



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:56 PM UTC

PDB ID : 3B3N / pdb_00003b3n
Title : Structure of neuronal NOS heme domain in complex with a inhibitor (+-)-N1-
-{cis-4'-[(6"-aminopyridin-2"-yl)methyl]pyrrolidin-3'-yl}ethane-1,2-diamine
Authors : Igarashi, J.; Li, H.; Poulos, T.L.
Deposited on : 2007-10-22
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 types of validation reports are described at

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

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

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

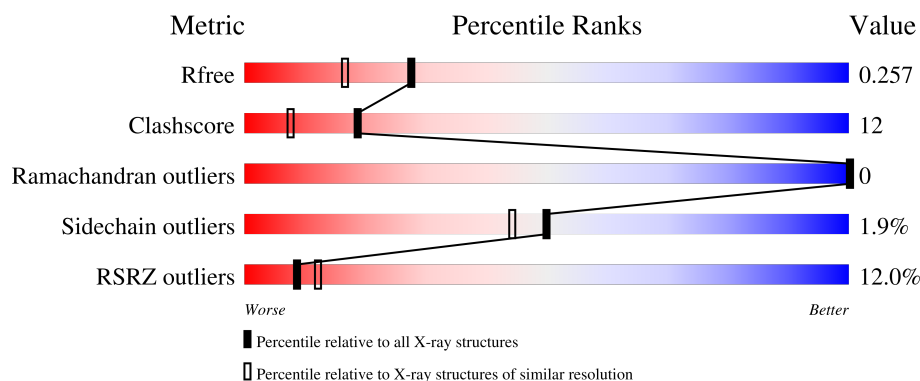
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	18% 67% 27% • •
1	B	422	5% 78% 18% • •

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7213 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.

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
			3345	2140	574	610	21			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).

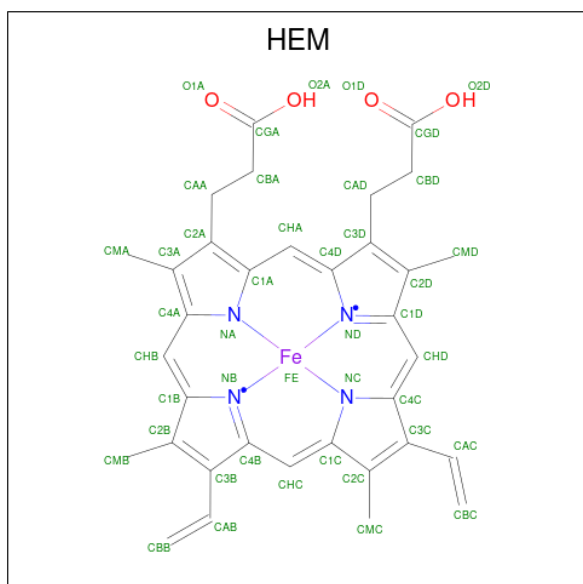


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



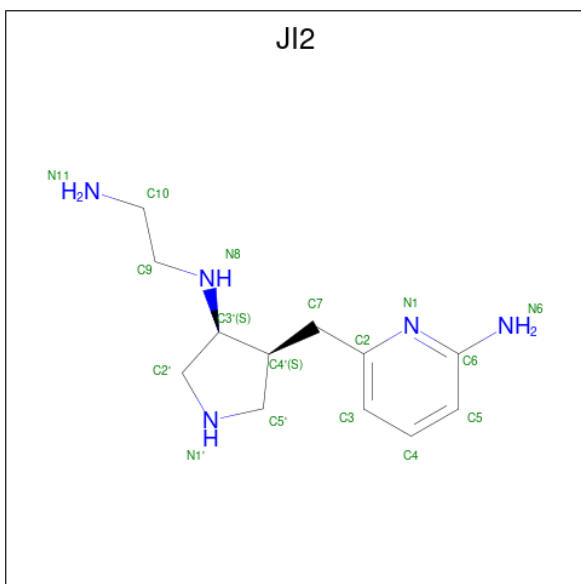
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



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

- Molecule 6 is N-[(3S,4S)-4-[(6-aminopyridin-2-yl)methyl]pyrrolidin-3-yl]ethane-1,2-diamine (CCD ID: JI2) (formula: C₁₂H₂₁N₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N		0	0
			17	12	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	0	0
			17	12	5		

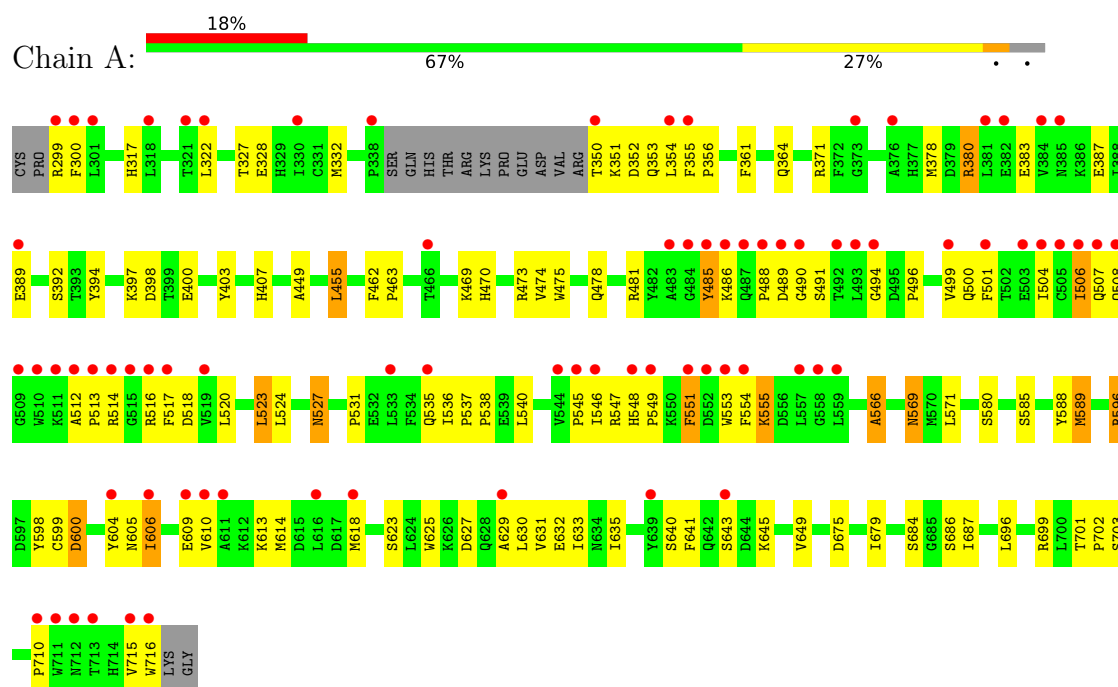
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	166	Total	O	0	0
			166	166		
7	B	226	Total	O	0	0
			226	226		

