



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 10:05 AM EST

PDB ID : 1MMV
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

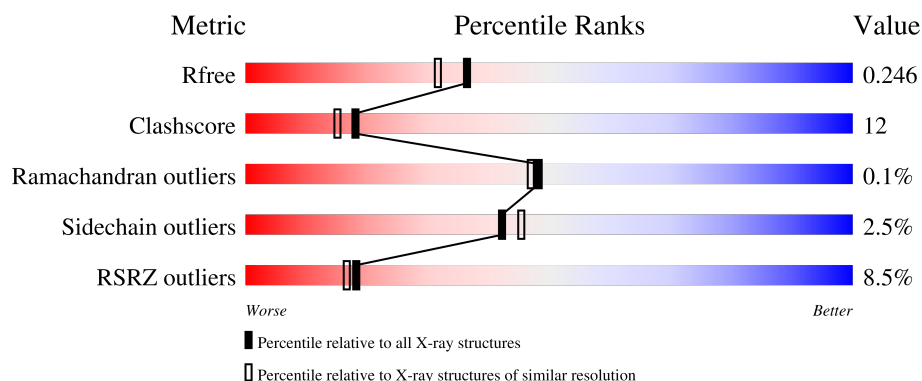
1 Overall quality at a glance

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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	
1	B	419	

2 Entry composition [i](#)

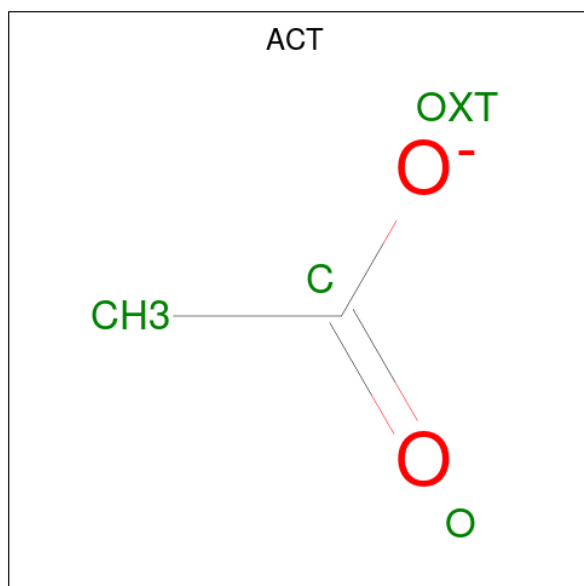
There are 7 unique types of molecules in this entry. The entry contains 7255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: ACT) (formula: C₂H₃O₂).

