



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:15 AM UTC

PDB ID : 1LZZ / pdb_00001lzz
Title : Rat neuronal NOS heme domain with N-isopropyl-N'-hydroxyguanidine bound
Authors : Li, H.; Shimizu, H.; Flinspach, M.; Jamal, J.; Yang, W.; Xian, M.; Cai, T.; Wen, E.Z.; Jia, Q.; Wang, P.G.; Poulos, T.L.
Deposited on : 2002-06-11
Resolution : 2.05 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

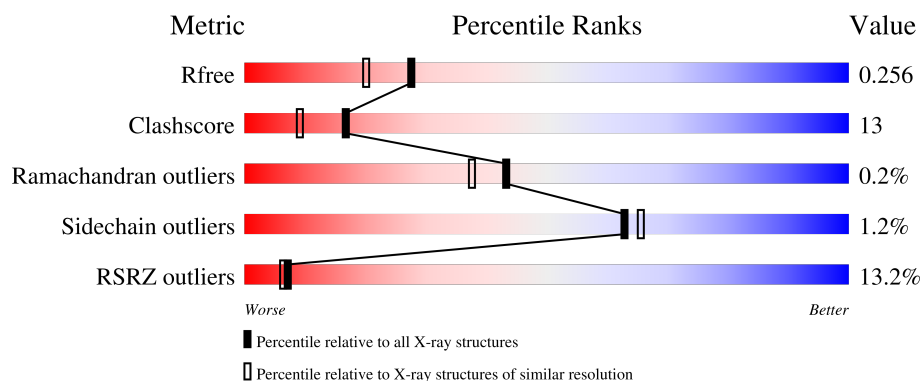
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	419	20% 64% 31% ..
1	B	419	6% 75% 22% ..

2 Entry composition [i](#)

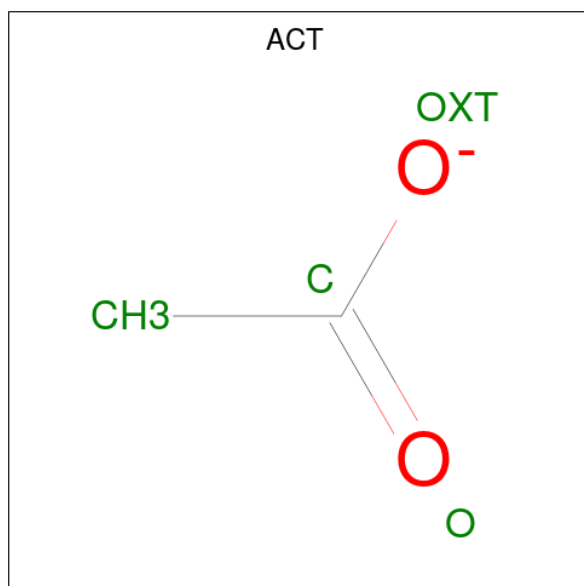
There are 7 unique types of molecules in this entry. The entry contains 7309 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	410	Total	C	N	O	S	0	0	0
			3340	2138	573	608	21			

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

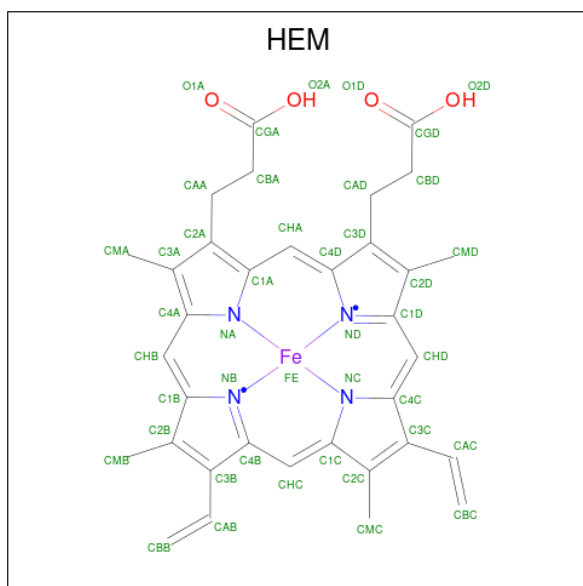


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

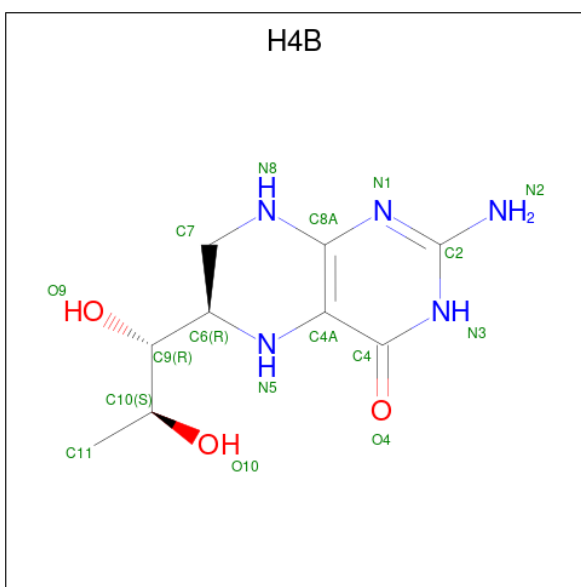
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

