



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:45 AM UTC

PDB ID : 3NLR / pdb_00003nlr
Title : Structure of neuronal nitric oxide synthase D597N/M336V mutant heme domain in complex with 6-{{(3'R,4'S)-3'-[2''-(3'''-fluorophenethylamino)ethoxy]pyrrolidin-4'-yl}methyl}-4-methylpyridin-2-amine
Authors : Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on : 2010-06-21
Resolution : 2.10 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

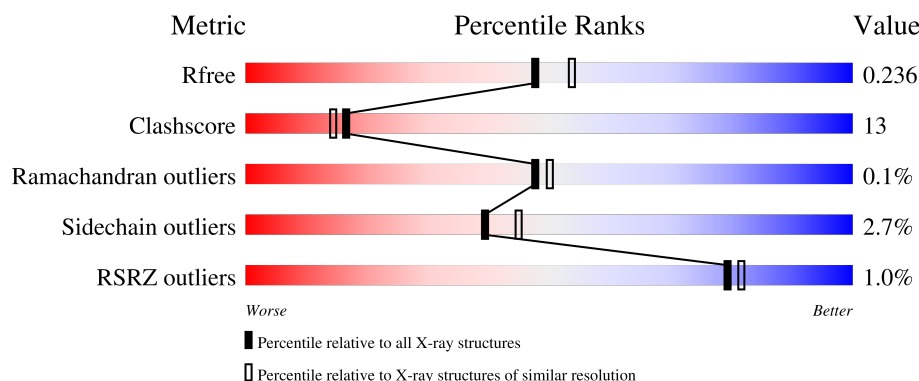
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	% 69% 26% ..
1	B	422	% 72% 24% ..

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7039 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.

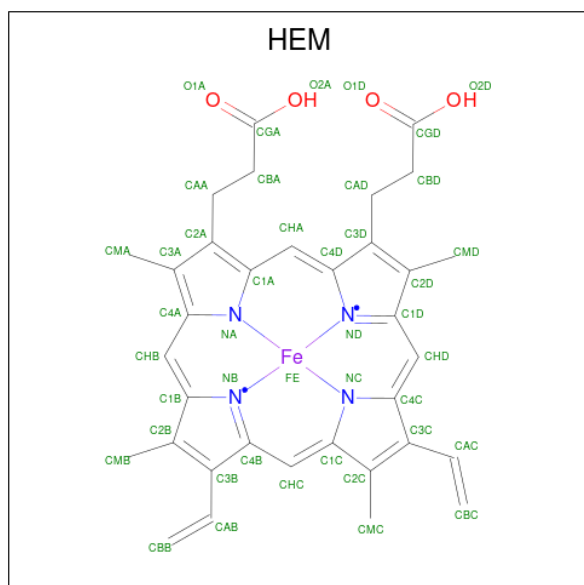
- Molecule 1 is a protein called Nitric oxide synthase, brain.

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	0	0
			3344	2140	575	609	20			

There are 4 discrepancies between the modelled and reference sequences:

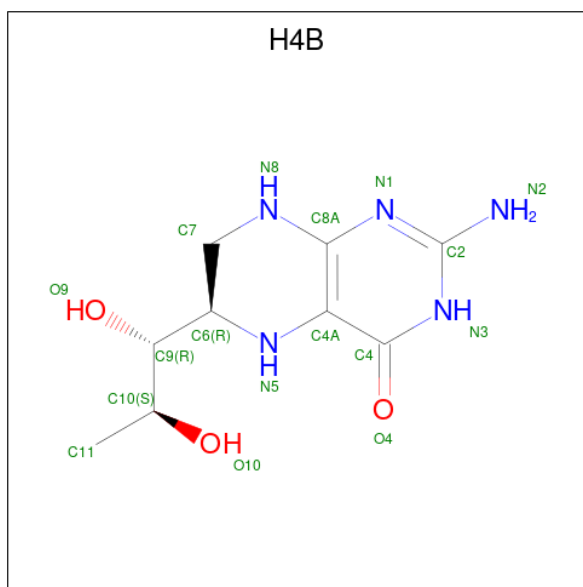
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	engineered mutation	UNP P29476
A	597	ASN	ASP	engineered mutation	UNP P29476
B	336	VAL	MET	engineered mutation	UNP P29476
B	597	ASN	ASP	engineered mutation	UNP P29476

