



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:09 PM UTC

PDB ID : 2G6I / pdb_00002g6i
Title : Structure of rat nNOS heme domain (BH2-bound) in the reduced form
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Deposited on : 2006-02-24
Resolution : 1.90 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

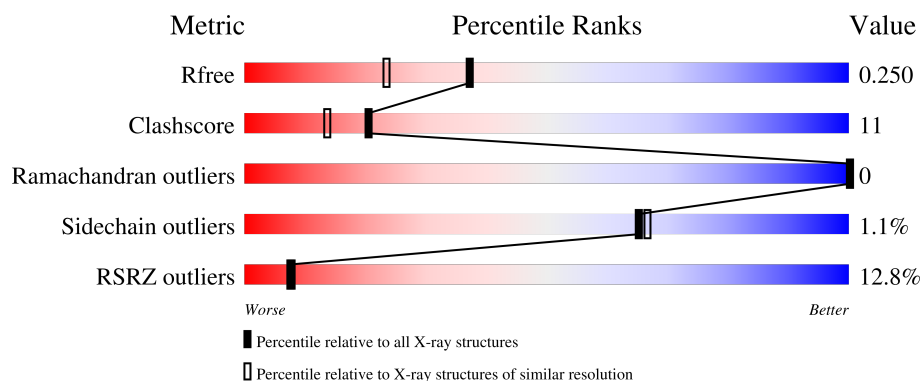
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	420	20% 70% 25% ..
1	B	420	5% 79% 18% ..

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7307 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
			3331	2132	571	607	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: $C_2H_3O_2^-$).

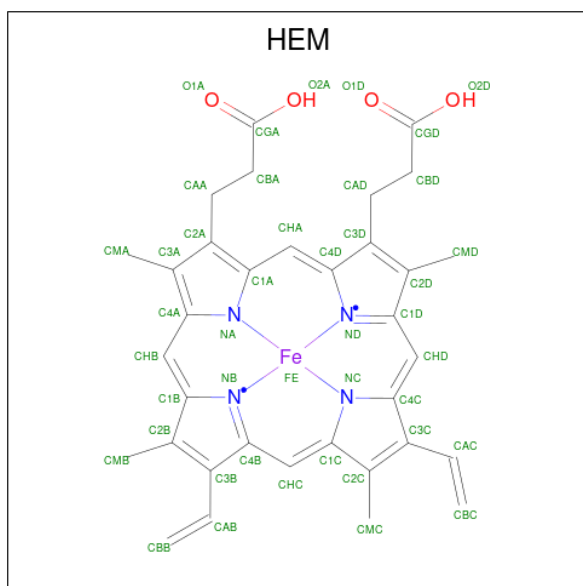


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

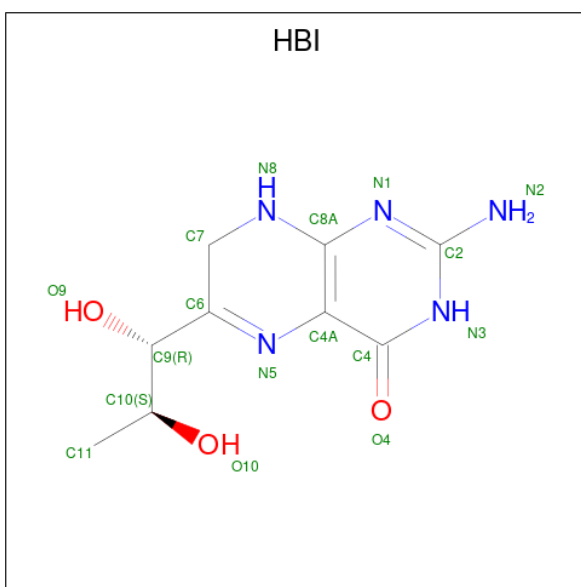
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

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



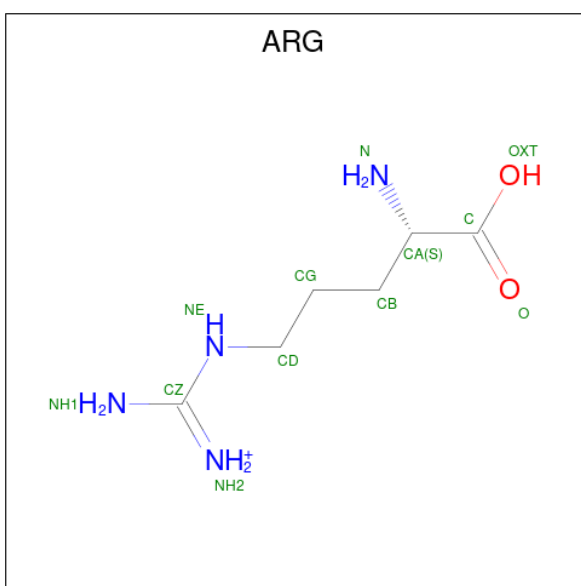
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 7,8-DIHYDROBIOPTERIN (CCD ID: HBI) (formula: $\text{C}_9\text{H}_{13}\text{N}_5\text{O}_3$).



