



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 11:16 PM EST

PDB ID : 1MMW
Title : Rat neuronal NOS heme domain with vinyl-L-NIO 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

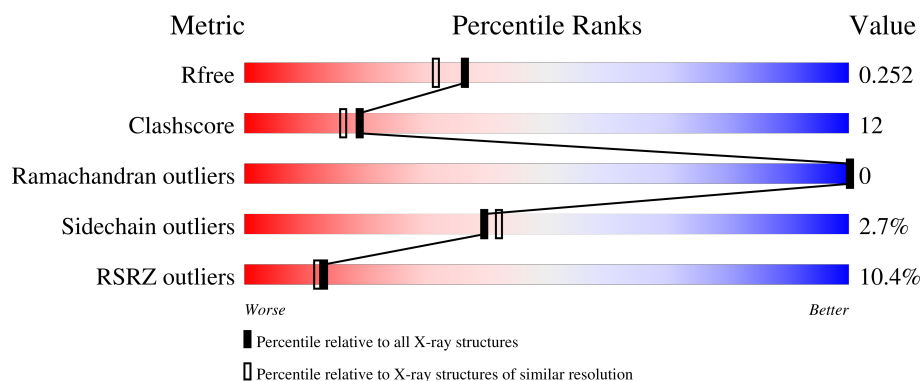
1 Overall quality at a glance

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	<div> <div>15%</div> <div>71%</div> <div>24%</div> <div>• •</div> </div>
1	B	419	<div> <div>5%</div> <div>77%</div> <div>20%</div> <div>•</div> </div>

2 Entry composition [i](#)

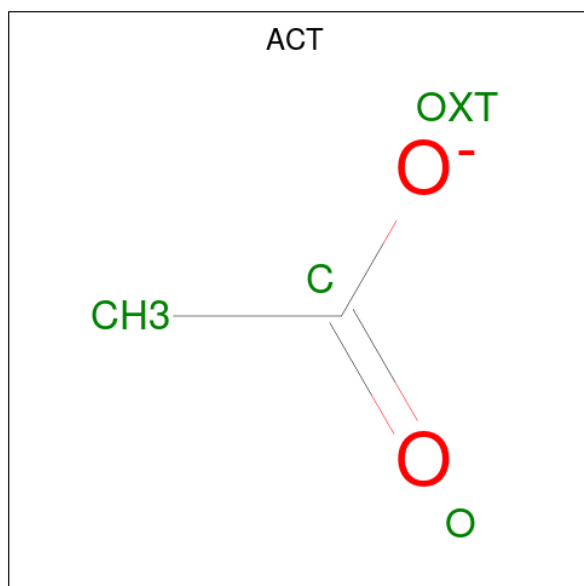
There are 7 unique types of molecules in this entry. The entry contains 7270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	410	Total	C	N	O	S	0	0	0
			3341	2138	573	609	21			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

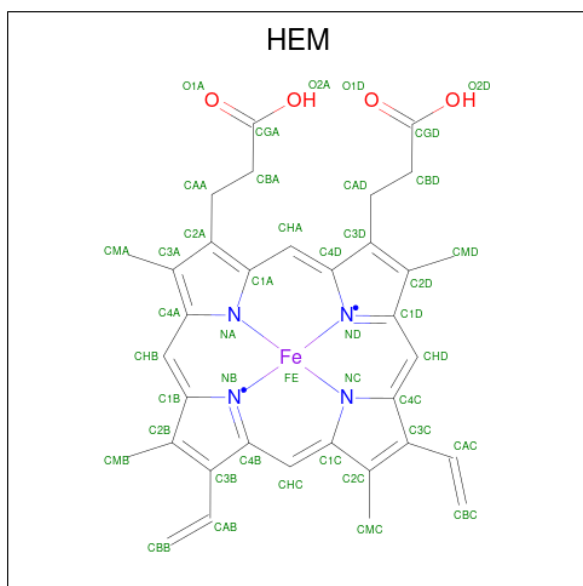


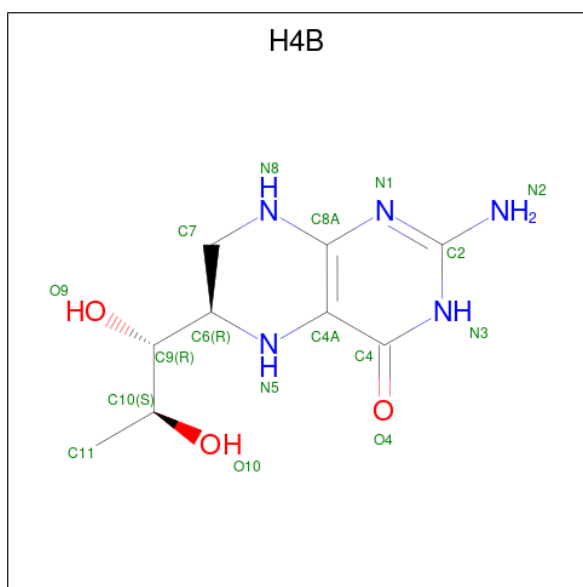
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

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

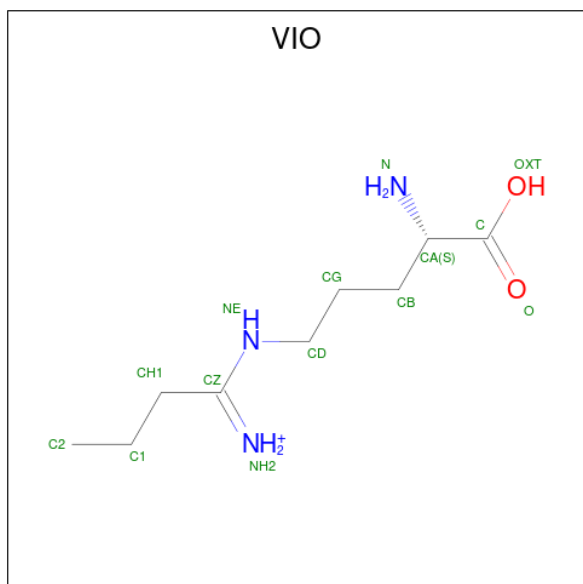
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 N5-(1-IMINO-3-BUTENYL)-L-ORNITHINE (three-letter code: VIO) (formula: $C_9H_{20}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	9	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	9	3	2		

