



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:31 AM EDT

PDB ID : 1OM4 / pdb_00001om4
Title : STRUCTURE OF RAT NEURONAL NOS HEME DOMAIN WITH L-ARGININE BOUND
Authors : Li, H.; Martasek, P.; Shimizu, H.; Masters, B.S.S.; Poulos, T.L.; Raman, C.S.
Deposited on : 2003-02-24
Resolution : 1.75 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

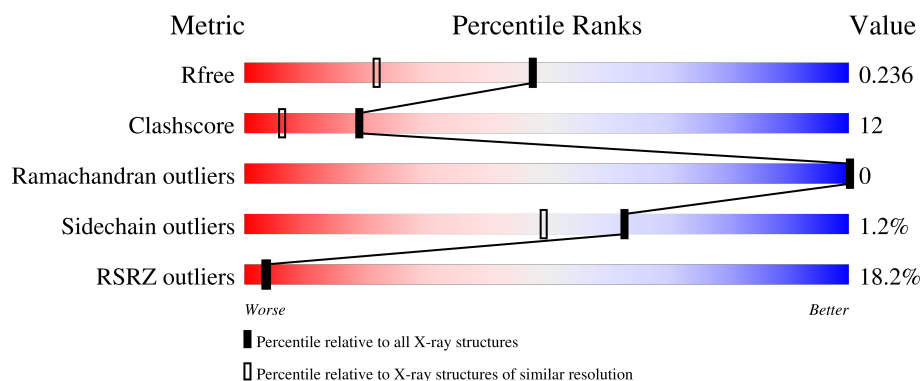
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	27% 69% 26% • •
1	B	422	8% 78% 18% •

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7483 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 ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



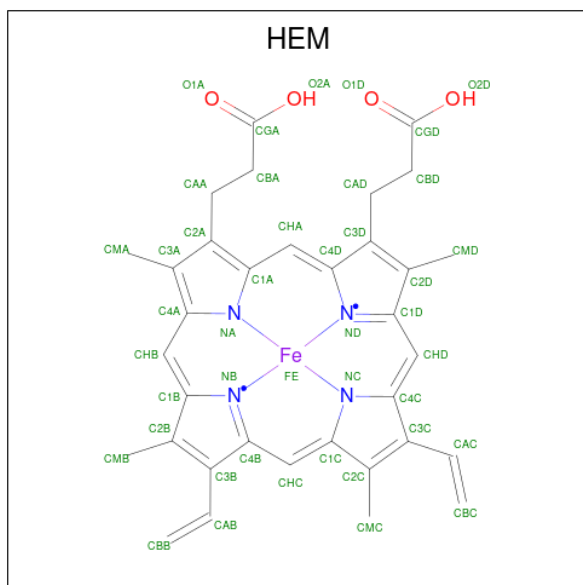
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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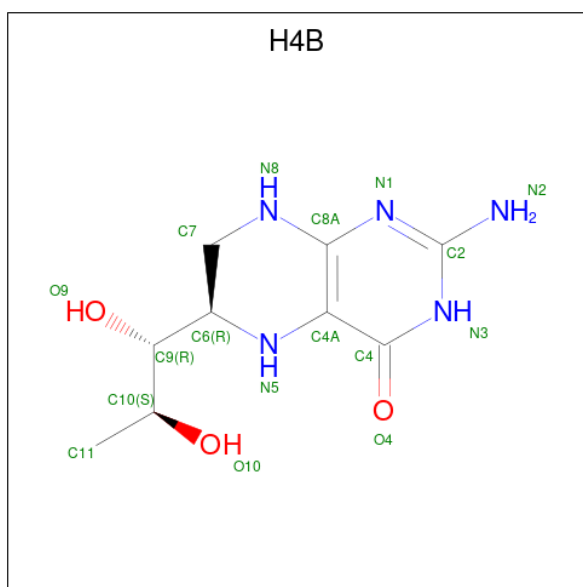
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



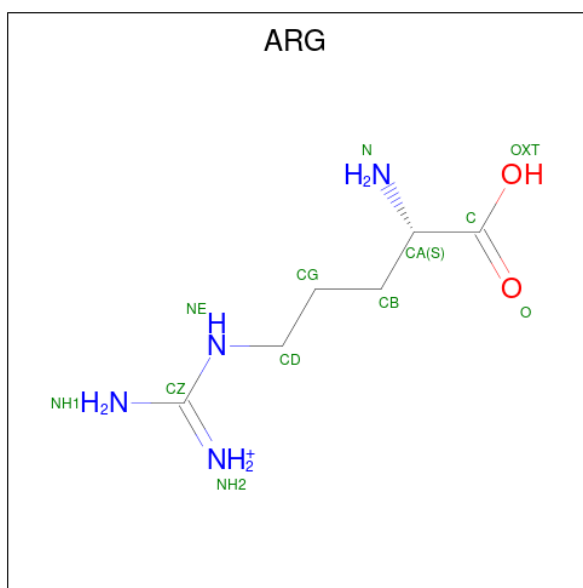
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	9	5	3		
5	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



