
1:A:307:GLU:HG3	8:B:1011:HOH:O	2.14	0.48
1:B:522:LEU:HB3	1:B:524:LEU:HD21	1.96	0.48
1:B:584:PHE:CD1	2:B:750:HEM:CAC	2.97	0.48
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.49	0.48
2:B:750:HEM:CMC	2:B:750:HEM:CBC	2.91	0.48
1:A:569:ASN:H	1:A:569:ASN:HD22	1.61	0.47
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.02	0.47
1:A:384:VAL:HG12	1:A:388:ILE:HD12	1.97	0.47
1:B:595:VAL:O	1:B:599:CYS:HB2	2.14	0.47
1:A:375:LYS:HG2	1:A:379:ASP:OD1	2.15	0.47
1:A:607:LEU:O	1:A:608:GLU:C	2.52	0.47
1:A:449:ALA:O	1:A:455:LEU:HA	2.15	0.46
1:B:512:ALA:HA	1:B:513:PRO:HD2	1.85	0.46
1:A:354:LEU:CD2	1:A:393:THR:HA	2.45	0.46
1:B:325:GLY:O	1:B:332:MET:HG3	2.16	0.46
1:A:328:GLU:OE2	1:B:328:GLU:OE2	2.33	0.46
2:B:750:HEM:CBC	2:B:750:HEM:HMC1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:SER:O	1:B:375:LYS:C	2.53	0.46
1:A:609:GLU:O	1:A:612:LYS:HB2	2.15	0.46
1:B:332:MET:HE2	1:B:338:PRO:HB3	1.98	0.46
1:A:418:ARG:O	1:A:419:ILE:C	2.54	0.45
1:B:419:ILE:HG23	1:B:420:GLN:HG2	1.97	0.45
1:B:504:ILE:O	1:B:508:GLN:HG2	2.17	0.45
1:A:596:ARG:O	1:A:600:ASP:HB2	2.17	0.45
1:B:409:TRP:HZ3	1:B:424:LEU:HB2	1.82	0.45
1:B:415:CYS:HB2	2:B:750:HEM:ND	2.32	0.44
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.52	0.44
1:B:495:ASP:OD2	1:B:603:ARG:NH2	2.38	0.44
1:A:595:VAL:O	1:A:599:CYS:HB2	2.18	0.43
1:B:703:SER:HA	8:B:1037:HOH:O	2.18	0.43
1:A:567:VAL:HB	1:A:584:PHE:CE1	2.54	0.43
2:B:750:HEM:HBA1	4:B:800:JSR:H7AA	2.00	0.43
1:A:445:HIS:C	1:A:445:HIS:CD2	2.92	0.43
1:A:674:ALA:HB3	1:A:695:MET:HB3	2.00	0.43
2:A:750:HEM:HBA1	4:A:800:JSR:H7AA	1.99	0.43
1:A:526:ALA:O	1:A:529:ASN:ND2	2.51	0.43
1:A:566:ALA:HA	1:A:584:PHE:O	2.19	0.43
1:A:384:VAL:HG12	1:A:388:ILE:CD1	2.49	0.42
1:B:475:TRP:CE2	1:B:531:PRO:HG3	2.55	0.42
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.55	0.42
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.83	0.42
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.34	0.42
1:A:317:HIS:O	1:A:320:SER:HB3	2.20	0.42
1:A:442:ILE:HG21	1:A:522:LEU:HD11	2.01	0.42
1:B:300:PHE:HD2	1:B:315:THR:CG2	2.33	0.42
1:B:302:LYS:HA	1:B:312:LEU:O	2.19	0.41
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	2.03	0.41
1:B:607:LEU:HA	1:B:607:LEU:HD23	1.83	0.41
1:A:593:ILE:HA	1:A:597:ASP:HB2	2.02	0.41
1:A:610:VAL:HG21	1:A:633:ILE:HD11	2.02	0.41
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.14	0.41
1:B:610:VAL:HG21	1:B:633:ILE:HD11	2.02	0.41
1:A:391:THR:O	1:A:392:SER:CB	2.69	0.41
1:A:561:TRP:CD1	1:A:593:ILE:HG12	2.56	0.41
1:A:300:PHE:CD2	1:A:315:THR:HG22	2.51	0.40
1:A:429:ALA:HB3	1:A:461:ILE:O	2.21	0.40
1:A:317:HIS:NE2	1:A:318:LEU:HG	2.35	0.40
1:B:409:TRP:CZ3	1:B:424:LEU:HB2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:LYS:NZ	1:B:642:GLN:HE22	2.19	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	403/422 (96%)	378 (94%)	24 (6%)	1 (0%)	47	58
1	B	407/422 (96%)	393 (97%)	13 (3%)	1 (0%)	47	58
All	All	810/844 (96%)	771 (95%)	37 (5%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	575	GLY
1	A	488	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	363/376 (96%)	344 (95%)	19 (5%)	23	32
1	B	365/376 (97%)	356 (98%)	9 (2%)	47	65
All	All	728/752 (97%)	700 (96%)	28 (4%)	33	47