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



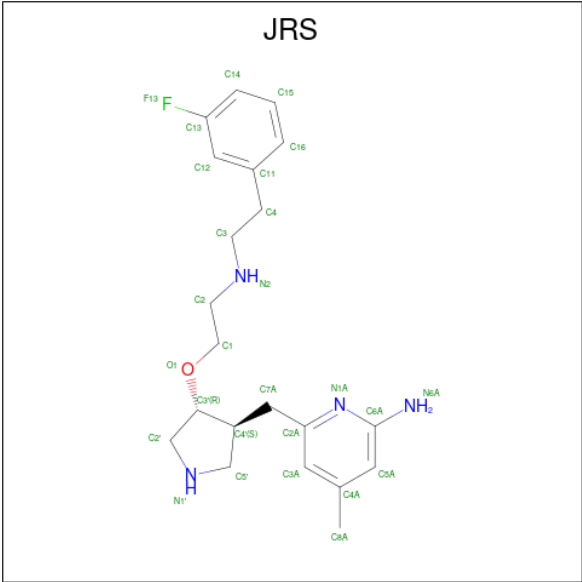
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



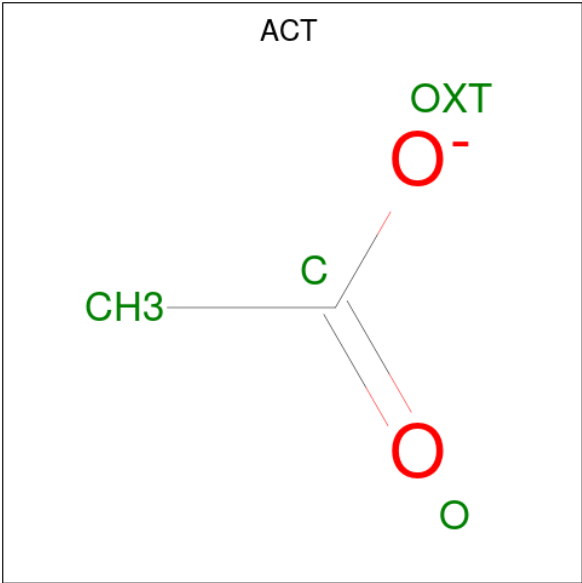
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-[(3S,4R)-4-(2-{[2-(3-fluorophenyl)ethyl]amino}ethoxy)pyrrolidin-3-yl]methyl-4-methylpyridin-2-amine (CCD ID: JRS) (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: C₂H₃O₂⁻).



