



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:58 AM UTC

PDB ID : 2G6H / pdb_00002g6h
Title : Structure of rat nNOS heme domain (BH4 bound) in the reduced form
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Deposited on : 2006-02-24
Resolution : 2.00 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

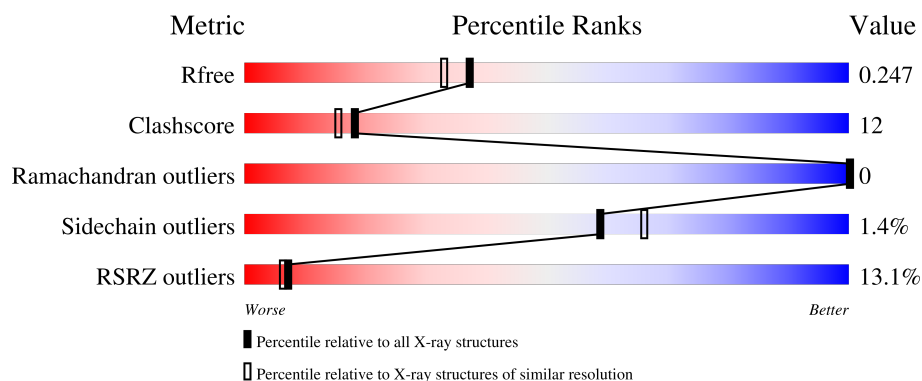
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	
1	B	420	

2 Entry composition [i](#)

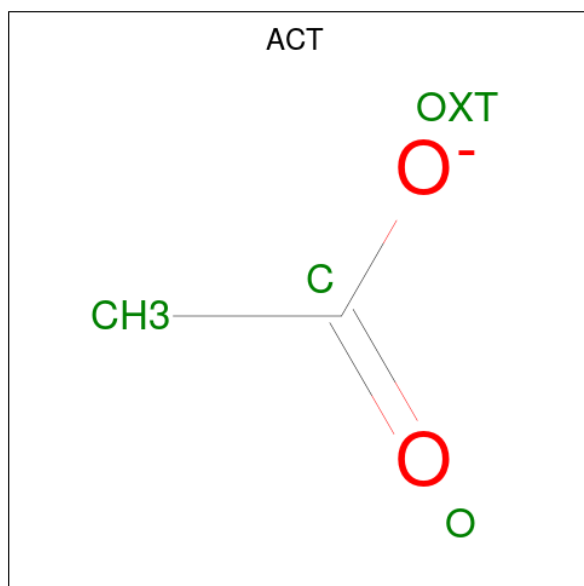
There are 7 unique types of molecules in this entry. The entry contains 7242 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	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: $C_2H_3O_2^-$).

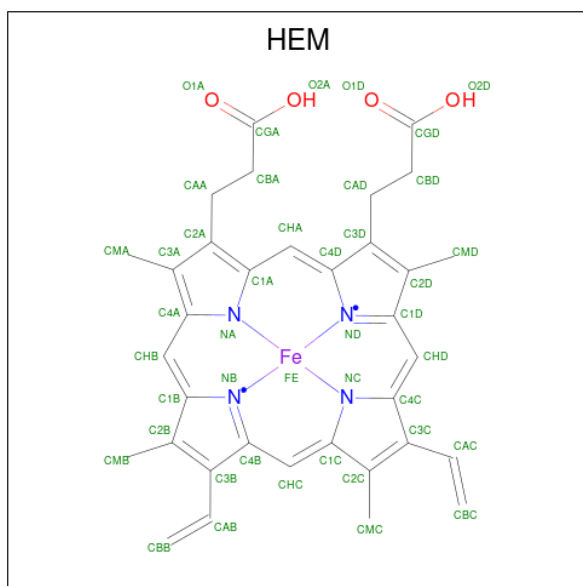


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

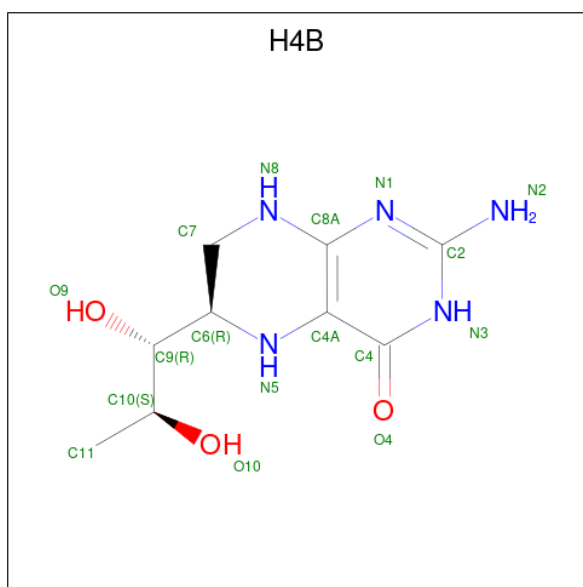
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

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



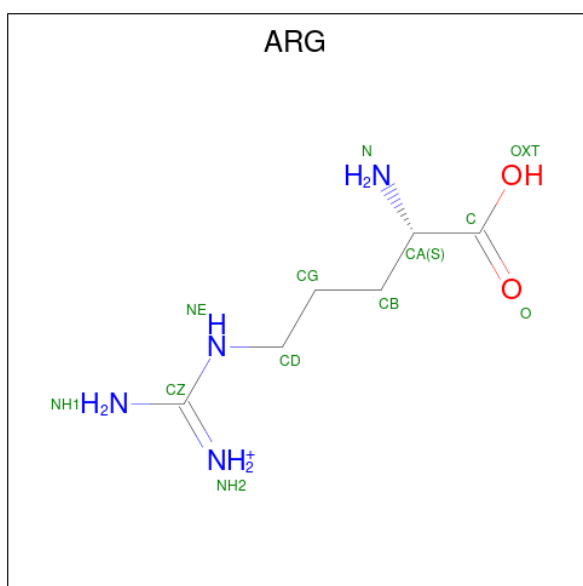
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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 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		