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 ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	6	4	2		
6	B	1	Total	C	N	O	0	0
			12	6	4	2		

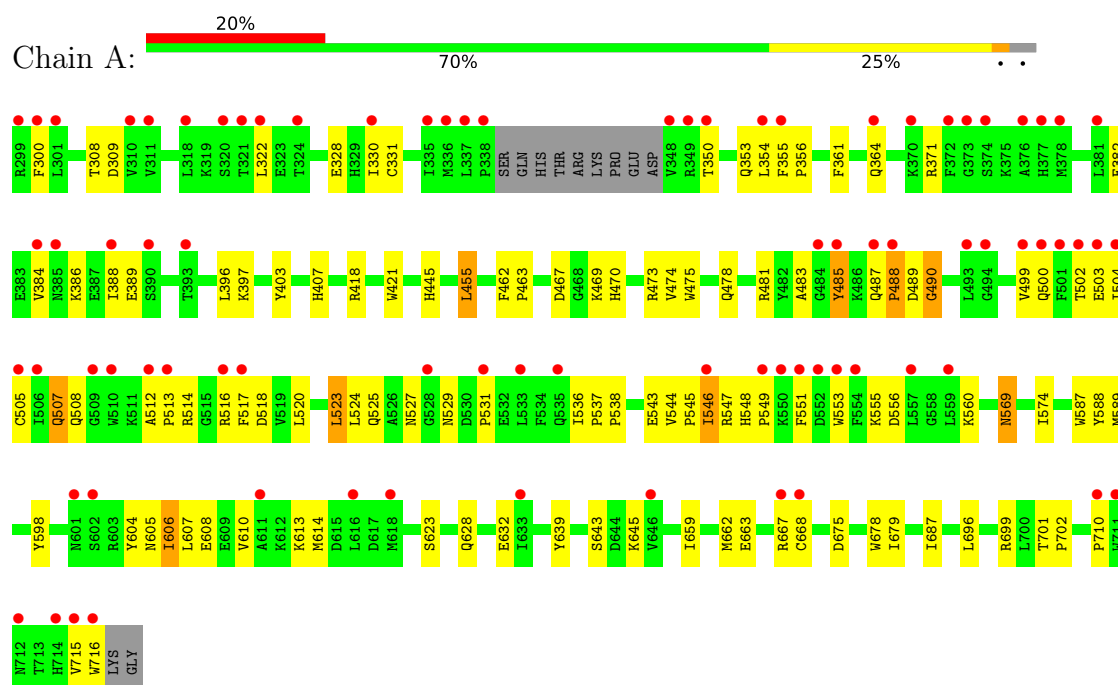
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	204	Total 204	O 204	0	0
7	B	274	Total 274	O 274	0	0

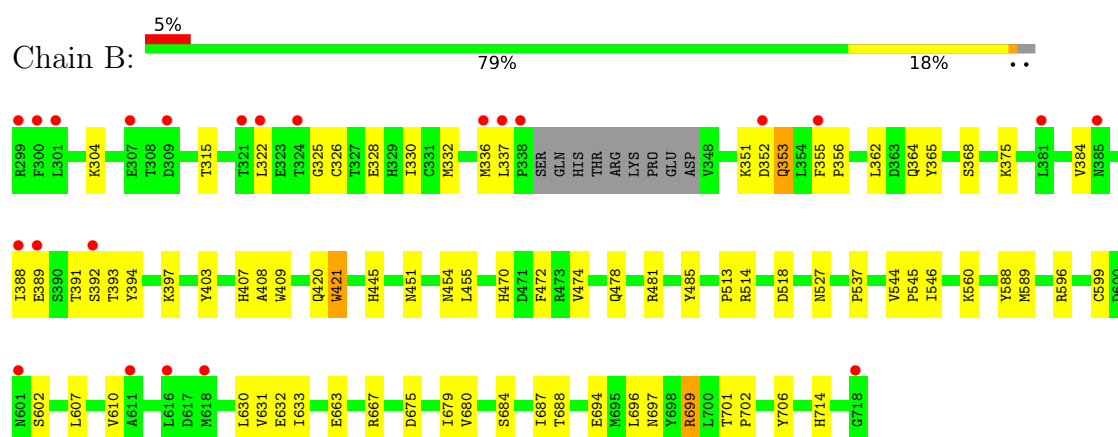
3 Residue-property plots

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, 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	51.60Å 110.58Å 164.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 1.90 49.24 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.24-1.90) 98.8 (49.24-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.263 0.210 , 0.250	Depositor DCC
R_{free} test set	3721 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7307	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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, HBI, ZN, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/3424	0.94	15/4645 (0.3%)
1	B	0.51	0/3438	0.97	18/4661 (0.4%)
All	All	0.49	0/6862	0.96	33/9306 (0.4%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-8.30	95.70	109.24
1	B	680	VAL	CA-C-N	8.29	125.72	119.66
1	B	680	VAL	C-N-CA	8.29	125.72	119.66
1	A	589	MET	N-CA-C	-8.12	96.01	109.24
1	A	588	TYR	N-CA-C	7.05	120.44	110.50
1	B	421	TRP	N-CA-C	6.59	119.31	111.33
1	A	474	VAL	N-CA-C	-6.25	98.73	107.80
1	B	588	TYR	N-CA-C	6.12	119.14	110.50
1	A	606	ILE	N-CA-C	6.03	117.90	112.17
1	B	474	VAL	N-CA-C	-5.97	98.53	107.37
1	A	421	TRP	N-CA-C	5.96	118.54	111.33
1	A	488	PRO	N-CA-C	-5.96	105.76	113.57
1	B	315	THR	N-CA-C	-5.90	106.69	114.31
1	B	455	LEU	N-CA-C	5.76	118.37	110.24
1	B	353	GLN	N-CA-C	5.63	118.36	111.82
1	B	397	LYS	N-CA-C	-5.55	103.06	110.55
1	B	699	ARG	N-CA-C	5.54	117.55	108.52
1	B	688	THR	N-CA-C	-5.52	101.98	110.32
1	A	397	LYS	N-CA-C	-5.43	103.22	110.55
1	A	623	SER	N-CA-C	-5.42	106.63	113.18
1	A	418	ARG	N-CA-C	5.33	119.41	113.01
1	A	546	ILE	N-CA-C	5.32	116.36	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	596	ARG	N-CA-C	5.30	118.08	111.24
1	A	513	PRO	N-CA-C	-5.29	107.86	114.20
1	B	408	ALA	N-CA-C	-5.28	105.52	111.28
1	B	472	PHE	N-CA-C	-5.27	100.66	109.24
1	A	354	LEU	N-CA-C	5.24	116.99	111.28
1	B	599	CYS	N-CA-C	5.17	120.44	113.72
1	A	490	GLY	N-CA-C	-5.15	108.95	115.08
1	B	714	HIS	N-CA-C	5.12	117.73	110.10
1	B	375	LYS	N-CA-C	-5.03	105.88	111.36
1	A	607	LEU	N-CA-C	5.01	116.44	110.97
1	A	455	LEU	N-CA-C	5.01	117.30	110.24

