



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:20 PM UTC

PDB ID : 4V3W / pdb_00004v3w
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with
2-(2-(1H-imidazol-1-yl)pyrimidin-4-yl)-N-(3- fluorophenethyl)ethan-1-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-10-20
Resolution : 2.13 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

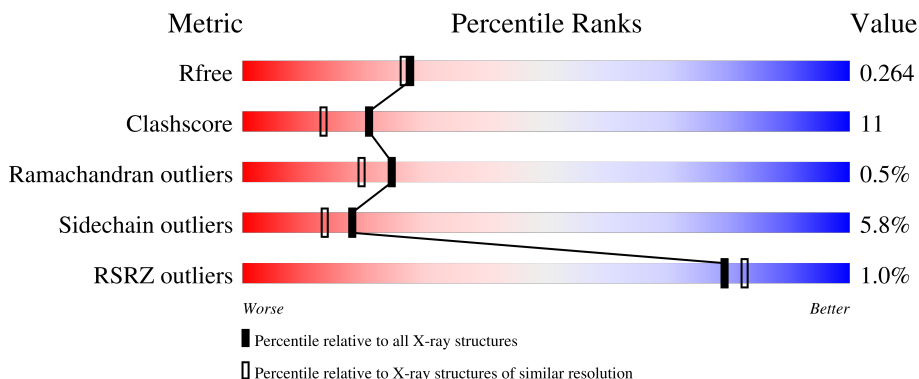
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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.

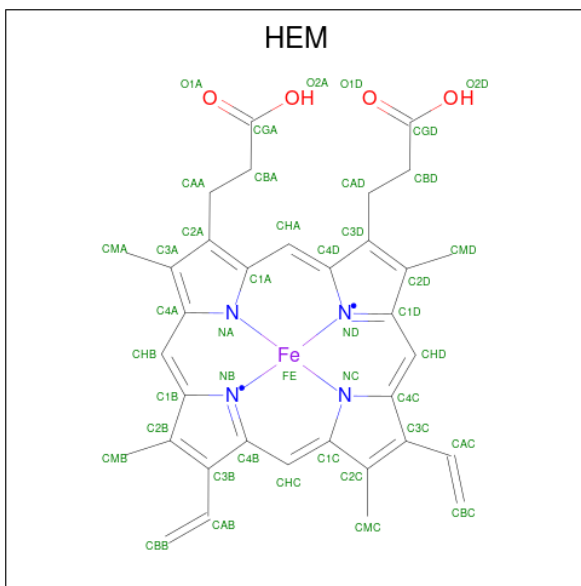
Mol	Chain	Length	Quality of chain
1	A	422	
1	B	422	

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.

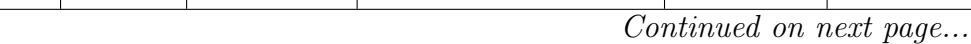
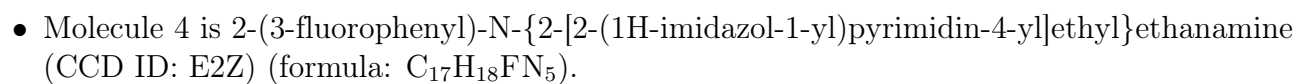
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total 3323	C 2127	N 567	O 607	S 22	0	2	1
1	B	411	Total 3354	C 2146	N 574	O 613	S 21	0	2	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	F	N	0	0
			23	17	1	5		

- 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		

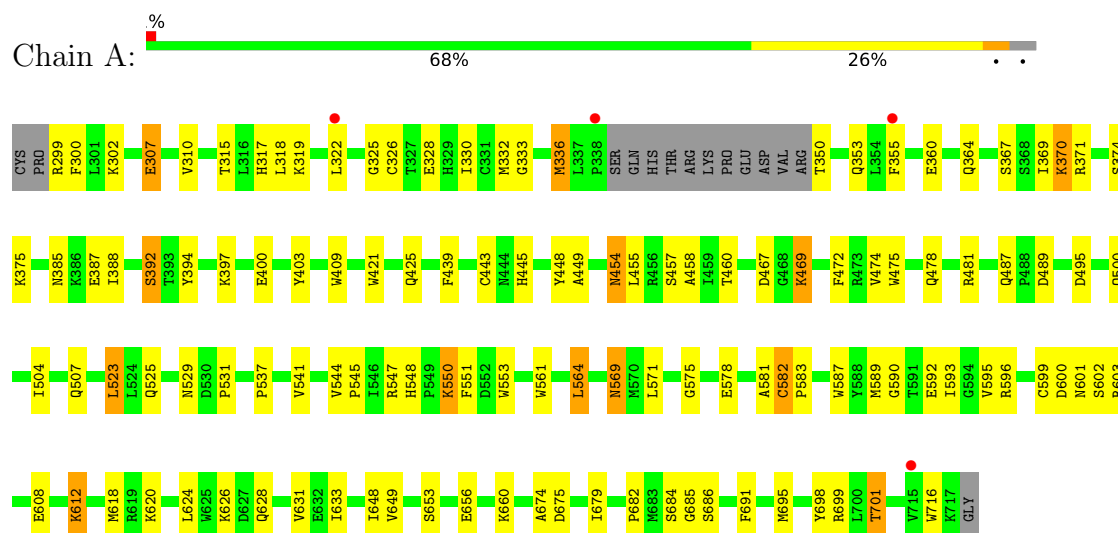
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	72	Total	O	0	0
			72	72		
7	B	80	Total	O	0	0
			80	80		

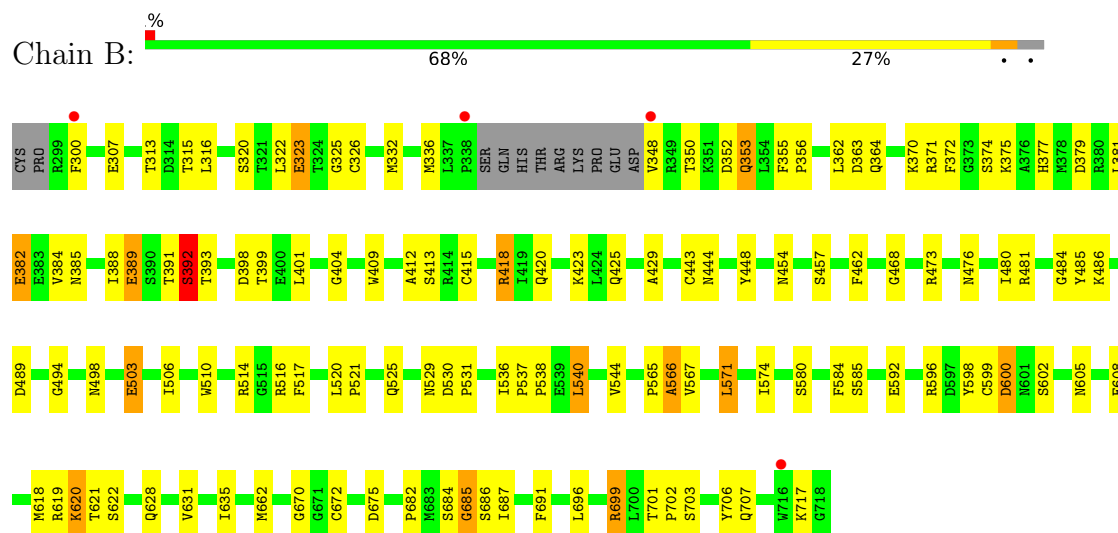
3 Residue-property plots [i](#)

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: 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	51.84Å 110.25Å 164.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.72 – 2.13 91.55 – 2.13	Depositor EDS
% Data completeness (in resolution range)	98.6 (91.72-2.13) 98.7 (91.55-2.13)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.206 , 0.265 0.206 , 0.264	Depositor DCC
R_{free} test set	2640 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.5	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	7004	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: H4B, ACT, E2Z, ZN, HEM

