



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:35 AM UTC

PDB ID : 3NLQ / pdb_00003nlq
Title : Structure of neuronal nitric oxide synthase D597N/M336V mutant heme domain in complex with 6-{{(3'R,4'R)-3'-[2''-(3'''-fluorophenethylamino)ethoxy]pyrrolidin-4'-yl}methyl}-4-methylpyridin-2-amine
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Deposited on : 2010-06-21
Resolution : 2.15 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

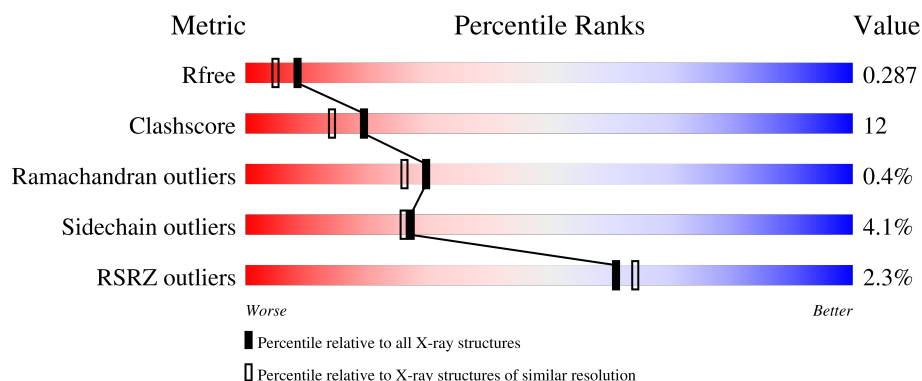
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 8 unique types of molecules in this entry. The entry contains 7063 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.

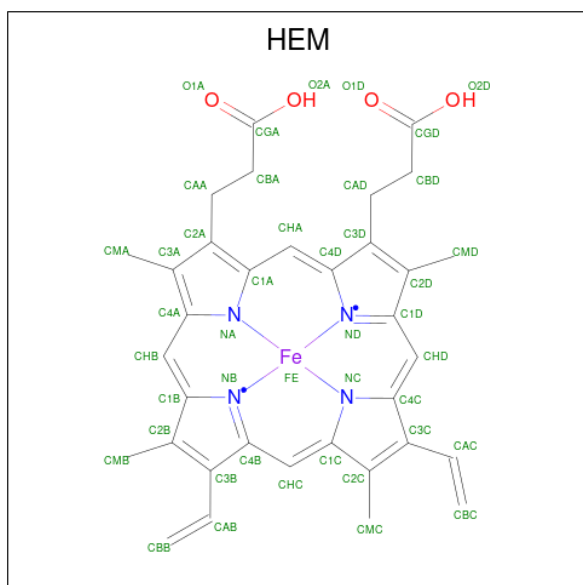
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3312	2121	567	604	20			
1	B	411	Total	C	N	O	S	0	1	0
			3350	2144	575	611	20			

There are 4 discrepancies between the modelled and reference sequences:

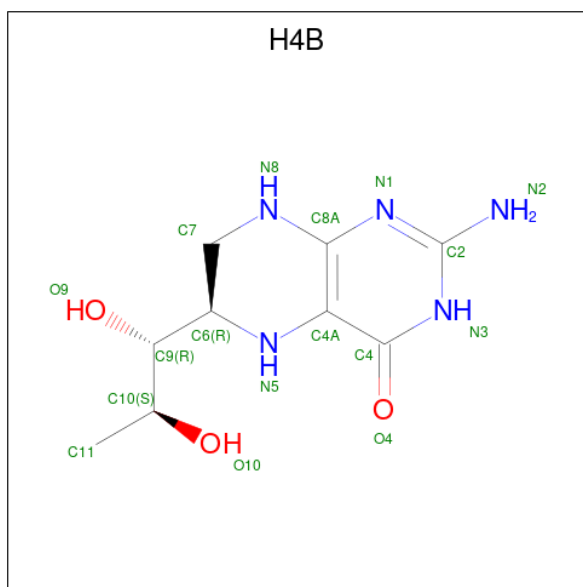
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	engineered mutation	UNP P29476
A	597	ASN	ASP	engineered mutation	UNP P29476
B	336	VAL	MET	engineered mutation	UNP P29476
B	597	ASN	ASP	engineered mutation	UNP P29476

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



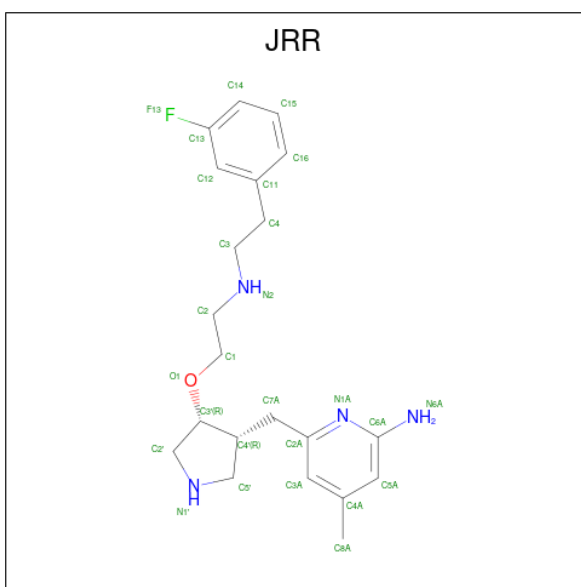
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



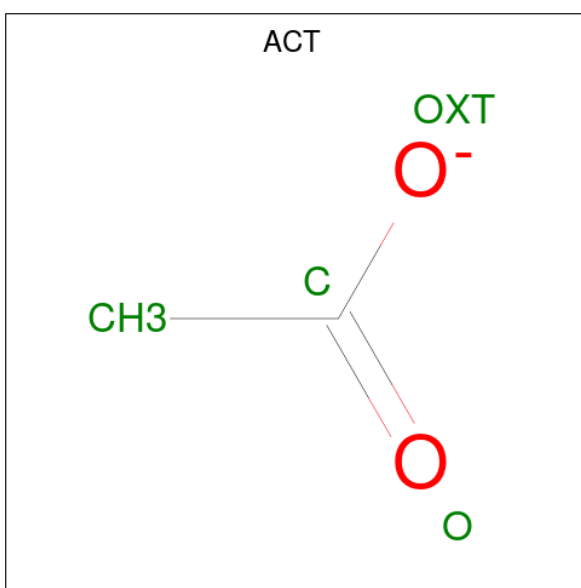
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-[[[(3R,4R)-4-(2-{[2-(3-fluorophenyl)ethyl]amino}ethoxy)pyrrolidin-3-yl]methyl]-4-methylpyridin-2-amine (CCD ID: JRR) (formula: $C_{21}H_{29}FN_4O$).



