



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:26 AM UTC

PDB ID : 4UPN / pdb_00004upn
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with N,N''-{[(2S)-3-aminopropane-1,2-diyl]bis(oxymethanediylbenzene-3,1-diyl)}di thiophene-2-carboximidamide
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-06-17
Resolution : 2.09 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

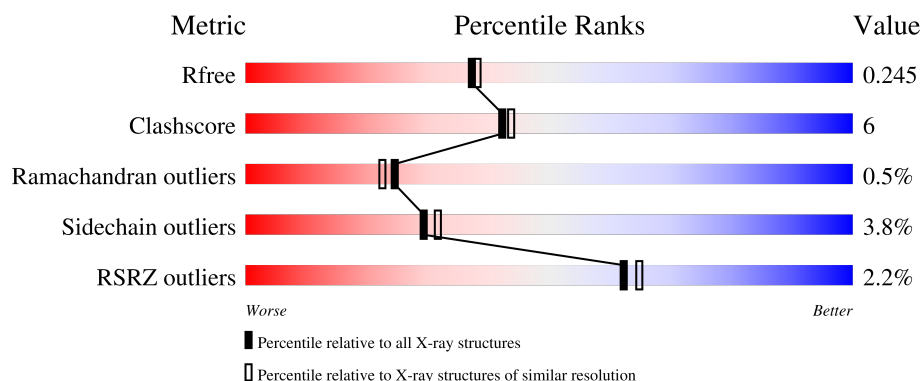
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	422	
1	B	422	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7073 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 NEURONAL NITRIC OXIDE SYNTHASE.

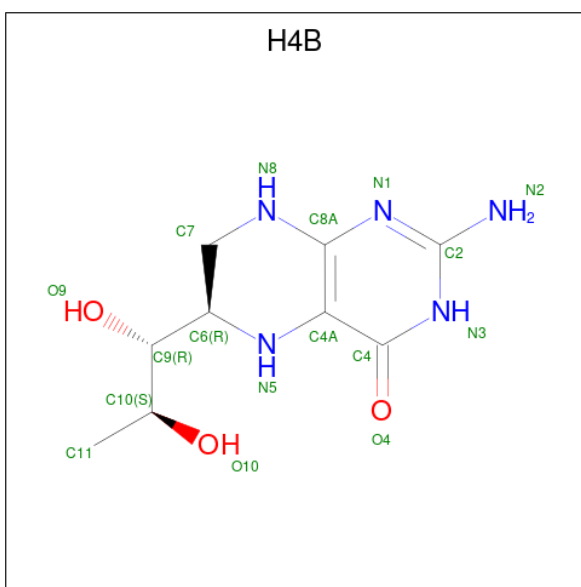
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	1
			3314	2121	567	605	21			
1	B	411	Total	C	N	O	S	0	0	0
			3345	2140	574	610	21			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



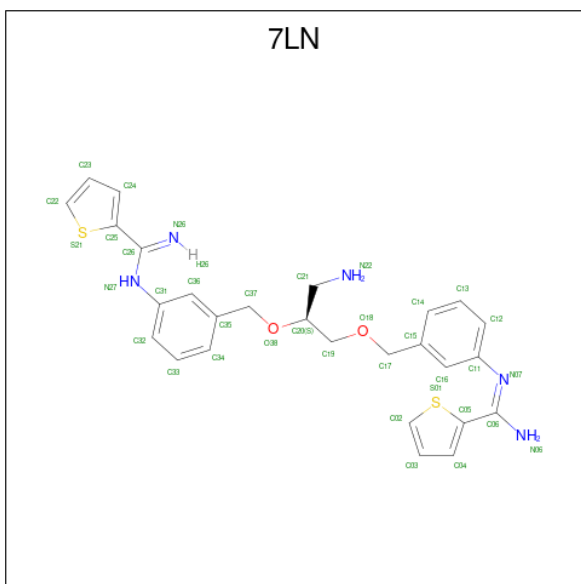
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 4 is N,N''-{[(2S)-3-aminopropane-1,2-diyl]bis(oxymethanediylbenzene-3,1-diyl)}di thiophene-2-carboximidamide (CCD ID: 7LN) (formula: C₂₇H₂₉N₅O₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			36	27	5	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			36	27	5	2	2		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

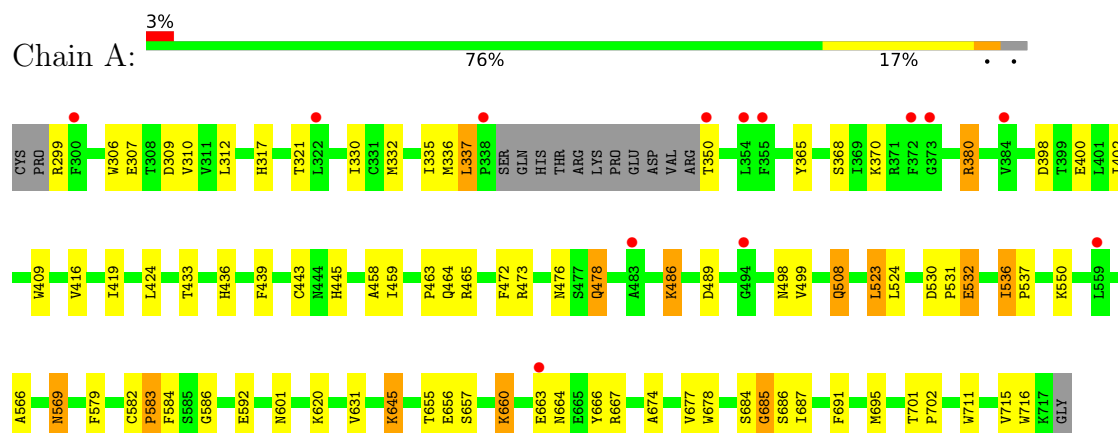
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	96	Total	O	0	0
			96	96		
7	B	117	Total	O	0	0
			117	117		

