



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 01:39 AM EDT

PDB ID : 3JTA
Title : Structure of neuronal nitric oxide synthase heme domain in the ferrous state complexed with N 5 -[4-(methylsulfanyl)butanimidoyl]-L-ornithine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2009-09-11
Resolution : 2.18 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

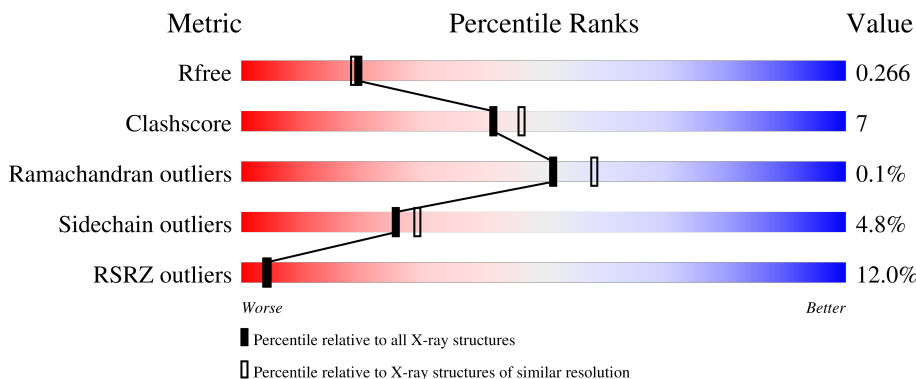
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	
1	B	422	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	JM6	A	800	-	-	X	-
4	JM6	B	800	-	-	X	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 6934 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
			Total	C	N	O	S			
1	A	407	Total 3322	C 2127	N 566	O 607	S 22	0	2	0
1	B	411	Total 3348	C 2142	N 574	O 610	S 22	0	1	0

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



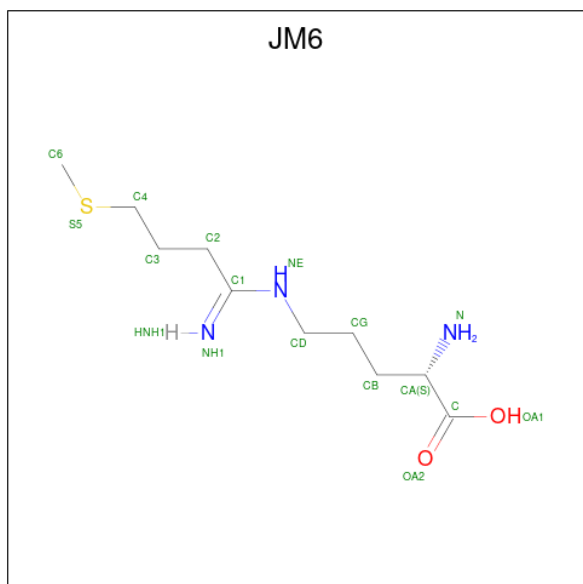
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (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 5 -[4-(methylsulfanyl)butanimidoyl]-L-ornithine (three-letter code: JM6) (formula: C₁₀H₂₁N₃O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			16	10	3	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	16	10	3	2	1	0	0

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



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

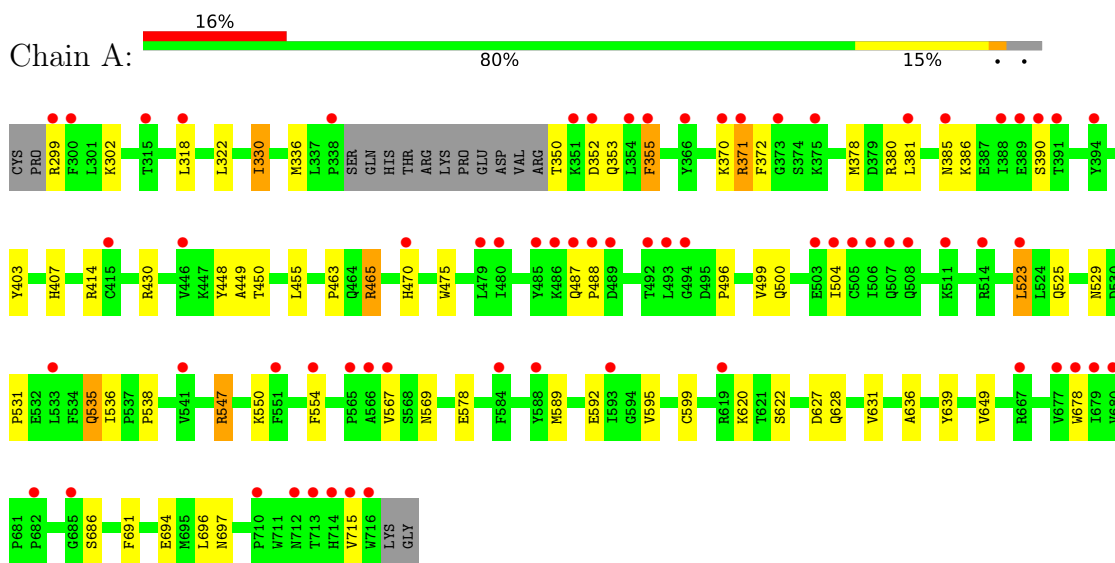
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	42	42	42	0	0
7	B	61	61	61	0	0