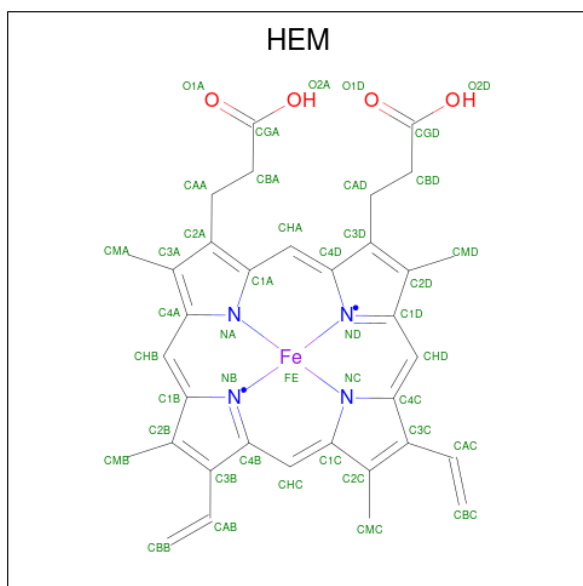


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

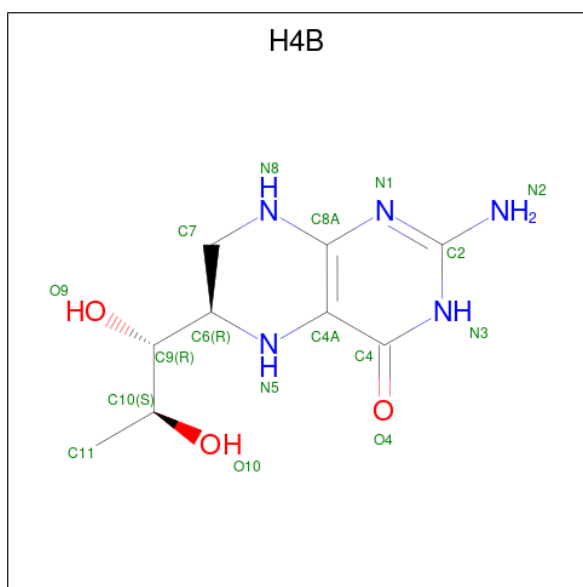
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

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



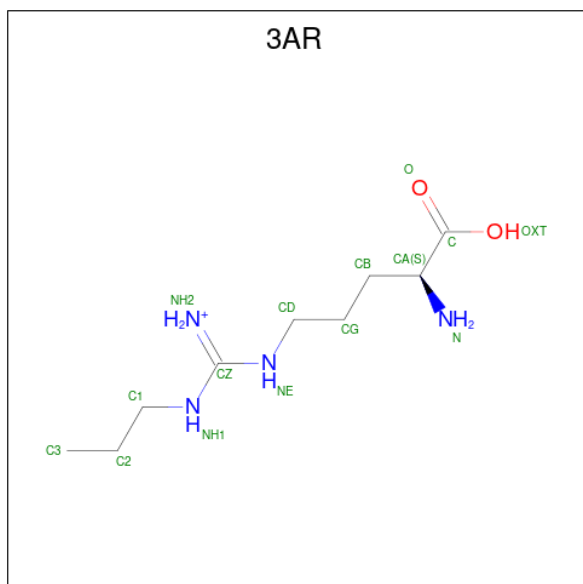
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: 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 (three-letter code: 3AR) (formula: $C_9H_{21}N_4O_2$).



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

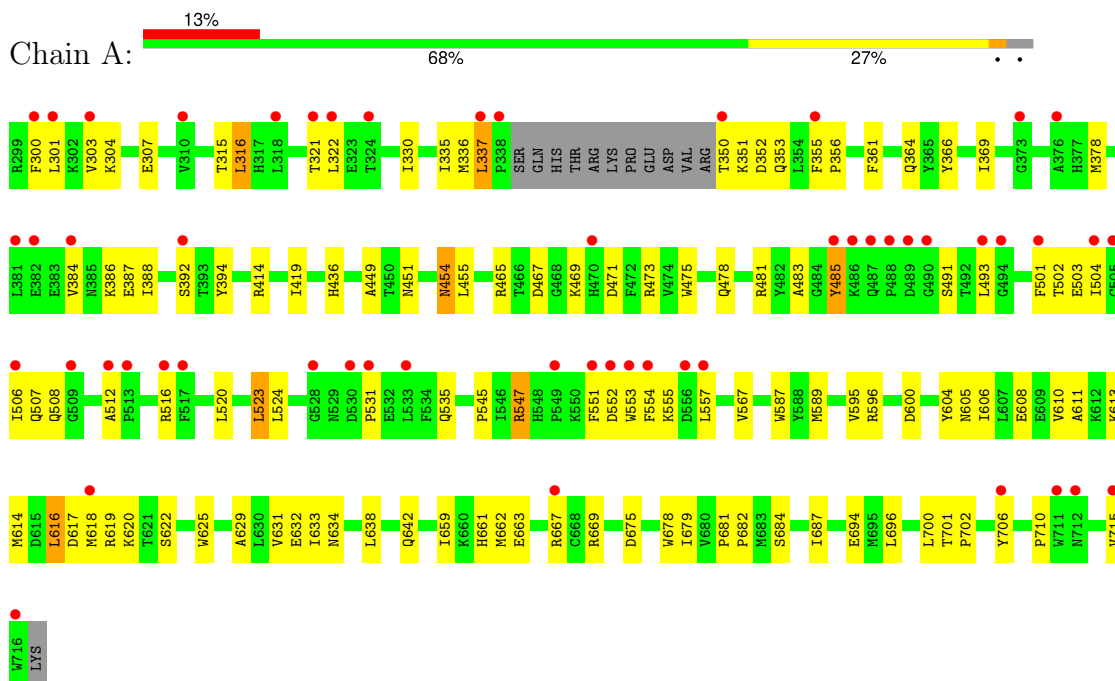
- Molecule 7 is water.

