



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:35 am BST

PDB ID : 3NLN
Title : Structure of neuronal nitric oxide synthase R349A mutant heme domain in complex with 6-{{(3'R,4'S)-3'-[2''-(3'''-fluorophenethylamino)ethoxy]pyrrolidin-4'-yl}methyl}-4-methylpyridin-2-amine
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Deposited on : 2010-06-21
Resolution : 2.00 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

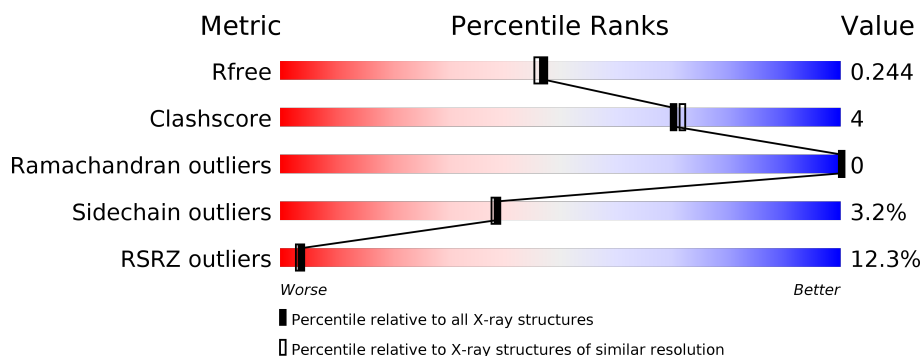
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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 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	<div> <div>17%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>••</div> </div> </div>
1	B	422	<div> <div>7%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7141 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.

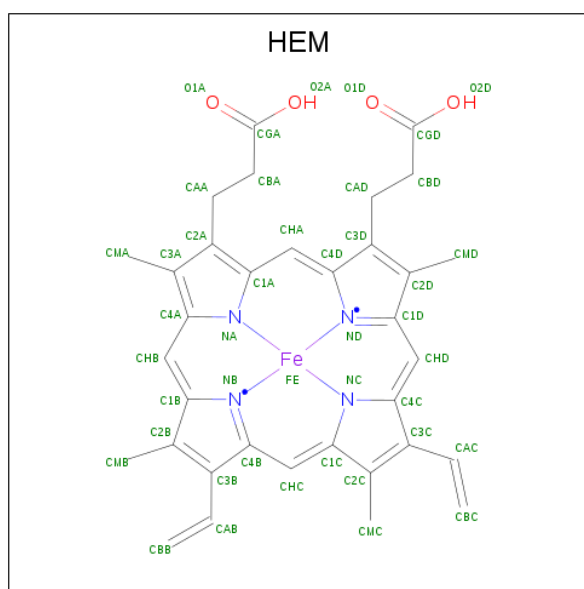
- Molecule 1 is a protein called Nitric oxide synthase, brain.

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: $C_{34}H_{32}FeN_4O_4$).



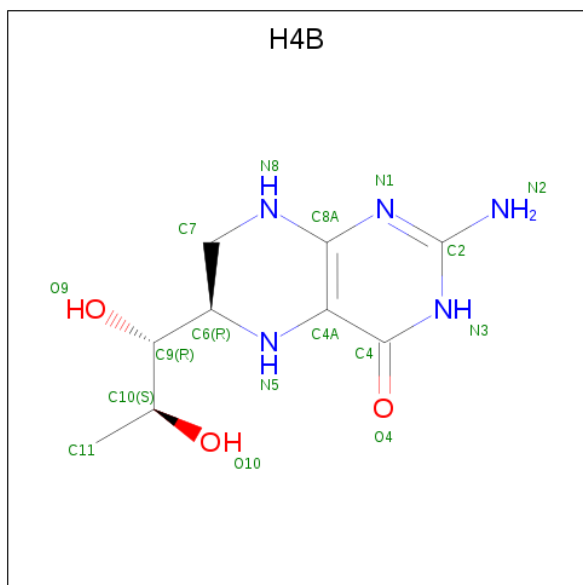
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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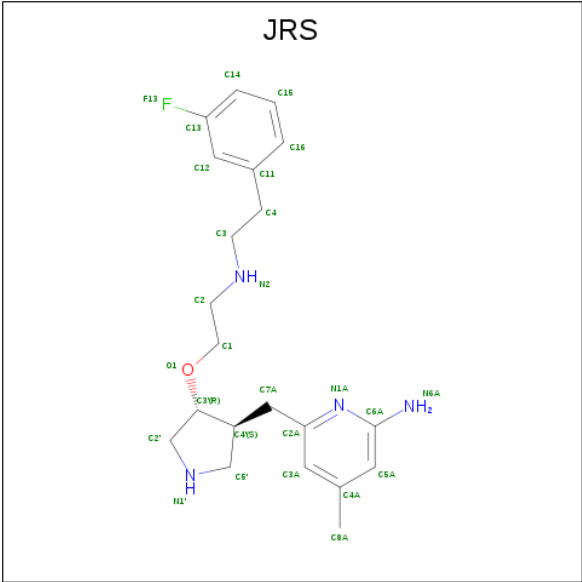
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



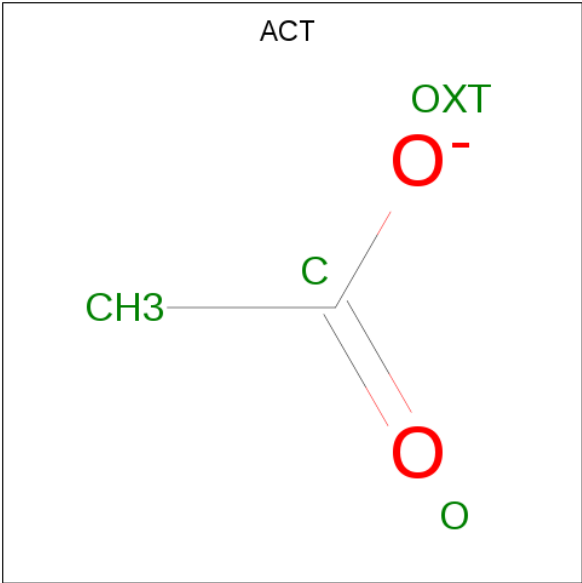
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-[(3S,4R)-4-(2-{[2-(3-fluorophenyl)ethyl]amino}ethoxy)pyrrolidin-3-yl]methyl-4-methylpyridin-2-amine (three-letter code: JRS) (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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

