



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:08 PM UTC

PDB ID : 3JX2 / pdb_00003jx2
Title : Structure of rat neuronal nitric oxide synthase D597N/M336V mutant heme domain in complex with N1-{(3'S,4'S)-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 : 2.10 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

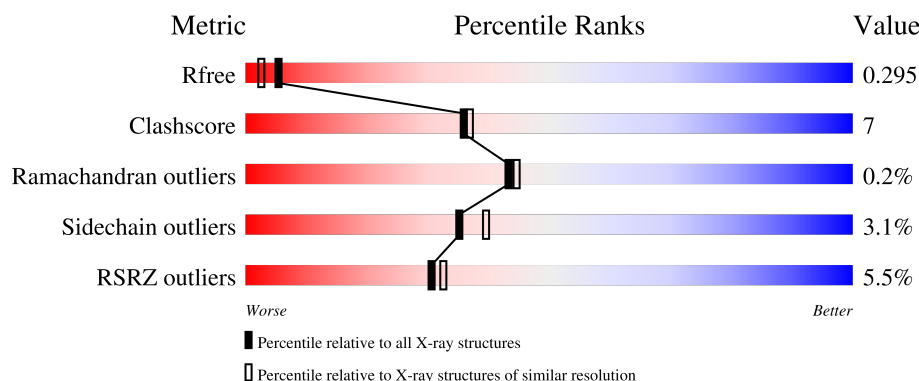
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	8% 80% 16% ..
1	B	422	2% 78% 18% ..

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
5	ACT	A	860	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7190 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.

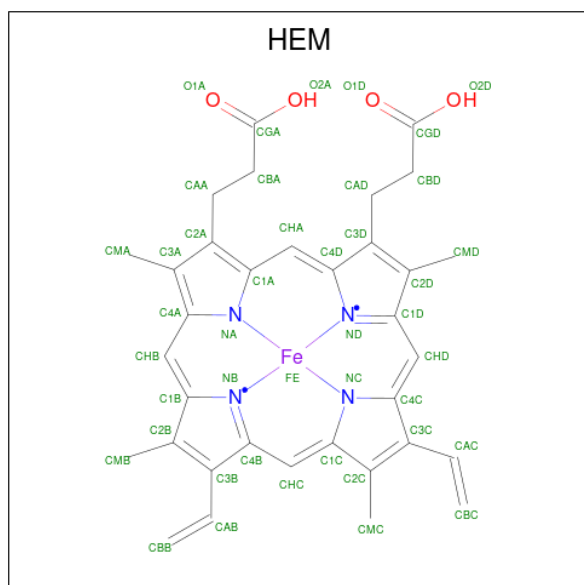
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3330	2132	572	606	20			
1	B	411	Total	C	N	O	S	0	0	0
			3344	2140	575	609	20			

There are 4 discrepancies between the modelled and reference sequences:

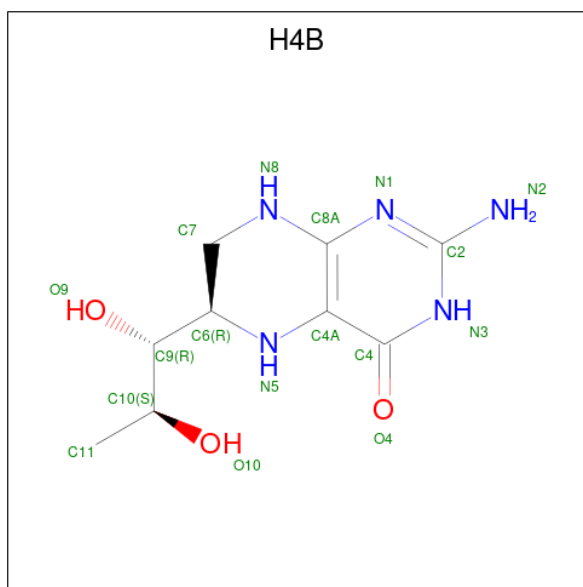
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	engineered mutation	UNP P29476
A	597	ASN	ASP	engineered mutation	UNP P29476
B	336	VAL	MET	engineered mutation	UNP P29476
B	597	ASN	ASP	engineered mutation	UNP P29476

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



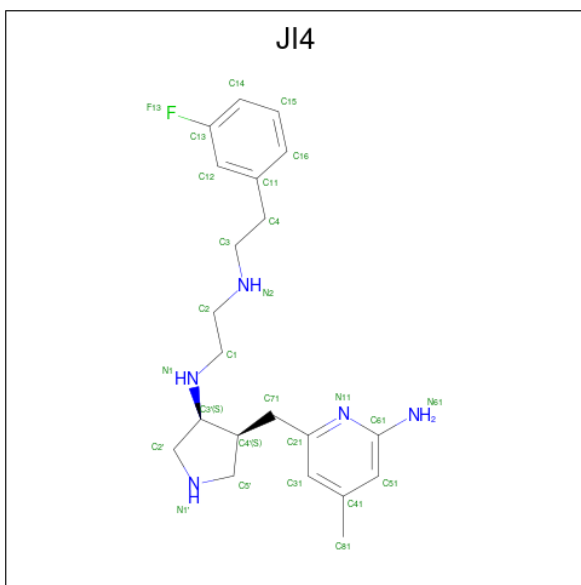
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



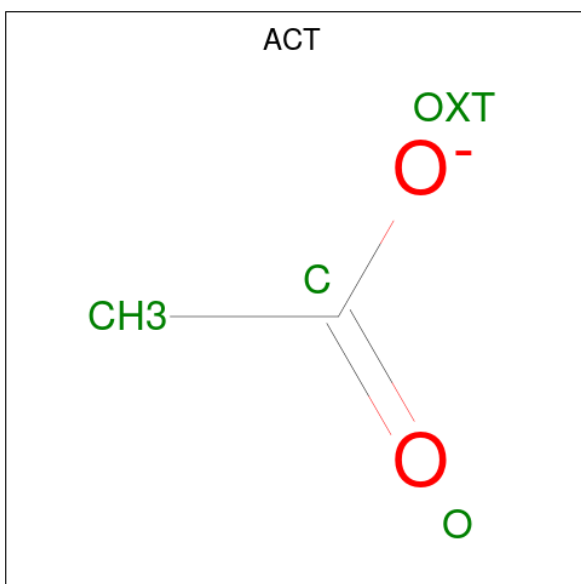
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- 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: $C_{21}H_{30}FN_5$).



