



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 01:03 PM EDT

PDB ID : 3JWV
Title : Structure of rat neuronal nitric oxide synthase R349A mutant heme domain in complex with N1-{(3'S,4'R)-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]pyrrolidin-3'-yl}-N2-(3'-fluorophenethyl)ethane-1,2-diamine
Authors : Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on : 2009-09-18
Resolution : 1.98 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 : 2.23.2
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) : 2.23.2

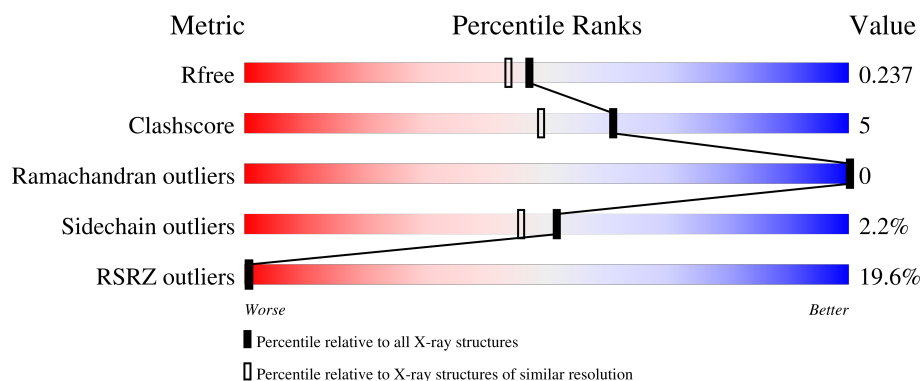
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	<div> <div>27%</div> <div>87%</div> <div>9%</div> <div>••</div> </div>
1	B	422	<div> <div>11%</div> <div>89%</div> <div>9%</div> <div>•</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7170 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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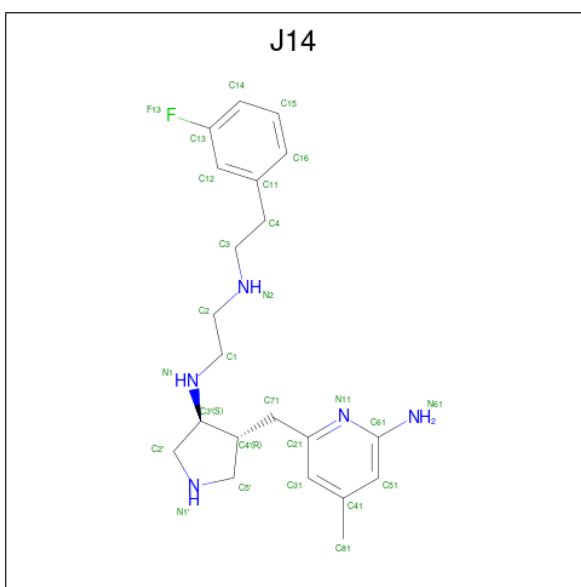
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



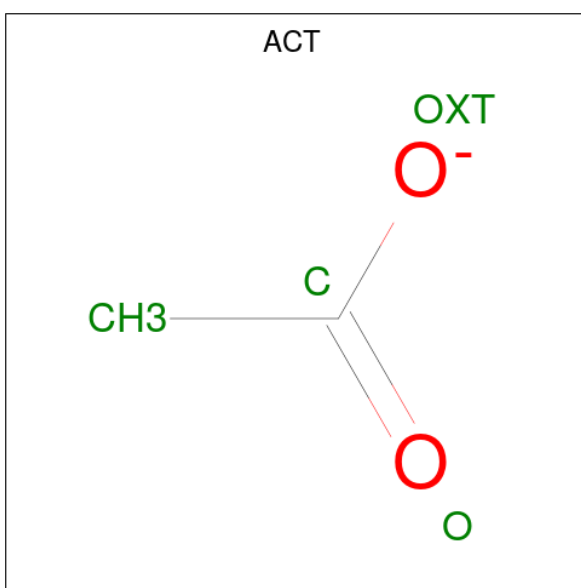
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-{(3S,4R)-4-[(6-amino-4-methylpyridin-2-yl)methyl]pyrrolidin-3-yl}-N'-[2-(3-fluorophenyl)ethyl]ethane-1,2-diamine (three-letter code: J14) (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 (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is ZINC ION (three-letter code: 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	137	Total 137	O 137	0	0
7	B	202	Total 202	O 202	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.91Å 111.90Å 164.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.86 – 1.98 40.86 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.86-1.98) 97.7 (40.86-1.98)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0089, CNS	Depositor
R, R_{free}	0.181 , 0.213 0.210 , 0.237	Depositor DCC
R_{free} test set	3299 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.3	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	7170	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: ZN, J14, ACT, H4B, 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	0.60	0/3406	0.63	1/4621 (0.0%)
1	B	0.65	0/3432	0.64	1/4654 (0.0%)
All	All	0.62	0/6838	0.64	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	A	547	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	B	596	ARG	NE-CZ-NH1	-5.19	117.70	120.30