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	1.10	5/3422 (0.1%)	1.27	18/4643 (0.4%)
1	B	1.35	18/3453 (0.5%)	1.40	28/4681 (0.6%)
All	All	1.23	23/6875 (0.3%)	1.33	46/9324 (0.5%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	566	ALA	C-O	8.70	1.34	1.24
1	B	503	GLU	N-CA	7.94	1.56	1.46
1	A	596	ARG	CZ-NH2	7.20	1.42	1.33
1	B	484	GLY	N-CA	7.13	1.53	1.45
1	B	600	ASP	CA-C	6.95	1.61	1.52
1	A	716	TRP	C-N	-6.60	1.24	1.33
1	B	571	LEU	N-CA	-6.60	1.38	1.46
1	B	371	ARG	NE-CZ	6.37	1.40	1.33
1	B	565	PRO	C-O	6.32	1.32	1.24
1	A	537	PRO	C-O	-6.24	1.17	1.24
1	B	544	VAL	CA-CB	6.00	1.58	1.54
1	B	670	GLY	N-CA	5.99	1.53	1.45
1	B	388	ILE	N-CA	-5.82	1.39	1.46
1	B	412	ALA	N-CA	5.81	1.53	1.46
1	A	474	VAL	C-O	5.61	1.30	1.24
1	B	401	LEU	N-CA	5.54	1.53	1.46
1	B	506	ILE	N-CA	5.44	1.52	1.46
1	B	457	SER	C-O	5.44	1.30	1.23
1	A	592	GLU	CG-CD	5.42	1.65	1.52
1	B	444	ASN	N-CA	5.41	1.53	1.46
1	B	670	GLY	CA-C	5.36	1.58	1.51
1	B	393	THR	CA-C	5.14	1.58	1.53
1	B	494	GLY	C-O	-5.10	1.17	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	ASP	CA-C-N	-12.72	107.11	120.85
1	B	530	ASP	C-N-CA	-12.72	107.11	120.85
1	B	536	ILE	CA-C-N	-9.84	110.25	120.38
1	B	536	ILE	C-N-CA	-9.84	110.25	120.38
1	B	315	THR	N-CA-C	-8.69	103.10	114.31
1	B	401	LEU	N-CA-C	-7.58	103.03	111.82
1	A	596	ARG	NE-CZ-NH1	-7.44	114.06	121.50
1	A	701	THR	CB-CA-C	7.43	120.02	108.88
1	A	592	GLU	N-CA-C	-6.90	103.76	111.28
1	A	564	LEU	CA-C-N	-6.89	111.23	119.84
1	A	564	LEU	C-N-CA	-6.89	111.23	119.84
1	B	520	LEU	CA-C-N	-6.74	113.85	120.52
1	B	520	LEU	C-N-CA	-6.74	113.85	120.52
1	B	429	ALA	N-CA-C	-6.53	103.64	112.26
1	A	541	VAL	CB-CA-C	-6.33	104.60	112.45
1	B	703	SER	N-CA-C	5.98	117.33	108.60
1	B	443	CYS	N-CA-C	-5.96	104.70	111.07
1	A	495	ASP	CA-C-N	-5.77	113.73	119.56
1	A	495	ASP	C-N-CA	-5.77	113.73	119.56
1	B	489	ASP	CA-C-N	-5.76	116.59	123.44
1	B	489	ASP	C-N-CA	-5.76	116.59	123.44
1	B	707	GLN	CA-C-N	-5.72	113.70	120.11
1	B	707	GLN	C-N-CA	-5.72	113.70	120.11
1	B	392	SER	N-CA-CB	-5.68	108.42	114.10
1	B	316	LEU	N-CA-C	5.67	119.01	111.75
1	B	468	GLY	N-CA-C	-5.62	107.89	115.36
1	A	474	VAL	CB-CA-C	-5.61	103.45	111.31
1	A	582	CYS	CA-C-N	-5.58	114.01	119.76
1	A	582	CYS	C-N-CA	-5.58	114.01	119.76
1	B	672	CYS	CA-C-N	-5.57	113.97	119.93
1	B	672	CYS	C-N-CA	-5.57	113.97	119.93
1	A	333	GLY	N-CA-C	5.57	120.67	113.27
1	B	592	GLU	N-CA-C	-5.51	105.27	111.28
1	A	633	ILE	N-CA-C	-5.40	105.11	110.62
1	B	413	SER	N-CA-C	5.37	119.09	112.54
1	A	457	SER	CA-CB-OG	-5.28	100.54	111.10
1	A	600	ASP	N-CA-C	-5.22	102.66	110.23
1	B	462	PHE	CA-C-N	-5.18	114.44	119.78
1	B	462	PHE	C-N-CA	-5.18	114.44	119.78
1	B	599	CYS	N-CA-C	5.18	120.45	113.72
1	B	336	MET	N-CA-C	5.14	116.88	111.28
1	A	537	PRO	CA-C-N	5.09	125.12	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	PRO	C-N-CA	5.09	125.12	119.32
1	A	569	ASN	N-CA-C	5.08	119.17	112.92
1	B	699	ARG	N-CA-C	5.03	116.89	107.99
1	B	418	ARG	N-CA-C	5.01	119.02	113.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3323	0	3231	78	0
1	B	3354	0	3270	72	0
2	A	43	0	30	4	0
2	B	43	0	30	11	0
3	A	17	0	15	3	0
3	B	17	0	15	0	0
4	A	23	0	18	1	0
4	B	23	0	18	1	0
5	A	4	0	3	1	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	72	0	0	0	0
7	B	80	0	0	6	0
All	All	7004	0	6633	149	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 11.