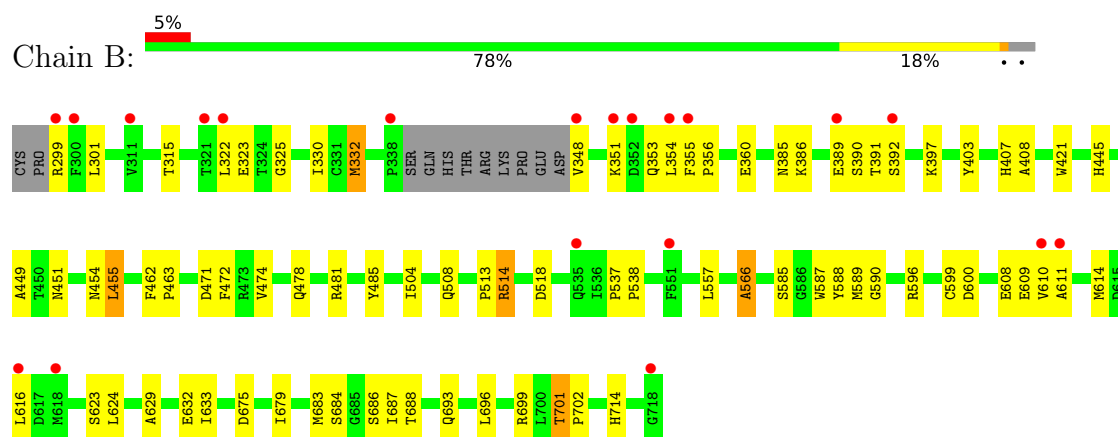
3 Residue-property plots

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



• Molecule 1: Nitric-oxide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.05Å 110.69Å 164.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 1.98 49.64 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.64-1.98) 98.7 (49.64-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.270 0.221 , 0.257	Depositor DCC
R_{free} test set	3301 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7213	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: ZN, ACT, H4B, JI2, 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	0.51	0/3406	1.00	14/4621 (0.3%)
1	B	0.56	0/3438	1.03	24/4661 (0.5%)
All	All	0.53	0/6844	1.02	38/9282 (0.4%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	MET	N-CA-C	-8.71	95.05	109.07
1	B	589	MET	N-CA-C	-8.28	95.74	109.24
1	B	566	ALA	N-CA-C	7.38	119.50	107.32
1	A	623	SER	N-CA-C	-7.34	104.30	113.18
1	B	421	TRP	N-CA-C	7.33	120.20	111.33
1	A	588	TYR	N-CA-C	7.06	120.45	110.50
1	A	566	ALA	N-CA-C	6.64	118.27	107.32
1	B	599	CYS	N-CA-C	6.51	121.38	113.38
1	A	455	LEU	N-CA-C	6.35	119.44	110.23
1	B	588	TYR	N-CA-C	6.24	119.29	110.50
1	A	354	LEU	N-CA-C	6.20	119.31	111.69
1	B	474	VAL	N-CA-C	-6.12	98.32	107.37
1	B	472	PHE	N-CA-C	-6.11	99.74	109.76
1	B	688	THR	N-CA-C	-6.10	101.11	110.32
1	B	354	LEU	N-CA-C	6.07	118.80	111.40
1	A	546	ILE	N-CA-C	5.99	116.73	107.99
1	B	714	HIS	N-CA-C	5.80	118.74	110.10
1	B	701	THR	N-CA-C	-5.76	102.16	110.40
1	A	606	ILE	N-CA-C	5.63	117.58	112.29
1	A	506	ILE	N-CA-C	-5.62	105.36	110.82
1	B	590	GLY	N-CA-C	5.61	119.43	112.64
1	B	623	SER	N-CA-C	-5.57	105.99	112.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	686	SER	N-CA-C	5.51	119.62	113.01
1	B	514	ARG	N-CA-C	5.50	118.78	111.30
1	A	596	ARG	N-CA-C	5.48	118.09	111.40
1	A	703	SER	N-CA-C	5.44	117.34	109.07
1	B	315	THR	N-CA-C	-5.44	107.29	114.31
1	B	596	ARG	N-CA-C	5.42	118.23	111.24
1	B	455	LEU	N-CA-C	5.38	118.03	110.23
1	B	600	ASP	N-CA-C	-5.30	103.14	110.35
1	A	686	SER	N-CA-C	5.28	119.35	113.01
1	B	408	ALA	N-CA-C	-5.21	105.60	111.28
1	B	471	ASP	N-CA-C	5.17	117.72	110.23
1	A	474	VAL	N-CA-C	-5.13	99.78	107.37
1	B	616	LEU	N-CA-C	-5.09	102.93	110.46
1	B	397	LYS	N-CA-C	-5.07	103.70	110.55
1	A	599	CYS	N-CA-C	5.03	119.56	113.38
1	B	693	GLN	N-CA-C	5.02	116.91	108.73

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	3313	0	3221	117	0
1	B	3345	0	3259	46	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	43	0	30	3	0
4	B	43	0	30	2	0
5	A	17	0	15	0	0
5	B	17	0	15	0	0
6	A	17	0	21	2	0
6	B	17	0	21	0	0
7	A	166	0	0	8	0
7	B	226	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7213	0	6618	160	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 12.