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

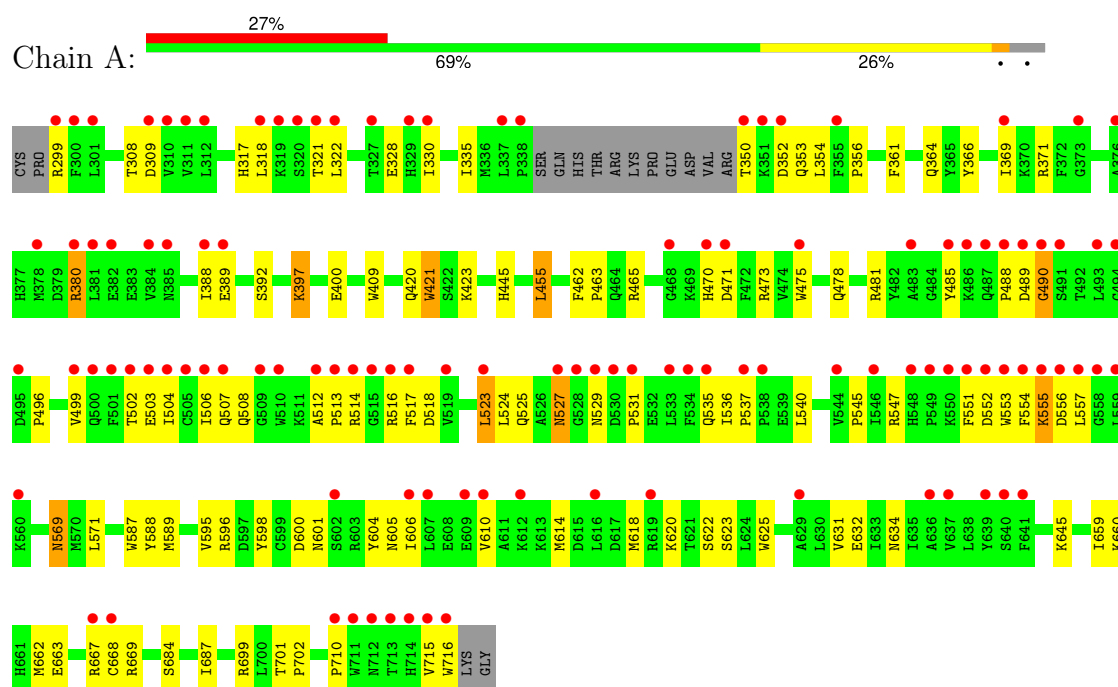
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	266	Total	O	0	0
			266	266		
8	B	394	Total	O	0	0
			394	394		

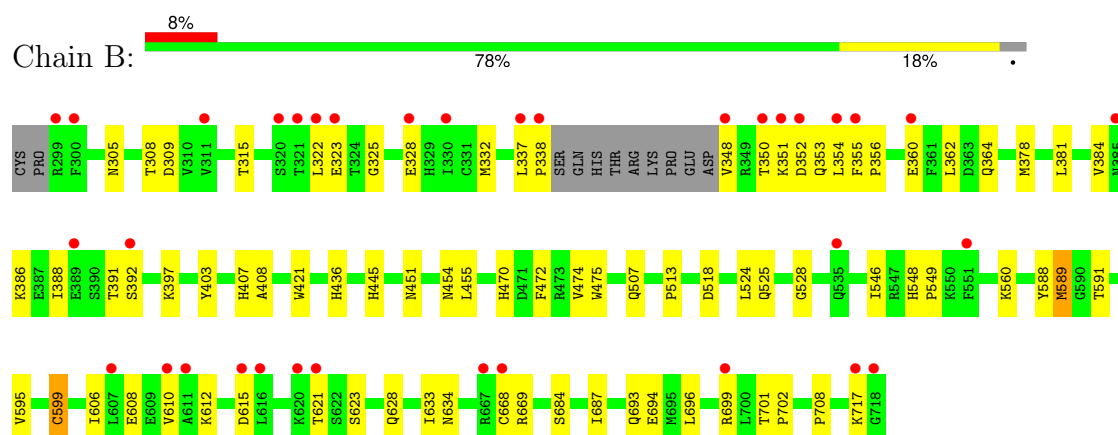
3 Residue-property plots [i](#)

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	51.89Å 110.19Å 164.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 1.75 29.98 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.98-1.75) 98.5 (29.98-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.245 0.212 , 0.236	Depositor DCC
R_{free} test set	5600 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7483	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, H4B, ACT, GOL, 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	0.34	0/3406	0.87	8/4621 (0.2%)
1	B	0.37	0/3438	0.89	12/4661 (0.3%)
All	All	0.36	0/6844	0.88	20/9282 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-8.11	96.02	109.24
1	A	589	MET	N-CA-C	-7.83	96.47	109.24
1	A	421	TRP	N-CA-C	6.89	119.67	111.33
1	B	474	VAL	N-CA-C	-6.81	98.05	107.99
1	B	421	TRP	N-CA-C	6.79	119.55	111.33
1	A	588	TYR	N-CA-C	6.13	119.14	110.50
1	A	490	GLY	N-CA-C	-6.12	106.96	114.92
1	B	588	TYR	N-CA-C	6.01	118.97	110.50
1	A	623	SER	N-CA-C	-5.82	106.14	113.18
1	B	408	ALA	N-CA-C	-5.65	105.12	111.28
1	A	455	LEU	N-CA-C	5.52	118.02	110.24
1	B	397	LYS	N-CA-C	-5.51	103.12	110.55
1	B	455	LEU	N-CA-C	5.40	117.85	110.24
1	A	397	LYS	N-CA-C	-5.39	103.28	110.55
1	B	315	THR	N-CA-C	-5.37	107.74	114.56
1	A	354	LEU	N-CA-C	5.35	116.92	111.14
1	B	472	PHE	N-CA-C	-5.29	100.61	109.24
1	B	623	SER	N-CA-C	-5.21	106.42	112.89
1	B	524	LEU	N-CA-C	5.20	117.44	109.07
1	B	599	CYS	N-CA-C	5.17	120.44	113.72