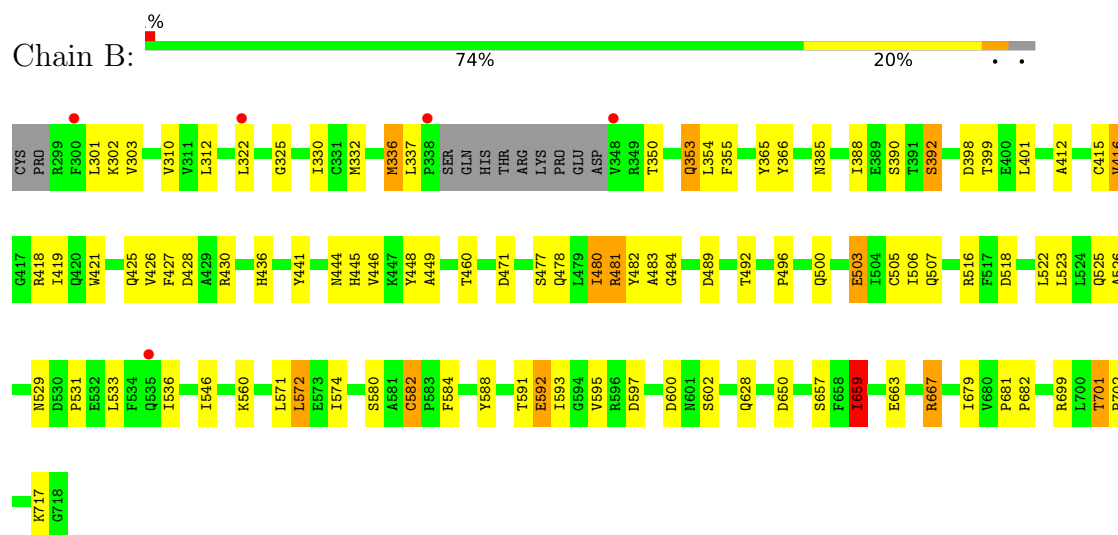
3 Residue-property plots [i](#)

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

• Molecule 1: NEURONAL NITRIC OXIDE SYNTHASE



• Molecule 1: NEURONAL NITRIC OXIDE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.07Å 111.27Å 165.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 2.09 49.38 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.38-2.09) 97.6 (49.38-2.09)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.199 , 0.245 0.202 , 0.245	Depositor DCC
R_{free} test set	2772 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7073	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, ACT, H4B, 7LN

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	1.16	17/3407 (0.5%)	1.13	11/4623 (0.2%)
1	B	1.46	38/3438 (1.1%)	1.25	20/4661 (0.4%)
All	All	1.32	55/6845 (0.8%)	1.19	31/9284 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	ILE	N-CA	8.56	1.58	1.46
1	A	416	VAL	C-O	8.22	1.35	1.24
1	B	446	VAL	CA-CB	8.17	1.65	1.54
1	A	532	GLU	C-O	8.09	1.34	1.23
1	B	471	ASP	C-O	8.04	1.33	1.23
1	B	506	ILE	N-CA	7.48	1.55	1.46
1	A	310	VAL	C-O	7.16	1.31	1.24
1	A	716	TRP	C-N	-7.15	1.23	1.33
1	B	572	LEU	N-CA	7.07	1.54	1.46
1	B	365	TYR	CA-C	6.99	1.61	1.52
1	B	310	VAL	C-O	6.88	1.30	1.24
1	B	419	ILE	N-CA	-6.83	1.38	1.46
1	A	566	ALA	C-O	-6.64	1.15	1.23
1	A	531	PRO	N-CA	6.63	1.52	1.46
1	B	418	ARG	C-O	-6.45	1.15	1.24
1	B	701	THR	C-O	-6.43	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	584	PHE	N-CA	6.40	1.53	1.45
1	B	415	CYS	C-O	6.33	1.31	1.24
1	B	416	VAL	CA-C	6.27	1.59	1.52
1	B	600	ASP	CA-C	6.27	1.60	1.52
1	A	711	TRP	N-CA	6.12	1.54	1.46
1	A	531	PRO	C-O	6.02	1.31	1.23
1	A	433	THR	N-CA	5.95	1.53	1.45
1	A	459	ILE	N-CA	-5.91	1.39	1.46
1	B	592	GLU	CA-C	5.80	1.60	1.52
1	B	571	LEU	N-CA	-5.74	1.39	1.46
1	B	426	VAL	CA-C	-5.72	1.45	1.52
1	B	398	ASP	CA-C	-5.72	1.45	1.52
1	B	526	ALA	C-O	5.69	1.30	1.24
1	B	444	ASN	C-O	-5.66	1.17	1.24
1	B	430	ARG	NE-CZ	5.59	1.39	1.33
1	B	448	TYR	N-CA	5.54	1.52	1.46
1	B	477	SER	C-O	-5.49	1.17	1.24
1	B	533	LEU	CA-CB	5.47	1.61	1.53
1	B	681	PRO	C-N	5.47	1.39	1.33
1	B	428	ASP	CA-CB	5.44	1.59	1.52
1	B	399	THR	N-CA	-5.40	1.39	1.46
1	A	660	LYS	N-CA	5.39	1.52	1.46
1	B	489	ASP	N-CA	5.34	1.53	1.46
1	A	424	LEU	N-CA	5.29	1.52	1.46
1	A	436	HIS	CA-C	5.28	1.59	1.52
1	B	505	CYS	CA-C	5.28	1.59	1.52
1	B	522	LEU	CA-CB	5.28	1.61	1.53
1	B	536	ILE	N-CA	-5.25	1.41	1.47
1	B	401	LEU	N-CA	5.24	1.52	1.46
1	B	503	GLU	N-CA	5.24	1.52	1.46
1	B	441	TYR	CE2-CZ	5.23	1.50	1.38
1	A	656	GLU	N-CA	5.14	1.52	1.46
1	B	427	PHE	CA-CB	5.13	1.60	1.53
1	B	446	VAL	N-CA	-5.12	1.40	1.46
1	B	523	LEU	CA-C	-5.09	1.46	1.53
1	B	412	ALA	N-CA	5.08	1.53	1.46
1	B	484	GLY	CA-C	5.04	1.56	1.51
1	A	458	ALA	CA-C	5.02	1.58	1.52
1	B	591	THR	C-O	-5.00	1.17	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	LEU	N-CA-C	7.63	119.39	111.14
1	A	530	ASP	CA-C-N	-7.43	112.83	120.85
1	A	530	ASP	C-N-CA	-7.43	112.83	120.85
1	B	659	ILE	N-CA-C	-6.81	103.85	110.72
1	A	536	ILE	CA-C-N	-6.42	113.77	120.38
1	A	536	ILE	C-N-CA	-6.42	113.77	120.38
1	B	536	ILE	CA-C-N	-6.40	113.78	120.38
1	B	536	ILE	C-N-CA	-6.40	113.78	120.38
1	B	449	ALA	N-CA-C	6.21	118.05	111.28
1	A	478	GLN	N-CA-C	-6.07	100.11	109.52
1	B	483	ALA	CA-C-N	5.97	125.71	121.65
1	B	483	ALA	C-N-CA	5.97	125.71	121.65
1	B	436	HIS	N-CA-C	-5.90	104.85	111.28
1	B	500	GLN	N-CA-C	5.80	118.07	111.11
1	B	425	GLN	CA-C-N	-5.73	115.67	123.12
1	B	425	GLN	C-N-CA	-5.73	115.67	123.12
1	B	667	ARG	N-CA-C	5.69	117.35	111.03
1	B	531	PRO	N-CA-C	5.64	120.14	111.57
1	A	583	PRO	CB-CA-C	-5.59	104.46	111.56
1	B	580	SER	N-CA-C	5.58	119.35	112.54
1	B	365	TYR	N-CA-C	-5.40	105.30	111.07
1	A	663	GLU	N-CA-C	5.39	117.91	111.71
1	A	645	LYS	N-CA-C	5.38	119.12	112.24
1	B	366	TYR	N-CA-C	5.37	116.93	111.14
1	A	586	GLY	N-CA-C	-5.36	100.47	113.18
1	B	421	TRP	N-CA-C	5.34	117.79	111.33
1	A	677	VAL	N-CA-C	5.33	116.70	110.62
1	B	582	CYS	CA-C-N	-5.18	114.38	119.93
1	B	582	CYS	C-N-CA	-5.18	114.38	119.93
1	B	480	ILE	N-CA-C	-5.02	100.30	107.78
1	A	655	THR	N-CA-C	-5.02	105.89	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	588	TYR	Peptide