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	3331	0	3243	105	0
1	B	3345	0	3259	50	0
2	A	4	0	3	0	0
2	B	4	0	3	1	0
3	A	1	0	0	0	0
4	A	43	0	30	1	0
4	B	43	0	30	2	0
5	A	17	0	13	1	0
5	B	17	0	13	0	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
7	A	204	0	0	13	0
7	B	274	0	0	6	0
All	All	7307	0	6618	150	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 11.

All (150) 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:602:SER:HB2	7:B:1075:HOH:O	1.61	0.99
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.42	0.97
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.39	0.88
1:A:520:LEU:HD22	7:A:982:HOH:O	1.78	0.82
1:A:549:PRO:HG3	1:A:639:TYR:CG	2.16	0.81
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.63	0.80
1:A:574:ILE:HG22	7:A:1061:HOH:O	1.81	0.80
1:B:699:ARG:HG2	1:B:699:ARG:HH11	1.51	0.74
1:A:699:ARG:HD2	7:A:1043:HOH:O	1.87	0.73
1:A:499:VAL:O	1:A:503:GLU:HG3	1.89	0.72
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.74	0.70
1:A:483:ALA:HA	1:A:520:LEU:HD21	1.74	0.70
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.55	0.69
1:B:355:PHE:HB2	1:B:356:PRO:HD3	1.76	0.67
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.08	0.67
1:A:556:ASP:O	7:A:1098:HOH:O	2.13	0.66
1:B:368:SER:OG	7:B:1071:HOH:O	2.12	0.66
1:A:569:ASN:HD22	1:A:569:ASN:H	1.45	0.65
1:A:355:PHE:HB2	1:A:356:PRO:HD3	1.79	0.64
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.80	0.64
1:A:538:PRO:HD3	7:A:1002:HOH:O	1.98	0.62
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.81	0.62
1:A:610:VAL:O	1:A:614:MET:HG3	1.99	0.62
1:A:545:PRO:HG2	1:A:547:ARG:NH2	2.15	0.61
1:B:364:GLN:NE2	7:B:1086:HOH:O	2.34	0.60
1:A:382:GLU:HG3	1:A:386:LYS:HE3	1.82	0.60
1:A:512:ALA:C	1:A:514:ARG:H	2.08	0.60
1:A:350:THR:OG1	1:A:353:GLN:HG3	2.02	0.59
1:A:716:TRP:H	1:A:716:TRP:CD1	2.21	0.59
1:A:322:LEU:HB2	1:A:699:ARG:HE	1.68	0.58
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.17	0.58
1:A:505:CYS:O	1:A:508:GLN:N	2.37	0.58
1:A:485:TYR:CZ	1:A:514:ARG:HA	2.39	0.57
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.19	0.57
1:A:569:ASN:HD22	1:A:569:ASN:N	2.03	0.57
1:A:687:ILE:HD12	1:B:607:LEU:HD11	1.87	0.56
1:A:483:ALA:CA	1:A:520:LEU:HD21	2.36	0.55
1:B:537:PRO:HA	7:B:978:HOH:O	2.06	0.55
1:B:699:ARG:HG2	1:B:699:ARG:NH1	2.22	0.55
1:A:467:ASP:OD2	1:A:469:LYS:HB2	2.05	0.55
1:A:516:ARG:HD3	1:A:517:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ILE:O	1:A:508:GLN:HG2	2.07	0.55
4:B:750:HEM:HMC1	4:B:750:HEM:HBC2	1.89	0.55
1:B:336:MET:C	1:B:337:LEU:HD23	2.32	0.55
1:A:608:GLU:N	7:A:1100:HOH:O	2.07	0.54
1:B:388:ILE:O	1:B:392:SER:N	2.33	0.54
1:A:485:TYR:OH	1:A:518:ASP:OD2	2.26	0.54
1:A:569:ASN:H	1:A:569:ASN:ND2	2.04	0.54
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.41	0.54
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.33	0.54
1:B:365:TYR:CD1	7:B:1071:HOH:O	2.53	0.53
1:A:396:LEU:HD21	7:A:1061:HOH:O	2.07	0.53
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.90	0.53
1:A:537:PRO:HA	7:A:1002:HOH:O	2.07	0.53
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.90	0.53
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.25	0.52
1:A:353:GLN:O	1:A:356:PRO:HD2	2.10	0.52
1:A:675:ASP:O	1:A:679:ILE:HG12	2.10	0.52
1:A:543:GLU:O	7:A:1096:HOH:O	2.19	0.51
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.92	0.51
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.92	0.51
1:A:512:ALA:C	1:A:514:ARG:N	2.69	0.50
4:B:750:HEM:HBC2	4:B:750:HEM:CMC	2.41	0.50
1:A:553:TRP:O	1:A:556:ASP:HB2	2.11	0.50
1:A:687:ILE:HG13	1:B:630:LEU:HD22	1.92	0.50
1:A:551:PHE:CD2	1:A:551:PHE:N	2.77	0.50
1:A:525:GLN:HG3	1:A:529:ASN:O	2.12	0.50
1:A:614:MET:CE	1:A:632:GLU:HG3	2.42	0.50
1:A:545:PRO:HG2	1:A:547:ARG:HH21	1.76	0.49
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.48	0.49
1:A:322:LEU:HB3	1:A:699:ARG:NH2	2.18	0.49
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.93	0.49
1:A:322:LEU:CB	1:A:699:ARG:HE	2.25	0.49