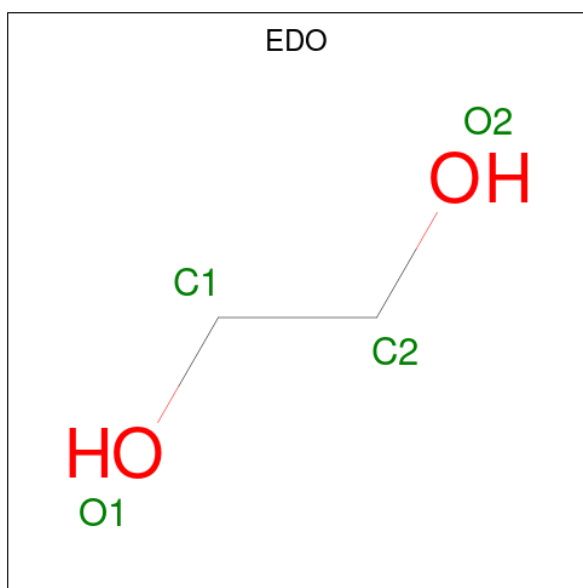
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	21	1	4	1		
4	B	1	Total	C	F	N	O	0	0
			27	21	1	4	1		

- 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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	91	Total	O	0	0
			91	91		
8	B	123	Total	O	0	0
			123	123		

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 111.23Å 163.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.82 – 2.15 37.82 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.82-2.15) 99.3 (37.82-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.204 , 0.259 0.248 , 0.287	Depositor DCC
R_{free} test set	2601 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7063	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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, JRR, ZN, H4B, ACT, EDO

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	0.87	1/3405 (0.0%)	1.03	8/4621 (0.2%)
1	B	1.21	20/3446 (0.6%)	1.22	17/4673 (0.4%)
All	All	1.06	21/6851 (0.3%)	1.13	25/9294 (0.3%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	566	ALA	C-O	9.87	1.35	1.23
1	B	499	VAL	CA-CB	-7.97	1.45	1.54
1	B	581	ALA	CA-CB	-7.86	1.41	1.53
1	A	466	THR	CA-C	7.12	1.55	1.52
1	B	498	ASN	CA-C	6.49	1.61	1.52
1	B	479	LEU	C-O	-6.47	1.16	1.24
1	B	459	ILE	C-O	-6.35	1.17	1.24
1	B	442	ILE	C-O	6.35	1.31	1.24
1	B	481	ARG	N-CA	-6.10	1.38	1.46
1	B	423	LYS	CA-C	-5.58	1.45	1.53
1	B	531	PRO	C-O	5.57	1.31	1.24
1	B	495	ASP	CA-CB	5.51	1.62	1.53
1	B	482	TYR	N-CA	5.50	1.53	1.45
1	B	483	ALA	CA-CB	-5.37	1.44	1.53
1	B	446	VAL	CA-CB	5.36	1.62	1.54
1	B	460	THR	CA-CB	5.22	1.60	1.53
1	B	499	VAL	N-CA	5.17	1.52	1.46
1	B	492	THR	N-CA	-5.17	1.39	1.45
1	B	437	GLY	N-CA	5.12	1.52	1.45
1	B	429	ALA	C-O	5.05	1.30	1.23
1	B	442	ILE	CG1-CD1	5.03	1.71	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	668	CYS	N-CA-C	8.31	121.46	111.82
1	B	530	ASP	CA-C-N	-8.26	109.51	119.84
1	B	530	ASP	C-N-CA	-8.26	109.51	119.84
1	A	680	VAL	CA-C-N	8.10	125.57	119.66
1	A	680	VAL	C-N-CA	8.10	125.57	119.66
1	B	426	VAL	CA-C-N	-7.97	111.37	122.93
1	B	426	VAL	C-N-CA	-7.97	111.37	122.93
1	B	437	GLY	N-CA-C	-7.92	103.22	112.73
1	B	517	PHE	N-CA-C	7.10	118.79	110.41
1	B	680	VAL	CA-C-N	7.06	124.82	119.66
1	B	680	VAL	C-N-CA	7.06	124.82	119.66
1	A	701	THR	CB-CA-C	6.34	118.70	108.87
1	B	679	ILE	N-CA-C	6.25	117.75	110.62
1	B	520	LEU	CA-C-N	6.16	126.67	120.14
1	B	520	LEU	C-N-CA	6.16	126.67	120.14
1	A	589	MET	N-CA-C	-6.07	99.76	109.96
1	B	536	ILE	CA-C-N	-6.00	114.20	120.38
1	B	536	ILE	C-N-CA	-6.00	114.20	120.38
1	A	487	GLN	CA-C-N	5.40	126.59	119.84
1	A	487	GLN	C-N-CA	5.40	126.59	119.84
1	B	471	ASP	N-CA-C	5.23	117.90	110.10
1	B	686	SER	N-CA-C	5.16	118.84	112.54
1	A	707	GLN	CA-C-N	-5.12	114.46	119.99
1	A	707	GLN	C-N-CA	-5.12	114.46	119.99
1	B	446	VAL	CB-CA-C	-5.12	104.22	112.16

