



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:05 AM UTC

PDB ID : 3JWS / pdb_00003jws
Title : Structure of neuronal nitric oxide synthase R349A mutant heme domain complexed with N1-[(3' S,4'S)-4'-((6"-amino-4"-methylpyridin-2"-yl)methyl)pyrrolidin-3'-yl]-N2-(3'-fluorophenethyl)ethane-1,2-diamine tetrahydrochloride
Authors : Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on : 2009-09-18
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

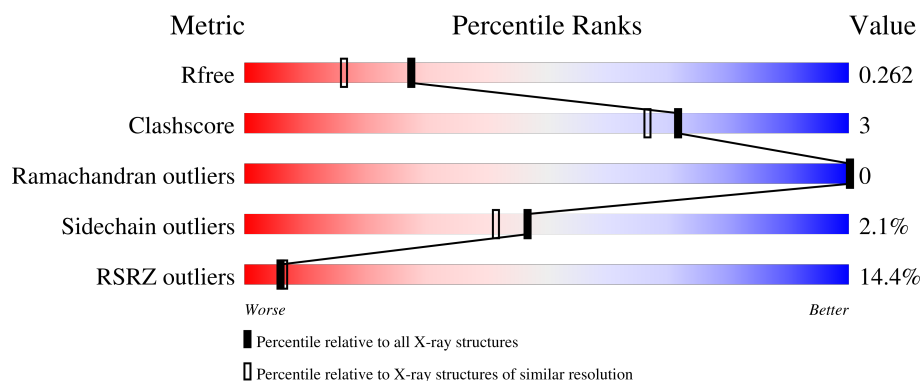
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	21% 85% 11% .
1	B	422	7% 91% 7% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7166 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.

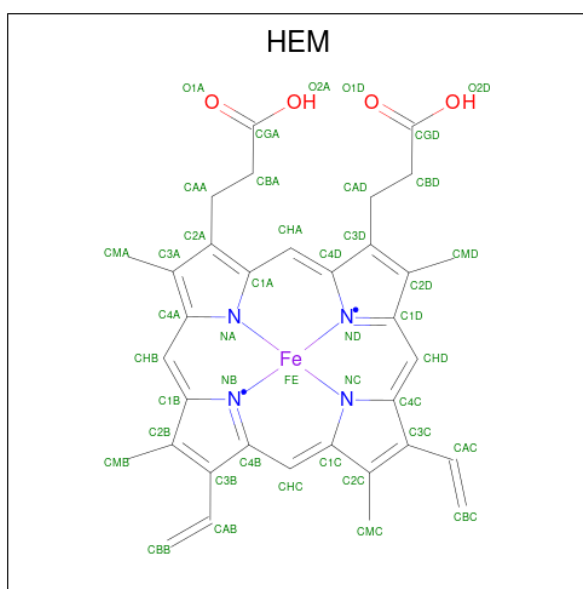
- Molecule 1 is a protein called Nitric oxide synthase, brain.

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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



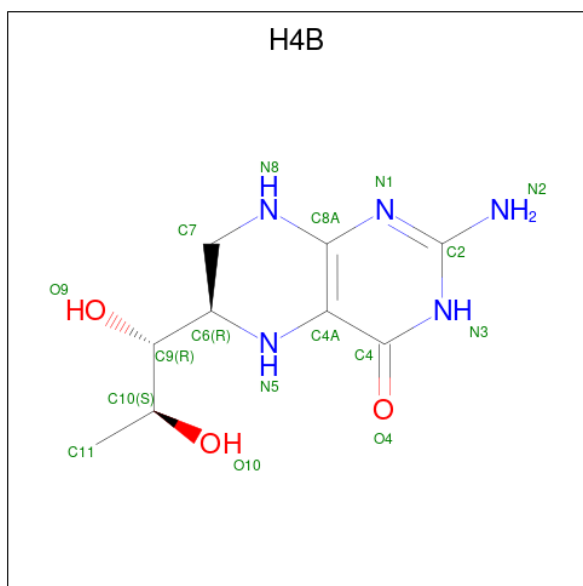
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

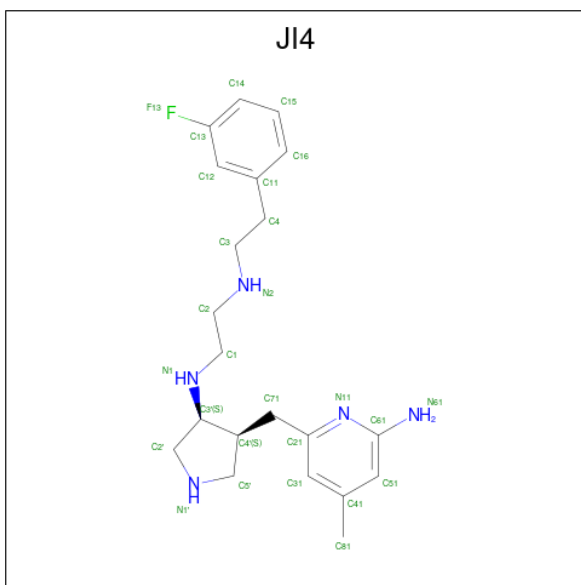
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



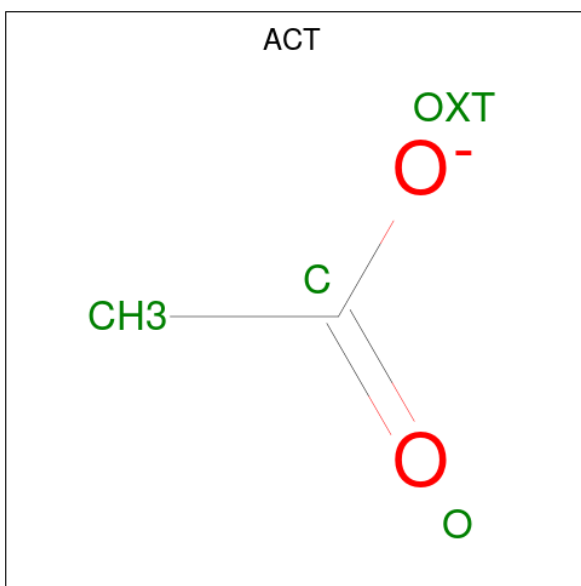
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-{(3S,4S)-4-[(6-amino-4-methylpyridin-2-yl)methyl]pyrrolidin-3-yl}-N'-[2-(3-fluorophenyl)ethyl]ethane-1,2-diamine (CCD ID: JI4) (formula: $C_{21}H_{30}FN_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			27	21	1	5		
4	B	1	Total	C	F	N	0	0
			27	21	1	5		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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 ZINC ION (CCD ID: ZN) (formula: Zn).