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	3313	0	3221	25	0
1	B	3339	0	3251	28	0
2	A	43	0	30	4	0
2	B	43	0	30	9	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	30	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	30	7	0
5	A	4	0	3	0	0
6	A	1	0	0	0	0
7	A	137	0	0	0	0
7	B	202	0	0	2	0
All	All	7170	0	6625	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (61) 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:567:VAL:CG2	4:B:800:J14:H5'A	1.84	1.07
1:A:567:VAL:HG22	4:A:800:J14:H5'A	1.41	0.98
1:B:706:TYR:OH	2:B:750:HEM:O1D	1.84	0.94
1:B:567:VAL:HG21	4:B:800:J14:H5'A	1.49	0.93
1:A:706:TYR:OH	2:A:750:HEM:O1D	1.92	0.88
1:A:567:VAL:CG2	4:A:800:J14:H5'A	2.09	0.82
1:B:567:VAL:HG22	4:B:800:J14:H5'A	1.59	0.82
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.68	0.75
1:B:567:VAL:HG21	4:B:800:J14:C5'	2.18	0.72
2:B:750:HEM:HHB	2:B:750:HEM:HBB2	1.71	0.72
1:A:567:VAL:CG2	4:A:800:J14:C5'	2.68	0.71
1:B:299:ARG:HG2	1:B:317:HIS:NE2	2.12	0.65
1:B:299:ARG:HB2	1:B:299:ARG:NH1	2.12	0.65
1:B:706:TYR:HH	2:B:750:HEM:CGD	2.06	0.65
1:B:567:VAL:CG2	4:B:800:J14:C5'	2.71	0.61
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.83	0.61
2:A:750:HEM:HBA1	4:A:800:J14:H71A	1.82	0.60
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.83	0.59
1:A:567:VAL:HG21	4:A:800:J14:H5'	1.85	0.59
2:B:750:HEM:CMC	2:B:750:HEM:HBC2	2.33	0.59
1:A:663:GLU:O	1:A:667:ARG:HG2	2.04	0.57
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.85	0.57
1:B:332:MET:CE	1:B:338:PRO:HB3	2.34	0.57
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.89	0.55
4:B:800:J14:H1A	7:B:1103:HOH:O	2.05	0.55
1:B:552:ASP:OD1	1:B:555:LYS:NZ	2.39	0.55
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.36	0.55
1:B:299:ARG:HB2	1:B:299:ARG:CZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.23	0.53
1:B:299:ARG:HB3	1:B:318:LEU:HD21	1.91	0.53
1:A:299:ARG:O	1:A:317:HIS:CE1	2.62	0.52
1:A:316:LEU:HD12	1:A:319:LYS:HD2	1.92	0.51
1:A:299:ARG:HG3	1:A:318:LEU:HD11	1.93	0.51
1:B:706:TYR:OH	2:B:750:HEM:CGD	2.54	0.51
1:A:596:ARG:NH2	1:A:600:ASP:OD2	2.43	0.50
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.11	0.50
1:B:332:MET:HE3	1:B:338:PRO:HB3	1.92	0.50
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.28	0.49
2:B:750:HEM:HBC2	2:B:750:HEM:HMC1	1.95	0.48
1:A:525:GLN:HG3	1:A:529:ASN:O	2.14	0.47
1:B:701:THR:HA	1:B:702:PRO:C	2.34	0.47
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.04	0.46
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.52	0.46
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.04	0.45
4:B:800:J14:H2A	7:B:1176:HOH:O	2.16	0.45
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.51	0.45
1:A:567:VAL:HG21	4:A:800:J14:C5'	2.41	0.44
1:B:300:PHE:HD2	1:B:315:THR:HG22	1.83	0.44
2:B:750:HEM:HBB2	2:B:750:HEM:CHC	2.42	0.43
1:A:567:VAL:CG2	4:A:800:J14:H5'	2.41	0.43
1:B:300:PHE:CD2	1:B:315:THR:HG22	2.54	0.42
1:B:356:PRO:O	1:B:360:GLU:HG3	2.20	0.42
1:B:389:GLU:HG2	1:B:390:SER:N	2.34	0.42
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.01	0.42
1:A:631:VAL:HG11	1:B:628:GLN:HG2	2.02	0.41
1:B:595:VAL:O	1:B:599:CYS:HB2	2.21	0.41
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.56	0.41
1:B:409:TRP:CH2	2:B:750:HEM:HMC3	2.56	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.94	0.41
2:B:750:HEM:HMC1	2:B:750:HEM:CBC	2.51	0.41
2:A:750:HEM:O2A	4:A:800:J14:H2'A	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%)	393 (98%)	10 (2%)	0	100	100
1	B	407/422 (96%)	402 (99%)	5 (1%)	0	100	100
All	All	810/844 (96%)	795 (98%)	15 (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%)	354 (98%)	9 (2%)	47	39
1	B	365/376 (97%)	358 (98%)	7 (2%)	57	50
All	All	728/752 (97%)	712 (98%)	16 (2%)	52	46

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	THR
1	A	380	ARG
1	A	454	ASN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS

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Mol	Chain	Res	Type
1	A	715	VAL
1	B	353	GLN
1	B	392	SER
1	B	540	LEU
1	B	547	ARG
1	B	552	ASP
1	B	620	LYS
1	B	697	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	454	ASN
1	A	569	ASN
1	A	605	ASN
1	A	697	ASN
1	A	714	HIS
1	B	364	GLN
1	B	385	ASN
1	B	454	ASN
1	B	507	GLN
1	B	535	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	2.04	8 (29%)	17,82,82	2.55	6 (35%)
5	ACT	A	860	-	1,3,3	1.57	0	0,3,3	-	-
3	H4B	B	760	-	16,18,18	1.13	1 (6%)	11,26,26	2.73	6 (54%)
4	J14	B	800	-	27,29,29	0.77	0	30,38,38	2.42	9 (30%)
3	H4B	A	760	-	16,18,18	1.04	1 (6%)	11,26,26	2.91	7 (63%)
4	J14	A	800	-	27,29,29	0.71	0	30,38,38	1.89	6 (20%)
2	HEM	B	750	1	27,50,50	2.22	9 (33%)	17,82,82	1.85	3 (17%)