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



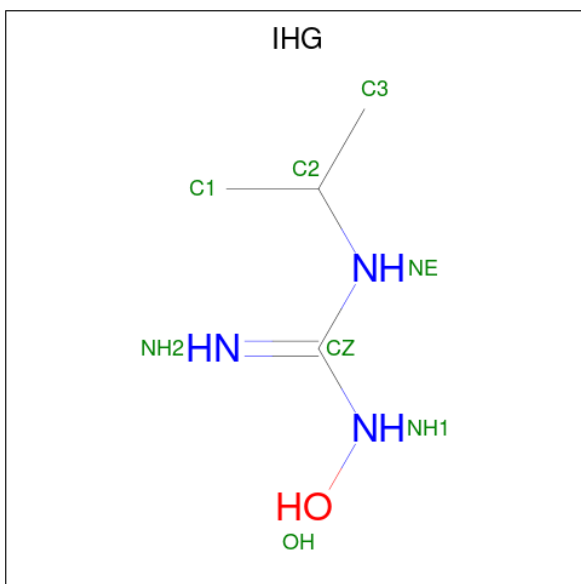
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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-ISOPROPYL-N'-HYDROXYGUANIDINE (CCD ID: IHG) (formula: $C_4H_{11}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			8	4	3	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	217	Total	O	0	0
			217	217		
7	B	294	Total	O	0	0
			294	294		

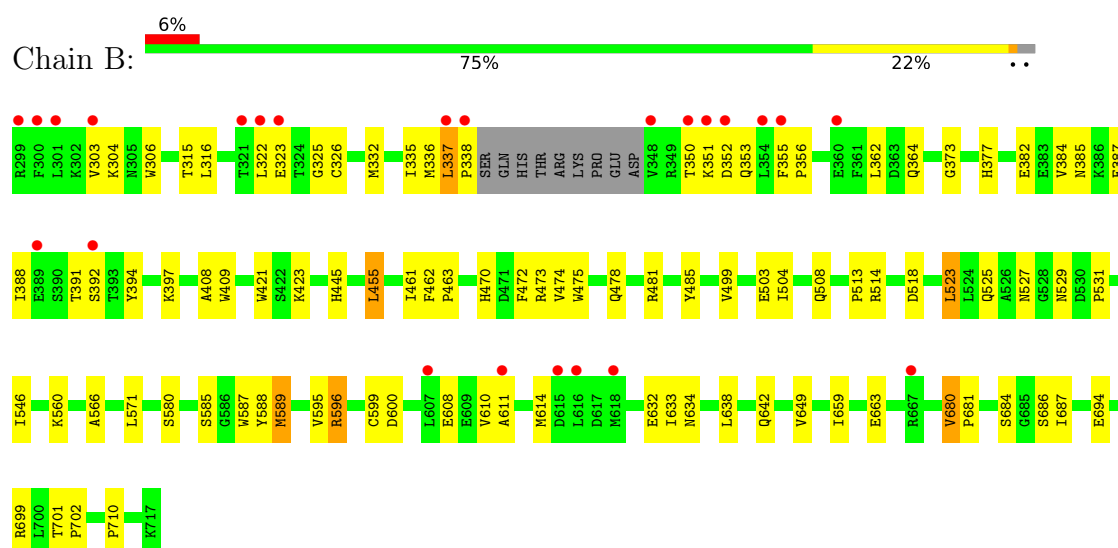
3 Residue-property plots [i](#)

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



• 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	52.02Å 111.11Å 163.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.42 – 2.05 38.42 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.42-2.05) 97.5 (38.42-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.05Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.266 0.219 , 0.256	Depositor DCC
R_{free} test set	2936 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7309	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: IHG, H4B, HEM, 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	0.37	0/3406	0.91	14/4621 (0.3%)
1	B	0.41	0/3433	0.90	15/4656 (0.3%)
All	All	0.39	0/6839	0.91	29/9277 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-8.93	94.69	109.24
1	A	589	MET	N-CA-C	-8.86	94.81	109.07
1	A	421	TRP	N-CA-C	7.39	120.27	111.33
1	A	354	LEU	N-CA-C	7.02	118.62	110.97
1	A	588	TYR	N-CA-C	6.93	119.78	110.35
1	B	596	ARG	N-CA-C	6.62	118.38	111.03
1	A	681	PRO	CA-C-N	6.59	126.73	119.87
1	A	681	PRO	C-N-CA	6.59	126.73	119.87
1	A	680	VAL	CA-C-N	6.56	124.45	119.66
1	A	680	VAL	C-N-CA	6.56	124.45	119.66
1	A	490	GLY	N-CA-C	-6.52	106.94	114.69
1	B	472	PHE	N-CA-C	-6.50	99.09	109.76
1	A	455	LEU	N-CA-C	6.01	118.71	110.24
1	B	455	LEU	N-CA-C	5.91	118.57	110.24
1	B	408	ALA	N-CA-C	-5.88	104.87	111.28
1	A	599	CYS	N-CA-C	5.87	120.60	113.38
1	A	623	SER	N-CA-C	-5.58	106.43	113.18
1	B	588	TYR	N-CA-C	5.44	118.17	110.50
1	B	397	LYS	N-CA-C	-5.39	103.27	110.55
1	B	315	THR	N-CA-C	-5.37	107.38	114.31
1	B	326	CYS	CA-CB-SG	5.37	126.74	114.40
1	B	599	CYS	N-CA-C	5.36	119.97	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	686	SER	N-CA-C	5.34	119.42	113.01
1	A	397	LYS	N-CA-C	-5.25	103.09	110.50
1	B	680	VAL	CA-C-N	5.23	123.48	119.66
1	B	680	VAL	C-N-CA	5.23	123.48	119.66
1	A	688	THR	N-CA-C	-5.23	103.59	110.39
1	B	474	VAL	N-CA-C	-5.23	99.63	107.37
1	B	461	ILE	N-CA-C	5.02	114.80	107.37

