



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:20 PM UTC

PDB ID : 1MMV / pdb_00001mmv
Title : Rat neuronal NOS heme domain with NG-propyl-L-arginine bound
Authors : Bretscher, L.E.; Li, H.; Poulos, T.L.; Griffith, O.W.
Deposited on : 2002-09-04
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

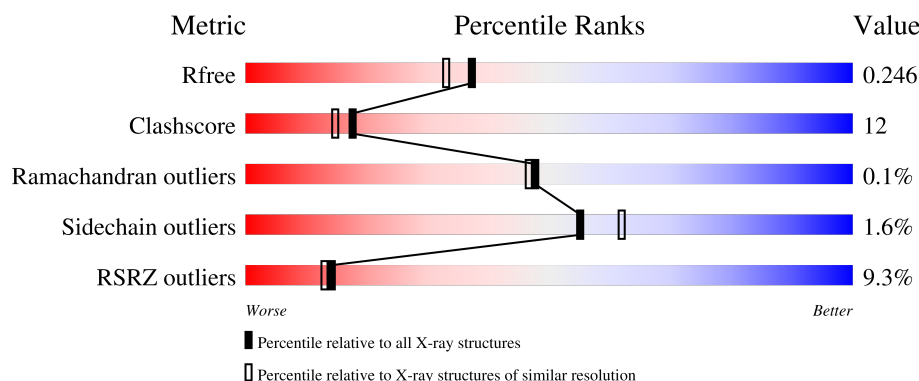
1 Overall quality at a glance

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	419	15% 66% 29% ..
1	B	419	4% 75% 21% ..

2 Entry composition [i](#)

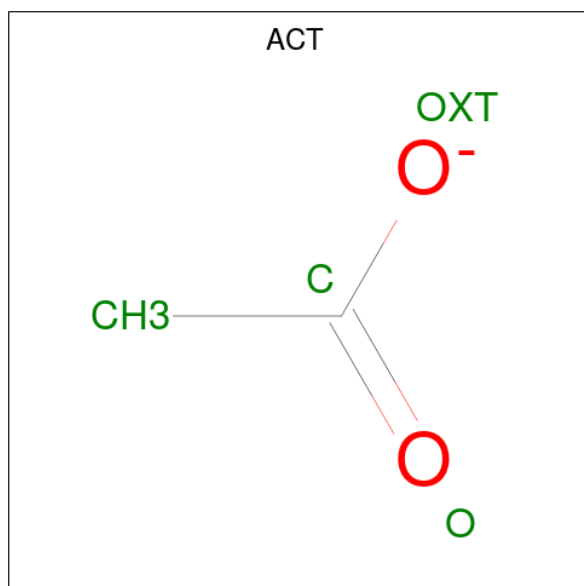
There are 7 unique types of molecules in this entry. The entry contains 7255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	409	Total	C	N	O	S	0	0	0
			3334	2133	572	608	21			

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

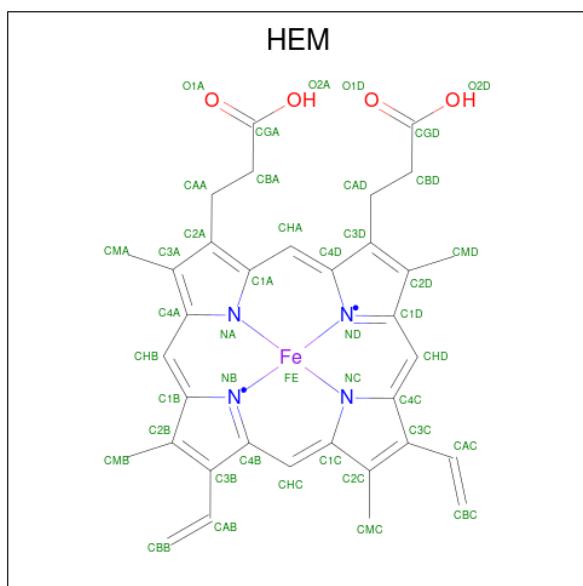


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

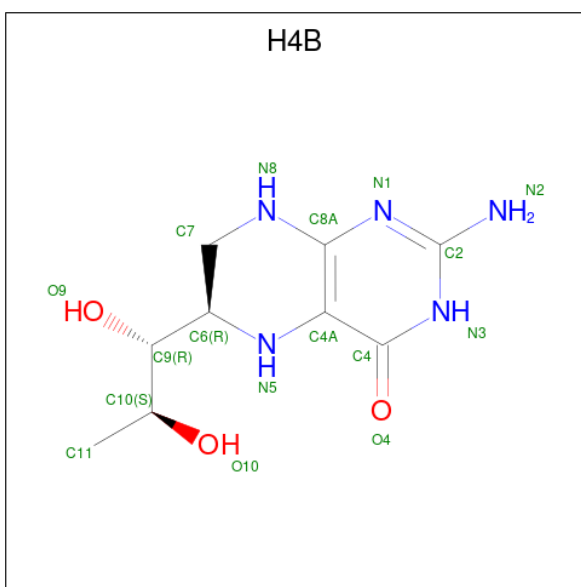
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

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



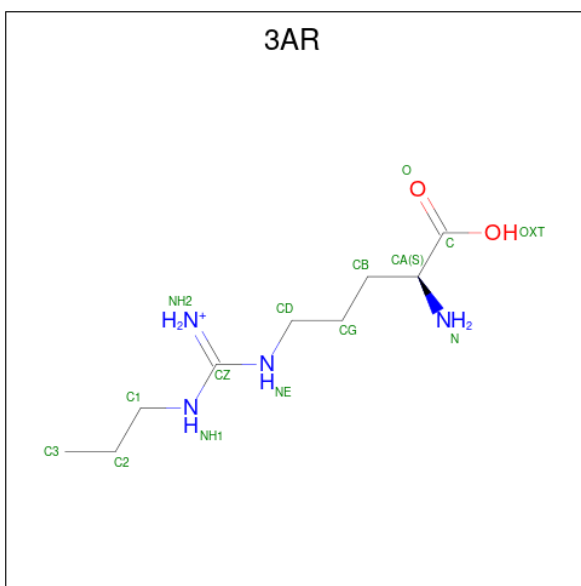
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