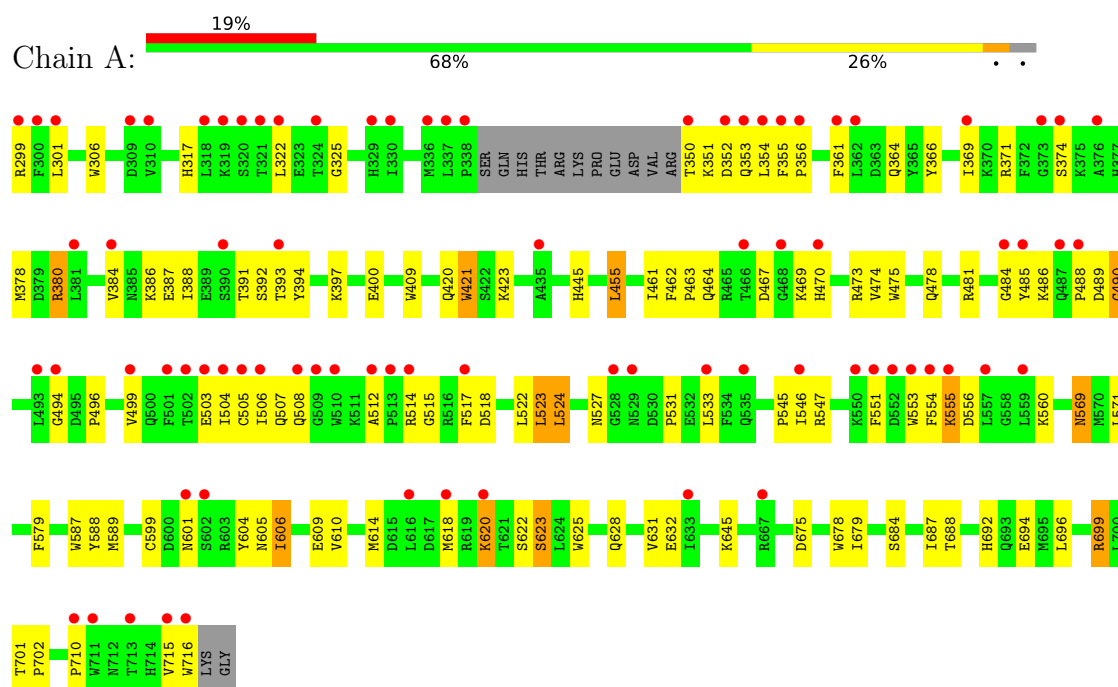
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	170	Total 170	O 170	0	0
7	B	261	Total 261	O 261	0	0

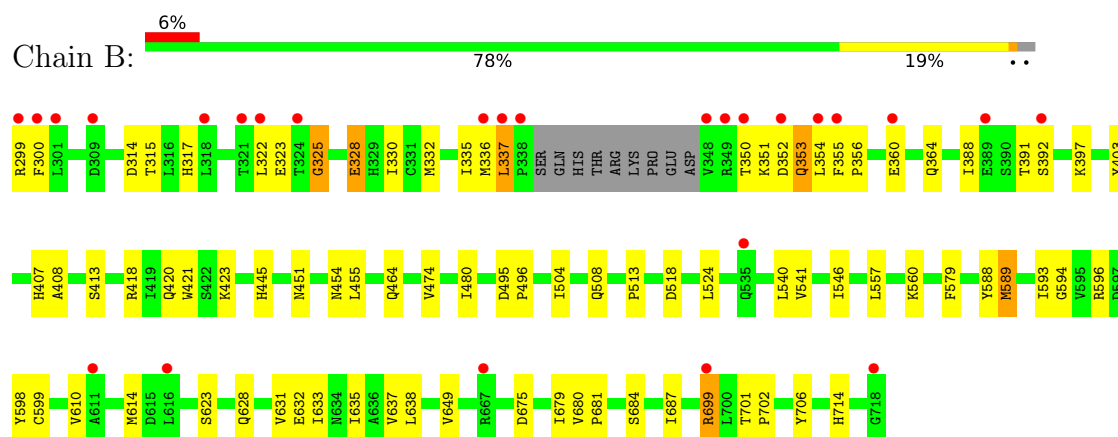
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric-oxide synthase, brain



- Molecule 1: Nitric-oxide synthase, brain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.80Å 110.96Å 164.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 2.00 49.13 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.13-2.00) 97.8 (49.13-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.256 0.210 , 0.247	Depositor DCC
R_{free} test set	3370 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7242	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 4.84% 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: 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	0.46	0/3406	0.97	16/4621 (0.3%)
1	B	0.51	0/3438	0.98	20/4661 (0.4%)
All	All	0.48	0/6844	0.98	36/9282 (0.4%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	N-CA-C	8.35	120.16	111.14
1	B	589	MET	N-CA-C	-8.22	95.85	109.24
1	A	606	ILE	N-CA-C	8.12	119.89	112.17
1	A	589	MET	N-CA-C	-8.06	96.10	109.24
1	A	397	LYS	N-CA-C	-7.58	101.09	110.41
1	B	421	TRP	N-CA-C	7.06	119.88	111.33
1	A	688	THR	N-CA-C	-6.84	101.50	110.39
1	A	588	TYR	N-CA-C	6.82	120.11	110.50
1	B	474	VAL	N-CA-C	-6.79	97.96	107.80
1	B	354	LEU	N-CA-C	6.46	118.20	111.03
1	B	599	CYS	N-CA-C	6.41	121.89	113.30
1	B	455	LEU	N-CA-C	6.32	119.40	110.23
1	A	421	TRP	N-CA-C	6.21	118.85	111.33
1	B	596	ARG	N-CA-C	6.19	117.90	111.03
1	A	599	CYS	N-CA-C	5.94	120.69	113.38
1	B	588	TYR	N-CA-C	5.88	119.19	110.48
1	B	325	GLY	N-CA-C	-5.87	106.97	114.37
1	A	325	GLY	N-CA-C	-5.77	107.10	114.37
1	B	699	ARG	N-CA-C	5.72	118.05	108.73
1	B	623	SER	N-CA-C	-5.68	106.31	113.18
1	A	474	VAL	N-CA-C	-5.66	99.73	107.99
1	B	524	LEU	N-CA-C	5.55	118.01	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	623	SER	N-CA-C	-5.51	106.51	113.18
1	B	397	LYS	N-CA-C	-5.51	103.11	110.55
1	B	408	ALA	N-CA-C	-5.45	105.34	111.28
1	A	461	ILE	N-CA-C	5.42	115.39	107.37
1	B	714	HIS	N-CA-C	5.34	118.06	110.10
1	B	413	SER	N-CA-C	5.32	117.83	111.71
1	A	699	ARG	N-CA-C	5.32	117.40	108.73
1	A	455	LEU	N-CA-C	5.23	117.81	110.23
1	A	490	GLY	N-CA-C	-5.19	107.35	114.67
1	B	315	THR	N-CA-C	-5.18	107.62	114.31
1	B	557	LEU	N-CA-C	-5.12	106.98	113.18
1	B	594	GLY	N-CA-C	5.02	118.75	112.73
1	B	418	ARG	N-CA-C	5.01	119.02	113.01
1	A	524	LEU	N-CA-C	5.01	117.97	109.76