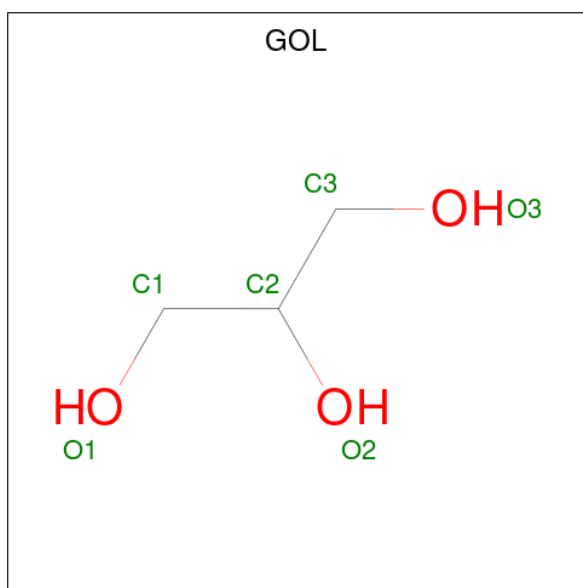
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			27	21	1	5		
4	B	1	Total	C	F	N	0	0
			27	21	1	5		

- 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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

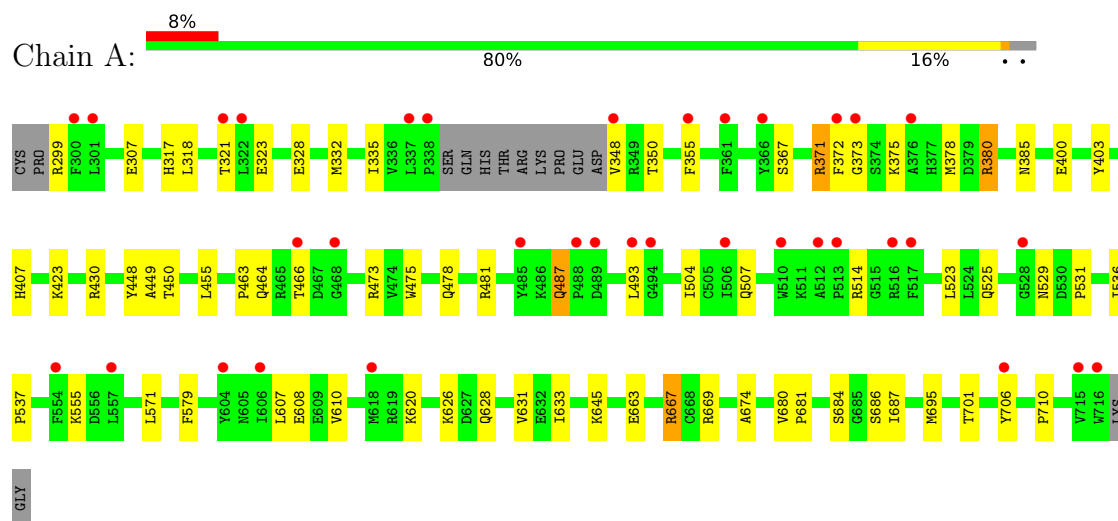
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	126	Total	O	0	0
			126	126		
8	B	195	Total	O	0	0
			195	195		

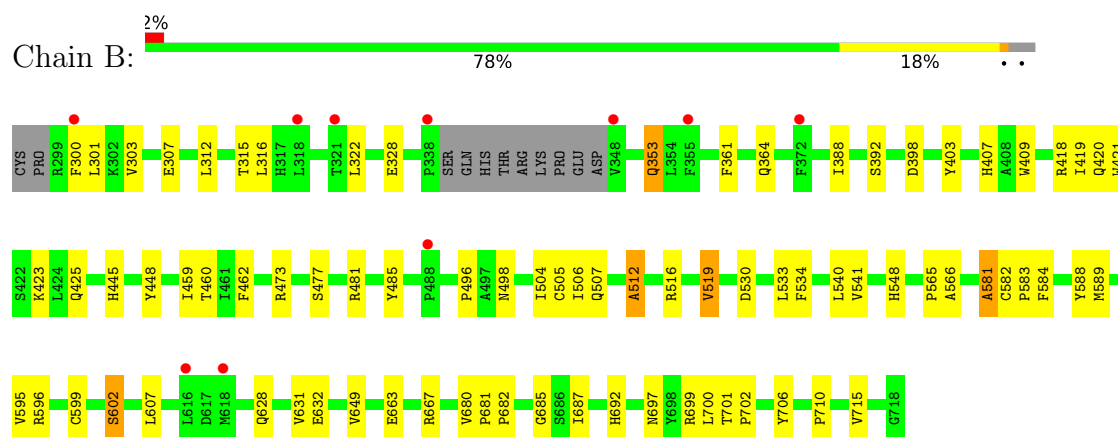
3 Residue-property plots [i](#)

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	51.69Å 110.80Å 164.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.83 – 2.10 46.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.83-2.10) 99.5 (46.83-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0089, CNS	Depositor
R, R_{free}	0.197 , 0.248 0.247 , 0.295	Depositor DCC
R_{free} test set	2768 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7190	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 5.97% 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: HEM, GOL, JI4, ZN, ACT, H4B

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	0.77	0/3423	0.95	3/4645 (0.1%)
1	B	0.96	3/3437 (0.1%)	1.05	6/4661 (0.1%)
All	All	0.87	3/6860 (0.0%)	1.00	9/9306 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	581	ALA	CA-CB	-6.03	1.44	1.52
1	B	519	VAL	C-O	-5.20	1.19	1.24
1	B	566	ALA	C-O	5.00	1.29	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ALA	CA-C-N	5.91	125.78	119.28
1	B	512	ALA	C-N-CA	5.91	125.78	119.28
1	B	421	TRP	N-CA-C	5.71	118.24	111.33
1	B	530	ASP	CA-C-N	-5.49	114.93	120.31
1	B	530	ASP	C-N-CA	-5.49	114.93	120.31
1	B	419	ILE	N-CA-C	-5.47	104.02	111.89
1	A	487	GLN	CA-C-N	5.43	126.63	119.84
1	A	487	GLN	C-N-CA	5.43	126.63	119.84
1	A	669	ARG	N-CA-C	-5.13	108.28	114.75