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

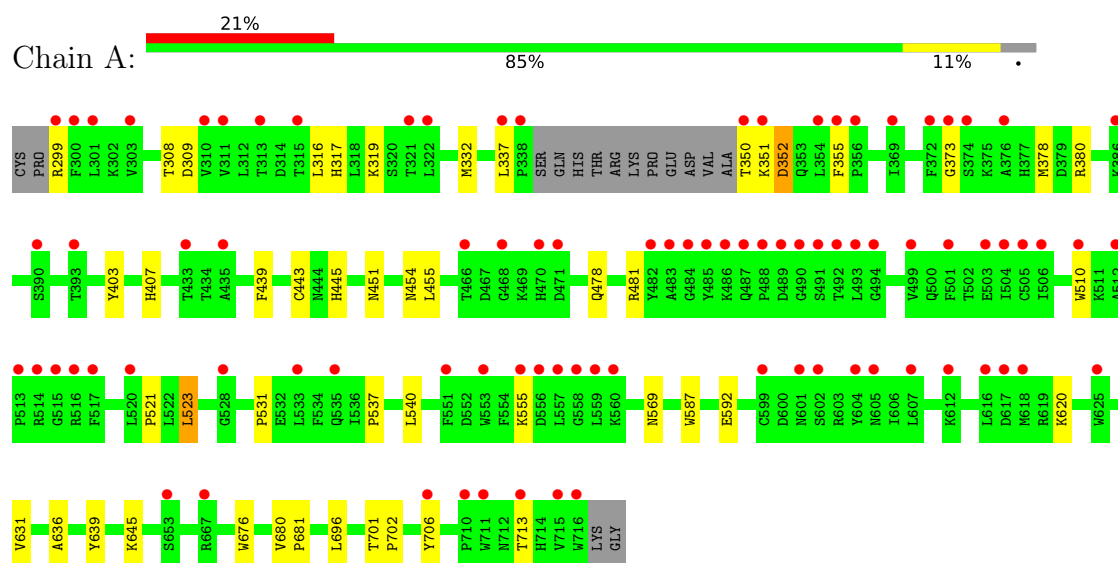
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	134	Total 134	O 134	0	0
7	B	197	Total 197	O 197	0	0

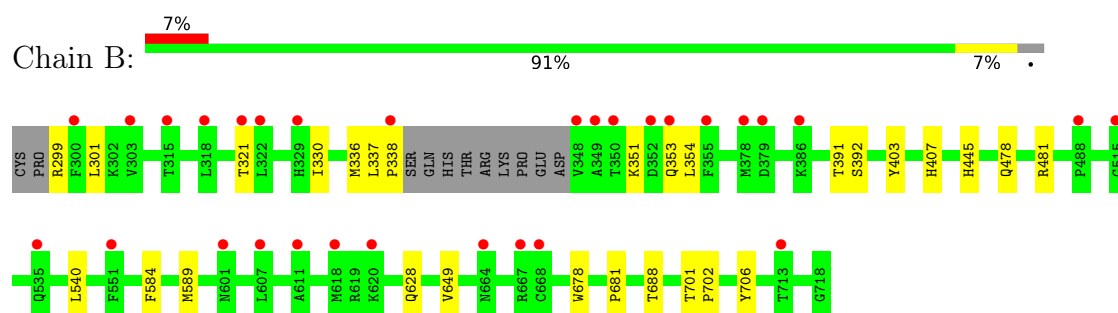
3 Residue-property plots [i](#)

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	51.94Å 112.19Å 164.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.92 – 1.95 43.92 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.92-1.95) 97.8 (43.92-1.95)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0089, CNS	Depositor
R, R_{free}	0.187 , 0.221 (Not available) , 0.262	Depositor DCC
R_{free} test set	3458 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7166	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: ACT, HEM, H4B, JI4, 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	0.66	0/3406	0.85	1/4621 (0.0%)
1	B	0.73	0/3432	0.85	1/4654 (0.0%)
All	All	0.70	0/6838	0.85	2/9275 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	LEU	N-CA-C	5.43	117.00	111.14
1	A	681	PRO	O-C-N	5.28	123.74	121.31

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	3313	0	3221	27	0
1	B	3339	0	3251	16	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	30	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	30	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	134	0	0	4	0
7	B	197	0	0	1	0
All	All	7166	0	6628	44	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 3.

All (44) 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:706:TYR:OH	2:B:750:HEM:O1D	1.90	0.89
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.60	0.82
1:A:636:ALA:C	7:A:1053:HOH:O	2.27	0.78
1:A:706:TYR:OH	2:A:750:HEM:O2D	2.03	0.76
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.75	0.69
1:B:351:LYS:HE2	1:B:392:SER:OG	1.99	0.63
1:A:636:ALA:O	7:A:1053:HOH:O	2.14	0.62
1:A:639:TYR:N	7:A:1053:HOH:O	2.32	0.61
1:A:373:GLY:HA2	1:A:378:MET:HE3	1.82	0.61
1:A:355:PHE:HB2	7:A:1024:HOH:O	2.02	0.60
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.85	0.58
1:A:706:TYR:OH	2:A:750:HEM:CGD	2.55	0.54
1:A:337:LEU:HG	4:A:800:JI4:F13	1.98	0.53
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.91	0.53
1:B:701:THR:HA	1:B:702:PRO:C	2.33	0.53
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.93	0.50
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.92	0.50
1:B:391:THR:O	1:B:392:SER:HB2	2.14	0.47
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.03	0.47
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.97	0.47
1:A:701:THR:HA	1:A:702:PRO:C	2.40	0.46
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.98	0.46
1:A:316:LEU:HD12	1:A:319:LYS:HD2	1.98	0.45
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.37	0.45
1:A:308:THR:O	1:A:309:ASP:HB2	2.16	0.45
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.00	0.44
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:HIS:C	1:B:445:HIS:CD2	2.96	0.43
1:B:337:LEU:HG	4:B:800:JI4:F13	2.08	0.43
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	2.01	0.43
1:B:338:PRO:HG3	7:B:1172:HOH:O	2.18	0.43
1:A:451:ASN:HB3	1:A:454:ASN:O	2.19	0.43
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.54	0.42
1:B:678:TRP:HH2	4:B:800:JI4:H4	1.84	0.42
1:A:445:HIS:C	1:A:445:HIS:CD2	2.97	0.42
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.08	0.42
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.13	0.41
1:B:584:PHE:CD1	2:B:750:HEM:CAC	3.04	0.41
1:A:696:LEU:HB3	1:B:330:ILE:HD11	2.01	0.41
1:A:352:ASP:OD2	1:A:352:ASP:N	2.54	0.41
1:B:681:PRO:HG2	1:B:688:THR:HG21	2.03	0.41
1:A:592:GLU:OE1	4:A:800:JI4:N11	2.54	0.40
1:A:299:ARG:O	1:A:317:HIS:CE1	2.74	0.40
1:B:589:MET:HA	1:B:649:VAL:O	2.22	0.40