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	107	0
1	B	3345	0	3259	66	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	0	0
5	A	17	0	15	1	0
5	B	17	0	15	0	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
7	A	170	0	0	7	0
7	B	261	0	0	10	0
All	All	7242	0	6600	162	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 (162) 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	1.46	0.97
1:B:638:LEU:HD12	7:B:1057:HOH:O	1.74	0.87
1:B:593:ILE:HG22	7:B:1003:HOH:O	1.78	0.84
1:B:350:THR:HG22	1:B:352:ASP:H	1.49	0.77
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.65	0.76
1:B:356:PRO:O	1:B:360:GLU:HG3	1.85	0.76
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.50	0.76
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.72	0.72
1:A:555:LYS:NZ	1:A:555:LYS:HB3	2.04	0.72
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.72	0.72
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.53	0.71
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.06	0.71
1:B:635:ILE:HA	7:B:1057:HOH:O	1.90	0.71
1:B:699:ARG:HG2	7:B:1019:HOH:O	1.91	0.70
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.06	0.69
1:A:546:ILE:HG12	1:A:560:LYS:HA	1.73	0.68
1:A:609:GLU:HG3	7:A:969:HOH:O	1.92	0.68
1:A:545:PRO:HG2	1:A:547:ARG:NH2	2.09	0.68
1:B:637:VAL:HG21	7:B:1003:HOH:O	1.96	0.66
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.78	0.65
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.13	0.64
1:A:692:HIS:ND1	7:A:1068:HOH:O	2.30	0.64
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.80	0.62
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.15	0.61
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.27	0.61
1:A:467:ASP:OD2	1:A:469:LYS:HB2	2.00	0.61
1:A:696:LEU:HD22	1:B:330:ILE:CD1	2.31	0.61
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.25	0.61
1:A:716:TRP:H	1:A:716:TRP:CD1	2.18	0.60
1:A:555:LYS:HB3	1:A:555:LYS:HZ3	1.65	0.60
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.37	0.60
1:A:545:PRO:HG2	1:A:547:ARG:HH21	1.64	0.60
1:A:605:ASN:ND2	7:A:1052:HOH:O	2.24	0.60
1:A:506:ILE:C	1:A:508:GLN:H	2.09	0.58
1:A:601:ASN:HB2	7:A:1053:HOH:O	2.04	0.57
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.34	0.57
1:B:323:GLU:O	1:B:699:ARG:HD3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ARG:HB3	1:B:299:ARG:HH11	1.68	0.56
1:A:610:VAL:O	1:A:614:MET:HG3	2.06	0.56
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.87	0.56
1:B:684:SER:HB3	1:B:687:ILE:HG12	1.87	0.55
1:A:553:TRP:O	1:A:556:ASP:HB2	2.07	0.55
1:A:524:LEU:O	1:A:531:PRO:HA	2.07	0.55
1:A:499:VAL:O	1:A:503:GLU:HG3	2.06	0.54
1:A:393:THR:OG1	1:A:394:TYR:N	2.40	0.54
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.89	0.54
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.89	0.54
1:B:351:LYS:HE2	1:B:392:SER:OG	2.08	0.54
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.43	0.53
1:A:350:THR:HB	1:A:353:GLN:CD	2.33	0.53
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.73	0.53
1:A:675:ASP:O	1:A:679:ILE:HG12	2.08	0.53
1:B:675:ASP:O	1:B:679:ILE:HG12	2.09	0.53
1:B:355:PHE:N	1:B:356:PRO:HD2	2.24	0.53
1:A:371:ARG:HH21	1:A:371:ARG:CG	2.22	0.52
1:A:355:PHE:N	1:A:356:PRO:HD2	2.24	0.52
1:A:506:ILE:C	1:A:508:GLN:N	2.65	0.52
1:A:420:GLN:OE1	1:A:423:LYS:HE2	2.10	0.52
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.25	0.52
1:B:350:THR:O	1:B:353:GLN:HG2	2.10	0.52
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.10	0.51
1:A:350:THR:HG22	1:A:352:ASP:H	1.74	0.51
1:A:374:SER:O	1:A:378:MET:HG2	2.11	0.51
1:A:322:LEU:CB	1:A:699:ARG:HE	2.23	0.50
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.92	0.50
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.94	0.50
1:B:420:GLN:HG2	2:B:861:ACT:H2	1.94	0.50
1:A:350:THR:HB	1:A:353:GLN:CG	2.41	0.50
1:B:388:ILE:O	1:B:392:SER:N	2.41	0.50
1:A:618:MET:HE3	1:A:625:TRP:CZ3	2.47	0.50
1:A:489:ASP:OD2	1:A:489:ASP:O	2.30	0.49
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.47	0.49
1:B:355:PHE:HB2	7:B:1001:HOH:O	2.11	0.49
1:B:445:HIS:C	1:B:445:HIS:CD2	2.91	0.49
1:A:504:ILE:O	1:A:508:GLN:HG2	2.13	0.49
1:A:678:TRP:HA	5:A:760:H4B:N1	2.28	0.48
1:B:328:GLU:H	1:B:328:GLU:CD	2.21	0.48
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:GLN:NE2	1:A:508:GLN:HA	2.28	0.48
1:A:322:LEU:HB2	1:A:699:ARG:HE	1.78	0.48
1:A:386:LYS:HD2	7:A:1027:HOH:O	2.13	0.48
1:A:620:LYS:HE3	1:A:622:SER:OG	2.13	0.48
1:A:505:CYS:O	1:A:508:GLN:HB2	2.13	0.48
1:B:701:THR:HA	1:B:702:PRO:C	2.39	0.48
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.30	0.47
1:A:306:TRP:CD2	1:B:336:MET:HE2	2.49	0.47
1:B:614:MET:CE	1:B:632:GLU:HG3	2.44	0.47
1:A:306:TRP:CG	1:B:336:MET:HE2	2.48	0.47
1:A:351:LYS:HE2	1:A:392:SER:HA	1.95	0.47
1:B:328:GLU:CD	1:B:328:GLU:N	2.73	0.47
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.45	0.46
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.44	0.46
1:B:364:GLN:NE2	7:B:1095:HOH:O	2.49	0.46
1:A:515:GLY:N	1:A:518:ASP:OD2	2.43	0.46
1:B:391:THR:O	1:B:392:SER:HB2	2.15	0.46
1:A:715:VAL:O	1:A:715:VAL:HG23	2.15	0.46
1:A:618:MET:HE3	1:A:625:TRP:CH2	2.50	0.46
1:B:337:LEU:HD22	1:B:706:TYR:CD1	2.50	0.46
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.98	0.45
1:B:299:ARG:NH1	1:B:299:ARG:CB	2.79	0.45
1:A:306:TRP:CE2	1:B:336:MET:HE2	2.51	0.45
1:A:488:PRO:C	1:A:490:GLY:N	2.74	0.45
1:A:384:VAL:O	1:A:388:ILE:HG13	2.16	0.45
1:A:569:ASN:ND2	1:A:569:ASN:H	2.14	0.45
1:A:350:THR:HB	1:A:353:GLN:HG3	1.99	0.45
1:A:485:TYR:CE1	1:A:514:ARG:HA	2.52	0.45
1:A:620:LYS:HE2	1:A:623:SER:HB3	1.97	0.45
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.48	0.45
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.82	0.44
1:A:484:GLY:O	1:A:499:VAL:HA	2.17	0.44
1:B:328:GLU:N	1:B:328:GLU:OE1	2.49	0.44
1:A:445:HIS:C	1:A:445:HIS:CD2	2.95	0.44
1:B:350:THR:HG22	1:B:352:ASP:N	2.25	0.44
1:A:571:LEU:C	1:A:571:LEU:HD23	2.42	0.44
1:B:325:GLY:O	1:B:332:MET:HG3	2.18	0.44
1:A:299:ARG:O	1:A:317:HIS:CE1	2.70	0.44
1:A:470:HIS:HA	1:A:527:ASN:O	2.17	0.44
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.83	0.44
1:A:551:PHE:CD2	1:A:551:PHE:N	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:O	1:A:364:GLN:HG2	2.16	0.44
1:B:451:ASN:HB3	1:B:454:ASN:O	2.17	0.44
1:A:701:THR:HA	1:A:702:PRO:C	2.43	0.44
1:B:314:ASP:OD1	1:B:317:HIS:ND1	2.43	0.44
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.89	0.44
1:B:589:MET:HA	1:B:649:VAL:O	2.18	0.43
1:B:598:TYR:CD1	7:B:1003:HOH:O	2.56	0.43
1:A:517:PHE:HB2	1:A:560:LYS:HE2	2.00	0.43
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.99	0.43
1:A:494:GLY:O	1:A:496:PRO:HD3	2.19	0.43
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.07	0.43
1:A:387:GLU:O	1:A:391:THR:OG1	2.36	0.43
1:A:391:THR:O	1:A:392:SER:OG	2.32	0.43
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.53	0.43
1:B:480:ILE:HD13	1:B:541:VAL:HG13	2.01	0.43
1:B:546:ILE:HG12	1:B:560:LYS:HA	2.01	0.42
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.49	0.42
1:A:514:ARG:HH21	1:A:514:ARG:HG3	1.85	0.42
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.54	0.42
1:A:556:ASP:O	7:A:1049:HOH:O	2.21	0.42
1:A:604:TYR:O	1:A:605:ASN:C	2.63	0.42
1:A:508:GLN:CA	1:A:508:GLN:HE21	2.33	0.42
1:A:522:LEU:O	1:A:533:LEU:HA	2.20	0.42
1:A:699:ARG:HD2	7:A:1015:HOH:O	2.19	0.42
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.55	0.42
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.84	0.41
1:A:507:GLN:O	1:A:507:GLN:HG2	2.19	0.41
1:B:504:ILE:O	1:B:508:GLN:HG2	2.20	0.41
1:A:628:GLN:HG2	1:B:631:VAL:HG11	2.02	0.41
1:A:486:LYS:HG3	1:A:499:VAL:HG11	2.03	0.41
1:A:555:LYS:HB3	1:A:555:LYS:HZ2	1.84	0.41
1:A:631:VAL:HG11	1:B:628:GLN:CG	2.50	0.41
1:B:423:LYS:NZ	7:B:1043:HOH:O	2.54	0.41
1:B:593:ILE:C	7:B:1003:HOH:O	2.64	0.41
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.03	0.41
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.51	0.41
1:B:353:GLN:HE21	1:B:353:GLN:HB3	1.53	0.41
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.48	0.41
1:B:300:PHE:CD1	1:B:300:PHE:N	2.88	0.41
1:B:495:ASP:HA	1:B:496:PRO:HD3	1.94	0.40
1:A:606:ILE:O	1:A:610:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:MET:C	1:B:337:LEU:HD23	2.46	0.40
1:A:569:ASN:N	1:A:569:ASN:HD22	2.19	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	403/420 (96%)	374 (93%)	29 (7%)	0	100	100
1	B	407/420 (97%)	397 (98%)	10 (2%)	0	100	100
All	All	810/840 (96%)	771 (95%)	39 (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	363/375 (97%)	357 (98%)	6 (2%)	53	60
1	B	366/375 (98%)	362 (99%)	4 (1%)	65	73
All	All	729/750 (97%)	719 (99%)	10 (1%)	59	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	ARG
1	A	523	LEU
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	B	328	GLU
1	B	337	LEU
1	B	353	GLN
1	B	540	LEU