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	3312	0	3223	66	0
1	B	3350	0	3267	87	0
2	A	43	0	30	5	0
2	B	43	0	30	10	0
3	A	17	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	0	0
4	A	27	0	29	3	0
4	B	27	0	29	3	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	4	0	6	0	0
7	A	1	0	0	0	0
8	A	91	0	0	2	0
8	B	123	0	0	4	0
All	All	7063	0	6650	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:500:GLN:HA	1:B:503:GLU:OE2	1.58	1.01
1:B:514:ARG:HH11	1:B:514:ARG:HG2	1.26	0.99
2:B:750:HEM:HMC2	2:B:750:HEM:HBC2	1.50	0.92
1:A:299:ARG:O	1:A:317:HIS:CE1	2.24	0.90
1:B:480:ILE:HA	8:B:1035:HOH:O	1.73	0.88
1:B:439:PHE:CE2	1:B:443:CYS:SG	2.74	0.80
1:B:514:ARG:HG2	1:B:514:ARG:NH1	1.96	0.76
1:A:299:ARG:O	1:A:317:HIS:HE1	1.67	0.76
1:B:481:ARG:HD3	1:B:498:ASN:HD21	1.51	0.76
1:B:659:ILE:O	1:B:663:GLU:HG3	1.88	0.74
1:B:481:ARG:HD3	1:B:498:ASN:ND2	2.05	0.72
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.04	0.71
1:B:663:GLU:O	1:B:667:ARG:HD2	1.90	0.70
1:A:486:LYS:HE2	1:A:499:VAL:HG11	1.73	0.69
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.75	0.69
1:B:409:TRP:CH2	2:B:750:HEM:HMC1	2.28	0.68
1:B:533:LEU:O	1:B:534:PHE:CG	2.46	0.68
1:B:525:GLN:HG3	1:B:529:ASN:O	1.94	0.68
1:B:587:TRP:H	2:B:750:HEM:HAB	1.59	0.68
1:B:501:PHE:CE2	1:B:505:CYS:SG	2.87	0.68
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.60	0.66
1:A:554:PHE:HB3	8:A:1087:HOH:O	1.96	0.65
2:B:750:HEM:HBA2	4:B:800:JRR:H4	1.78	0.64
1:A:686:SER:OG	1:B:682:PRO:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:LEU:HD12	1:B:494:GLY:N	2.14	0.63
1:B:592[A]:GLU:OE1	4:B:800:JRR:H16	1.99	0.62
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.35	0.62
1:A:299:ARG:HG3	1:A:318:LEU:HD11	1.82	0.61
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.35	0.61
1:A:317:HIS:O	1:A:320:SER:HB3	2.01	0.60
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.84	0.59
1:B:445:HIS:C	1:B:445:HIS:CD2	2.81	0.59
1:A:569:ASN:O	1:A:707:GLN:HG3	2.02	0.59
2:B:750:HEM:HBA1	2:B:750:HEM:HMA2	1.85	0.59
1:A:492:THR:HG21	1:A:496:PRO:HB3	1.85	0.59
1:A:667:ARG:NH1	1:A:668:CYS:SG	2.76	0.59
1:B:499:VAL:O	1:B:503:GLU:HG3	2.03	0.58
1:B:473:ARG:HD3	1:B:580:SER:HB2	1.86	0.58
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.86	0.57
1:B:595:VAL:O	1:B:599:CYS:HB2	2.04	0.57
1:A:321:THR:HG23	1:A:322:LEU:HG	1.86	0.57
1:A:304:LYS:O	1:A:694:GLU:HG3	2.05	0.57
1:B:510:TRP:CD1	1:B:521:PRO:HG3	2.40	0.57
1:A:323:GLU:HG2	1:B:328:GLU:HB3	1.86	0.56
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.87	0.56
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.68	0.56
1:A:500:GLN:O	1:A:504:ILE:HG13	2.07	0.55
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.89	0.55
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.89	0.55
1:B:388:ILE:O	1:B:392:SER:N	2.40	0.55
1:A:478:GLN:HA	1:A:566:ALA:O	2.07	0.54
1:B:425:GLN:HG2	1:B:448:TYR:CZ	2.42	0.54
1:B:304:LYS:O	1:B:694:GLU:HG3	2.07	0.54
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.42	0.53
1:A:507:GLN:O	1:A:507:GLN:HG2	2.08	0.53
1:A:299:ARG:HG3	1:A:318:LEU:CD1	2.39	0.53
1:B:409:TRP:CE2	2:B:750:HEM:C2C	2.97	0.53
1:B:607:LEU:HD13	1:B:626:LYS:HG2	1.90	0.53
2:A:750:HEM:HBA2	4:A:800:JRR:H4	1.90	0.53
1:B:514:ARG:NH1	1:B:514:ARG:CG	2.70	0.52
1:A:317:HIS:O	1:A:320:SER:CB	2.58	0.52
1:B:439:PHE:CZ	1:B:443:CYS:SG	3.03	0.51
1:A:371:ARG:NH2	1:A:371:ARG:HG2	2.26	0.51
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.10	0.51
1:B:533:LEU:C	1:B:534:PHE:CG	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLU:O	1:A:391:THR:OG1	2.25	0.50
1:B:505:CYS:O	1:B:506:ILE:C	2.53	0.50
1:B:514:ARG:HH11	1:B:514:ARG:CG	2.08	0.50
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.93	0.50
1:B:476:ASN:ND2	1:B:501:PHE:CZ	2.80	0.50
1:A:536:ILE:O	1:A:537:PRO:C	2.54	0.50
1:B:567:VAL:HB	1:B:584:PHE:CE1	2.47	0.49
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.94	0.49
1:A:487:GLN:O	1:A:490:GLY:N	2.45	0.49
1:A:371:ARG:HH21	1:A:371:ARG:HG2	1.78	0.49
1:A:675:ASP:O	1:A:679:ILE:HG12	2.12	0.49
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.43	0.49
1:B:481:ARG:NH1	1:B:498:ASN:OD1	2.45	0.49
1:B:567:VAL:HB	1:B:584:PHE:CZ	2.48	0.49
2:A:750:HEM:O2D	4:A:800:JRR:N1A	2.46	0.49
1:B:478:GLN:HA	1:B:566:ALA:O	2.12	0.48
1:B:624:LEU:O	1:B:628:GLN:HG3	2.13	0.48
1:B:366:TYR:HD2	1:B:371:ARG:HB2	1.77	0.48
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.76	0.48
1:A:665:GLU:CB	1:A:672:CYS:HB2	2.43	0.48
2:B:750:HEM:HMC2	2:B:750:HEM:CBC	2.33	0.48
1:B:481:ARG:CD	1:B:498:ASN:HD21	2.23	0.46
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.50	0.46
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.48	0.46
1:B:495:ASP:HB2	1:B:604:TYR:CE1	2.50	0.46
1:A:299:ARG:O	1:A:317:HIS:NE2	2.49	0.45
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.99	0.45
2:A:750:HEM:O2A	4:A:800:JRR:H2'A	2.16	0.45
1:B:299:ARG:CZ	1:B:299:ARG:HB3	2.47	0.45
1:B:566:ALA:HA	1:B:584:PHE:O	2.16	0.45
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.99	0.45
1:A:460:THR:O	1:A:583:PRO:HD2	2.17	0.45
1:B:302:LYS:HA	1:B:312:LEU:O	2.17	0.45
1:B:314:ASP:OD1	1:B:314:ASP:C	2.60	0.45
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.51	0.45
1:A:352:ASP:OD2	1:A:352:ASP:N	2.48	0.45
1:B:498:ASN:O	1:B:499:VAL:C	2.59	0.45
1:B:496:PRO:HD2	1:B:603:ARG:HA	1.98	0.45
1:B:582:CYS:O	1:B:583:PRO:C	2.59	0.45
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.45
1:B:477:SER:HA	1:B:569:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.99	0.44
1:A:370:LYS:HB2	1:A:370:LYS:HE3	1.85	0.44
1:A:606:ILE:O	1:A:610:VAL:HG23	2.18	0.44
1:B:439:PHE:HZ	1:B:537:PRO:HD3	1.82	0.44
1:A:303:VAL:HG23	1:A:312:LEU:HB2	1.99	0.43
1:A:449:ALA:O	1:A:455:LEU:HA	2.18	0.43
1:B:425:GLN:HG2	1:B:448:TYR:CE2	2.53	0.43
1:A:709:ASP:HB3	1:A:711:TRP:CE2	2.54	0.43
1:B:416:VAL:HB	8:B:1001:HOH:O	2.19	0.43
1:B:455:LEU:HD12	1:B:455:LEU:N	2.33	0.43
2:B:750:HEM:O2D	4:B:800:JRR:N1A	2.51	0.43
1:A:708:PRO:O	1:A:709:ASP:C	2.62	0.43
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.07	0.42
1:B:409:TRP:CZ2	2:B:750:HEM:HMC1	2.53	0.42
1:B:568:SER:C	8:B:1004:HOH:O	2.62	0.42
1:A:418:ARG:C	1:A:420:GLN:N	2.75	0.42
1:A:321:THR:HG23	1:A:322:LEU:N	2.34	0.42
1:A:549:PRO:C	1:A:550:LYS:HG2	2.43	0.42
1:B:416:VAL:HG23	1:B:679:ILE:HG23	2.00	0.42
1:B:631:VAL:HG22	1:B:683:MET:HE1	2.01	0.42
1:A:418:ARG:C	1:A:420:GLN:H	2.27	0.42
1:A:445:HIS:C	1:A:445:HIS:CD2	2.96	0.42
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.92	0.42
1:B:589:MET:HA	1:B:649:VAL:O	2.18	0.42
1:A:440:ASN:ND2	8:A:1057:HOH:O	2.43	0.42
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.55	0.42
1:A:510:TRP:CE3	1:A:512:ALA:HB2	2.54	0.42
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.02	0.42
1:B:391:THR:O	1:B:392:SER:HB2	2.19	0.42
1:B:409:TRP:CH2	2:B:750:HEM:CMC	3.00	0.41
1:B:388:ILE:O	1:B:392:SER:HA	2.21	0.41
1:A:590:GLY:HA3	1:A:638:LEU:HD21	2.01	0.41
1:B:449:ALA:O	1:B:455:LEU:HA	2.20	0.41
1:A:685:GLY:O	1:A:691:PHE:HB2	2.20	0.41
1:A:709:ASP:HA	1:A:710:PRO:HD3	1.96	0.41
1:B:418:ARG:C	1:B:420:GLN:N	2.74	0.41
1:B:505:CYS:O	1:B:507:GLN:N	2.54	0.41
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.56	0.41
1:B:567:VAL:O	1:B:583:PRO:HA	2.21	0.41
1:A:694:GLU:HB3	1:B:335:ILE:HD13	2.02	0.41
1:B:510:TRP:CG	1:B:521:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:HIS:O	1:B:408:ALA:C	2.63	0.41
1:B:412:ALA:O	1:B:418:ARG:CZ	2.69	0.41
1:B:455:LEU:N	1:B:455:LEU:CD1	2.83	0.40
1:A:492:THR:HG21	1:A:496:PRO:CB	2.50	0.40
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.40
1:B:447:LYS:HG2	8:B:1095:HOH:O	2.22	0.40
1:B:493:LEU:HD12	1:B:493:LEU:C	2.46	0.40
1:A:321:THR:HG23	1:A:322:LEU:H	1.85	0.40
1:B:710:PRO:HD2	1:B:711:TRP:CE3	2.57	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	403/422 (96%)	381 (94%)	21 (5%)	1 (0%)	43	44
1	B	408/422 (97%)	379 (93%)	27 (7%)	2 (0%)	24	20
All	All	811/844 (96%)	760 (94%)	48 (6%)	3 (0%)	30	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	GLY
1	B	685	GLY
1	A	709	ASP