There are no symmetry-related clashes.

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	403/422 (96%)	396 (98%)	7 (2%)	0	100	100
1	B	407/422 (96%)	402 (99%)	5 (1%)	0	100	100
All	All	810/844 (96%)	798 (98%)	12 (2%)	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	363/376 (96%)	353 (97%)	10 (3%)	38	30
1	B	365/376 (97%)	360 (99%)	5 (1%)	59	56
All	All	728/752 (97%)	713 (98%)	15 (2%)	47	41

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	THR
1	A	351	LYS
1	A	352	ASP
1	A	380	ARG
1	A	523	LEU
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	713	THR
1	B	299	ARG
1	B	321	THR
1	B	336	MET
1	B	353	GLN
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	A	454	ASN
1	A	527	ASN
1	A	569	ASN
1	A	601	ASN
1	A	605	ASN
1	A	642	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN
1	B	407	HIS
1	B	425	GLN
1	B	454	ASN
1	B	500	GLN
1	B	507	GLN
1	B	508	GLN
1	B	527	ASN
1	B	535	GLN
1	B	697	ASN
1	B	707	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
3	H4B	B	761	-	17,18,18	1.19	3 (17%)	14,26,26	1.62	4 (28%)
2	HEM	B	750	1	50,50,50	1.96	11 (22%)	67,82,82	1.36	6 (8%)
2	HEM	A	750	1	50,50,50	2.03	11 (22%)	67,82,82	1.33	8 (11%)
4	JI4	A	800	-	28,29,29	0.63	0	29,38,38	1.56	5 (17%)
3	H4B	A	760	-	17,18,18	0.99	1 (5%)	14,26,26	2.03	6 (42%)
4	JI4	B	800	-	28,29,29	0.64	0	29,38,38	1.99	7 (24%)
5	ACT	B	861	-	3,3,3	0.76	0	3,3,3	0.82	0
5	ACT	A	860	-	3,3,3	0.85	0	3,3,3	0.76	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
3	H4B	B	761	-	-	0/8/17/17	0/2/2/2
2	HEM	B	750	1	-	0/14/54/54	-
2	HEM	A	750	1	-	2/14/54/54	-
4	JI4	A	800	-	-	1/13/23/23	0/3/3/3
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	JI4	B	800	-	-	1/13/23/23	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3D-C2D	7.48	1.52	1.36
2	A	750	HEM	C3D-C2D	7.12	1.52	1.36
2	B	750	HEM	FE-ND	5.06	2.10	1.94
2	A	750	HEM	FE-ND	4.89	2.10	1.94
2	A	750	HEM	FE-NB	4.75	2.09	1.94
2	A	750	HEM	FE-NA	4.13	2.08	1.95
2	B	750	HEM	FE-NA	3.97	2.08	1.95
2	B	750	HEM	FE-NC	3.88	2.08	1.95
2	A	750	HEM	FE-NC	3.49	2.06	1.95
2	A	750	HEM	CMB-C2B	3.18	1.57	1.50
2	B	750	HEM	CAC-C3C	2.96	1.55	1.47
2	A	750	HEM	CAB-C3B	2.95	1.55	1.47
2	A	750	HEM	CMD-C2D	2.81	1.56	1.50
2	B	750	HEM	CMB-C2B	2.80	1.56	1.50
2	B	750	HEM	CAB-C3B	2.73	1.54	1.47
2	A	750	HEM	CAC-C3C	2.73	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	CMC-C2C	2.71	1.56	1.50
2	B	750	HEM	FE-NB	2.69	2.03	1.94
2	B	750	HEM	CMD-C2D	2.61	1.56	1.50
3	B	761	H4B	O4-C4	2.58	1.28	1.23
2	A	750	HEM	CMA-C3A	2.52	1.55	1.50
3	B	761	H4B	C4-N3	-2.51	1.34	1.38
2	B	750	HEM	CMA-C3A	2.39	1.55	1.50
3	A	760	H4B	C2-N2	2.23	1.39	1.34
3	B	761	H4B	C7-C6	2.23	1.54	1.52
2	B	750	HEM	C2A-C3A	-2.04	1.33	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	JI4	C61-N11-C21	5.79	122.40	118.07
4	B	800	JI4	C1-N1-C3'	5.29	121.76	114.05
2	B	750	HEM	CBA-CAA-C2A	-4.95	98.86	112.53
3	A	760	H4B	C2-N1-C8A	4.73	121.71	113.36
2	B	750	HEM	C4D-ND-C1D	4.37	110.38	105.21
2	A	750	HEM	C4D-ND-C1D	4.21	110.19	105.21
4	A	800	JI4	C61-N11-C21	3.82	120.93	118.07
4	A	800	JI4	C1-N1-C3'	3.75	119.51	114.05
2	A	750	HEM	CBD-CAD-C3D	-3.69	102.33	112.53
2	A	750	HEM	CBA-CAA-C2A	-3.50	102.84	112.53
3	B	761	H4B	C2-N1-C8A	3.34	119.26	113.36
4	A	800	JI4	C5'-N1'-C2'	3.18	113.35	105.45
2	B	750	HEM	CBD-CAD-C3D	-3.15	103.83	112.53
4	B	800	JI4	C31-C21-N11	-3.12	119.17	122.73
4	B	800	JI4	C5'-N1'-C2'	2.96	112.80	105.45
4	A	800	JI4	C71-C21-N11	2.90	120.12	116.57
4	B	800	JI4	C71-C21-N11	2.84	120.04	116.57
4	A	800	JI4	C31-C21-N11	-2.77	119.57	122.73
3	A	760	H4B	C4-C4A-N5	2.70	123.62	116.27
2	A	750	HEM	CHD-C4C-NC	2.69	127.38	124.45
2	B	750	HEM	C2A-C1A-NA	-2.69	107.17	110.15
3	B	761	H4B	C2-N3-C4	-2.59	120.41	125.11
3	A	760	H4B	N2-C2-N3	2.48	122.00	116.76
2	A	750	HEM	CMD-C2D-C1D	2.36	128.72	125.03
2	B	750	HEM	C3B-C4B-NB	-2.34	107.79	109.47
3	A	760	H4B	C4A-C4-N3	2.33	118.53	112.13
3	A	760	H4B	N3-C2-N1	-2.31	119.10	123.32
2	B	750	HEM	CAD-C3D-C4D	2.30	128.70	124.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	C1D-C2D-C3D	-2.21	104.66	106.98
3	B	761	H4B	C4A-C4-N3	2.20	118.16	112.13
2	A	750	HEM	CHC-C1C-NC	2.17	126.81	124.45
4	B	800	JI4	C51-C41-C31	2.13	120.48	118.11
4	B	800	JI4	C2'-C3'-N1	-2.08	110.03	113.73
3	A	760	H4B	O4-C4-C4A	-2.06	122.30	127.26
2	A	750	HEM	C2A-C1A-NA	-2.04	107.89	110.15
3	B	761	H4B	C4-C4A-N5	2.00	121.72	116.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