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	3314	0	3221	46	0
1	B	3345	0	3259	34	0
2	A	43	0	30	5	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	36	0	28	8	0
4	B	36	0	28	4	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	96	0	0	6	0
7	B	117	0	0	2	0
All	All	7073	0	6632	85	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 6.

All (85) 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)
4:A:800:7LN:H24	4:A:800:7LN:H36	1.63	0.80
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.64	0.79
4:B:800:7LN:H23	7:B:2096:HOH:O	1.82	0.78
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.76	0.67
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.76	0.67
1:A:592:GLU:OE1	4:A:800:7LN:N07	2.31	0.64
4:A:800:7LN:H36	4:A:800:7LN:C24	2.29	0.61
1:B:325:GLY:O	1:B:332:MET:HG3	2.00	0.61
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.67	0.59
1:A:601:ASN:HB2	7:A:2072:HOH:O	2.02	0.59
1:A:337:LEU:HD21	4:A:800:7LN:H33	1.86	0.57
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.87	0.55
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.87	0.55
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.07	0.54
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.01	0.53
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.43	0.53
1:B:388:ILE:O	1:B:392:SER:N	2.39	0.53
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:800:7LN:H24	4:A:800:7LN:C36	2.36	0.52
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.38	0.51
1:B:584:PHE:CD2	2:B:750:HEM:CAC	2.94	0.50
4:A:800:7LN:C12	4:A:800:7LN:C05	2.87	0.50
1:A:523:LEU:C	1:A:524:LEU:HD23	2.37	0.49
1:A:701:THR:OG1	1:A:702:PRO:HA	2.11	0.49
1:B:572:LEU:HD21	1:B:574:ILE:HD11	1.95	0.49
1:A:321:THR:HG22	7:A:2003:HOH:O	2.12	0.49
1:A:684:SER:O	1:A:685:GLY:C	2.54	0.49
1:A:299:ARG:O	1:A:317:HIS:CE1	2.66	0.49
1:B:445:HIS:C	1:B:445:HIS:CD2	2.91	0.49
1:B:701:THR:HA	1:B:702:PRO:C	2.37	0.49
1:B:525:GLN:HG3	1:B:529:ASN:O	2.13	0.48
1:B:416:VAL:HG23	1:B:679:ILE:HG23	1.95	0.48
2:B:750:HEM:CMC	2:B:750:HEM:HBC2	2.44	0.48
2:B:750:HEM:C4B	4:B:800:7LN:S01	3.08	0.47
1:A:464:GLN:HB3	1:A:579:PHE:CE1	2.50	0.46
1:A:306:TRP:CE2	1:B:336:MET:HE3	2.50	0.46
1:B:350:THR:OG1	1:B:353:GLN:NE2	2.48	0.46
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.46	0.46
1:A:445:HIS:C	1:A:445:HIS:CD2	2.93	0.46
1:B:592:GLU:OE1	4:B:800:7LN:N07	2.49	0.46
1:B:492:THR:HG21	1:B:496:PRO:HG3	1.98	0.45
1:A:337:LEU:HD21	4:A:800:7LN:C33	2.45	0.45
1:A:473:ARG:HD3	7:A:2047:HOH:O	2.16	0.45
1:B:593:ILE:HA	1:B:597:ASP:HB2	1.99	0.45
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.52	0.45
1:A:664:ASN:OD1	1:A:667:ARG:NH2	2.50	0.45
1:A:330:ILE:O	1:A:330:ILE:HG23	2.16	0.45
1:A:409:TRP:CH2	2:A:750:HEM:HMC1	2.52	0.45
1:A:657:SER:HB2	7:A:2025:HOH:O	2.17	0.45
1:B:478:GLN:HB2	1:B:481:ARG:HG3	2.00	0.44
1:A:498:ASN:O	1:A:499:VAL:C	2.60	0.44
1:A:409:TRP:CE2	2:A:750:HEM:C2C	3.06	0.44
1:A:463:PRO:HG2	1:A:472:PHE:CZ	2.53	0.44
1:A:657:SER:CB	7:A:2025:HOH:O	2.66	0.44
1:B:336:MET:HE2	1:B:336:MET:HB2	1.94	0.43
1:B:460:THR:O	1:B:582:CYS:HA	2.18	0.43
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.33	0.43
1:A:486:LYS:HE3	1:A:486:LYS:HB2	1.90	0.43
1:A:365:TYR:O	1:A:368:SER:OG	2.27	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ILE:O	1:A:537:PRO:C	2.61	0.42
1:B:657:SER:HB2	7:B:2028:HOH:O	2.19	0.42
1:A:686:SER:HA	1:A:691:PHE:CG	2.54	0.42
1:A:398:ASP:O	1:A:402:ILE:HD12	2.19	0.42
1:B:496:PRO:HB2	1:B:602:SER:O	2.19	0.42
1:B:546:ILE:HG12	1:B:560:LYS:HA	2.02	0.42
1:A:476:ASN:HB3	1:A:478:GLN:O	2.20	0.42
1:A:508:GLN:HA	1:A:508:GLN:HE21	1.85	0.42
1:A:569:ASN:HD22	1:A:569:ASN:H	1.66	0.42
1:B:659:ILE:HD13	1:B:659:ILE:HA	1.94	0.42
1:A:312:LEU:HB3	1:A:666:TYR:CD2	2.55	0.41
1:A:332:MET:O	1:A:335:ILE:HG12	2.20	0.41
1:A:686:SER:OG	1:B:682:PRO:HB2	2.20	0.41
4:A:800:7LN:C23	7:A:2070:HOH:O	2.68	0.41
1:B:650:ASP:OD1	1:B:650:ASP:C	2.63	0.41
4:B:800:7LN:C12	4:B:800:7LN:C05	2.98	0.41
1:B:482:TYR:HA	1:B:518:ASP:O	2.21	0.41
1:A:306:TRP:CD1	1:B:336:MET:CE	3.04	0.41
1:B:303:VAL:HG23	1:B:312:LEU:HB2	2.03	0.41
1:A:582:CYS:N	1:A:583:PRO:CD	2.83	0.41
1:A:684:SER:HB3	1:A:687:ILE:HD11	2.03	0.41
1:A:701:THR:HA	1:A:702:PRO:C	2.46	0.40
1:A:686:SER:OG	1:B:595:VAL:CG1	2.70	0.40
1:B:302:LYS:HA	1:B:312:LEU:O	2.21	0.40
1:A:306:TRP:CG	1:B:336:MET:HE3	2.57	0.40
1:A:336:MET:HE3	1:A:678:TRP:HZ2	1.87	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	404/422 (96%)	388 (96%)	12 (3%)	4 (1%)	12	9
1	B	407/422 (96%)	393 (97%)	14 (3%)	0	100	100
All	All	811/844 (96%)	781 (96%)	26 (3%)	4 (0%)	24	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP
1	A	685	GLY
1	A	309	ASP
1	A	465	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/377 (96%)	348 (96%)	15 (4%)	27	29
1	B	366/377 (97%)	353 (96%)	13 (4%)	31	34
All	All	729/754 (97%)	701 (96%)	28 (4%)	29	32