All (160) 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:A:523:LEU:HD22	1:A:531:PRO:HB2	1.45	0.94
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.47	0.80
1:A:614:MET:O	7:A:1065:HOH:O	2.01	0.79
1:A:332:MET:HE2	1:B:696:LEU:HD21	1.69	0.74
4:B:750:HEM:HMC2	4:B:750:HEM:HBC2	1.69	0.73
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.52	0.73
1:A:627:ASP:O	1:A:631:VAL:HG23	1.88	0.73
1:A:555:LYS:NZ	1:A:555:LYS:HB3	2.07	0.70
1:A:613:LYS:O	7:A:1064:HOH:O	2.09	0.69
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.74	0.69
1:A:516:ARG:HD3	1:A:517:PHE:HE1	1.58	0.69
1:A:350:THR:HG22	1:A:352:ASP:H	1.60	0.66
1:A:328:GLU:H	1:A:328:GLU:CD	2.03	0.66
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.59	0.66
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.79	0.65
1:A:569:ASN:HD22	1:A:569:ASN:H	1.44	0.64
1:A:596:ARG:O	1:A:600:ASP:HB2	1.99	0.63
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.81	0.61
1:A:350:THR:HB	1:A:353:GLN:CD	2.24	0.61
1:B:391:THR:O	1:B:392:SER:HB2	2.01	0.61
1:A:514:ARG:HH21	1:A:514:ARG:HG3	1.68	0.58
1:B:356:PRO:O	1:B:360:GLU:HG3	2.03	0.58
1:B:355:PHE:N	1:B:356:PRO:HD2	2.18	0.58
1:A:551:PHE:CD2	1:A:551:PHE:N	2.71	0.58
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.19	0.57
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.39	0.57
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.86	0.56
1:A:545:PRO:HG2	1:A:547:ARG:NH2	2.21	0.56
1:B:386:LYS:HD3	7:B:1205:HOH:O	2.06	0.55
1:A:675:ASP:O	1:A:679:ILE:HG12	2.06	0.55
1:B:325:GLY:O	1:B:332:MET:HG3	2.07	0.55
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.89	0.54
1:A:569:ASN:HD22	1:A:569:ASN:N	2.04	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.89	0.54
1:B:386:LYS:O	1:B:389:GLU:HG2	2.08	0.54
1:A:378:MET:HA	1:A:378:MET:HE2	1.88	0.54
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.07	0.54
1:A:350:THR:HB	1:A:353:GLN:CG	2.38	0.54
1:A:598:TYR:O	1:A:606:ILE:HG12	2.09	0.53
1:A:606:ILE:O	1:A:610:VAL:HG23	2.08	0.53
1:B:348:VAL:HG12	7:B:1230:HOH:O	2.08	0.53
1:A:355:PHE:N	1:A:356:PRO:HD2	2.24	0.53
1:A:545:PRO:HG2	1:A:547:ARG:HH21	1.72	0.53
1:A:350:THR:HB	1:A:353:GLN:HG3	1.89	0.53
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.34	0.53
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.90	0.53
1:A:500:GLN:O	1:A:504:ILE:HG13	2.08	0.53
1:A:501:PHE:CD2	1:A:520:LEU:HD13	2.45	0.52
1:A:569:ASN:H	1:A:569:ASN:ND2	2.05	0.52
1:A:716:TRP:H	1:A:716:TRP:CD1	2.27	0.52
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.74	0.52
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.24	0.52
1:A:489:ASP:C	1:A:491:SER:H	2.17	0.52
1:A:551:PHE:N	1:A:551:PHE:HD2	2.08	0.52
1:A:610:VAL:O	1:A:614:MET:HG3	2.10	0.51
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.92	0.51
1:A:516:ARG:HD3	1:A:517:PHE:CE1	2.43	0.51
1:A:488:PRO:C	1:A:490:GLY:H	2.18	0.51
1:B:351:LYS:HE3	1:B:392:SER:OG	2.10	0.51
1:A:380:ARG:NH1	1:A:397:LYS:HG2	2.24	0.51
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.74	0.51
4:A:750:HEM:O2D	6:A:800:JI2:N11	2.44	0.50
1:A:555:LYS:HB3	1:A:555:LYS:HZ2	1.76	0.50
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.27	0.50
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.46	0.50
1:A:696:LEU:HD22	1:B:330:ILE:CD1	2.41	0.50
1:B:538:PRO:HD3	7:B:1212:HOH:O	2.12	0.50
1:A:489:ASP:OD2	1:A:489:ASP:O	2.31	0.49
1:A:554:PHE:HB3	7:A:965:HOH:O	2.13	0.49
1:B:323:GLU:HG3	7:B:1175:HOH:O	2.12	0.49
1:A:371:ARG:HH21	1:A:371:ARG:CG	2.24	0.49
1:A:555:LYS:HB3	1:A:555:LYS:HZ3	1.78	0.49
1:B:614:MET:CE	1:B:632:GLU:HG3	2.42	0.49
1:A:571:LEU:C	1:A:571:LEU:HD23	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.95	0.49
1:A:485:TYR:OH	1:A:518:ASP:OD2	2.31	0.48
1:A:535:GLN:NE2	7:A:994:HOH:O	2.45	0.48
1:B:587:TRP:H	4:B:750:HEM:HAB	1.77	0.48
1:A:494:GLY:O	1:A:496:PRO:HD3	2.13	0.48
1:A:332:MET:HE2	1:B:696:LEU:CD2	2.41	0.48
1:B:701:THR:HA	1:B:702:PRO:C	2.39	0.48
1:A:351:LYS:HE2	1:A:392:SER:CB	2.44	0.48
1:A:536:ILE:O	1:A:537:PRO:C	2.54	0.48
1:A:614:MET:CE	1:A:632:GLU:HG3	2.44	0.48
1:B:566:ALA:HB2	1:B:585:SER:HB3	1.96	0.48
1:A:486:LYS:HE2	1:A:499:VAL:HG11	1.97	0.47
1:A:610:VAL:HG21	1:A:633:ILE:CD1	2.43	0.47
1:A:506:ILE:C	1:A:508:GLN:N	2.70	0.47
1:A:551:PHE:CE1	1:A:614:MET:HE3	2.42	0.47
1:A:715:VAL:O	1:A:715:VAL:HG23	2.14	0.47
1:B:504:ILE:O	1:B:508:GLN:HG2	2.15	0.47
1:A:387:GLU:OE1	1:A:394:TYR:HA	2.15	0.46
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.80	0.46
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.32	0.46
1:A:635:ILE:HG13	1:B:624:LEU:HD12	1.97	0.46
4:A:750:HEM:HBA2	6:A:800:JI2:H72	1.98	0.46
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.31	0.46
1:A:322:LEU:HB3	1:A:699:ARG:NH2	2.24	0.46
1:A:640:SER:O	1:A:643:SER:N	2.47	0.46
1:A:589:MET:HA	1:A:649:VAL:O	2.16	0.45
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.98	0.45
1:B:614:MET:HE3	1:B:632:GLU:HG3	1.98	0.45
1:B:445:HIS:C	1:B:445:HIS:CD2	2.95	0.45
1:A:524:LEU:O	1:A:531:PRO:HA	2.16	0.45
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.97	0.45
1:A:504:ILE:O	1:A:508:GLN:HG2	2.16	0.45
1:A:614:MET:HA	7:A:1064:HOH:O	2.15	0.45
1:B:299:ARG:HB3	1:B:299:ARG:HH11	1.81	0.45
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.80	0.45
1:B:451:ASN:HB3	1:B:454:ASN:O	2.17	0.44
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.52	0.44
1:B:478:GLN:HB2	1:B:481:ARG:CG	2.47	0.44
1:A:299:ARG:O	1:A:317:HIS:CE1	2.70	0.44
1:B:449:ALA:O	1:B:455:LEU:HA	2.18	0.44
1:A:553:TRP:CE3	1:A:613:LYS:HD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:ALA:O	1:A:630:LEU:C	2.61	0.43
1:A:701:THR:HA	1:A:702:PRO:C	2.43	0.43
1:A:361:PHE:O	1:A:364:GLN:HG2	2.17	0.43
1:A:322:LEU:HB2	1:A:699:ARG:HE	1.83	0.43
1:A:507:GLN:O	1:A:507:GLN:HG2	2.18	0.43
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.07	0.43
1:B:537:PRO:HA	7:B:1212:HOH:O	2.18	0.43
1:B:608:GLU:O	1:B:611:ALA:HB3	2.19	0.43
1:A:569:ASN:N	1:A:569:ASN:ND2	2.66	0.43
1:A:604:TYR:O	1:A:605:ASN:C	2.62	0.43
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.48	0.43
1:B:629:ALA:O	1:B:633:ILE:HG13	2.18	0.43
1:A:614:MET:HE3	1:A:632:GLU:HG3	2.01	0.43
1:A:506:ILE:C	1:A:508:GLN:H	2.25	0.42
1:B:389:GLU:HG3	1:B:390:SER:N	2.35	0.42
1:A:473:ARG:HD2	1:A:580:SER:HB2	2.01	0.42
1:A:640:SER:O	1:A:641:PHE:C	2.63	0.42
1:B:675:ASP:O	1:B:679:ILE:HG12	2.20	0.42
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.50	0.42
1:A:566:ALA:HB2	1:A:585:SER:HB3	2.01	0.42
1:A:300:PHE:CD1	1:A:300:PHE:N	2.88	0.42
1:A:397:LYS:O	1:A:398:ASP:C	2.62	0.42
1:A:469:LYS:C	1:A:470:HIS:ND1	2.78	0.42
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.86	0.42
1:B:299:ARG:NH1	1:B:299:ARG:CB	2.83	0.42
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.35	0.42
1:A:523:LEU:HA	1:A:523:LEU:HD23	1.84	0.42
1:A:322:LEU:CB	1:A:699:ARG:HE	2.33	0.41
1:A:684:SER:HB3	1:A:687:ILE:HG12	2.02	0.41
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.50	0.41
1:A:609:GLU:HG3	7:A:1048:HOH:O	2.19	0.41
1:B:557:LEU:HD23	1:B:609:GLU:OE1	2.21	0.41
1:A:350:THR:HG22	1:A:352:ASP:N	2.31	0.41
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.50	0.41
1:B:355:PHE:N	1:B:356:PRO:CD	2.83	0.41
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.50	0.41
1:A:449:ALA:O	1:A:455:LEU:HA	2.21	0.41
1:B:610:VAL:HG21	1:B:633:ILE:HD11	2.03	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.41
1:A:383:GLU:HG3	7:A:1050:HOH:O	2.20	0.40
1:A:488:PRO:C	1:A:490:GLY:N	2.76	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:PHE:HD1	1:A:553:TRP:CZ2	2.40	0.40
1:A:618:MET:HA	1:A:625:TRP:CD1	2.56	0.40
1:A:627:ASP:OD2	1:B:683:MET:HE2	2.22	0.40
1:A:643:SER:HA	7:A:1051:HOH:O	2.21	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	403/422 (96%)	372 (92%)	31 (8%)	0	100	100
1	B	407/422 (96%)	396 (97%)	11 (3%)	0	100	100
All	All	810/844 (96%)	768 (95%)	42 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	363/377 (96%)	351 (97%)	12 (3%)	33	23
1	B	366/377 (97%)	364 (100%)	2 (0%)	81	79
All	All	729/754 (97%)	715 (98%)	14 (2%)	50	44