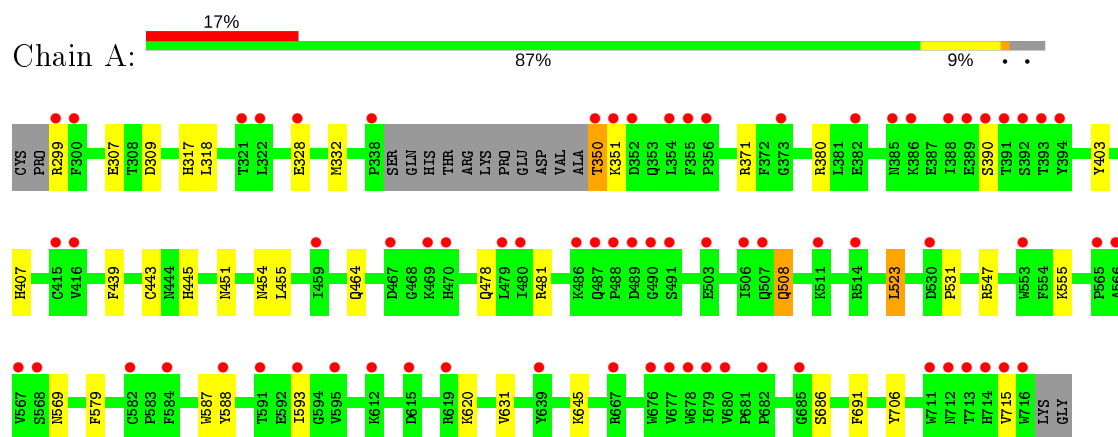
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	123	Total 123	O 123	0	0
7	B	183	Total 183	O 183	0	0

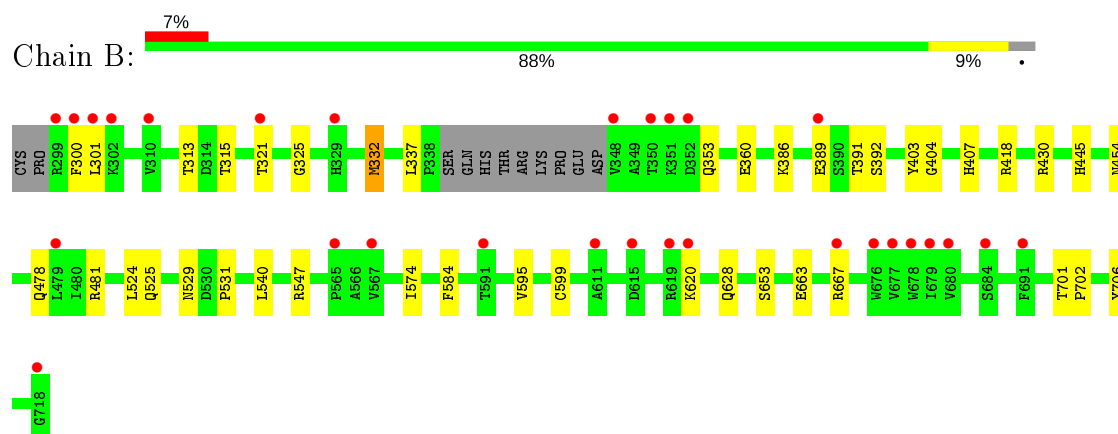
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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	51.95Å 112.19Å 164.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.20 – 2.00 38.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.20-2.00) 98.8 (38.67-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.187 , 0.225 0.208 , 0.244	Depositor DCC
R_{free} test set	3236 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.4	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	7141	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 3.72% 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, ZN, JRS, H4B, ACT

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	0.67	0/3406	0.65	0/4621
1	B	0.71	0/3432	0.70	2/4654 (0.0%)
All	All	0.69	0/6838	0.67	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	418	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	430	ARG	NE-CZ-NH1	5.53	123.06	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	20	0
1	B	3339	0	3251	21	0
2	A	43	0	30	7	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	29	4	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	123	0	0	2	0
7	B	183	0	0	1	0
All	All	7141	0	6626	48	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 4.