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	GLU
1	A	337	LEU
1	A	350	THR
1	A	370	LYS
1	A	380	ARG
1	A	486	LYS
1	A	508	GLN
1	A	523	LEU
1	A	532	GLU
1	A	550	LYS
1	A	569	ASN
1	A	620	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	645	LYS
1	A	660	LYS
1	A	715	VAL
1	B	330	ILE
1	B	336	MET
1	B	337	LEU
1	B	353	GLN
1	B	390	SER
1	B	392	SER
1	B	480	ILE
1	B	481	ARG
1	B	503	GLU
1	B	507	GLN
1	B	516	ARG
1	B	659	ILE
1	B	717	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	454	ASN
1	A	508	GLN
1	A	527	ASN
1	A	569	ASN
1	A	697	ASN
1	A	712	ASN
1	B	353	GLN
1	B	364	GLN
1	B	454	ASN
1	B	535	GLN
1	B	601	ASN
1	B	642	GLN
1	B	697	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [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$
2	HEM	B	750	1	50,50,50	1.61	9 (18%)	67,82,82	2.31	24 (35%)
5	ACT	B	860	-	3,3,3	0.49	0	3,3,3	1.70	1 (33%)
3	H4B	B	760	-	17,18,18	1.47	2 (11%)	14,26,26	1.63	3 (21%)
2	HEM	A	750	1	50,50,50	1.50	9 (18%)	67,82,82	1.84	23 (34%)
4	7LN	B	800	-	38,39,39	1.36	4 (10%)	44,51,51	2.21	11 (25%)
4	7LN	A	800	-	38,39,39	1.22	4 (10%)	44,51,51	1.84	7 (15%)
3	H4B	A	760	-	17,18,18	2.02	3 (17%)	14,26,26	2.70	7 (50%)
5	ACT	A	860	-	3,3,3	0.76	0	3,3,3	1.06	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
2	HEM	B	750	1	-	4/14/54/54	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
2	HEM	A	750	1	-	4/14/54/54	-
4	7LN	B	800	-	-	12/23/29/29	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	7LN	A	800	-	-	7/23/29/29	0/4/4/4
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C1B-NB	-5.15	1.31	1.40
3	A	760	H4B	C8A-N1	-5.14	1.28	1.36
4	B	800	7LN	C03-C02	4.77	1.51	1.34
2	A	750	HEM	FE-NB	4.67	2.09	1.94
2	B	750	HEM	C1C-C2C	-4.45	1.36	1.45
3	B	760	H4B	O4-C4	4.09	1.31	1.23
4	A	800	7LN	C25-C26	3.36	1.51	1.45
4	A	800	7LN	C11-N07	-3.25	1.36	1.42
4	A	800	7LN	C06-N07	3.19	1.37	1.31
3	A	760	H4B	C7-N8	3.18	1.49	1.46
4	B	800	7LN	C11-N07	-3.16	1.37	1.42
2	A	750	HEM	CHC-C1C	3.09	1.44	1.38
2	B	750	HEM	C3B-C4B	2.94	1.50	1.44
2	A	750	HEM	C2A-C3A	-2.89	1.31	1.38
4	B	800	7LN	C13-C14	2.87	1.43	1.38
2	A	750	HEM	CHB-C4A	2.71	1.45	1.39
3	B	760	H4B	C4-N3	-2.58	1.34	1.38
2	B	750	HEM	C1D-ND	-2.51	1.33	1.38
2	B	750	HEM	CAD-C3D	2.47	1.57	1.51
4	B	800	7LN	C25-C26	2.39	1.49	1.45
2	B	750	HEM	O1D-CGD	2.29	1.29	1.22
2	B	750	HEM	CMD-C2D	2.29	1.55	1.50
2	A	750	HEM	C1B-NB	-2.22	1.36	1.40
2	A	750	HEM	C4C-NC	-2.22	1.35	1.39
2	A	750	HEM	FE-NC	2.17	2.02	1.95
3	A	760	H4B	C11-C10	2.11	1.57	1.51
2	B	750	HEM	C1D-C2D	2.09	1.48	1.44
4	A	800	7LN	C31-N27	-2.09	1.37	1.41
2	A	750	HEM	C1C-NC	2.08	1.43	1.39
2	A	750	HEM	C1C-C2C	-2.04	1.41	1.45
2	B	750	HEM	FE-NC	2.02	2.01	1.95