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	363/377 (96%)	347 (96%)	16 (4%)	25	23
1	B	367/377 (97%)	353 (96%)	14 (4%)	29	29
All	All	730/754 (97%)	700 (96%)	30 (4%)	27	26

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	VAL
1	A	319	LYS
1	A	350	THR
1	A	352	ASP
1	A	371	ARG
1	A	380	ARG
1	A	477	SER
1	A	504	ILE
1	A	507	GLN
1	A	508	GLN
1	A	555	LYS
1	A	608	GLU
1	A	620	LYS
1	A	645	LYS
1	A	701	THR
1	A	707	GLN
1	B	300	PHE
1	B	303	VAL
1	B	330	ILE
1	B	382	GLU
1	B	481	ARG
1	B	493	LEU
1	B	500	GLN
1	B	516	ARG
1	B	523	LEU
1	B	532	GLU
1	B	535	GLN
1	B	540	LEU
1	B	667	ARG
1	B	715	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	A	353	GLN
1	A	395	GLN
1	A	407	HIS
1	A	440	ASN
1	A	454	ASN
1	A	478	GLN
1	A	508	GLN
1	A	628	GLN
1	A	642	GLN
1	A	697	ASN
1	A	712	ASN
1	B	385	ASN
1	B	407	HIS
1	B	454	ASN
1	B	470	HIS
1	B	487	GLN
1	B	527	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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
3	H4B	A	760	-	17,18,18	1.32	3 (17%)	14,26,26	2.31	5 (35%)
3	H4B	B	760	-	17,18,18	1.52	3 (17%)	14,26,26	1.89	5 (35%)
5	ACT	B	860	-	3,3,3	0.90	0	3,3,3	0.30	0
2	HEM	A	750	1	50,50,50	1.98	10 (20%)	67,82,82	1.51	13 (19%)
6	EDO	A	890	-	3,3,3	0.62	0	2,2,2	0.45	0
2	HEM	B	750	1	50,50,50	1.85	9 (18%)	67,82,82	1.31	8 (11%)
5	ACT	A	860	-	3,3,3	0.74	0	3,3,3	0.93	0
4	JRR	A	800	-	28,29,29	1.05	1 (3%)	29,38,38	2.19	11 (37%)
4	JRR	B	800	-	28,29,29	0.88	0	29,38,38	2.19	11 (37%)

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
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
3	H4B	B	760	-	-	1/8/17/17	0/2/2/2
2	HEM	A	750	1	-	2/14/54/54	-
6	EDO	A	890	-	-	0/1/1/1	-
2	HEM	B	750	1	-	5/14/54/54	-
4	JRR	A	800	-	-	5/13/23/23	0/3/3/3
4	JRR	B	800	-	-	1/13/23/23	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3D-C2D	7.55	1.53	1.36
2	A	750	HEM	C3D-C2D	7.27	1.52	1.36
2	A	750	HEM	FE-NC	5.09	2.12	1.95
2	B	750	HEM	FE-NC	4.20	2.09	1.95
2	B	750	HEM	FE-NA	3.76	2.07	1.95
2	A	750	HEM	FE-ND	3.62	2.06	1.94
2	B	750	HEM	FE-ND	3.55	2.05	1.94
3	B	760	H4B	O4-C4	3.50	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	CMC-C2C	3.42	1.57	1.50
2	A	750	HEM	CAB-C3B	3.36	1.56	1.47
3	B	760	H4B	C7-N8	3.36	1.49	1.46
2	B	750	HEM	CMC-C2C	3.02	1.57	1.50
2	A	750	HEM	FE-NB	3.00	2.04	1.94
2	B	750	HEM	CMB-C2B	2.93	1.56	1.50
3	A	760	H4B	C7-N8	2.76	1.49	1.46
4	A	800	JRR	C2A-N1A	2.73	1.39	1.34
2	B	750	HEM	CAB-C3B	2.73	1.54	1.47
2	B	750	HEM	CAC-C3C	2.71	1.54	1.47
2	A	750	HEM	FE-NA	2.68	2.04	1.95
2	A	750	HEM	CMA-C3A	2.59	1.56	1.50
2	B	750	HEM	CMA-C3A	2.50	1.55	1.50
2	A	750	HEM	C2A-C3A	-2.31	1.32	1.38
3	A	760	H4B	C2-N2	2.26	1.39	1.34
2	A	750	HEM	CAC-C3C	2.22	1.53	1.47
3	B	760	H4B	C7-C6	2.17	1.54	1.52
3	A	760	H4B	C4-N3	-2.09	1.34	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	JRR	C6A-N1A-C2A	6.98	123.29	118.07
3	A	760	H4B	C2-N1-C8A	5.52	123.11	113.36
4	A	800	JRR	C7A-C2A-N1A	4.61	122.21	116.57
4	B	800	JRR	C11-C12-C13	4.42	122.60	118.75
2	A	750	HEM	CBA-CAA-C2A	-4.31	100.60	112.53
4	A	800	JRR	N6A-C6A-N1A	4.08	123.16	116.59
2	B	750	HEM	C4D-ND-C1D	4.03	109.98	105.21
3	B	760	H4B	C2-N1-C8A	4.01	120.44	113.36
2	A	750	HEM	C4D-ND-C1D	3.99	109.93	105.21
4	A	800	JRR	C6A-N1A-C2A	3.94	121.02	118.07
4	A	800	JRR	C2'-C3'-C4'	3.76	108.75	103.22
4	A	800	JRR	C3-C4-C11	-3.57	104.78	112.83
2	A	750	HEM	C4C-C3C-C2C	3.53	109.88	106.81
2	A	750	HEM	C3B-C2B-C1B	3.34	108.92	106.41
4	B	800	JRR	C14-C13-C12	-3.20	119.00	123.23
2	A	750	HEM	CBD-CAD-C3D	-3.02	104.19	112.53
2	B	750	HEM	CBA-CAA-C2A	-2.97	104.32	112.53
4	A	800	JRR	F13-C13-C14	2.93	123.25	118.55
3	A	760	H4B	N3-C2-N1	-2.81	118.17	123.32
2	B	750	HEM	CAA-CBA-CGA	-2.80	106.25	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	C4-C4A-N5	2.80	123.89	116.27
4	B	800	JRR	C2'-C3'-C4'	-2.76	99.17	103.22
4	A	800	JRR	C5'-N1'-C2'	2.72	112.22	105.45
4	B	800	JRR	C5A-C4A-C3A	2.69	121.11	118.11
3	A	760	H4B	C4A-C4-N3	2.68	119.49	112.13
3	B	760	H4B	O4-C4-C4A	-2.57	121.07	127.26
2	A	750	HEM	CBC-CAC-C3C	-2.55	114.77	127.53
4	B	800	JRR	C3-C4-C11	-2.52	107.16	112.83
4	A	800	JRR	C3A-C2A-N1A	-2.51	119.87	122.73
4	A	800	JRR	C16-C15-C14	-2.45	117.09	120.24
3	B	760	H4B	C4A-C4-N3	2.38	118.66	112.13
4	B	800	JRR	C8A-C4A-C3A	-2.36	117.73	120.92
2	B	750	HEM	CHA-C4D-ND	2.35	127.28	124.37
2	B	750	HEM	C4A-CHB-C1B	-2.35	120.73	126.25
2	B	750	HEM	CHC-C4B-NB	2.28	126.88	124.42
4	B	800	JRR	C5'-N1'-C2'	2.26	111.07	105.45
2	B	750	HEM	CBD-CAD-C3D	-2.26	106.28	112.53
2	B	750	HEM	C4B-C3B-C2B	2.24	109.34	107.28
4	A	800	JRR	F13-C13-C12	-2.24	115.10	118.28
4	A	800	JRR	C4-C11-C12	-2.21	116.83	120.54
3	B	760	H4B	C2-N3-C4	-2.18	121.16	125.11
2	A	750	HEM	C1A-CHA-C4D	-2.14	121.20	126.25
4	B	800	JRR	F13-C13-C14	2.14	121.98	118.55
2	A	750	HEM	O1A-CGA-CBA	-2.13	116.32	123.09
2	A	750	HEM	C3B-C4B-NB	-2.13	107.94	109.47
3	A	760	H4B	C11-C10-C9	-2.13	109.50	112.11
4	B	800	JRR	C1-O1-C3'	2.12	118.75	113.90
2	A	750	HEM	CHA-C4D-ND	2.07	126.93	124.37
3	B	760	H4B	N2-C2-N3	2.07	121.12	116.76
2	A	750	HEM	C4D-C3D-C2D	-2.06	103.89	106.89
4	B	800	JRR	C5A-C6A-N1A	-2.06	117.65	121.76
2	A	750	HEM	C4C-NC-C1C	2.05	109.17	105.82
2	A	750	HEM	C2B-C1B-NB	-2.01	107.53	109.84