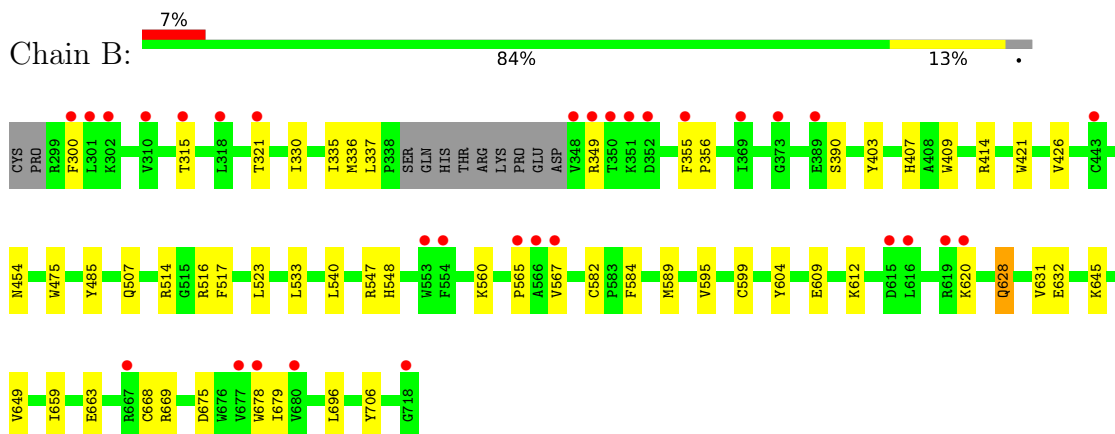
3 Residue-property plots [i](#)

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	51.84Å 111.50Å 164.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.21 – 2.18 40.80 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.6 (41.21-2.18) 98.7 (40.80-2.17)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.5.0089, CNS	Depositor
R, R_{free}	0.190 , 0.245 0.216 , 0.266	Depositor DCC
R_{free} test set	2540 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6934	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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, H4B, JM6, ACT, 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	0.91	2/3421 (0.1%)	0.84	0/4641
1	B	0.93	3/3444 (0.1%)	0.81	2/4669 (0.0%)
All	All	0.92	5/6865 (0.1%)	0.83	2/9310 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	PHE	CG-CD1	7.04	1.49	1.38
1	A	372	PHE	CE1-CZ	6.67	1.50	1.37
1	B	604	TYR	CD1-CE1	5.62	1.47	1.39
1	B	426	VAL	CB-CG2	5.27	1.64	1.52
1	B	582	CYS	CB-SG	5.12	1.91	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	533	LEU	CB-CG-CD1	-5.11	102.31	111.00