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	3330	0	3245	45	0
1	B	3344	0	3261	51	0
2	A	43	0	30	9	0
2	B	43	0	30	8	0
3	A	17	0	15	0	0
3	B	17	0	15	1	0
4	A	27	0	30	1	0
4	B	27	0	30	2	0
5	A	4	0	3	2	0
5	B	4	0	3	0	0
6	A	6	0	8	0	0
6	B	6	0	8	2	0
7	A	1	0	0	0	0
8	A	126	0	0	2	0
8	B	195	0	0	4	0
All	All	7190	0	6678	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (99) 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:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.59	0.82
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.65	0.78
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.00	0.74
1:A:348:VAL:HG11	1:A:466:THR:O	1.87	0.74
3:B:760:H4B:HN5	6:B:880:GOL:H32	1.53	0.72
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.72	0.69
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.58	0.69
1:A:706:TYR:OH	2:A:750:HEM:O1D	2.06	0.68
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.77	0.67
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.10	0.67
1:B:460:THR:O	1:B:583:PRO:HD2	1.97	0.63
1:B:595:VAL:O	1:B:599:CYS:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:750:HEM:O2A	8:B:1039:HOH:O	2.16	0.60
1:A:525:GLN:HG3	1:A:529:ASN:O	2.02	0.59
2:A:750:HEM:HBA1	4:A:800:JI4:H71A	1.84	0.58
1:B:706:TYR:CZ	4:B:800:JI4:H12	2.38	0.58
2:A:750:HEM:HBB2	2:A:750:HEM:CHC	2.34	0.57
1:B:425:GLN:HG2	1:B:448:TYR:CZ	2.40	0.57
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.69	0.57
2:A:750:HEM:HMB3	5:A:860:ACT:H3	1.87	0.56
1:B:505:CYS:O	1:B:506:ILE:C	2.49	0.56
1:B:398:ASP:HB2	8:B:1103:HOH:O	2.05	0.56
1:A:323:GLU:HG2	1:B:328:GLU:HB3	1.89	0.55
1:A:663:GLU:O	1:A:667:ARG:HG2	2.07	0.55
1:B:462:PHE:HB2	1:B:581:ALA:HB3	1.89	0.54
1:B:596:ARG:HH22	6:B:880:GOL:H2	1.72	0.54
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.08	0.53
2:B:750:HEM:HBA1	4:B:800:JI4:H71A	1.91	0.52
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.90	0.52
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.92	0.52
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.91	0.52
1:A:450:THR:HA	1:A:455:LEU:HD22	1.93	0.51
1:B:533:LEU:O	1:B:534:PHE:CG	2.63	0.51
1:A:307:GLU:HG3	8:B:1052:HOH:O	2.10	0.51
1:B:485:TYR:HE2	1:B:512:ALA:HB1	1.76	0.50
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.67	0.50
1:B:409:TRP:CZ3	2:B:750:HEM:HMC3	2.48	0.49
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.43	0.48
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.47	0.48
2:A:750:HEM:HMB3	5:A:860:ACT:CH3	2.43	0.48
1:B:459:ILE:HD11	1:B:582:CYS:HB2	1.96	0.48
1:B:303:VAL:HG23	1:B:312:LEU:HB2	1.95	0.47
1:B:584:PHE:CD1	2:B:750:HEM:HAC	2.50	0.47
2:A:750:HEM:O2A	8:A:1021:HOH:O	2.21	0.47
1:B:519:VAL:HG21	1:B:541:VAL:HG11	1.96	0.47
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.97	0.47
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.97	0.47
1:B:425:GLN:HG2	1:B:448:TYR:CE2	2.49	0.46
1:A:607:LEU:HD13	1:A:626:LYS:HG2	1.97	0.46
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.96	0.46
1:B:418:ARG:C	1:B:420:GLN:N	2.73	0.46
1:B:481:ARG:NE	1:B:498:ASN:HD21	2.14	0.46
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.98	0.45
1:B:316:LEU:HD21	1:B:700:LEU:HD11	1.98	0.45
1:A:332:MET:HE1	1:B:301:LEU:CD2	2.42	0.45
2:A:750:HEM:HHC	2:A:750:HEM:CBB	2.42	0.45
1:B:663:GLU:O	1:B:667:ARG:HD2	2.17	0.45
1:A:571:LEU:C	1:A:571:LEU:HD23	2.42	0.45
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.06	0.44
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.52	0.44
1:B:473:ARG:CZ	1:B:710:PRO:HG3	2.48	0.44
1:A:430:ARG:O	1:A:463:PRO:HG3	2.18	0.44
1:A:373:GLY:HA2	1:A:378:MET:HE3	2.00	0.43
1:B:353:GLN:HE21	1:B:353:GLN:HB3	1.63	0.43
1:A:299:ARG:HA	8:A:1034:HOH:O	2.18	0.43
1:B:307:GLU:HG2	1:B:692:HIS:CG	2.54	0.43
1:B:409:TRP:CH2	2:B:750:HEM:HMC3	2.54	0.43
1:B:565:PRO:HB3	1:B:588:TYR:CZ	2.53	0.43
1:A:686:SER:OG	1:B:595:VAL:HG12	2.19	0.43
1:B:445:HIS:CD2	1:B:445:HIS:C	2.97	0.43
1:A:299:ARG:O	1:A:317:HIS:CE1	2.72	0.43
1:B:361:PHE:HA	1:B:364:GLN:HE21	1.84	0.43
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.90	0.42
1:A:686:SER:HB3	1:B:682:PRO:HB2	2.00	0.42
1:B:589:MET:HA	1:B:649:VAL:O	2.19	0.42
1:B:701:THR:HA	1:B:702:PRO:C	2.43	0.42
1:B:584:PHE:CD1	2:B:750:HEM:CAC	3.03	0.42
1:A:367:SER:HA	1:A:372:PHE:HB2	2.01	0.42
1:A:449:ALA:O	1:A:455:LEU:HA	2.20	0.42
1:A:536:ILE:O	1:A:537:PRO:C	2.63	0.42
1:A:448:TYR:CD2	1:A:448:TYR:C	2.97	0.41
1:A:610:VAL:HG21	1:A:633:ILE:HD11	2.01	0.41
1:A:487:GLN:HE22	1:A:493:LEU:HD22	1.85	0.41
1:B:388:ILE:O	1:B:392:SER:N	2.47	0.41
1:A:332:MET:HB3	1:A:335:ILE:HG13	2.03	0.41
1:B:496:PRO:HB2	1:B:602:SER:O	2.20	0.41
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.55	0.41
1:A:423:LYS:HB2	1:A:423:LYS:HE2	1.87	0.41
1:B:300:PHE:CD2	1:B:315:THR:HG22	2.56	0.41
1:B:473:ARG:HA	1:B:473:ARG:HD2	1.83	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.95	0.41
1:A:323:GLU:HA	1:B:328:GLU:O	2.21	0.41
1:B:303:VAL:CG2	1:B:312:LEU:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:ASN:HD22	1:B:697:ASN:HA	1.70	0.41
1:B:607:LEU:HB2	8:B:1023:HOH:O	2.21	0.40
1:B:409:TRP:CZ2	2:B:750:HEM:CHC	3.05	0.40
1:A:299:ARG:HG3	1:A:318:LEU:HD11	2.03	0.40
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.54	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	405/422 (96%)	390 (96%)	15 (4%)	0	100	100
1	B	407/422 (96%)	390 (96%)	15 (4%)	2 (0%)	24	22
All	All	812/844 (96%)	780 (96%)	30 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	685	GLY
1	B	504	ILE

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	365/377 (97%)	350 (96%)	15 (4%)	27	29
1	B	366/377 (97%)	358 (98%)	8 (2%)	45	53
All	All	731/754 (97%)	708 (97%)	23 (3%)	35	39