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	THR
1	A	380	ARG
1	A	389	GLU
1	A	485	TYR
1	A	523	LEU
1	A	527	ASN
1	A	538	PRO
1	A	551	PHE
1	A	555	LYS
1	A	569	ASN
1	A	600	ASP
1	A	645	LYS
1	B	332	MET
1	B	353	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	407	HIS
1	A	425	GLN
1	A	454	ASN
1	A	487	GLN
1	A	507	GLN
1	A	508	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	628	GLN
1	B	364	GLN
1	B	385	ASN
1	B	407	HIS
1	B	440	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	697	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
6	JI2	A	800	-	17,18,18	2.20	5 (29%)	16,23,23	2.49	6 (37%)
6	JI2	B	800	-	17,18,18	2.34	5 (29%)	16,23,23	2.46	4 (25%)
5	H4B	A	760	-	17,18,18	1.71	3 (17%)	14,26,26	2.05	4 (28%)
2	ACT	B	860	-	3,3,3	1.01	0	3,3,3	0.64	0
2	ACT	A	860	-	3,3,3	0.99	0	3,3,3	0.79	0
4	HEM	B	750	1	50,50,50	1.25	4 (8%)	67,82,82	1.20	6 (8%)
5	H4B	B	760	-	17,18,18	1.90	3 (17%)	14,26,26	1.90	4 (28%)
4	HEM	A	750	1	50,50,50	1.29	4 (8%)	67,82,82	1.26	9 (13%)