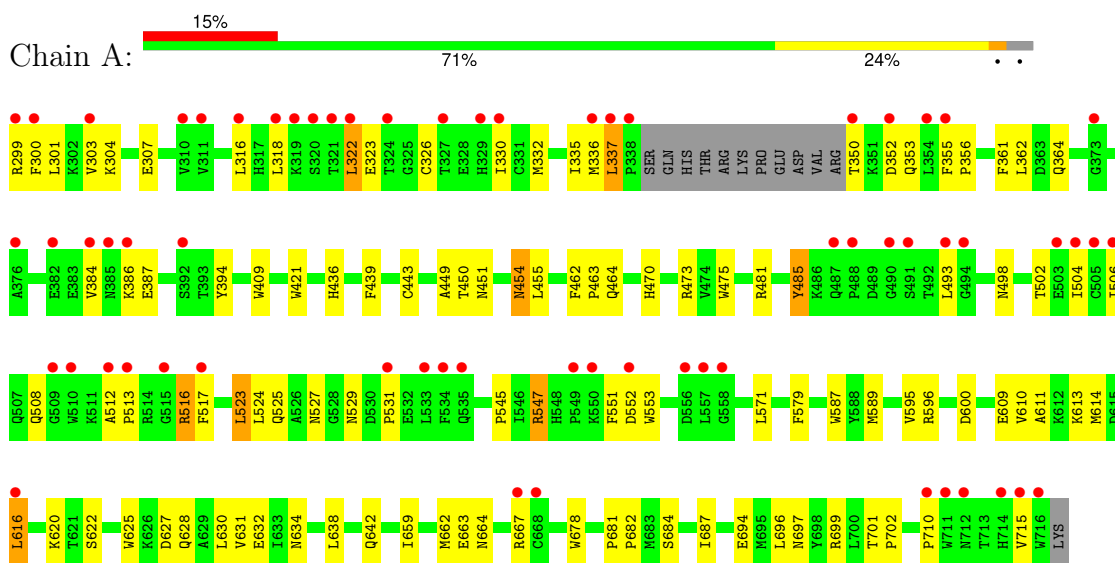
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	203	Total	O	0	0
			203	203		
7	B	256	Total	O	0	0
			256	256		

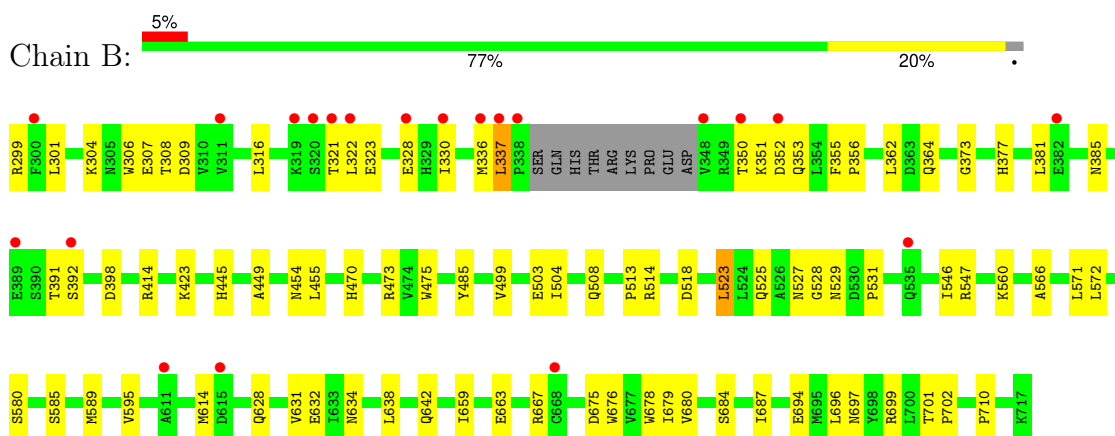
3 Residue-property plots

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	51.69Å 109.98Å 164.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.25 – 2.00 34.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.9 (34.25-2.00) 93.0 (34.25-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.266 0.220 , 0.252	Depositor DCC
R_{free} test set	3013 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7270	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: ACT, H4B, ZN, HEM, VIO

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	0.32	0/3406	0.58	1/4621 (0.0%)
1	B	0.35	0/3434	0.61	1/4656 (0.0%)
All	All	0.33	0/6840	0.60	2/9277 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-5.86	95.19	111.00
1	A	589	MET	N-CA-C	-5.72	95.56	111.00