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

- Molecule 6 is N-OMEGA-PROPYL-L-ARGININE (CCD ID: 3AR) (formula: $C_9H_{21}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			15	9	4	2		
6	B	1	Total	C	N	O	0	0
			15	9	4	2		

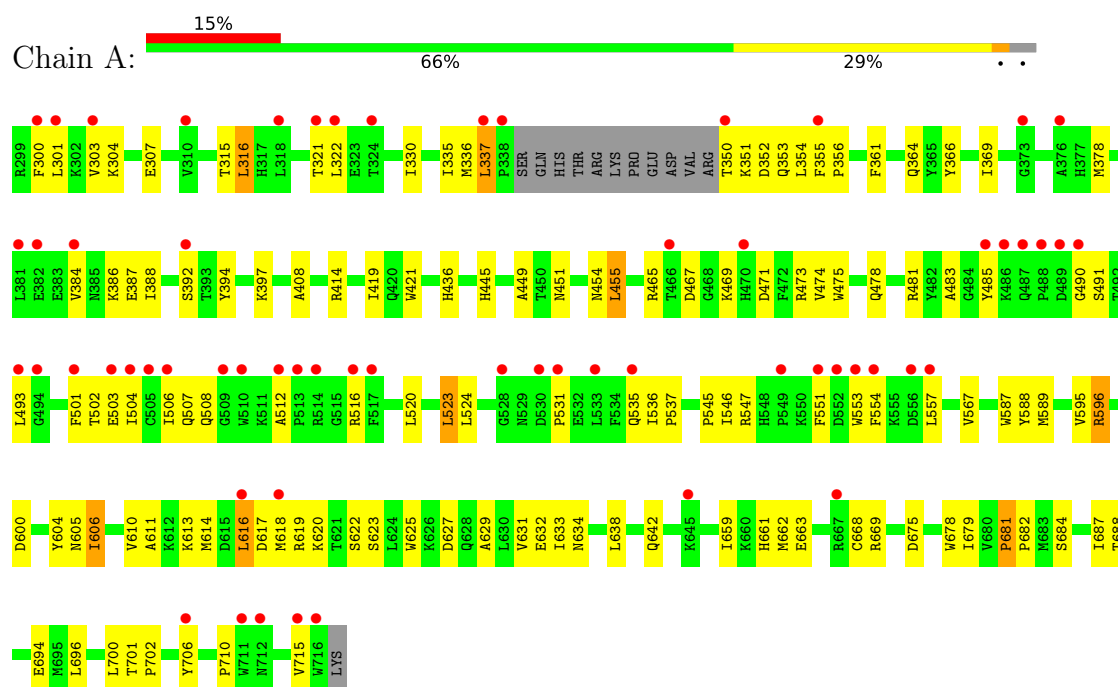
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	209	Total 209	O 209	0	0
7	B	240	Total 240	O 240	0	0

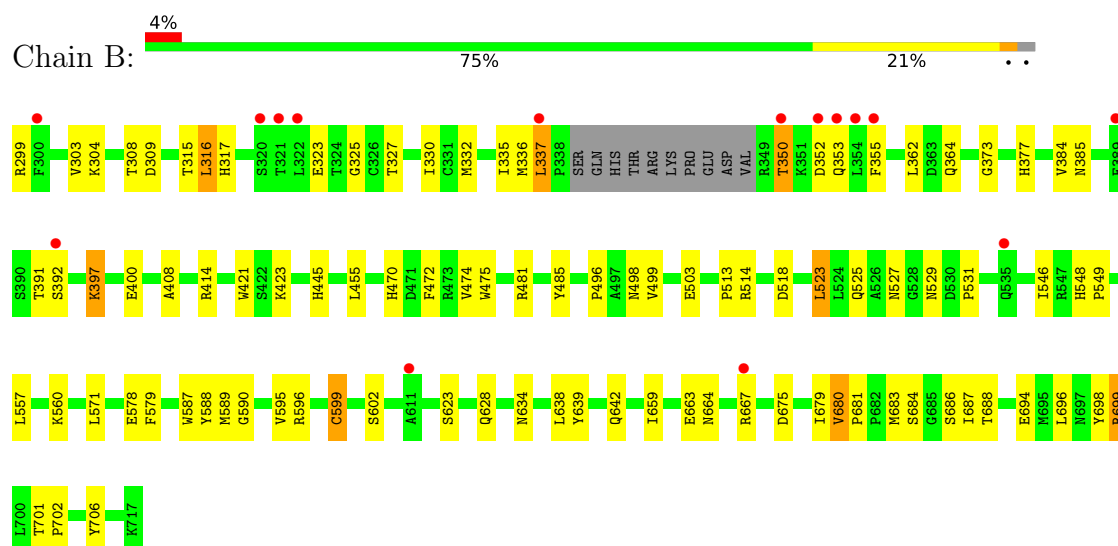
3 Residue-property plots

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	51.59Å 110.36Å 164.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.91 – 2.00 30.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.91-2.00) 96.8 (30.91-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.256 0.215 , 0.246	Depositor DCC
R_{free} test set	3121 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.0	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	7255	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: ACT, 3AR, ZN, HEM, H4B