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

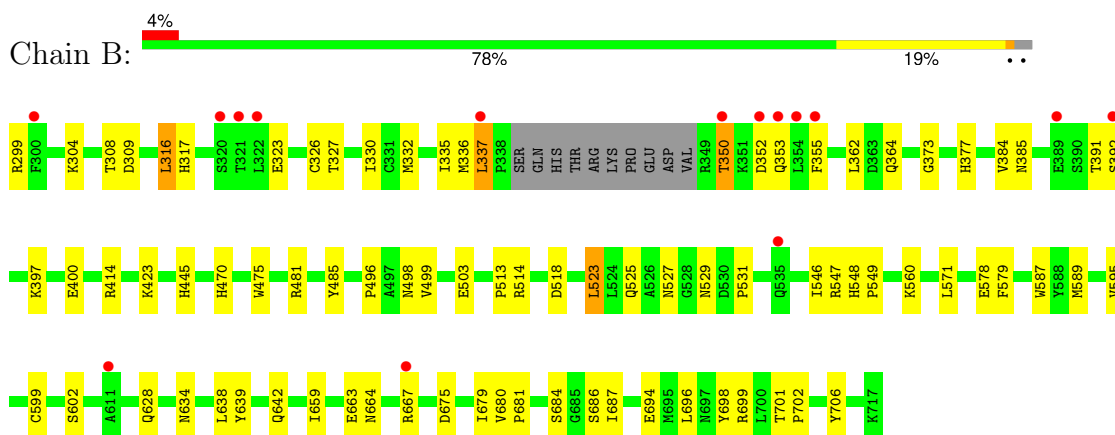
3 Residue-property plots

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H4B, HEM, 3AR, ZN, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/3406	0.57	1/4621 (0.0%)
1	B	0.34	0/3427	0.60	2/4646 (0.0%)
All	All	0.34	0/6833	0.59	3/9267 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-5.84	95.24	111.00
1	A	589	MET	N-CA-C	-5.65	95.75	111.00
1	B	326	CYS	CA-CB-SG	5.07	123.13	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	98	0
1	B	3334	0	3247	63	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	7255	0	6604	161	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 (161) 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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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:A:551:PHE:HE1	1:A:614:MET:HE3	1.75	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:B:336:MET:HE2	5:B:2760:H4B:H9	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:MET:HA	1:A:378:MET:CE	2.41	0.50
1:B:414:ARG:NH1	1:B:706:TYR:OH	2.44	0.50
1:B:701:THR:HA	1:B:702:PRO:C	2.31	0.50
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.93	0.50
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:614:MET:HE3	1:A:632:GLU:HG3	1.95	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:B:475:TRP:HB2	1:B:523:LEU:HB3	1.95	0.48
1:A:706:TYR:OH	4:A:1750:HEM:O1D	2.19	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: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: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: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: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:316:LEU:HD11	1:A:669:ARG:CD	2.44	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:701:THR:HA	1:A:702:PRO:C	2.38	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:B:445:HIS:CD2	1:B:445:HIS:C	2.92	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: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:B:513:PRO:HG2	1:B:518:ASP:CG	2.39	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:350:THR:HB	1:B:353:GLN:CD	2.39	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:B:571:LEU:HD12	1:B:579:PHE:C	2.40	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:A:353:GLN:C	1:A:356:PRO:HD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:VAL:HG11	1:A:694:GLU:O	2.21	0.41
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
4:B:2750:HEM:HMC1	4:B:2750:HEM:HBC2	2.02	0.41
1:A:604:TYR:O	1:A:605:ASN:C	2.59	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:B:317:HIS:HB3	1:B:698:TYR:CE2	2.56	0.40
1:A:608:GLU:HA	1:A:618:MET:HE3	2.03	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%)	44	42
All	All	808/838 (96%)	767 (95%)	40 (5%)	1 (0%)	48	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	THR