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	353	GLN
1	A	364	GLN
1	A	425	GLN
1	A	454	ASN
1	A	507	GLN
1	A	508	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	425	GLN
1	B	454	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 [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
5	H4B	A	760	-	17,18,18	1.71	4 (23%)	14,26,26	2.03	4 (28%)
6	ARG	A	770	-	10,11,11	0.91	0	9,13,13	0.49	0
2	ACT	A	860	-	3,3,3	0.91	0	3,3,3	0.88	0
4	HEM	B	750	1	50,50,50	1.37	8 (16%)	67,82,82	0.98	4 (5%)
5	H4B	B	761	-	17,18,18	1.54	3 (17%)	14,26,26	2.00	4 (28%)
4	HEM	A	750	1	50,50,50	1.62	9 (18%)	67,82,82	1.07	4 (5%)
2	ACT	B	861	-	3,3,3	1.09	0	3,3,3	0.63	0
6	ARG	B	771	-	10,11,11	0.83	0	9,13,13	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
6	ARG	A	770	-	-	0/11/11/11	-
4	HEM	B	750	1	-	1/14/54/54	-
5	H4B	B	761	-	-	0/8/17/17	0/2/2/2
4	HEM	A	750	1	-	2/14/54/54	-
6	ARG	B	771	-	-	1/11/11/11	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	760	H4B	C4A-N5	4.11	1.47	1.37
4	A	750	HEM	FE-NB	4.11	2.07	1.94
4	A	750	HEM	FE-ND	3.73	2.06	1.94
5	B	761	H4B	C4A-N5	3.64	1.46	1.37
4	B	750	HEM	FE-NA	3.42	2.06	1.95
4	A	750	HEM	FE-NA	3.24	2.05	1.95
4	B	750	HEM	FE-ND	3.23	2.04	1.94
4	A	750	HEM	CAB-C3B	-3.23	1.38	1.47
5	A	760	H4B	C6-N5	3.10	1.53	1.47
5	B	761	H4B	C6-N5	3.00	1.52	1.47
4	A	750	HEM	CHD-C4C	2.69	1.43	1.38
4	A	750	HEM	CMD-C2D	2.69	1.56	1.50
4	B	750	HEM	CAB-C3B	-2.67	1.40	1.47
4	A	750	HEM	CAC-C3C	-2.57	1.40	1.47
5	A	760	H4B	C7-N8	2.57	1.49	1.46
4	A	750	HEM	C4A-NA	-2.36	1.35	1.39
4	B	750	HEM	CHD-C4C	2.20	1.42	1.38
5	B	761	H4B	C4-N3	2.20	1.43	1.38
4	B	750	HEM	CAC-C3C	-2.18	1.41	1.47
5	A	760	H4B	C4-N3	2.10	1.42	1.38
4	B	750	HEM	FE-NC	2.07	2.02	1.95
4	A	750	HEM	CMA-C3A	2.06	1.55	1.50
4	B	750	HEM	FE-NB	2.04	2.01	1.94
4	B	750	HEM	O2A-CGA	-2.02	1.24	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	760	H4B	C2-N1-C8A	5.29	122.70	113.36
5	B	761	H4B	C2-N1-C8A	5.03	122.24	113.36
5	A	760	H4B	N3-C2-N1	-3.13	117.60	123.32
5	A	760	H4B	O10-C10-C9	-3.09	104.66	109.77
4	A	750	HEM	CBA-CAA-C2A	-3.05	104.09	112.53
5	B	761	H4B	N3-C2-N1	-2.93	117.97	123.32
5	B	761	H4B	O9-C9-C6	2.84	116.09	109.28
5	B	761	H4B	O10-C10-C9	-2.75	105.22	109.77
4	B	750	HEM	CMB-C2B-C1B	2.49	128.92	125.03
4	A	750	HEM	CAB-C3B-C2B	-2.33	120.86	128.43
4	A	750	HEM	CHC-C4B-NB	-2.30	121.95	124.42
4	A	750	HEM	C1D-C2D-C3D	-2.26	104.60	106.98
4	B	750	HEM	C3C-C2C-C1C	-2.23	104.93	107.05
4	B	750	HEM	CAB-C3B-C2B	-2.21	121.25	128.43
5	A	760	H4B	O9-C9-C6	2.11	114.34	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	750	HEM	CBA-CAA-C2A	-2.08	106.78	112.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