All (149) 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)
2:B:750:HEM:HMC2	2:B:750:HEM:HBC2	1.34	1.08
1:B:596:ARG:NH2	1:B:600:ASP:OD2	1.98	0.95
1:B:537:PRO:HG2	1:B:540:LEU:HD22	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:MET:HE2	3:A:760:H4B:O4	1.77	0.85
1:A:336:MET:CE	3:A:760:H4B:O4	2.28	0.81
1:A:350:THR:N	1:A:353:GLN:HE21	1.83	0.76
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.73	0.70
1:B:364:GLN:NE2	7:B:2003:HOH:O	2.24	0.69
1:B:391:THR:O	1:B:392:SER:HB2	1.92	0.69
1:A:571:LEU:HD21	1:A:578:GLU:HB3	1.74	0.69
1:A:336:MET:HE3	3:A:760:H4B:HN5	1.59	0.68
1:A:487:GLN:HB2	1:A:489:ASP:HB3	1.78	0.66
1:A:328:GLU:HB3	1:B:323:GLU:HG2	1.78	0.65
1:B:398:ASP:HB2	7:B:2008:HOH:O	1.95	0.65
1:A:454:ASN:C	1:A:454:ASN:HD22	2.07	0.63
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.28	0.63
1:B:608:GLU:HG3	1:B:618:MET:HE1	1.80	0.63
2:A:750:HEM:HBC2	2:A:750:HEM:HMC1	1.81	0.63
1:B:415:CYS:HB2	2:B:750:HEM:C4D	2.34	0.63
1:B:415:CYS:HB2	2:B:750:HEM:ND	2.12	0.63
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.17	0.62
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.34	0.61
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.82	0.61
1:A:589:MET:HA	1:A:649:VAL:O	2.00	0.61
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.83	0.61
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.37	0.60
1:B:355:PHE:CE2	1:B:385:ASN:HB2	2.37	0.59
1:B:353:GLN:O	1:B:356:PRO:HG2	2.02	0.59
1:A:487:GLN:C	1:A:489:ASP:H	2.11	0.58
1:B:404:GLY:HA3	1:B:574:ILE:HD13	1.84	0.58
1:B:620:LYS:HE3	1:B:620:LYS:HA	1.86	0.58
1:B:391:THR:O	1:B:392:SER:CB	2.51	0.58
1:B:325:GLY:O	1:B:332:MET:HE2	2.05	0.57
1:B:375:LYS:NZ	1:B:379:ASP:OD2	2.37	0.56
1:B:350:THR:O	1:B:353:GLN:HG2	2.05	0.56
1:B:596:ARG:HH21	1:B:600:ASP:CG	2.08	0.56
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.87	0.56
1:A:350:THR:N	1:A:353:GLN:NE2	2.53	0.56
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.42	0.55
1:B:619:ARG:HH11	1:B:619:ARG:HB2	1.71	0.55
1:A:325:GLY:O	1:A:332:MET:HG3	2.07	0.53
1:B:701:THR:HB	1:B:702:PRO:HA	1.90	0.53
1:B:619:ARG:HB2	1:B:619:ARG:NH1	2.24	0.53
1:A:307[B]:GLU:OE1	1:B:602:SER:OG	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ILE:O	1:A:392:SER:HA	2.07	0.53
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.91	0.53
1:B:476:ASN:HB3	7:B:2039:HOH:O	2.08	0.53
1:B:701:THR:HA	1:B:702:PRO:C	2.34	0.53
1:B:409:TRP:CE2	2:B:750:HEM:C2C	2.97	0.52
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.90	0.52
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.91	0.52
1:A:388:ILE:O	1:A:392:SER:N	2.43	0.52
1:B:525:GLN:HG3	1:B:529:ASN:O	2.10	0.51
1:A:369:ILE:O	1:A:370:LYS:HE3	2.10	0.51
1:A:601:ASN:HB2	1:B:307[B]:GLU:CD	2.35	0.51
1:A:487:GLN:C	1:A:489:ASP:N	2.66	0.51
1:A:603:ARG:HH11	1:A:603:ARG:HG3	1.76	0.51
1:B:374:SER:O	1:B:377:HIS:HB3	2.11	0.50
1:A:525:GLN:HG3	1:A:529:ASN:O	2.12	0.50
1:A:500:GLN:O	1:A:504:ILE:HG13	2.12	0.49
1:A:460:THR:O	1:A:583:PRO:HD2	2.12	0.49
1:B:481:ARG:NE	1:B:498:ASN:HD21	2.11	0.49
1:A:317:HIS:CE1	1:A:318:LEU:HG	2.48	0.49
1:A:350:THR:OG1	1:A:353:GLN:NE2	2.45	0.49
1:A:550:LYS:HA	1:A:550:LYS:NZ	2.28	0.48
1:A:439:PHE:CE1	1:A:443:CYS:SG	3.07	0.48
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.78	0.48
2:A:750:HEM:O1D	4:A:800:E2Z:N19	2.46	0.48
1:B:382:GLU:HA	1:B:382:GLU:OE1	2.12	0.48
1:B:418:ARG:C	1:B:420:GLN:H	2.22	0.48
1:B:571:LEU:C	1:B:571:LEU:HD23	2.38	0.47
1:B:385:ASN:O	1:B:389:GLU:HG2	2.14	0.47
1:B:353:GLN:HG2	1:B:353:GLN:H	1.40	0.47
1:B:448:TYR:CD1	1:B:448:TYR:C	2.92	0.47
1:A:364:GLN:HG3	1:A:403:TYR:OH	2.14	0.47
1:A:686:SER:HA	1:A:691:PHE:CG	2.49	0.47
1:B:307[B]:GLU:HA	1:B:307[B]:GLU:OE1	2.15	0.47
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.50	0.47
1:B:684:SER:O	1:B:685:GLY:C	2.59	0.46
1:A:675:ASP:O	1:A:679:ILE:HG12	2.15	0.46
1:A:561:TRP:CD1	1:A:593:ILE:HD13	2.51	0.46
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.74	0.46
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.98	0.46
1:B:454:ASN:ND2	7:B:2026:HOH:O	2.49	0.46
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:GLY:HA2	1:A:648:ILE:HD11	1.99	0.45
2:B:750:HEM:C1A	4:B:800:E2Z:H02	2.52	0.45
1:A:425:GLN:HG2	1:A:448:TYR:CE2	2.52	0.45
1:B:686:SER:HA	1:B:691:PHE:CG	2.51	0.45
1:A:300:PHE:CD1	1:A:300:PHE:N	2.85	0.44
1:A:455:LEU:HD13	1:A:564:LEU:HD12	1.98	0.44
1:A:445:HIS:CD2	1:A:445:HIS:C	2.95	0.44
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.52	0.44
2:A:750:HEM:HMC1	2:A:750:HEM:CBC	2.47	0.44
1:B:706:TYR:OH	2:B:750:HEM:O2D	2.19	0.44
1:B:567:VAL:HB	1:B:584:PHE:CZ	2.52	0.44
1:A:317:HIS:C	1:A:319:LYS:H	2.25	0.44
1:B:363:ASP:HB3	1:B:372:PHE:HE1	1.82	0.44
1:B:415:CYS:HB2	2:B:750:HEM:C1D	2.52	0.44
2:B:750:HEM:HMC2	2:B:750:HEM:CBC	2.22	0.44
1:B:516:ARG:HG2	1:B:517:PHE:CE2	2.53	0.44
1:A:469:LYS:CE	1:A:469:LYS:HA	2.47	0.44
1:A:472:PHE:O	1:A:581:ALA:HB2	2.18	0.43
1:A:603:ARG:HG3	1:A:603:ARG:NH1	2.33	0.43
1:B:322:LEU:HB2	1:B:699:ARG:HB2	2.00	0.43
1:B:619:ARG:HH11	1:B:619:ARG:CB	2.30	0.43
1:B:567:VAL:HB	1:B:584:PHE:CE1	2.53	0.43
2:B:750:HEM:HBD1	2:B:750:HEM:HHA	1.99	0.43
1:B:418:ARG:C	1:B:420:GLN:N	2.75	0.43
1:A:467:ASP:OD1	1:A:467:ASP:C	2.61	0.43
1:A:674:ALA:HB3	1:A:695:MET:HB3	2.01	0.43
1:A:322:LEU:CB	1:A:699:ARG:HE	2.31	0.42
1:A:449:ALA:O	1:A:455:LEU:HA	2.19	0.42
1:A:682:PRO:HB2	1:B:686:SER:HB3	2.01	0.42
1:A:612:LYS:HG3	1:A:618:MET:SD	2.59	0.42
1:B:566:ALA:HB2	1:B:585:SER:HB3	2.00	0.42
1:A:624:LEU:HD12	1:B:635:ILE:HG13	2.02	0.42
1:B:473:ARG:HD2	1:B:580:SER:O	2.20	0.42
1:A:326:CYS:HB3	1:B:326:CYS:HB3	2.01	0.42
1:A:454:ASN:C	1:A:454:ASN:ND2	2.74	0.42
1:A:317:HIS:HA	1:A:698:TYR:CE2	2.55	0.42
1:A:587:TRP:CZ2	5:A:860:ACT:H1	2.54	0.42
1:B:370:LYS:HZ3	1:B:370:LYS:HG3	1.64	0.42
1:A:322:LEU:HB2	1:A:699:ARG:CB	2.45	0.41
1:A:425:GLN:O	1:A:458:ALA:HA	2.20	0.41
1:A:467:ASP:OD1	1:A:469:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:VAL:HA	1:A:545:PRO:HD2	1.82	0.41
1:B:353:GLN:HE21	1:B:353:GLN:HB3	1.68	0.41
1:B:399:THR:HG23	7:B:2008:HOH:O	2.21	0.41
1:A:684:SER:O	1:A:685:GLY:C	2.62	0.41
1:A:548:HIS:CE1	1:A:550:LYS:HB3	2.56	0.41
1:A:561:TRP:CD1	1:A:593:ILE:CD1	3.03	0.41
1:A:397:LYS:HB2	1:A:400:GLU:HG3	2.02	0.41
1:A:582:CYS:O	1:A:583:PRO:C	2.62	0.41
1:B:300:PHE:HB3	1:B:313:THR:CG2	2.50	0.41
1:A:595:VAL:O	1:A:599:CYS:HB2	2.21	0.41
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.36	0.41
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.03	0.41
1:B:537:PRO:O	1:B:538:PRO:C	2.63	0.41
1:B:675:ASP:OD1	1:B:675:ASP:C	2.64	0.41
1:B:425:GLN:HG2	1:B:448:TYR:CZ	2.55	0.40
1:A:547:ARG:HD3	1:A:547:ARG:H	1.86	0.40
1:B:598:TYR:O	1:B:605:ASN:N	2.55	0.40
1:B:662:MET:HE3	7:B:2073:HOH:O	2.20	0.40
1:A:330:ILE:HD11	1:B:696:LEU:HB3	2.03	0.40
1:A:374:SER:O	1:A:375:LYS:C	2.63	0.40
1:B:485:TYR:CE2	1:B:514:ARG:HA	2.57	0.40
1:A:388:ILE:O	1:A:392:SER:CA	2.69	0.40
1:A:686:SER:OG	1:B:682:PRO:HB2	2.22	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	406/422 (96%)	382 (94%)	22 (5%)	2 (0%)	24	19
1	B	409/422 (97%)	386 (94%)	21 (5%)	2 (0%)	24	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	815/844 (97%)	768 (94%)	43 (5%)	4 (0%)	24 19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	352	ASP
1	A	575	GLY
1	A	392	SER
1	B	685	GLY