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	3322	0	3232	52	0
1	B	3348	0	3264	26	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	16	0	19	13	0
4	B	16	0	19	10	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	42	0	0	5	0
7	B	61	0	0	0	0
All	All	6934	0	6630	94	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 (94) 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)
4:A:800:JM6:H6A	4:A:800:JM6:H2	1.37	1.06
4:A:800:JM6:HD	4:A:800:JM6:H4A	1.45	0.98
4:A:800:JM6:H2	4:A:800:JM6:C6	1.95	0.94
4:A:800:JM6:H4A	4:A:800:JM6:CD	1.98	0.92
1:A:371:ARG:CG	1:A:371:ARG:HH21	1.85	0.89
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.52	0.89
1:A:371:ARG:HH21	1:A:371:ARG:HG2	1.38	0.87
1:A:355:PHE:CZ	1:A:385:ASN:HB2	2.17	0.79
1:A:567:VAL:HG23	4:A:800:JM6:H6	1.68	0.76
1:B:567:VAL:H	4:B:800:JM6:H6B	1.51	0.75
1:A:350:THR:HG22	1:A:352:ASP:H	1.52	0.73
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.72	0.71
1:A:535:GLN:HE22	1:A:538:PRO:HD3	1.54	0.71
4:B:800:JM6:H4A	4:B:800:JM6:CD	2.22	0.70
1:A:636:ALA:C	7:A:128:HOH:O	2.29	0.70
4:A:800:JM6:HD	4:A:800:JM6:C4	2.20	0.70
2:A:750:HEM:NB	4:A:800:JM6:H3A	2.06	0.70
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.76	0.67
1:A:636:ALA:O	7:A:128:HOH:O	2.12	0.66
4:B:800:JM6:H4A	4:B:800:JM6:HDA	1.77	0.66
2:B:750:HEM:CMC	2:B:750:HEM:HBC2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:VAL:HG23	4:A:800:JM6:C6	2.25	0.66
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.78	0.64
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.78	0.63
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.25	0.60
1:A:371:ARG:HG2	1:A:371:ARG:NH2	2.13	0.58
1:A:465:ARG:CD	1:A:578:GLU:OE1	2.52	0.58
2:B:750:HEM:HBC2	2:B:750:HEM:HMC1	1.85	0.57
4:B:800:JM6:H4A	4:B:800:JM6:NE	2.18	0.57
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.87	0.57
1:B:675:ASP:O	1:B:679:ILE:HG12	2.04	0.57
1:A:639:TYR:N	7:A:128:HOH:O	2.37	0.57
4:A:800:JM6:HD	4:A:800:JM6:H6	1.87	0.57
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.40	0.57
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.87	0.57
1:A:639:TYR:HB3	7:A:128:HOH:O	2.06	0.56
1:A:554:PHE:HB3	7:A:108:HOH:O	2.04	0.56
1:B:300:PHE:HD2	1:B:315:THR:HG22	1.71	0.56
1:B:565:PRO:HG2	4:B:800:JM6:H2A	1.87	0.56
1:A:525:GLN:HG3	1:A:529:ASN:O	2.06	0.56
1:B:517:PHE:HB2	1:B:560:LYS:HE2	1.88	0.55
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.89	0.55
1:A:355:PHE:CE2	1:A:385:ASN:ND2	2.75	0.54
1:A:487:GLN:CB	1:A:488:PRO:HD2	2.37	0.54
1:A:547:ARG:HD3	1:A:547:ARG:H	1.73	0.53
1:B:595:VAL:O	1:B:599:CYS:HB2	2.09	0.52
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.90	0.52
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.92	0.50
4:A:800:JM6:HD	4:A:800:JM6:C6	2.42	0.50
1:A:465:ARG:HD2	1:A:578:GLU:OE1	2.12	0.49
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.47	0.49
1:A:592:GLU:OE1	4:A:800:JM6:NE	2.45	0.49
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.48	0.49
1:A:500:GLN:O	1:A:504:ILE:HG13	2.13	0.48
2:B:750:HEM:C4B	4:B:800:JM6:H3A	2.49	0.48
4:A:800:JM6:H4A	4:A:800:JM6:HDA	1.92	0.47
1:A:686:SER:HA	1:A:691:PHE:CG	2.48	0.47
1:B:584:PHE:CE1	4:B:800:JM6:S5	3.08	0.47
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.95	0.47
1:A:370:LYS:HB2	1:A:370:LYS:HE3	1.71	0.47
1:A:430:ARG:O	1:A:463:PRO:HG3	2.14	0.47
1:A:448:TYR:CD2	1:A:448:TYR:C	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ALA:O	1:A:455:LEU:HA	2.15	0.47
1:A:535:GLN:NE2	1:A:536:ILE:O	2.48	0.47
1:A:299:ARG:HG3	1:A:318:LEU:CD2	2.45	0.46
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.97	0.46
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.78	0.46
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.51	0.45
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.50	0.45
1:A:589:MET:HA	1:A:649:VAL:O	2.15	0.45
1:B:517:PHE:CB	1:B:560:LYS:HE2	2.47	0.45
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.47	0.44
2:B:750:HEM:NC	4:B:800:JM6:H4	2.32	0.44
2:B:750:HEM:HMC1	2:B:750:HEM:CBC	2.46	0.43
1:A:414:ARG:HD3	1:A:678:TRP:CD2	2.53	0.43
1:A:450:THR:O	1:A:455:LEU:HD23	2.18	0.43
1:B:584:PHE:HE1	4:B:800:JM6:S5	2.42	0.43
1:B:589:MET:HA	1:B:649:VAL:O	2.18	0.43
1:A:686:SER:HA	1:A:691:PHE:CB	2.49	0.43
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.01	0.42
1:A:595:VAL:O	1:A:599:CYS:HB2	2.20	0.42
2:A:750:HEM:C1B	4:A:800:JM6:H3A	2.55	0.42
1:A:487:GLN:HB3	1:A:488:PRO:CD	2.47	0.41
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.08	0.41
1:B:659:ILE:O	1:B:663:GLU:HG3	2.21	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.41
1:A:336:MET:CE	1:A:678:TRP:HZ2	2.34	0.41
1:A:350:THR:N	1:A:353:GLN:HE21	2.18	0.41
1:A:627:ASP:O	1:A:631:VAL:HG23	2.21	0.41
1:B:706:TYR:OH	2:B:750:HEM:O1D	2.16	0.41
1:B:355:PHE:N	1:B:356:PRO:HD2	2.36	0.40
1:A:385:ASN:O	1:A:386:LYS:C	2.58	0.40
1:A:465:ARG:HD3	1:A:578:GLU:OE1	2.19	0.40
1:B:565:PRO:HB2	4:B:800:JM6:H2	2.03	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%)	385 (95%)	19 (5%)	1 (0%)	47	52
1	B	408/422 (97%)	397 (97%)	11 (3%)	0	100	100
All	All	813/844 (96%)	782 (96%)	30 (4%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	LEU

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%)	346 (95%)	19 (5%)	23	26
1	B	367/377 (97%)	350 (95%)	17 (5%)	27	31
All	All	732/754 (97%)	696 (95%)	36 (5%)	25	28

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	LYS
1	A	330	ILE
1	A	355	PHE
1	A	371	ARG
1	A	378	MET
1	A	380	ARG
1	A	381	LEU
1	A	390	SER
1	A	465	ARG
1	A	470	HIS
1	A	523	LEU

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Mol	Chain	Res	Type
1	A	535	GLN
1	A	547	ARG
1	A	550	LYS
1	A	569	ASN
1	A	620	LYS
1	A	622	SER
1	A	697	ASN
1	A	715	VAL
1	B	321	THR
1	B	336	MET
1	B	337	LEU
1	B	349	ARG
1	B	390	SER
1	B	454	ASN
1	B	507	GLN
1	B	516	ARG
1	B	540	LEU
1	B	547	ARG
1	B	609	GLU
1	B	612	LYS
1	B	620	LYS
1	B	628	GLN
1	B	645	LYS
1	B	668[A]	CYS
1	B	668[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	385	ASN
1	A	454	ASN
1	A	535	GLN
1	A	569	ASN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	454	ASN
1	B	470	HIS
1	B	535	GLN
1	B	601	ASN