1:B:393:THR:HG23	1:B:394:TYR:N	2.27	0.48
1:A:507:GLN:OE1	1:A:507:GLN:C	2.57	0.48
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.79	0.48
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.94	0.48
1:B:304:LYS:O	1:B:694:GLU:HG3	2.14	0.48
1:B:336:MET:O	1:B:337:LEU:HD23	2.14	0.48
1:B:352:ASP:HA	7:B:1050:HOH:O	2.13	0.48
1:B:391:THR:O	1:B:392:SER:HB2	2.14	0.48
1:B:445:HIS:C	1:B:445:HIS:CD2	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:THR:HA	1:A:702:PRO:C	2.40	0.47
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.95	0.47
1:A:502:THR:HA	7:A:982:HOH:O	2.14	0.47
1:A:508:GLN:NE2	1:A:508:GLN:HA	2.30	0.47
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.50	0.47
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.45	0.47
1:A:606:ILE:O	1:A:610:VAL:HG23	2.14	0.47
1:B:355:PHE:HZ	1:B:389:GLU:HG2	1.80	0.47
1:A:371:ARG:HG3	1:A:371:ARG:NH2	2.28	0.47
1:A:598:TYR:O	1:A:606:ILE:HG12	2.15	0.47
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.45	0.46
1:A:678:TRP:HA	5:A:760:HBI:N1	2.30	0.46
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.97	0.46
1:B:337:LEU:HD22	1:B:706:TYR:CD1	2.49	0.46
1:A:659:ILE:O	1:A:663:GLU:HG3	2.15	0.46
1:A:445:HIS:C	1:A:445:HIS:CD2	2.94	0.46
1:B:325:GLY:O	1:B:332:MET:HE2	2.16	0.46
1:A:328:GLU:HA	1:B:326:CYS:O	2.16	0.45
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.30	0.45
1:A:536:ILE:O	1:A:537:PRO:C	2.57	0.45
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.45
1:A:549:PRO:HG3	1:A:639:TYR:CD1	2.52	0.45
1:A:553:TRP:CE3	1:A:613:LYS:HD2	2.52	0.45
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.04	0.45
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.32	0.45
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.52	0.45
1:A:488:PRO:C	1:A:490:GLY:H	2.25	0.45
1:A:384:VAL:O	1:A:388:ILE:HG13	2.16	0.45
1:A:361:PHE:O	1:A:364:GLN:HG2	2.16	0.45
1:A:544:VAL:HB	7:A:1059:HOH:O	2.16	0.45
1:A:308:THR:O	1:A:309:ASP:HB2	2.17	0.44
1:A:488:PRO:C	1:A:490:GLY:N	2.75	0.44
1:A:382:GLU:O	1:A:386:LYS:HG3	2.18	0.44
1:A:300:PHE:CD1	1:A:300:PHE:N	2.86	0.44
1:A:569:ASN:N	1:A:569:ASN:ND2	2.65	0.44
1:A:643:SER:OG	7:A:1101:HOH:O	2.21	0.44
1:A:604:TYR:O	1:A:605:ASN:C	2.61	0.44
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.33	0.44
1:A:696:LEU:HB3	1:B:330:ILE:HD11	1.98	0.44
1:A:330:ILE:HD11	1:B:696:LEU:HD22	2.00	0.44
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:VAL:O	1:A:715:VAL:HG13	2.18	0.44
1:A:546:ILE:HG12	1:A:560:LYS:HA	2.00	0.44
1:A:524:LEU:O	1:A:531:PRO:HA	2.18	0.43
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.99	0.43
1:B:675:ASP:O	1:B:679:ILE:HG12	2.18	0.43
1:A:701:THR:OG1	1:A:702:PRO:HA	2.18	0.43
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.07	0.43
1:B:351:LYS:HE3	1:B:392:SER:OG	2.20	0.42
1:B:420:GLN:HG2	2:B:861:ACT:H2	2.00	0.42
1:A:331:CYS:HB3	1:B:697:ASN:HB3	2.02	0.42
1:A:716:TRP:CD1	1:A:716:TRP:N	2.88	0.42
1:B:328:GLU:N	1:B:328:GLU:OE1	2.52	0.41
1:A:614:MET:HE3	1:A:632:GLU:HG3	2.01	0.41
1:B:388:ILE:HA	1:B:393:THR:O	2.21	0.41
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.36	0.41
1:A:483:ALA:CB	1:A:520:LEU:HD21	2.50	0.41
1:A:489:ASP:OD2	1:A:489:ASP:O	2.38	0.41
1:A:555:LYS:N	7:A:1097:HOH:O	2.37	0.41
1:A:508:GLN:CA	1:A:508:GLN:HE21	2.33	0.41
1:B:699:ARG:NH1	1:B:699:ARG:CG	2.83	0.41
1:A:473:ARG:HH22	1:A:710:PRO:HD3	1.84	0.41
1:A:483:ALA:HB2	1:A:520:LEU:CD2	2.51	0.41
1:A:667:ARG:HG3	1:A:668:CYS:N	2.36	0.41
1:B:544:VAL:HA	1:B:545:PRO:HD3	1.90	0.41
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.51	0.40
1:A:500:GLN:O	1:A:504:ILE:HG13	2.21	0.40
1:B:451:ASN:HB3	1:B:454:ASN: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	405/420 (96%)	381 (94%)	24 (6%)	0	100	100
1	B	407/420 (97%)	390 (96%)	17 (4%)	0	100	100
All	All	812/840 (97%)	771 (95%)	41 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/375 (97%)	358 (98%)	7 (2%)	50	47
1	B	366/375 (98%)	365 (100%)	1 (0%)	86	88
All	All	731/750 (98%)	723 (99%)	8 (1%)	65	67