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	363/375 (97%)	350 (96%)	13 (4%)	30	30
1	B	365/375 (97%)	360 (99%)	5 (1%)	62	68
All	All	728/750 (97%)	710 (98%)	18 (2%)	42	45

All (18) 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	454	ASN
1	A	485	TYR
1	A	493	LEU
1	A	523	LEU
1	A	547	ARG
1	A	552	ASP
1	A	555	LYS
1	A	616	LEU
1	A	662	MET
1	A	667	ARG
1	B	316	LEU
1	B	337	LEU
1	B	423	LYS
1	B	523	LEU
1	B	547	ARG

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	407	HIS
1	A	425	GLN
1	A	451	ASN

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Mol	Chain	Res	Type
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	425	GLN
1	B	451	ASN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	527	ASN
1	B	535	GLN
1	B	634	ASN
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
5	H4B	A	1760	-	16,18,18	2.24	4 (25%)	14,26,26	3.85	9 (64%)
4	HEM	B	2750	1	42,50,50	1.28	5 (11%)	46,82,82	1.45	2 (4%)
4	HEM	A	1750	1	42,50,50	1.18	4 (9%)	46,82,82	1.48	4 (8%)
6	3AR	B	2785	-	10,14,14	1.16	1 (10%)	13,16,16	1.46	2 (15%)
5	H4B	B	2760	-	16,18,18	2.30	4 (25%)	14,26,26	3.88	9 (64%)
2	ACT	A	1860	-	3,3,3	0.92	0	3,3,3	0.84	0
2	ACT	B	2860	-	3,3,3	1.03	0	3,3,3	0.74	0
6	3AR	A	1785	-	10,14,14	1.11	0	13,16,16	1.41	2 (15%)

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	1760	-	-	0/8/17/17	0/2/2/2
4	HEM	B	2750	1	-	4/12/54/54	-
4	HEM	A	1750	1	-	4/12/54/54	-
6	3AR	B	2785	-	-	5/15/15/15	-
5	H4B	B	2760	-	-	0/8/17/17	0/2/2/2
6	3AR	A	1785	-	-	4/15/15/15	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2760	H4B	C4-N3	5.57	1.42	1.33
5	A	1760	H4B	C4-N3	5.35	1.42	1.33
5	A	1760	H4B	C4A-N5	4.66	1.47	1.37
5	B	2760	H4B	C6-N5	4.34	1.53	1.45
5	B	2760	H4B	C4A-N5	4.27	1.46	1.37
5	A	1760	H4B	C6-N5	4.12	1.53	1.45
4	B	2750	HEM	CAB-C3B	-2.96	1.39	1.47
4	A	1750	HEM	C3C-CAC	-2.79	1.41	1.47
4	A	1750	HEM	CAB-C3B	-2.59	1.40	1.47
4	B	2750	HEM	C3C-C2C	-2.58	1.36	1.40
4	B	2750	HEM	CHB-C1B	2.53	1.40	1.34
4	B	2750	HEM	C3C-C4C	2.42	1.44	1.41
6	B	2785	3AR	OXT-C	-2.22	1.23	1.30
4	A	1750	HEM	C3C-C4C	2.22	1.44	1.41
5	B	2760	H4B	C8A-N1	2.17	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1750	HEM	CHA-C4D	2.17	1.39	1.34
5	A	1760	H4B	C8A-N1	2.11	1.38	1.34
4	B	2750	HEM	CHA-C4D	2.03	1.39	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2760	H4B	C8A-C4A-C4	9.13	122.81	114.50
5	A	1760	H4B	C8A-C4A-C4	8.74	122.45	114.50
4	B	2750	HEM	CBA-CAA-C2A	-6.43	101.73	112.54
5	A	1760	H4B	C2-N3-C4	6.33	124.77	115.96
5	B	2760	H4B	C2-N3-C4	6.21	124.60	115.96
4	A	1750	HEM	CBA-CAA-C2A	-5.92	102.58	112.54
5	A	1760	H4B	N1-C2-N3	-4.86	118.03	125.48
5	B	2760	H4B	N1-C2-N3	-4.83	118.08	125.48
5	A	1760	H4B	C4A-C4-N3	-4.00	113.82	123.91
5	B	2760	H4B	C4A-C4-N3	-3.98	113.86	123.91
5	A	1760	H4B	N2-C2-N1	3.54	122.53	117.22
5	B	2760	H4B	N2-C2-N1	3.44	122.38	117.22
5	A	1760	H4B	C2-N1-C8A	3.41	122.70	114.59
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	B	2760	H4B	C2-N1-C8A	3.29	122.42	114.59
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	C4A-N5-C6	-2.95	113.12	121.16
5	B	2760	H4B	C4A-N5-C6	-2.81	113.50	121.16
6	B	2785	3AR	C1-NH1-CZ	-2.58	118.73	123.46
4	A	1750	HEM	C4B-CHC-C1C	2.51	125.88	122.56
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
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