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Mol	Chain	Res	Type
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 [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$
2	HEM	B	750	1	41,50,50	2.03	11 (26%)	45,82,82	1.73	7 (15%)
3	H4B	B	760	-	16,18,18	1.64	3 (18%)	11,26,26	2.55	5 (45%)
5	ACT	B	860	-	3,3,3	0.90	0	3,3,3	0.50	0
4	JM6	A	800	-	13,15,15	0.96	0	13,17,17	1.80	3 (23%)
2	HEM	A	750	1	41,50,50	1.93	10 (24%)	45,82,82	2.12	13 (28%)
3	H4B	A	760	-	16,18,18	1.13	2 (12%)	11,26,26	2.93	6 (54%)
4	JM6	B	800	-	13,15,15	0.83	0	13,17,17	1.56	3 (23%)
5	ACT	A	860	-	3,3,3	0.74	0	3,3,3	0.93	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
2	HEM	B	750	1	-	0/12/54/54	-
3	H4B	B	760	-	-	1/8/17/17	0/2/2/2
4	JM6	A	800	-	-	5/15/16/16	-
2	HEM	A	750	1	-	0/12/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	JM6	B	800	-	-	3/15/16/16	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3D-C2D	6.96	1.51	1.36
2	A	750	HEM	C3D-C2D	6.75	1.51	1.36
2	B	750	HEM	C3C-C2C	-4.57	1.34	1.40
3	B	760	H4B	C7-C6	4.17	1.56	1.52
2	B	750	HEM	FE-ND	3.46	2.14	1.96
3	B	760	H4B	C4-N3	3.32	1.38	1.33
2	A	750	HEM	CMA-C3A	3.20	1.58	1.51
2	A	750	HEM	C3C-C2C	-3.16	1.36	1.40
2	A	750	HEM	C3C-CAC	2.99	1.53	1.47
2	A	750	HEM	CMC-C2C	2.97	1.58	1.51
2	A	750	HEM	CAB-C3B	2.96	1.55	1.47
2	A	750	HEM	FE-ND	2.84	2.10	1.96
2	B	750	HEM	C3C-CAC	2.82	1.53	1.47
2	B	750	HEM	CMD-C2D	2.65	1.56	1.50
2	A	750	HEM	FE-NB	2.58	2.09	1.96
2	A	750	HEM	CMD-C2D	2.52	1.56	1.50
2	B	750	HEM	CMB-C2B	2.49	1.56	1.50
2	B	750	HEM	CMC-C2C	2.48	1.57	1.51
2	B	750	HEM	CAB-C3B	2.40	1.54	1.47
2	A	750	HEM	O1D-CGD	2.34	1.29	1.22
2	B	750	HEM	CMA-C3A	2.31	1.56	1.51
3	B	760	H4B	C7-N8	2.29	1.48	1.44
2	B	750	HEM	C4A-NA	2.22	1.40	1.36
2	B	750	HEM	CAD-C3D	2.11	1.56	1.51
3	A	760	H4B	C4-N3	2.10	1.36	1.33
3	A	760	H4B	C2-N2	2.09	1.38	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBA-CAA-C2A	-6.50	101.53	112.62
2	A	750	HEM	C4D-ND-C1D	5.26	110.51	105.07
2	B	750	HEM	CBA-CAA-C2A	-5.24	103.67	112.62
3	B	760	H4B	C8A-C4A-C4	5.13	119.13	114.57
2	A	750	HEM	CBD-CAD-C3D	-4.80	99.30	112.63
3	A	760	H4B	C4-C4A-N5	4.32	122.75	119.12
3	A	760	H4B	N1-C2-N3	-4.23	118.79	125.42
3	B	760	H4B	C4-C4A-N5	4.16	122.61	119.12
3	A	760	H4B	C8A-C4A-C4	3.86	118.00	114.57
2	B	750	HEM	C4D-ND-C1D	3.80	109.00	105.07
4	A	800	JM6	C6-S5-C4	3.79	113.41	100.40
3	A	760	H4B	C2-N3-C4	3.69	121.79	115.93
3	A	760	H4B	C2-N1-C8A	3.53	122.45	114.54
2	B	750	HEM	C4C-CHD-C1D	3.37	127.01	122.56
2	A	750	HEM	CMD-C2D-C1D	3.26	130.01	125.04
2	B	750	HEM	CBD-CAD-C3D	-3.23	103.65	112.63
2	A	750	HEM	CMC-C2C-C3C	3.18	130.63	124.68
4	A	800	JM6	C4-C3-C2	-3.13	103.59	113.38
2	A	750	HEM	C1D-C2D-C3D	-3.09	103.71	106.96
4	B	800	JM6	C6-S5-C4	3.08	110.98	100.40
2	A	750	HEM	CHA-C4D-ND	3.07	128.17	124.38
2	B	750	HEM	C2C-C3C-C4C	3.04	109.02	106.90
4	A	800	JM6	C3-C4-S5	-3.04	99.03	113.06
2	B	750	HEM	C1D-C2D-C3D	-2.94	103.86	106.96
2	A	750	HEM	C4C-CHD-C1D	2.88	126.36	122.56
3	A	760	H4B	N2-C2-N3	2.81	121.63	117.25
3	B	760	H4B	C2-N3-C4	2.80	120.37	115.93
2	A	750	HEM	C2C-C3C-C4C	2.79	108.84	106.90
2	A	750	HEM	C4B-CHC-C1C	2.77	126.21	122.56
4	B	800	JM6	C4-C3-C2	-2.75	104.78	113.38
3	B	760	H4B	N1-C2-N3	-2.35	121.73	125.42
3	B	760	H4B	C2-N1-C8A	2.24	119.55	114.54
2	A	750	HEM	CHC-C4B-C3B	2.23	127.99	124.57
2	A	750	HEM	C1B-NB-C4B	2.16	107.30	105.07
2	B	750	HEM	CHC-C4B-C3B	2.15	127.87	124.57
4	B	800	JM6	OA1-C-CA	2.14	120.67	113.38
2	A	750	HEM	C3C-C4C-NC	-2.01	107.14	110.94