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	1/3406 (0.0%)	0.90	16/4621 (0.3%)
1	B	0.41	0/3427	0.92	18/4646 (0.4%)
All	All	0.39	1/6833 (0.0%)	0.91	34/9267 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	668	CYS	C-N	-5.94	1.24	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-8.59	95.24	109.24
1	A	589	MET	N-CA-C	-8.27	95.75	109.07
1	A	421	TRP	N-CA-C	7.02	119.83	111.33
1	A	623	SER	N-CA-C	-6.71	105.06	113.18
1	A	688	THR	N-CA-C	-6.48	101.97	110.39
1	B	421	TRP	N-CA-C	6.39	119.06	111.33
1	A	490	GLY	N-CA-C	-6.21	106.85	114.92
1	A	546	ILE	N-CA-C	6.19	117.03	107.99
1	A	354	LEU	N-CA-C	6.09	117.72	111.14
1	B	680	VAL	CA-C-N	6.09	124.11	119.66
1	B	680	VAL	C-N-CA	6.09	124.11	119.66
1	A	474	VAL	N-CA-C	-5.97	99.14	107.80
1	B	596	ARG	N-CA-C	5.92	117.60	111.03
1	B	408	ALA	N-CA-C	-5.82	104.94	111.28
1	B	557	LEU	N-CA-C	-5.79	106.17	113.18
1	B	474	VAL	N-CA-C	-5.76	98.85	107.37
1	B	590	GLY	N-CA-C	5.75	119.84	112.83
1	B	472	PHE	N-CA-C	-5.74	100.34	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	LYS	N-CA-C	-5.68	103.03	110.53
1	A	681	PRO	CA-C-N	5.45	126.17	120.12
1	A	681	PRO	C-N-CA	5.45	126.17	120.12
1	B	588	TYR	N-CA-C	5.38	118.88	110.32
1	A	408	ALA	N-CA-C	-5.38	105.42	111.28
1	B	599	CYS	N-CA-C	5.36	120.68	113.72
1	B	688	THR	N-CA-C	-5.31	102.30	110.32
1	A	588	TYR	N-CA-C	5.31	118.33	110.48
1	B	699	ARG	N-CA-C	5.25	117.80	109.24
1	B	315	THR	N-CA-C	-5.20	107.61	114.31
1	A	596	ARG	N-CA-C	5.14	117.87	111.24
1	A	606	ILE	N-CA-C	5.14	117.92	112.83
1	B	623	SER	N-CA-C	-5.09	106.57	112.89
1	B	397	LYS	N-CA-C	-5.08	103.82	110.53
1	B	455	LEU	N-CA-C	5.03	117.34	110.24
1	A	455	LEU	N-CA-C	5.02	117.31	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	3313	0	3221	102	0
1	B	3334	0	3247	65	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	43	0	30	5	0
4	B	43	0	30	6	0
5	A	17	0	15	0	0
5	B	17	0	15	2	0
6	A	15	0	20	2	0
6	B	15	0	20	2	0
7	A	209	0	0	8	0
7	B	240	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7255	0	6604	166	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 (166) 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	1.35	1.07
1:B:373:GLY:H	1:B:377:HIS:HD2	1.03	1.00
1:B:523:LEU:HD22	1:B:531:PRO:HB2	1.47	0.94
1:B:373:GLY:H	1:B:377:HIS:CD2	1.93	0.85
1:A:378:MET:HA	1:A:378:MET:HE2	1.61	0.83
1:A:350:THR:HB	1:A:353:GLN:HG3	1.66	0.77
4:A:1750:HEM:HBA2	6:A:1785:3AR:HD2	1.66	0.77
4:B:2750:HEM:HBD1	7:B:3067:HOH:O	1.83	0.76
4:B:2750:HEM:HBC2	4:B:2750:HEM:HMC2	1.73	0.71
1:B:706:TYR:OH	4:B:2750:HEM:O1D	2.09	0.69
1:B:549:PRO:HG3	1:B:639:TYR:CG	2.28	0.68
1:B:325:GLY:O	1:B:332:MET:HE2	1.93	0.68
1:A:596:ARG:O	1:A:600:ASP:HB2	1.94	0.68
1:A:595:VAL:HG23	1:A:634:ASN:HD21	1.58	0.68
1:B:499:VAL:O	1:B:503:GLU:HG3	1.93	0.67
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.76	0.66
1:B:659:ILE:O	1:B:663:GLU:HG3	1.96	0.65
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.77	0.65
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.12	0.64
1:A:316:LEU:HD11	1:A:669:ARG:HD3	1.80	0.64
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.80	0.63
4:A:1750:HEM:HBC2	4:A:1750:HEM:HMC2	1.81	0.63
1:A:350:THR:HG22	1:A:352:ASP:H	1.65	0.62
1:B:664:ASN:O	1:B:667:ARG:HG2	2.00	0.62
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.82	0.61
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.82	0.61
1:B:587:TRP:H	4:B:2750:HEM:HAB	1.66	0.61
1:A:304:LYS:O	1:A:694:GLU:HG3	2.01	0.60
1:A:321:THR:HG23	1:A:322:LEU:N	2.16	0.60
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.83	0.60
1:A:675:ASP:O	1:A:679:ILE:HG12	2.02	0.60
1:A:467:ASP:OD2	1:A:469:LYS:HB2	2.01	0.60
1:B:373:GLY:N	1:B:377:HIS:HD2	1.88	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.85	0.59
4:A:1750:HEM:HBD1	7:A:2039:HOH:O	2.02	0.59
1:A:620:LYS:HE3	1:A:622:SER:OG	2.03	0.59
1:A:682:PRO:HG3	7:A:1862:HOH:O	2.02	0.59
1:B:323:GLU:O	1:B:699:ARG:HD3	2.03	0.58
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.19	0.58
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.86	0.58
1:B:391:THR:O	1:B:392:SER:HB2	2.04	0.58
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.86	0.58
1:A:516:ARG:HH11	1:A:516:ARG:HG3	1.69	0.57
1:A:350:THR:HB	1:A:353:GLN:CG	2.34	0.57
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.86	0.57
1:B:337:LEU:N	1:B:337:LEU:HD23	2.20	0.57
1:A:706:TYR:OH	4:A:1750:HEM:O1D	2.19	0.57
1:A:491:SER:HB2	7:A:2055:HOH:O	2.05	0.56
1:B:350:THR:HG22	1:B:352:ASP:H	1.70	0.56
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.40	0.56
1:B:701:THR:HA	1:B:702:PRO:C	2.31	0.55
1:A:524:LEU:O	1:A:531:PRO:HA	2.06	0.55
1:A:659:ILE:O	1:A:663:GLU:HG3	2.07	0.55
1:A:595:VAL:HG11	1:A:682:PRO:HB2	1.89	0.54
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.22	0.54
1:A:436:HIS:HB2	7:A:1955:HOH:O	2.08	0.54
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.89	0.54
1:B:336:MET:HE2	5:B:2760:H4B:H9	1.89	0.54
1:A:307:GLU:HG3	7:B:2905:HOH:O	2.08	0.53
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.37	0.53
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.89	0.53
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.73	0.53
1:A:351:LYS:HE2	1:A:392:SER:CB	2.38	0.53