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

Mol	Chain	Res	Type
1	A	321	THR
1	A	328	GLU
1	A	350	THR
1	A	371	ARG
1	A	375	LYS
1	A	380	ARG
1	A	504	ILE
1	A	507	GLN
1	A	514	ARG
1	A	555	LYS
1	A	608	GLU
1	A	620	LYS
1	A	645	LYS
1	A	667	ARG
1	A	701	THR
1	B	353	GLN
1	B	423	LYS
1	B	477	SER
1	B	507	GLN
1	B	516	ARG
1	B	540	LEU
1	B	602	SER
1	B	715	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	527	ASN
1	A	628	GLN
1	A	642	GLN
1	A	664	ASN
1	A	697	ASN
1	A	707	GLN

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Mol	Chain	Res	Type
1	A	712	ASN
1	A	714	HIS
1	B	364	GLN
1	B	395	GLN
1	B	420	GLN
1	B	454	ASN
1	B	500	GLN
1	B	508	GLN
1	B	535	GLN
1	B	642	GLN
1	B	664	ASN
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 oligosaccharides 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	$\# Z > 2$
6	GOL	A	880	-	5,5,5	0.45	0	5,5,5	0.24	0
3	H4B	B	760	-	17,18,18	1.27	2 (11%)	14,26,26	1.82	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	750	1	50,50,50	2.04	11 (22%)	67,82,82	1.56	8 (11%)
2	HEM	B	750	1	50,50,50	2.00	12 (24%)	67,82,82	1.59	13 (19%)
5	ACT	B	860	-	3,3,3	0.80	0	3,3,3	0.99	0
6	GOL	B	880	-	5,5,5	0.36	0	5,5,5	0.20	0
4	JI4	A	800	-	28,29,29	0.74	2 (7%)	29,38,38	1.87	8 (27%)
4	JI4	B	800	-	28,29,29	0.72	0	29,38,38	1.67	7 (24%)
3	H4B	A	760	-	17,18,18	0.91	0	14,26,26	1.77	4 (28%)
5	ACT	A	860	-	3,3,3	0.81	0	3,3,3	0.86	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
6	GOL	A	880	-	-	2/4/4/4	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
2	HEM	A	750	1	-	1/14/54/54	-
2	HEM	B	750	1	-	2/14/54/54	-
6	GOL	B	880	-	-	2/4/4/4	-
4	JI4	A	800	-	-	1/13/23/23	0/3/3/3
4	JI4	B	800	-	-	5/13/23/23	0/3/3/3
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	7.45	1.52	1.36
2	B	750	HEM	C3D-C2D	7.07	1.52	1.36
2	B	750	HEM	FE-NC	6.10	2.15	1.95
2	A	750	HEM	FE-NA	5.75	2.14	1.95
2	B	750	HEM	FE-NA	5.00	2.11	1.95
2	A	750	HEM	FE-ND	4.37	2.08	1.94
2	A	750	HEM	FE-NC	4.01	2.08	1.95
2	A	750	HEM	CMC-C2C	3.33	1.57	1.50
2	A	750	HEM	FE-NB	3.17	2.04	1.94
2	B	750	HEM	CMB-C2B	3.11	1.57	1.50
2	B	750	HEM	FE-ND	2.97	2.04	1.94
2	B	750	HEM	CAC-C3C	2.80	1.54	1.47
3	B	760	H4B	C7-C6	2.80	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	CAB-C3B	2.71	1.54	1.47
2	B	750	HEM	CMA-C3A	2.65	1.56	1.50
2	A	750	HEM	C2A-C3A	-2.48	1.32	1.38
2	B	750	HEM	CAB-C3B	2.43	1.53	1.47
2	A	750	HEM	CMB-C2B	2.42	1.55	1.50
2	B	750	HEM	CMC-C2C	2.36	1.55	1.50
2	B	750	HEM	CMD-C2D	2.35	1.55	1.50
3	B	760	H4B	O4-C4	2.26	1.27	1.23
2	A	750	HEM	C3B-C2B	-2.24	1.32	1.37
2	B	750	HEM	CHB-C4A	-2.16	1.34	1.39
4	A	800	JI4	C12-C13	2.10	1.41	1.37
2	B	750	HEM	O1D-CGD	2.02	1.28	1.22
2	A	750	HEM	CAC-C3C	2.02	1.52	1.47
4	A	800	JI4	C14-C13	2.01	1.41	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	C4D-ND-C1D	5.14	111.29	105.21
2	A	750	HEM	CBA-CAA-C2A	-4.61	99.78	112.53
2	B	750	HEM	CBA-CAA-C2A	-4.39	100.39	112.53
3	A	760	H4B	C2-N1-C8A	4.20	120.77	113.36
2	B	750	HEM	CHB-C1B-NB	4.14	129.48	124.37
4	B	800	JI4	C1-N1-C3'	4.00	119.88	114.05
4	B	800	JI4	C61-N11-C21	3.94	121.01	118.07
2	B	750	HEM	C3B-C4B-NB	-3.92	106.65	109.47
3	B	760	H4B	C2-N1-C8A	3.90	120.23	113.36
4	A	800	JI4	C71-C21-N11	3.78	121.20	116.57
2	B	750	HEM	C4D-ND-C1D	3.74	109.63	105.21
4	A	800	JI4	C1-N1-C3'	3.57	119.25	114.05
4	A	800	JI4	C61-N11-C21	3.50	120.69	118.07
2	A	750	HEM	CHA-C4D-ND	3.50	128.70	124.37
2	A	750	HEM	CBD-CAD-C3D	-3.48	102.90	112.53
2	A	750	HEM	C4C-C3C-C2C	3.36	109.73	106.81
4	A	800	JI4	C5'-N1'-C2'	3.33	113.72	105.45
4	B	800	JI4	C31-C21-N11	-3.14	119.16	122.73
3	B	760	H4B	C11-C10-C9	-2.93	108.53	112.11
2	B	750	HEM	C1D-C2D-C3D	-2.92	103.91	106.98
2	B	750	HEM	CMD-C2D-C1D	2.90	129.56	125.03
4	A	800	JI4	C31-C21-N11	-2.88	119.44	122.73
4	A	800	JI4	C14-C13-C12	-2.82	119.51	123.23
2	B	750	HEM	CHA-C4D-ND	2.82	127.85	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	JI4	C2-C1-N1	-2.78	106.53	111.06
2	A	750	HEM	CMD-C2D-C1D	2.67	129.21	125.03
4	A	800	JI4	C81-C41-C31	-2.61	117.39	120.92
3	A	760	H4B	C4A-C4-N3	2.54	119.12	112.13
2	B	750	HEM	CAD-CBD-CGD	-2.51	107.00	113.67
4	B	800	JI4	C5'-N1'-C2'	2.40	111.42	105.45
3	A	760	H4B	C2-N3-C4	-2.40	120.77	125.11
2	B	750	HEM	C2A-C1A-NA	-2.37	107.52	110.15
4	B	800	JI4	C14-C13-C12	-2.37	120.10	123.23
3	B	760	H4B	C2-N3-C4	-2.36	120.82	125.11
4	B	800	JI4	C3-C4-C11	-2.36	107.51	112.83
3	A	760	H4B	C4-C4A-N5	2.35	122.68	116.27
3	B	760	H4B	C4A-C4-N3	2.32	118.49	112.13
4	B	800	JI4	C2'-C3'-N1	2.19	117.64	113.73
2	B	750	HEM	CHB-C1B-C2B	-2.18	120.75	126.95
2	B	750	HEM	C4C-C3C-C2C	2.14	108.67	106.81
2	B	750	HEM	C4C-NC-C1C	2.09	109.23	105.82
2	A	750	HEM	C4C-NC-C1C	2.06	109.17	105.82
3	B	760	H4B	C4-C4A-N5	2.03	121.81	116.27
2	B	750	HEM	C4B-C3B-C2B	2.03	109.15	107.28
2	A	750	HEM	CMB-C2B-C1B	2.02	128.19	125.03

There are no chirality outliers.