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 1	Zn 1	0	0

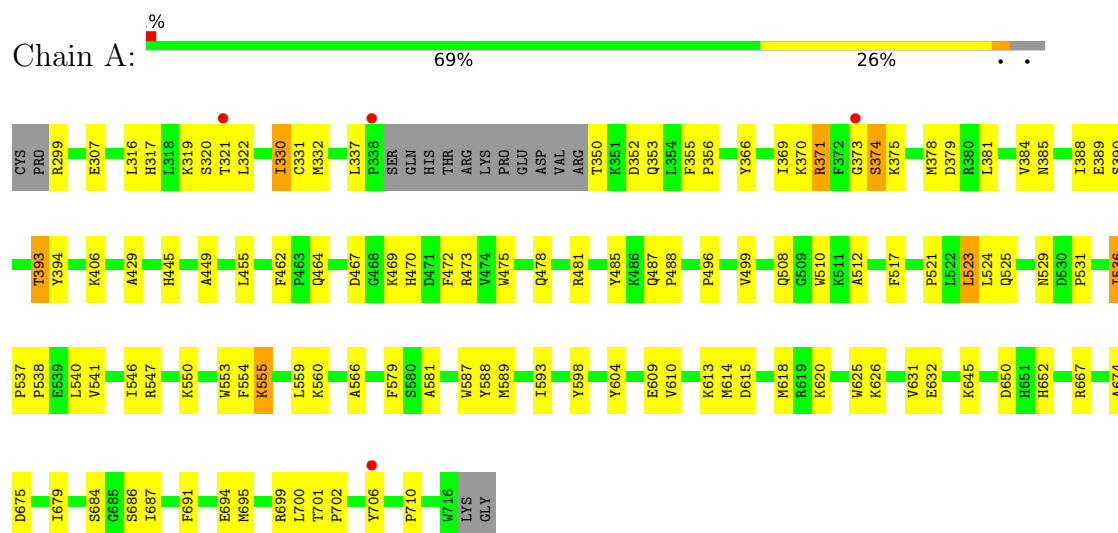
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	87	Total 87	O 87	0	0
7	B	113	Total 113	O 113	0	0

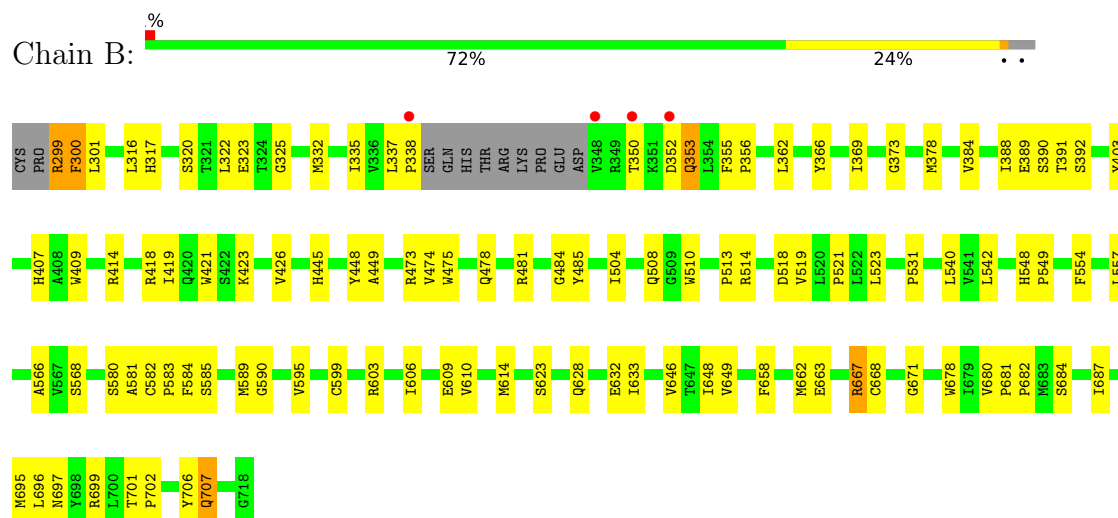
3 Residue-property plots

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

• Molecule 1: Nitric oxide synthase, brain



• Molecule 1: Nitric oxide synthase, brain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.45Å 110.58Å 164.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.56 – 2.10 40.56 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (40.56-2.10) 93.7 (40.56-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0069, CNS	Depositor
R, R_{free}	0.186 , 0.235 0.187 , 0.236	Depositor DCC
R_{free} test set	2574 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.6	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	0.97	EDS
Total number of atoms	7039	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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: ACT, HEM, JRS, ZN, H4B