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	365/377 (97%)	340 (93%)	25 (7%)	14 9
1	B	368/377 (98%)	350 (95%)	18 (5%)	22 18
All	All	733/754 (97%)	690 (94%)	43 (6%)	18 13

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	ARG
1	A	302	LYS
1	A	307[A]	GLU
1	A	307[B]	GLU
1	A	310	VAL
1	A	315	THR
1	A	336	MET
1	A	360	GLU
1	A	367	SER
1	A	370	LYS
1	A	371	ARG
1	A	454	ASN
1	A	469	LYS
1	A	507	GLN

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Mol	Chain	Res	Type
1	A	523	LEU
1	A	550	LYS
1	A	569	ASN
1	A	602	SER
1	A	608	GLU
1	A	612	LYS
1	A	620	LYS
1	A	653	SER
1	A	656	GLU
1	A	660	LYS
1	A	701	THR
1	B	320	SER
1	B	323	GLU
1	B	348	VAL
1	B	353	GLN
1	B	381	LEU
1	B	382	GLU
1	B	389	GLU
1	B	392	SER
1	B	423	LYS
1	B	480	ILE
1	B	486	LYS
1	B	503	GLU
1	B	531	PRO
1	B	540	LEU
1	B	620	LYS
1	B	621	THR
1	B	622	SER
1	B	717	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	A	353	GLN
1	A	436	HIS
1	A	454	ASN
1	A	487	GLN
1	A	508	GLN
1	A	527	ASN
1	A	605	ASN
1	A	642	GLN

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Mol	Chain	Res	Type
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	436	HIS
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	605	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 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	1,4	50,50,50	1.51	10 (20%)	67,82,82	1.96	16 (23%)
4	E2Z	A	800	2	25,25,25	1.59	6 (24%)	30,32,32	3.49	16 (53%)
4	E2Z	B	800	2	25,25,25	1.25	2 (8%)	30,32,32	4.55	14 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H4B	B	760	-	17,18,18	0.91	1 (5%)	14,26,26	2.03	5 (35%)
2	HEM	A	750	1,4	50,50,50	1.63	9 (18%)	67,82,82	1.81	16 (23%)
5	ACT	B	860	-	3,3,3	0.91	0	3,3,3	0.43	0
5	ACT	A	860	-	3,3,3	0.83	0	3,3,3	0.84	0
3	H4B	A	760	-	17,18,18	0.96	0	14,26,26	2.58	9 (64%)

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	-	2/14/54/54	-
4	E2Z	A	800	2	-	0/12/12/12	0/3/3/3
4	E2Z	B	800	2	-	1/12/12/12	0/3/3/3
3	H4B	B	760	-	-	3/8/17/17	0/2/2/2
2	HEM	A	750	1,4	-	1/14/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	FE-NB	4.20	2.07	1.94
2	A	750	HEM	C1B-NB	-3.76	1.33	1.40
2	A	750	HEM	FE-NC	3.70	2.07	1.95
2	A	750	HEM	C4D-ND	-3.65	1.33	1.40
4	A	800	E2Z	C4'-C3'	3.64	1.44	1.37
2	B	750	HEM	FE-NC	3.55	2.06	1.95
4	B	800	E2Z	C16-N11	3.17	1.41	1.34
2	B	750	HEM	FE-NB	2.96	2.04	1.94
2	B	750	HEM	C3C-C4C	-2.84	1.41	1.46
2	B	750	HEM	C1B-NB	-2.84	1.35	1.40
2	B	750	HEM	C4D-ND	-2.81	1.35	1.40
4	A	800	E2Z	C12-N03	-2.80	1.35	1.41
2	B	750	HEM	C1C-C2C	-2.68	1.40	1.45
4	A	800	E2Z	C02-N01	2.54	1.38	1.32
4	A	800	E2Z	C5'-C6'	2.52	1.43	1.38
2	A	750	HEM	C3C-C2C	2.50	1.42	1.37
2	B	750	HEM	C1D-ND	-2.48	1.34	1.38
4	A	800	E2Z	C2'-C3'	2.42	1.41	1.37
2	A	750	HEM	C3D-C2D	-2.38	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	E2Z	C6'-C1'	2.22	1.43	1.38
2	A	750	HEM	C1D-ND	-2.22	1.34	1.38
2	B	750	HEM	O1D-CGD	2.19	1.29	1.22
4	B	800	E2Z	C04-N03	-2.17	1.34	1.38
2	B	750	HEM	FE-ND	-2.10	1.88	1.94
3	B	760	H4B	C2-N1	2.09	1.38	1.33
2	B	750	HEM	C4B-NB	-2.08	1.34	1.38
2	A	750	HEM	C1A-C2A	-2.06	1.40	1.44
2	A	750	HEM	C1C-C2C	-2.03	1.41	1.45