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

Mol	Chain	Res	Type
1	A	321	THR
1	A	327	THR
1	A	337	LEU
1	A	352	ASP
1	A	371	ARG
1	A	382	GLU
1	A	481	ARG
1	A	486	LYS
1	A	489	ASP
1	A	507	GLN
1	A	523	LEU
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	615	ASP
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	351	LYS
1	B	353	GLN
1	B	392	SER
1	B	398	ASP
1	B	481	ARG
1	B	540	LEU
1	B	547	ARG
1	B	555	LYS
1	B	667	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	A	454	ASN
1	A	527	ASN
1	A	535	GLN
1	A	569	ASN
1	A	642	GLN
1	A	697	ASN
1	B	353	GLN
1	B	364	GLN

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Mol	Chain	Res	Type
1	B	385	ASN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	601	ASN
1	B	605	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	750	1	27,50,50	2.02	7 (25%)	17,82,82	2.17	6 (35%)
2	HEM	B	750	1	27,50,50	2.30	12 (44%)	17,82,82	1.62	4 (23%)
6	EDO	A	891	-	3,3,3	0.47	0	2,2,2	0.57	0
5	ACT	A	860	-	1,3,3	1.49	0	0,3,3	0.00	-
5	ACT	B	860	-	1,3,3	3.30	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H4B	B	760	-	16,18,18	1.35	3 (18%)	11,26,26	2.99	6 (54%)
4	JSR	A	800	-	28,29,29	0.99	1 (3%)	31,38,38	1.90	5 (16%)
6	EDO	A	890	-	3,3,3	0.86	0	2,2,2	0.31	0
3	H4B	A	760	-	16,18,18	1.09	2 (12%)	11,26,26	3.53	6 (54%)
4	JSR	B	800	-	28,29,29	1.07	2 (7%)	31,38,38	2.31	7 (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	A	750	1	-	1/6/54/54	-
2	HEM	B	750	1	-	1/6/54/54	-
6	EDO	A	891	-	-	1/1/1/1	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	JSR	A	800	-	-	6/13/23/23	0/3/3/3
6	EDO	A	890	-	-	1/1/1/1	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	JSR	B	800	-	-	8/13/23/23	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3D-C2D	5.16	1.53	1.37
2	A	750	HEM	C3D-C2D	4.64	1.51	1.37
2	B	750	HEM	C3B-C2B	-4.50	1.34	1.40
2	A	750	HEM	C3B-C2B	-4.29	1.34	1.40
2	B	750	HEM	C3C-C2C	-4.04	1.34	1.40
2	A	750	HEM	C3C-C2C	-3.63	1.35	1.40
2	A	750	HEM	C3B-CAB	3.55	1.55	1.47
2	B	750	HEM	CAA-C2A	3.31	1.56	1.52
5	B	860	ACT	CH3-C	3.30	1.52	1.48
2	B	750	HEM	C3C-CAC	3.18	1.54	1.47
2	B	750	HEM	CAD-C3D	3.04	1.57	1.52
2	B	750	HEM	CMC-C2C	2.89	1.58	1.51
3	B	760	H4B	C7-N8	2.61	1.49	1.44
2	A	750	HEM	C3C-CAC	2.61	1.53	1.47
4	B	800	JSR	C12-C13	2.59	1.42	1.37
2	A	750	HEM	CMC-C2C	2.55	1.57	1.51
2	A	750	HEM	CAA-C2A	2.51	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	760	H4B	C4-N3	2.47	1.37	1.33
3	A	760	H4B	C4-N3	2.38	1.37	1.33
4	A	800	JSR	C12-C13	2.34	1.41	1.37
2	B	750	HEM	C3B-CAB	2.31	1.52	1.47
4	B	800	JSR	C14-C13	2.19	1.41	1.37
2	B	750	HEM	C1C-C2C	2.15	1.47	1.42
3	B	760	H4B	C4A-C8A	-2.13	1.37	1.41
3	A	760	H4B	C2-N2	2.09	1.38	1.33
2	B	750	HEM	CMD-C2D	2.07	1.55	1.51
2	B	750	HEM	C4A-CHB	-2.05	1.35	1.41
2	B	750	HEM	CMB-C2B	2.04	1.56	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	JSR	C3A-C2A-N1A	-7.14	115.33	122.90
4	B	800	JSR	C6A-N1A-C2A	7.02	123.42	118.10
4	A	800	JSR	C6A-N1A-C2A	6.34	122.91	118.10
3	A	760	H4B	C4-C4A-N5	5.98	124.14	119.12
3	A	760	H4B	C4-C4A-C8A	5.63	119.57	114.57
4	A	800	JSR	C3A-C2A-N1A	-5.34	117.24	122.90
3	B	760	H4B	C4-C4A-N5	5.28	123.55	119.12
2	A	750	HEM	CBA-CAA-C2A	-4.84	103.55	112.49
3	A	760	H4B	N2-C2-N3	4.34	124.00	117.25
3	B	760	H4B	C4-C4A-C8A	4.33	118.41	114.57
3	B	760	H4B	N3-C2-N1	-4.21	118.82	125.42
3	A	760	H4B	N3-C2-N1	-4.03	119.10	125.42
3	B	760	H4B	C2-N1-C8A	4.02	123.55	114.54
3	A	760	H4B	C2-N1-C8A	3.96	123.42	114.54
2	A	750	HEM	C4C-C3C-C2C	3.79	109.55	106.90
3	A	760	H4B	C4-N3-C2	3.19	120.99	115.93
2	B	750	HEM	C4C-C3C-C2C	3.07	109.05	106.90
2	A	750	HEM	C4A-C3A-C2A	3.06	109.13	107.00
4	B	800	JSR	C4A-C3A-C2A	3.01	122.29	120.32
4	B	800	JSR	C2A-C7A-C4'	2.89	125.05	115.55
2	B	750	HEM	CBD-CAD-C3D	-2.82	107.29	112.48
4	B	800	JSR	C14-C13-C12	-2.76	119.71	123.29
2	A	750	HEM	CMC-C2C-C3C	2.66	129.65	124.68
2	A	750	HEM	C3C-C4C-NC	-2.64	105.97	110.94
2	B	750	HEM	C1D-C2D-C3D	-2.52	105.24	107.00
4	A	800	JSR	C14-C13-C12	-2.51	120.04	123.29
3	B	760	H4B	C4-N3-C2	2.48	119.87	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	JSR	O1-C3'-C2'	-2.38	105.08	111.42
3	B	760	H4B	N2-C2-N3	2.34	120.90	117.25
2	B	750	HEM	CBA-CAA-C2A	-2.33	108.19	112.49
4	A	800	JSR	C3-N2-C2	2.13	123.51	113.45
2	A	750	HEM	CAA-CBA-CGA	2.08	116.16	112.67
4	B	800	JSR	C7A-C2A-C3A	2.04	125.38	121.04
4	A	800	JSR	C5'-N1'-C2'	2.01	110.17	105.42