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	105	0
1	B	3340	0	3256	69	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	2	0
4	B	43	0	30	2	0
5	A	17	0	15	0	0
5	B	17	0	15	0	0
6	A	8	0	11	0	0
6	B	8	0	11	0	0
7	A	217	0	0	8	0
7	B	294	0	0	7	0
All	All	7309	0	6595	171	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 13.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:LEU:HD22	1:B:531:PRO:HB2	1.51	0.91
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.55	0.87
1:B:373:GLY:H	1:B:377:HIS:HD2	1.25	0.85
1:B:350:THR:HB	1:B:353:GLN:OE1	1.82	0.79
4:B:750:HEM:HMC2	4:B:750:HEM:HBC2	1.64	0.79
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.68	0.74
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.03	0.74
1:B:595:VAL:HG23	1:B:634:ASN:HD21	1.56	0.70
1:B:336:MET:HB3	1:B:337:LEU:HD23	1.73	0.69
1:A:620:LYS:HE3	1:A:622:SER:OG	1.93	0.69
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.08	0.68
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.19	0.67
1:A:595:VAL:HG11	1:A:682:PRO:HB2	1.77	0.66
1:B:382:GLU:HG3	7:B:2087:HOH:O	1.95	0.65
1:A:350:THR:HB	1:A:353:GLN:HG3	1.77	0.65
1:B:337:LEU:HD23	1:B:337:LEU:N	2.12	0.65
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.79	0.64
1:A:307:GLU:HG3	7:B:1925:HOH:O	1.98	0.63
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.81	0.63
1:B:323:GLU:O	1:B:699:ARG:HD3	1.99	0.63
1:A:545:PRO:HG2	1:A:547:ARG:HH11	1.62	0.62
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.15	0.60
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.84	0.60
1:A:516:ARG:HG2	1:A:517:PHE:CE1	2.37	0.59
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.84	0.59
1:A:350:THR:HG22	1:A:352:ASP:H	1.68	0.58
1:B:304:LYS:O	1:B:694:GLU:HG3	2.03	0.58
1:B:332:MET:HE3	1:B:338:PRO:HB2	1.85	0.57
1:B:455:LEU:HD12	1:B:587:TRP:HB3	1.87	0.57
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.40	0.57
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.33	0.57
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.69	0.56
1:B:391:THR:O	1:B:392:SER:HB2	2.05	0.56
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.36	0.56
1:B:325:GLY:O	1:B:332:MET:HE2	2.06	0.56
1:A:627:ASP:O	1:A:631:VAL:HG23	2.05	0.56
1:A:336:MET:HE2	1:B:306:TRP:CG	2.41	0.56
1:B:701:THR:HA	1:B:702:PRO:C	2.31	0.56
1:A:595:VAL:HG23	1:A:634:ASN:HD21	1.71	0.55
1:A:621:THR:HG22	7:A:1062:HOH:O	2.05	0.55
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.87	0.55
1:A:407:HIS:CE1	1:A:410:ARG:HH11	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:LEU:O	1:B:642:GLN:HG3	2.07	0.55
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.23	0.54
1:A:350:THR:HB	1:A:353:GLN:CG	2.38	0.54
1:B:355:PHE:N	1:B:356:PRO:HD2	2.22	0.54
1:A:589:MET:HA	1:A:649:VAL:O	2.08	0.54
1:A:596:ARG:O	1:A:600:ASP:HB2	2.08	0.53
1:A:486:LYS:NZ	1:A:499:VAL:HG11	2.24	0.53
1:A:504:ILE:O	1:A:508:GLN:HB2	2.09	0.53
1:B:504:ILE:O	1:B:508:GLN:HG2	2.09	0.53
1:A:614:MET:CE	1:A:632:GLU:HG3	2.39	0.53
1:B:350:THR:HG22	1:B:352:ASP:H	1.74	0.53
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.39	0.52
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.39	0.52
1:B:499:VAL:O	1:B:503:GLU:HG3	2.10	0.52
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.45	0.52
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.92	0.52
1:B:478:GLN:HB2	1:B:481:ARG:CG	2.40	0.52
1:A:378:MET:HA	1:A:378:MET:HE2	1.91	0.52
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.91	0.52
1:B:608:GLU:HG3	7:B:2080:HOH:O	2.10	0.52
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.25	0.51
1:A:684:SER:O	1:A:687:ILE:HG12	2.10	0.51
1:B:455:LEU:HD12	1:B:587:TRP:CB	2.41	0.51
1:A:682:PRO:HG3	7:A:902:HOH:O	2.09	0.51
1:A:715:VAL:O	1:A:715:VAL:HG23	2.11	0.51
1:A:336:MET:HE2	1:B:306:TRP:CD2	2.46	0.51
1:A:361:PHE:O	1:A:364:GLN:HG2	2.11	0.50
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.26	0.50
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.93	0.50
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.46	0.50
1:A:716:TRP:H	1:A:716:TRP:CD1	2.29	0.50
1:B:373:GLY:H	1:B:377:HIS:CD2	2.16	0.50
1:A:621:THR:HG23	7:A:1064:HOH:O	2.12	0.50
1:B:659:ILE:O	1:B:663:GLU:HG3	2.12	0.50
1:A:510:TRP:HZ2	7:A:977:HOH:O	1.95	0.49
1:A:659:ILE:O	1:A:663:GLU:HG3	2.12	0.49
1:A:675:ASP:O	1:A:679:ILE:HG12	2.12	0.49
1:A:353:GLN:O	1:A:356:PRO:HG2	2.12	0.49
1:A:374:SER:O	1:A:378:MET:HG2	2.12	0.49
1:A:355:PHE:N	1:A:356:PRO:HD2	2.28	0.49
1:B:571:LEU:HD13	1:B:580:SER:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ASP:HA	7:B:2143:HOH:O	2.13	0.49