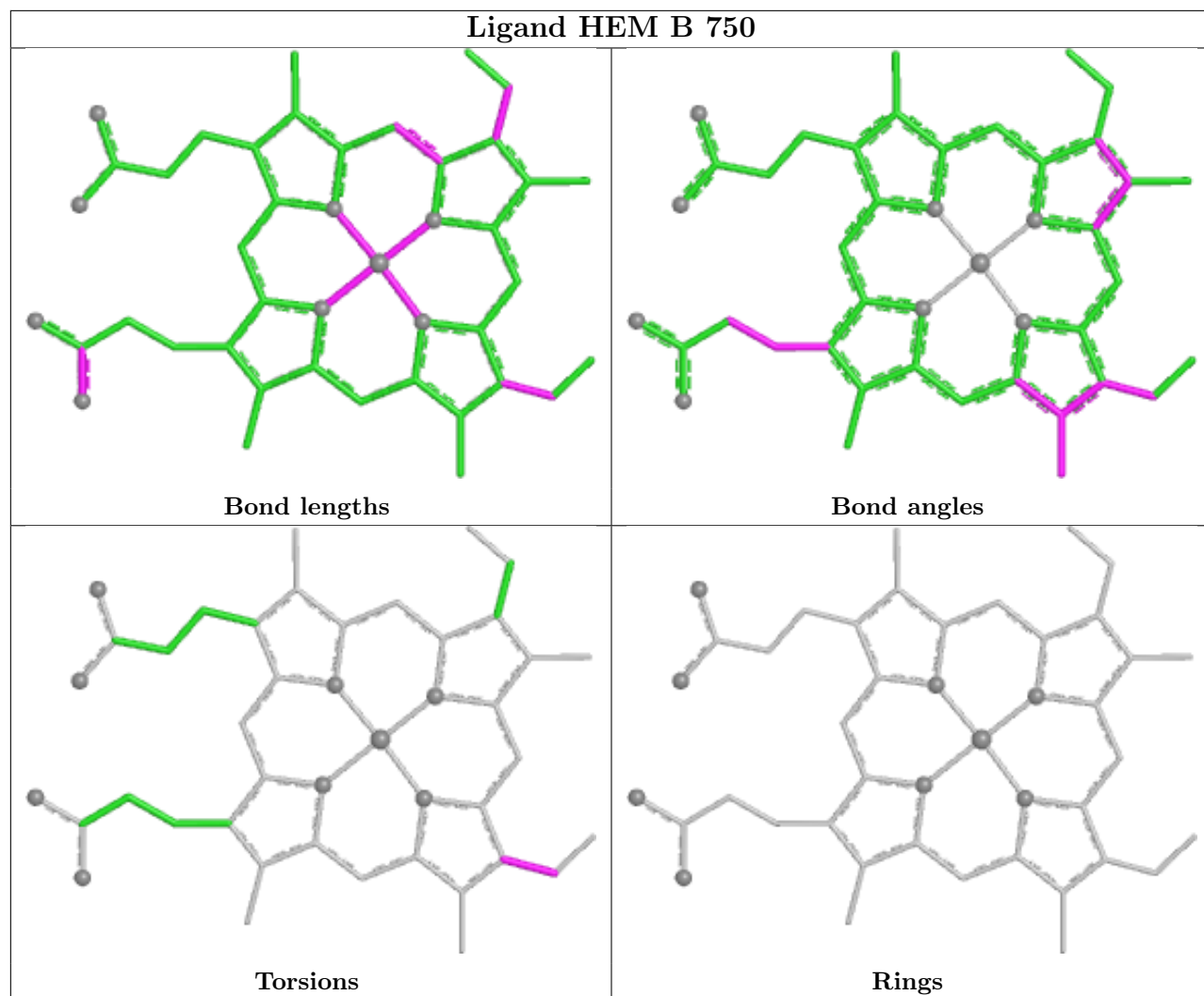
Mol	Chain	Res	Type	Atoms
4	B	750	HEM	C4B-C3B-CAB-CBB
6	B	771	ARG	O-C-CA-N
4	A	750	HEM	CAD-CBD-CGD-O2D
4	A	750	HEM	CAD-CBD-CGD-O1D