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	102	0
1	B	3345	0	3259	59	0
2	A	1	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	43	0	30	2	0
4	B	43	0	30	0	0
5	A	17	0	15	0	0
5	B	17	0	15	0	0
6	A	6	0	8	3	0
6	B	6	0	8	3	0
7	B	24	0	24	0	0
8	A	266	0	0	7	0
8	B	394	0	0	9	0
All	All	7483	0	6616	159	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 (159) 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	1.42	1.01
1:B:475:TRP:HE1	1:B:525:GLN:HE21	1.18	0.86
1:A:554:PHE:O	1:A:557:LEU:HD12	1.79	0.81
1:B:668:CYS:HB3	8:B:1191:HOH:O	1.86	0.74
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.70	0.74
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.70	0.73
1:A:669:ARG:HH21	6:A:880:GOL:H32	1.53	0.71
1:A:504:ILE:O	1:A:508:GLN:HG2	1.90	0.70
1:A:660:LYS:HE2	8:A:1164:HOH:O	1.91	0.69
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.57	0.68
1:B:323:GLU:O	1:B:699:ARG:HD3	1.95	0.67
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.11	0.66
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.79	0.65
1:B:669:ARG:HH21	6:B:881:GOL:C1	2.11	0.64
1:B:475:TRP:HE1	1:B:525:GLN:NE2	1.95	0.63
1:A:350:THR:HG22	1:A:352:ASP:H	1.65	0.61
1:A:361:PHE:O	1:A:364:GLN:HG2	2.00	0.61
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.81	0.61
1:A:620:LYS:HE3	1:A:622:SER:OG	2.00	0.61
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.30	0.60
1:A:601:ASN:HB2	8:A:1161:HOH:O	2.01	0.60
1:A:328:GLU:H	1:A:328:GLU:CD	2.11	0.58
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.28	0.58
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.84	0.58
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.19	0.58
1:A:618:MET:HE3	1:A:625:TRP:CZ3	2.39	0.58
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.85	0.58
1:B:355:PHE:N	1:B:356:PRO:HD2	2.18	0.57
1:A:659:ILE:O	1:A:663:GLU:HG3	2.04	0.57
1:A:555:LYS:NZ	1:A:555:LYS:HB3	2.19	0.57
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.33	0.56
1:A:524:LEU:O	1:A:531:PRO:HA	2.05	0.56
1:B:356:PRO:O	1:B:360:GLU:HG3	2.06	0.56
1:A:499:VAL:O	1:A:503:GLU:HG3	2.06	0.56
1:B:615:ASP:HA	8:B:1186:HOH:O	2.05	0.56
1:A:321:THR:HG21	8:A:1064:HOH:O	2.05	0.56
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.36	0.55
1:A:321:THR:HG23	1:A:322:LEU:HG	1.88	0.55
1:A:569:ASN:HD22	1:A:569:ASN:H	1.54	0.55
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.36	0.55
1:B:669:ARG:HH21	6:B:881:GOL:H11	1.70	0.55
1:A:614:MET:CE	1:A:632:GLU:HG3	2.36	0.55
1:B:328:GLU:N	1:B:328:GLU:OE1	2.39	0.54
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.72	0.54
1:A:380:ARG:NH1	1:A:397:LYS:HG2	2.23	0.54
1:A:555:LYS:HB3	1:A:555:LYS:HZ2	1.73	0.53
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.38	0.53
1:A:715:VAL:O	1:A:715:VAL:HG23	2.09	0.53
1:A:716:TRP:H	1:A:716:TRP:CD1	2.26	0.52
1:B:378:MET:HE2	1:B:378:MET:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.75	0.52
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.92	0.52
1:A:669:ARG:NH2	6:A:880:GOL:H32	2.24	0.52
1:B:351:LYS:HE2	1:B:392:SER:HA	1.92	0.52
1:B:305:ASN:HD22	1:B:693:GLN:NE2	2.08	0.51
1:A:554:PHE:HA	1:A:557:LEU:HD12	1.91	0.51
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.92	0.51
1:A:308:THR:O	1:A:309:ASP:HB2	2.11	0.51
1:A:701:THR:HA	1:A:702:PRO:C	2.37	0.50
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.11	0.50
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.94	0.50
1:A:518:ASP:OD1	8:A:1158:HOH:O	2.20	0.49
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.93	0.49
1:B:391:THR:O	1:B:392:SER:HB2	2.11	0.49
1:A:321:THR:HG23	1:A:322:LEU:N	2.28	0.49
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.93	0.49
1:B:669:ARG:NH2	6:B:881:GOL:H11	2.27	0.48
1:A:322:LEU:HB2	1:A:699:ARG:HE	1.78	0.48
1:A:420:GLN:OE1	1:A:423:LYS:HE2	2.13	0.48
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.94	0.48
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.48	0.48
4:A:750:HEM:HMC1	4:A:750:HEM:HBC2	1.96	0.48
1:A:321:THR:HG23	1:A:322:LEU:H	1.79	0.47
1:A:525:GLN:HG3	1:A:529:ASN:O	2.14	0.47
1:A:595:VAL:HG23	1:A:634:ASN:HD21	1.79	0.47
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.96	0.47