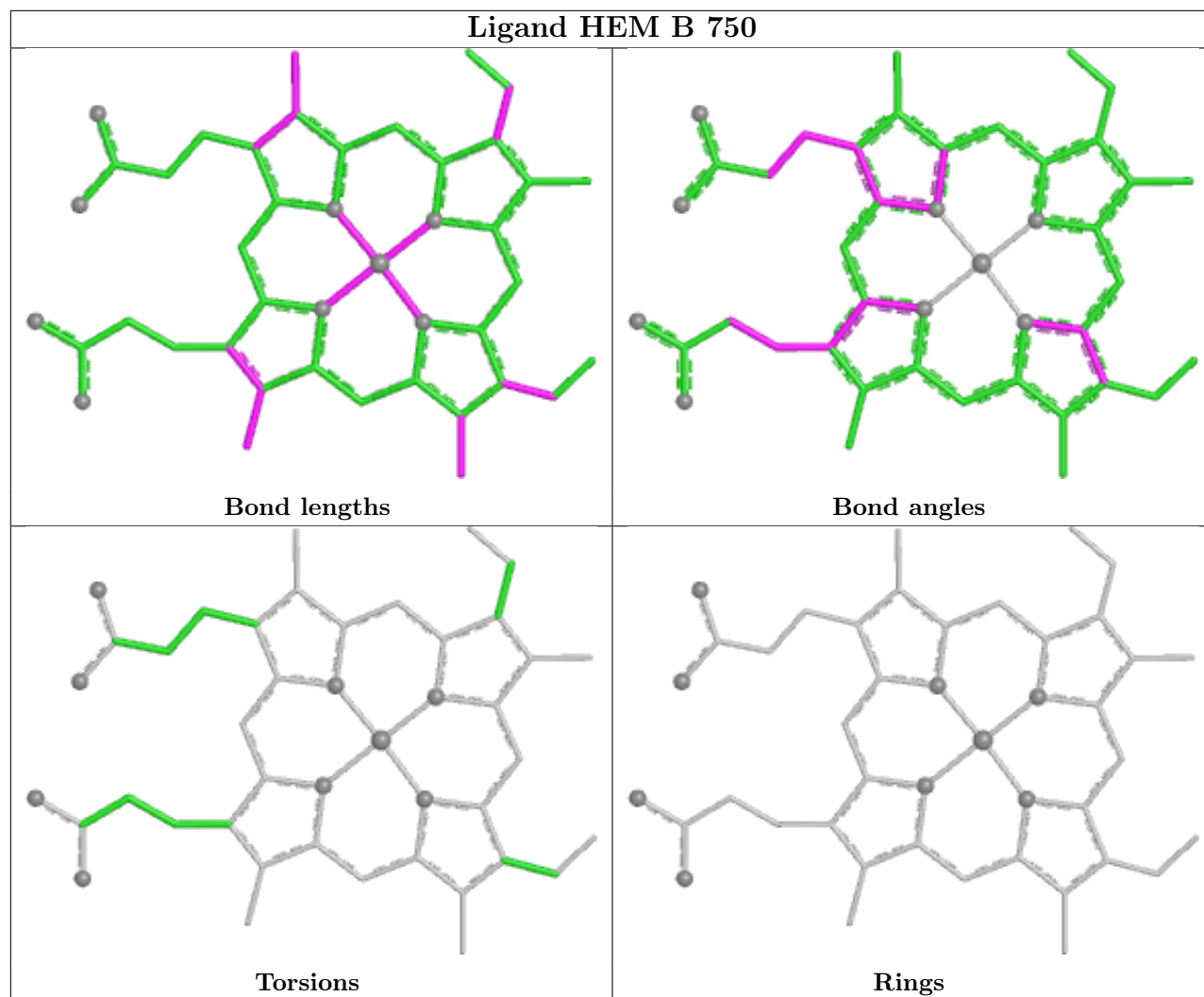
Mol	Chain	Res	Type	Atoms
4	A	800	JI4	C2-C1-N1-C3'
4	B	800	JI4	C2-C1-N1-C3'
2	A	750	HEM	C2A-CAA-CBA-CGA
2	A	750	HEM	C4B-C3B-CAB-CBB