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	E2Z	N11-C12-N03	14.25	122.62	115.11
4	B	800	E2Z	C12-N13-C14	9.12	122.51	115.23
4	B	800	E2Z	N11-C12-N13	-8.69	117.28	126.12
4	A	800	E2Z	C12-N13-C14	8.61	122.10	115.23
4	B	800	E2Z	C16-N11-C12	8.39	123.36	115.13
4	B	800	E2Z	C04-N03-C02	7.99	118.24	106.40
4	A	800	E2Z	N11-C12-N13	-7.75	118.24	126.12
4	A	800	E2Z	C04-N03-C02	6.20	115.60	106.40
4	A	800	E2Z	C16-N11-C12	5.57	120.59	115.13
2	A	750	HEM	CHC-C4B-NB	4.98	129.79	124.42
4	A	800	E2Z	N13-C12-N03	4.98	124.24	115.44
2	B	750	HEM	CHC-C4B-NB	4.98	129.78	124.42
4	B	800	E2Z	C12-N03-C04	-4.87	119.71	126.67
3	A	760	H4B	O10-C10-C9	-4.82	101.79	109.77
2	A	750	HEM	C1B-NB-C4B	4.78	110.87	105.21
2	B	750	HEM	C1B-NB-C4B	4.77	110.85	105.21
3	A	760	H4B	C2-N1-C8A	4.67	121.61	113.36
4	A	800	E2Z	C12-N03-C04	-4.62	120.08	126.67
4	B	800	E2Z	C05-N01-C02	4.41	113.94	105.47
2	B	750	HEM	C3B-C4B-NB	-4.40	106.31	109.47
2	A	750	HEM	CHA-C4D-ND	4.39	129.79	124.37
4	A	800	E2Z	N11-C12-N03	4.36	117.41	115.11
2	B	750	HEM	CHA-C4D-ND	4.34	129.74	124.37
4	B	800	E2Z	N03-C02-N01	-4.32	100.06	111.13
4	A	800	E2Z	C21-C1'-C2'	-4.14	113.58	120.54
2	B	750	HEM	CHA-C4D-C3D	-4.03	117.80	125.23
4	A	800	E2Z	F7'-C3'-C4'	3.95	124.87	118.55
2	B	750	HEM	CHB-C1B-NB	3.70	128.94	124.37
2	B	750	HEM	C4C-CHD-C1D	-3.63	118.31	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	750	HEM	CHD-C1D-ND	3.57	128.26	124.42
3	B	760	H4B	C11-C10-C9	-3.44	107.91	112.11
4	B	800	E2Z	C15-C16-N11	-3.40	119.80	123.97
4	B	800	E2Z	C05-C04-N03	-3.39	100.56	106.70
2	B	750	HEM	CHD-C4C-NC	3.30	128.05	124.45
2	B	750	HEM	CHD-C1D-C2D	-3.21	119.96	125.03
4	A	800	E2Z	N03-C02-N01	-3.20	102.92	111.13
2	A	750	HEM	CHA-C4D-C3D	-3.19	119.35	125.23
3	B	760	H4B	O4-C4-C4A	-3.15	119.66	127.26
2	A	750	HEM	CMD-C2D-C1D	3.13	129.93	125.03
2	A	750	HEM	CHD-C1D-ND	3.12	127.78	124.42
3	B	760	H4B	C2-N1-C8A	3.12	118.87	113.36
2	B	750	HEM	O2A-CGA-CBA	2.97	123.39	114.00
2	A	750	HEM	C1A-CHA-C4D	-2.90	119.43	126.25
4	A	800	E2Z	C17-C14-N13	2.90	120.45	116.06
2	A	750	HEM	CHD-C1D-C2D	-2.89	120.46	125.03
2	B	750	HEM	CMC-C2C-C1C	2.89	129.82	124.73
3	B	760	H4B	C2-N3-C4	-2.89	119.88	125.11
2	B	750	HEM	C1A-CHA-C4D	-2.87	119.49	126.25
2	A	750	HEM	CBD-CAD-C3D	-2.80	104.78	112.53
4	A	800	E2Z	C18-C17-C14	-2.74	102.74	112.56
3	A	760	H4B	C11-C10-C9	-2.68	108.83	112.11
4	A	800	E2Z	C4'-C3'-C2'	-2.67	119.71	123.23
4	B	800	E2Z	N13-C12-N03	2.63	120.08	115.44
3	B	760	H4B	C4A-C4-N3	2.59	119.23	112.13
3	A	760	H4B	C2-N3-C4	-2.58	120.43	125.11
2	A	750	HEM	CHB-C1B-NB	2.58	127.56	124.37
2	B	750	HEM	O2A-CGA-O1A	-2.57	116.73	123.33
2	A	750	HEM	O2D-CGD-CBD	2.54	122.03	114.00
4	B	800	E2Z	C6'-C1'-C2'	2.52	122.02	118.55
3	A	760	H4B	O4-C4-C4A	-2.48	121.27	127.26
2	A	750	HEM	O2A-CGA-CBA	2.43	121.67	114.00
3	A	760	H4B	N2-C2-N3	2.42	121.86	116.76
2	A	750	HEM	C4C-CHD-C1D	-2.41	120.89	126.02
2	B	750	HEM	O2D-CGD-O1D	-2.40	117.15	123.33
3	A	760	H4B	C4A-C4-N3	2.35	118.59	112.13
3	A	760	H4B	O9-C9-C10	2.32	113.56	109.14
4	A	800	E2Z	C6'-C1'-C2'	2.28	121.70	118.55
3	A	760	H4B	C4-C4A-N5	2.26	122.42	116.27
2	A	750	HEM	C4C-NC-C1C	2.25	109.49	105.82
2	B	750	HEM	C4A-CHB-C1B	-2.21	121.05	126.25
4	A	800	E2Z	C05-C04-N03	-2.20	102.73	106.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CMA-C3A-C4A	2.17	128.72	125.42
4	B	800	E2Z	C12-N03-C02	-2.16	122.04	126.20
4	B	800	E2Z	C16-C15-C14	-2.16	114.49	116.68
2	A	750	HEM	C3B-C4B-NB	-2.10	107.96	109.47
4	A	800	E2Z	F7'-C3'-C2'	-2.02	115.42	118.28

There are no chirality outliers.

All (7) torsion outliers are listed below:

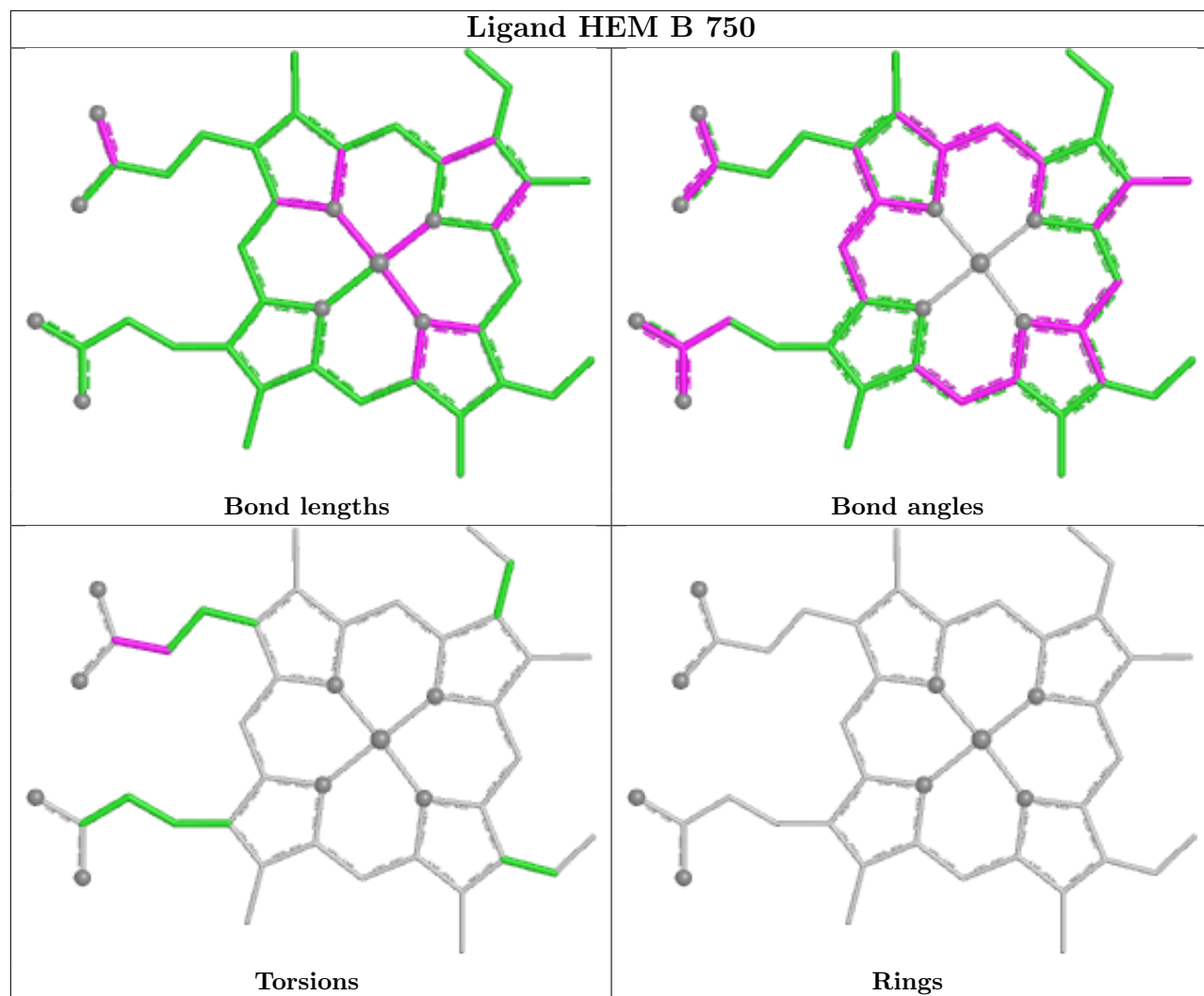
Mol	Chain	Res	Type	Atoms
3	B	760	H4B	O10-C10-C9-O9
3	B	760	H4B	C11-C10-C9-O9
2	B	750	HEM	CAD-CBD-CGD-O2D
2	B	750	HEM	CAD-CBD-CGD-O1D
3	B	760	H4B	O10-C10-C9-C6
4	B	800	E2Z	C17-C18-N19-C20
2	A	750	HEM	CAD-CBD-CGD-O2D