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.96	0.47
1:A:350:THR:HB	1:A:353:GLN:CD	2.40	0.47
1:A:553:TRP:HA	1:A:556:ASP:OD2	2.14	0.46
1:B:606:ILE:HD11	1:B:633:ILE:HD13	1.97	0.46
1:B:717:LYS:NZ	8:B:1181:HOH:O	2.48	0.46
1:B:386:LYS:HD3	8:B:1122:HOH:O	2.16	0.46
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.46
1:A:535:GLN:NE2	8:A:1159:HOH:O	2.49	0.46
1:A:299:ARG:O	1:A:317:HIS:CE1	2.69	0.46
1:A:465:ARG:HG3	1:A:471:ASP:OD1	2.15	0.46
1:A:569:ASN:H	1:A:569:ASN:ND2	2.13	0.46
1:A:571:LEU:C	1:A:571:LEU:HD23	2.41	0.46
1:B:436:HIS:HB2	8:B:1060:HOH:O	2.17	0.45
1:A:701:THR:HG23	8:A:985:HOH:O	2.16	0.45
1:B:445:HIS:C	1:B:445:HIS:CD2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:ARG:HH21	6:A:880:GOL:C3	2.24	0.45
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.97	0.45
1:B:350:THR:HG22	1:B:352:ASP:H	1.82	0.45
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.05	0.45
1:A:554:PHE:C	1:A:557:LEU:HD12	2.42	0.44
1:B:364:GLN:NE2	8:B:982:HOH:O	2.49	0.44
1:B:589:MET:HE3	1:B:591:THR:OG1	2.18	0.44
1:B:308:THR:O	1:B:309:ASP:HB2	2.18	0.44
1:B:595:VAL:HG23	1:B:634:ASN:HD21	1.83	0.44
1:A:502:THR:O	1:A:506:ILE:HG13	2.17	0.43
1:B:708:PRO:HG2	8:B:1199:HOH:O	2.18	0.43
1:A:353:GLN:O	1:A:356:PRO:HD2	2.18	0.43
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.00	0.43
1:A:507:GLN:O	1:A:507:GLN:HG2	2.18	0.43
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.88	0.43
1:A:569:ASN:HD22	1:A:569:ASN:N	2.11	0.43
1:A:598:TYR:O	1:A:606:ILE:HG12	2.18	0.43
1:A:514:ARG:HH21	1:A:514:ARG:HG3	1.82	0.43
1:B:348:VAL:HG13	1:B:348:VAL:O	2.19	0.43
1:B:378:MET:HE2	1:B:381:LEU:HD12	1.99	0.43
1:B:388:ILE:O	1:B:392:SER:N	2.48	0.43
1:A:388:ILE:O	1:A:392:SER:N	2.52	0.43
1:A:445:HIS:CD2	1:A:445:HIS:C	2.97	0.43
1:B:337:LEU:O	1:B:338:PRO:C	2.60	0.43
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.00	0.43
1:B:325:GLY:O	1:B:332:MET:HG3	2.18	0.43
1:A:667:ARG:NH1	1:A:668:CYS:SG	2.92	0.43
1:A:536:ILE:O	1:A:537:PRO:C	2.60	0.42
1:B:608:GLU:O	1:B:612:LYS:HG3	2.19	0.42
1:A:335:ILE:HD13	1:B:694:GLU:HB3	2.00	0.42
1:A:604:TYR:O	1:A:605:ASN:C	2.62	0.42
1:A:470:HIS:HB3	1:A:527:ASN:HD22	1.81	0.42
1:A:516:ARG:HD3	1:A:517:PHE:HE1	1.85	0.42
1:B:595:VAL:O	1:B:599:CYS:HB2	2.20	0.42
1:B:621:THR:HG22	8:B:1141:HOH:O	2.19	0.42
1:A:489:ASP:OD2	1:A:489:ASP:O	2.37	0.42
1:A:545:PRO:HG2	1:A:547:ARG:NH2	2.33	0.42
1:A:596:ARG:O	1:A:600:ASP:HB2	2.19	0.42
1:A:516:ARG:HD3	1:A:517:PHE:CE1	2.54	0.42
8:A:1160:HOH:O	1:B:628:GLN:NE2	2.53	0.42
1:A:350:THR:HB	1:A:353:GLN:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:PHE:N	1:B:356:PRO:CD	2.82	0.41
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.50	0.41
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.01	0.41
1:A:488:PRO:C	1:A:490:GLY:N	2.78	0.41
1:A:684:SER:O	1:A:687:ILE:HG12	2.20	0.41
1:A:322:LEU:CB	1:A:699:ARG:HE	2.33	0.41
1:A:551:PHE:CD2	1:A:551:PHE:N	2.87	0.41
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.55	0.41
1:A:506:ILE:C	1:A:508:GLN:N	2.78	0.41
1:A:554:PHE:CA	1:A:557:LEU:HD12	2.51	0.41
1:A:610:VAL:O	1:A:614:MET:HG3	2.21	0.41
1:B:470:HIS:HA	1:B:528:GLY:HA3	2.03	0.41
1:A:552:ASP:O	1:A:555:LYS:HG2	2.21	0.41
1:B:354:LEU:C	1:B:356:PRO:HD2	2.46	0.41
1:B:507:GLN:NE2	8:B:1214:HOH:O	2.54	0.41
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.55	0.41
1:A:507:GLN:HE21	1:A:507:GLN:HB3	1.67	0.40
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.56	0.40
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.36	0.40
1:A:350:THR:HB	1:A:353:GLN:HG3	2.04	0.40
1:A:353:GLN:C	1:A:356:PRO:HD2	2.46	0.40
4:A:750:HEM:HBC2	4:A:750:HEM:CMC	2.52	0.40
1:B:350:THR:HG22	1:B:351:LYS:N	2.35	0.40
1:A:554:PHE:HA	1:A:557:LEU:CD1	2.51	0.40
1:B:451:ASN:HB3	1:B:454:ASN:O	2.22	0.40
1:B:684:SER:HB3	1:B:687:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/422 (96%)	388 (96%)	15 (4%)	0	100	100
1	B	407/422 (96%)	397 (98%)	10 (2%)	0	100	100
All	All	810/844 (96%)	785 (97%)	25 (3%)	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	363/377 (96%)	355 (98%)	8 (2%)	45	26
1	B	366/377 (97%)	365 (100%)	1 (0%)	86	83
All	All	729/754 (97%)	720 (99%)	9 (1%)	63	49