All (48) 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)
2:A:750:HEM:O2D	4:A:800:JRS:H2	1.69	0.91
1:A:706:TYR:OH	2:A:750:HEM:O1D	1.89	0.90
1:B:706:TYR:OH	2:B:750:HEM:O1D	1.93	0.86
2:B:750:HEM:O2D	4:B:800:JRS:H2	1.90	0.71
1:A:328:GLU:OE2	7:A:1049:HOH:O	2.09	0.70
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.77	0.67
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.79	0.65
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.78	0.65
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.79	0.64
2:B:750:HEM:HBA1	4:B:800:JRS:H7AA	1.80	0.61
1:B:706:TYR:CZ	4:B:800:JRS:H16	2.36	0.60
1:B:391:THR:O	1:B:392:SER:HB2	2.04	0.57
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.86	0.57
1:A:508:GLN:HA	1:A:508:GLN:HE21	1.70	0.55
2:A:750:HEM:HBA1	4:A:800:JRS:H7AA	1.89	0.55
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.37	0.55
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.90	0.53
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.91	0.53
1:A:299:ARG:O	1:A:317:HIS:CE1	2.62	0.52
1:A:350:THR:HG22	1:A:351:LYS:H	1.73	0.52
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.41	0.51
1:B:701:THR:HA	1:B:702:PRO:C	2.32	0.49
1:B:300:PHE:CD2	1:B:315:THR:HG22	2.49	0.48
1:A:307:GLU:HG3	7:B:1045:HOH:O	2.14	0.48
1:B:706:TYR:OH	2:B:750:HEM:CGD	2.61	0.47
2:A:750:HEM:HMC1	2:A:750:HEM:HBC2	1.97	0.47
1:B:584:PHE:CD1	2:B:750:HEM:CAC	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:PHE:CD1	2:B:750:HEM:HAC	2.50	0.46
1:B:404:GLY:HA3	1:B:574:ILE:HD13	1.99	0.45
1:A:332:MET:HE3	1:B:301:LEU:HD22	1.99	0.44
1:B:337:LEU:HG	4:B:800:JRS:H15	2.00	0.44
1:A:451:ASN:HB3	1:A:454:ASN:O	2.18	0.44
1:B:595:VAL:O	1:B:599:CYS:HB2	2.18	0.44
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.53	0.43
1:B:325:GLY:O	1:B:332:MET:HG3	2.19	0.43
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.07	0.43
1:B:445:HIS:C	1:B:445:HIS:CD2	2.92	0.43
1:B:525:GLN:HG3	1:B:529:ASN:O	2.19	0.43
2:A:750:HEM:O2A	7:A:1083:HOH:O	2.21	0.42
1:B:524:LEU:O	1:B:531:PRO:HA	2.20	0.42
1:A:299:ARG:HG3	1:A:318:LEU:HD11	2.01	0.42
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.56	0.41
1:A:686:SER:HA	1:A:691:PHE:CG	2.55	0.41
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.14	0.41
1:B:386:LYS:O	1:B:389:GLU:HG2	2.21	0.41
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.36	0.40
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.40
1:A:445:HIS:C	1:A:445:HIS:CD2	2.94	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%)	395 (98%)	8 (2%)	0	100	100
1	B	407/422 (96%)	397 (98%)	10 (2%)	0	100	100
All	All	810/844 (96%)	792 (98%)	18 (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%)	350 (96%)	13 (4%)	35	34
1	B	365/376 (97%)	355 (97%)	10 (3%)	44	46
All	All	728/752 (97%)	705 (97%)	23 (3%)	39	38

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	ASP
1	A	350	THR
1	A	371	ARG
1	A	380	ARG
1	A	390	SER
1	A	508	GLN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	313	THR
1	B	321	THR
1	B	332	MET
1	B	353	GLN
1	B	360	GLU
1	B	454	ASN
1	B	540	LEU
1	B	547	ARG
1	B	620	LYS
1	B	653	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	ASN
1	A	454	ASN
1	A	508	GLN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	B	353	GLN
1	B	364	GLN
1	B	385	ASN
1	B	440	ASN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	527	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 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	$\# Z > 2$
4	JRS	A	800	-	28,29,29	0.67	0	31,38,38	1.48	3 (9%)
4	JRS	B	800	-	28,29,29	0.74	0	31,38,38	1.37	3 (9%)
3	H4B	B	760	-	16,18,18	1.22	2 (12%)	11,26,26	2.74	4 (36%)
2	HEM	A	750	1	27,50,50	2.08	9 (33%)	17,82,82	2.14	5 (29%)
5	ACT	B	860	-	1,3,3	1.51	0	0,3,3	0.00	-
5	ACT	A	860	-	1,3,3	1.49	0	0,3,3	0.00	-
2	HEM	B	750	1	27,50,50	2.08	6 (22%)	17,82,82	2.18	3 (17%)
3	H4B	A	760	-	16,18,18	1.30	3 (18%)	11,26,26	3.13	7 (63%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	JRS	A	800	-	-	4/13/23/23	0/3/3/3
4	JRS	B	800	-	-	2/13/23/23	0/3/3/3
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
2	HEM	A	750	1	-	1/6/54/54	-
2	HEM	B	750	1	-	1/6/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3B-C2B	-4.76	1.33	1.40
2	A	750	HEM	C3D-C2D	4.65	1.51	1.37
2	A	750	HEM	C3C-C2C	-4.49	1.34	1.40
2	B	750	HEM	C3D-C2D	4.40	1.50	1.37
2	B	750	HEM	C3C-C2C	-4.10	1.34	1.40
2	A	750	HEM	C3B-C2B	-3.61	1.35	1.40
2	B	750	HEM	C3C-CAC	3.59	1.55	1.47
2	A	750	HEM	C3C-CAC	3.06	1.54	1.47
2	A	750	HEM	C3B-CAB	3.00	1.54	1.47
2	B	750	HEM	C3B-CAB	2.90	1.53	1.47
3	B	760	H4B	C7-C6	2.89	1.55	1.52
3	A	760	H4B	C4-N3	2.79	1.37	1.33
3	A	760	H4B	C2-N2	2.63	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	CMD-C2D	2.50	1.56	1.51
2	A	750	HEM	CAD-C3D	2.49	1.56	1.52
2	A	750	HEM	CMC-C2C	2.45	1.57	1.51
3	B	760	H4B	C7-N8	2.35	1.48	1.44
3	A	760	H4B	C4-C4A	-2.35	1.38	1.41
2	A	750	HEM	CMA-C3A	2.15	1.56	1.51
2	A	750	HEM	CMB-C2B	2.01	1.56	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	760	H4B	C4-C4A-C8A	6.28	120.14	114.57
2	B	750	HEM	CBD-CAD-C3D	-5.51	102.33	112.48
2	A	750	HEM	CBD-CAD-C3D	-5.25	102.81	112.48
2	B	750	HEM	CAD-CBD-CGD	-4.79	104.63	112.67
4	A	800	JRS	C6A-N1A-C2A	4.62	121.60	118.10
3	A	760	H4B	C4-C4A-C8A	4.51	118.57	114.57
3	A	760	H4B	C4-N3-C2	4.42	122.95	115.93
3	A	760	H4B	N3-C2-N1	-4.36	118.59	125.42
3	B	760	H4B	C4-N3-C2	4.17	122.56	115.93
3	A	760	H4B	C4-C4A-N5	4.12	122.58	119.12
4	A	800	JRS	C3A-C2A-N1A	-3.91	118.75	122.90
4	B	800	JRS	C6A-N1A-C2A	3.80	120.98	118.10
3	A	760	H4B	N2-C2-N3	3.78	123.14	117.25
4	B	800	JRS	C3A-C2A-N1A	-3.60	119.08	122.90
2	B	750	HEM	C1D-C2D-C3D	-3.56	104.52	107.00
2	A	750	HEM	CMA-C3A-C4A	-3.39	123.25	128.46
2	A	750	HEM	C4C-C3C-C2C	3.10	109.06	106.90
3	A	760	H4B	C2-N1-C8A	2.90	121.03	114.54
2	A	750	HEM	C4A-C3A-C2A	2.72	108.89	107.00
3	B	760	H4B	N3-C2-N1	-2.70	121.18	125.42
4	A	800	JRS	C3-C4-C11	-2.64	106.75	112.87
3	B	760	H4B	C4A-C4-N3	-2.42	117.14	124.01
4	B	800	JRS	C3'-C2'-N1'	2.20	108.89	105.20
3	A	760	H4B	C4A-C4-N3	-2.08	118.10	124.01
2	A	750	HEM	C1D-C2D-C3D	-2.04	105.58	107.00