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	750	HEM	C3D-CAD-CBD-CGD
2	B	750	HEM	C2A-CAA-CBA-CGA
4	A	800	JSR	C3'-C4'-C7A-C2A
4	A	800	JSR	C5'-C4'-C7A-C2A
4	B	800	JSR	C2'-C3'-O1-C1
4	B	800	JSR	N2-C3-C4-C11
4	B	800	JSR	N1A-C2A-C7A-C4'
4	B	800	JSR	C3'-C4'-C7A-C2A
4	B	800	JSR	C5'-C4'-C7A-C2A
4	B	800	JSR	O1-C1-C2-N2
4	A	800	JSR	O1-C1-C2-N2
4	A	800	JSR	C4-C3-N2-C2
4	A	800	JSR	C1-C2-N2-C3
4	B	800	JSR	C1-C2-N2-C3
6	A	891	EDO	O1-C1-C2-O2
4	B	800	JSR	C4-C3-N2-C2
4	A	800	JSR	C2-C1-O1-C3'
6	A	890	EDO	O1-C1-C2-O2

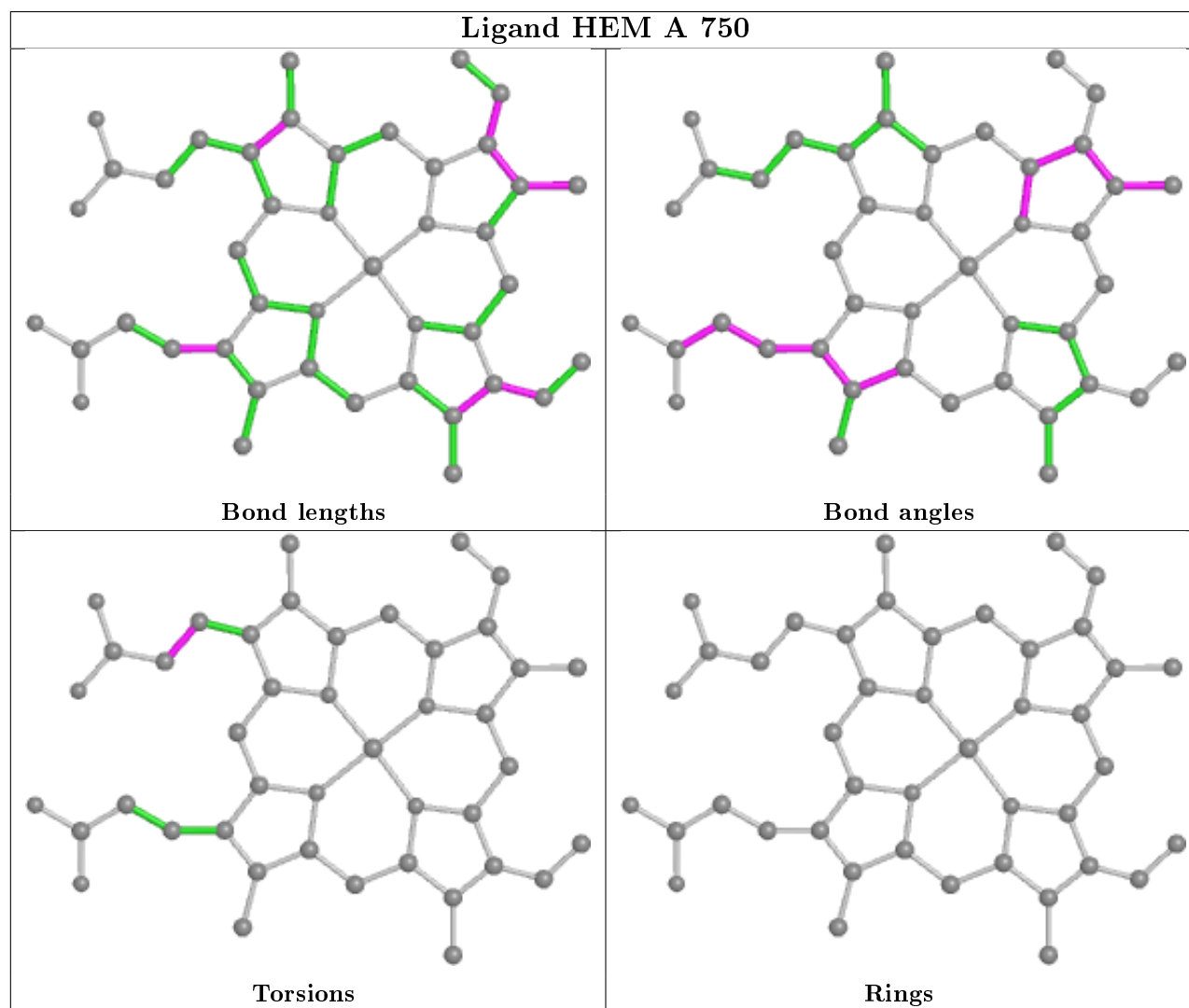
There are no ring outliers.