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	750	HEM	C2B-C3B-CAB-CBB
4	A	800	JRR	C5'-C4'-C7A-C2A
4	A	800	JRR	C4-C3-N2-C2
4	B	800	JRR	C1-C2-N2-C3

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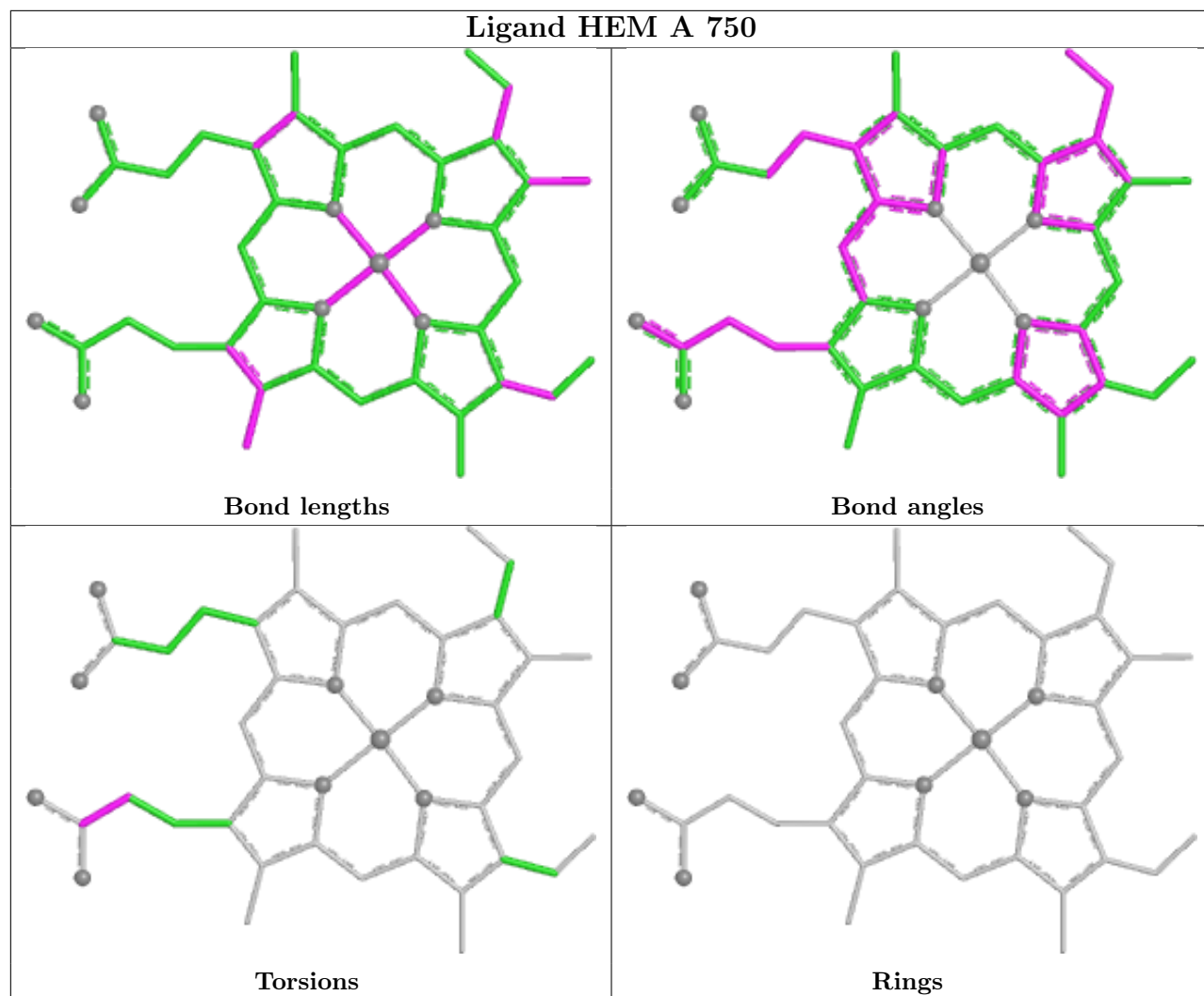
Mol	Chain	Res	Type	Atoms
2	B	750	HEM	C4B-C3B-CAB-CBB
3	B	760	H4B	C7-C6-C9-O9
4	A	800	JRR	C2-C1-O1-C3'
4	A	800	JRR	N1A-C2A-C7A-C4'
2	B	750	HEM	CAA-CBA-CGA-O2A
2	B	750	HEM	CAA-CBA-CGA-O1A
2	A	750	HEM	CAA-CBA-CGA-O2A
4	A	800	JRR	C1-C2-N2-C3
2	A	750	HEM	CAA-CBA-CGA-O1A
2	B	750	HEM	C3A-C2A-CAA-CBA