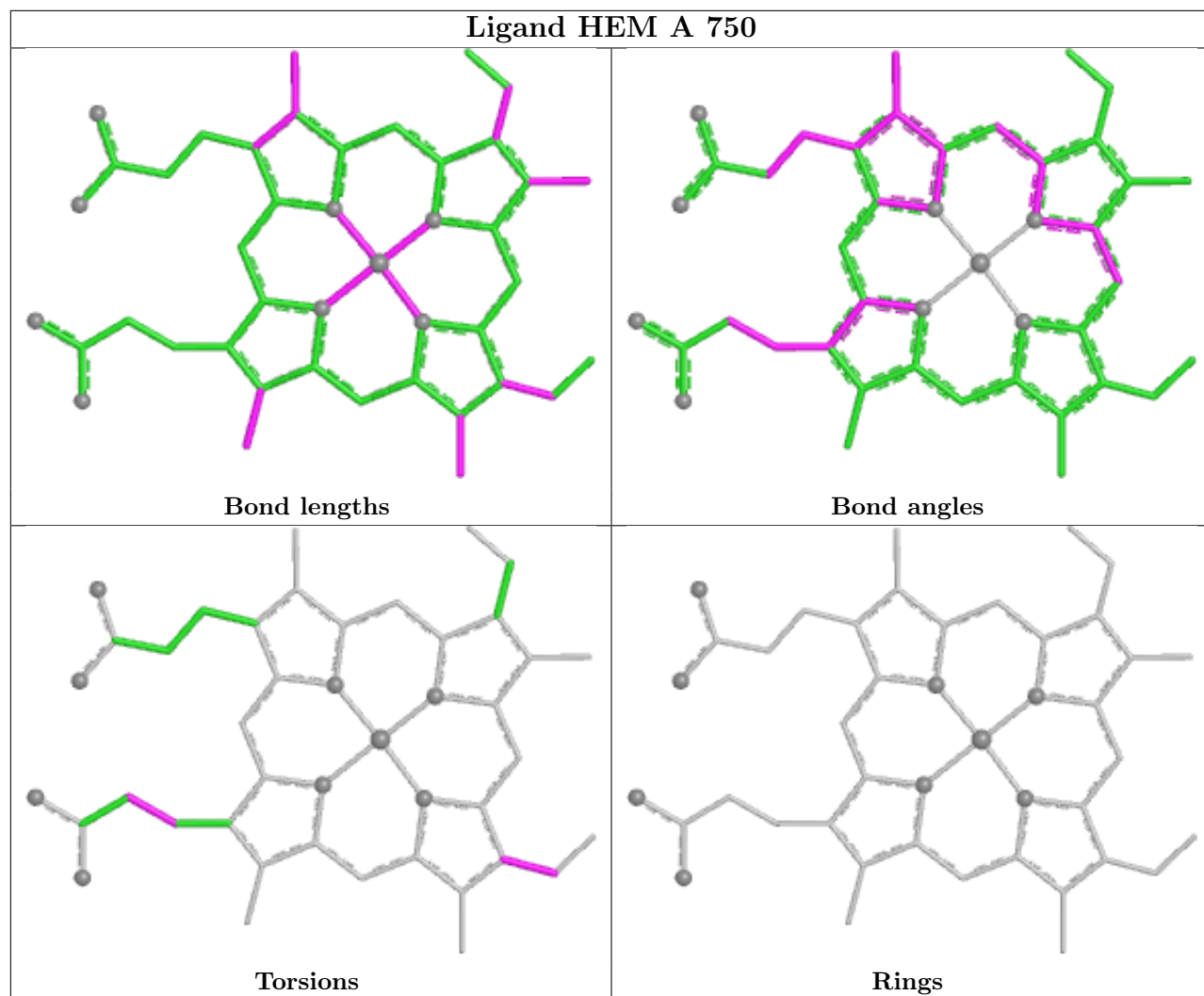
There are no ring outliers.

4 monomers are involved in 12 short contacts:

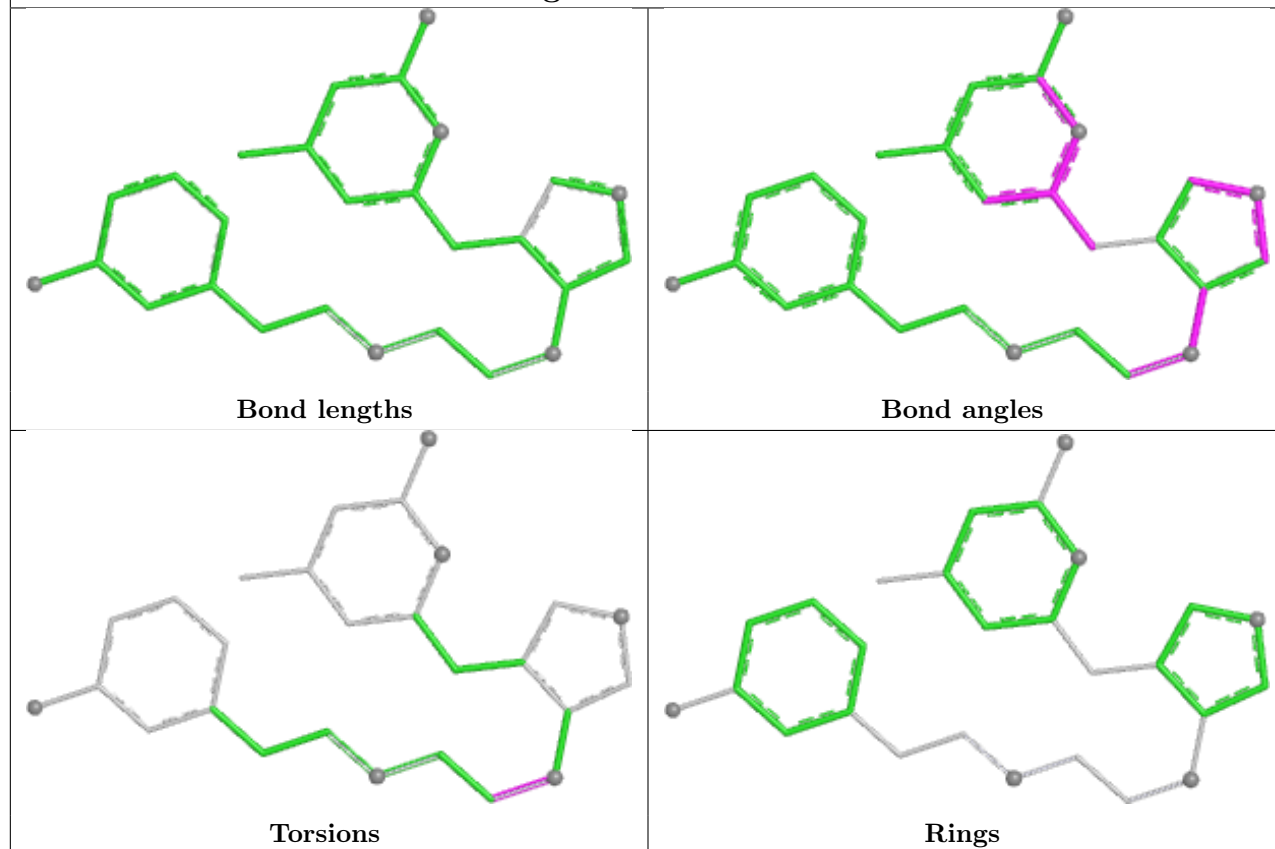
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	HEM	3	0
2	A	750	HEM	5	0
4	A	800	JI4	2	0
4	B	800	JI4	2	0