All (13) torsion outliers are listed below:

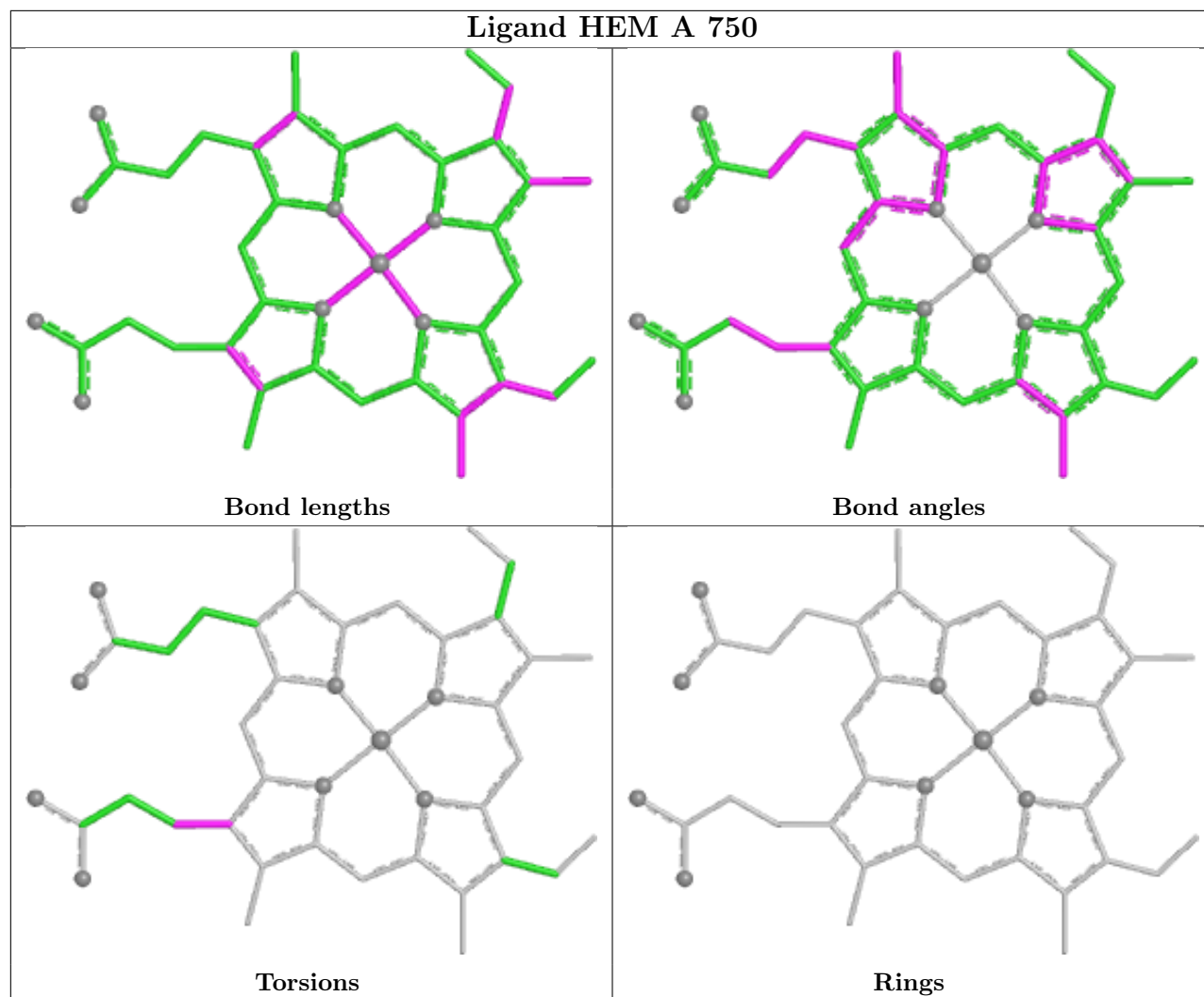
Mol	Chain	Res	Type	Atoms
4	A	800	JI4	C2-C1-N1-C3'
4	B	800	JI4	C2-C1-N1-C3'
6	A	880	GOL	O1-C1-C2-C3
6	B	880	GOL	O1-C1-C2-C3
6	A	880	GOL	O1-C1-C2-O2
6	B	880	GOL	O1-C1-C2-O2
4	B	800	JI4	C16-C11-C4-C3
4	B	800	JI4	C12-C11-C4-C3
2	B	750	HEM	C4B-C3B-CAB-CBB
2	B	750	HEM	C2A-CAA-CBA-CGA
4	B	800	JI4	C4-C3-N2-C2
4	B	800	JI4	C2'-C3'-N1-C1
2	A	750	HEM	C1A-C2A-CAA-CBA