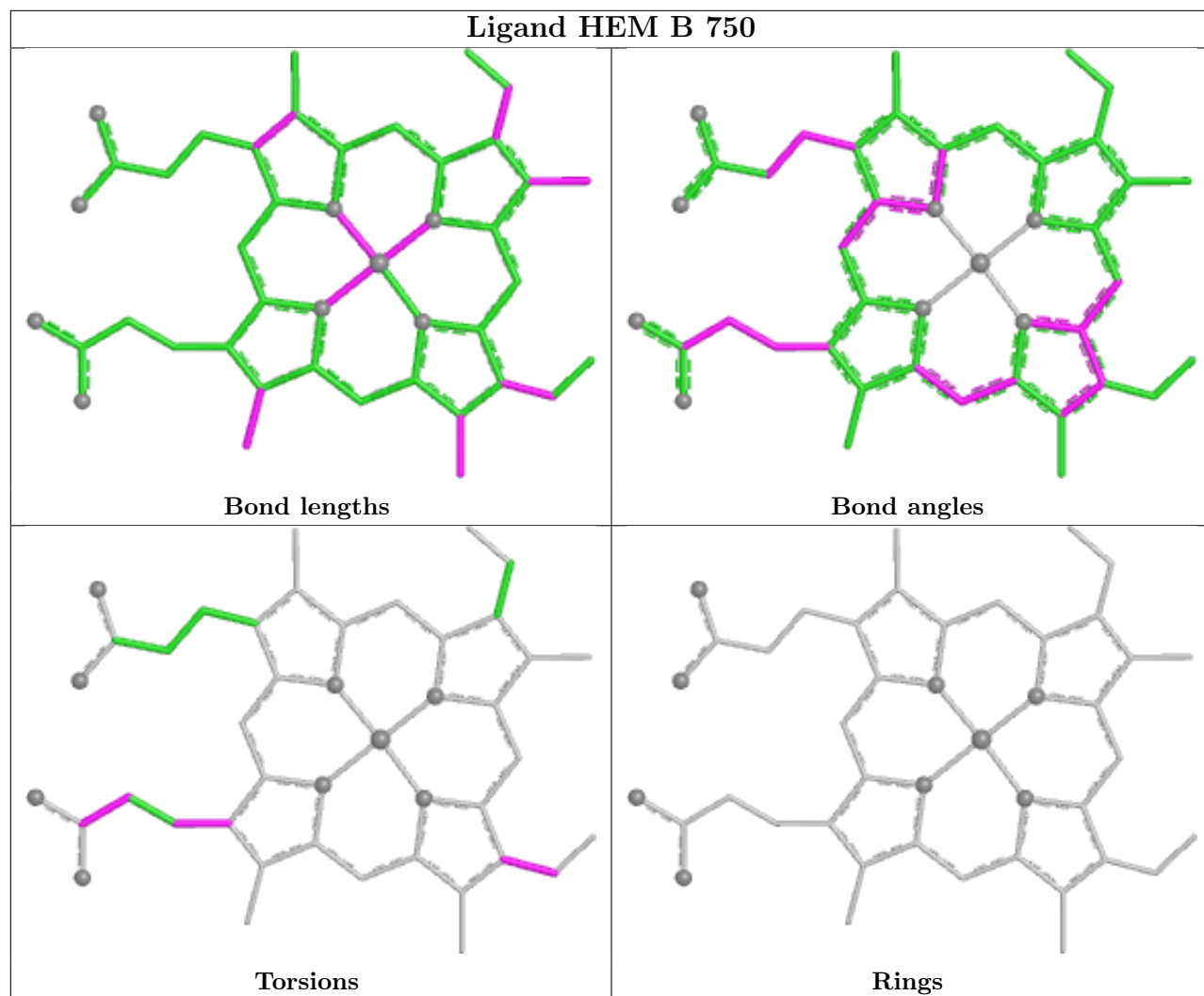
There are no ring outliers.

4 monomers are involved in 16 short contacts:

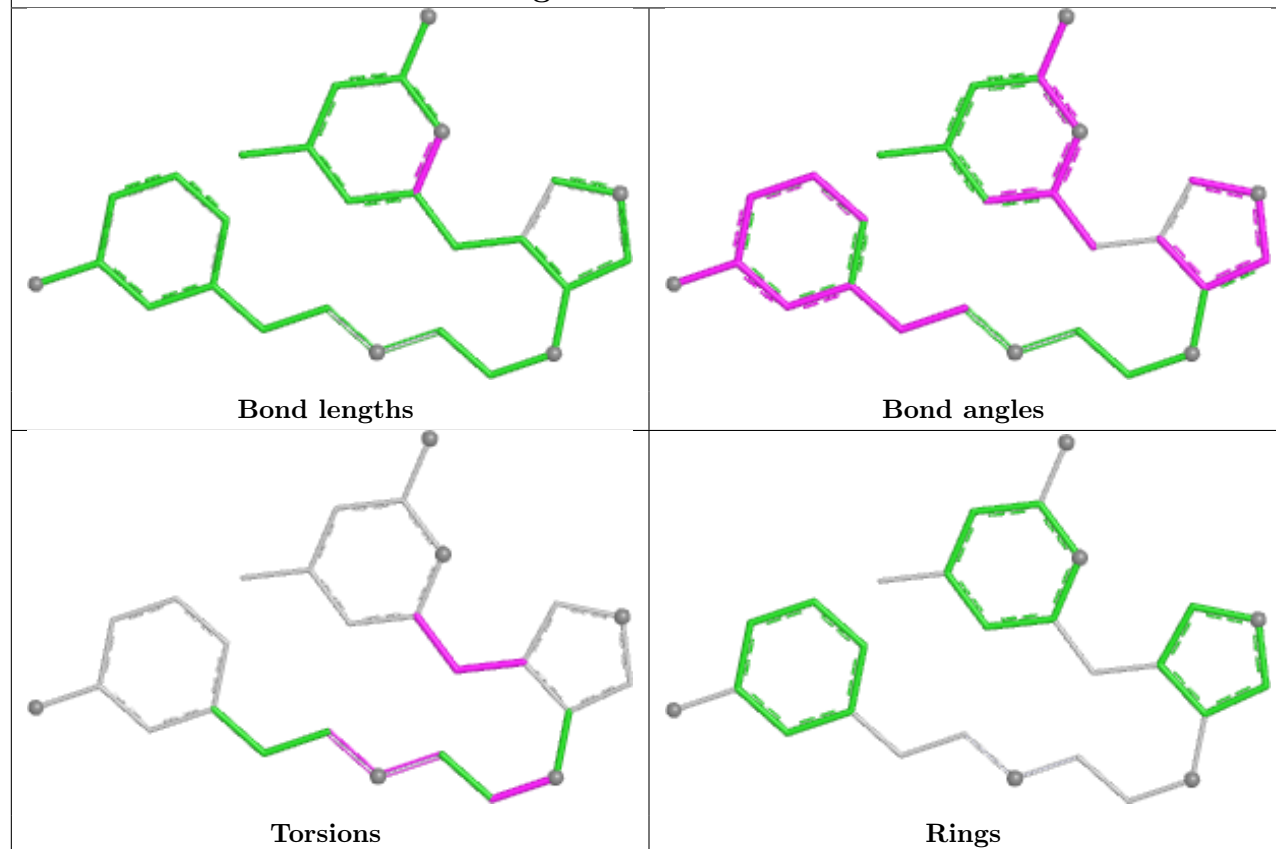
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	5	0
2	B	750	HEM	10	0
4	A	800	JRR	3	0
4	B	800	JRR	3	0

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.