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	JI2	A	800	-	-	0/8/18/18	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	JI2	B	800	-	-	1/8/18/18	0/2/2/2
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	HEM	B	750	1	-	2/14/54/54	-
5	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	HEM	A	750	1	-	2/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	800	JI2	C7-C4'	4.87	1.59	1.53
6	A	800	JI2	C7-C4'	4.70	1.59	1.53
5	A	760	H4B	C4A-N5	4.59	1.48	1.37
6	B	800	JI2	C4-C3	4.56	1.46	1.38
5	B	760	H4B	C4A-N5	4.51	1.48	1.37
5	B	760	H4B	C6-N5	4.32	1.55	1.47
6	A	800	JI2	C4-C3	4.22	1.46	1.38
6	B	800	JI2	C4-C5	3.99	1.45	1.38
6	A	800	JI2	C4-C5	3.69	1.45	1.38
5	A	760	H4B	C6-N5	3.69	1.54	1.47
6	B	800	JI2	C3-C2	3.53	1.46	1.38
4	B	750	HEM	CAB-C3B	-3.03	1.39	1.47
6	A	800	JI2	C3-C2	3.01	1.45	1.38
4	A	750	HEM	CHC-C1C	2.89	1.44	1.38
6	A	800	JI2	C2-N1	2.73	1.39	1.34
4	A	750	HEM	FE-NB	2.73	2.03	1.94
5	B	760	H4B	C7-N8	2.64	1.49	1.46
6	B	800	JI2	C2-N1	2.61	1.39	1.34
4	A	750	HEM	CMB-C2B	2.45	1.55	1.50
4	B	750	HEM	FE-NB	2.41	2.02	1.94
4	B	750	HEM	CMB-C2B	2.40	1.55	1.50
4	A	750	HEM	CAB-C3B	-2.36	1.41	1.47
5	A	760	H4B	C4-N3	2.21	1.43	1.38
4	B	750	HEM	CHD-C4C	2.06	1.42	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	800	JI2	C6-N1-C2	8.08	124.11	118.07
6	A	800	JI2	C6-N1-C2	7.86	123.95	118.07
5	A	760	H4B	C2-N1-C8A	5.54	123.14	113.36
5	B	760	H4B	C2-N1-C8A	5.20	122.53	113.36
5	A	760	H4B	N3-C2-N1	-3.05	117.73	123.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	750	HEM	CHC-C4B-NB	-2.98	121.22	124.42
5	B	760	H4B	N3-C2-N1	-2.79	118.21	123.32
4	A	750	HEM	CAB-C3B-C2B	-2.71	119.62	128.43
4	A	750	HEM	CMB-C2B-C1B	2.60	129.09	125.03
6	A	800	JI2	C2'-C3'-N8	-2.55	109.20	113.73
5	A	760	H4B	O10-C10-C9	-2.54	105.57	109.77
5	B	760	H4B	O10-C10-C9	-2.52	105.59	109.77
6	A	800	JI2	C5'-C4'-C3'	-2.50	99.64	103.97
4	A	750	HEM	C3B-C4B-NB	2.49	111.26	109.47
6	B	800	JI2	C5'-C4'-C3'	-2.48	99.66	103.97
6	B	800	JI2	C2'-C3'-N8	-2.43	109.41	113.73
4	B	750	HEM	C2B-C1B-NB	2.41	112.61	109.84
5	A	760	H4B	O9-C9-C6	2.38	114.99	109.28
4	B	750	HEM	C4A-NA-C1A	-2.32	102.05	105.82
4	B	750	HEM	C3D-C4D-ND	2.30	112.69	110.17
4	A	750	HEM	C2A-C1A-NA	2.28	112.68	110.15
5	B	760	H4B	O9-C9-C6	2.23	114.62	109.28
4	B	750	HEM	CMB-C2B-C1B	2.15	128.40	125.03
6	B	800	JI2	C9-N8-C3'	2.14	117.17	114.05
4	A	750	HEM	C2B-C1B-NB	2.12	112.28	109.84
6	A	800	JI2	N6-C6-N1	2.10	119.96	116.59
6	A	800	JI2	C5-C6-N1	-2.09	119.31	121.83
4	B	750	HEM	CBA-CAA-C2A	-2.06	106.83	112.53
6	A	800	JI2	C9-N8-C3'	2.06	117.05	114.05
4	A	750	HEM	CHD-C1D-ND	-2.03	122.24	124.42
4	A	750	HEM	CAA-C2A-C3A	2.02	131.60	127.07
4	A	750	HEM	CAB-C3B-C4B	2.02	133.31	124.39
4	B	750	HEM	C4A-C3A-C2A	-2.02	104.51	106.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