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	750	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
4	A	800	JRS	C1-C2-N2-C3
4	B	800	JRS	C1-C2-N2-C3
4	A	800	JRS	O1-C1-C2-N2
2	B	750	HEM	C2A-CAA-CBA-CGA
4	A	800	JRS	N2-C3-C4-C11
4	B	800	JRS	N2-C3-C4-C11
4	A	800	JRS	C2-C1-O1-C3'

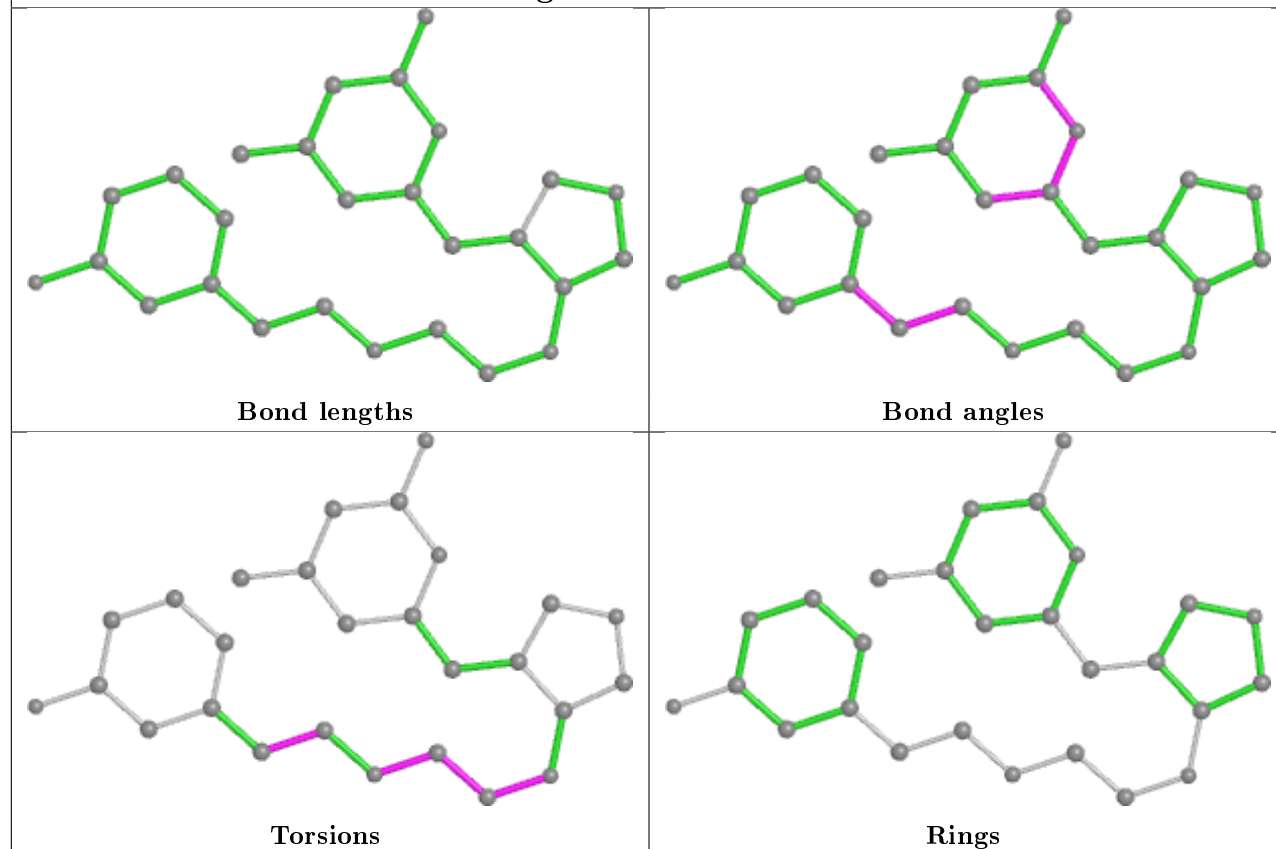
There are no ring outliers.