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.

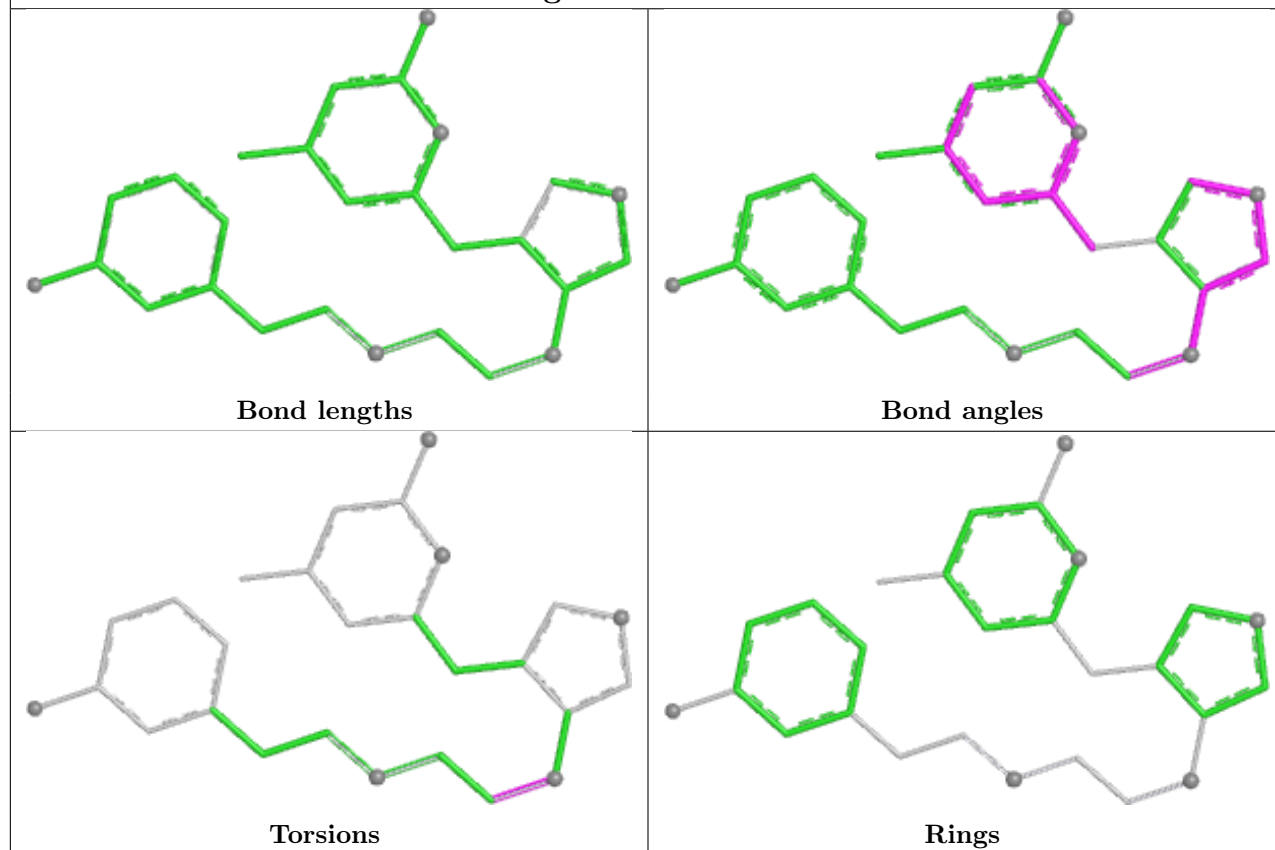




Ligand JI4 A 800



Ligand JI4 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%)	1.20	88 (21%) 2 2	26, 51, 96, 119	0
1	B	411/422 (97%)	0.62	30 (7%) 21 24	26, 40, 64, 88	0
All	All	818/844 (96%)	0.90	118 (14%) 6 6	26, 45, 88, 119	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	ALA	6.0
1	A	513	PRO	5.4
1	A	321	THR	4.8
1	A	528	GLY	4.8
1	A	470	HIS	4.6
1	A	493	LEU	4.5
1	A	510	TRP	4.4
1	A	485	TYR	4.3
1	A	338	PRO	4.2
1	A	715	VAL	4.1
1	A	716	TRP	4.1
1	A	506	ILE	4.1
1	B	348	VAL	4.0
1	A	706	TYR	4.0
1	B	322	LEU	4.0
1	A	625	TRP	4.0
1	A	466	THR	3.9
1	A	487	GLN	3.9
1	A	350	THR	3.9
1	A	488	PRO	3.7
1	B	349	ALA	3.6
1	B	300	PHE	3.6
1	A	559	LEU	3.5
1	B	318	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	558	GLY	3.5
1	A	483	ALA	3.5
1	A	515	GLY	3.4
1	A	376	ALA	3.4
1	A	517	PHE	3.4
1	A	468	GLY	3.4
1	B	350	THR	3.4
1	A	618	MET	3.3
1	A	490	GLY	3.3
1	A	386	LYS	3.1
1	B	321	THR	3.1
1	A	369	ILE	3.0
1	A	514	ARG	3.0
1	B	329	HIS	3.0
1	A	484	GLY	3.0
1	B	611	ALA	3.0
1	A	300	PHE	2.9
1	A	491	SER	2.9
1	A	372	PHE	2.9
1	A	390	SER	2.8
1	B	535	GLN	2.8
1	A	504	ILE	2.8
1	A	311	VAL	2.8
1	A	355	PHE	2.7
1	A	471	ASP	2.7
1	A	599	CYS	2.7
1	B	713	THR	2.6
1	A	556	ASP	2.6
1	A	503	GLU	2.6
1	A	653	SER	2.6
1	A	533	LEU	2.6
1	A	602	SER	2.6
1	A	713	THR	2.6
1	A	354	LEU	2.5
1	A	489	ASP	2.5
1	B	620	LYS	2.5
1	B	515	GLY	2.5
1	A	322	LEU	2.5
1	A	494	GLY	2.5
1	A	551	PHE	2.4
1	A	557	LEU	2.4
1	B	352	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	711	TRP	2.4
1	A	535	GLN	2.4
1	A	492	THR	2.4
1	A	516	ARG	2.4
1	A	482	TYR	2.4
1	B	379	ASP	2.4