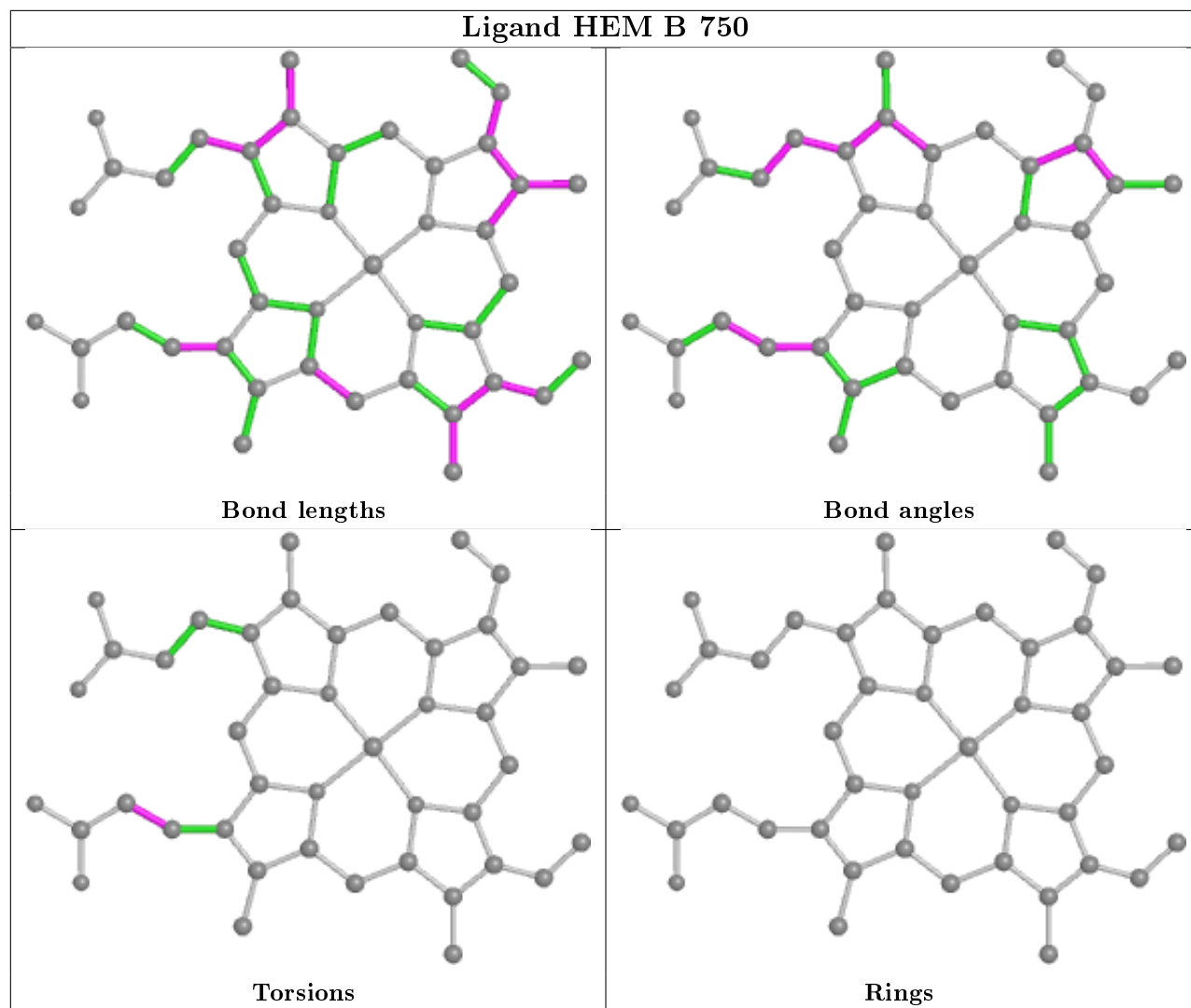
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	2	0
2	B	750	HEM	7	0
4	A	800	JSR	5	0
4	B	800	JSR	6	0