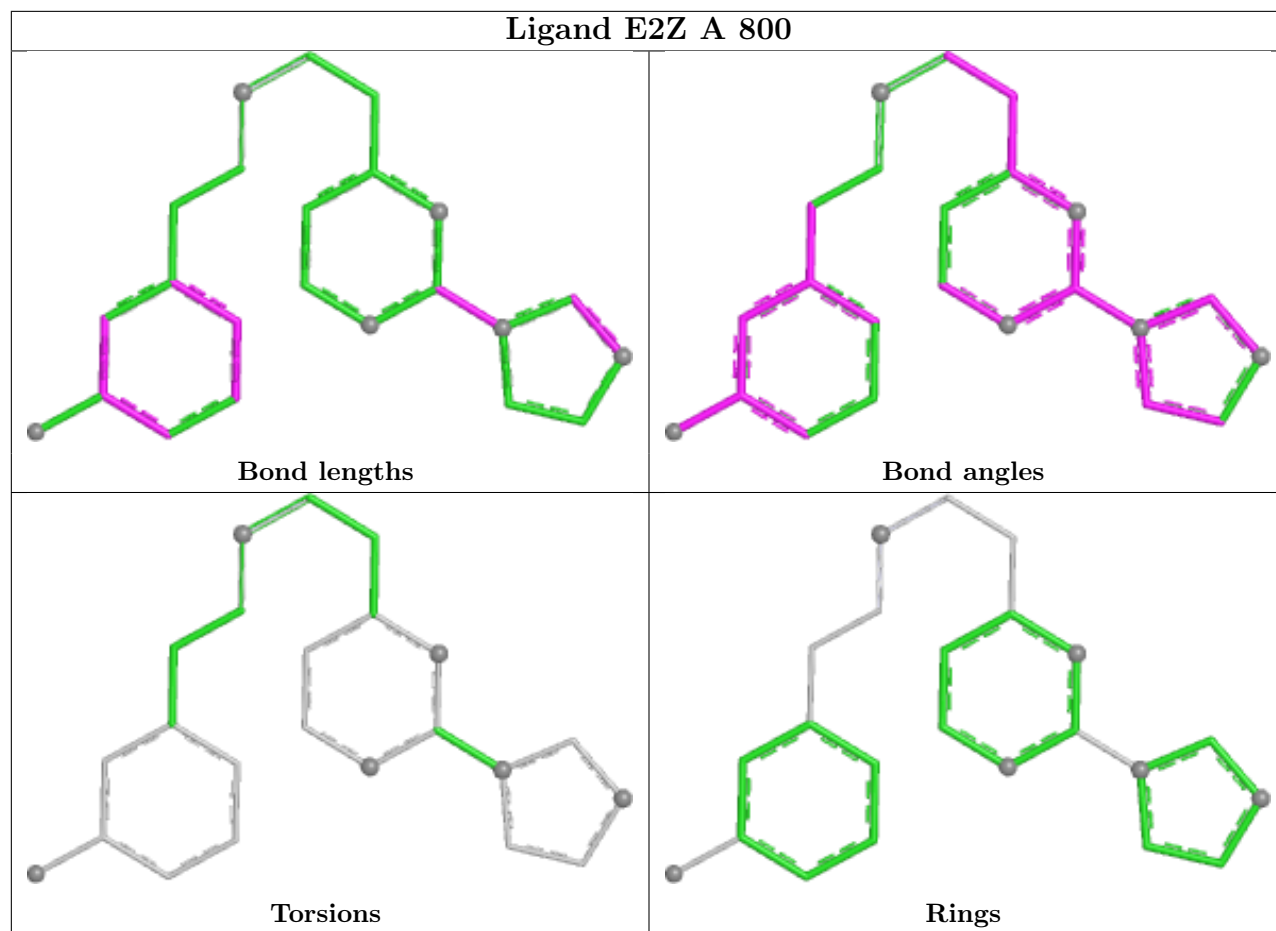
There are no ring outliers.

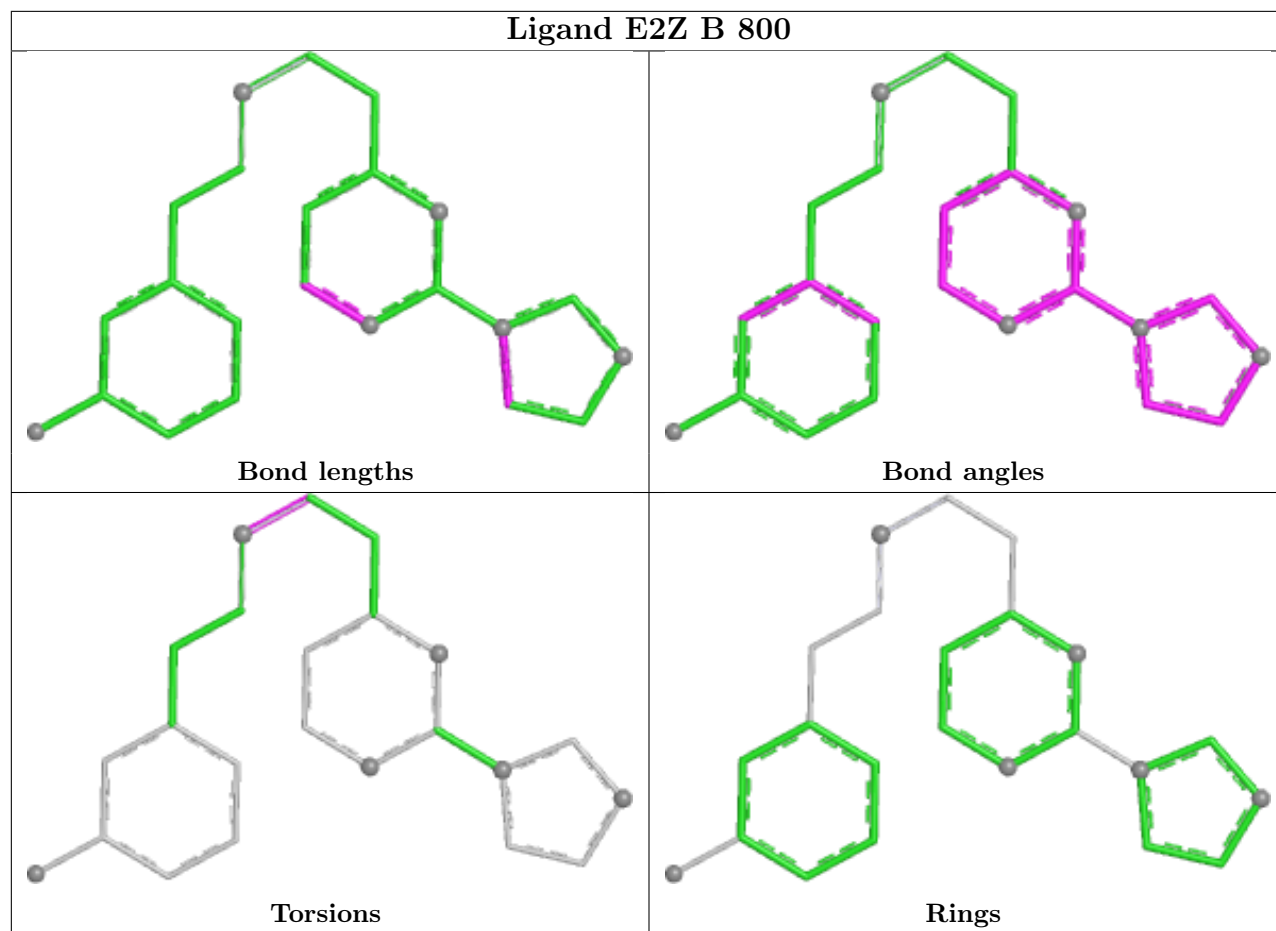
6 monomers are involved in 19 short contacts:

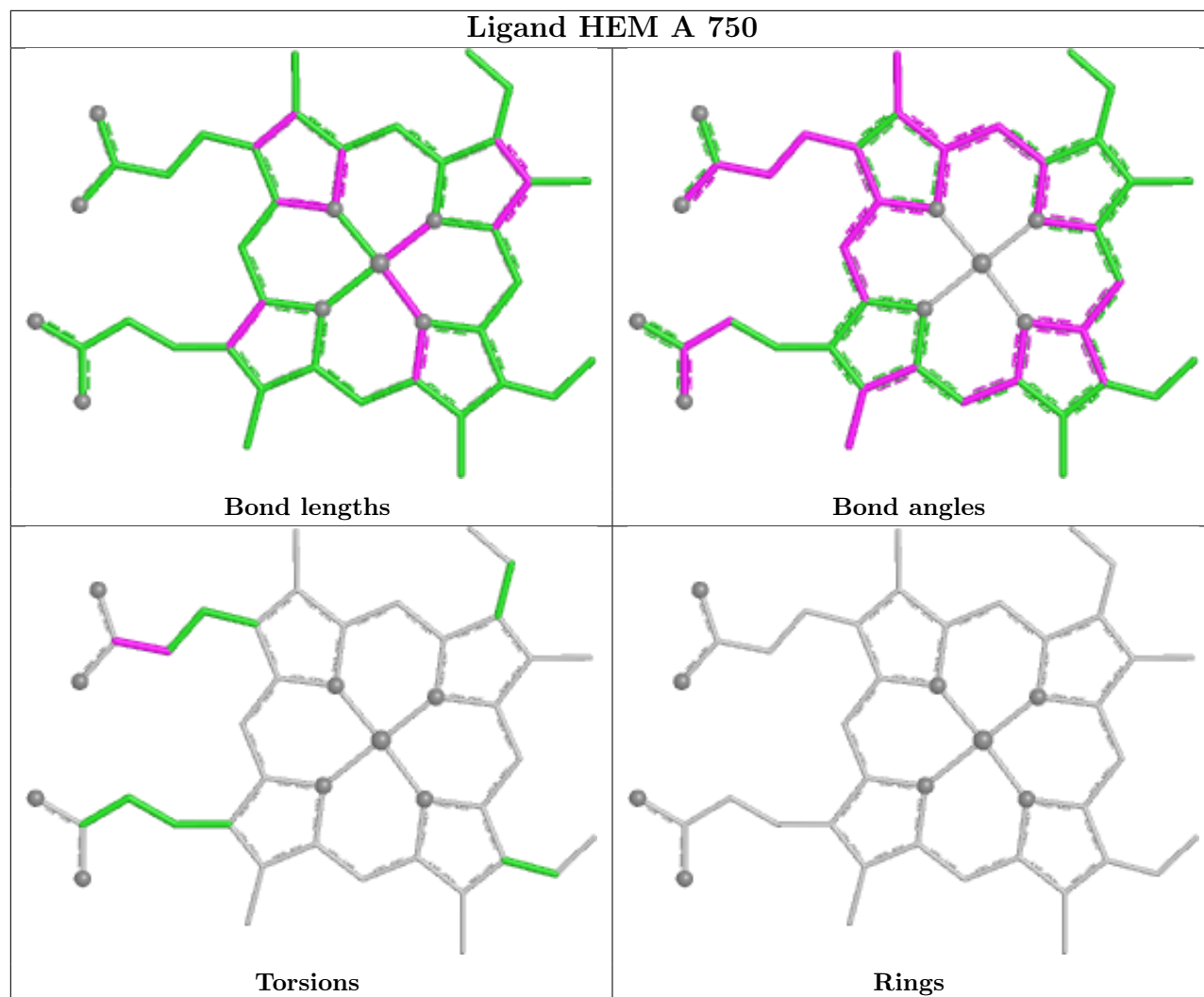
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	HEM	11	0
4	A	800	E2Z	1	0
4	B	800	E2Z	1	0
2	A	750	HEM	4	0
5	A	860	ACT	1	0
3	A	760	H4B	3	0

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.









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%)	0.28	4 (0%) 79 83	32, 53, 82, 105	2 (0%)
1	B	411/422 (97%)	0.13	4 (0%) 79 83	28, 45, 70, 93	3 (0%)
All	All	819/844 (97%)	0.20	8 (0%) 79 83	28, 49, 79, 105	5 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	4.0
1	B	338	PRO	3.6
1	A	355	PHE	3.1
1	B	300	PHE	2.7
1	A	322	LEU	2.5
1	A	715	VAL	2.5
1	A	338	PRO	2.4
1	B	716	TRP	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,

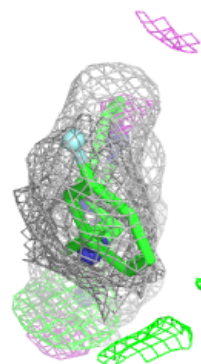
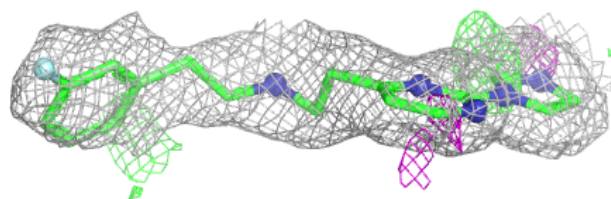
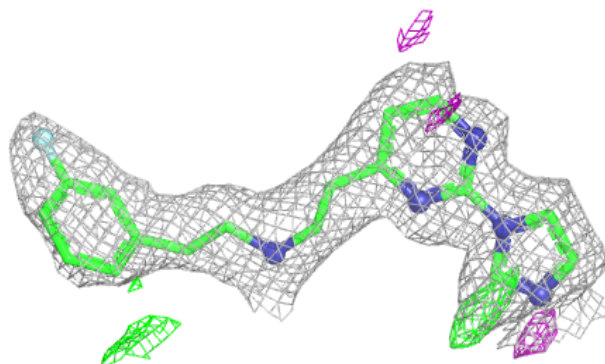
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	H4B	A	760	17/17	0.83	0.17	58,70,87,96	0
5	ACT	B	860	4/4	0.86	0.17	60,67,68,69	0
4	E2Z	B	800	23/23	0.89	0.11	36,39,63,63	0
5	ACT	A	860	4/4	0.89	0.19	90,90,91,95	0
4	E2Z	A	800	23/23	0.89	0.11	40,42,65,69	0
3	H4B	B	760	17/17	0.90	0.10	50,54,55,55	0
2	HEM	A	750	43/43	0.97	0.07	38,40,43,46	0
2	HEM	B	750	43/43	0.98	0.07	32,34,42,45	0
6	ZN	A	900	1/1	0.99	0.03	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.