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

Mol	Chain	Res	Type
1	A	380	ARG
1	A	389	GLU
1	A	523	LEU
1	A	527	ASN
1	A	555	LYS
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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	425	GLN
1	A	451	ASN
1	A	454	ASN

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Mol	Chain	Res	Type
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	601	ASN
1	A	605	ASN
1	A	634	ASN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN
1	B	425	GLN
1	B	451	ASN
1	B	454	ASN
1	B	507	GLN
1	B	525	GLN
1	B	527	ASN
1	B	535	GLN
1	B	601	ASN
1	B	634	ASN
1	B	693	GLN
1	B	697	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	B	761	-	17,18,18	1.61	3 (17%)	14,26,26	1.93	4 (28%)
6	GOL	B	881	-	5,5,5	0.24	0	5,5,5	0.24	0
7	ARG	B	770	-	10,11,11	0.79	0	9,13,13	0.56	0
6	GOL	A	880	-	5,5,5	0.31	0	5,5,5	0.26	0
4	HEM	A	750	1	50,50,50	1.13	5 (10%)	67,82,82	1.01	1 (1%)
3	ACT	B	861	-	3,3,3	0.93	0	3,3,3	0.72	0
7	ARG	B	771	-	10,11,11	0.76	0	9,13,13	0.62	0
3	ACT	A	860	-	3,3,3	0.94	0	3,3,3	0.83	0
4	HEM	B	750	1	50,50,50	1.07	3 (6%)	67,82,82	1.11	4 (5%)
5	H4B	A	760	-	17,18,18	1.47	2 (11%)	14,26,26	2.02	4 (28%)

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	B	761	-	-	0/8/17/17	0/2/2/2
6	GOL	B	881	-	-	0/4/4/4	-
7	ARG	B	770	-	-	1/11/11/11	-
6	GOL	A	880	-	-	2/4/4/4	-
4	HEM	A	750	1	-	1/14/54/54	-
7	ARG	B	771	-	-	1/11/11/11	-
4	HEM	B	750	1	-	0/14/54/54	-
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	761	H4B	C4A-N5	3.82	1.46	1.37
5	A	760	H4B	C4A-N5	3.65	1.46	1.37
5	A	760	H4B	C6-N5	3.45	1.53	1.47
5	B	761	H4B	C6-N5	3.43	1.53	1.47
4	A	750	HEM	CAB-C3B	-2.68	1.40	1.47
4	B	750	HEM	CAB-C3B	-2.47	1.40	1.47
4	A	750	HEM	CAC-C3C	-2.38	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	750	HEM	FE-ND	2.26	2.01	1.94
4	B	750	HEM	CAC-C3C	-2.22	1.41	1.47
4	A	750	HEM	CHD-C4C	2.16	1.42	1.38
4	B	750	HEM	FE-NA	2.16	2.02	1.95
4	A	750	HEM	FE-NA	2.05	2.01	1.95
5	B	761	H4B	C7-C6	2.05	1.54	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	760	H4B	C2-N1-C8A	5.30	122.71	113.36
5	B	761	H4B	C2-N1-C8A	4.97	122.12	113.36
5	A	760	H4B	O10-C10-C9	-3.11	104.62	109.77
5	B	761	H4B	O10-C10-C9	-3.11	104.62	109.77
5	A	760	H4B	N3-C2-N1	-2.99	117.85	123.32
5	B	761	H4B	N3-C2-N1	-2.88	118.05	123.32
4	B	750	HEM	C3B-C2B-C1B	2.88	108.57	106.41
4	A	750	HEM	C3B-C4B-NB	2.63	111.35	109.47
5	B	761	H4B	O9-C9-C6	2.17	114.47	109.28
5	A	760	H4B	O9-C9-C6	2.17	114.47	109.28
4	B	750	HEM	C4B-C3B-C2B	-2.15	105.31	107.28
4	B	750	HEM	C3B-C4B-NB	2.14	111.01	109.47
4	B	750	HEM	CAB-C3B-C2B	-2.13	121.50	128.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