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	92	0
1	B	3341	0	3256	72	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	2	0
4	B	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	17	0	15	1	0
5	B	17	0	15	0	0
6	A	14	0	19	0	0
6	B	14	0	19	0	0
7	A	203	0	0	5	0
7	B	256	0	0	5	0
All	All	7270	0	6611	156	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 (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:HB2	1:B:699:ARG:HH11	1.14	1.05
1:B:373:GLY:H	1:B:377:HIS:HD2	1.06	0.98
1:B:523:LEU:HD22	1:B:531:PRO:HB2	1.46	0.94
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.51	0.92
1:A:322:LEU:HD13	1:A:323:GLU:H	1.36	0.91
1:A:322:LEU:HB2	1:A:699:ARG:HH11	1.36	0.90
1:B:322:LEU:HD13	1:B:323:GLU:H	1.38	0.88
1:B:322:LEU:HG	1:B:699:ARG:HD3	1.59	0.84
1:B:322:LEU:HB2	1:B:699:ARG:NH1	1.94	0.83
1:A:506:ILE:HD11	1:A:512:ALA:HB2	1.64	0.80
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.66	0.77
1:B:322:LEU:HD13	1:B:323:GLU:N	1.99	0.76
1:B:350:THR:HB	1:B:353:GLN:OE1	1.86	0.76
1:A:436:HIS:ND1	7:A:2053:HOH:O	2.20	0.74
1:A:659:ILE:O	1:A:663:GLU:HG3	1.88	0.73
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.70	0.73
1:A:322:LEU:CB	1:A:699:ARG:HD3	2.19	0.72
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.71	0.71
1:A:350:THR:HB	1:A:353:GLN:HG3	1.72	0.71
1:B:322:LEU:CB	1:B:699:ARG:HH11	1.98	0.71
1:A:350:THR:HG22	1:A:352:ASP:H	1.56	0.71
1:A:664:ASN:HA	1:A:667:ARG:NH1	2.06	0.70
7:A:1879:HOH:O	1:B:337:LEU:HD23	1.91	0.70
1:B:373:GLY:H	1:B:377:HIS:CD2	1.98	0.70
1:B:322:LEU:CG	1:B:699:ARG:HD3	2.20	0.70
1:A:322:LEU:HD13	1:A:323:GLU:N	2.07	0.69
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:HG	1:A:699:ARG:HD3	1.76	0.68
1:A:638:LEU:O	1:A:642:GLN:HG3	1.95	0.66
1:B:322:LEU:CB	1:B:699:ARG:HD3	2.26	0.65
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.11	0.64
1:A:304:LYS:O	1:A:694:GLU:HG3	1.98	0.64
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.81	0.63
1:A:595:VAL:HG23	1:A:634:ASN:HD21	1.63	0.63
4:A:1750:HEM:HMC1	4:A:1750:HEM:HBC2	1.82	0.62
1:A:595:VAL:HG11	1:A:682:PRO:HB2	1.82	0.61
1:B:659:ILE:O	1:B:663:GLU:HG3	2.00	0.61
1:A:322:LEU:CG	1:A:699:ARG:HD3	2.32	0.60
1:A:322:LEU:HB3	1:A:699:ARG:HD3	1.84	0.60
1:A:682:PRO:HG3	7:A:1862:HOH:O	2.02	0.59
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.33	0.59
1:A:361:PHE:O	1:A:364:GLN:HG2	2.03	0.58
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.84	0.58
1:B:499:VAL:O	1:B:503:GLU:HG3	2.05	0.57
1:A:620:LYS:HE3	1:A:622:SER:OG	2.04	0.57
1:B:336:MET:HE1	7:B:2968:HOH:O	2.05	0.57
1:A:504:ILE:O	1:A:508:GLN:HB2	2.05	0.56
1:B:337:LEU:HD23	1:B:337:LEU:N	2.19	0.56
1:B:595:VAL:HG23	1:B:634:ASN:HD21	1.71	0.56
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.36	0.56
1:B:391:THR:O	1:B:392:SER:HB2	2.04	0.56
1:A:609:GLU:HG3	7:A:2060:HOH:O	2.06	0.56
1:B:663:GLU:O	1:B:667:ARG:HD2	2.06	0.55
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.22	0.55
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.87	0.55
1:A:451:ASN:HB3	1:A:454:ASN:O	2.06	0.55
1:B:638:LEU:O	1:B:642:GLN:HG3	2.06	0.55
1:B:355:PHE:N	1:B:356:PRO:HD2	2.22	0.54
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.90	0.54
1:A:524:LEU:O	1:A:531:PRO:HA	2.08	0.54
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.37	0.54
1:A:350:THR:HB	1:A:353:GLN:CG	2.38	0.53
1:B:299:ARG:HB3	1:B:299:ARG:HH11	1.73	0.53
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.28	0.53
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.90	0.53
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.44	0.52
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.24	0.52
1:B:675:ASP:O	1:B:679:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.45	0.51
1:B:525:GLN:HG3	1:B:529:ASN:O	2.10	0.51
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.91	0.51
1:A:715:VAL:O	1:A:715:VAL:HG23	2.11	0.51
1:B:398:ASP:HB2	7:B:3027:HOH:O	2.10	0.50
1:B:504:ILE:O	1:B:508:GLN:HG2	2.12	0.50
1:B:473:ARG:NH2	1:B:710:PRO:HD3	2.27	0.50
1:B:322:LEU:HG	1:B:699:ARG:CD	2.38	0.50
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.93	0.50