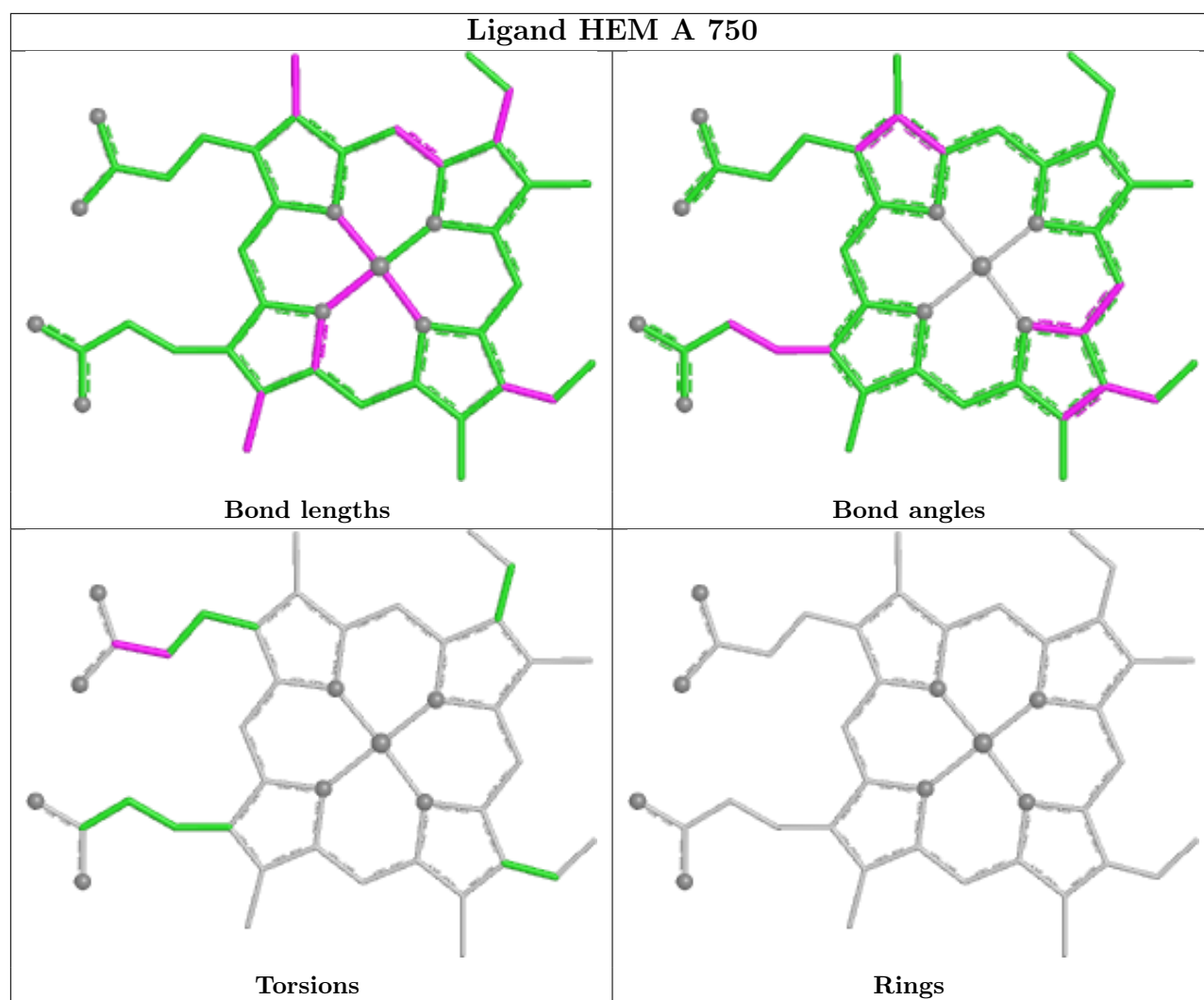
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	760	H4B	1	0
4	A	750	HEM	1	0
2	B	861	ACT	1	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	407/420 (96%)	1.05	81 (19%) 3 2	21, 42, 71, 87	0
1	B	411/420 (97%)	0.36	26 (6%) 26 24	21, 32, 59, 76	0
All	All	818/840 (97%)	0.70	107 (13%) 7 6	21, 36, 67, 87	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	PHE	5.2
1	A	716	TRP	4.4
1	B	322	LEU	4.4
1	A	321	THR	4.2
1	A	504	ILE	4.1
1	B	321	THR	4.1
1	A	551	PHE	4.1
1	A	715	VAL	4.0
1	A	322	LEU	3.9
1	B	350	THR	3.9
1	A	493	LEU	3.8
1	A	355	PHE	3.8
1	A	554	PHE	3.8
1	B	338	PRO	3.7
1	A	338	PRO	3.7
1	B	348	VAL	3.6
1	A	711	TRP	3.6
1	A	350	THR	3.5
1	A	506	ILE	3.5
1	B	300	PHE	3.5
1	A	373	GLY	3.5
1	A	318	LEU	3.5
1	A	513	PRO	3.4
1	A	381	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	352	ASP	3.3
1	A	488	PRO	3.3
1	A	528	GLY	3.2
1	A	533	LEU	3.2
1	A	487	GLN	3.1
1	B	337	LEU	3.1
1	B	611	ALA	3.1
1	A	557	LEU	3.1
1	A	301	LEU	3.0
1	A	376	ALA	3.0
1	A	510	TRP	3.0
1	A	512	ALA	2.9
1	A	324	THR	2.9
1	A	501	PHE	2.9
1	A	352	ASP	2.8
1	A	494	GLY	2.8
1	A	299	ARG	2.7
1	A	618	MET	2.7
1	A	509	GLY	2.7
1	A	499	VAL	2.7
1	A	484	GLY	2.7
1	A	393	THR	2.7
1	B	301	LEU	2.7
1	A	553	TRP	2.7
1	A	535	GLN	2.6
1	A	319	LYS	2.6
1	B	718	GLY	2.6
1	A	384	VAL	2.5
1	A	529	ASN	2.5
1	A	555	LYS	2.5
1	B	324	THR	2.5
1	A	337	LEU	2.5
1	A	559	LEU	2.5
1	A	485	TYR	2.5
1	A	552	ASP	2.5
1	A	330	ILE	2.5
1	A	667	ARG	2.4
1	A	713	THR	2.4
1	B	299	ARG	2.4
1	A	503	GLU	2.4
1	A	353	GLN	2.4
1	A	505	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	309	ASP	2.3
1	A	470	HIS	2.3
1	A	320	SER	2.3
1	A	374	SER	2.3
1	A	354	LEU	2.3
1	A	616	LEU	2.3
1	B	699	ARG	2.3
1	A	361	PHE	2.3
1	A	435	ALA	2.3
1	A	550	LYS	2.3
1	B	336	MET	2.3
1	A	329	HIS	2.2
1	B	360	GLU	2.2
1	A	633	ILE	2.2
1	A	508	GLN	2.2
1	A	602	SER	2.2
1	B	349	ARG	2.2
1	A	710	PRO	2.2
1	B	389	GLU	2.2
1	B	309	ASP	2.2
1	B	392	SER	2.2
1	A	466	THR	2.2
1	A	502	THR	2.2
1	A	517	PHE	2.1
1	A	546	ILE	2.1
1	A	468	GLY	2.1
1	A	362	LEU	2.1
1	B	354	LEU	2.1
1	B	535	GLN	2.1
1	A	390	SER	2.1
1	B	616	LEU	2.1
1	A	356	PRO	2.1
1	B	667	ARG	2.1
1	A	310	VAL	2.1
1	A	336	MET	2.1
1	A	601	ASN	2.1
1	A	369	ILE	2.1
1	B	318	LEU	2.0
1	A	514	ARG	2.0
1	B	355	PHE	2.0
1	A	620	LYS	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](#)