7:A:1898:HOH:O	1:B:337:LEU:HD23	2.09	0.52
1:B:304:LYS:O	1:B:694:GLU:HG3	2.09	0.52
1:B:595:VAL:HG23	1:B:634:ASN:HD21	1.73	0.52
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.39	0.52
4:B:2750:HEM:HBA2	6:B:2785:3AR:HD2	1.92	0.52
1:A:361:PHE:O	1:A:364:GLN:HG2	2.09	0.51
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.24	0.51
1:A:353:GLN:O	1:A:356:PRO:HD2	2.11	0.51
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.40	0.51
1:B:414:ARG:NH1	1:B:706:TYR:OH	2.44	0.50
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:VAL:O	1:A:614:MET:HG3	2.11	0.50
1:B:332:MET:HB3	1:B:335:ILE:HG13	1.94	0.50
1:A:715:VAL:O	1:A:715:VAL:HG23	2.12	0.50
1:A:300:PHE:CD2	1:A:315:THR:HG22	2.46	0.50
1:A:595:VAL:HG23	1:A:634:ASN:ND2	2.26	0.49
1:A:504:ILE:O	1:A:508:GLN:HB2	2.12	0.49
1:A:321:THR:HG23	1:A:322:LEU:H	1.76	0.49
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.75	0.49
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.42	0.49
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.28	0.49
1:A:617:ASP:OD1	1:A:619:ARG:NE	2.42	0.49
1:B:299:ARG:HB3	1:B:299:ARG:HH11	1.77	0.49
1:A:337:LEU:HD12	1:A:337:LEU:O	2.13	0.48
1:A:701:THR:HA	1:A:702:PRO:C	2.38	0.48
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.95	0.48
1:B:445:HIS:C	1:B:445:HIS:CD2	2.92	0.48
1:B:675:ASP:O	1:B:679:ILE:HG12	2.13	0.48
1:B:638:LEU:O	1:B:642:GLN:HG3	2.13	0.48
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.44	0.48
1:A:330:ILE:CD1	1:B:696:LEU:HD22	2.42	0.48
1:A:618:MET:HE3	1:A:625:TRP:CZ3	2.48	0.48
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.49	0.47
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.49	0.47
1:A:414:ARG:HD3	1:A:678:TRP:CD2	2.49	0.47
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.96	0.47
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.97	0.47
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.39	0.47
1:B:350:THR:HB	1:B:353:GLN:CD	2.39	0.47
1:B:684:SER:HB3	1:B:687:ILE:HG12	1.96	0.47
1:A:483:ALA:HB1	1:A:502:THR:CG2	2.45	0.47
1:B:571:LEU:HD12	1:B:579:PHE:C	2.40	0.47
1:A:535:GLN:NE2	7:A:2020:HOH:O	2.49	0.46
1:B:316:LEU:HB3	1:B:698:TYR:OH	2.15	0.46
1:A:553:TRP:CE3	1:A:613:LYS:HD3	2.50	0.46
1:A:449:ALA:O	1:A:455:LEU:HA	2.15	0.46
1:A:353:GLN:C	1:A:356:PRO:HD2	2.40	0.46
1:A:614:MET:CE	1:A:632:GLU:HG3	2.46	0.46
1:B:364:GLN:NE2	7:B:3043:HOH:O	2.48	0.45
1:A:516:ARG:HG3	1:A:516:ARG:NH1	2.31	0.45
1:A:604:TYR:O	1:A:605:ASN:C	2.59	0.45
1:A:316:LEU:HD11	1:A:669:ARG:CD	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ALA:HA	1:A:616:LEU:HD11	1.98	0.45
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.15	0.45
1:A:303:VAL:CG1	1:A:694:GLU:O	2.65	0.45
1:A:629:ALA:O	1:A:633:ILE:HG13	2.17	0.45
1:A:507:GLN:O	1:A:507:GLN:HG2	2.16	0.45
1:A:567:VAL:HG23	6:A:1785:3AR:H32	1.99	0.44
1:B:308:THR:O	1:B:309:ASP:HB2	2.16	0.44
1:B:336:MET:CE	5:B:2760:H4B:H9	2.47	0.44
1:A:445:HIS:C	1:A:445:HIS:CD2	2.95	0.44
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.53	0.44
1:A:316:LEU:HD22	1:A:700:LEU:HD11	1.99	0.44
1:A:451:ASN:HB3	1:A:454:ASN:O	2.17	0.44
1:B:525:GLN:HG3	1:B:529:ASN:O	2.17	0.43
1:A:502:THR:O	1:A:506:ILE:HG13	2.18	0.43
1:B:496:PRO:HB2	1:B:602:SER:O	2.18	0.43
1:B:571:LEU:HD11	1:B:578:GLU:HB3	2.01	0.43
1:A:321:THR:CG2	1:A:322:LEU:N	2.82	0.43
1:A:638:LEU:O	1:A:642:GLN:HG3	2.18	0.43
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.83	0.43
1:A:536:ILE:O	1:A:537:PRO:C	2.60	0.43
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.53	0.43
1:A:606:ILE:HA	7:A:1948:HOH:O	2.18	0.42
1:A:386:LYS:HA	1:A:386:LYS:HD3	1.87	0.42
1:A:627:ASP:OD2	1:B:683:MET:HE2	2.20	0.42
1:A:551:PHE:CD2	1:A:551:PHE:N	2.86	0.42
1:B:327:THR:OG1	1:B:330:ILE:HG22	2.19	0.42
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.90	0.42
1:A:503:GLU:HG3	7:A:2054:HOH:O	2.19	0.42
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.01	0.42
1:A:300:PHE:HD2	1:A:315:THR:HG22	1.84	0.42
1:A:682:PRO:HB3	1:B:686:SER:HB3	2.02	0.42
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.02	0.41
4:A:1750:HEM:HBC2	4:A:1750:HEM:CMC	2.49	0.41
1:A:501:PHE:CD2	1:A:520:LEU:HD13	2.53	0.41
1:A:681:PRO:HA	1:A:682:PRO:HD3	1.77	0.41
1:B:481:ARG:HD3	1:B:498:ASN:ND2	2.36	0.41
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.50	0.41
1:B:397:LYS:HB2	1:B:400:GLU:HG3	2.02	0.41
1:A:384:VAL:O	1:A:388:ILE:HG13	2.21	0.41
4:B:2750:HEM:CBA	6:B:2785:3AR:HD2	2.50	0.41
1:A:303:VAL:HG11	1:A:694:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ILE:HB	1:A:661:HIS:HB2	2.03	0.41
1:A:465:ARG:NE	1:A:471:ASP:OD2	2.47	0.41
1:B:548:HIS:ND1	1:B:549:PRO:HD2	2.36	0.41
1:B:571:LEU:HD12	1:B:579:PHE:O	2.21	0.41
1:A:506:ILE:C	1:A:508:GLN:H	2.29	0.40
1:B:595:VAL:O	1:B:599:CYS:HB2	2.21	0.40
1:A:350:THR:HG22	1:A:352:ASP:N	2.35	0.40
1:A:554:PHE:O	1:A:557:LEU:HD12	2.20	0.40
1:A:506:ILE:C	1:A:508:GLN:N	2.79	0.40
1:B:317:HIS:HB3	1:B:698:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/419 (96%)	378 (94%)	25 (6%)	0	100	100
1	B	405/419 (97%)	389 (96%)	15 (4%)	1 (0%)	43	42
All	All	808/838 (96%)	767 (95%)	40 (5%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	THR