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Mol	Chain	Res	Type	Atoms
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

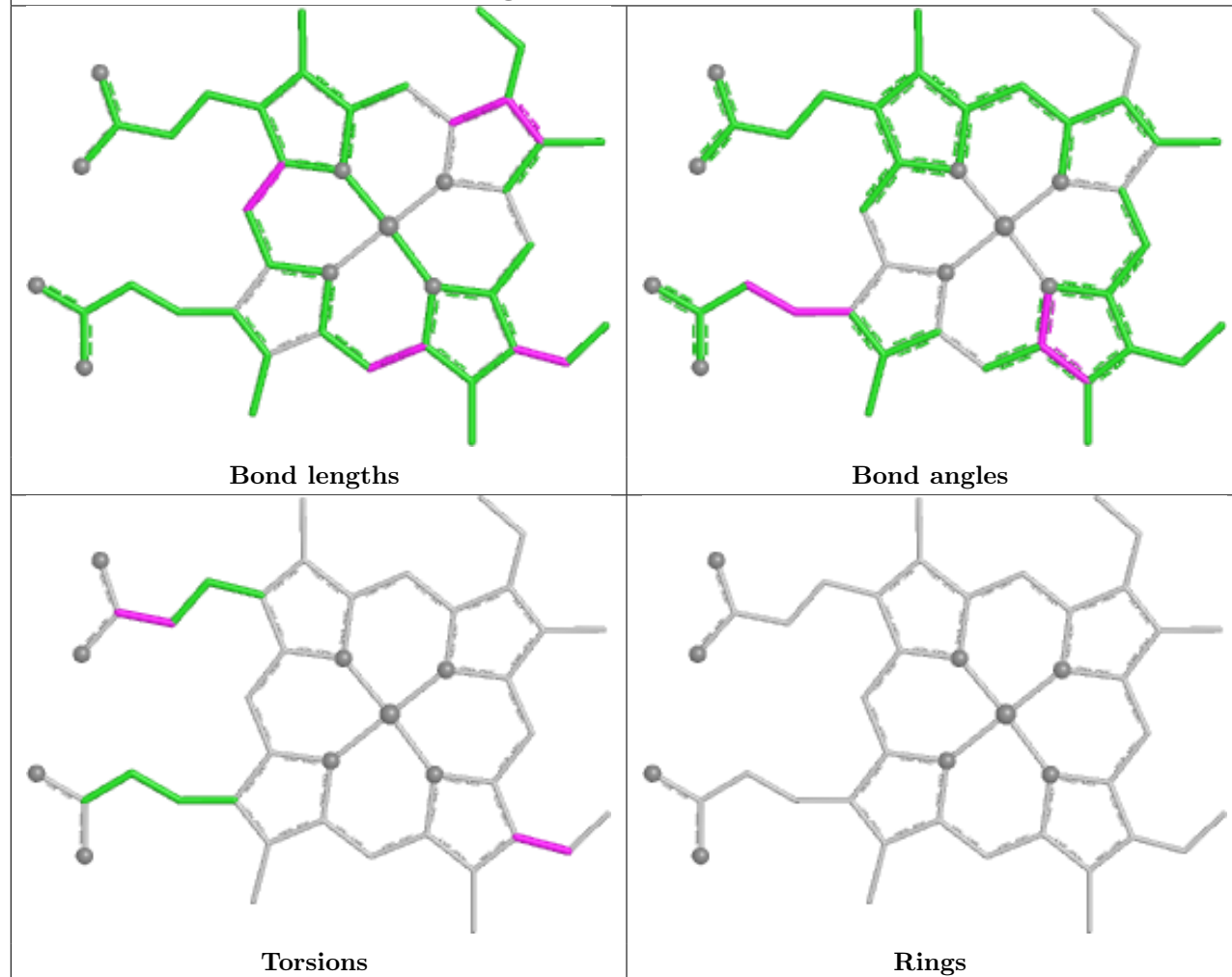
There are no ring outliers.