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800	JM6	NH1-C1-NE-CD

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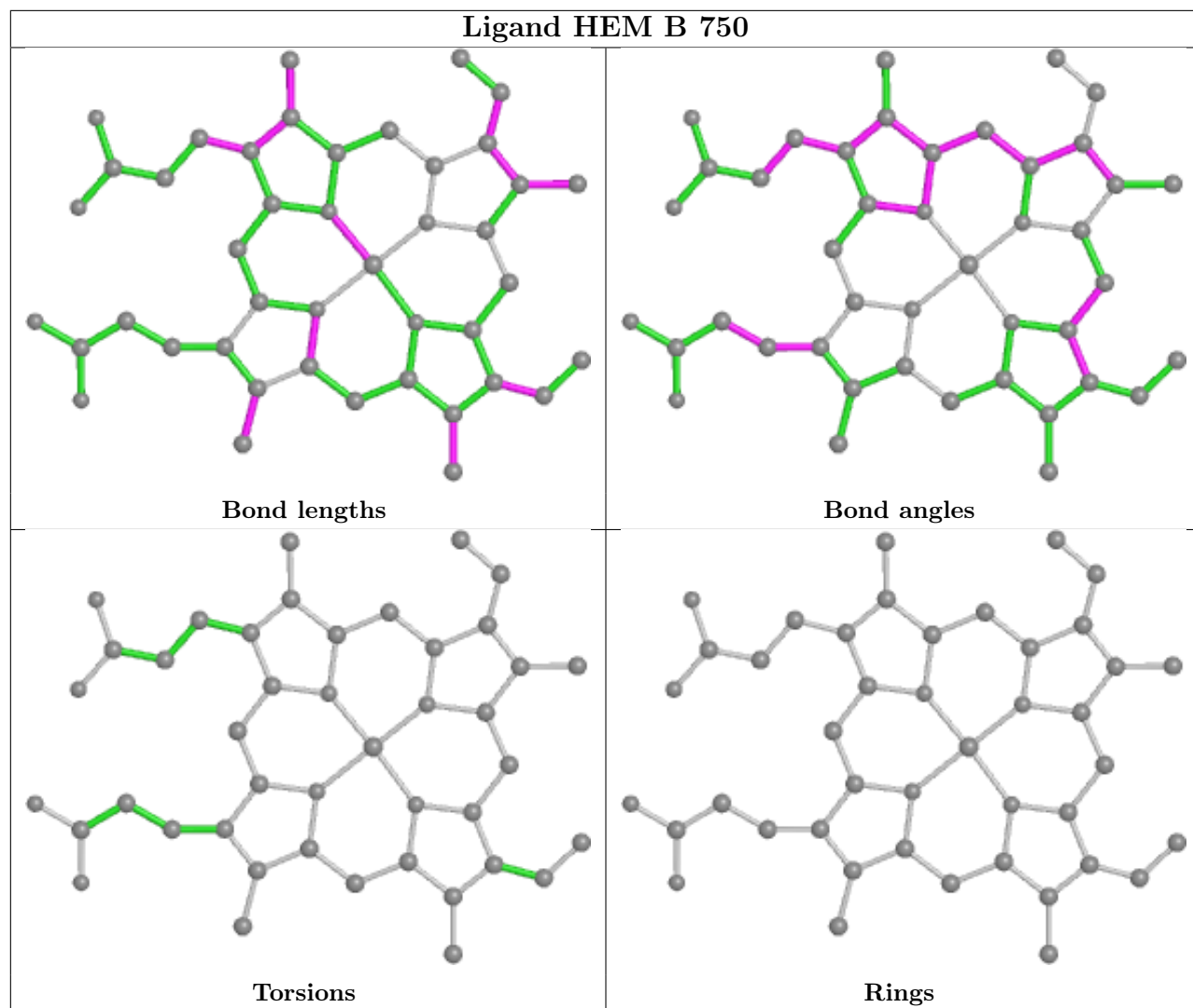
Mol	Chain	Res	Type	Atoms
4	A	800	JM6	C2-C1-NE-CD
4	A	800	JM6	NE-CD-CG-CB
4	B	800	JM6	C2-C3-C4-S5
4	B	800	JM6	C3-C4-S5-C6
4	A	800	JM6	CA-CB-CG-CD
3	B	760	H4B	O10-C10-C9-O9
4	B	800	JM6	C2-C1-NE-CD
4	A	800	JM6	C1-C2-C3-C4