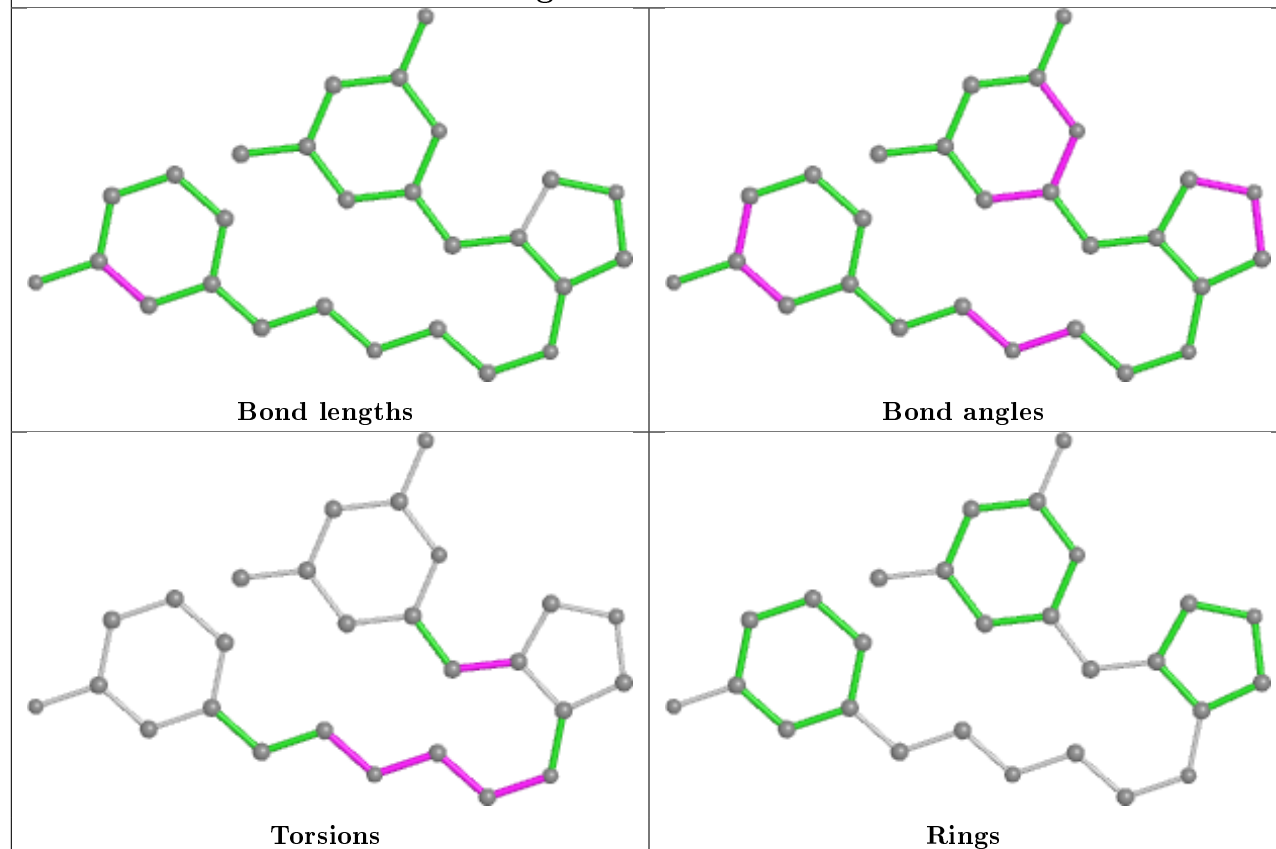
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