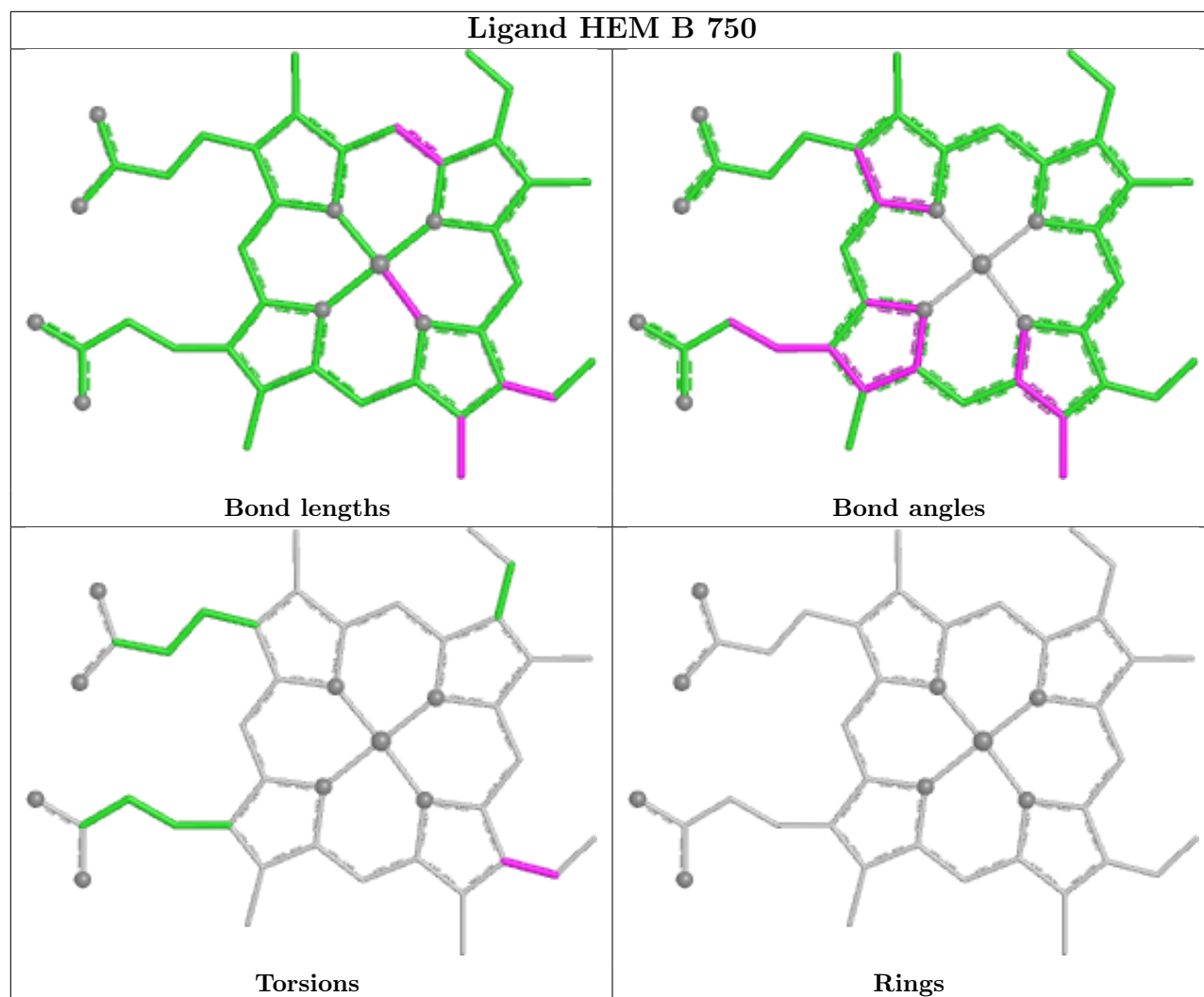
Mol	Chain	Res	Type	Atoms
4	B	750	HEM	C2B-C3B-CAB-CBB
6	B	800	JI2	C2'-C3'-N8-C9
4	B	750	HEM	C4B-C3B-CAB-CBB
4	A	750	HEM	CAA-CBA-CGA-O2A
4	A	750	HEM	CAA-CBA-CGA-O1A