1:A:467:ASP:OD1	1:A:469:LYS:HB2	2.13	0.49
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.95	0.48
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.96	0.48
1:A:350:THR:HG22	1:A:352:ASP:N	2.27	0.48
1:B:336:MET:HB3	1:B:337:LEU:CD2	2.43	0.48
1:B:351:LYS:HE2	1:B:392:SER:OG	2.14	0.48
1:A:604:TYR:O	1:A:605:ASN:C	2.57	0.48
1:A:714:HIS:ND1	7:A:1095:HOH:O	2.35	0.48
1:A:638:LEU:O	1:A:642:GLN:HG3	2.13	0.48
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.44	0.48
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.49	0.47
1:A:701:THR:HA	1:A:702:PRO:C	2.39	0.47
1:A:524:LEU:O	1:A:531:PRO:HA	2.15	0.47
1:B:462:PHE:HB3	1:B:463:PRO:HD2	1.96	0.47
1:B:699:ARG:HG2	7:B:2048:HOH:O	2.13	0.47
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.97	0.47
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.50	0.47
1:A:350:THR:HB	1:A:353:GLN:CD	2.40	0.46
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.45	0.46
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.30	0.46
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.97	0.46
1:B:388:ILE:O	1:B:392:SER:N	2.38	0.46
1:A:483:ALA:HB2	1:A:520:LEU:CD2	2.45	0.46
1:A:566:ALA:HB2	1:A:585:SER:HB3	1.98	0.46
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.46	0.46
1:B:566:ALA:HB2	1:B:585:SER:HB3	1.99	0.45
1:B:595:VAL:HG23	1:B:634:ASN:ND2	2.29	0.45
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.99	0.45
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.99	0.45
1:A:322:LEU:HB3	1:A:699:ARG:NH1	2.31	0.45
1:A:571:LEU:C	1:A:571:LEU:HD23	2.42	0.44
1:A:323:GLU:O	1:A:699:ARG:HD3	2.16	0.44
1:A:709:ASP:HB2	1:A:712:ASN:ND2	2.32	0.44
1:B:525:GLN:HG3	1:B:529:ASN:O	2.16	0.44
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.53	0.44
1:B:387:GLU:OE2	1:B:394:TYR:HA	2.18	0.44
1:A:462:PHE:HB3	1:A:463:PRO:HD2	1.99	0.44
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.85	0.44
1:B:364:GLN:NE2	7:B:2112:HOH:O	2.50	0.44
1:A:423:LYS:HB3	7:A:1065:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:MET:HE1	1:A:632:GLU:HG3	2.00	0.43
1:B:546:ILE:HG12	1:B:560:LYS:HA	2.00	0.43
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.18	0.43
1:A:610:VAL:O	1:A:614:MET:HG3	2.18	0.43
1:A:551:PHE:CE1	1:A:614:MET:HE3	2.53	0.43
1:A:300:PHE:CD1	1:A:300:PHE:N	2.87	0.43
1:A:415:CYS:HB2	4:A:750:HEM:ND	2.33	0.43
1:A:494:GLY:O	1:A:496:PRO:HD3	2.19	0.43
1:A:549:PRO:HB3	1:A:639:TYR:CD1	2.54	0.43
1:A:630:LEU:HD22	1:B:687:ILE:HD13	2.00	0.43
1:B:596:ARG:O	1:B:600:ASP:HB2	2.19	0.43
1:A:388:ILE:O	1:A:392:SER:N	2.48	0.43
1:B:445:HIS:CD2	1:B:445:HIS:C	2.97	0.43
1:B:684:SER:CB	1:B:687:ILE:HD11	2.44	0.43
1:A:536:ILE:O	1:A:537:PRO:C	2.60	0.42
1:A:549:PRO:HB3	1:A:639:TYR:CE1	2.54	0.42
1:A:502:THR:O	1:A:506:ILE:HG12	2.18	0.42
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.49	0.42
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.54	0.42
1:A:506:ILE:C	1:A:508:GLN:N	2.77	0.42
1:B:614:MET:CE	1:B:632:GLU:HG3	2.50	0.42
1:B:473:ARG:NH2	1:B:710:PRO:HD3	2.34	0.42
1:B:589:MET:HA	1:B:649:VAL:O	2.20	0.42
1:B:337:LEU:N	1:B:337:LEU:CD2	2.80	0.42
1:A:303:VAL:CG1	1:A:694:GLU:O	2.67	0.42
1:A:384:VAL:O	1:A:388:ILE:HG13	2.20	0.41
1:A:610:VAL:HG21	1:A:633:ILE:CD1	2.50	0.41
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.56	0.41
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.85	0.41
1:A:554:PHE:HB3	7:A:953:HOH:O	2.19	0.41
1:B:610:VAL:HG21	1:B:633:ILE:HD11	2.02	0.41
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.55	0.41
1:A:686:SER:HA	1:A:691:PHE:CG	2.55	0.41
1:A:522:LEU:O	1:A:533:LEU:HA	2.21	0.41
1:B:608:GLU:O	1:B:611:ALA:HB3	2.21	0.41
4:B:750:HEM:HBC2	4:B:750:HEM:CMC	2.43	0.41
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.02	0.40
1:A:552:ASP:O	1:A:555:LYS:HG2	2.21	0.40
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.93	0.40
1:A:449:ALA:O	1:A:455:LEU:HA	2.22	0.40
1:A:549:PRO:O	1:A:550:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:MET:HE3	1:B:338:PRO:CB	2.49	0.40
1:A:634:ASN:HB3	7:A:1044:HOH:O	2.21	0.40
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.57	0.40
1:B:304:LYS:NZ	7:B:2140:HOH:O	2.54	0.40
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.36	0.40
1:B:523:LEU:HD23	1:B:523:LEU:HA	1.91	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	403/419 (96%)	375 (93%)	26 (6%)	2 (0%)	24	16
1	B	406/419 (97%)	390 (96%)	16 (4%)	0	100	100
All	All	809/838 (96%)	765 (95%)	42 (5%)	2 (0%)	43	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	605	ASN
1	A	550	LYS