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%)	356 (98%)	7 (2%)	50	56
1	B	365/375 (97%)	360 (99%)	5 (1%)	59	66
All	All	728/750 (97%)	716 (98%)	12 (2%)	55	62

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	336	MET
1	A	337	LEU
1	A	493	LEU
1	A	523	LEU
1	A	616	LEU
1	A	662	MET
1	B	303	VAL
1	B	316	LEU
1	B	337	LEU
1	B	423	LYS
1	B	523	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) 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
1	A	500	GLN
1	A	634	ASN
1	A	697	ASN
1	B	364	GLN
1	B	377	HIS
1	B	385	ASN
1	B	451	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN

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Mol	Chain	Res	Type
1	B	628	GLN
1	B	634	ASN
1	B	642	GLN
1	B	664	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	$\# Z > 2$
4	HEM	A	1750	1	50,50,50	1.08	4 (8%)	67,82,82	1.06	3 (4%)
2	ACT	A	1860	-	3,3,3	0.92	0	3,3,3	0.84	0
5	H4B	B	2760	-	17,18,18	1.64	2 (11%)	14,26,26	1.96	4 (28%)
6	3AR	A	1785	-	10,14,14	1.11	0	13,16,16	1.41	2 (15%)
6	3AR	B	2785	-	10,14,14	1.16	1 (10%)	13,16,16	1.46	2 (15%)
2	ACT	B	2860	-	3,3,3	1.03	0	3,3,3	0.74	0
4	HEM	B	2750	1	50,50,50	1.05	2 (4%)	67,82,82	1.10	2 (2%)
5	H4B	A	1760	-	17,18,18	1.55	2 (11%)	14,26,26	2.01	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
4	HEM	A	1750	1	-	4/14/54/54	-
5	H4B	B	2760	-	-	0/8/17/17	0/2/2/2
6	3AR	A	1785	-	-	4/15/15/15	-
6	3AR	B	2785	-	-	5/15/15/15	-
4	HEM	B	2750	1	-	4/14/54/54	-
5	H4B	A	1760	-	-	0/8/17/17	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1760	H4B	C4A-N5	4.06	1.47	1.37
5	B	2760	H4B	C4A-N5	3.73	1.46	1.37
5	B	2760	H4B	C6-N5	3.57	1.53	1.47
5	A	1760	H4B	C6-N5	3.36	1.53	1.47
4	B	2750	HEM	CAB-C3B	-2.96	1.39	1.47
4	A	1750	HEM	CAB-C3B	-2.59	1.40	1.47
4	A	1750	HEM	CAC-C3C	-2.39	1.41	1.47
6	B	2785	3AR	OXT-C	-2.22	1.23	1.30
4	A	1750	HEM	FE-NB	2.21	2.01	1.94
4	A	1750	HEM	CMC-C2C	2.16	1.55	1.50
4	B	2750	HEM	FE-NA	2.04	2.01	1.95