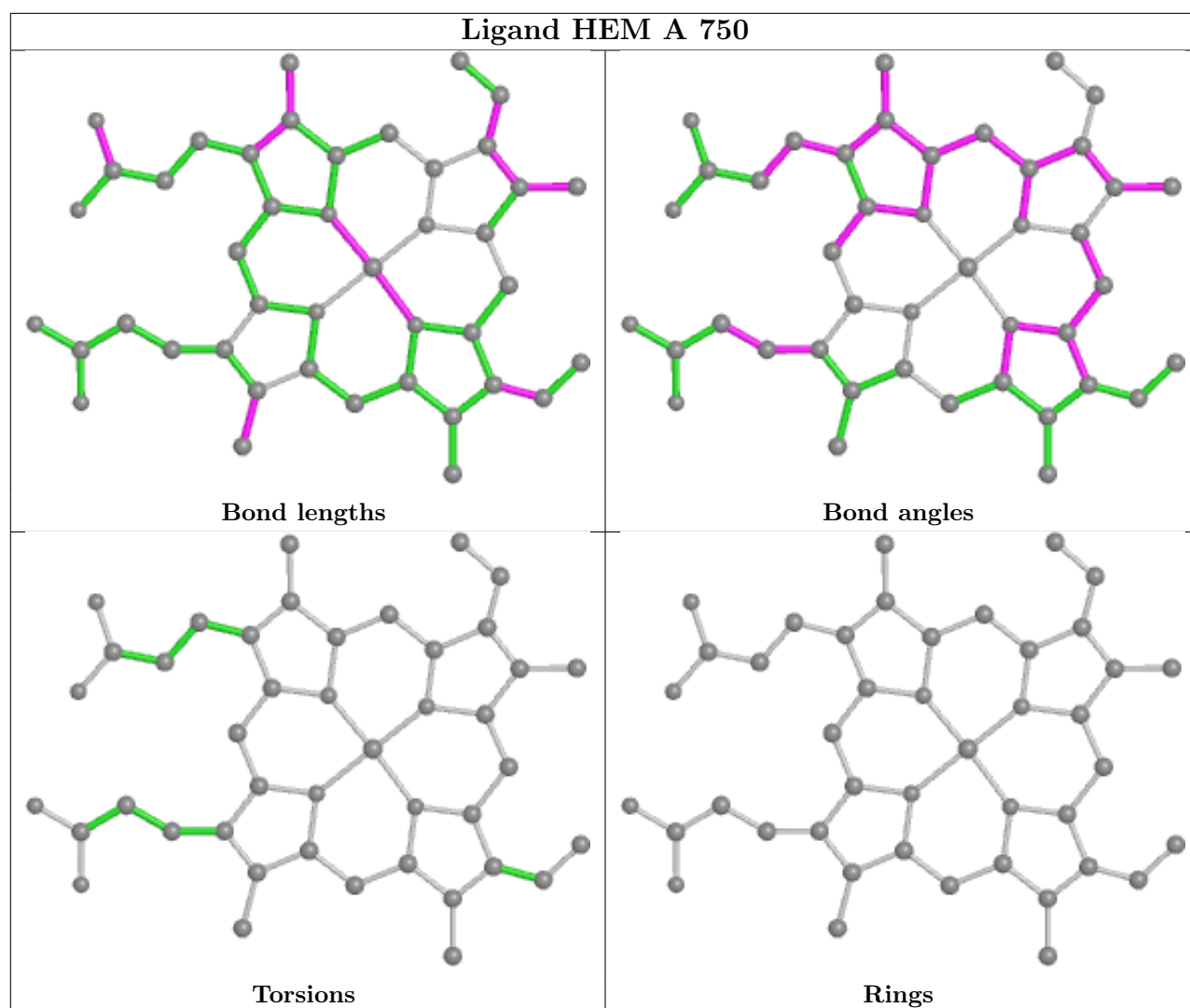
There are no ring outliers.

4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	HEM	6	0
4	A	800	JM6	13	0
2	A	750	HEM	5	0
4	B	800	JM6	10	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.