4 monomers are involved in 16 short contacts:

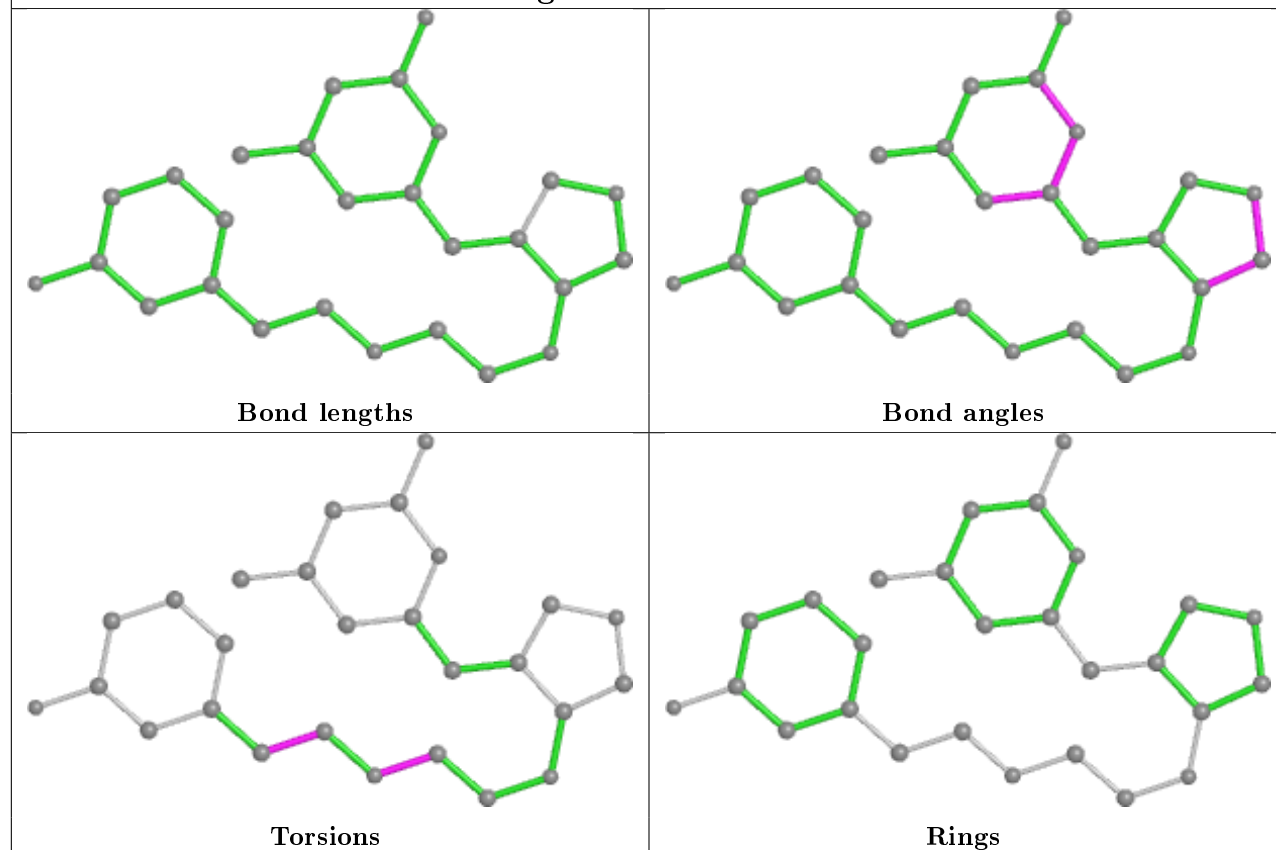
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	JRS	2	0
4	B	800	JRS	4	0
2	A	750	HEM	7	0
2	B	750	HEM	7	0

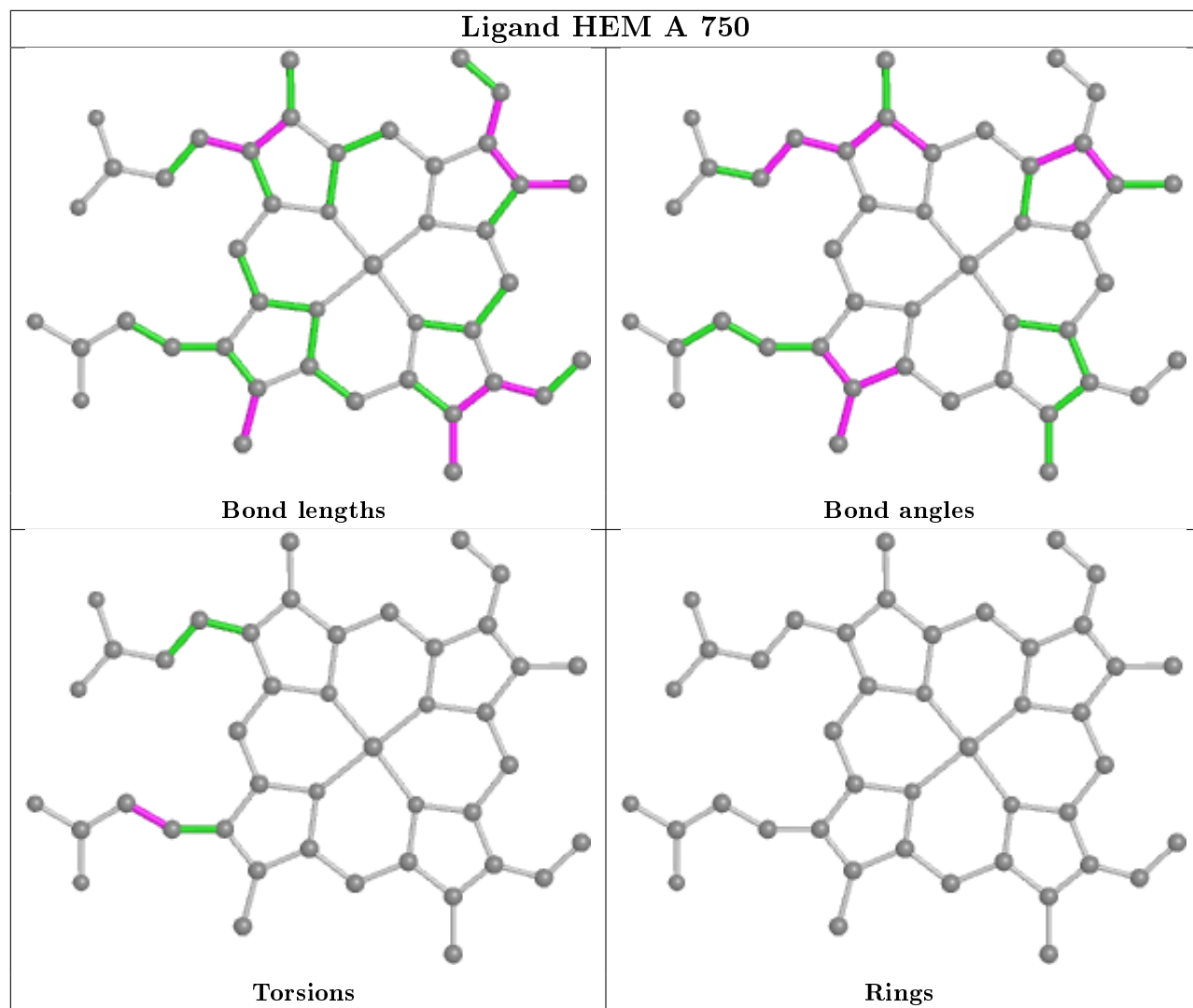
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