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	363/375 (97%)	359 (99%)	4 (1%)	65	68
1	B	366/375 (98%)	361 (99%)	5 (1%)	59	60
All	All	729/750 (97%)	720 (99%)	9 (1%)	63	65

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	493	LEU
1	A	523	LEU
1	A	527	ASN
1	B	303	VAL
1	B	316	LEU
1	B	337	LEU
1	B	423	LYS
1	B	523	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	HIS
1	A	420	GLN
1	A	425	GLN
1	A	451	ASN
1	A	454	ASN
1	A	500	GLN
1	A	527	ASN
1	A	601	ASN
1	A	605	ASN
1	A	634	ASN
1	A	697	ASN
1	A	707	GLN
1	B	364	GLN
1	B	377	HIS
1	B	407	HIS
1	B	451	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	634	ASN

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Mol	Chain	Res	Type
1	B	664	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	$\# Z > 2$
4	HEM	B	750	1	50,50,50	1.10	3 (6%)	67,82,82	1.02	2 (2%)
6	IHG	A	830	-	6,7,7	1.57	1 (16%)	7,8,8	2.28	1 (14%)
5	H4B	A	760	-	17,18,18	1.68	4 (23%)	14,26,26	2.01	4 (28%)
2	ACT	A	860	-	3,3,3	1.03	0	3,3,3	0.82	0
5	H4B	B	1760	-	17,18,18	1.55	2 (11%)	14,26,26	2.01	4 (28%)
4	HEM	A	750	1	50,50,50	1.19	6 (12%)	67,82,82	1.10	4 (5%)
2	ACT	B	1860	-	3,3,3	1.07	0	3,3,3	0.75	0
6	IHG	B	1830	-	6,7,7	1.74	1 (16%)	7,8,8	2.38	1 (14%)

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	HEM	B	750	1	-	0/14/54/54	-
6	IHG	A	830	-	-	0/4/6/6	-
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	H4B	B	1760	-	-	0/8/17/17	0/2/2/2
4	HEM	A	750	1	-	0/14/54/54	-
6	IHG	B	1830	-	-	0/4/6/6	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	760	H4B	C4A-N5	3.86	1.46	1.37
5	B	1760	H4B	C4A-N5	3.63	1.46	1.37
5	A	760	H4B	C6-N5	3.59	1.53	1.47
6	B	1830	IHG	OH-NH1	-3.43	1.31	1.40
6	A	830	IHG	OH-NH1	-3.14	1.32	1.40
5	B	1760	H4B	C6-N5	3.01	1.52	1.47
4	B	750	HEM	CAB-C3B	-2.61	1.40	1.47
4	A	750	HEM	CAC-C3C	-2.51	1.40	1.47
4	A	750	HEM	FE-ND	2.34	2.02	1.94
4	A	750	HEM	CHD-C4C	2.34	1.42	1.38
5	A	760	H4B	C7-N8	2.31	1.48	1.46
4	A	750	HEM	FE-NB	2.29	2.02	1.94
4	B	750	HEM	CAC-C3C	-2.29	1.41	1.47
4	A	750	HEM	CAB-C3B	-2.25	1.41	1.47
5	A	760	H4B	C4-N3	2.14	1.42	1.38
4	A	750	HEM	CMC-C2C	2.12	1.55	1.50
4	B	750	HEM	C3B-C4B	2.05	1.48	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1830	IHG	C2-NE-CZ	-6.03	112.07	124.06
6	A	830	IHG	C2-NE-CZ	-5.84	112.45	124.06
5	A	760	H4B	C2-N1-C8A	5.26	122.65	113.36
5	B	1760	H4B	C2-N1-C8A	5.15	122.45	113.36
5	B	1760	H4B	O10-C10-C9	-3.27	104.36	109.77
5	A	760	H4B	O10-C10-C9	-3.08	104.67	109.77
5	A	760	H4B	N3-C2-N1	-3.03	117.78	123.32
5	B	1760	H4B	N3-C2-N1	-2.91	117.99	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	750	HEM	C3D-C4D-ND	2.52	112.93	110.17
5	B	1760	H4B	O9-C9-C6	2.50	115.26	109.28
4	A	750	HEM	CHC-C4B-NB	-2.31	121.94	124.42
4	A	750	HEM	CAB-C3B-C2B	-2.24	121.14	128.43
4	B	750	HEM	C3B-C4B-NB	2.16	111.02	109.47
5	A	760	H4B	O9-C9-C6	2.13	114.39	109.28
4	A	750	HEM	CHD-C1D-ND	-2.11	122.15	124.42
4	B	750	HEM	CHB-C1B-C2B	-2.04	121.15	126.95

There are no chirality outliers.