1	B	338	PRO	2.4
1	B	353	GLN	2.4
1	A	612	LYS	2.4
1	A	520	LEU	2.3
1	B	355	PHE	2.3
1	A	393	THR	2.3
1	A	710	PRO	2.3
1	A	555	LYS	2.3
1	A	617	ASP	2.3
1	A	373	GLY	2.3
1	A	310	VAL	2.3
1	A	301	LEU	2.3
1	A	607	LEU	2.3
1	A	433	THR	2.3
1	A	601	ASN	2.3
1	A	315	THR	2.3
1	B	618	MET	2.3
1	A	486	LYS	2.3
1	A	299	ARG	2.2
1	A	505	CYS	2.2
1	A	351	LYS	2.2
1	A	337	LEU	2.2
1	B	315	THR	2.2
1	B	668	CYS	2.2
1	A	435	ALA	2.2
1	B	551	PHE	2.1
1	A	553	TRP	2.1
1	A	303	VAL	2.1
1	A	374	SER	2.1
1	A	356	PRO	2.1
1	B	601	ASN	2.1
1	B	607	LEU	2.1
1	A	501	PHE	2.1
1	A	313	THR	2.1
1	B	303	VAL	2.1
1	A	616	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	667	ARG	2.1
1	B	667	ARG	2.1
1	B	386	LYS	2.0
1	B	378	MET	2.0
1	A	605	ASN	2.0
1	B	488	PRO	2.0
1	A	560	LYS	2.0
1	A	604	TYR	2.0
1	B	664	ASN	2.0
1	A	499	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

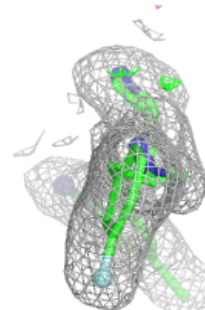
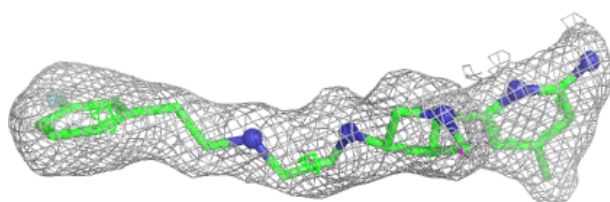
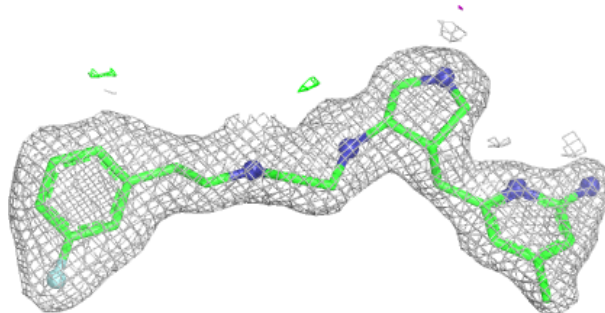
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	A	860	4/4	0.91	0.12	54,55,56,56	0
4	J14	B	800	27/27	0.92	0.09	33,36,57,59	0
4	J14	A	800	27/27	0.92	0.09	34,39,65,67	0
5	ACT	B	861	4/4	0.94	0.11	51,52,52,52	0
3	H4B	A	760	17/17	0.95	0.07	29,32,37,39	0
3	H4B	B	761	17/17	0.95	0.07	26,30,34,36	0
2	HEM	A	750	43/43	0.97	0.08	29,31,43,45	0
2	HEM	B	750	43/43	0.97	0.08	26,30,44,48	0
6	ZN	A	900	1/1	0.99	0.02	36,36,36,36	0

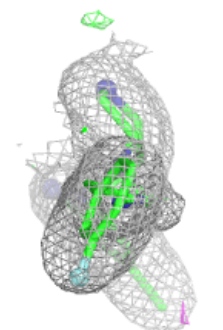
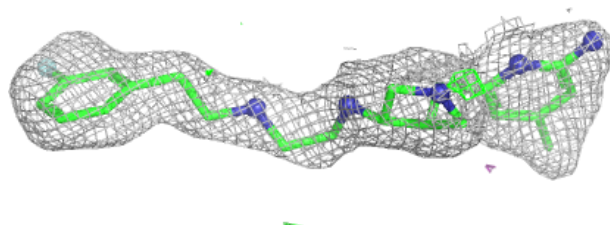
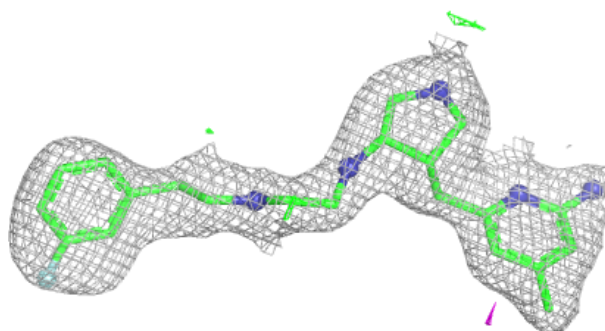
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JI4 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)