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%)	0.97	67 (16%) 1 1	41, 70, 119, 146	0
1	B	411/422 (97%)	0.53	31 (7%) 14 15	40, 59, 86, 111	0
All	All	818/844 (96%)	0.75	98 (11%) 4 4	40, 64, 110, 146	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	8.0
1	A	715	VAL	7.1
1	B	300	PHE	5.8
1	A	486	LYS	5.4
1	A	366	TYR	5.4
1	B	352	ASP	5.3
1	B	718	GLY	5.3
1	A	390	SER	5.0
1	A	355	PHE	4.8
1	B	348	VAL	4.3
1	A	488	PRO	4.2
1	B	350	THR	4.1
1	B	351	LYS	4.1
1	A	375	LYS	3.9
1	A	371	ARG	3.9
1	A	566	ALA	3.8
1	A	712	ASN	3.8
1	A	551	PHE	3.8
1	B	566	ALA	3.7
1	A	713	THR	3.6
1	A	299	ARG	3.6
1	A	370	LYS	3.6
1	A	508	GLN	3.6
1	A	503	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	385	ASN	3.5
1	B	619	ARG	3.5
1	A	352	ASP	3.4
1	A	315	THR	3.3
1	A	480	ILE	3.3
1	A	678	TRP	3.3
1	A	485	TYR	3.3
1	A	388	ILE	3.3
1	A	565	PRO	3.3
1	A	554	PHE	3.3
1	B	567	VAL	3.2
1	A	714	HIS	3.2
1	B	554	PHE	3.1
1	A	593	ILE	3.1
1	B	667	ARG	3.1
1	A	584	PHE	3.1
1	A	506	ILE	3.1
1	A	394	TYR	3.0
1	A	567	VAL	3.0
1	A	479	LEU	3.0
1	A	588	TYR	3.0
1	A	494	GLY	3.0
1	B	615	ASP	3.0
1	A	389	GLU	2.9
1	A	351	LYS	2.9
1	A	381	LEU	2.9
1	B	310	VAL	2.8
1	B	389	GLU	2.7
1	A	300	PHE	2.7
1	B	349	ARG	2.7
1	A	354	LEU	2.7
1	A	619	ARG	2.6
1	A	338	PRO	2.6
1	B	620	LYS	2.6
1	A	533	LEU	2.6
1	A	677	VAL	2.6
1	A	507	GLN	2.5
1	B	301	LEU	2.5
1	B	443	CYS	2.5
1	B	677	VAL	2.5
1	A	492	THR	2.5
1	A	373	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	302	LYS	2.5
1	A	391	THR	2.4
1	B	318	LEU	2.4
1	B	678	TRP	2.4
1	A	511	LYS	2.4
1	A	505	CYS	2.3
1	A	679	ILE	2.3
1	A	487	GLN	2.3
1	A	667	ARG	2.3
1	A	415	CYS	2.3
1	A	318	LEU	2.3
1	B	321	THR	2.3
1	B	315	THR	2.2
1	A	446	VAL	2.2
1	A	541	VAL	2.2
1	A	470	HIS	2.2
1	A	489	ASP	2.2
1	A	523	LEU	2.2
1	B	680	VAL	2.2
1	A	680	VAL	2.2
1	B	616	LEU	2.2
1	A	682	PRO	2.1
1	A	514	ARG	2.1
1	B	355	PHE	2.1
1	B	565	PRO	2.1
1	A	493	LEU	2.1
1	A	504	ILE	2.1
1	B	369	ILE	2.0
1	A	710	PRO	2.0
1	A	685	GLY	2.0
1	B	553	TRP	2.0
1	B	373	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](#)

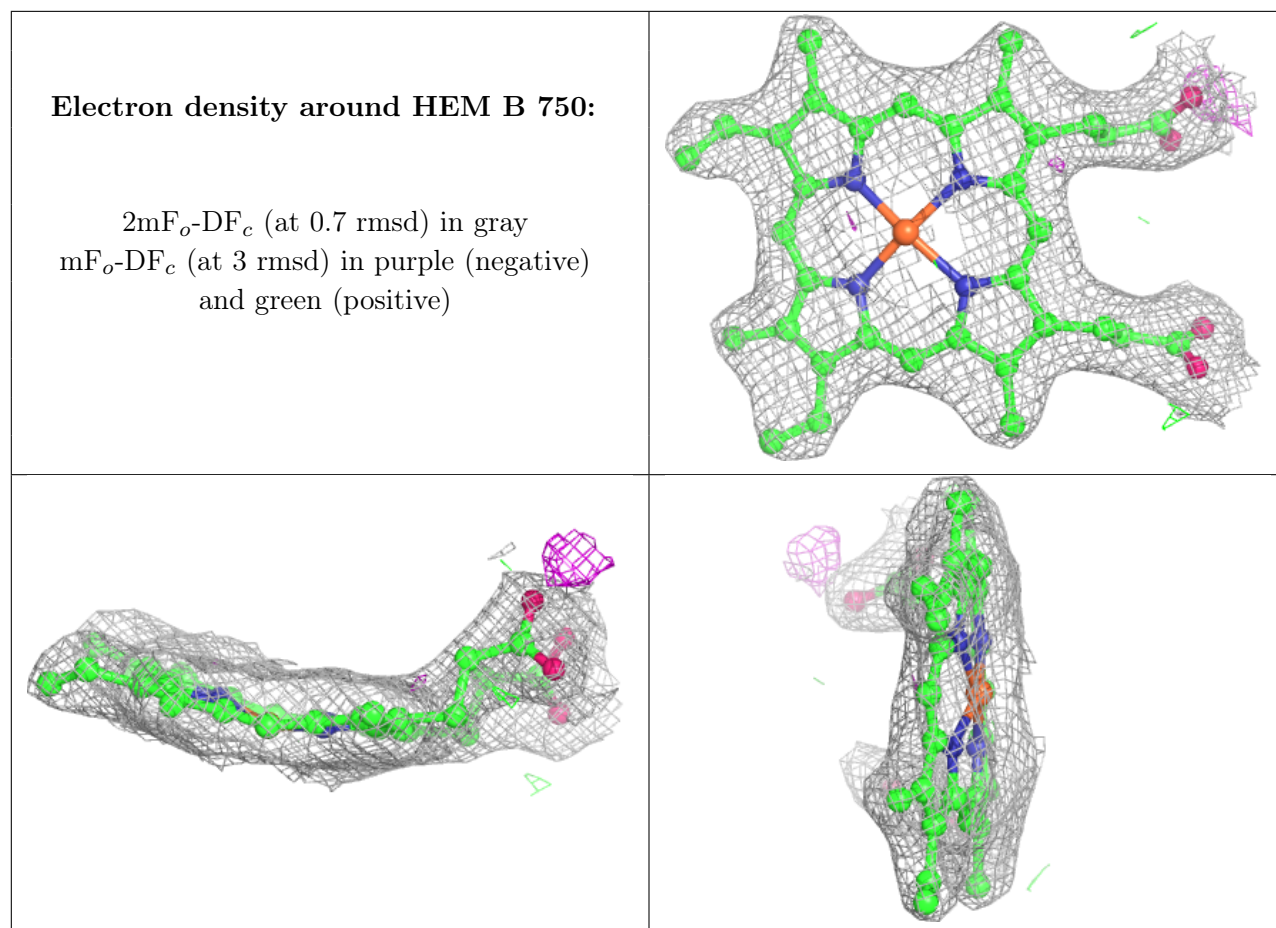
There are no monosaccharides in this entry.