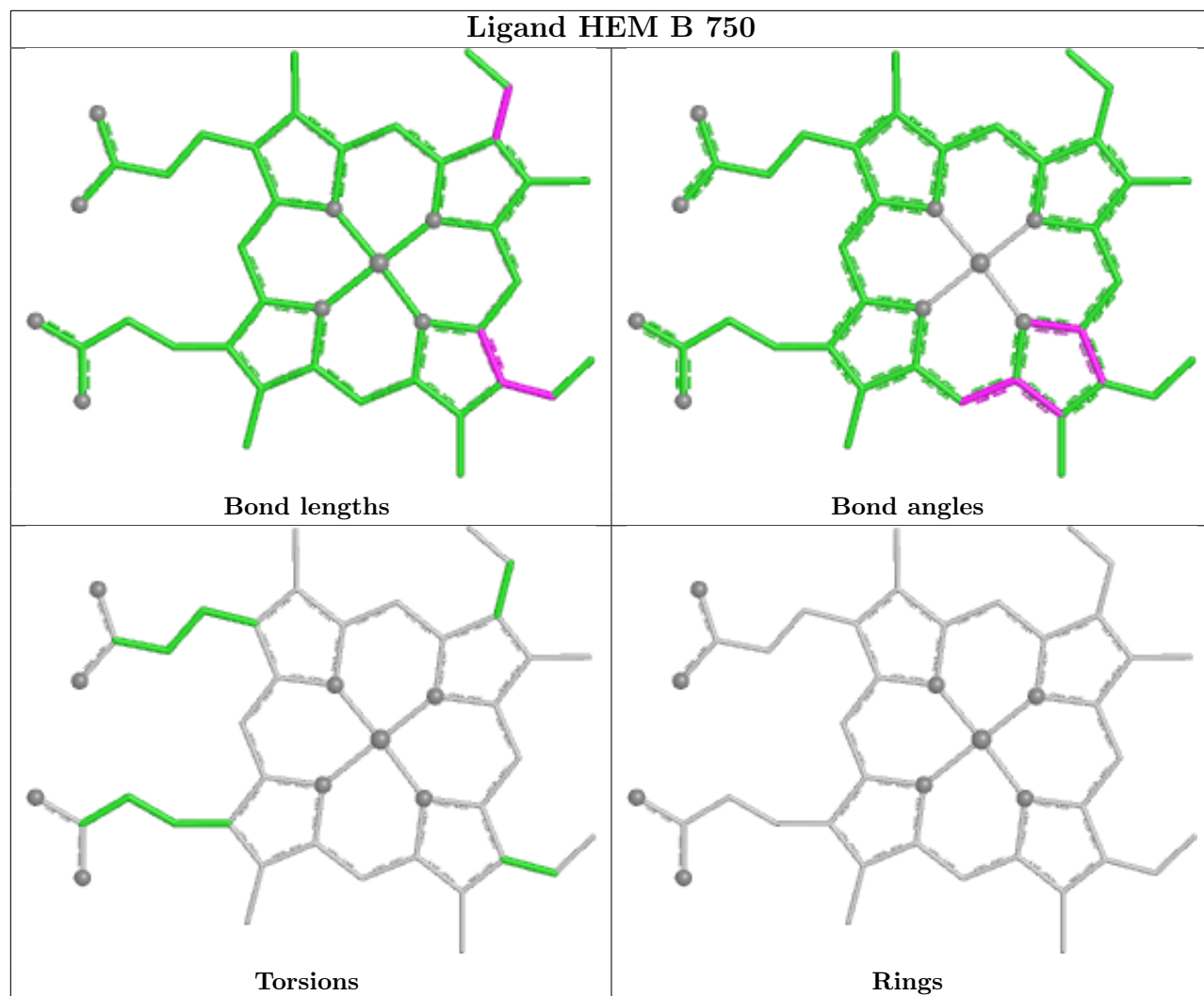
There are no torsion outliers.

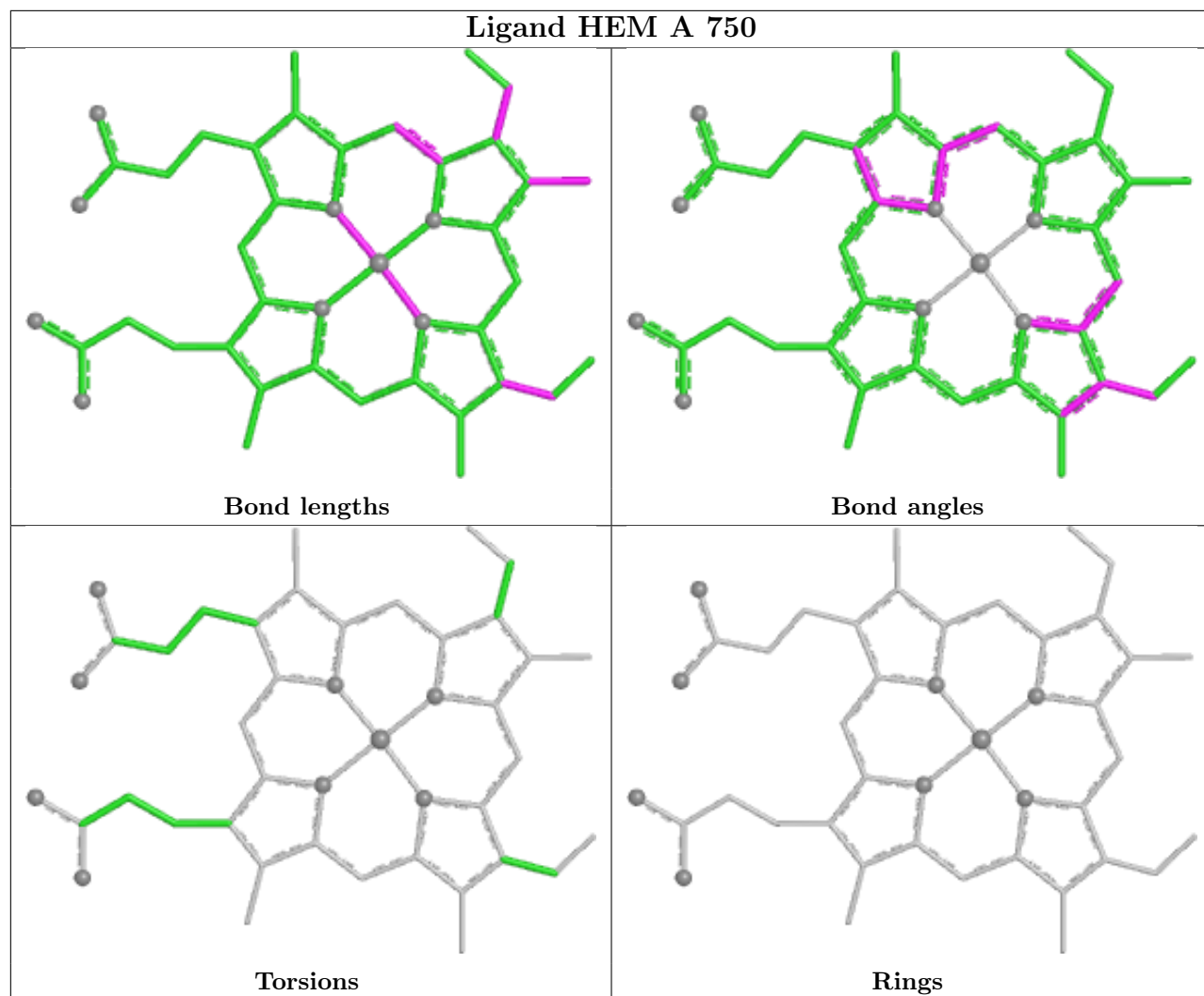
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	750	HEM	2	0
4	A	750	HEM	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.