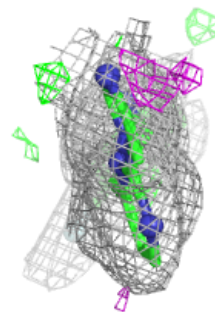
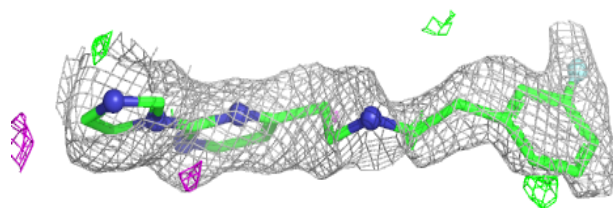
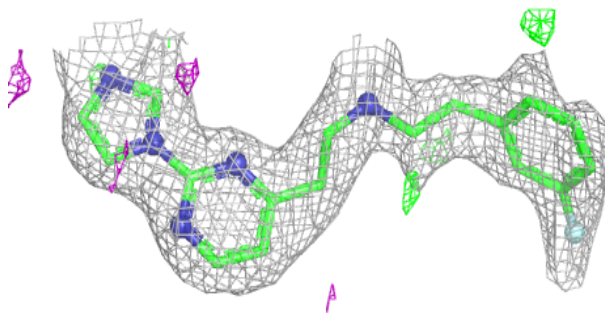
Electron density around E2Z B 800:

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



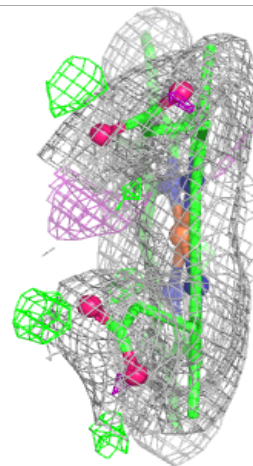
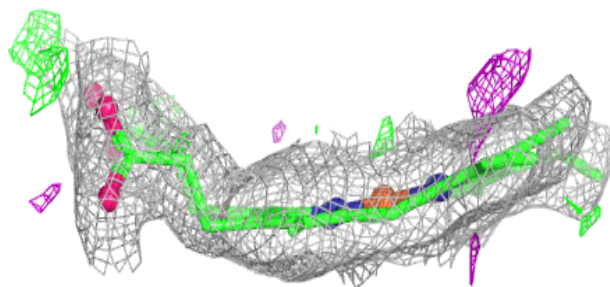
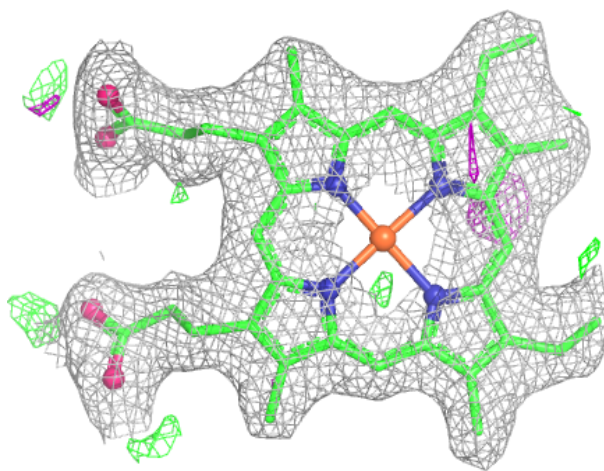
Electron density around E2Z A 800:

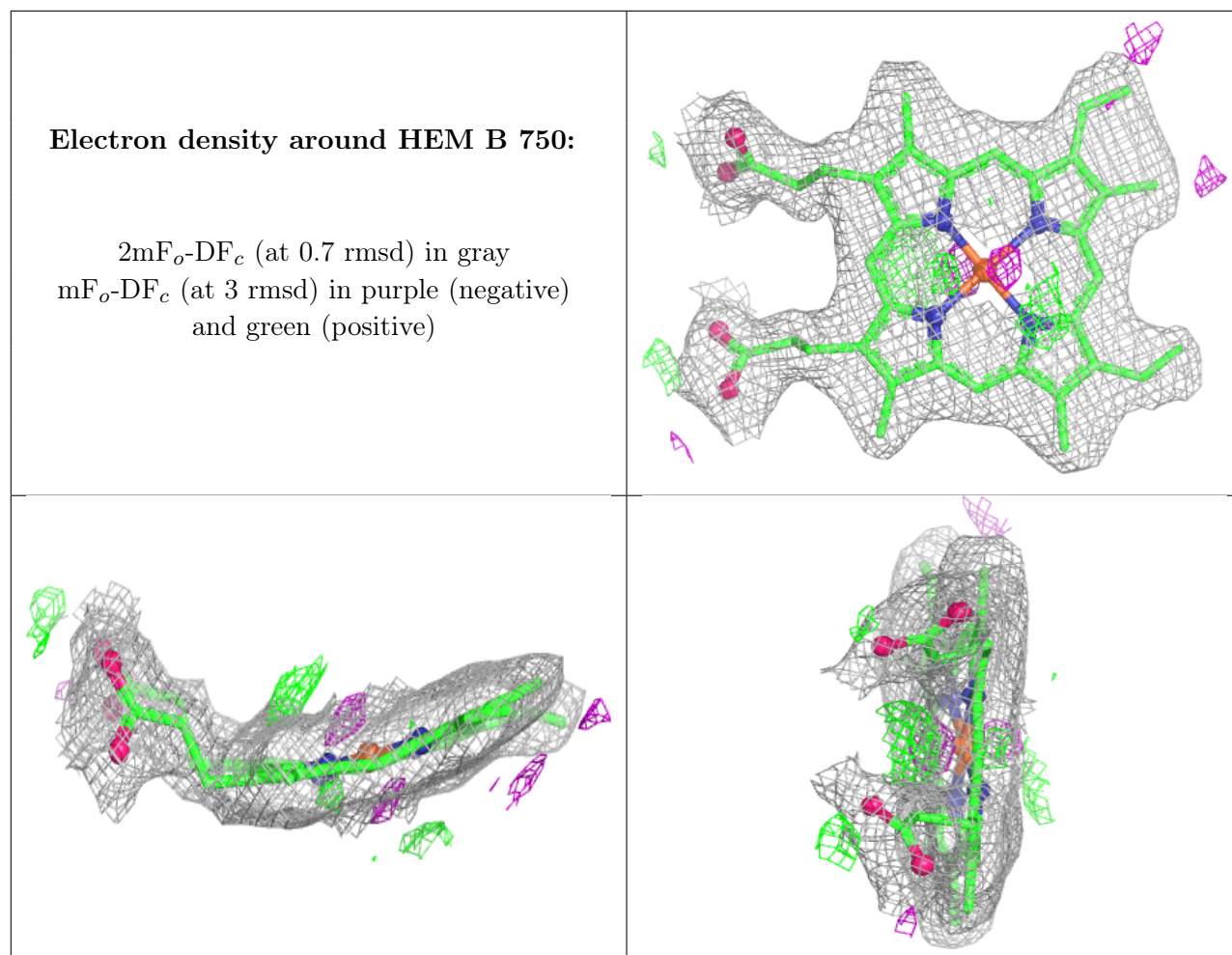
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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.