1:A:614:MET:CE	1:A:632:GLU:HG3	2.42	0.50
1:A:330:ILE:CD1	1:B:696:LEU:HD22	2.40	0.50
1:B:304:LYS:O	1:B:694:GLU:HG3	2.13	0.49
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.94	0.49
1:A:355:PHE:N	1:A:356:PRO:HD2	2.28	0.48
1:B:470:HIS:HA	1:B:528:GLY:HA3	1.95	0.48
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.48	0.48
1:A:596:ARG:O	1:A:600:ASP:HB2	2.13	0.48
1:B:566:ALA:HB2	1:B:585:SER:HB3	1.96	0.48
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.78	0.48
1:A:322:LEU:CD1	1:A:323:GLU:N	2.76	0.47
1:B:307:GLU:HG3	7:B:2989:HOH:O	2.13	0.47
1:A:667:ARG:HD3	7:A:1988:HOH:O	2.14	0.47
1:B:364:GLN:NE2	7:B:3057:HOH:O	2.47	0.47
1:B:321:THR:HG23	1:B:322:LEU:N	2.30	0.47
1:B:322:LEU:HB3	1:B:699:ARG:HD3	1.97	0.47
1:A:322:LEU:HB2	1:A:699:ARG:NH1	2.18	0.47
1:A:337:LEU:HD12	1:A:337:LEU:O	2.16	0.46
4:B:2750:HEM:CMC	4:B:2750:HEM:HBC2	2.45	0.46
1:A:299:ARG:O	1:A:318:LEU:HD21	2.16	0.46
1:B:308:THR:O	1:B:309:ASP:HB2	2.15	0.46
1:A:506:ILE:C	1:A:508:GLN:H	2.18	0.46
1:A:627:ASP:O	1:A:631:VAL:HG23	2.16	0.45
1:B:350:THR:HG22	1:B:352:ASP:H	1.80	0.45
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.45	0.45
1:A:614:MET:HE1	1:A:632:GLU:HG3	1.99	0.45
1:A:332:MET:HB3	1:A:335:ILE:HG13	1.97	0.45
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.47	0.45
4:B:2750:HEM:HBC2	4:B:2750:HEM:HMC1	1.98	0.45
1:A:450:THR:HA	1:A:455:LEU:HD22	1.98	0.45
1:A:303:VAL:CG1	1:A:694:GLU:O	2.66	0.44
1:B:362:LEU:HD12	1:B:381:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.52	0.44
1:A:630:LEU:HD22	1:B:687:ILE:HD13	1.99	0.44
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.99	0.44
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.32	0.44
1:A:610:VAL:O	1:A:614:MET:HG3	2.16	0.44
1:A:506:ILE:C	1:A:508:GLN:N	2.71	0.44
1:A:696:LEU:HB3	1:B:330:ILE:HD11	1.99	0.44
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.87	0.43
1:B:701:THR:HA	1:B:702:PRO:C	2.39	0.43
1:A:336:MET:HB3	1:B:306:TRP:CZ2	2.53	0.43
1:B:350:THR:HG22	1:B:351:LYS:N	2.33	0.43
1:A:330:ILE:HD13	1:B:301:LEU:HD13	2.01	0.43
1:B:571:LEU:HD12	1:B:572:LEU:N	2.32	0.43
1:A:303:VAL:HG11	1:A:694:GLU:O	2.19	0.43
1:A:362:LEU:HD11	1:A:384:VAL:HG21	2.00	0.43
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.33	0.43
1:A:525:GLN:HG3	1:A:529:ASN:O	2.18	0.43
4:A:1750:HEM:HBC2	4:A:1750:HEM:CMC	2.48	0.43
1:A:386:LYS:HD3	1:A:386:LYS:HA	1.86	0.42
1:A:481:ARG:HD3	1:A:498:ASN:HD21	1.84	0.42
1:A:553:TRP:CE3	1:A:613:LYS:HD3	2.53	0.42
1:A:307:GLU:HG3	7:B:2916:HOH:O	2.18	0.42
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.13	0.42
1:A:502:THR:O	1:A:506:ILE:HG12	2.18	0.42
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.49	0.42
1:A:571:LEU:C	1:A:571:LEU:HD23	2.40	0.42
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.02	0.42
1:B:445:HIS:CD2	1:B:445:HIS:C	2.94	0.42
1:A:516:ARG:HG2	1:A:517:PHE:CE1	2.55	0.42
1:A:678:TRP:HA	5:A:1760:H4B:N1	2.34	0.41
1:A:701:THR:HA	1:A:702:PRO:C	2.40	0.41
1:A:462:PHE:HB3	1:A:463:PRO:HD2	2.03	0.41
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.55	0.41
1:B:614:MET:CE	1:B:632:GLU:HG3	2.51	0.41
1:B:322:LEU:HD12	1:B:323:GLU:O	2.20	0.41
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.21	0.41
1:A:300:PHE:CD1	1:A:300:PHE:N	2.88	0.41
1:A:449:ALA:O	1:A:455:LEU:HA	2.21	0.41
1:A:611:ALA:HB1	1:A:616:LEU:HD11	2.02	0.41
1:B:676:TRP:CZ2	1:B:680:VAL:HG21	2.56	0.41
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:CD1	1:B:323:GLU:N	2.79	0.40
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.56	0.40
1:A:681:PRO:HA	1:A:682:PRO:HD3	1.76	0.40
1:B:449:ALA:O	1:B:455:LEU:HA	2.22	0.40
1:A:326:CYS:O	1:B:328:GLU:HA	2.21	0.40
1:B:571:LEU:HD13	1:B:580:SER:HA	2.04	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%)	382 (95%)	21 (5%)	0	100	100
1	B	406/419 (97%)	392 (97%)	14 (3%)	0	100	100
All	All	809/838 (96%)	774 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/375 (97%)	350 (96%)	13 (4%)	30	30
1	B	366/375 (98%)	359 (98%)	7 (2%)	52	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	729/750 (97%)	709 (97%)	20 (3%)	40	42