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	-	0/6/54/54	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	J14	B	800	-	-	8/13/23/23	0/3/3/3
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	J14	A	800	-	-	10/13/23/23	0/3/3/3
2	HEM	B	750	1	-	1/6/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3B-C2B	-5.07	1.33	1.40
2	A	750	HEM	C3D-C2D	4.84	1.52	1.37
2	B	750	HEM	C3C-C2C	-4.65	1.33	1.40
2	B	750	HEM	C3D-C2D	4.54	1.51	1.37
2	A	750	HEM	C3B-C2B	-4.20	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3C-C2C	-3.86	1.35	1.40
2	B	750	HEM	C3C-CAC	3.55	1.55	1.47
2	A	750	HEM	C3B-CAB	3.45	1.55	1.47
2	B	750	HEM	C3B-CAB	3.43	1.54	1.47
2	A	750	HEM	C3C-CAC	3.35	1.54	1.47
2	B	750	HEM	CAA-C2A	2.37	1.55	1.52
2	B	750	HEM	CMA-C3A	2.19	1.56	1.51
2	B	750	HEM	CMD-C2D	2.18	1.56	1.51
2	A	750	HEM	CMC-C2C	2.18	1.56	1.51
2	A	750	HEM	CMA-C3A	2.16	1.56	1.51
3	B	760	H4B	C7-C6	2.11	1.54	1.52
3	A	760	H4B	C2-N2	2.05	1.38	1.33
2	B	750	HEM	CMB-C2B	2.02	1.56	1.51
2	A	750	HEM	CMD-C2D	2.01	1.55	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	J14	C61-N11-C21	7.35	123.67	118.10
4	B	800	J14	C31-C21-N11	-5.74	116.81	122.90
3	A	760	H4B	C4-C4A-C8A	5.65	119.59	114.57
2	A	750	HEM	CBA-CAA-C2A	-5.60	102.17	112.49
3	B	760	H4B	C4-C4A-C8A	5.41	119.37	114.57
2	A	750	HEM	CBD-CAD-C3D	-5.34	102.64	112.48
4	A	800	J14	C61-N11-C21	5.15	122.00	118.10
4	B	800	J14	C2'-C3'-N1	-4.99	104.84	113.73
4	A	800	J14	C31-C21-N11	-4.48	118.14	122.90
4	A	800	J14	C1-N1-C3'	4.44	120.49	114.20
2	B	750	HEM	C1D-C2D-C3D	-4.36	103.96	107.00
2	B	750	HEM	CBD-CAD-C3D	-4.24	104.67	112.48
4	B	800	J14	C1-N1-C3'	4.01	119.88	114.20
3	A	760	H4B	C4-N3-C2	3.99	122.27	115.93
2	A	750	HEM	C1D-C2D-C3D	-3.93	104.26	107.00
3	A	760	H4B	N3-C2-N1	-3.79	119.48	125.42
3	B	760	H4B	N3-C2-N1	-3.70	119.62	125.42
3	B	760	H4B	C4-N3-C2	3.59	121.64	115.93
4	A	800	J14	C2'-C3'-N1	-2.86	108.64	113.73
3	B	760	H4B	C2-N1-C8A	2.76	120.73	114.54
3	A	760	H4B	N2-C2-N3	2.76	121.54	117.25
2	A	750	HEM	C4C-C3C-C2C	2.74	108.81	106.90
3	A	760	H4B	C2-N1-C8A	2.73	120.65	114.54
4	B	800	J14	C2-C1-N1	2.69	115.44	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	C4-C4A-N5	2.67	121.36	119.12
4	A	800	J14	C5'-N1'-C2'	2.63	111.63	105.42
4	B	800	J14	C5'-N1'-C2'	2.63	111.62	105.42
4	A	800	J14	C2-C1-N1	2.59	115.28	111.06
2	B	750	HEM	CAD-CBD-CGD	-2.46	108.55	112.67
3	B	760	H4B	C4-C4A-N5	2.39	121.12	119.12
3	B	760	H4B	N2-C2-N3	2.26	120.77	117.25
4	B	800	J14	C21-C71-C4'	2.18	122.72	115.55
4	B	800	J14	C14-C13-C12	-2.18	120.46	123.29
4	B	800	J14	C71-C21-C31	2.15	125.62	121.04
2	A	750	HEM	CMC-C2C-C3C	2.13	128.66	124.68
3	A	760	H4B	C4A-C4-N3	-2.11	118.03	124.01
2	A	750	HEM	CMD-C2D-C3D	2.06	128.83	124.94

There are no chirality outliers.

All (19) torsion outliers are listed below:

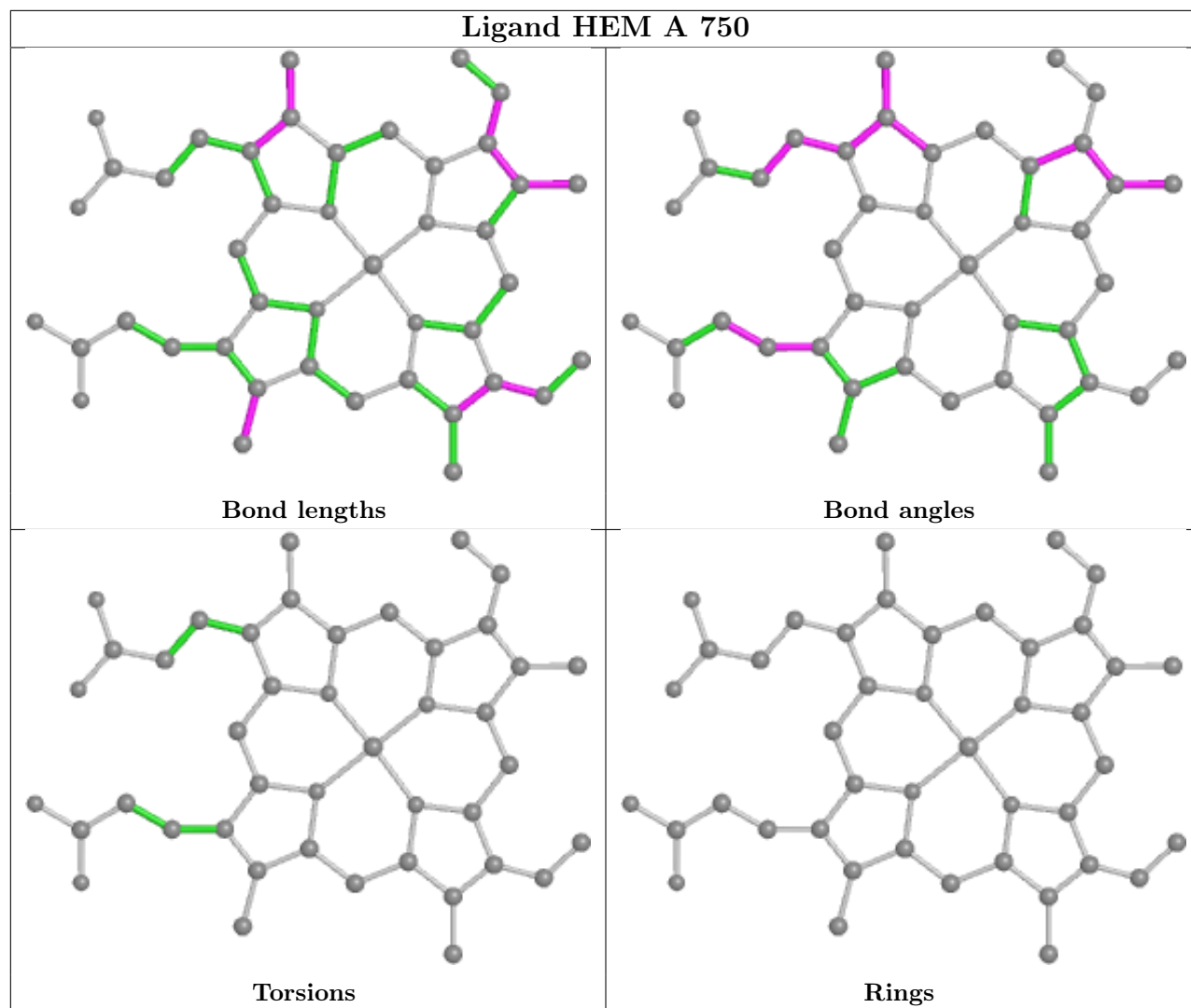
Mol	Chain	Res	Type	Atoms
2	B	750	HEM	C2A-CAA-CBA-CGA
4	A	800	J14	C2-C1-N1-C3'
4	A	800	J14	N2-C3-C4-C11
4	A	800	J14	N11-C21-C71-C4'
4	A	800	J14	C3'-C4'-C71-C21
4	A	800	J14	C5'-C4'-C71-C21
4	B	800	J14	N2-C3-C4-C11
4	B	800	J14	N11-C21-C71-C4'
4	A	800	J14	N1-C1-C2-N2
4	B	800	J14	N1-C1-C2-N2
4	B	800	J14	C2-C1-N1-C3'
4	A	800	J14	C4-C3-N2-C2
4	A	800	J14	C1-C2-N2-C3
4	B	800	J14	C1-C2-N2-C3
4	A	800	J14	C16-C11-C4-C3
4	A	800	J14	C12-C11-C4-C3
4	B	800	J14	C16-C11-C4-C3
4	B	800	J14	C12-C11-C4-C3
4	B	800	J14	C31-C21-C71-C4'

There are no ring outliers.

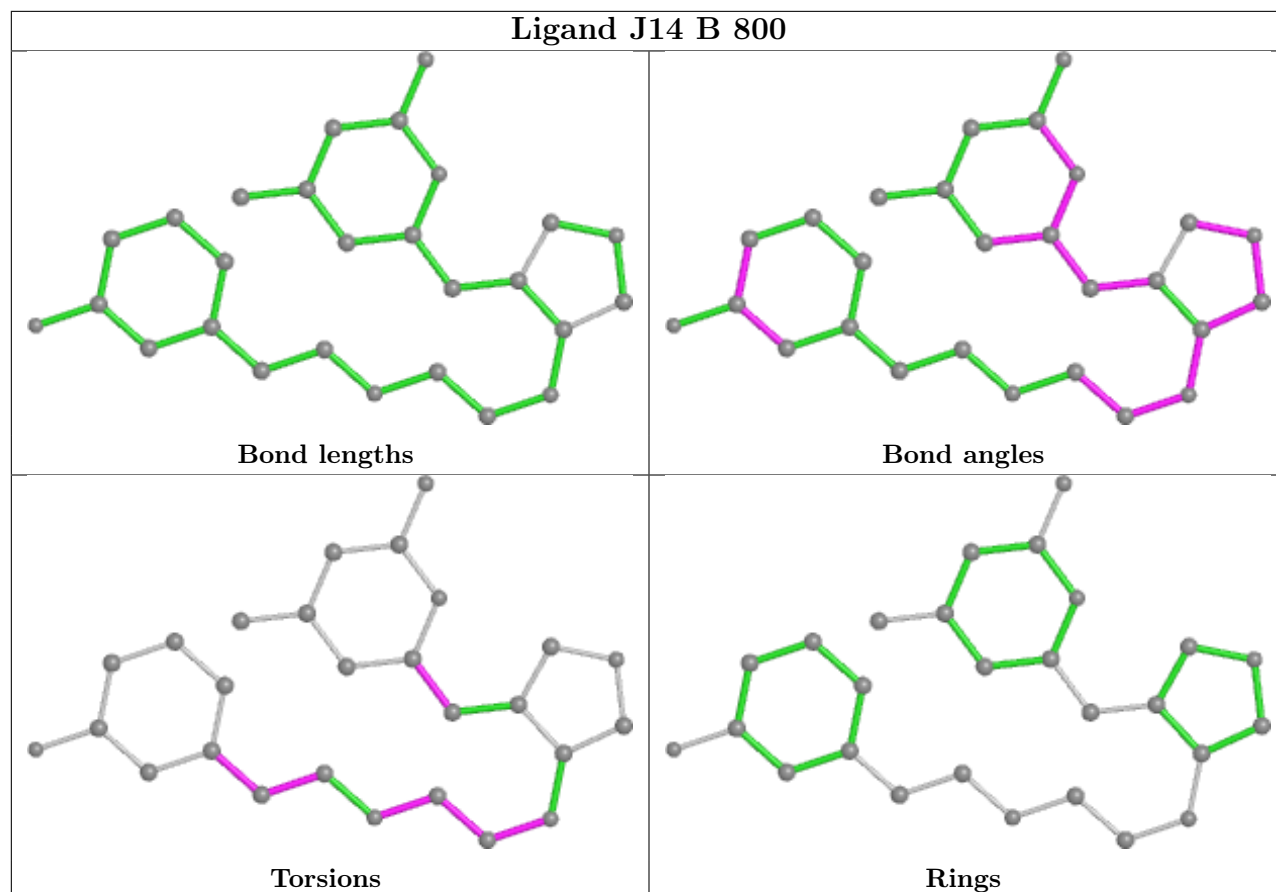
4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	4	0
4	B	800	J14	7	0
4	A	800	J14	8	0
2	B	750	HEM	9	0