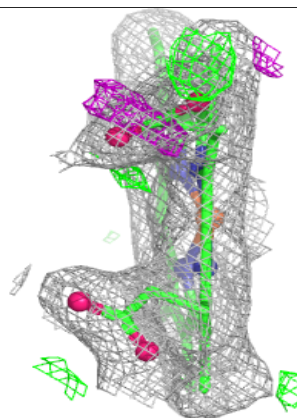
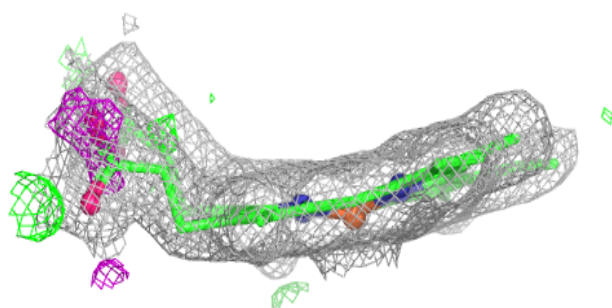
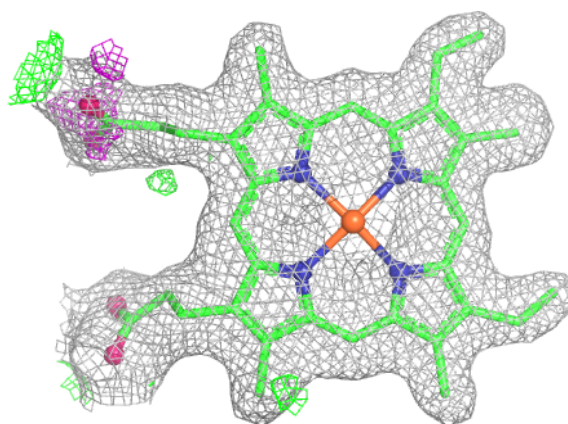
**Electron density around JI4 A 800:**

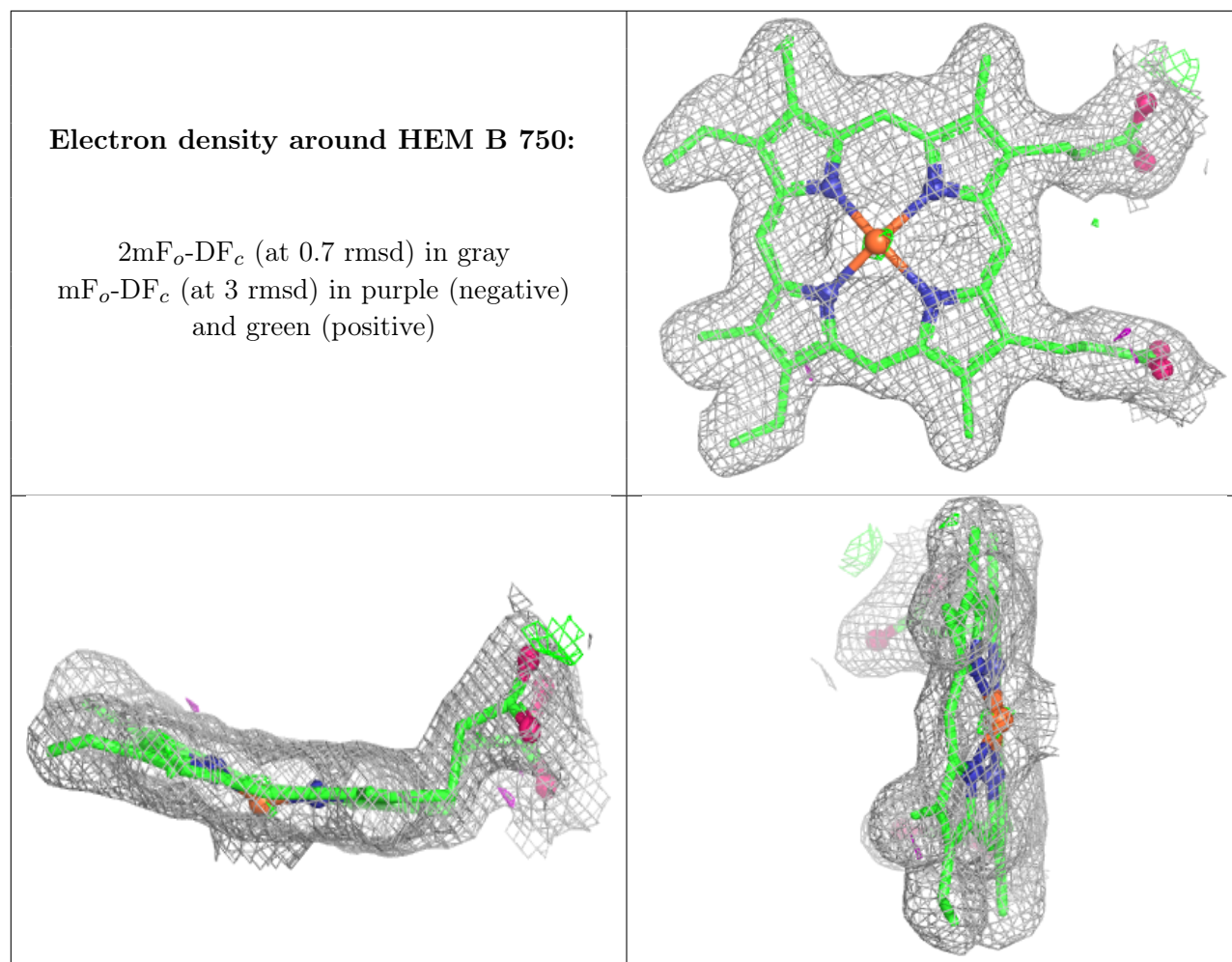
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.