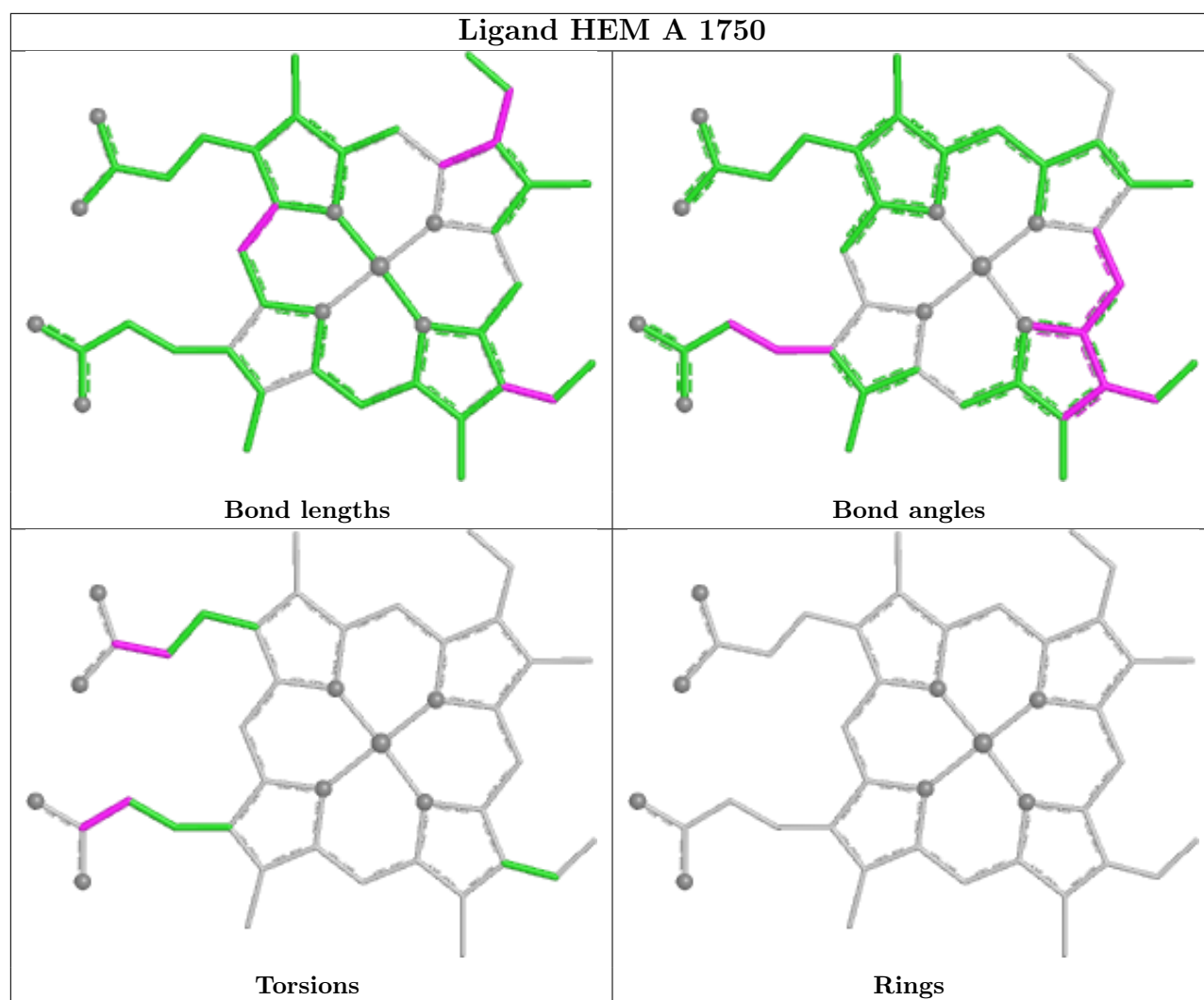
5 monomers are involved in 14 short contacts:

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

Ligand HEM B 2750





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%)	0.70	54 (13%) 8 7	20, 40, 71, 87	0
1	B	409/419 (97%)	0.11	15 (3%) 45 43	18, 32, 60, 89	0
All	All	816/838 (97%)	0.40	69 (8%) 18 17	18, 36, 64, 89	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	THR	5.9
1	A	322	LEU	5.8
1	A	715	VAL	4.9
1	B	350	THR	4.4
1	B	322	LEU	4.3
1	B	352	ASP	4.3
1	A	486	LYS	4.1
1	A	300	PHE	4.0
1	A	321	THR	3.7
1	A	355	PHE	3.6
1	B	392	SER	3.5
1	A	716	TRP	3.4
1	A	505	CYS	3.3
1	A	493	LEU	3.3
1	A	512	ALA	3.2
1	A	350	THR	3.2
1	A	552	ASP	3.2
1	A	310	VAL	3.2
1	A	488	PRO	3.2
1	A	338	PRO	3.1
1	A	506	ILE	3.1
1	A	513	PRO	3.1
1	A	303	VAL	3.0
1	A	551	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	485	TYR	2.8
1	B	300	PHE	2.8
1	A	533	LEU	2.7
1	B	611	ALA	2.7
1	B	353	GLN	2.7
1	A	301	LEU	2.7
1	A	324	THR	2.7
1	A	504	ILE	2.7
1	A	382	GLU	2.6
1	A	528	GLY	2.5
1	A	509	GLY	2.5
1	A	384	VAL	2.5
1	B	354	LEU	2.5
1	A	376	ALA	2.5
1	A	554	PHE	2.5
1	A	557	LEU	2.5
1	A	556	ASP	2.4
1	B	667	ARG	2.4
1	A	392	SER	2.4
1	B	320	SER	2.4
1	B	389	GLU	2.3
1	A	706	TYR	2.3
1	A	337	LEU	2.3
1	A	470	HIS	2.3
1	A	667	ARG	2.3
1	A	494	GLY	2.3
1	A	553	TRP	2.3
1	A	487	GLN	2.3
1	A	490	GLY	2.2
1	A	517	PHE	2.2
1	A	530	ASP	2.2
1	B	337	LEU	2.2
1	A	531	PRO	2.2
1	A	549	PRO	2.2
1	A	373	GLY	2.2
1	A	516	ARG	2.2
1	B	355	PHE	2.1
1	A	711	TRP	2.1
1	A	712	ASN	2.1
1	B	535	GLN	2.1
1	A	381	LEU	2.1
1	A	618	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	489	ASP	2.0
1	A	318	LEU	2.0
1	A	501	PHE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