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1760	H4B	C2-N1-C8A	5.29	122.70	113.36
5	B	2760	H4B	C2-N1-C8A	5.13	122.42	113.36
4	B	2750	HEM	CBA-CAA-C2A	-3.91	101.73	112.53
4	A	1750	HEM	CBA-CAA-C2A	-3.60	102.58	112.53
6	B	2785	3AR	NH1-CZ-NE	3.39	124.04	119.28
6	A	1785	3AR	NH1-CZ-NE	3.33	123.95	119.28
5	A	1760	H4B	O10-C10-C9	-3.28	104.33	109.77
5	B	2760	H4B	O10-C10-C9	-3.19	104.50	109.77
5	A	1760	H4B	N3-C2-N1	-2.89	118.03	123.32
5	B	2760	H4B	N3-C2-N1	-2.86	118.08	123.32
6	B	2785	3AR	C1-NH1-CZ	-2.58	118.73	123.46
6	A	1785	3AR	C1-NH1-CZ	-2.37	119.11	123.46
4	B	2750	HEM	C2B-C1B-NB	2.29	112.47	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1750	HEM	CAB-C3B-C2B	-2.11	121.56	128.43
4	A	1750	HEM	C3B-C4B-NB	2.05	110.94	109.47
5	B	2760	H4B	O9-C9-C6	2.04	114.16	109.28
5	A	1760	H4B	O9-C9-C6	2.01	114.10	109.28

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2750	HEM	C2B-C3B-CAB-CBB
6	B	2785	3AR	NE-CZ-NH1-C1
6	B	2785	3AR	NH2-CZ-NH1-C1
6	B	2785	3AR	CA-CB-CG-CD
6	A	1785	3AR	NE-CD-CG-CB
6	A	1785	3AR	CA-CB-CG-CD
6	B	2785	3AR	NE-CD-CG-CB
6	B	2785	3AR	NH1-C1-C2-C3
4	B	2750	HEM	C4B-C3B-CAB-CBB
6	A	1785	3AR	NE-CZ-NH1-C1
6	A	1785	3AR	NH2-CZ-NH1-C1
4	A	1750	HEM	CAD-CBD-CGD-O2D
4	A	1750	HEM	CAA-CBA-CGA-O2A
4	A	1750	HEM	CAA-CBA-CGA-O1A
4	A	1750	HEM	CAD-CBD-CGD-O1D
4	B	2750	HEM	CAD-CBD-CGD-O2D
4	B	2750	HEM	CAD-CBD-CGD-O1D

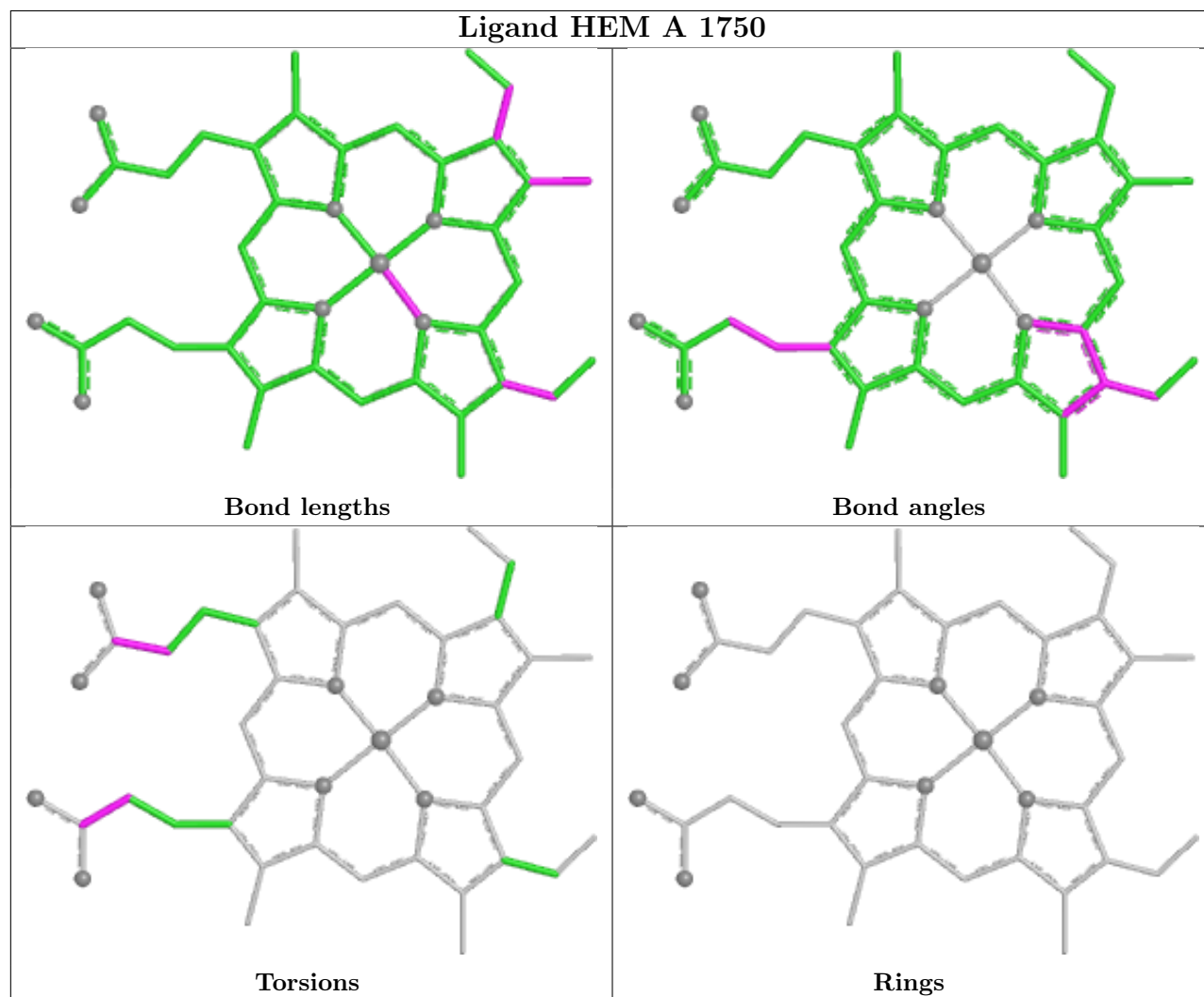
There are no ring outliers.