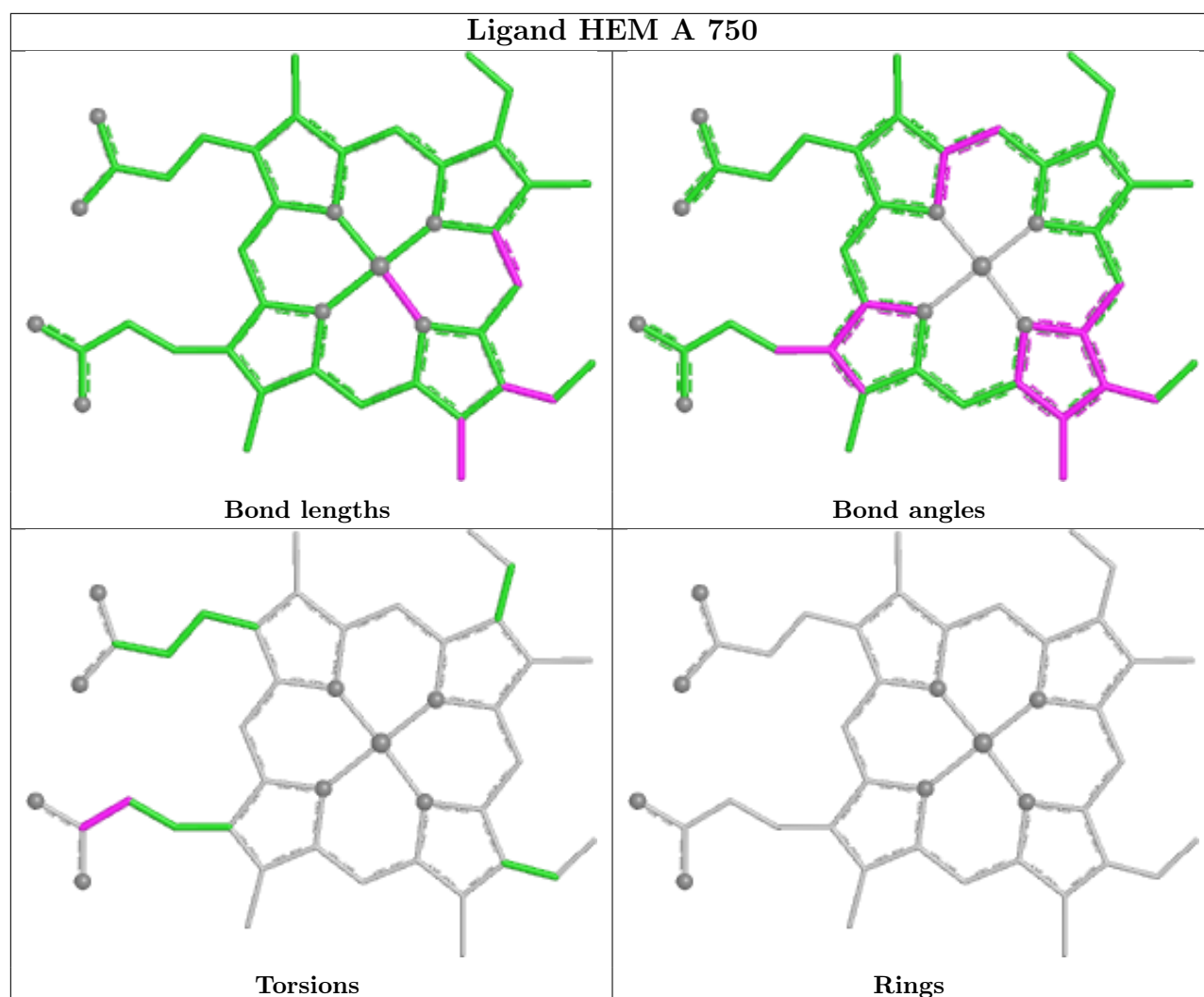
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	800	JI2	2	0
4	B	750	HEM	2	0
4	A	750	HEM	3	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%)	0.99	78 (19%) 3 4	21, 40, 67, 83	0
1	B	411/422 (97%)	0.34	20 (4%) 35 44	19, 32, 56, 68	0
All	All	818/844 (96%)	0.66	98 (11%) 9 12	19, 36, 63, 83	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	4.6
1	A	513	PRO	4.4
1	A	493	LEU	4.3
1	A	355	PHE	4.0
1	A	504	ILE	4.0
1	A	517	PHE	4.0
1	A	300	PHE	4.0
1	B	300	PHE	4.0
1	A	551	PHE	3.9
1	A	715	VAL	3.8
1	A	506	ILE	3.8
1	A	488	PRO	3.7
1	A	553	TRP	3.7
1	B	348	VAL	3.7
1	B	322	LEU	3.6
1	A	515	GLY	3.5
1	A	557	LEU	3.5
1	A	494	GLY	3.5
1	A	485	TYR	3.5
1	B	321	THR	3.4
1	A	512	ALA	3.4
1	A	616	LEU	3.4
1	A	610	VAL	3.3
1	B	355	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	499	VAL	3.2
1	A	322	LEU	3.2
1	A	554	PHE	3.2
1	B	352	ASP	3.2
1	A	510	TRP	3.1
1	B	611	ALA	3.1
1	A	559	LEU	3.1
1	A	338	PRO	3.1
1	A	711	TRP	3.1
1	B	616	LEU	3.0
1	A	545	PRO	3.0
1	A	501	PHE	3.0
1	A	321	THR	3.0
1	A	505	CYS	3.0
1	A	508	GLN	3.0
1	A	509	GLY	2.9
1	B	389	GLU	2.8
1	A	487	GLN	2.8
1	B	718	GLY	2.8
1	A	544	VAL	2.8
1	A	350	THR	2.7
1	A	301	LEU	2.7
1	A	299	ARG	2.7
1	A	514	ARG	2.7
1	B	354	LEU	2.6
1	A	558	GLY	2.6
1	A	489	ASP	2.6
1	A	381	LEU	2.6
1	A	373	GLY	2.6
1	A	511	LYS	2.6
1	A	483	ALA	2.6
1	A	713	THR	2.5
1	B	351	LYS	2.5
1	A	385	ASN	2.5
1	A	548	HIS	2.5
1	A	710	PRO	2.5
1	A	490	GLY	2.4
1	A	330	ILE	2.4
1	A	519	VAL	2.4
1	A	484	GLY	2.4
1	A	618	MET	2.4
1	A	611	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	516	ARG	2.3
1	A	384	VAL	2.3
1	A	552	ASP	2.3
1	A	503	GLU	2.3
1	A	318	LEU	2.3
1	B	551	PHE	2.3
1	B	311	VAL	2.3
1	A	492	THR	2.3
1	B	618	MET	2.3
1	A	629	ALA	2.3
1	A	466	THR	2.3
1	A	639	TYR	2.2
1	B	338	PRO	2.2
1	A	606	ILE	2.2
1	A	354	LEU	2.2
1	A	643	SER	2.2
1	A	546	ILE	2.2
1	A	486	LYS	2.2
1	A	533	LEU	2.2
1	A	535	GLN	2.2
1	B	535	GLN	2.2
1	A	389	GLU	2.2
1	B	392	SER	2.2
1	A	712	ASN	2.1
1	A	376	ALA	2.1
1	A	507	GLN	2.1
1	A	382	GLU	2.1
1	B	610	VAL	2.1
1	A	549	PRO	2.1
1	B	299	ARG	2.1
1	A	604	TYR	2.0
1	A	609	GLU	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