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	GLU
1	A	485	TYR
1	A	507	GLN
1	A	523	LEU
1	A	569	ASN
1	A	645	LYS
1	A	662	MET
1	B	353	GLN

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	425	GLN
1	A	436	HIS
1	A	454	ASN
1	A	508	GLN
1	A	527	ASN

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Mol	Chain	Res	Type
1	A	569	ASN
1	A	697	ASN
1	B	329	HIS
1	B	364	GLN
1	B	385	ASN
1	B	407	HIS
1	B	425	GLN
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 [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 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	ARG	A	770	-	10,11,11	0.88	0	9,13,13	0.46	0
5	HBI	B	761	-	15,18,18	2.47	4 (26%)	14,26,26	1.99	3 (21%)
2	ACT	A	860	-	3,3,3	0.95	0	3,3,3	0.81	0
4	HEM	A	750	1	50,50,50	1.49	9 (18%)	67,82,82	1.07	3 (4%)
6	ARG	B	771	-	10,11,11	0.86	1 (10%)	9,13,13	0.58	0
2	ACT	B	861	-	3,3,3	1.05	0	3,3,3	0.66	0
5	HBI	A	760	-	15,18,18	2.52	4 (26%)	14,26,26	2.07	3 (21%)
4	HEM	B	750	1	50,50,50	1.33	7 (14%)	67,82,82	1.13	4 (5%)

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	ARG	A	770	-	-	1/11/11/11	-
5	HBI	B	761	-	-	0/4/17/17	0/2/2/2
4	HEM	A	750	1	-	0/14/54/54	-
6	ARG	B	771	-	-	1/11/11/11	-
5	HBI	A	760	-	-	0/4/17/17	0/2/2/2
4	HEM	B	750	1	-	0/14/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	760	HBI	C6-N5	7.00	1.39	1.28
5	B	761	HBI	C6-N5	6.41	1.38	1.28
5	B	761	HBI	C7-N8	4.90	1.53	1.45
5	A	760	HBI	C7-N8	4.52	1.52	1.45
4	A	750	HEM	FE-NB	3.84	2.06	1.94
4	A	750	HEM	FE-ND	3.62	2.06	1.94
5	B	761	HBI	C7-C6	2.95	1.53	1.49
4	A	750	HEM	CAB-C3B	-2.85	1.39	1.47
4	B	750	HEM	FE-NA	2.85	2.04	1.95
4	A	750	HEM	CMC-C2C	2.83	1.56	1.50
4	B	750	HEM	FE-ND	2.83	2.03	1.94
5	A	760	HBI	C7-C6	2.79	1.53	1.49
4	B	750	HEM	CAD-C3D	2.77	1.58	1.51
4	B	750	HEM	CHB-C1B	2.62	1.43	1.38
4	A	750	HEM	CHD-C4C	2.61	1.43	1.38
4	A	750	HEM	CHC-C1C	2.51	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	750	HEM	CAB-C3B	-2.48	1.40	1.47
5	A	760	HBI	C4-N3	2.40	1.43	1.38
4	A	750	HEM	CAC-C3C	-2.31	1.41	1.47
4	A	750	HEM	CMA-C3A	2.19	1.55	1.50
4	B	750	HEM	C2A-C3A	-2.18	1.33	1.38
6	B	771	ARG	OXT-C	-2.17	1.23	1.30
5	B	761	HBI	C8A-N1	2.15	1.39	1.36
4	A	750	HEM	FE-NA	2.09	2.02	1.95
4	B	750	HEM	CMB-C2B	2.09	1.55	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	760	HBI	C2-N1-C8A	5.68	123.39	113.36
5	B	761	HBI	C2-N1-C8A	5.39	122.87	113.36
5	A	760	HBI	N3-C2-N1	-3.23	117.41	123.32
4	A	750	HEM	CBD-CAD-C3D	-3.16	103.80	112.53
4	B	750	HEM	CBA-CAA-C2A	-3.00	104.24	112.53
5	B	761	HBI	N3-C2-N1	-2.99	117.84	123.32
4	B	750	HEM	C4C-C3C-C2C	-2.58	104.57	106.81
4	A	750	HEM	C3C-C2C-C1C	-2.54	104.64	107.05
5	A	760	HBI	C4A-N5-C6	2.41	121.26	116.08
5	B	761	HBI	C4A-N5-C6	2.37	121.17	116.08
4	A	750	HEM	CAB-C3B-C2B	-2.23	121.17	128.43
4	B	750	HEM	C4D-C3D-C2D	-2.23	103.65	106.89
4	B	750	HEM	CBD-CAD-C3D	-2.15	106.58	112.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	770	ARG	O-C-CA-N
6	B	771	ARG	O-C-CA-N

There are no ring outliers.