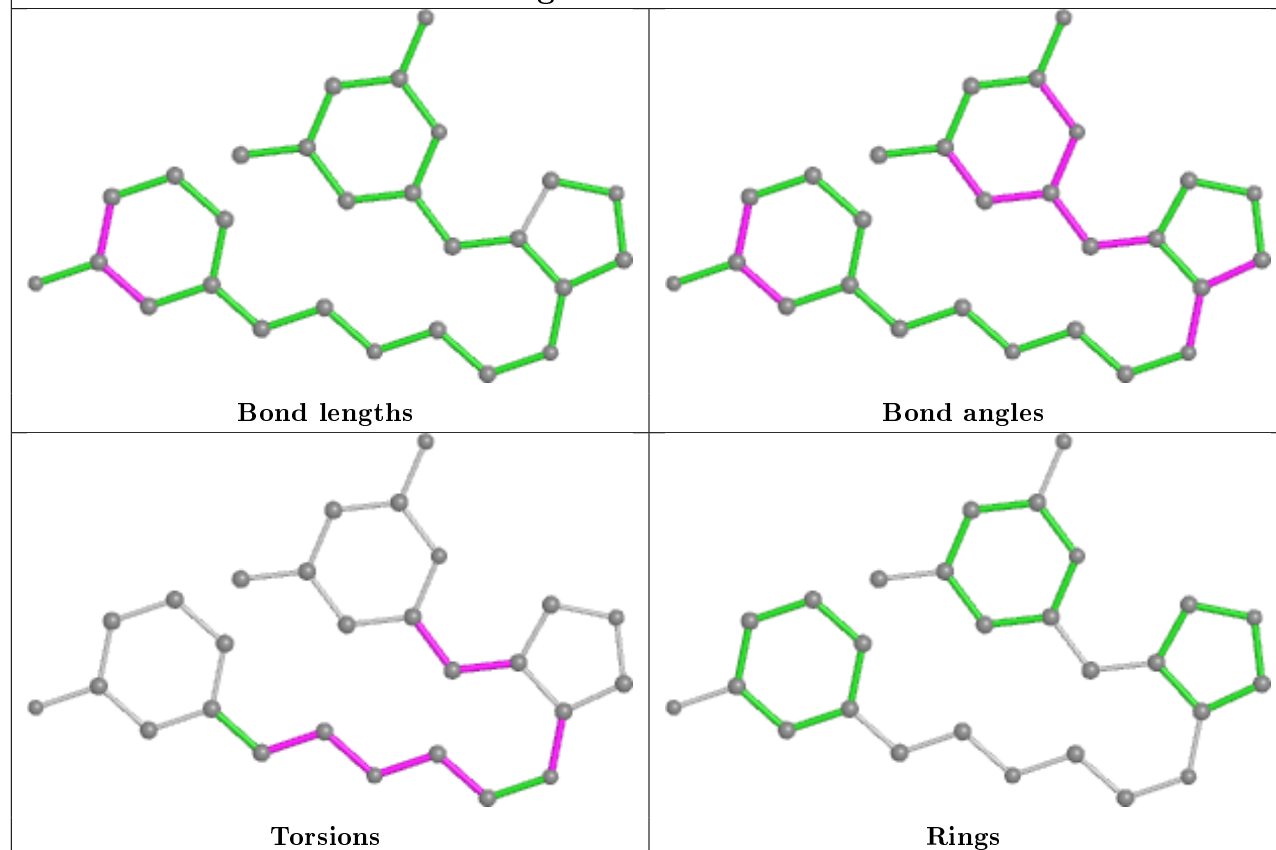




Ligand JSR A 800



Ligand JSR B 800



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%)	0.91	71 (17%)  	40, 71, 127, 163	0
1	B	411/422 (97%)	0.44	35 (8%)  	40, 60, 89, 115	0
All	All	818/844 (96%)	0.67	106 (12%)  	40, 64, 117, 163	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	6.3
1	A	352	ASP	6.3
1	A	716	TRP	5.9
1	A	715	VAL	5.7
1	B	300	PHE	5.7
1	A	351	LYS	5.0
1	B	348	VAL	4.9
1	A	713	THR	4.8
1	B	351	LYS	4.6
1	A	389	GLU	4.5
1	B	350	THR	4.4
1	A	390	SER	4.4
1	A	354	LEU	4.3
1	B	680	VAL	4.2
1	A	486	LYS	4.1
1	A	490	GLY	4.1
1	A	470	HIS	4.1
1	A	485	TYR	4.0
1	A	714	HIS	3.9
1	A	619	ARG	3.9
1	B	667	ARG	3.9
1	A	712	ASN	3.8
1	B	329	HIS	3.8
1	A	678	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	352	ASP	3.7
1	A	479	LEU	3.7
1	B	718	GLY	3.6
1	B	677	VAL	3.6
1	B	619	ARG	3.6
1	A	415	CYS	3.6
1	A	618	MET	3.5
1	A	507	GLN	3.5
1	A	503	GLU	3.5
1	A	355	PHE	3.5
1	A	710	PRO	3.4
1	A	388	ILE	3.4
1	A	680	VAL	3.4
1	A	553	TRP	3.3
1	A	677	VAL	3.3
1	A	489	ASP	3.3
1	A	567	VAL	3.2
1	A	353	GLN	3.2
1	A	682	PRO	3.2
1	A	391	THR	3.1
1	B	591	THR	3.1
1	A	300	PHE	3.1
1	B	299	ARG	3.0
1	A	506	ILE	3.0
1	A	505	CYS	3.0
1	A	394	TYR	3.0
1	A	350	THR	2.9
1	B	717	LYS	2.8
1	A	591	THR	2.8
1	A	416	VAL	2.8
1	B	310	VAL	2.8
1	B	309	ASP	2.8
1	A	385	ASN	2.8
1	A	681	PRO	2.7
1	A	480	ILE	2.7
1	B	493	LEU	2.7
1	A	676	TRP	2.7
1	A	356	PRO	2.5
1	B	615	ASP	2.5
1	A	551	PHE	2.5
1	B	349	ALA	2.5
1	A	555	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	469	LYS	2.5
1	B	311	VAL	2.5
1	A	511	LYS	2.4
1	A	679	ILE	2.4
1	B	375	LYS	2.4
1	A	491	SER	2.4
1	B	566	ALA	2.4
1	A	487	GLN	2.4
1	A	588	TYR	2.3
1	B	392	SER	2.3
1	B	715	VAL	2.3
1	B	327	THR	2.3
1	B	676	TRP	2.3
1	B	618	MET	2.3
1	A	565	PRO	2.3
1	A	381	LEU	2.3
1	B	561	TRP	2.3
1	A	392	SER	2.3
1	A	643	SER	2.3
1	A	452	LYS	2.3
1	A	566	ALA	2.3
1	B	691	PHE	2.2
1	B	621	THR	2.2
1	A	318	LEU	2.2
1	A	611	ALA	2.2
1	A	711	TRP	2.2
1	A	453	GLY	2.2
1	B	308	THR	2.1
1	A	299	ARG	2.1
1	B	678	TRP	2.1
1	A	386	LYS	2.1
1	A	612	LYS	2.1
1	A	593	ILE	2.1
1	A	683	MET	2.1
1	A	568	SER	2.1
1	B	312	LEU	2.0
1	B	593	ILE	2.0
1	A	466	THR	2.0
1	A	557	LEU	2.0
1	B	302	LYS	2.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