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	7LN	C25-C26-N27	9.15	134.27	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	C2-N1-C8A	7.03	125.77	113.36
4	A	800	7LN	C25-C26-N27	6.94	129.88	116.12
2	B	750	HEM	CHC-C4B-NB	5.91	130.79	124.42
2	B	750	HEM	CHA-C4D-C3D	-5.00	116.00	125.23
4	A	800	7LN	C24-C25-C26	4.73	137.99	128.65
2	B	750	HEM	C2D-C1D-ND	4.56	115.18	109.90
2	B	750	HEM	C4D-ND-C1D	-4.53	99.84	105.21
2	B	750	HEM	C3B-C4B-NB	-4.53	106.21	109.47
2	B	750	HEM	CMD-C2D-C1D	4.25	131.67	125.03
2	A	750	HEM	CMB-C2B-C1B	4.18	131.56	125.03
2	A	750	HEM	C4C-C3C-C2C	4.17	110.43	106.81
2	B	750	HEM	C3D-C4D-ND	4.02	114.58	110.17
2	B	750	HEM	CHD-C1D-C2D	-3.89	118.89	125.03
2	B	750	HEM	CHA-C4D-ND	3.80	129.06	124.37
2	A	750	HEM	CHA-C4D-ND	3.79	129.06	124.37
4	B	800	7LN	C06-C05-S01	-3.79	113.97	120.29
4	B	800	7LN	C11-N07-C06	3.69	125.56	119.19
2	B	750	HEM	C2B-C1B-NB	3.64	114.02	109.84
2	B	750	HEM	C3B-C2B-C1B	-3.61	103.70	106.41
2	B	750	HEM	C4A-NA-C1A	-3.52	100.08	105.82
2	A	750	HEM	C1A-CHA-C4D	-3.52	117.98	126.25
4	A	800	7LN	C26-C25-S21	-3.49	114.35	120.28
2	A	750	HEM	CMB-C2B-C3B	-3.45	120.08	128.43
4	B	800	7LN	C13-C12-C11	3.43	124.21	119.75
4	B	800	7LN	C24-C25-C26	3.37	135.31	128.65
2	B	750	HEM	CMB-C2B-C1B	3.33	130.24	125.03
2	A	750	HEM	CHA-C4D-C3D	-3.31	119.13	125.23
3	A	760	H4B	N2-C2-N3	3.27	123.66	116.76
2	B	750	HEM	C4C-CHD-C1D	-3.17	119.27	126.02
4	A	800	7LN	C02-S01-C05	-3.09	86.78	92.33
3	A	760	H4B	C2-N3-C4	-3.08	119.52	125.11
4	A	800	7LN	C17-O18-C19	-2.88	106.21	112.66
4	B	800	7LN	C26-C25-S21	-2.85	115.43	120.28
2	B	750	HEM	C1A-CHA-C4D	-2.85	119.56	126.25
4	B	800	7LN	C14-C15-C16	2.84	122.47	118.55
2	B	750	HEM	C1D-C2D-C3D	-2.81	104.03	106.98
2	B	750	HEM	O2D-CGD-CBD	2.80	122.83	114.00
4	B	800	7LN	C12-C13-C14	-2.76	116.70	120.24
3	A	760	H4B	O9-C9-C10	-2.73	103.94	109.14
2	A	750	HEM	CHC-C4B-NB	2.73	127.36	124.42
2	A	750	HEM	CAA-C2A-C1A	2.72	130.25	124.94
4	A	800	7LN	C06-C05-S01	-2.72	115.77	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CAD-CBD-CGD	-2.71	106.47	113.67
2	B	750	HEM	CHB-C1B-C2B	-2.70	119.28	126.95
2	A	750	HEM	CHC-C1C-NC	2.66	127.35	124.45
3	A	760	H4B	C4-C4A-N5	2.63	123.43	116.27
2	A	750	HEM	CHB-C1B-NB	2.55	127.52	124.37
3	B	760	H4B	C11-C10-C9	-2.52	109.03	112.11
2	B	750	HEM	CBA-CAA-C2A	-2.48	105.68	112.53
2	A	750	HEM	CAA-C2A-C3A	-2.48	121.52	127.07
4	A	800	7LN	N06-C06-N07	-2.44	121.20	125.74
3	B	760	H4B	N2-C2-N3	2.42	121.87	116.76
4	B	800	7LN	C34-C35-C36	2.40	121.86	118.55
2	B	750	HEM	C1B-NB-C4B	2.37	108.01	105.21
2	A	750	HEM	CMA-C3A-C4A	2.36	129.01	125.42
2	A	750	HEM	O2D-CGD-CBD	2.34	121.39	114.00
5	B	860	ACT	O-C-CH3	-2.31	113.07	122.53
4	B	800	7LN	N06-C06-N07	-2.26	121.54	125.74
2	A	750	HEM	C1B-NB-C4B	2.24	107.86	105.21
2	A	750	HEM	C3B-C2B-C1B	2.24	108.09	106.41
3	A	760	H4B	C4A-C4-N3	2.24	118.28	112.13
4	B	800	7LN	C04-C05-S01	2.23	116.43	111.23
2	A	750	HEM	CBA-CAA-C2A	-2.23	106.37	112.53
2	B	750	HEM	C3A-C4A-NA	2.21	113.69	110.14
3	B	760	H4B	O4-C4-C4A	-2.20	121.94	127.26
2	A	750	HEM	C4A-NA-C1A	-2.18	102.27	105.82
2	A	750	HEM	C1C-CHC-C4B	-2.16	121.42	126.02
2	A	750	HEM	C3C-C2C-C1C	-2.12	105.03	107.05
2	B	750	HEM	C2A-C1A-NA	2.12	112.50	110.15
2	B	750	HEM	O2A-CGA-O1A	-2.08	117.99	123.33
2	B	750	HEM	CHD-C4C-NC	2.07	126.71	124.45
3	A	760	H4B	O4-C4-N3	-2.04	116.28	120.11
2	A	750	HEM	CHA-C1A-C2A	-2.03	120.86	125.30
2	A	750	HEM	CHA-C1A-NA	2.03	127.53	123.86
2	A	750	HEM	CAA-CBA-CGA	2.00	118.97	113.67