4 monomers are involved in 5 short contacts:

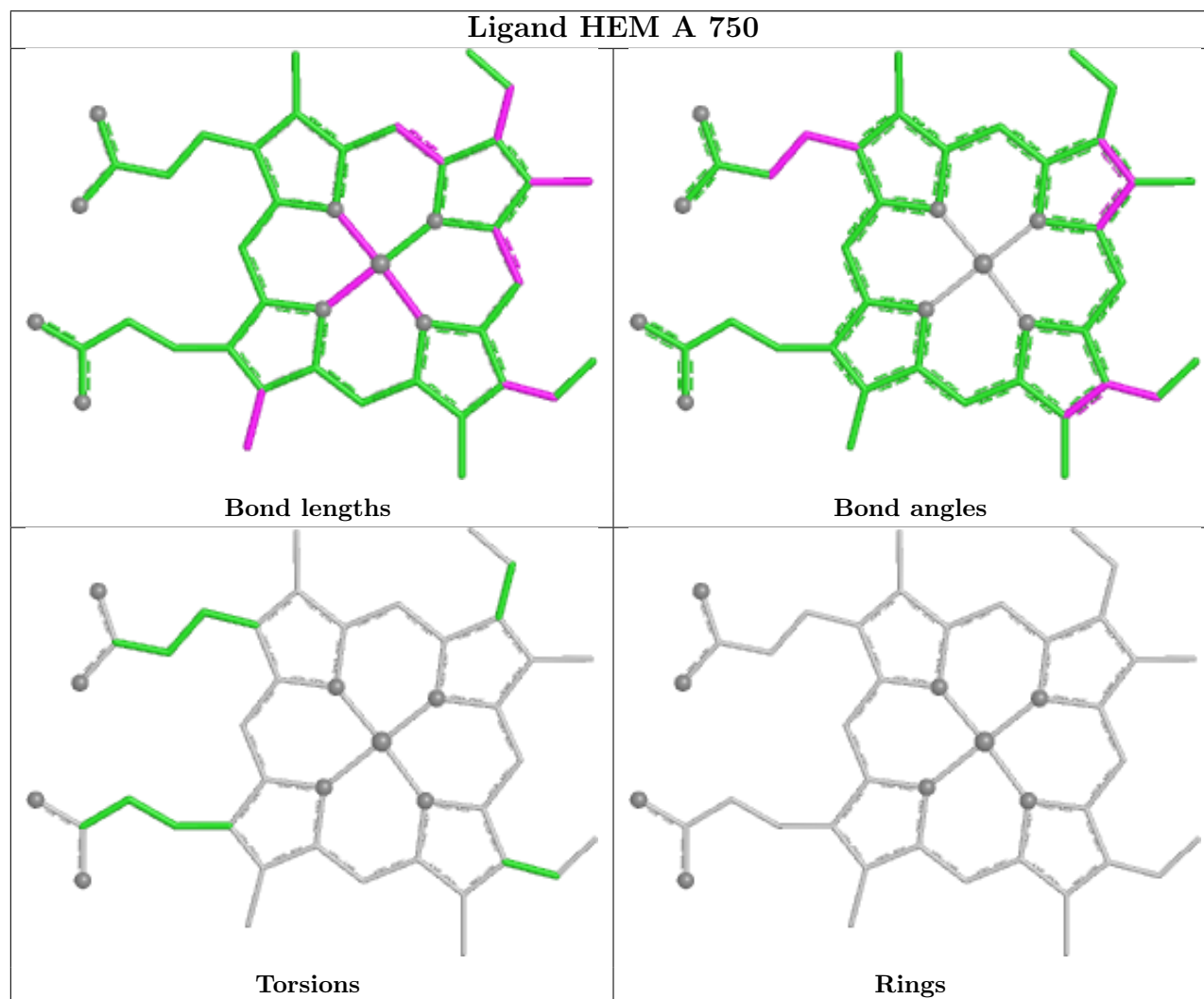
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	750	HEM	1	0
2	B	861	ACT	1	0
5	A	760	HBI	1	0