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	322	LEU
1	A	337	LEU
1	A	454	ASN
1	A	485	TYR
1	A	493	LEU
1	A	516	ARG
1	A	523	LEU
1	A	547	ARG
1	A	552	ASP
1	A	616	LEU
1	A	662	MET
1	A	697	ASN
1	B	316	LEU
1	B	337	LEU
1	B	423	LYS
1	B	454	ASN
1	B	523	LEU
1	B	547	ARG
1	B	697	ASN

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	364	GLN
1	A	407	HIS
1	A	425	GLN
1	A	436	HIS
1	A	451	ASN
1	A	454	ASN
1	A	527	ASN
1	A	634	ASN
1	A	697	ASN
1	B	364	GLN
1	B	377	HIS
1	B	425	GLN

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Mol	Chain	Res	Type
1	B	451	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	529	ASN
1	B	535	GLN
1	B	634	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	42,50,50	1.36	5 (11%)	46,82,82	1.30	6 (13%)
5	H4B	A	1760	-	16,18,18	2.24	4 (25%)	14,26,26	3.93	9 (64%)
5	H4B	B	2760	-	16,18,18	2.24	5 (31%)	14,26,26	3.93	9 (64%)
4	HEM	B	2750	1	42,50,50	1.33	4 (9%)	46,82,82	1.30	4 (8%)
6	VIO	A	1780	-	12,13,13	2.11	3 (25%)	10,15,15	1.73	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	VIO	B	2780	-	12,13,13	1.96	4 (33%)	10,15,15	1.45	2 (20%)
2	ACT	A	1860	-	3,3,3	0.93	0	3,3,3	0.83	0
2	ACT	B	2860	-	3,3,3	0.96	0	3,3,3	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	1750	1	-	1/12/54/54	-
5	H4B	A	1760	-	-	0/8/17/17	0/2/2/2
5	H4B	B	2760	-	-	0/8/17/17	0/2/2/2
6	VIO	A	1780	-	-	4/13/14/14	-
6	VIO	B	2780	-	-	3/13/14/14	-
4	HEM	B	2750	1	-	1/12/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1780	VIO	CH1-CZ	5.54	1.56	1.50
5	B	2760	H4B	C4-N3	5.33	1.42	1.33
5	A	1760	H4B	C4-N3	5.29	1.42	1.33
5	A	1760	H4B	C4A-N5	4.72	1.47	1.37
6	B	2780	VIO	CH1-CZ	4.67	1.55	1.50
5	B	2760	H4B	C6-N5	4.28	1.53	1.45
5	A	1760	H4B	C6-N5	4.21	1.53	1.45
5	B	2760	H4B	C4A-N5	4.21	1.46	1.37
4	B	2750	HEM	C3C-C2C	-3.83	1.35	1.40
4	A	1750	HEM	C3C-C4C	3.16	1.46	1.41
6	B	2780	VIO	CZ-NH2	3.12	1.34	1.27
6	A	1780	VIO	CZ-NH2	2.90	1.33	1.27
4	A	1750	HEM	C1A-NA	2.88	1.42	1.36
4	A	1750	HEM	CAB-C3B	-2.87	1.39	1.47
4	B	2750	HEM	CAB-C3B	-2.84	1.39	1.47
4	B	2750	HEM	CHB-C1B	2.70	1.41	1.34
4	A	1750	HEM	C3C-CAC	-2.65	1.41	1.47
4	A	1750	HEM	CHB-C1B	2.47	1.40	1.34
6	A	1780	VIO	C2-C1	-2.44	1.32	1.50
6	B	2780	VIO	C2-C1	-2.42	1.33	1.50
5	A	1760	H4B	C8A-N1	2.34	1.38	1.34
4	B	2750	HEM	C3C-C4C	2.18	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2780	VIO	OXT-C	-2.05	1.24	1.30
5	B	2760	H4B	C7-N8	2.04	1.48	1.44
5	B	2760	H4B	C7-C6	2.00	1.54	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2760	H4B	C8A-C4A-C4	9.23	122.90	114.50
5	A	1760	H4B	C8A-C4A-C4	8.74	122.45	114.50
5	A	1760	H4B	C2-N3-C4	6.51	125.01	115.96
5	B	2760	H4B	C2-N3-C4	6.19	124.56	115.96
5	A	1760	H4B	N1-C2-N3	-5.11	117.65	125.48
5	B	2760	H4B	N1-C2-N3	-4.76	118.18	125.48
5	B	2760	H4B	C4A-C4-N3	-4.04	113.71	123.91
5	A	1760	H4B	C4A-C4-N3	-3.95	113.93	123.91
5	A	1760	H4B	N2-C2-N1	3.81	122.94	117.22
5	B	2760	H4B	N2-C2-N1	3.49	122.45	117.22
4	B	2750	HEM	CBA-CAA-C2A	-3.45	106.74	112.54
5	A	1760	H4B	C2-N1-C8A	3.39	122.65	114.59
5	B	2760	H4B	C2-N1-C8A	3.34	122.53	114.59
5	A	1760	H4B	C4A-N5-C6	-3.25	112.31	121.16
5	B	2760	H4B	O10-C10-C9	-3.24	104.41	109.77
5	A	1760	H4B	O10-C10-C9	-3.09	104.66	109.77
5	B	2760	H4B	C4A-N5-C6	-3.06	112.84	121.16
4	A	1750	HEM	C4B-CHC-C1C	2.92	126.41	122.56
6	A	1780	VIO	NE-CZ-NH2	-2.91	114.42	121.36
4	B	2750	HEM	C4B-CHC-C1C	2.73	126.16	122.56
6	A	1780	VIO	C2-C1-CH1	2.66	123.94	112.69
6	B	2780	VIO	C2-C1-CH1	2.65	123.88	112.69
4	B	2750	HEM	C3B-C4B-NB	2.64	111.36	109.47
6	B	2780	VIO	NE-CZ-NH2	-2.59	115.19	121.36
4	A	1750	HEM	CAB-C3B-C2B	-2.49	120.34	128.43
4	B	2750	HEM	C2C-C3C-C4C	-2.44	105.20	106.90
4	A	1750	HEM	C3B-C4B-NB	2.41	111.20	109.47
4	A	1750	HEM	CBD-CAD-C3D	-2.41	105.88	112.53
5	A	1760	H4B	O9-C9-C6	2.37	114.96	109.28
4	A	1750	HEM	CBA-CAA-C2A	-2.31	108.65	112.54
5	B	2760	H4B	O9-C9-C6	2.21	114.58	109.28
4	A	1750	HEM	CAB-C3B-C4B	2.00	133.24	124.39