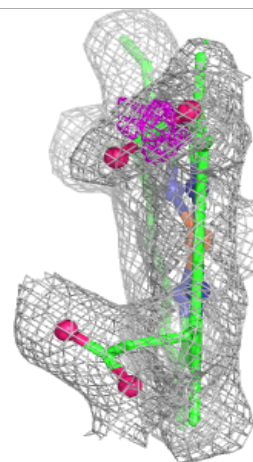
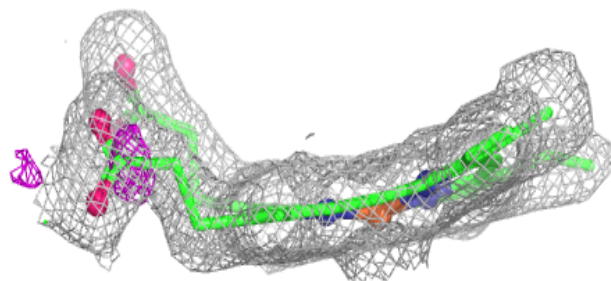
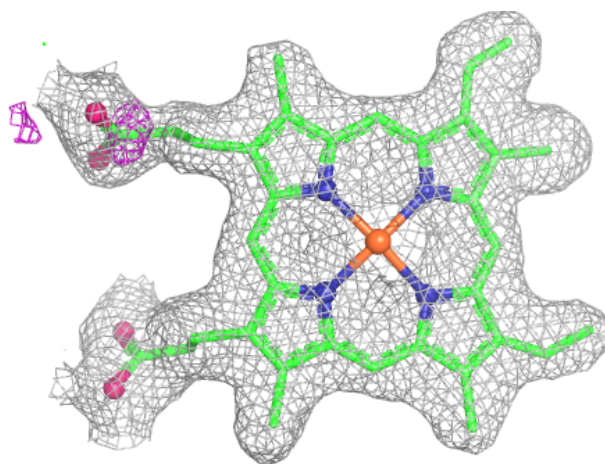
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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	1.00	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.

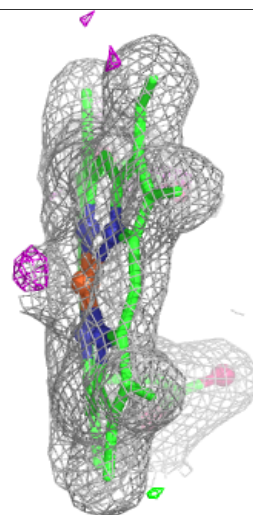
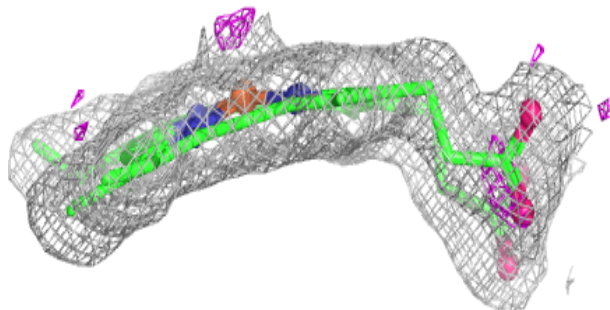
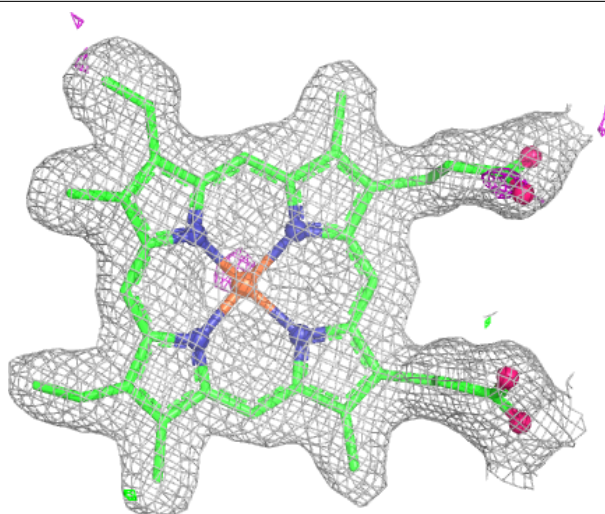
Electron density around HEM A 1750:

$2mF_o-DF_c$ (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.