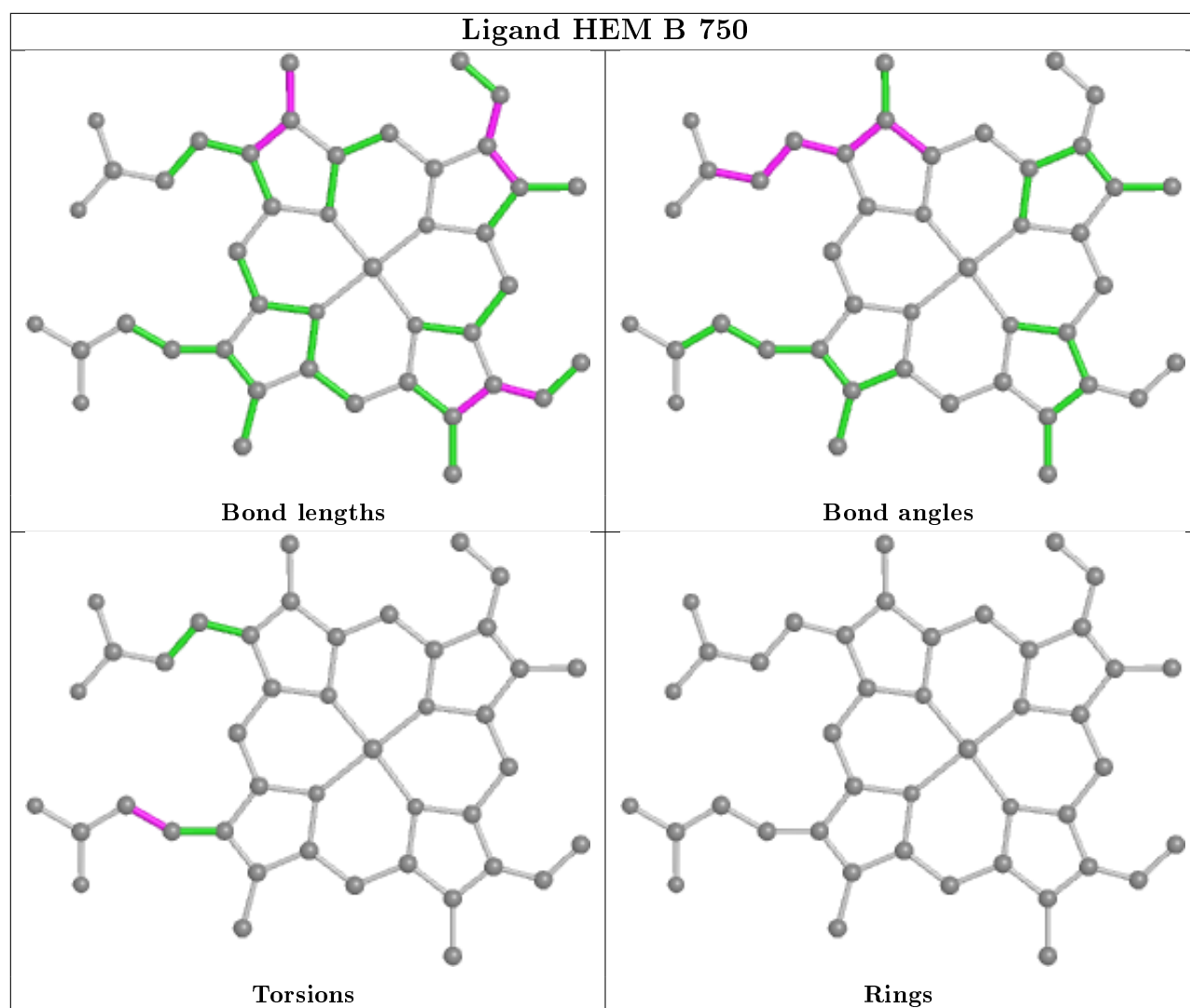
Ligand JRS A 800



Ligand JRS 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%)	0.92	72 (17%) 1 1	30, 56, 103, 131	0
1	B	411/422 (97%)	0.40	29 (7%) 16 15	30, 45, 71, 95	0
All	All	818/844 (96%)	0.66	101 (12%) 4 3	30, 50, 95, 131	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	6.6
1	B	350	THR	6.4
1	A	506	ILE	6.1
1	A	352	ASP	5.8
1	A	716	TRP	5.8
1	A	715	VAL	5.7
1	A	488	PRO	5.7
1	B	348	VAL	4.9
1	A	390	SER	4.9
1	A	487	GLN	4.6
1	A	355	PHE	4.6
1	A	389	GLU	4.5
1	A	388	ILE	4.5
1	A	350	THR	4.5
1	A	486	LYS	4.3
1	B	619	ARG	4.3
1	A	351	LYS	4.2
1	A	619	ARG	4.2
1	B	299	ARG	4.1
1	B	667	ARG	4.0
1	A	393	THR	4.0
1	A	470	HIS	3.9
1	A	507	GLN	3.9
1	A	321	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	713	THR	3.7
1	A	567	VAL	3.6
1	A	489	ASP	3.5
1	B	351	LYS	3.5
1	A	322	LEU	3.5
1	B	591	THR	3.5
1	B	620	LYS	3.4
1	B	321	THR	3.4
1	A	615	ASP	3.3
1	A	591	THR	3.3
1	B	389	GLU	3.3
1	A	391	THR	3.2
1	A	300	PHE	3.2
1	A	612	LYS	3.2
1	A	503	GLU	3.0
1	A	682	PRO	3.0
1	A	490	GLY	2.9
1	A	685	GLY	2.9
1	B	680	VAL	2.9
1	B	567	VAL	2.9
1	B	677	VAL	2.9
1	A	714	HIS	2.9
1	A	354	LEU	2.9
1	A	415	CYS	2.9
1	A	491	SER	2.8
1	A	299	ARG	2.8
1	A	678	TRP	2.8
1	A	679	ILE	2.7
1	B	310	VAL	2.7
1	A	712	ASN	2.7
1	A	677	VAL	2.7
1	A	479	LEU	2.7
1	A	582	CYS	2.6
1	A	416	VAL	2.5
1	A	459	ILE	2.5
1	B	352	ASP	2.5
1	B	301	LEU	2.5
1	A	584	PHE	2.5
1	A	514	ARG	2.5
1	A	511	LYS	2.5
1	B	678	TRP	2.5