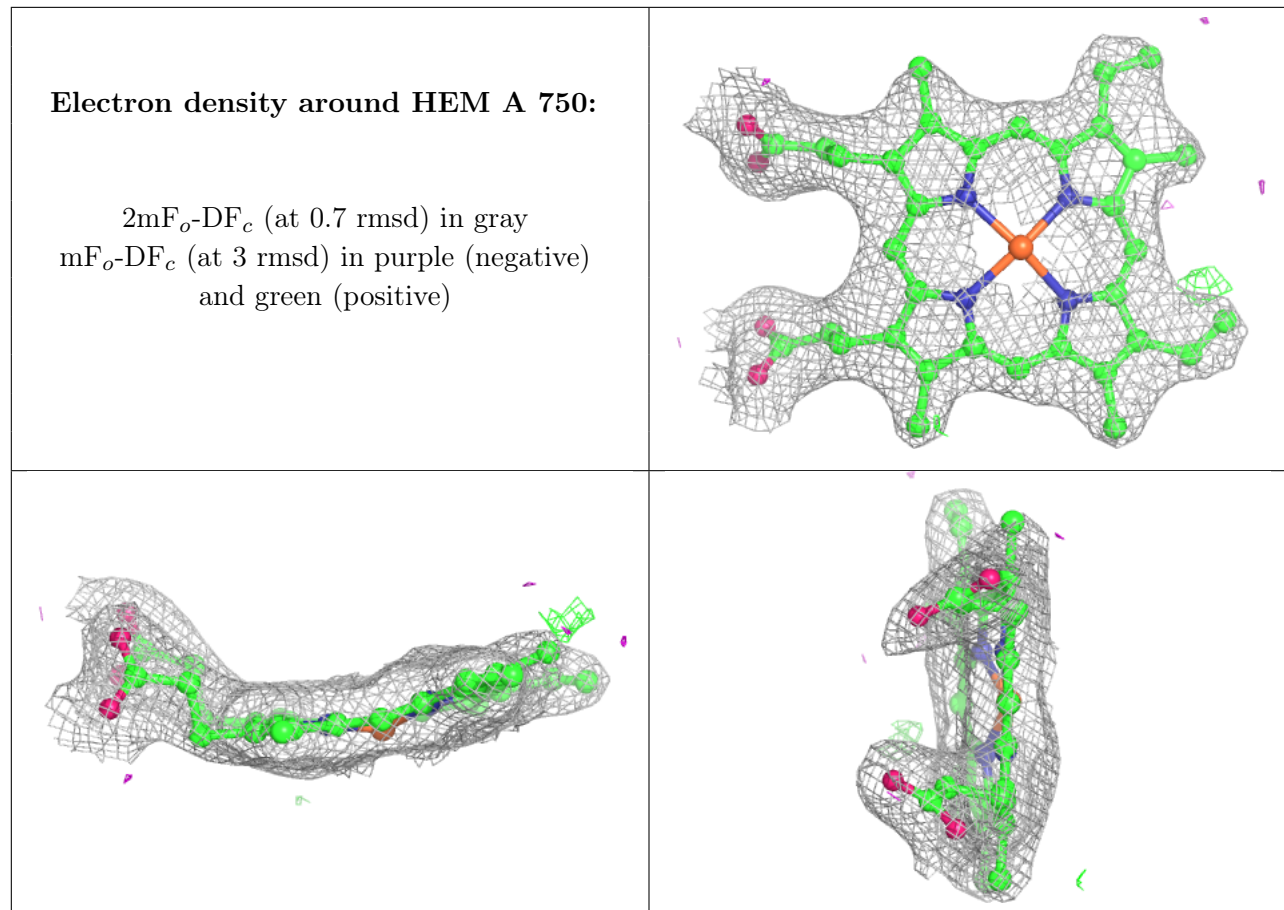
6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	860	4/4	0.89	0.32	93,95,95,96	0
4	JM6	B	800	16/16	0.91	0.24	39,56,93,94	0
4	JM6	A	800	16/16	0.92	0.33	47,59,90,94	0
5	ACT	B	860	4/4	0.94	0.14	77,81,81,84	0
3	H4B	A	760	17/17	0.95	0.18	43,49,53,56	0
3	H4B	B	760	17/17	0.96	0.18	40,43,47,51	0
6	ZN	A	900	1/1	0.96	0.10	55,55,55,55	0
2	HEM	B	750	43/43	0.97	0.16	37,43,50,55	0
2	HEM	A	750	43/43	0.98	0.21	44,48,52,57	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.