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	2780	VIO	C2-C1-CH1-CZ
6	A	1780	VIO	C2-C1-CH1-CZ
4	A	1750	HEM	C4B-C3B-CAB-CBB
6	A	1780	VIO	CH1-CZ-NE-CD
6	B	2780	VIO	CH1-CZ-NE-CD
6	A	1780	VIO	C1-CH1-CZ-NE
4	B	2750	HEM	C4B-C3B-CAB-CBB
6	A	1780	VIO	O-C-CA-N
6	B	2780	VIO	O-C-CA-N

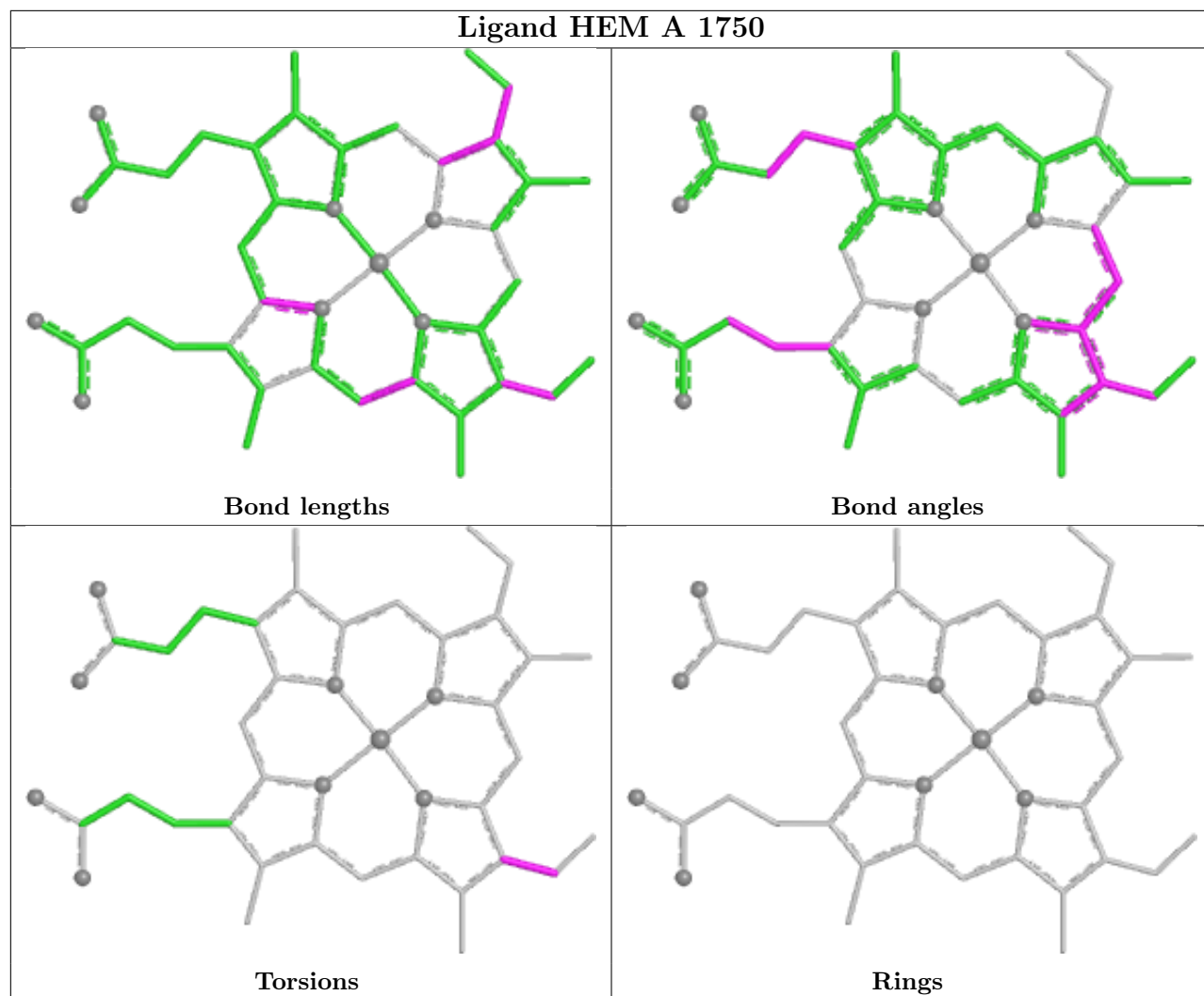
There are no ring outliers.