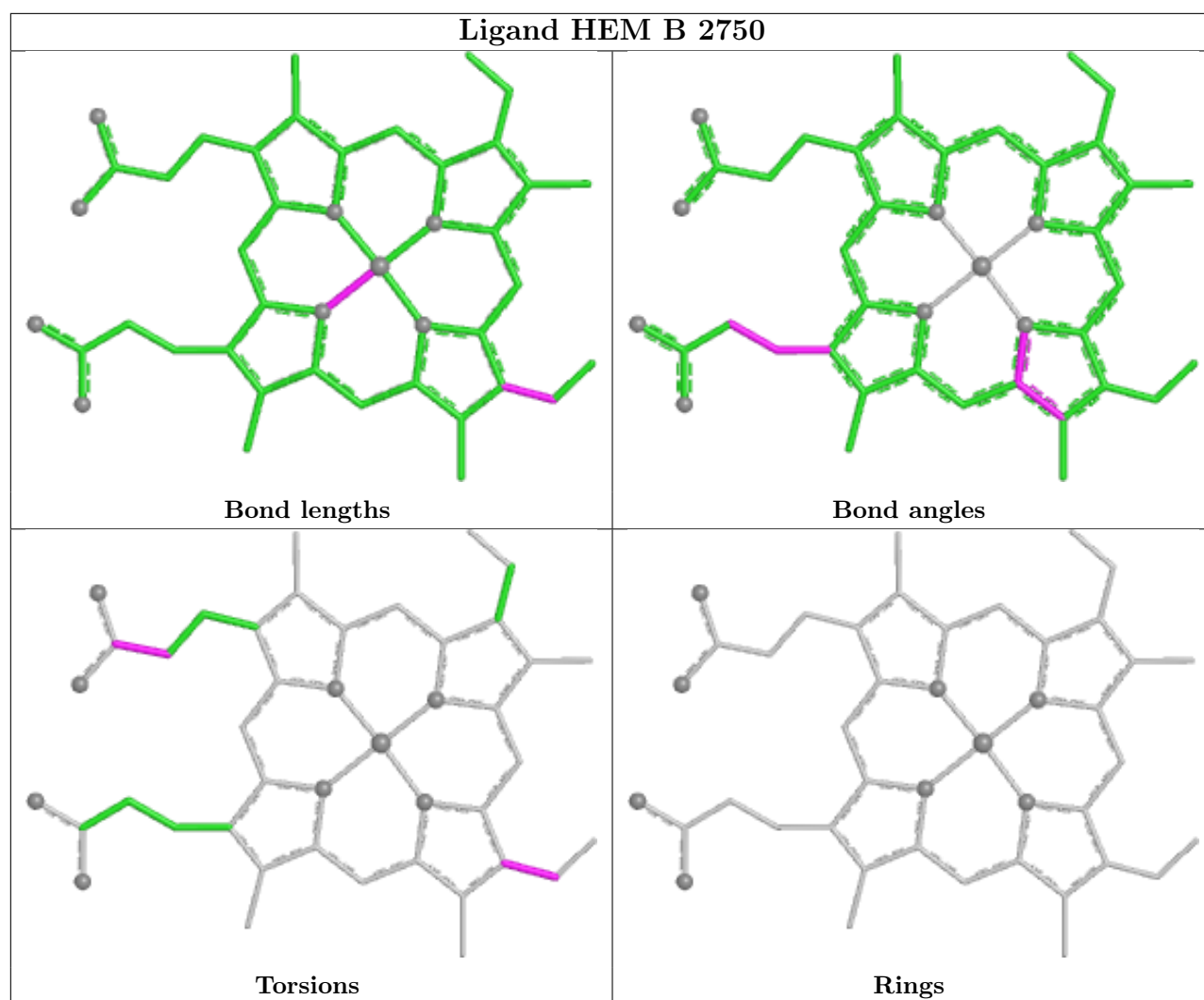
5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1750	HEM	5	0
5	B	2760	H4B	2	0
6	A	1785	3AR	2	0
6	B	2785	3AR	2	0
4	B	2750	HEM	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/419 (97%)	0.81	61 (14%) 5 5	20, 40, 71, 87	0
1	B	409/419 (97%)	0.21	15 (3%) 45 44	18, 32, 60, 89	0
All	All	816/838 (97%)	0.51	76 (9%) 14 13	18, 36, 64, 89	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	THR	6.0
1	A	322	LEU	6.0
1	A	715	VAL	5.1
1	B	350	THR	4.6
1	B	322	LEU	4.5
1	B	352	ASP	4.4
1	A	300	PHE	4.2
1	A	486	LYS	4.2
1	A	321	THR	3.8
1	A	355	PHE	3.8
1	B	392	SER	3.6
1	A	716	TRP	3.6
1	A	493	LEU	3.5
1	A	505	CYS	3.5
1	A	512	ALA	3.4
1	A	350	THR	3.4
1	A	310	VAL	3.4
1	A	488	PRO	3.3
1	A	552	ASP	3.3
1	A	338	PRO	3.3
1	A	506	ILE	3.2
1	A	513	PRO	3.2
1	A	303	VAL	3.1
1	A	551	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	485	TYR	3.0
1	B	300	PHE	3.0
1	A	533	LEU	2.9
1	B	611	ALA	2.9
1	A	301	LEU	2.8
1	A	324	THR	2.8
1	A	504	ILE	2.8
1	B	353	GLN	2.8
1	A	528	GLY	2.7
1	A	509	GLY	2.7
1	A	382	GLU	2.7
1	A	384	VAL	2.7
1	A	376	ALA	2.6
1	A	554	PHE	2.6
1	B	354	LEU	2.6
1	A	557	LEU	2.6
1	A	556	ASP	2.5
1	A	392	SER	2.5
1	B	667	ARG	2.5
1	A	706	TYR	2.5
1	B	320	SER	2.5
1	A	337	LEU	2.5
1	A	553	TRP	2.5
1	A	470	HIS	2.4
1	A	494	GLY	2.4
1	B	389	GLU	2.4
1	A	667	ARG	2.4
1	A	490	GLY	2.4
1	A	517	PHE	2.4
1	A	487	GLN	2.3
1	A	711	TRP	2.3
1	A	373	GLY	2.3
1	B	337	LEU	2.3
1	B	355	PHE	2.3
1	A	531	PRO	2.3
1	A	549	PRO	2.3
1	A	530	ASP	2.3
1	A	516	ARG	2.2
1	A	712	ASN	2.2
1	A	381	LEU	2.2
1	A	501	PHE	2.2
1	B	535	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	318	LEU	2.2
1	A	618	MET	2.2
1	A	489	ASP	2.1
1	A	466	THR	2.1
1	A	535	GLN	2.1
1	A	510	TRP	2.1
1	A	616	LEU	2.0
1	A	645	LYS	2.0
1	A	503	GLU	2.0
1	A	514	ARG	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](#)