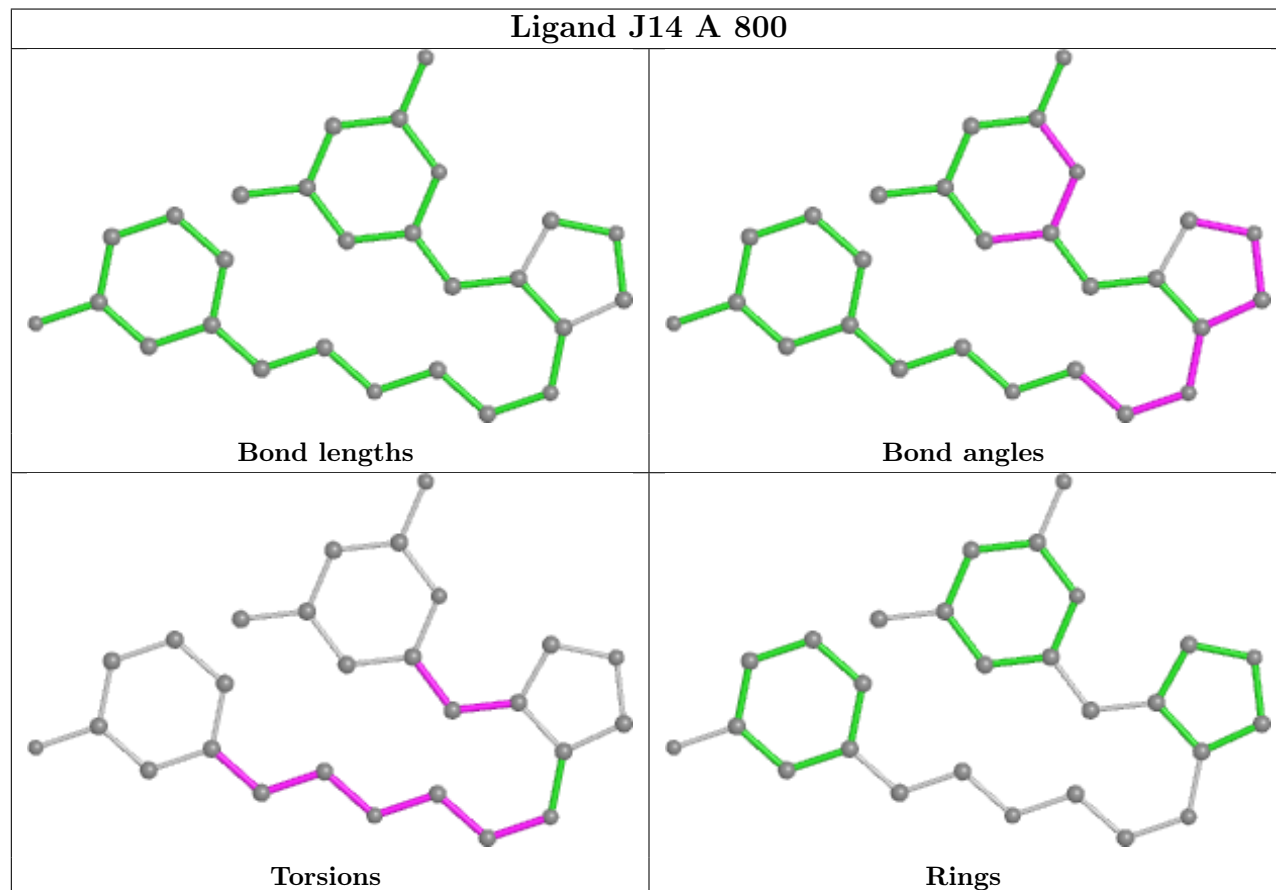
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