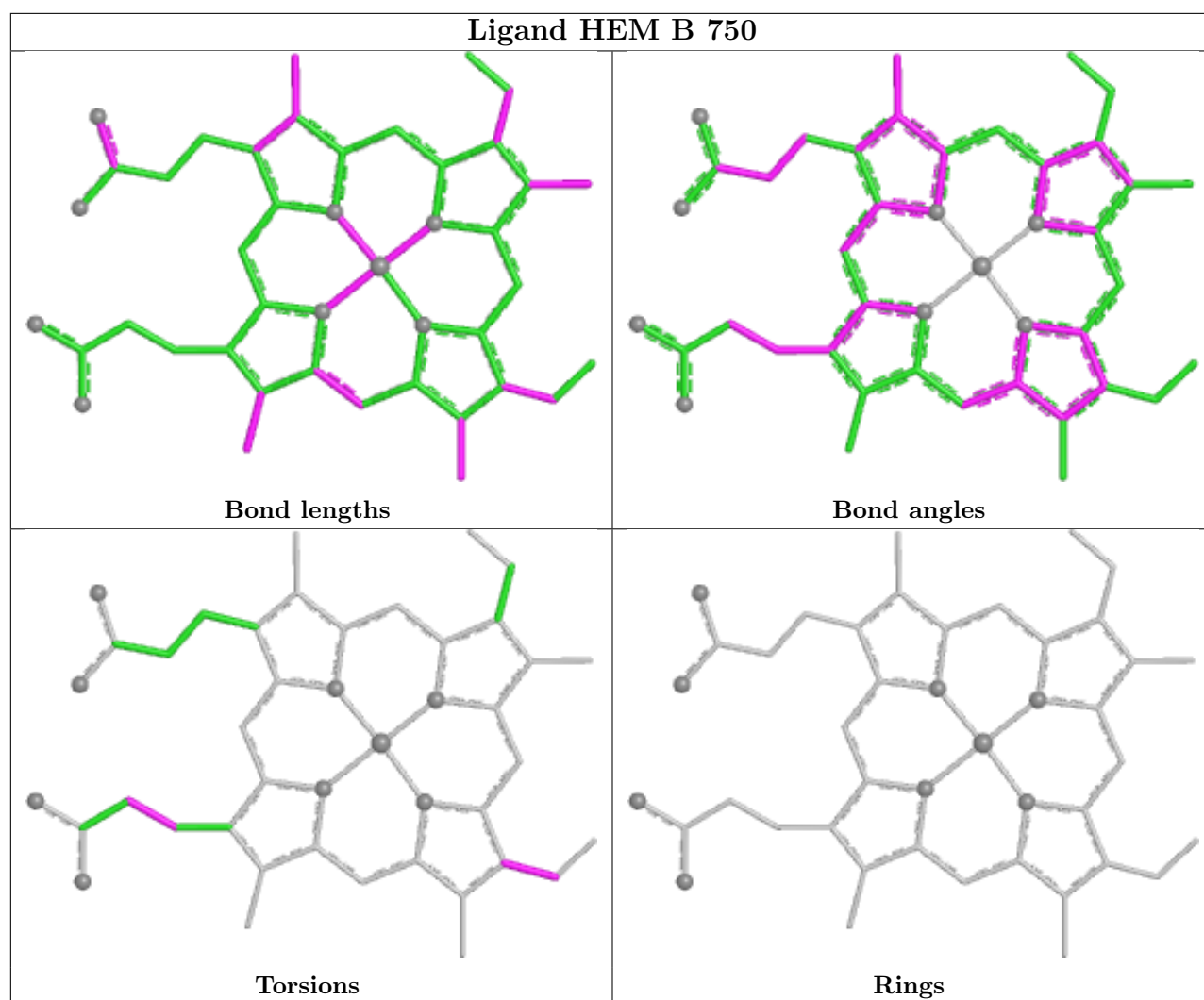
There are no ring outliers.

7 monomers are involved in 20 short contacts:

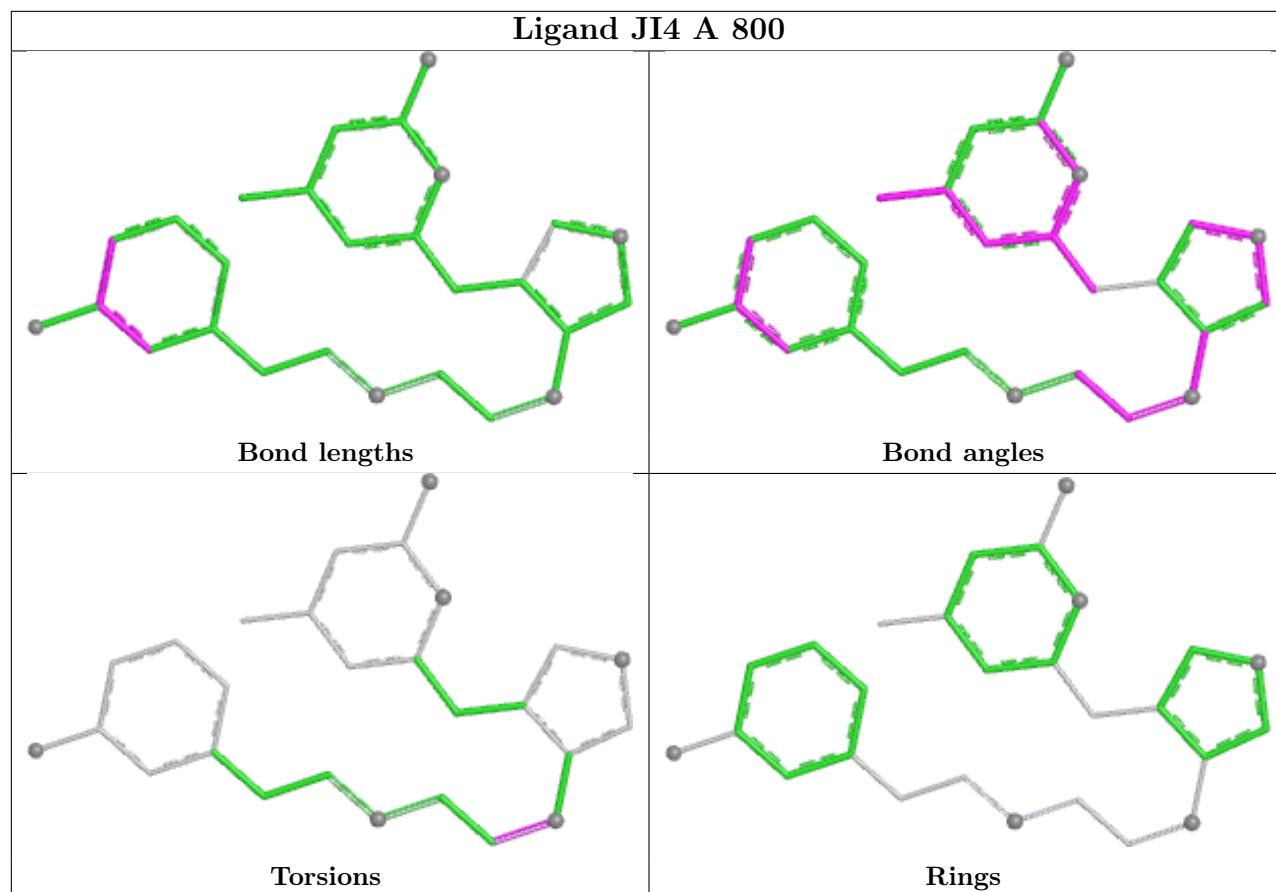
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	760	H4B	1	0
2	A	750	HEM	9	0
2	B	750	HEM	8	0
6	B	880	GOL	2	0
4	A	800	JI4	1	0
4	B	800	JI4	2	0
5	A	860	ACT	2	0

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.