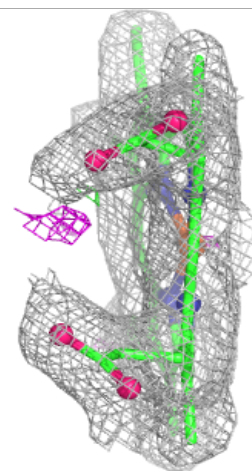
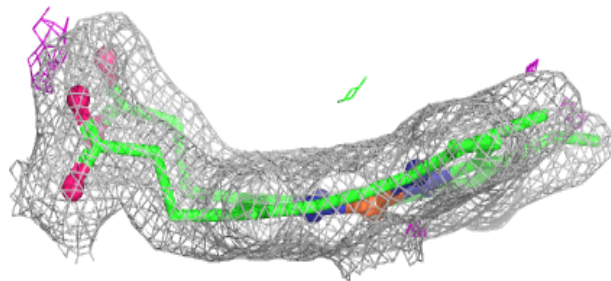
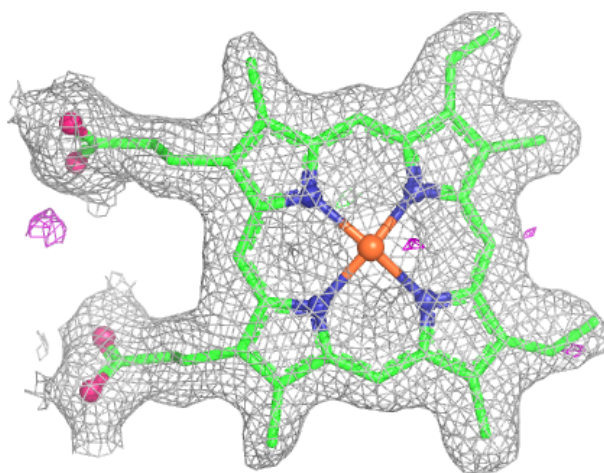
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