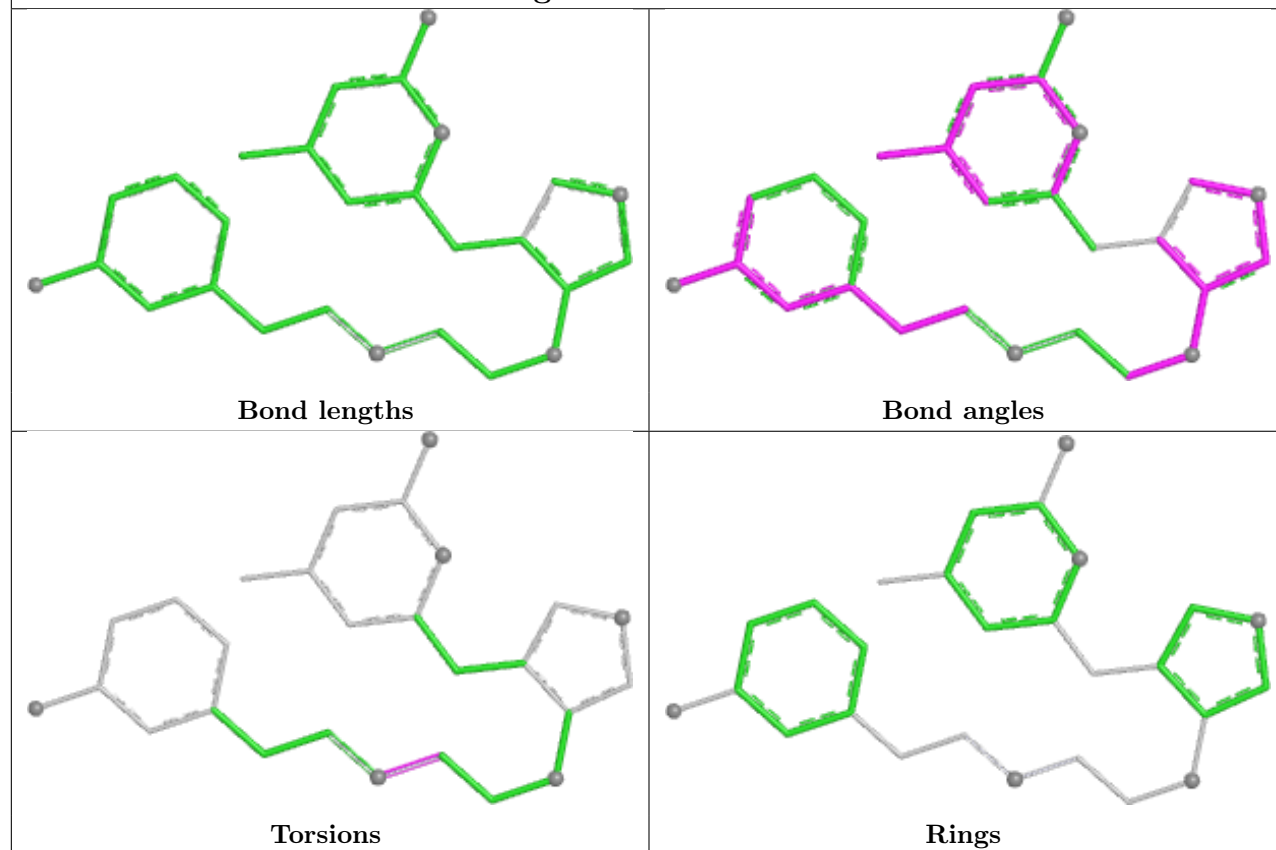




Ligand JRR A 800



Ligand JRR B 800



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	407/422 (96%)	0.38	14 (3%) 48 52	34, 64, 121, 153	0
1	B	411/422 (97%)	0.22	5 (1%) 76 79	22, 53, 89, 112	1 (0%)
All	All	818/844 (96%)	0.30	19 (2%) 61 64	22, 58, 110, 153	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	3.3
1	B	715	VAL	3.0
1	A	300	PHE	2.8
1	A	488	PRO	2.7
1	A	338	PRO	2.7
1	A	361	PHE	2.4
1	A	372	PHE	2.4
1	A	330	ILE	2.4
1	A	322	LEU	2.3
1	A	716	TRP	2.3
1	A	706	TYR	2.2
1	A	483	ALA	2.1
1	A	713	THR	2.1
1	B	338	PRO	2.1
1	B	488	PRO	2.1
1	A	493	LEU	2.0
1	A	557	LEU	2.0
1	A	350	THR	2.0
1	B	706	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

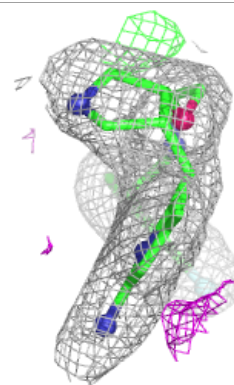
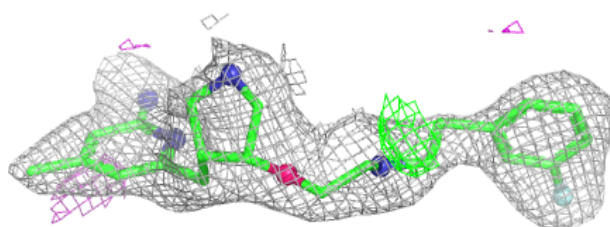
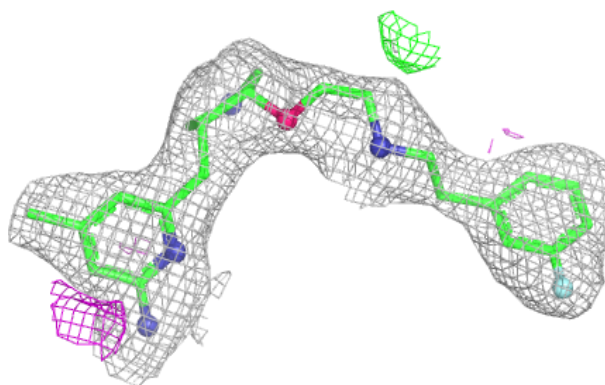
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	JRR	A	800	27/27	0.87	0.10	47,54,61,63	0
5	ACT	B	860	4/4	0.87	0.18	79,81,82,83	0
6	EDO	A	890	4/4	0.87	0.13	49,50,51,52	0
4	JRR	B	800	27/27	0.89	0.10	38,49,58,60	0
5	ACT	A	860	4/4	0.90	0.17	84,86,86,88	0
3	H4B	B	760	17/17	0.93	0.08	29,38,44,49	0
3	H4B	A	760	17/17	0.94	0.08	33,38,46,47	0
2	HEM	A	750	43/43	0.96	0.09	36,41,50,54	0
2	HEM	B	750	43/43	0.97	0.07	38,45,49,53	0
7	ZN	A	900	1/1	0.99	0.03	51,51,51,51	0