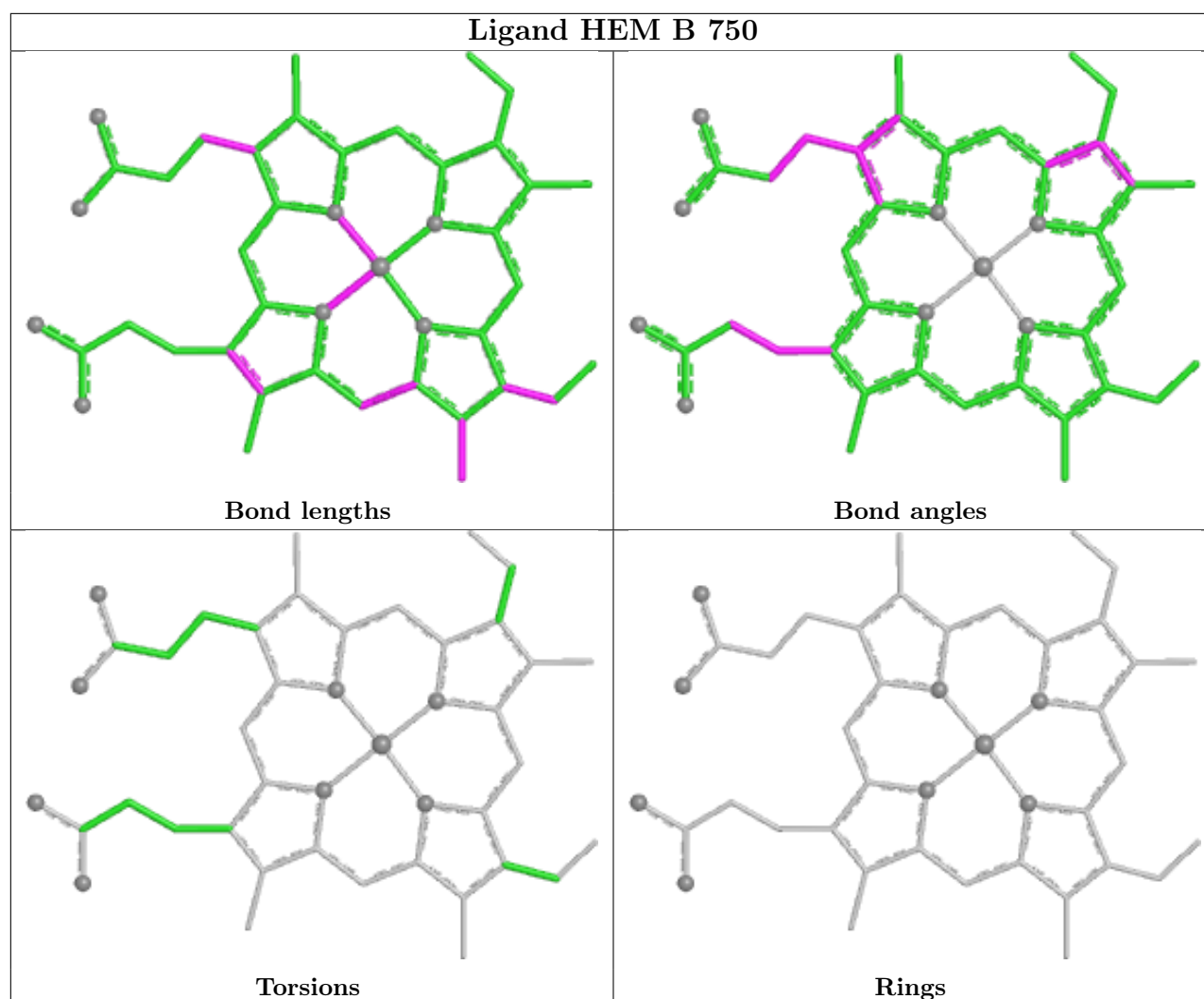
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	750	HEM	2	0

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	409/420 (97%)	1.03	82 (20%) 3 2	21, 42, 68, 83	0
1	B	411/420 (97%)	0.38	23 (5%) 30 32	22, 33, 55, 72	0
All	All	820/840 (97%)	0.71	105 (12%) 7 8	21, 37, 64, 83	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	5.3
1	A	300	PHE	5.0
1	A	506	ILE	4.3
1	B	321	THR	4.2
1	A	493	LEU	4.2
1	A	554	PHE	4.1
1	A	372	PHE	4.1
1	A	551	PHE	4.0
1	A	711	TRP	4.0
1	B	338	PRO	3.9
1	A	338	PRO	3.9
1	A	384	VAL	3.9
1	B	322	LEU	3.8
1	A	716	TRP	3.8
1	B	718	GLY	3.7
1	B	300	PHE	3.5
1	B	337	LEU	3.5
1	A	373	GLY	3.4
1	A	348	VAL	3.4
1	A	512	ALA	3.4
1	A	710	PRO	3.3
1	A	310	VAL	3.2
1	A	488	PRO	3.2
1	A	712	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	355	PHE	3.2
1	A	505	CYS	3.1
1	A	321	THR	3.1
1	A	535	GLN	3.0
1	A	715	VAL	3.0
1	A	354	LEU	3.0
1	A	299	ARG	3.0
1	A	510	TRP	3.0
1	A	503	GLU	3.0
1	A	320	SER	2.9
1	B	355	PHE	2.9
1	A	381	LEU	2.9
1	A	528	GLY	2.9
1	A	501	PHE	2.9
1	B	611	ALA	2.9
1	A	385	ASN	2.8
1	A	667	ARG	2.8
1	A	553	TRP	2.8
1	A	557	LEU	2.8
1	A	485	TYR	2.7
1	B	352	ASP	2.7
1	B	385	ASN	2.7
1	A	376	ALA	2.7
1	A	616	LEU	2.7
1	B	616	LEU	2.7
1	A	301	LEU	2.6
1	A	324	THR	2.6
1	A	550	LYS	2.6
1	A	318	LEU	2.6
1	A	337	LEU	2.5
1	A	601	ASN	2.5
1	A	611	ALA	2.5
1	A	517	PHE	2.5
1	A	502	THR	2.5
1	A	509	GLY	2.4
1	A	330	ILE	2.4
1	A	513	PRO	2.4
1	A	336	MET	2.4
1	A	370	LYS	2.4
1	A	335	ILE	2.4
1	A	388	ILE	2.4
1	A	668	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	559	LEU	2.4
1	A	552	ASP	2.4
1	A	350	THR	2.4
1	A	499	VAL	2.3
1	A	349	ARG	2.3
1	A	533	LEU	2.3
1	B	601	ASN	2.3
1	A	393	THR	2.3
1	A	531	PRO	2.3
1	A	504	ILE	2.3
1	A	633	ILE	2.3
1	B	389	GLU	2.3
1	A	487	GLN	2.3
1	A	549	PRO	2.2
1	A	364	GLN	2.2
1	A	618	MET	2.2
1	A	546	ILE	2.2
1	A	516	ARG	2.2
1	B	301	LEU	2.2
1	B	392	SER	2.2
1	B	388	ILE	2.2
1	A	377	HIS	2.2
1	A	714	HIS	2.2
1	B	309	ASP	2.2
1	A	602	SER	2.1
1	A	494	GLY	2.1
1	B	381	LEU	2.1
1	B	324	THR	2.1
1	B	336	MET	2.1
1	B	618	MET	2.1
1	A	311	VAL	2.1
1	A	374	SER	2.0
1	A	390	SER	2.0
1	A	500	GLN	2.0
1	B	299	ARG	2.0
1	B	307	GLU	2.0
1	A	378	MET	2.0
1	A	484	GLY	2.0
1	A	646	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