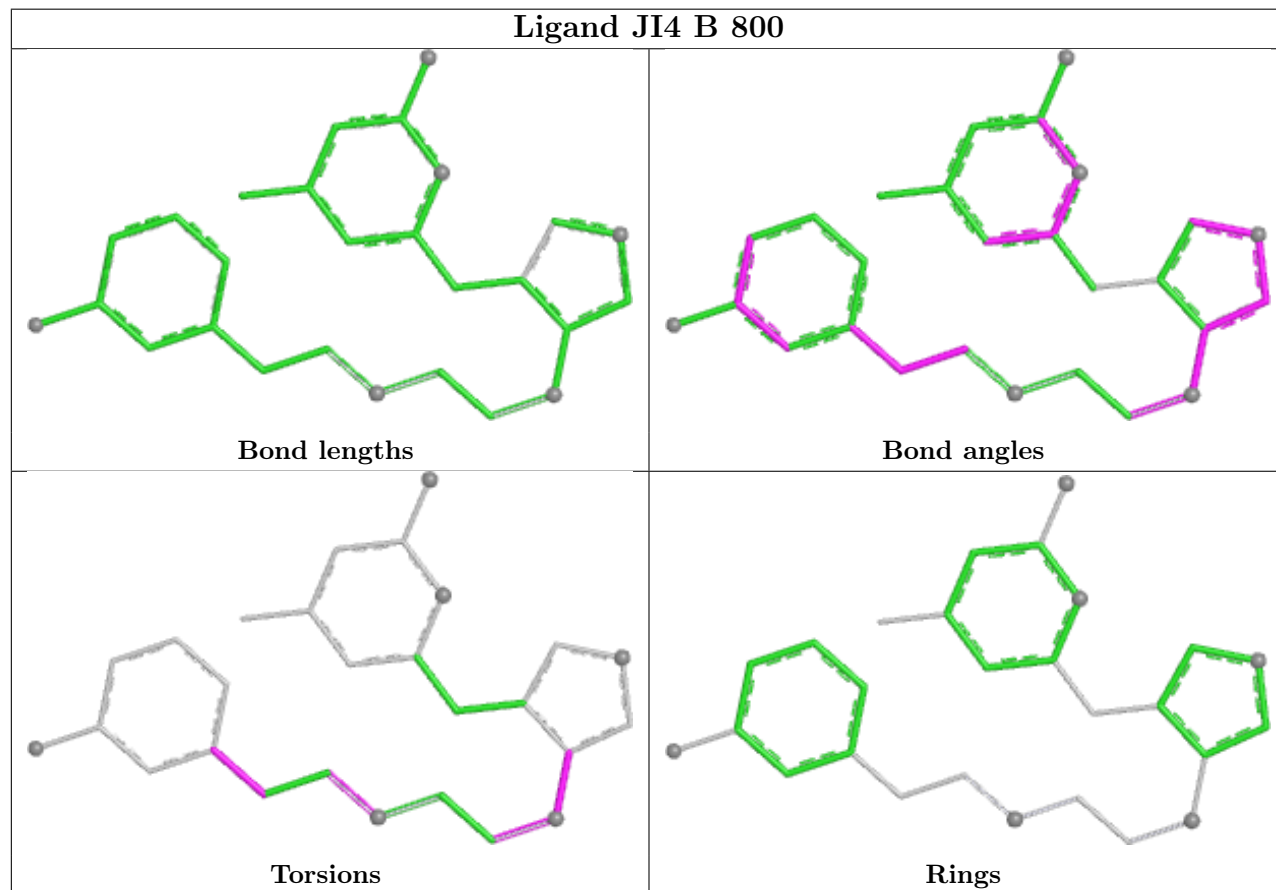




Ligand JI4 A 800



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	409/422 (96%)	0.69	35 (8%) 16 17	29, 57, 107, 131	0
1	B	411/422 (97%)	0.37	10 (2%) 59 62	25, 45, 76, 98	0
All	All	820/844 (97%)	0.53	45 (5%) 30 32	25, 50, 98, 131	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	PHE	3.6
1	A	716	TRP	3.6
1	A	485	TYR	3.3
1	B	348	VAL	3.2
1	A	338	PRO	3.1
1	A	494	GLY	3.1
1	A	618	MET	3.1
1	A	376	ALA	2.9
1	A	510	TRP	2.9
1	B	338	PRO	2.8
1	A	372	PHE	2.7
1	B	616	LEU	2.6
1	A	493	LEU	2.6
1	A	488	PRO	2.6
1	A	517	PHE	2.5
1	A	466	THR	2.5
1	A	489	ASP	2.5
1	B	488	PRO	2.5
1	B	300	PHE	2.4
1	A	512	ALA	2.4
1	A	606	ILE	2.3
1	A	706	TYR	2.3
1	A	468	GLY	2.3
1	B	318	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	618	MET	2.3
1	B	355	PHE	2.3
1	B	321	THR	2.3
1	A	348	VAL	2.2
1	A	715	VAL	2.2
1	A	557	LEU	2.2
1	A	604	TYR	2.2
1	A	361	PHE	2.2
1	A	506	ILE	2.2
1	A	366	TYR	2.2
1	A	301	LEU	2.1
1	A	516	ARG	2.1
1	A	322	LEU	2.1
1	A	355	PHE	2.1
1	A	321	THR	2.1
1	B	372	PHE	2.1
1	A	337	LEU	2.0
1	A	513	PRO	2.0
1	A	373	GLY	2.0
1	A	554	PHE	2.0
1	A	528	GLY	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
6	GOL	B	880	6/6	0.80	0.20	88,89,89,89	0
6	GOL	A	880	6/6	0.84	0.14	58,61,63,64	0

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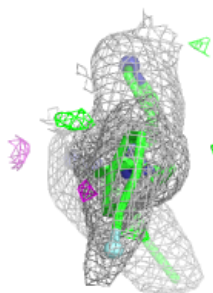
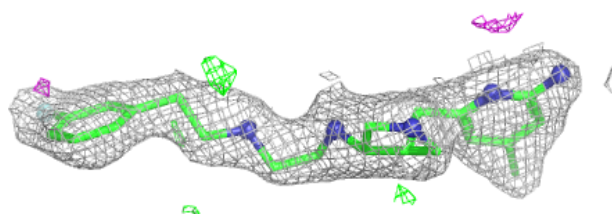
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	B	860	4/4	0.87	0.14	59,60,60,61	0
4	JI4	A	800	27/27	0.89	0.11	34,44,69,71	0
4	JI4	B	800	27/27	0.89	0.11	29,41,72,73	0
5	ACT	A	860	4/4	0.89	0.12	64,66,66,67	0
3	H4B	B	760	17/17	0.94	0.07	24,30,40,43	0
3	H4B	A	760	17/17	0.95	0.07	31,34,40,41	0
2	HEM	A	750	43/43	0.97	0.07	30,35,46,50	0
2	HEM	B	750	43/43	0.97	0.07	30,35,42,49	0
7	ZN	A	900	1/1	0.99	0.03	41,41,41,41	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.