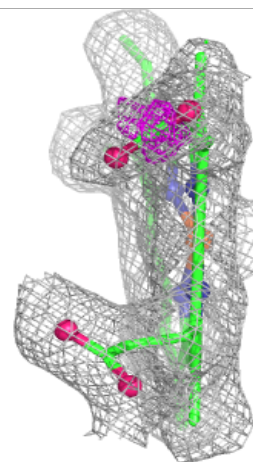
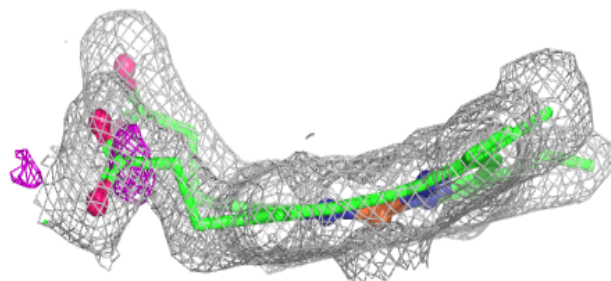
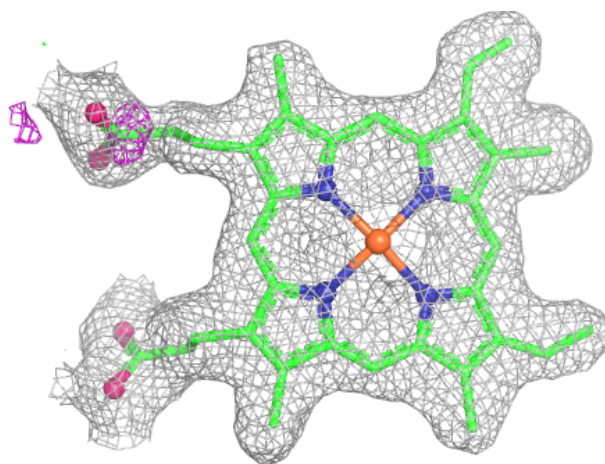
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	1860	4/4	0.91	0.14	40,43,44,44	0
2	ACT	B	2860	4/4	0.94	0.08	33,33,35,37	0
5	H4B	A	1760	17/17	0.94	0.07	26,29,33,34	0
5	H4B	B	2760	17/17	0.95	0.07	23,26,33,34	0
6	3AR	A	1785	15/15	0.95	0.07	22,25,27,30	0
6	3AR	B	2785	15/15	0.95	0.07	17,23,28,28	0
4	HEM	A	1750	43/43	0.97	0.07	23,27,34,39	0
4	HEM	B	2750	43/43	0.98	0.06	20,23,34,42	0
3	ZN	A	900	1/1	0.99	0.04	34,34,34,34	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.

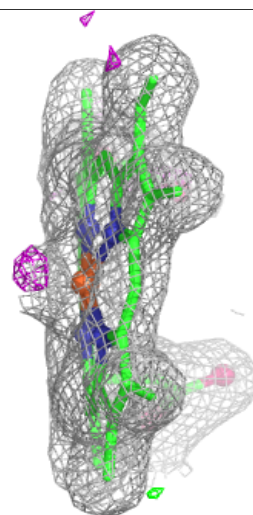
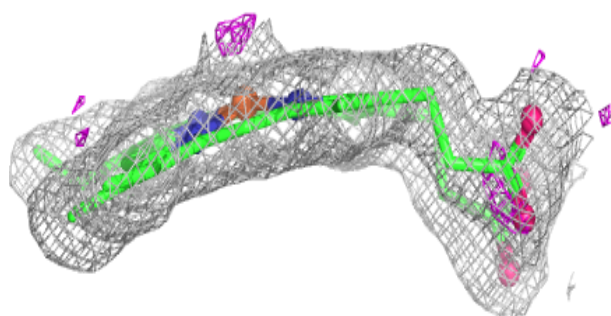
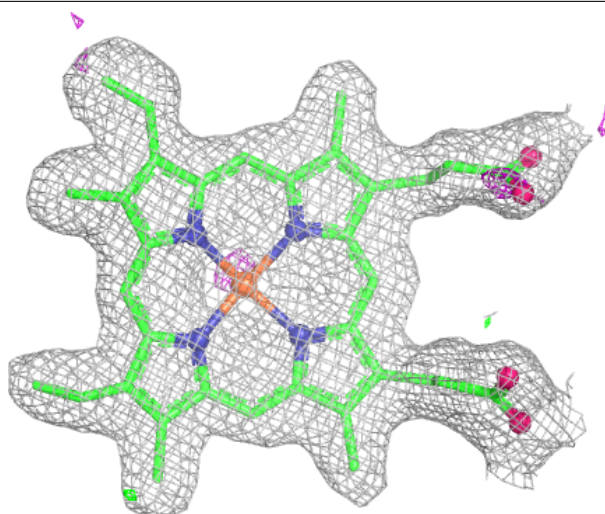
Electron density around HEM A 1750:

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



Electron density around HEM B 2750:

$2mF_o-DF_c$ (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.