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800	7LN	N06-C06-N07-C11
4	A	800	7LN	C05-C06-N07-C11
4	B	800	7LN	N26-C26-N27-C31
4	B	800	7LN	N06-C06-N07-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	800	7LN	C05-C06-N07-C11
4	A	800	7LN	C15-C17-O18-C19
4	B	800	7LN	O18-C19-C20-C21
4	A	800	7LN	C19-C20-C21-N22
4	B	800	7LN	C19-C20-C21-N22
2	A	750	HEM	C4B-C3B-CAB-CBB
2	B	750	HEM	C4B-C3B-CAB-CBB
4	B	800	7LN	O18-C19-C20-O38
4	A	800	7LN	C04-C05-C06-N06
4	B	800	7LN	C04-C05-C06-N06
4	A	800	7LN	O18-C19-C20-C21
4	B	800	7LN	C36-C31-N27-C26
4	B	800	7LN	C32-C31-N27-C26
2	A	750	HEM	C2D-C3D-CAD-CBD
2	A	750	HEM	CAD-CBD-CGD-O1D
4	B	800	7LN	C35-C37-O38-C20
2	B	750	HEM	C2D-C3D-CAD-CBD
4	B	800	7LN	C25-C26-N27-C31
2	A	750	HEM	CAD-CBD-CGD-O2D
4	B	800	7LN	C12-C11-N07-C06
2	B	750	HEM	CAD-CBD-CGD-O1D
2	B	750	HEM	CAD-CBD-CGD-O2D
4	A	800	7LN	C12-C11-N07-C06

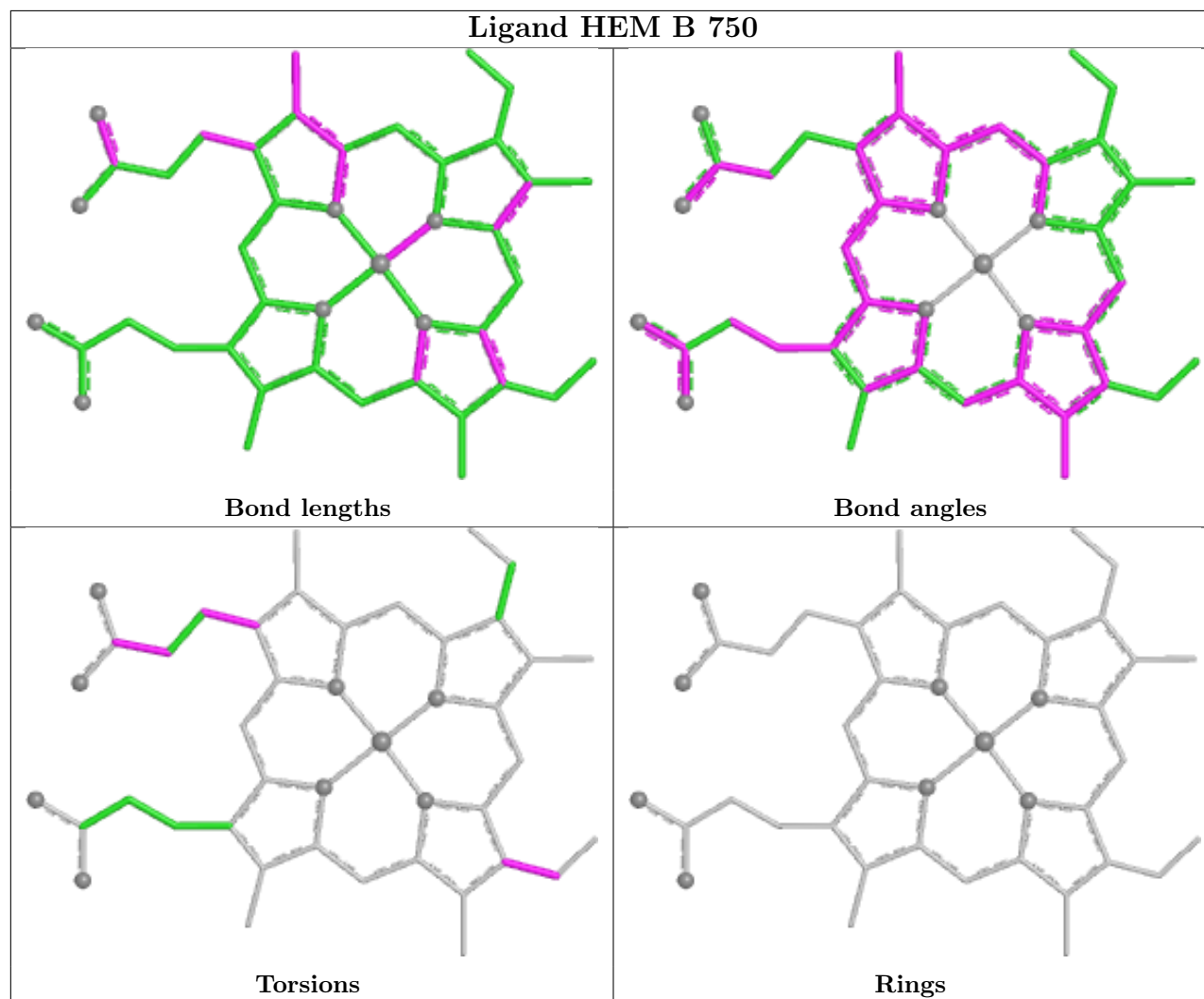
There are no ring outliers.