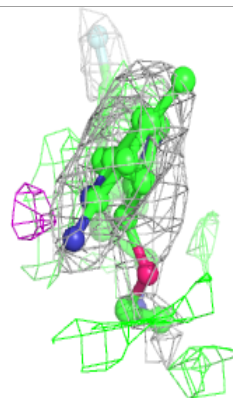
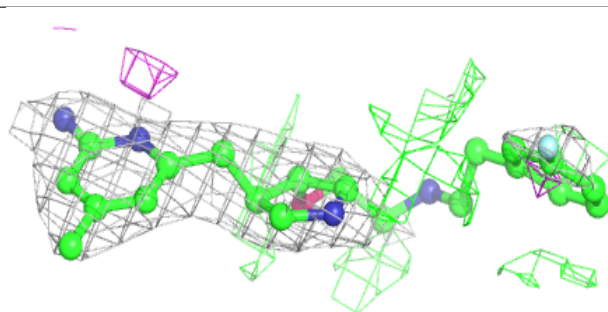
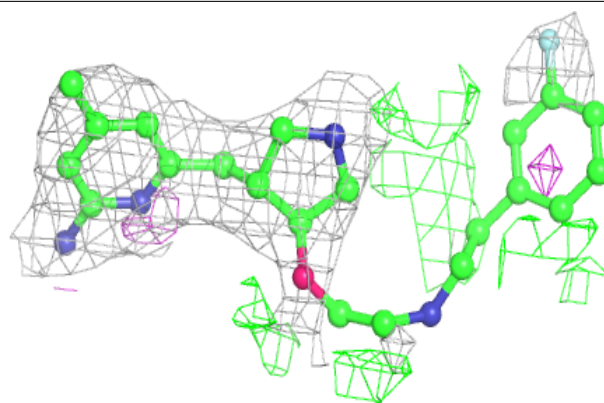
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	890	4/4	0.66	0.41	59,60,61,61	0
4	JSR	A	800	27/27	0.79	0.57	60,90,136,138	0
6	EDO	A	891	4/4	0.83	0.16	66,68,68,68	0
4	JSR	B	800	27/27	0.86	0.40	64,88,107,108	0
5	ACT	A	860	4/4	0.88	0.26	71,73,73,75	0
5	ACT	B	860	4/4	0.89	0.17	73,77,78,79	0
3	H4B	A	760	17/17	0.95	0.26	53,57,61,61	0
2	HEM	A	750	43/43	0.97	0.26	40,47,70,77	0
3	H4B	B	760	17/17	0.97	0.25	48,52,59,64	0
2	HEM	B	750	43/43	0.97	0.18	42,46,66,72	0
7	ZN	A	900	1/1	0.99	0.10	54,54,54,54	0