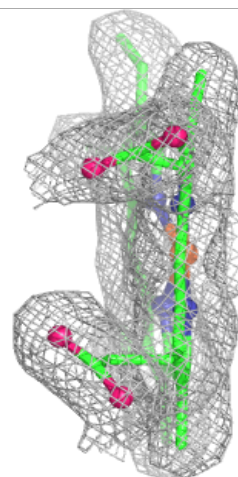
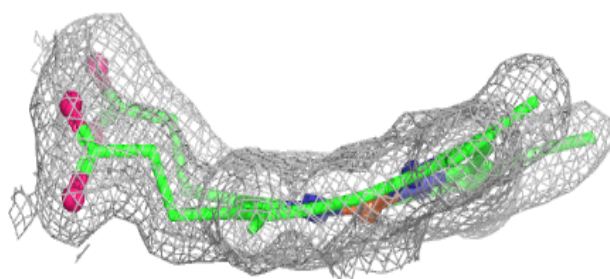
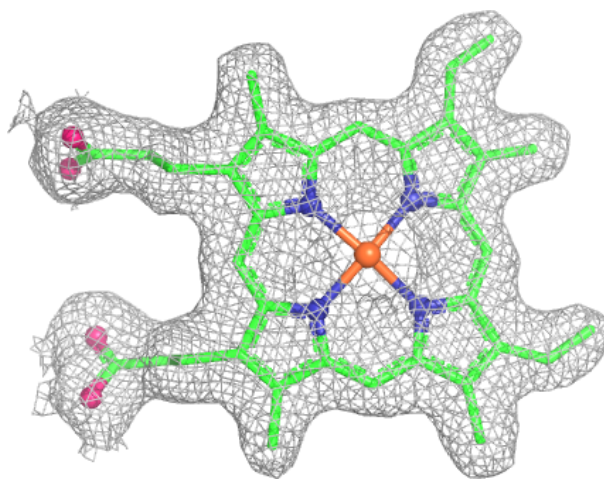
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

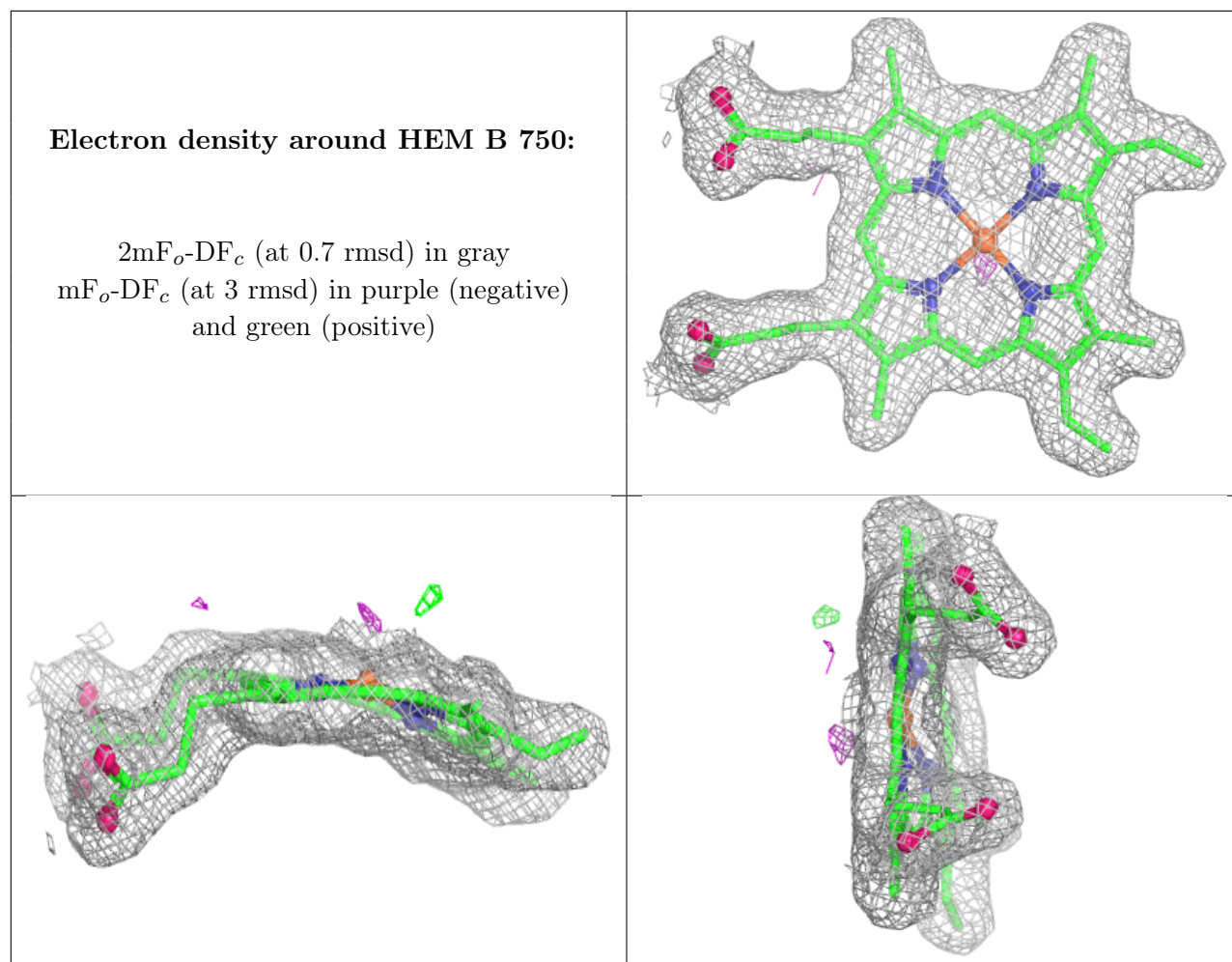
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACT	A	860	4/4	0.91	0.15	51,51,51,52	0
6	JI2	B	800	17/17	0.94	0.08	25,28,37,37	0
5	H4B	A	760	17/17	0.95	0.06	20,25,27,27	0
6	JI2	A	800	17/17	0.95	0.07	24,26,35,37	0
2	ACT	B	860	4/4	0.95	0.07	36,37,37,37	0
5	H4B	B	760	17/17	0.96	0.06	20,24,28,29	0
4	HEM	A	750	43/43	0.98	0.06	18,24,28,29	0
4	HEM	B	750	43/43	0.98	0.06	19,23,29,30	0
3	ZN	A	900	1/1	1.00	0.01	29,29,29,29	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 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 ⓘ

There are no such residues in this entry.