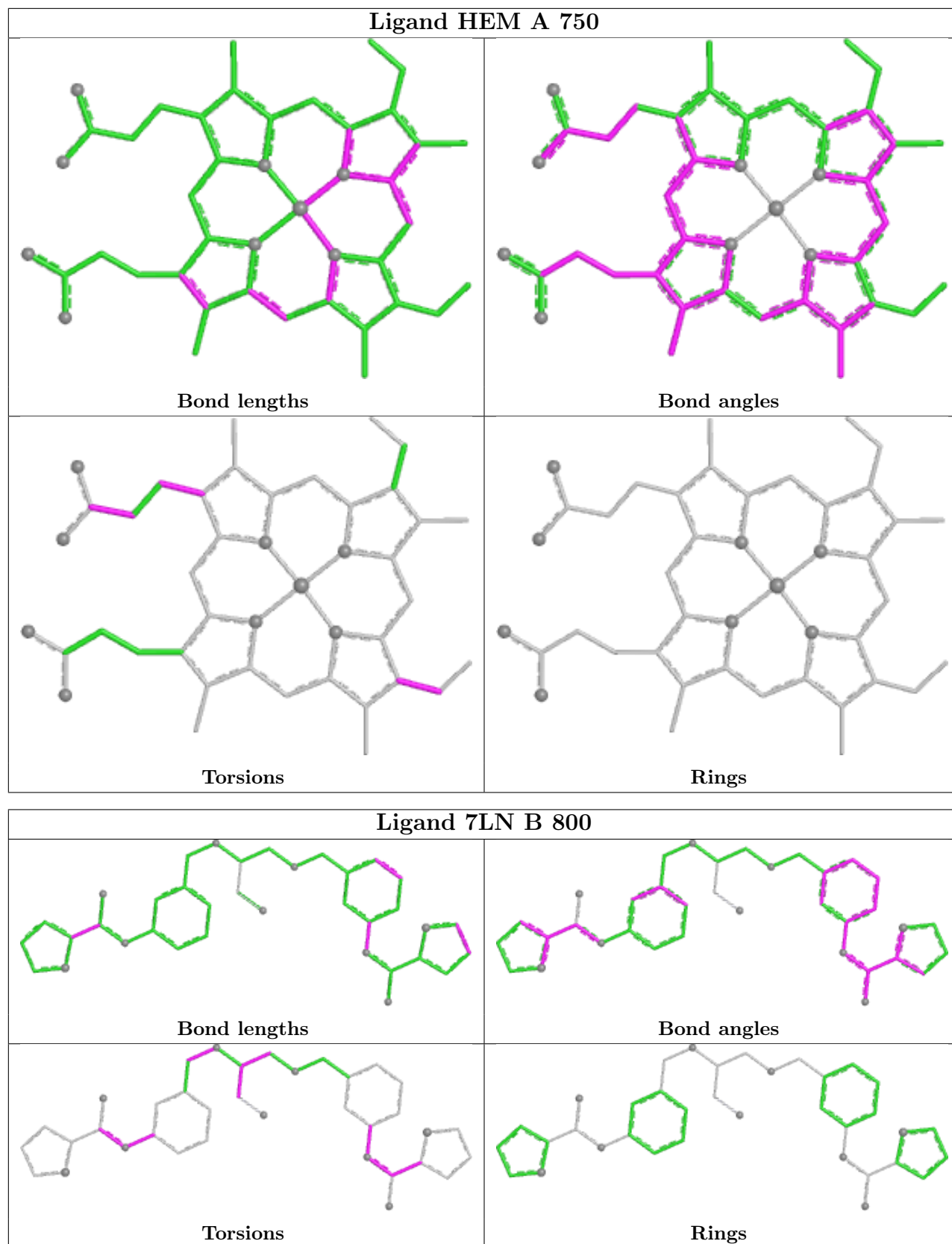
4 monomers are involved in 20 short contacts:

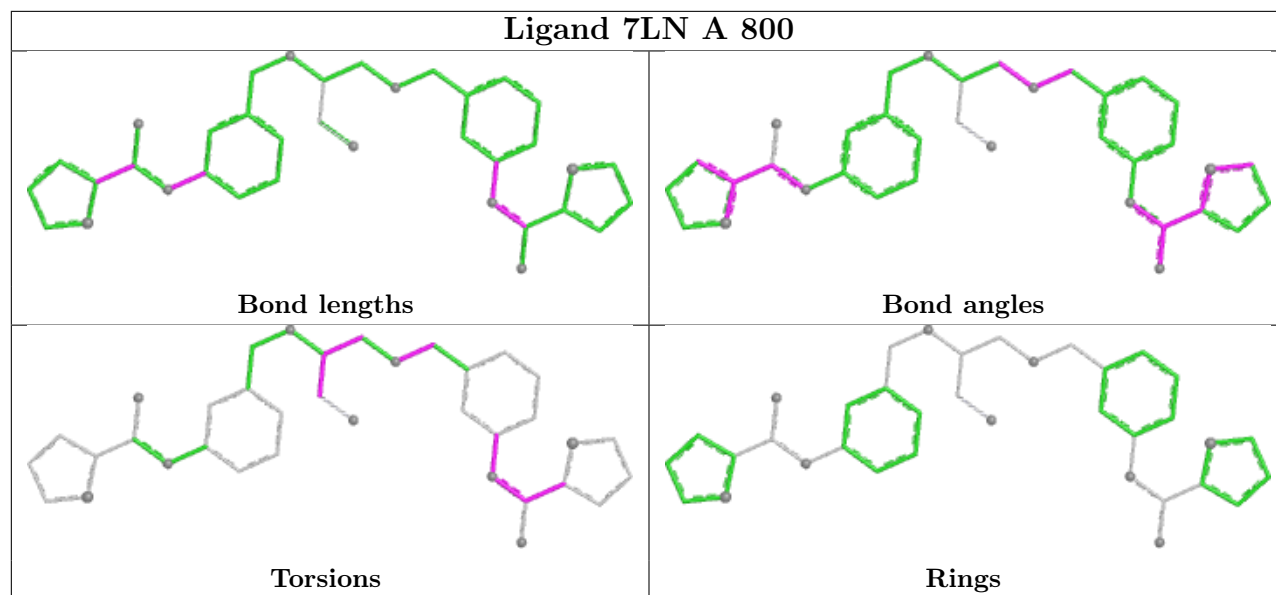
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	HEM	4	0
2	A	750	HEM	5	0
4	B	800	7LN	4	0
4	A	800	7LN	8	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	408/422 (96%)	0.52	13 (3%) 50 53	33, 59, 105, 132	0
1	B	411/422 (97%)	0.17	5 (1%) 76 78	31, 47, 76, 99	0
All	All	819/844 (97%)	0.35	18 (2%) 62 65	31, 52, 97, 132	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	PHE	3.8
1	A	338	PRO	3.4
1	B	300	PHE	3.3
1	B	348	VAL	3.3
1	B	338	PRO	3.3
1	A	350	THR	3.2
1	A	355	PHE	3.2
1	A	322	LEU	3.0
1	A	373	GLY	2.9
1	A	483	ALA	2.9
1	A	384	VAL	2.5
1	B	535	GLN	2.5
1	A	372	PHE	2.5
1	A	494	GLY	2.5
1	A	354	LEU	2.1
1	A	559	LEU	2.1
1	B	322	LEU	2.1
1	A	663	GLU	2.1

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](#)

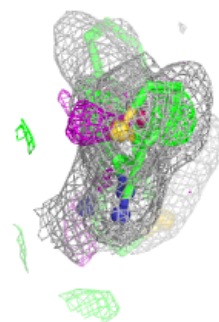
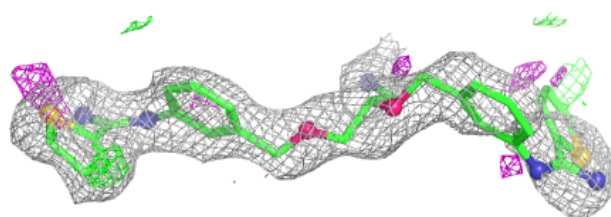
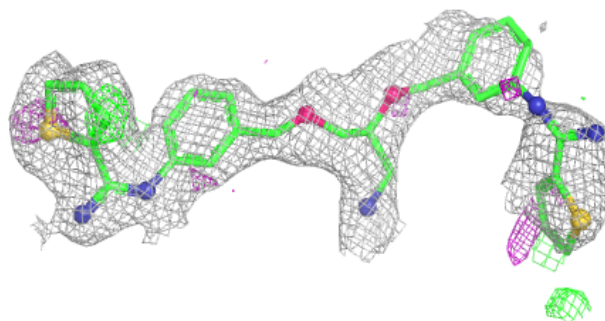
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	7LN	B	800	36/36	0.89	0.14	36,58,109,110	0
5	ACT	A	860	4/4	0.91	0.18	60,63,64,64	0
4	7LN	A	800	36/36	0.93	0.11	37,65,129,132	0
3	H4B	B	760	17/17	0.94	0.07	36,39,41,42	0
5	ACT	B	860	4/4	0.94	0.15	55,58,59,59	0
3	H4B	A	760	17/17	0.95	0.06	35,37,38,38	0
2	HEM	B	750	43/43	0.97	0.08	32,33,41,45	0
2	HEM	A	750	43/43	0.98	0.06	33,36,42,44	0
6	ZN	A	1717	1/1	0.99	0.04	55,55,55,55	0