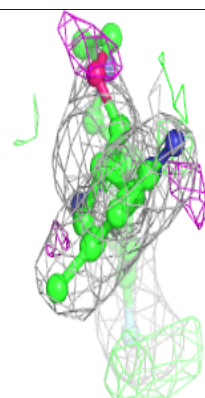
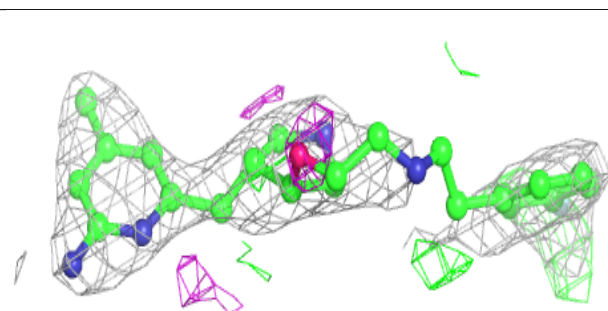
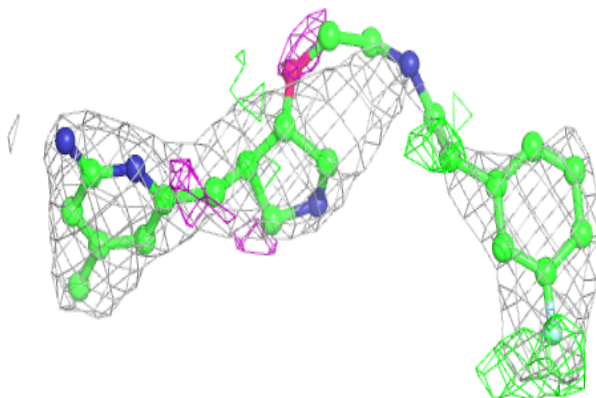
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around JSR A 800:

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

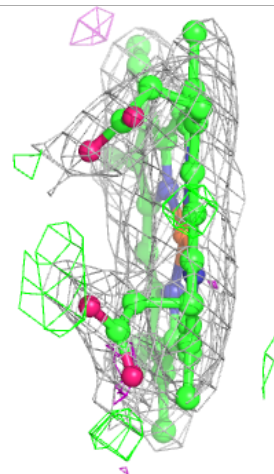
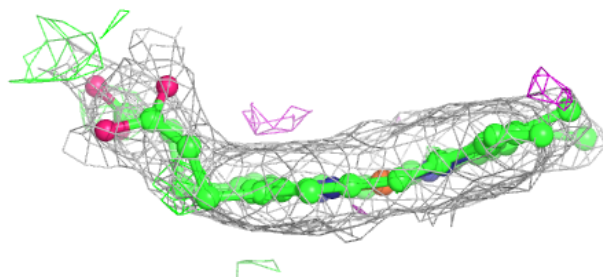
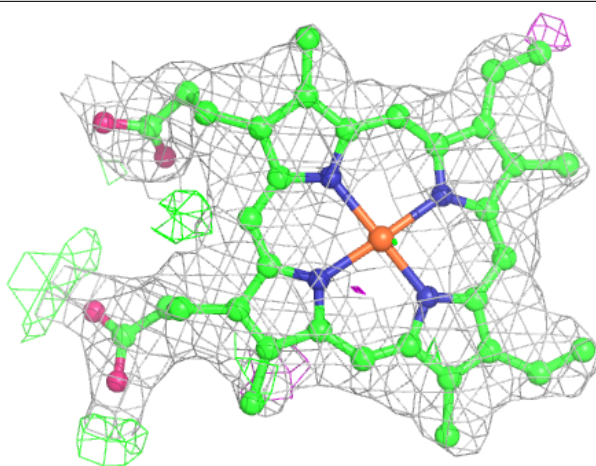
**Electron density around JSR B 800:**

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



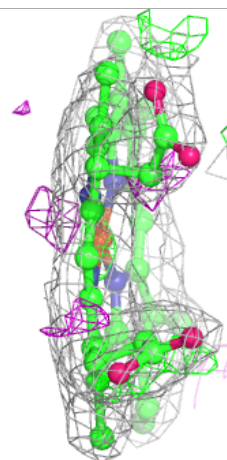
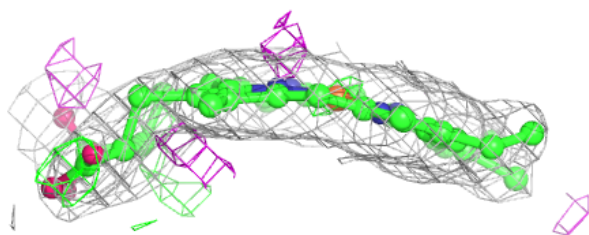
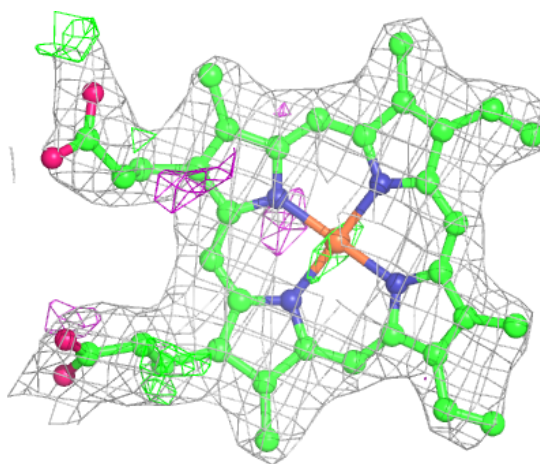
Electron density around HEM A 750:

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



Electron density around HEM B 750:

$2mF_o-DF_c$ (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.