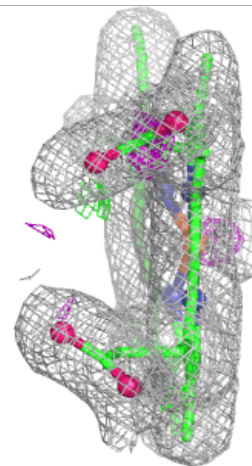
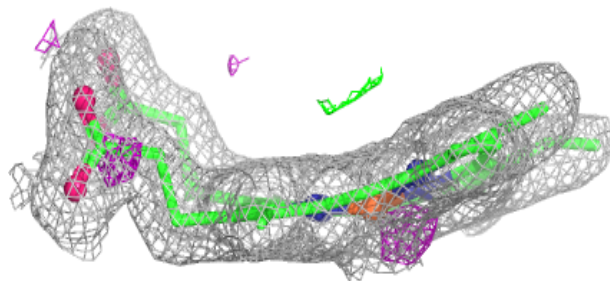
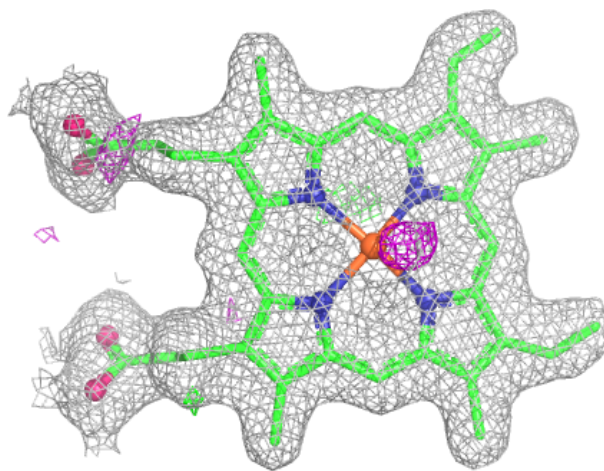
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	861	4/4	0.86	0.17	51,51,51,52	0
2	ACT	A	860	4/4	0.89	0.14	55,57,57,58	0
6	ARG	A	770	12/12	0.94	0.07	24,27,29,30	0
6	ARG	B	771	12/12	0.96	0.06	22,24,27,29	0
5	HBI	A	760	17/17	0.97	0.05	22,24,32,32	0
5	HBI	B	761	17/17	0.97	0.05	21,23,30,30	0
4	HEM	A	750	43/43	0.98	0.06	21,25,27,30	0
4	HEM	B	750	43/43	0.98	0.06	20,24,28,34	0
3	ZN	A	900	1/1	0.99	0.08	37,37,37,37	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.

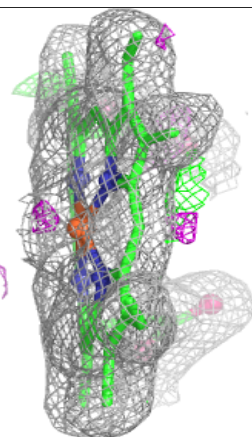
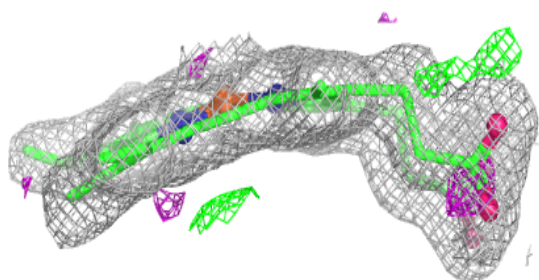
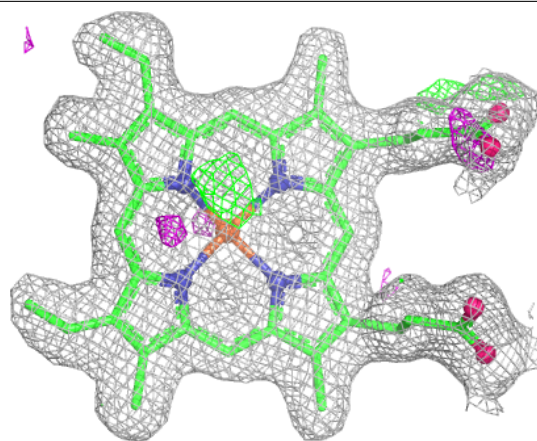
Electron density around HEM A 750:

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



Electron density around HEM B 750:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.