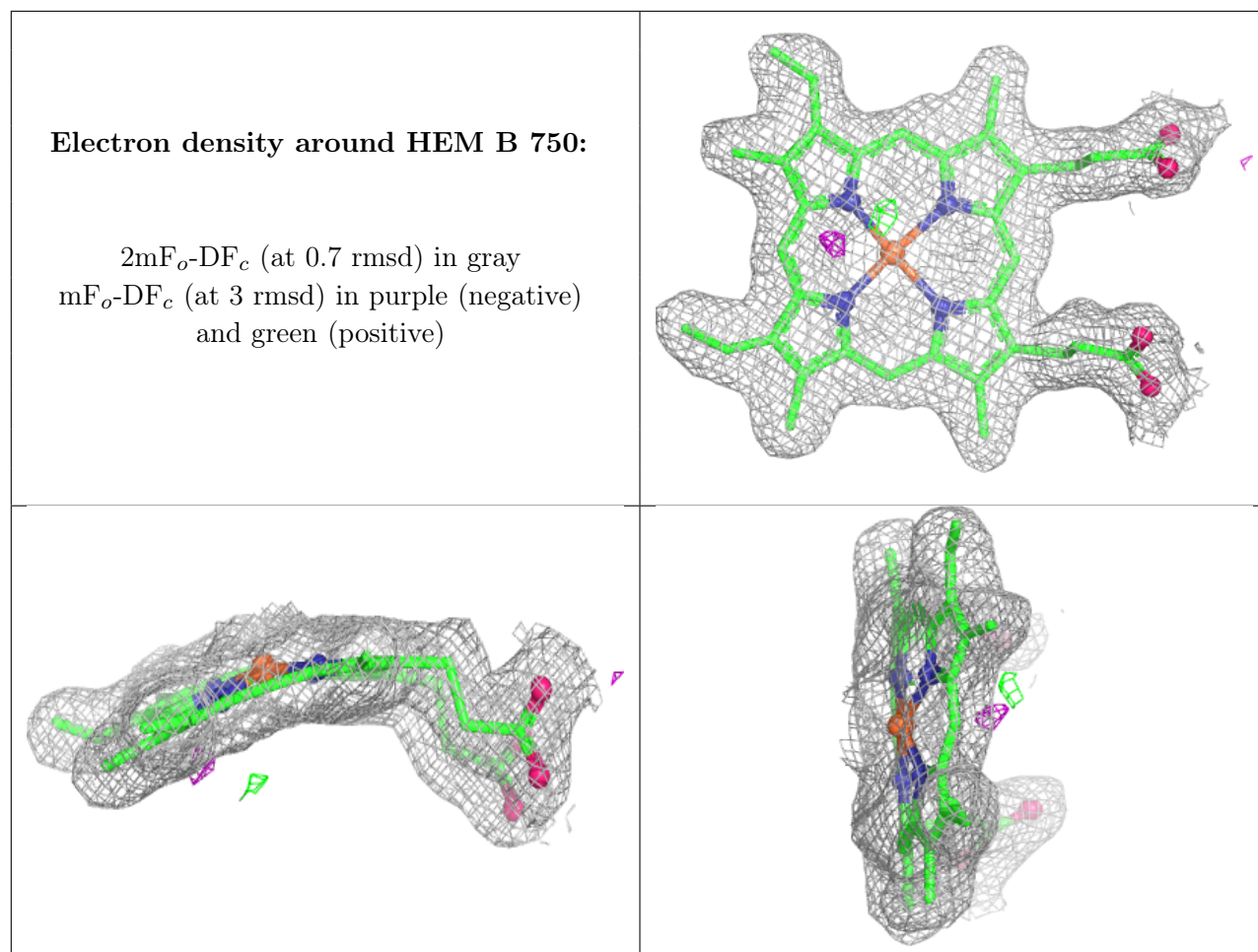
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	B	861	4/4	0.83	0.20	47,49,50,50	0
2	ACT	A	860	4/4	0.85	0.16	59,60,60,61	0
6	ARG	A	770	12/12	0.94	0.07	25,28,30,30	0
5	H4B	A	760	17/17	0.95	0.07	21,26,31,32	0
5	H4B	B	761	17/17	0.96	0.06	20,23,28,29	0
6	ARG	B	771	12/12	0.97	0.05	17,19,26,27	0
4	HEM	A	750	43/43	0.98	0.06	22,25,27,32	0
4	HEM	B	750	43/43	0.98	0.07	19,23,27,32	0
3	ZN	A	900	1/1	1.00	0.06	35,35,35,35	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.