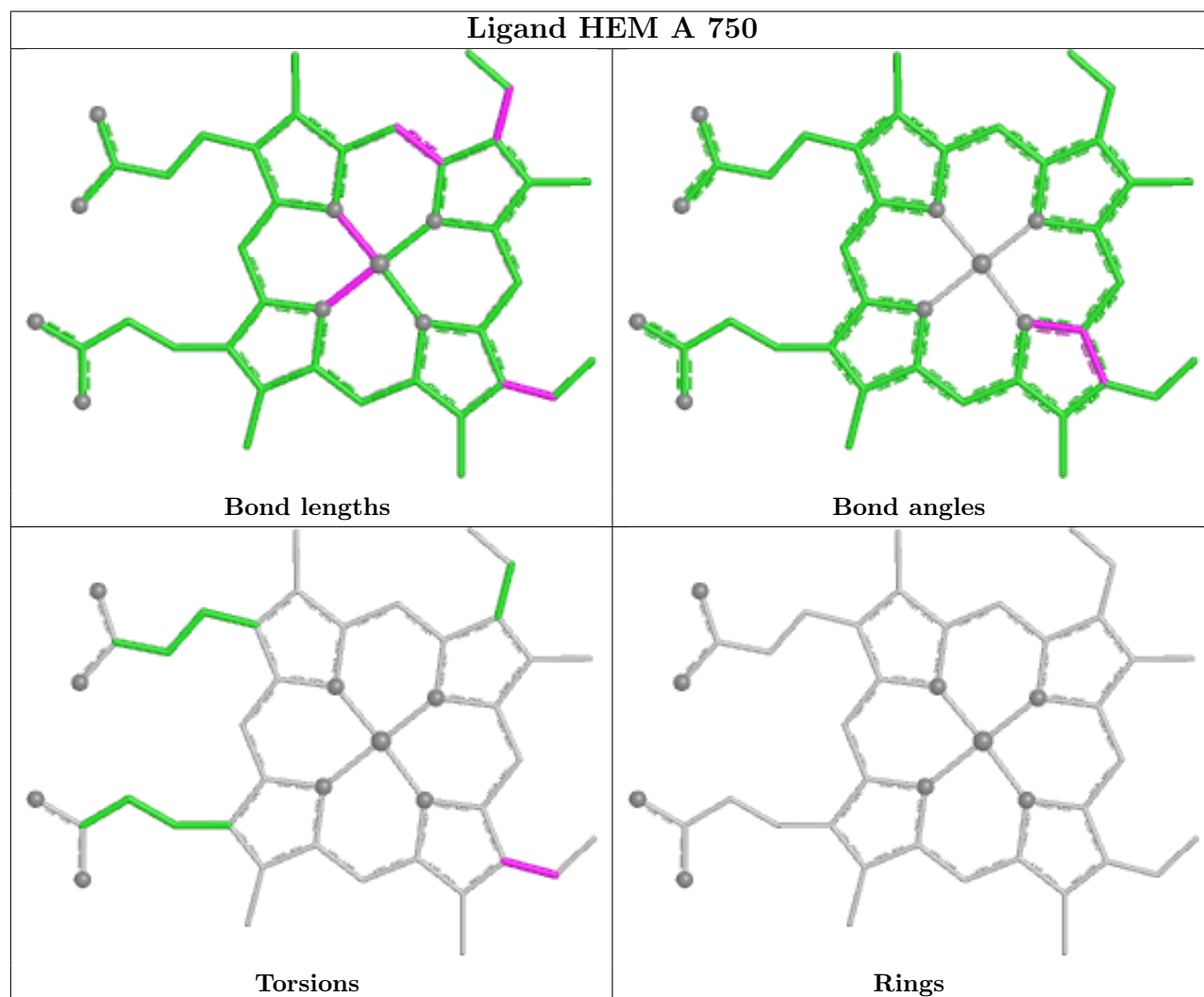
Mol	Chain	Res	Type	Atoms
6	A	880	GOL	O1-C1-C2-C3
4	A	750	HEM	C4B-C3B-CAB-CBB
6	A	880	GOL	O1-C1-C2-O2
7	B	770	ARG	O-C-CA-N
7	B	771	ARG	O-C-CA-N