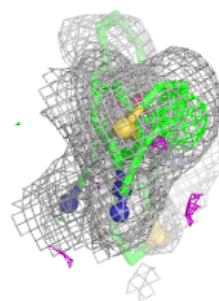
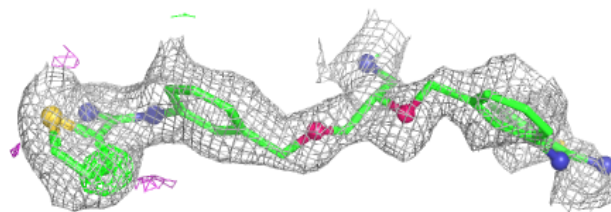
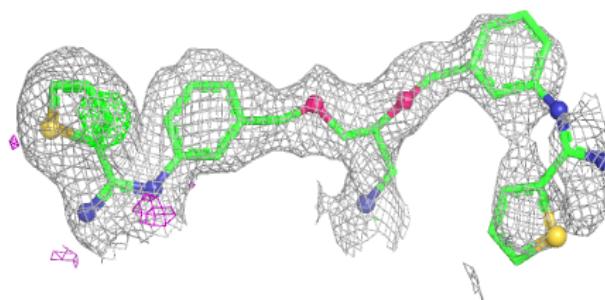
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 7LN B 800:

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

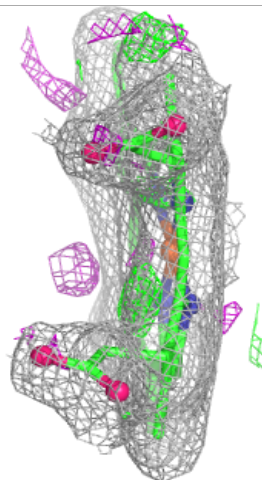
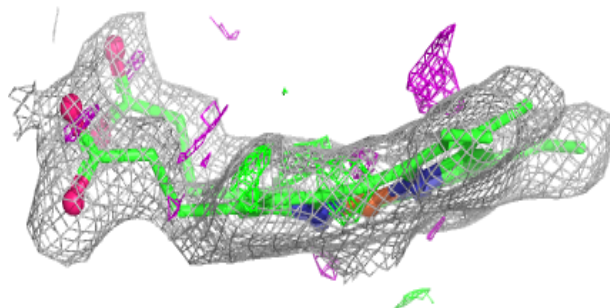
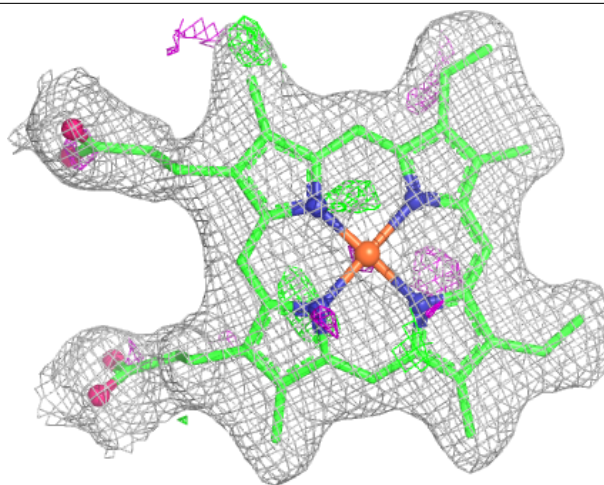
**Electron density around 7LN A 800:**

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



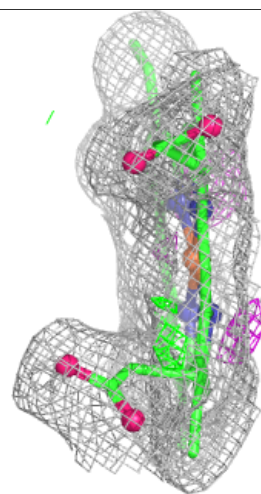
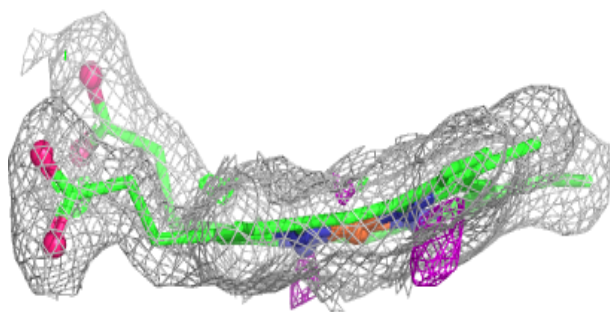
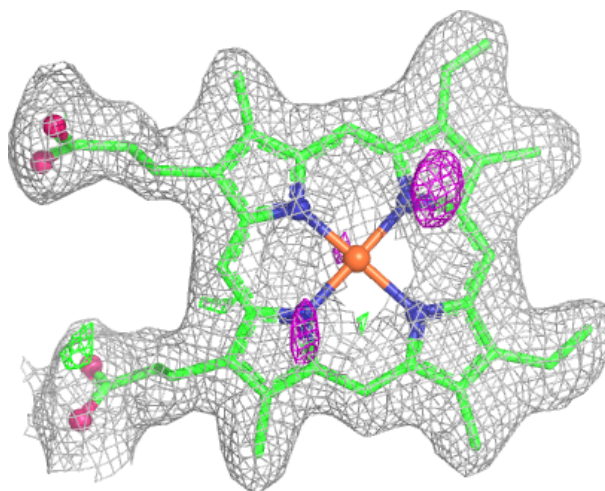
Electron density around HEM B 750:

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



Electron density around HEM A 750:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.