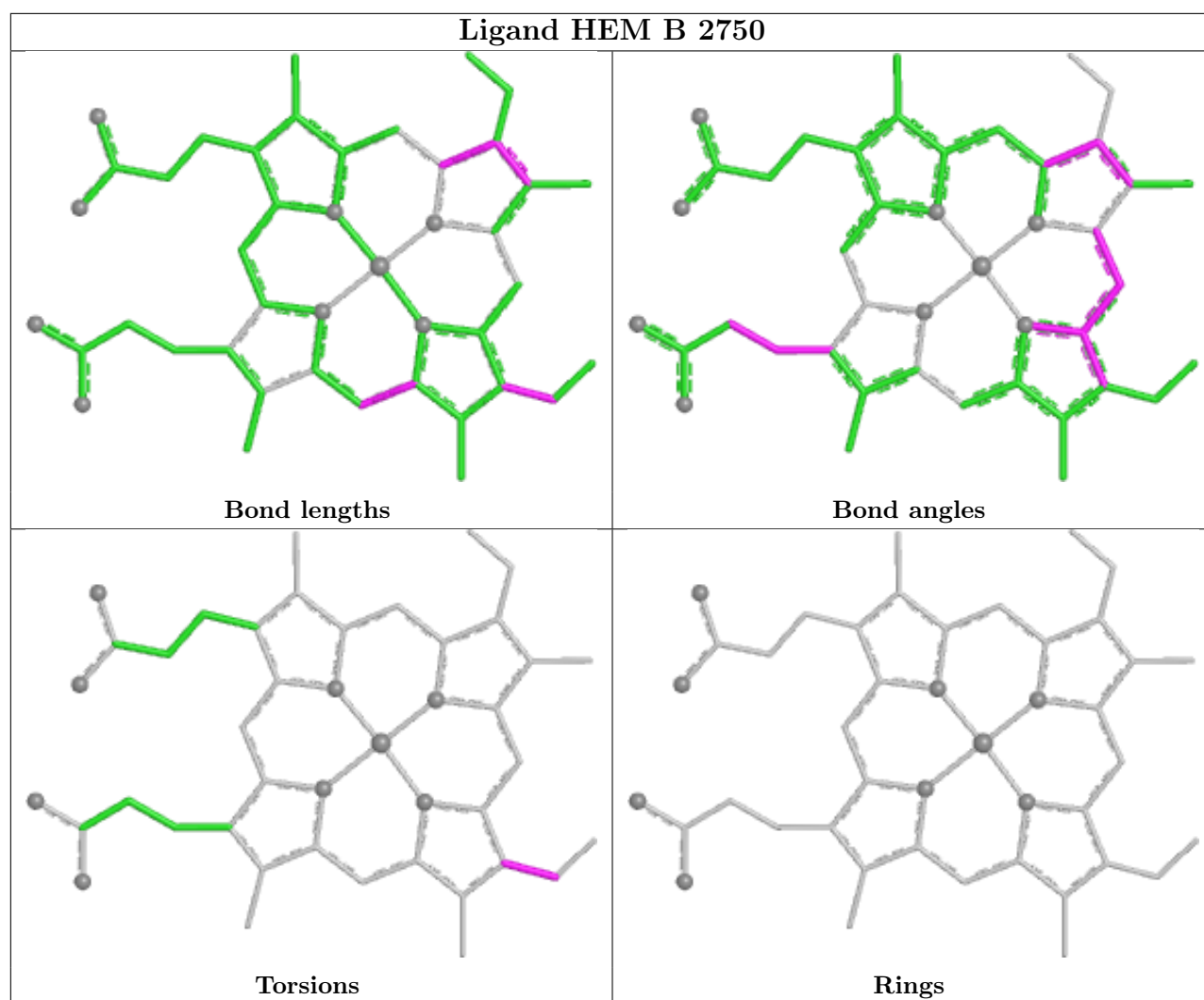
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1750	HEM	2	0
5	A	1760	H4B	1	0
4	B	2750	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.

Ligand HEM A 1750





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%)	0.92	64 (15%) 6 5	25, 42, 66, 79	0
1	B	410/419 (97%)	0.41	21 (5%) 34 32	23, 34, 60, 70	0
All	All	817/838 (97%)	0.66	85 (10%) 13 12	23, 37, 64, 79	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	6.9
1	B	322	LEU	6.9
1	A	321	THR	5.0
1	B	321	THR	4.8
1	A	330	ILE	4.5
1	A	303	VAL	4.2
1	B	350	THR	3.9
1	A	382	GLU	3.8
1	B	348	VAL	3.8
1	A	487	GLN	3.7
1	A	510	TRP	3.7
1	A	373	GLY	3.6
1	A	338	PRO	3.6
1	A	710	PRO	3.5
1	B	338	PRO	3.4
1	A	512	ALA	3.3
1	A	384	VAL	3.3
1	A	715	VAL	3.3
1	A	488	PRO	3.3
1	A	556	ASP	3.3
1	A	300	PHE	3.2
1	B	300	PHE	3.2
1	A	533	LEU	3.2
1	A	320	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	513	PRO	3.2
1	A	324	THR	3.1
1	A	327	THR	3.1
1	B	389	GLU	3.0
1	A	490	GLY	3.0
1	A	318	LEU	3.0
1	A	316	LEU	2.9
1	A	350	THR	2.9
1	A	716	TRP	2.8
1	A	506	ILE	2.7
1	A	549	PRO	2.7
1	B	330	ILE	2.7
1	B	392	SER	2.6
1	A	355	PHE	2.6
1	A	376	ALA	2.6
1	A	505	CYS	2.6
1	B	320	SER	2.6
1	B	615	ASP	2.5
1	A	336	MET	2.5
1	A	329	HIS	2.5
1	A	552	ASP	2.5
1	A	535	GLN	2.5
1	A	493	LEU	2.5
1	A	494	GLY	2.5
1	A	517	PHE	2.5
1	A	504	ILE	2.5
1	A	712	ASN	2.4
1	A	667	ARG	2.4
1	A	668	CYS	2.4
1	B	668	CYS	2.4
1	B	337	LEU	2.4
1	A	711	TRP	2.4
1	A	491	SER	2.3
1	A	352	ASP	2.3
1	A	557	LEU	2.3
1	A	310	VAL	2.2
1	A	311	VAL	2.2
1	B	336	MET	2.2
1	A	509	GLY	2.2
1	A	385	ASN	2.2
1	B	382	GLU	2.2
1	A	531	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	319	LYS	2.2
1	B	319	LYS	2.2
1	A	299	ARG	2.2
1	B	311	VAL	2.2
1	A	392	SER	2.1
1	A	714	HIS	2.1
1	A	558	GLY	2.1
1	B	535	GLN	2.1
1	A	386	LYS	2.1
1	B	352	ASP	2.1
1	A	337	LEU	2.1
1	A	354	LEU	2.1
1	A	616	LEU	2.1
1	A	515	GLY	2.0
1	B	611	ALA	2.0
1	A	534	PHE	2.0
1	A	503	GLU	2.0
1	B	328	GLU	2.0
1	A	550	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	0.92	0.12	51,51,51,51	0
5	H4B	A	1760	17/17	0.93	0.08	28,29,31,31	0
2	ACT	B	2860	4/4	0.94	0.06	35,35,35,36	0
5	H4B	B	2760	17/17	0.95	0.07	27,28,32,33	0