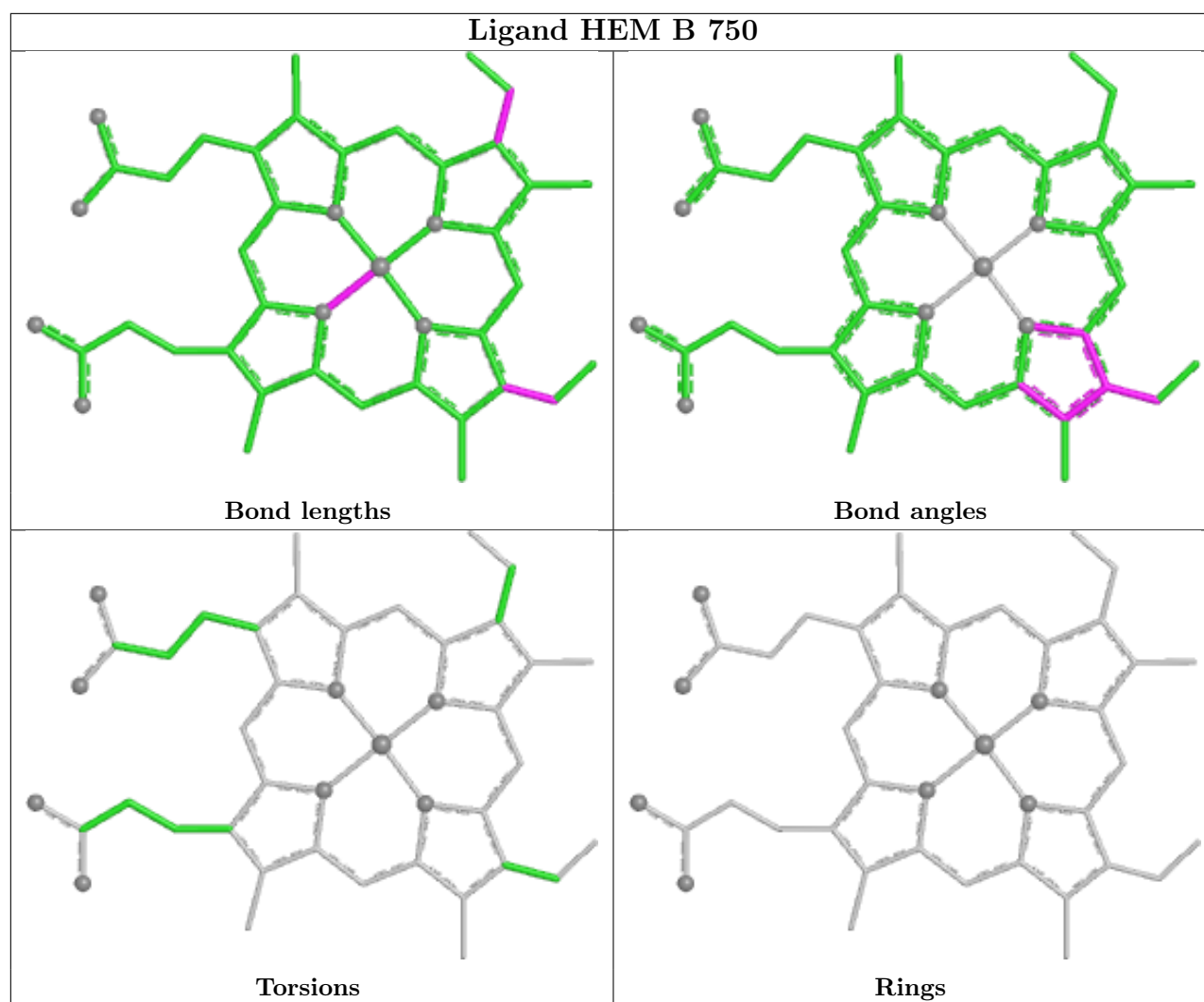
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	881	GOL	3	0
6	A	880	GOL	3	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	407/422 (96%)	1.33	114 (28%) 1 1	16, 34, 70, 93	0
1	B	411/422 (97%)	0.54	35 (8%) 16 20	15, 26, 55, 75	0
All	All	818/844 (96%)	0.93	149 (18%) 3 4	15, 29, 62, 93	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	THR	5.8
1	B	348	VAL	5.7
1	A	517	PHE	5.6
1	A	321	THR	5.4
1	A	300	PHE	5.4
1	A	322	LEU	5.3
1	B	321	THR	5.2
1	A	553	TRP	5.0
1	A	490	GLY	4.8
1	A	355	PHE	4.8
1	A	320	SER	4.7
1	A	505	CYS	4.6
1	A	513	PRO	4.6
1	A	488	PRO	4.4
1	B	322	LEU	4.3
1	A	549	PRO	4.2
1	A	487	GLN	4.2
1	A	350	THR	4.1
1	A	716	TRP	4.1
1	A	486	LYS	4.1
1	B	616	LEU	4.1
1	A	551	PHE	4.1
1	A	506	ILE	4.1
1	A	715	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	3.9
1	A	711	TRP	3.8
1	B	389	GLU	3.8
1	A	504	ILE	3.7
1	A	382	GLU	3.7
1	A	373	GLY	3.7
1	A	381	LEU	3.7
1	A	538	PRO	3.7
1	A	528	GLY	3.7
1	A	552	ASP	3.7
1	A	493	LEU	3.6
1	A	491	SER	3.6
1	B	338	PRO	3.6
1	A	485	TYR	3.6
1	A	512	ALA	3.6
1	B	392	SER	3.6
1	A	510	TRP	3.5
1	A	494	GLY	3.5
1	A	710	PRO	3.5
1	B	718	GLY	3.5
1	A	712	ASN	3.5
1	A	533	LEU	3.4
1	A	515	GLY	3.4
1	B	611	ALA	3.4
1	A	556	ASP	3.3
1	A	557	LEU	3.3
1	A	519	VAL	3.3
1	A	550	LYS	3.2
1	A	535	GLN	3.2
1	B	352	ASP	3.2
1	A	509	GLY	3.2
1	A	502	THR	3.2
1	B	355	PHE	3.2
1	A	318	LEU	3.1
1	B	300	PHE	3.1
1	A	310	VAL	3.0
1	A	376	ALA	3.0
1	A	559	LEU	3.0
1	B	337	LEU	3.0
1	A	530	ASP	3.0
1	A	299	ARG	3.0
1	A	713	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	378	MET	2.9
1	A	499	VAL	2.9
1	B	607	LEU	2.9
1	A	389	GLU	2.9
1	A	534	PHE	2.9
1	A	554	PHE	2.9
1	A	544	VAL	2.9
1	A	610	VAL	2.9
1	A	503	GLU	2.9
1	A	475	TRP	2.9
1	A	501	PHE	2.8
1	A	667	ARG	2.8
1	B	620	LYS	2.8
1	A	514	ARG	2.8
1	A	500	GLN	2.8
1	A	639	TYR	2.8
1	A	668	CYS	2.8
1	A	640	SER	2.8
1	B	621	THR	2.7
1	A	352	ASP	2.7
1	B	551	PHE	2.7
1	B	328	GLU	2.7
1	A	351	LYS	2.7
1	A	636	ALA	2.7
1	B	354	LEU	2.6
1	B	360	GLU	2.6
1	A	311	VAL	2.6
1	A	319	LYS	2.6
1	A	301	LEU	2.6
1	A	470	HIS	2.6
1	A	637	VAL	2.6
1	A	602	SER	2.6
1	A	483	ALA	2.6
1	A	471	ASP	2.5
1	A	337	LEU	2.5
1	A	489	ASP	2.5
1	B	351	LYS	2.5
1	A	529	ASN	2.5
1	B	323	GLU	2.5
1	A	527	ASN	2.4
1	A	507	GLN	2.4
1	A	537	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	384	VAL	2.4
1	B	610	VAL	2.4
1	B	385	ASN	2.4
1	A	607	LEU	2.4
1	A	385	ASN	2.3
1	A	609	GLU	2.3
1	A	329	HIS	2.3
1	B	330	ILE	2.3
1	A	612	LYS	2.3
1	B	320	SER	2.3
1	B	717	LYS	2.3
1	B	311	VAL	2.3
1	A	629	ALA	2.2
1	B	667	ARG	2.2
1	A	468	GLY	2.2
1	A	546	ILE	2.2
1	A	548	HIS	2.2
1	A	523	LEU	2.2
1	A	369	ILE	2.2
1	A	531	PRO	2.2
1	A	312	LEU	2.2
1	A	330	ILE	2.2
1	A	327	THR	2.2
1	A	616	LEU	2.1
1	B	699	ARG	2.1
1	A	641	PHE	2.1
1	A	388	ILE	2.1
1	A	714	HIS	2.1
1	A	555	LYS	2.1
1	A	558	GLY	2.1
1	A	516	ARG	2.1
1	A	619	ARG	2.1
1	B	535	GLN	2.0
1	A	309	ASP	2.0
1	A	495	ASP	2.0
1	A	380	ARG	2.0
1	B	299	ARG	2.0
1	B	668	CYS	2.0
1	A	560	LYS	2.0
1	A	606	ILE	2.0
1	B	615	ASP	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](#)