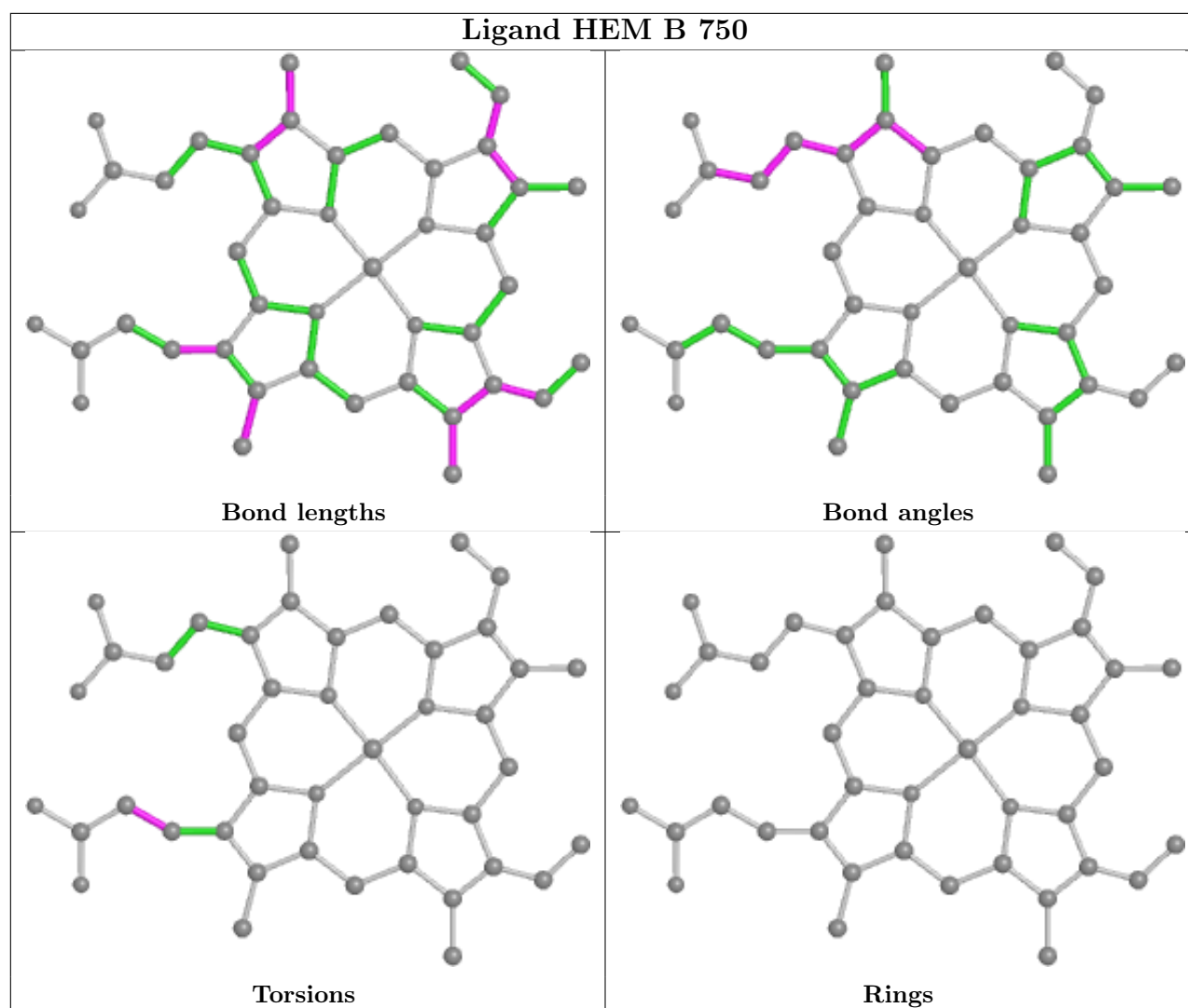


Ligand J14 B 800



Ligand J14 A 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%)	1.37	115 (28%) 0 0	29, 57, 107, 139	0
1	B	411/422 (97%)	0.71	45 (10%) 5 6	29, 44, 68, 91	0
All	All	818/844 (96%)	1.04	160 (19%) 1 1	29, 49, 99, 139	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	9.0
1	B	300	PHE	7.3
1	A	488	PRO	7.1
1	B	350	THR	6.7
1	A	715	VAL	6.6
1	A	355	PHE	6.2
1	A	388	ILE	6.0
1	B	348	VAL	5.6
1	A	619	ARG	5.3
1	A	506	ILE	5.3
1	A	486	LYS	5.1
1	A	507	GLN	4.8
1	A	390	SER	4.8
1	B	321	THR	4.8
1	B	619	ARG	4.4
1	B	611	ALA	4.4
1	A	351	LYS	4.3
1	A	713	THR	4.3
1	A	389	GLU	4.2
1	A	490	GLY	4.2
1	A	479	LEU	4.1
1	A	508	GLN	4.0
1	A	352	ASP	4.0
1	B	352	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	469	LYS	3.9
1	A	714	HIS	3.9
1	B	351	LYS	3.8
1	A	493	LEU	3.8
1	A	553	TRP	3.8
1	A	470	HIS	3.8
1	B	677	VAL	3.8
1	A	487	GLN	3.7
1	A	491	SER	3.7
1	A	567	VAL	3.7
1	A	300	PHE	3.7
1	A	494	GLY	3.7
1	A	551	PHE	3.6
1	A	480	ILE	3.6
1	B	479	LEU	3.6
1	A	392	SER	3.5
1	A	677	VAL	3.5
1	A	509	GLY	3.4
1	A	678	TRP	3.4
1	B	567	VAL	3.4
1	A	492	THR	3.4
1	A	373	GLY	3.4
1	B	349	ALA	3.3
1	B	299	ARG	3.3
1	A	503	GLU	3.3
1	A	711	TRP	3.3
1	B	318	LEU	3.3
1	A	541	VAL	3.2
1	B	355	PHE	3.2
1	A	382	GLU	3.2
1	A	499	VAL	3.2
1	B	620	LYS	3.2
1	A	712	ASN	3.2
1	B	718	GLY	3.2
1	A	584	PHE	3.2
1	A	386	LYS	3.1
1	B	676	TRP	3.1
1	A	415	CYS	3.1
1	A	570	MET	3.1
1	B	480	ILE	3.0
1	A	511	LYS	3.0
1	A	679	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	485	TYR	2.9
1	A	528	GLY	2.9
1	A	680	VAL	2.9
1	A	582	CYS	2.9
1	A	566	ALA	2.9
1	B	553	TRP	2.9
1	B	310	VAL	2.9
1	A	593	ILE	2.9
1	A	612	LYS	2.9
1	A	442	ILE	2.8
1	A	416	VAL	2.8
1	B	564	LEU	2.8
1	B	566	ALA	2.8
1	A	369	ILE	2.8
1	B	442	ILE	2.8
1	A	510	TRP	2.8
1	A	676	TRP	2.8
1	A	391	THR	2.7
1	A	588	TYR	2.7
1	B	680	VAL	2.7
1	A	537	PRO	2.7
1	B	591	THR	2.7
1	A	385	ASN	2.7
1	A	371	ARG	2.7
1	A	591	THR	2.7
1	A	489	ASP	2.6
1	A	366	TYR	2.6
1	B	386	LYS	2.6
1	A	514	ARG	2.6
1	A	483	ALA	2.5
1	B	389	GLU	2.5
1	A	322	LEU	2.5
1	A	319	LYS	2.5
1	A	609	GLU	2.5
1	A	706	TYR	2.5
1	A	565	PRO	2.4
1	A	568	SER	2.4
1	A	616	LEU	2.4
1	A	682	PRO	2.4
1	A	517	PHE	2.4
1	A	590	GLY	2.4
1	A	564	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	299	ARG	2.4
1	B	667	ARG	2.4
1	A	446	VAL	2.4
1	B	568	SER	2.3
1	A	533	LEU	2.3
1	A	372	PHE	2.3
1	A	394	TYR	2.3
1	B	615	ASP	2.3
1	A	393	THR	2.3
1	B	588	TYR	2.3
1	A	555	LYS	2.3
1	A	519	VAL	2.3
1	A	459	ILE	2.3
1	B	679	ILE	2.3
1	B	493	LEU	2.3
1	B	565	PRO	2.2
1	A	691	PHE	2.2
1	B	391	THR	2.2
1	B	678	TRP	2.2
1	A	540	LEU	2.2
1	A	557	LEU	2.2
1	A	561	TRP	2.2
1	A	681	PRO	2.2
1	A	611	ALA	2.2
1	B	353	GLN	2.2
1	A	376	ALA	2.1
1	A	482	TYR	2.1
1	A	562	TYR	2.1
1	B	443	CYS	2.1
1	B	541	VAL	2.1
1	A	618	MET	2.1
1	A	615	ASP	2.1
1	A	370	LYS	2.1
1	A	550	LYS	2.1
1	A	384	VAL	2.1
1	A	667	ARG	2.1
1	B	329	HIS	2.1
1	A	704	PHE	2.1
1	B	551	PHE	2.1
1	B	446	VAL	2.1
1	A	423	LYS	2.1
1	A	542	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	586	GLY	2.1
1	A	685	GLY	2.1
1	A	378	MET	2.0
1	A	585	SER	2.0
1	B	392	SER	2.0
1	B	550	LYS	2.0
1	A	581	ALA	2.0
1	A	552	ASP	2.0
1	A	520	LEU	2.0
1	A	315	THR	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](#)