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	407/419 (97%)	1.01	84 (20%) 2 2	20, 41, 61, 76	0
1	B	410/419 (97%)	0.30	24 (5%) 28 28	19, 30, 52, 65	0
All	All	817/838 (97%)	0.65	108 (13%) 7 6	19, 34, 59, 76	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	554	PHE	4.3
1	A	716	TRP	4.0
1	A	355	PHE	4.0
1	B	300	PHE	3.9
1	A	486	LYS	3.9
1	A	300	PHE	3.8
1	A	513	PRO	3.7
1	A	501	PHE	3.7
1	A	321	THR	3.4
1	B	348	VAL	3.4
1	A	556	ASP	3.4
1	A	715	VAL	3.3
1	A	303	VAL	3.3
1	B	321	THR	3.2
1	A	519	VAL	3.2
1	A	517	PHE	3.1
1	A	373	GLY	3.1
1	A	551	PHE	3.1
1	A	557	LEU	3.1
1	B	350	THR	3.0
1	A	338	PRO	3.0
1	A	301	LEU	3.0
1	A	546	ILE	3.0
1	A	490	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	504	ILE	3.0
1	A	488	PRO	3.0
1	A	510	TRP	3.0
1	A	489	ASP	2.9
1	A	493	LEU	2.9
1	A	558	GLY	2.9
1	A	381	LEU	2.8
1	B	337	LEU	2.8
1	A	485	TYR	2.8
1	A	711	TRP	2.8
1	B	355	PHE	2.8
1	A	506	ILE	2.8
1	A	322	LEU	2.7
1	B	351	LYS	2.7
1	A	354	LEU	2.7
1	A	710	PRO	2.7
1	A	350	THR	2.7
1	A	384	VAL	2.7
1	A	552	ASP	2.7
1	A	553	TRP	2.7
1	B	389	GLU	2.6
1	B	352	ASP	2.6
1	A	337	LEU	2.6
1	A	522	LEU	2.6
1	A	535	GLN	2.6
1	B	354	LEU	2.6
1	A	483	ALA	2.6
1	B	360	GLU	2.5
1	A	533	LEU	2.5
1	A	610	VAL	2.5
1	B	611	ALA	2.5
1	A	559	LEU	2.5
1	B	322	LEU	2.5
1	A	324	THR	2.5
1	A	618	MET	2.5
1	A	492	THR	2.4
1	B	392	SER	2.4
1	B	616	LEU	2.4
1	A	491	SER	2.4
1	B	338	PRO	2.4
1	A	514	ARG	2.4
1	B	299	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	714	HIS	2.4
1	A	482	TYR	2.3
1	A	487	GLN	2.3
1	A	712	ASN	2.3
1	A	523	LEU	2.3
1	B	615	ASP	2.3
1	A	499	VAL	2.3
1	A	544	VAL	2.3
1	A	393	THR	2.3
1	A	502	THR	2.3
1	A	484	GLY	2.3
1	A	520	LEU	2.3
1	A	667	ARG	2.3
1	A	516	ARG	2.3
1	B	667	ARG	2.3
1	A	512	ALA	2.3
1	A	505	CYS	2.2
1	A	614	MET	2.2
1	A	362	LEU	2.2
1	A	528	GLY	2.2
1	A	497	ALA	2.2
1	A	536	ILE	2.2
1	A	515	GLY	2.2
1	A	376	ALA	2.2
1	A	509	GLY	2.1
1	A	318	LEU	2.1
1	A	531	PRO	2.1
1	B	303	VAL	2.1
1	A	524	LEU	2.1
1	B	618	MET	2.1
1	B	323	GLU	2.1
1	A	548	HIS	2.1
1	A	611	ALA	2.1
1	A	378	MET	2.1
1	A	382	GLU	2.1
1	A	555	LYS	2.1
1	A	377	HIS	2.0
1	A	466	THR	2.0
1	B	301	LEU	2.0
1	B	607	LEU	2.0
1	A	352	ASP	2.0
1	A	470	HIS	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](#)