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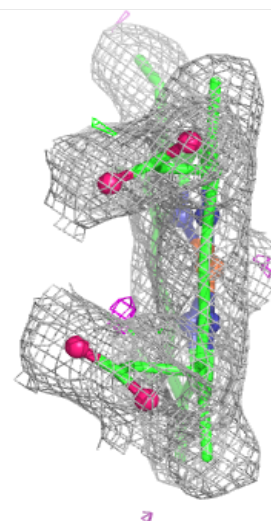
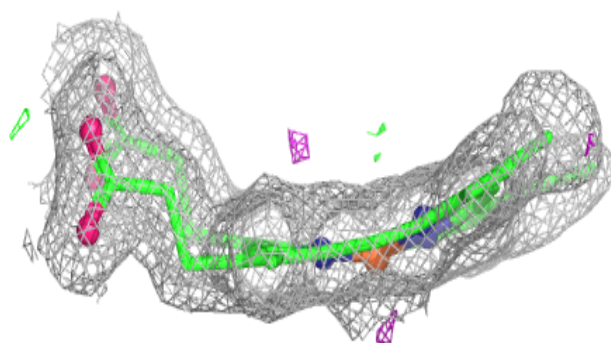
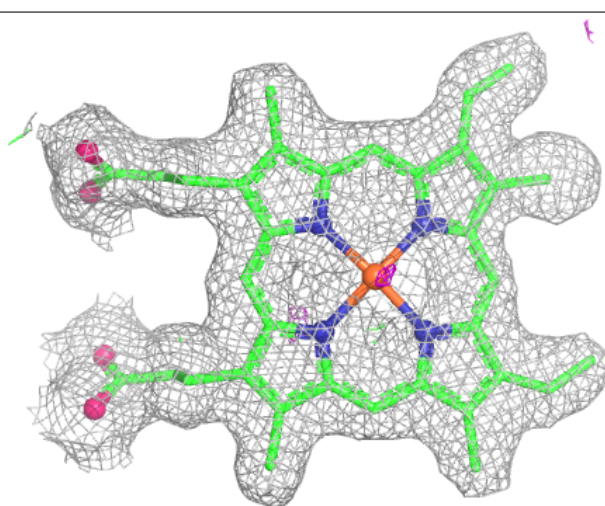
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	VIO	A	1780	14/14	0.95	0.07	26,27,30,31	0
6	VIO	B	2780	14/14	0.96	0.06	22,24,29,29	0
4	HEM	A	1750	43/43	0.97	0.06	25,27,27,27	0
4	HEM	B	2750	43/43	0.98	0.07	23,25,27,28	0
3	ZN	A	900	1/1	0.99	0.06	55,55,55,55	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.

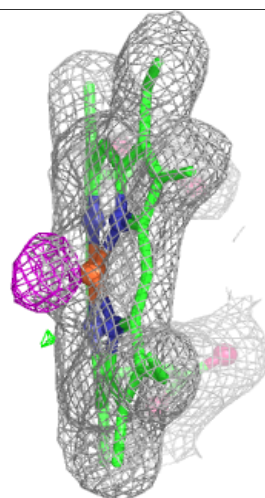
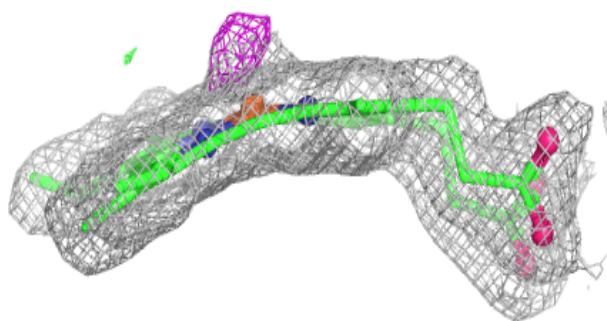
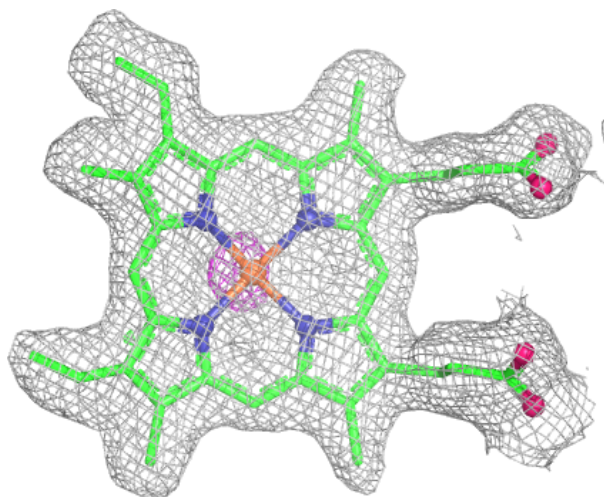
Electron density around HEM A 1750:

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 [i](#)

There are no such residues in this entry.