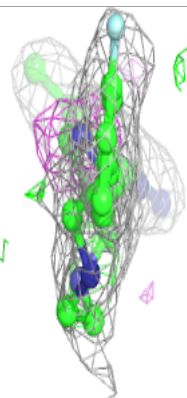
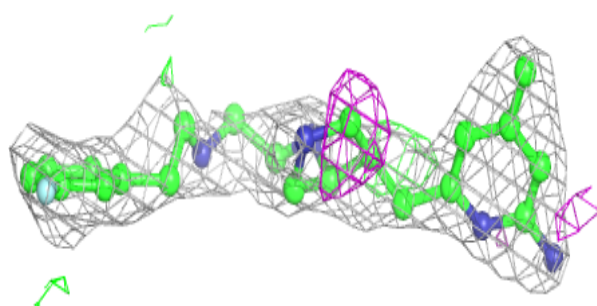
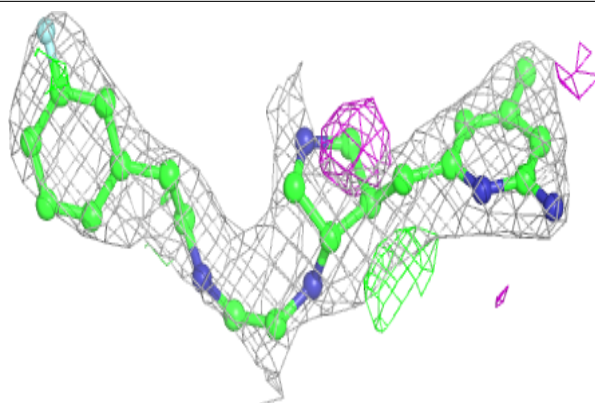
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	J14	B	800	27/27	0.84	0.30	51,73,84,85	0
4	J14	A	800	27/27	0.85	0.38	44,75,108,110	0
5	ACT	A	860	4/4	0.94	0.18	63,65,65,65	0
3	H4B	B	760	17/17	0.95	0.19	36,38,41,41	0
3	H4B	A	760	17/17	0.96	0.18	37,41,45,46	0
2	HEM	B	750	43/43	0.97	0.16	31,35,51,55	0
2	HEM	A	750	43/43	0.97	0.21	32,36,54,56	0
6	ZN	A	900	1/1	0.99	0.12	38,38,38,38	0

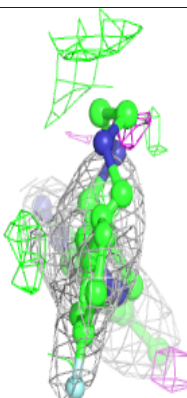
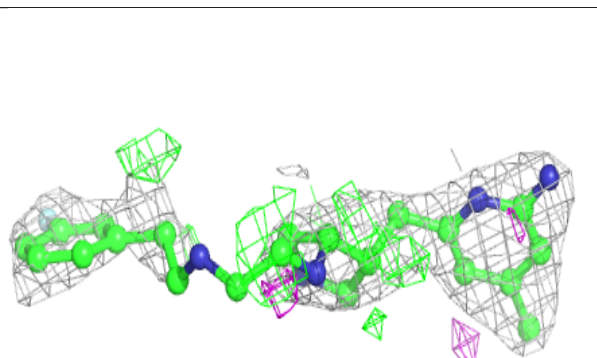
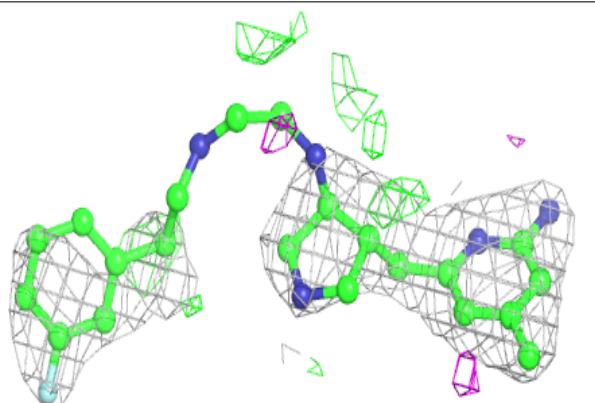
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around J14 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)