1	A	392	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	676	TRP	2.4
1	A	711	TRP	2.4
1	A	394	TYR	2.4
1	A	385	ASN	2.4
1	B	679	ILE	2.4
1	B	329	HIS	2.4
1	A	338	PRO	2.4
1	A	667	ARG	2.4
1	A	553	TRP	2.4
1	A	356	PRO	2.3
1	A	566	ALA	2.3
1	A	593	ILE	2.3
1	A	469	LYS	2.3
1	B	611	ALA	2.2
1	A	382	GLU	2.2
1	A	565	PRO	2.2
1	B	302	LYS	2.2
1	B	676	TRP	2.2
1	A	386	LYS	2.2
1	A	680	VAL	2.2
1	A	639	TYR	2.2
1	B	684	SER	2.2
1	B	479	LEU	2.2
1	B	615	ASP	2.1
1	A	568	SER	2.1
1	A	595	VAL	2.1
1	B	691	PHE	2.1
1	A	588	TYR	2.1
1	B	565	PRO	2.1
1	A	480	ILE	2.1
1	A	373	GLY	2.1
1	A	328	GLU	2.0
1	B	718	GLY	2.0
1	A	467	ASP	2.0
1	A	530	ASP	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

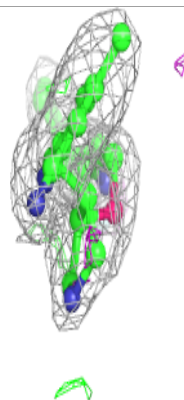
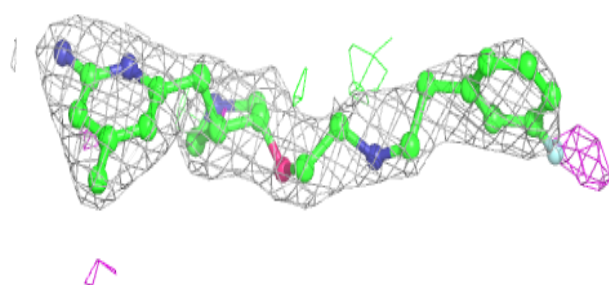
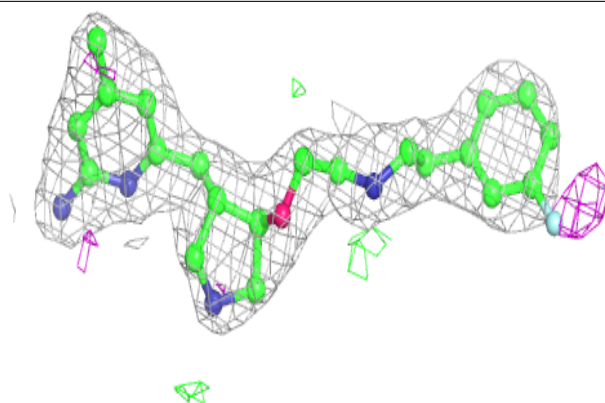
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	JRS	A	800	27/27	0.87	0.27	35,49,75,79	0
4	JRS	B	800	27/27	0.90	0.22	37,48,61,70	0
5	ACT	A	860	4/4	0.95	0.19	65,66,67,68	0
3	H4B	A	760	17/17	0.96	0.21	36,38,43,45	0
3	H4B	B	760	17/17	0.97	0.20	34,36,38,41	0
2	HEM	B	750	43/43	0.97	0.17	31,35,51,56	0
2	HEM	A	750	43/43	0.97	0.22	29,35,52,61	0
5	ACT	B	860	4/4	0.98	0.14	63,63,64,65	0
6	ZN	A	900	1/1	0.99	0.08	39,39,39,39	0

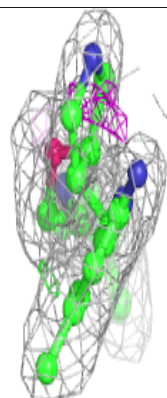
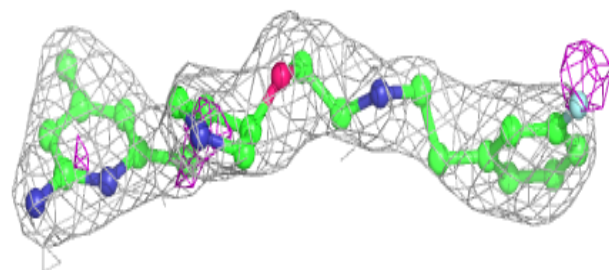
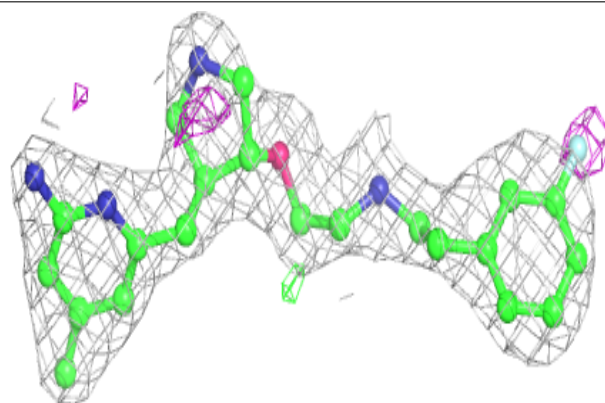
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JRS 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)