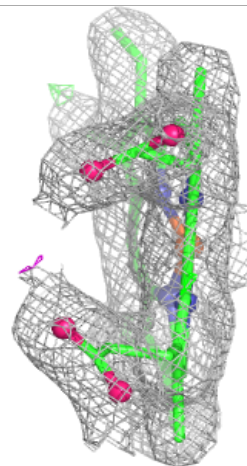
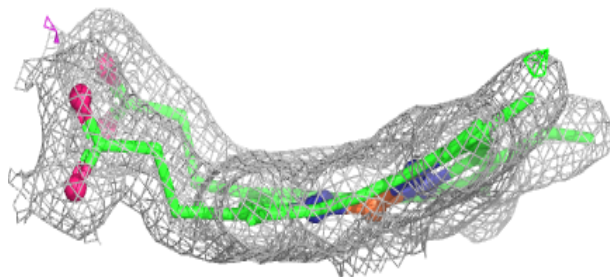
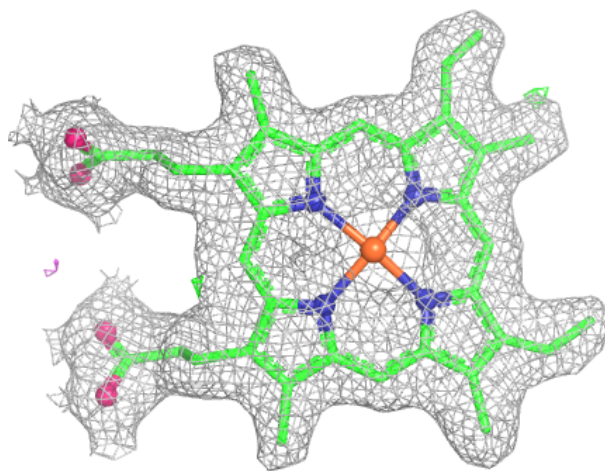
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

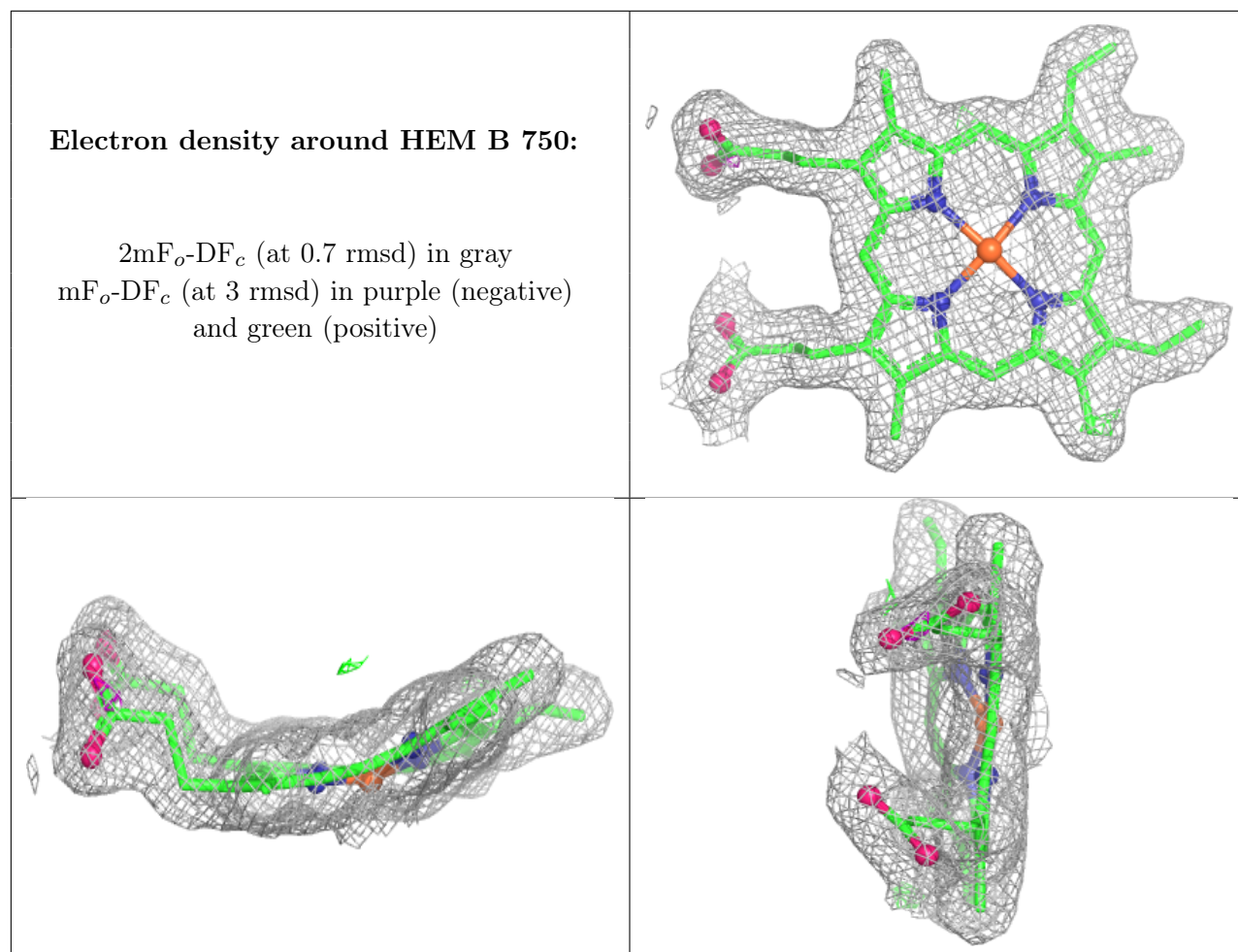
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	IHG	B	1830	8/8	0.84	0.13	32,32,32,33	0
6	IHG	A	830	8/8	0.90	0.10	29,30,30,30	0
2	ACT	A	860	4/4	0.92	0.19	46,46,46,46	0
2	ACT	B	1860	4/4	0.93	0.11	32,32,32,32	0
5	H4B	A	760	17/17	0.94	0.07	25,26,27,28	0
5	H4B	B	1760	17/17	0.96	0.06	19,20,22,22	0
4	HEM	A	750	43/43	0.98	0.06	19,20,21,22	0
4	HEM	B	750	43/43	0.98	0.06	18,20,22,24	0
3	ZN	A	900	1/1	1.00	0.02	33,33,33,33	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 [i](#)

There are no such residues in this entry.