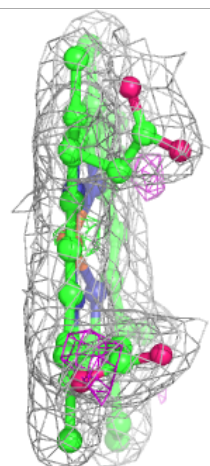
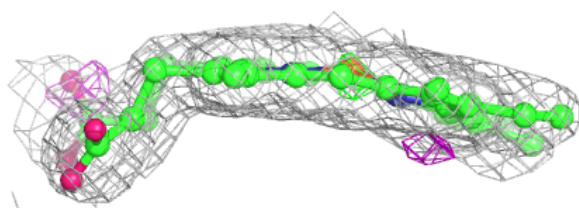
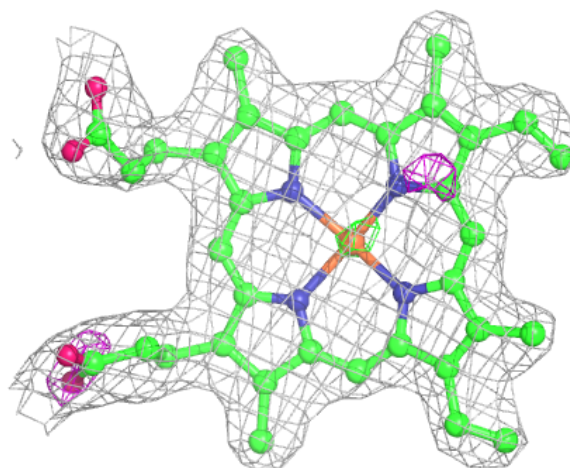
**Electron density around J14 A 800:**

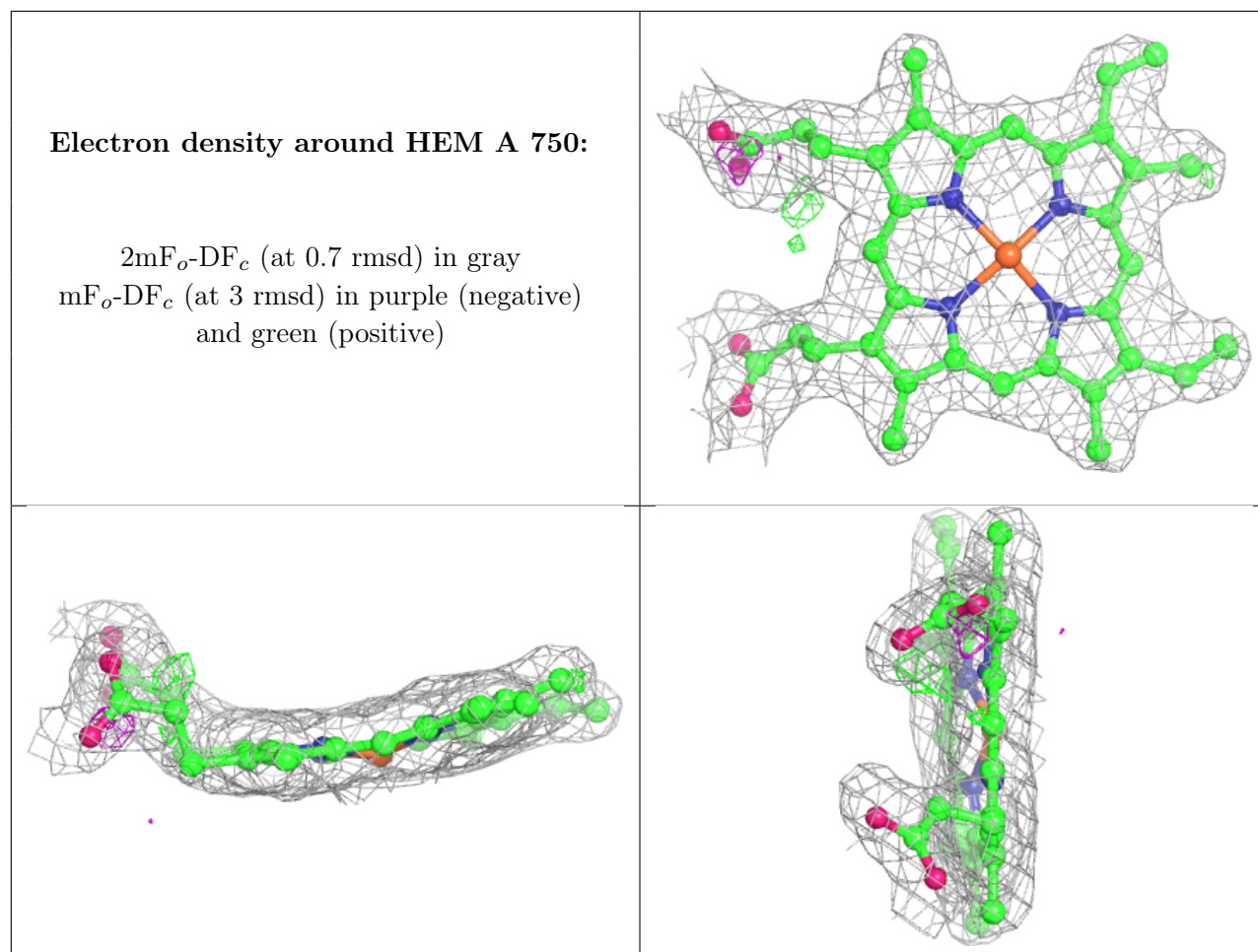
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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.