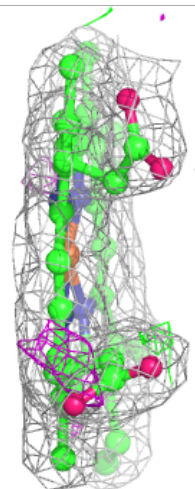
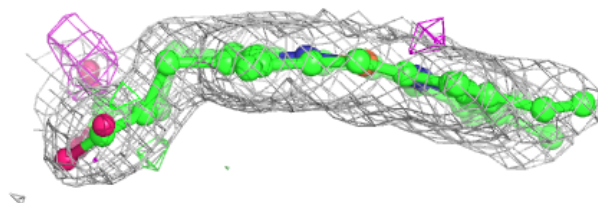
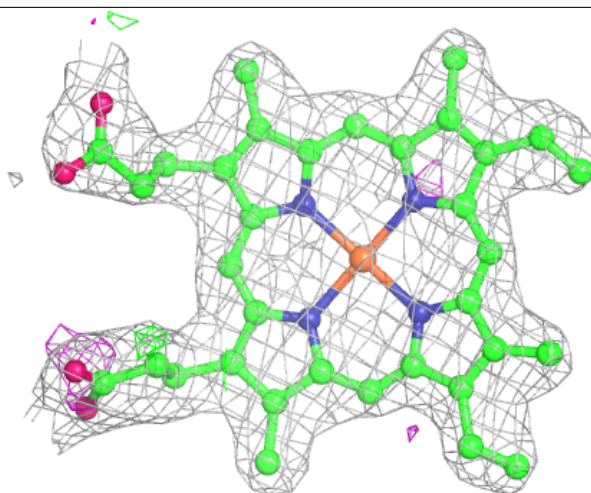
**Electron density around JRS B 800:**

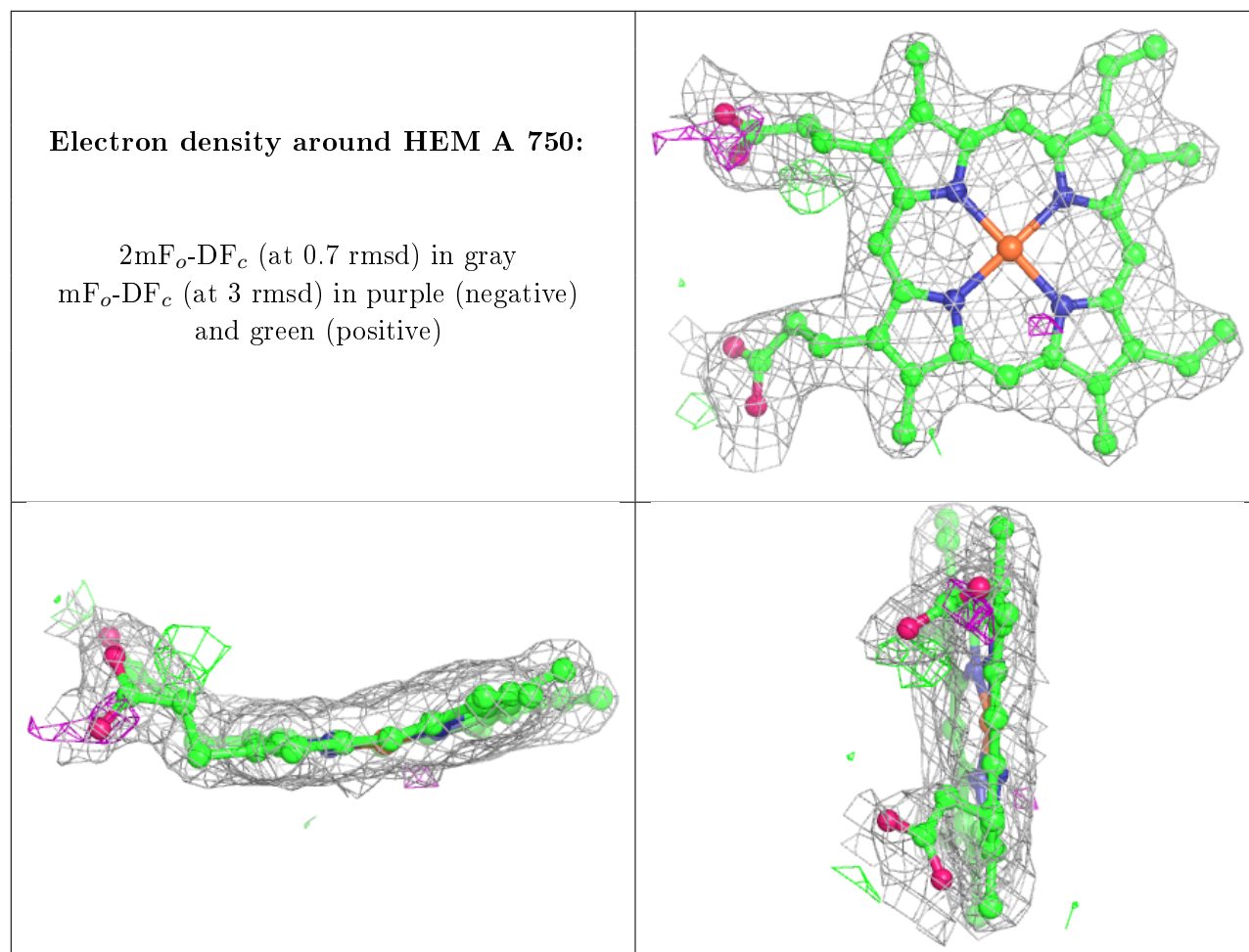
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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 ⓘ

There are no such residues in this entry.