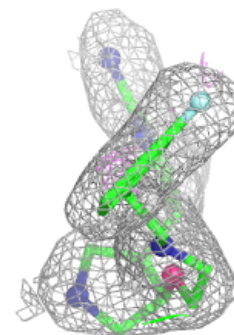
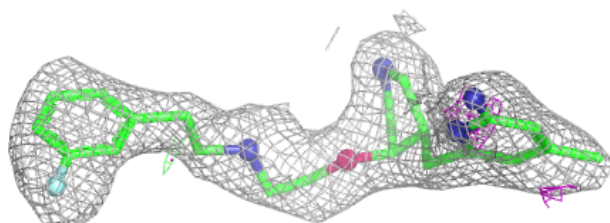
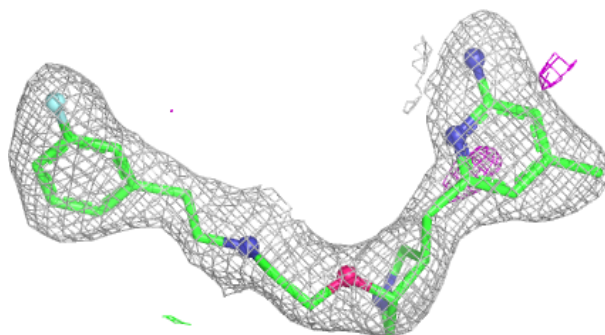
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JRR 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)

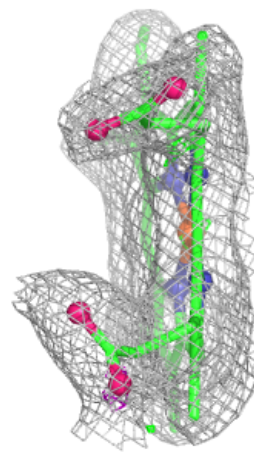
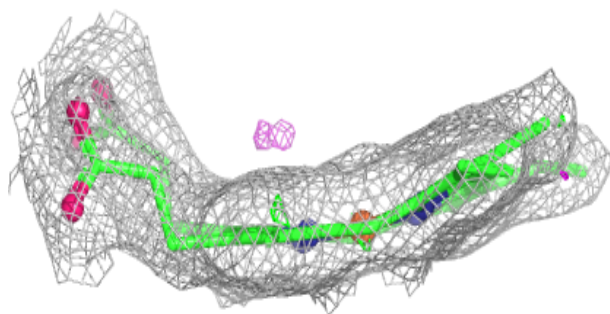
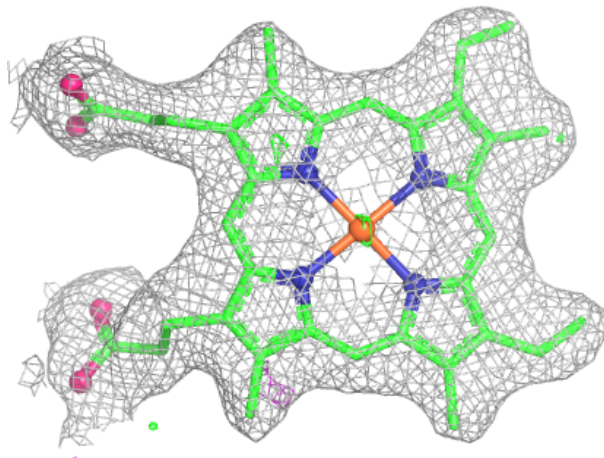
**Electron density around JRR B 800:**

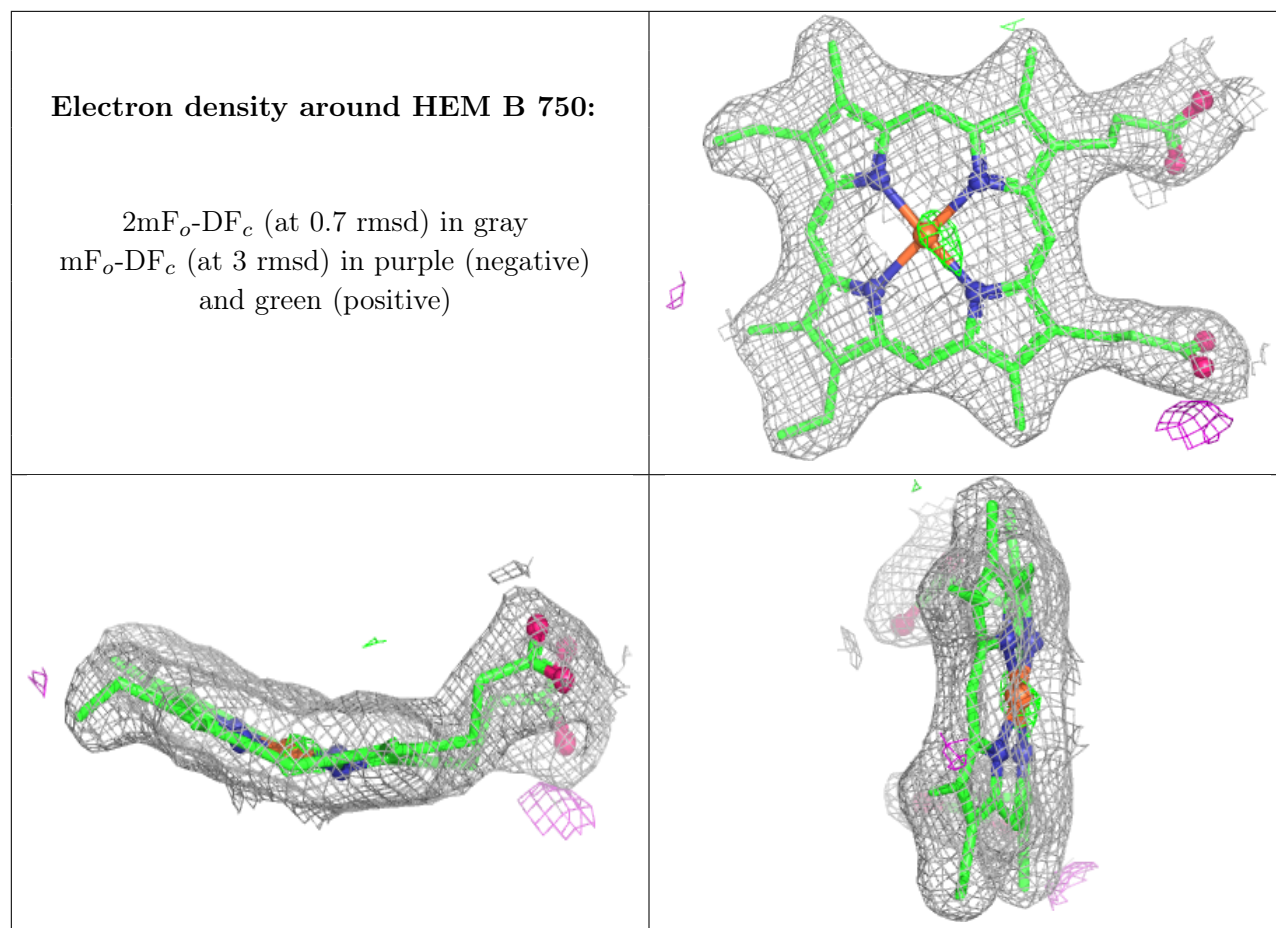
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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 ⓘ

There are no such residues in this entry.