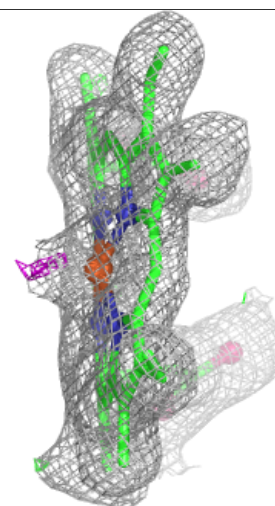
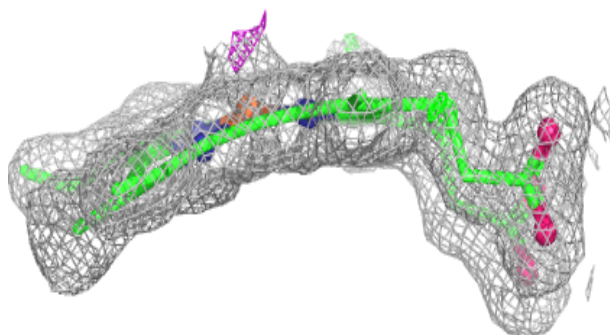
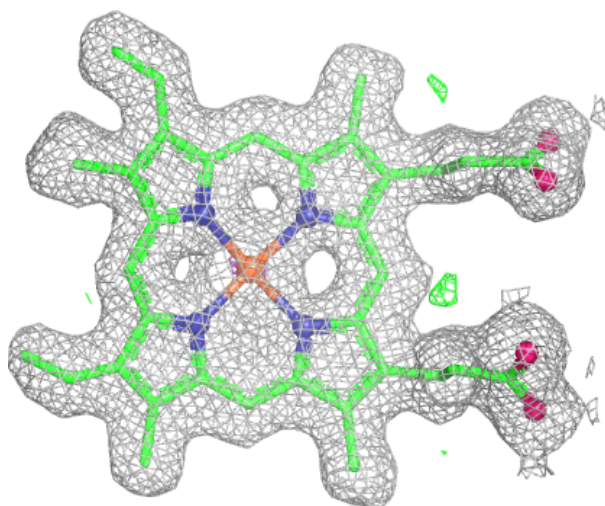
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	B	881	6/6	0.77	0.13	43,43,44,47	0
6	GOL	A	880	6/6	0.83	0.11	52,53,53,55	0
7	ARG	B	770	12/12	0.91	0.09	21,28,29,29	0
7	ARG	B	771	12/12	0.95	0.07	21,24,26,27	0
3	ACT	A	860	4/4	0.96	0.09	35,36,37,37	0
3	ACT	B	861	4/4	0.96	0.07	30,30,31,31	0
5	H4B	A	760	17/17	0.96	0.06	16,19,22,24	0
5	H4B	B	761	17/17	0.96	0.06	16,17,23,23	0
4	HEM	A	750	43/43	0.98	0.06	17,20,23,26	0
4	HEM	B	750	43/43	0.98	0.06	13,17,22,25	0
2	ZN	A	900	1/1	0.99	0.03	25,25,25,25	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.

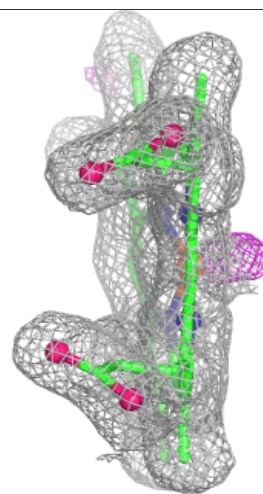
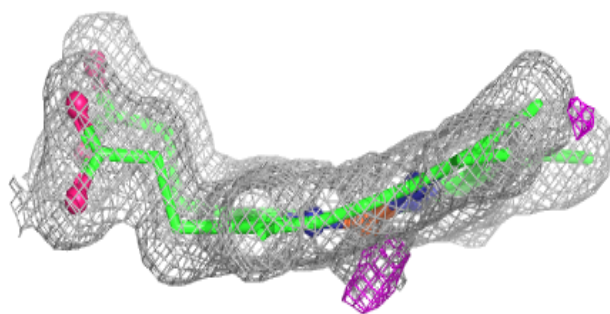
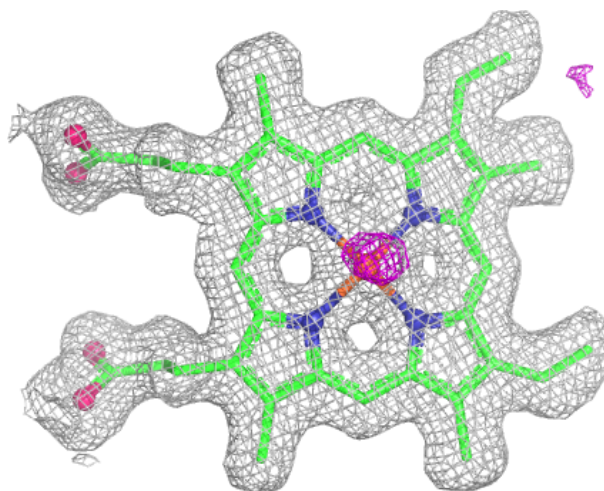
Electron density around HEM A 750:

$2mF_o-DF_c$ (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.