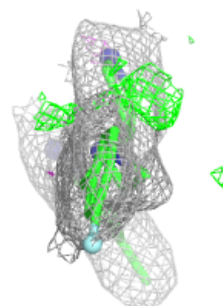
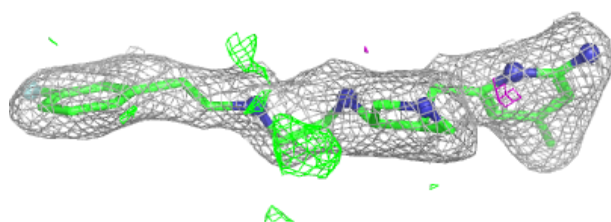
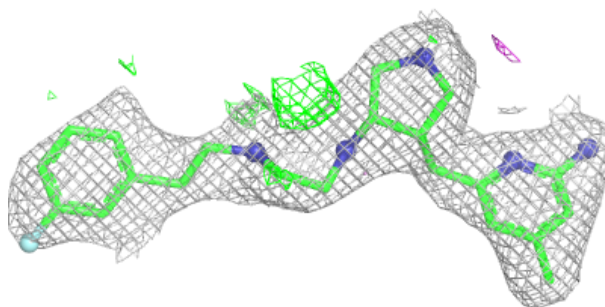
Electron density around JI4 A 800:

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



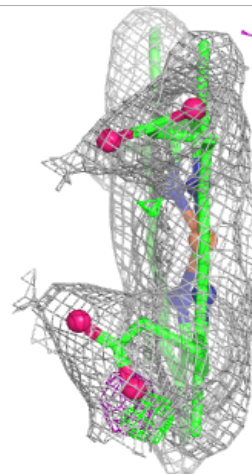
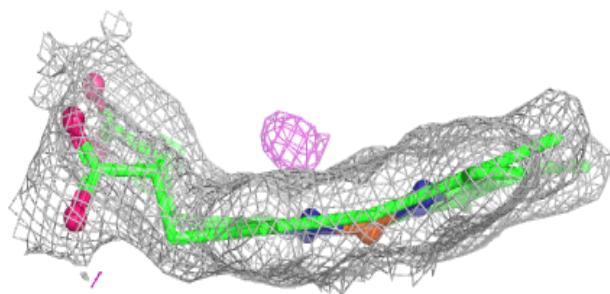
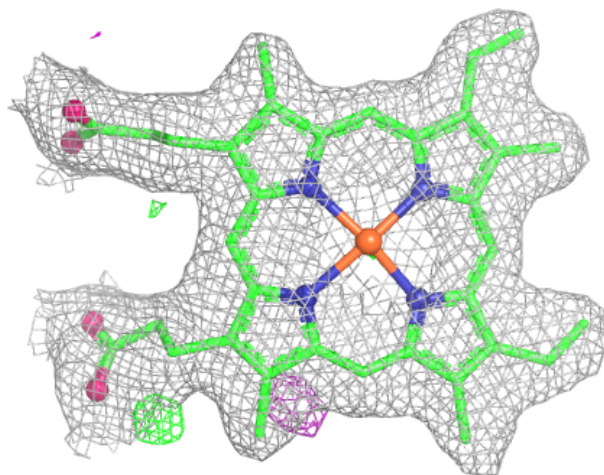
Electron density around JI4 B 800:

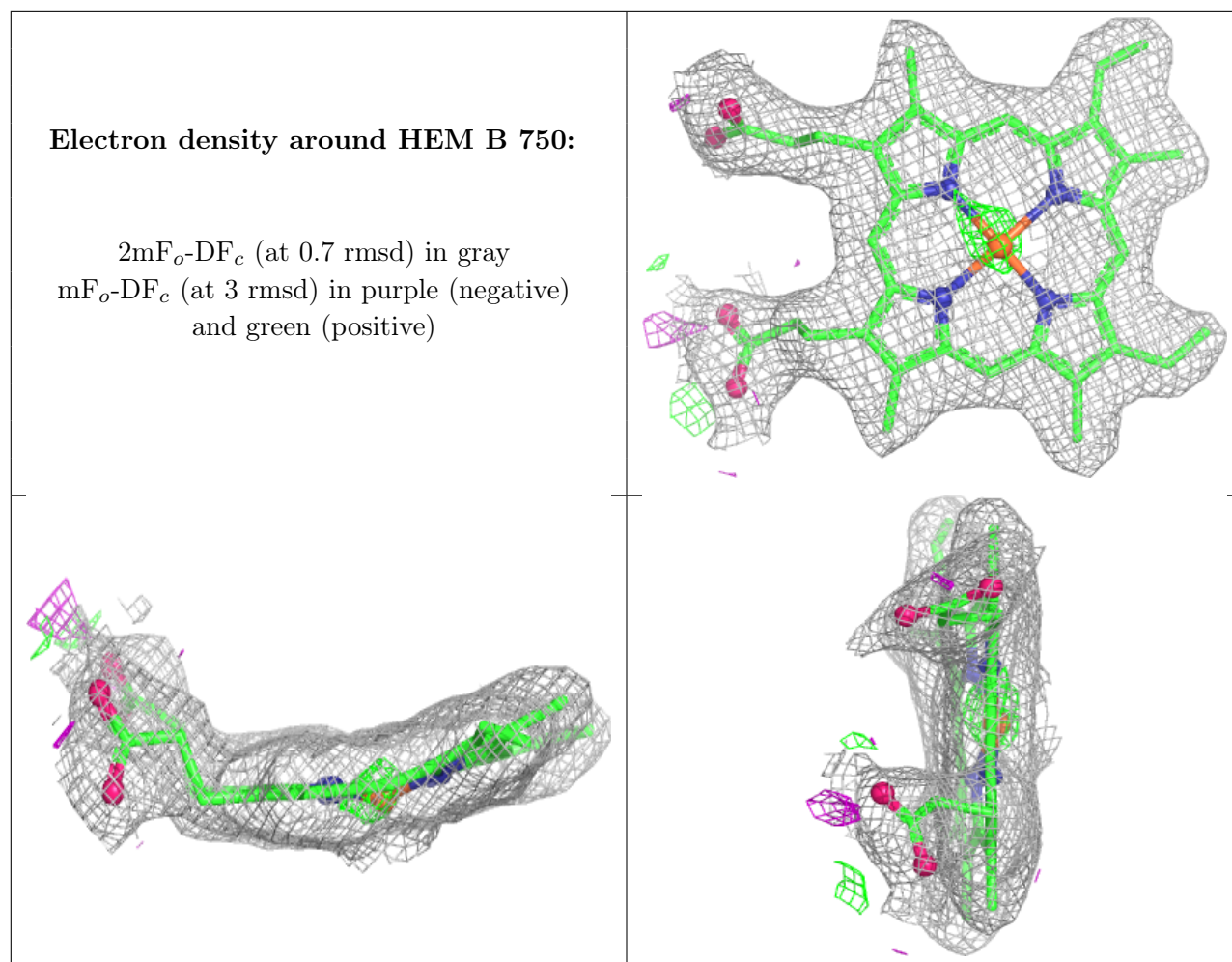
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.