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	1.02	0/3405	1.12	10/4621 (0.2%)
1	B	1.10	4/3437 (0.1%)	1.14	6/4661 (0.1%)
All	All	1.06	4/6842 (0.1%)	1.13	16/9282 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	581	ALA	CA-CB	-6.64	1.43	1.53
1	B	484	GLY	N-CA	6.57	1.52	1.45
1	B	519	VAL	C-O	-6.31	1.17	1.24
1	B	603	ARG	CA-C	5.83	1.56	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	707	GLN	CA-C-N	-6.97	113.13	120.03
1	B	707	GLN	C-N-CA	-6.97	113.13	120.03
1	B	623	SER	N-CA-C	-6.62	105.03	113.23
1	A	330	ILE	N-CA-C	6.18	116.50	108.35
1	B	418	ARG	N-CA-C	5.83	120.00	113.01
1	A	547	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	A	589	MET	N-CA-C	-5.73	100.34	109.96
1	A	547	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	A	541	VAL	CB-CA-C	-5.62	105.49	112.45
1	A	429	ALA	N-CA-C	-5.61	105.12	112.41
1	B	426	VAL	CA-C-N	-5.51	115.39	123.00
1	B	426	VAL	C-N-CA	-5.51	115.39	123.00
1	A	536	ILE	CA-C-N	-5.45	114.77	120.38
1	A	536	ILE	C-N-CA	-5.45	114.77	120.38
1	A	618	MET	N-CA-C	-5.43	106.53	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	LYS	N-CA-C	-5.18	105.72	111.36

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	89	0
1	B	3344	0	3261	77	0
2	A	43	0	30	10	0
2	B	43	0	30	9	0
3	A	17	0	15	0	0
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	1	0	0	0	0
7	A	87	0	0	8	0
7	B	113	0	0	5	0
All	All	7039	0	6638	174	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 13.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.45	0.99
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.49	0.93
1:B:299:ARG:HD2	7:B:74:HOH:O	1.79	0.82
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.62	0.81
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.62	0.81
1:B:706:TYR:OH	2:B:750:HEM:O1D	1.99	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:PHE:HB3	7:A:8:HOH:O	1.85	0.74
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.70	0.74
1:A:307:GLU:HG3	7:B:41:HOH:O	1.87	0.73
1:A:322:LEU:HD12	7:A:119:HOH:O	1.89	0.73
1:A:467:ASP:OD2	1:A:469:LYS:HB2	1.91	0.69
1:B:658:PHE:CE2	1:B:662:MET:HE3	2.30	0.67
2:A:750:HEM:O2D	4:A:800:JRS:H3A	1.96	0.66
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.23	0.66
1:B:391:THR:O	1:B:392:SER:HB2	1.97	0.64
1:B:299:ARG:HB3	1:B:299:ARG:CZ	2.28	0.64
2:B:750:HEM:O2D	4:B:800:JRS:H3A	1.98	0.64
1:B:668:CYS:HB3	7:B:43:HOH:O	1.96	0.64
1:A:706:TYR:OH	2:A:750:HEM:O1D	2.13	0.63
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.81	0.63
1:A:375:LYS:NZ	1:A:379:ASP:OD1	2.32	0.63
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.13	0.62
2:B:750:HEM:CMC	2:B:750:HEM:HBC2	2.29	0.62
1:B:325:GLY:O	1:B:332:MET:HE2	1.99	0.62
1:B:355:PHE:N	1:B:356:PRO:HD2	2.15	0.62
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.29	0.62
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.24	0.62
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.82	0.61
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.83	0.61
1:B:388:ILE:O	1:B:392:SER:N	2.32	0.61
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.16	0.60
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.84	0.60
1:A:508:GLN:HA	1:A:508:GLN:OE1	2.00	0.59
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.68	0.59
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.85	0.59
1:A:337:LEU:HD21	4:A:800:JRS:H15	1.85	0.58
1:B:701:THR:HA	1:B:702:PRO:C	2.28	0.58
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.38	0.58
1:A:598:TYR:HA	7:A:82:HOH:O	2.04	0.57
1:A:699:ARG:HB3	7:A:119:HOH:O	2.05	0.57
1:B:389:GLU:HG3	1:B:390:SER:N	2.20	0.56
1:A:536:ILE:O	1:A:537:PRO:C	2.48	0.55
1:A:449:ALA:O	1:A:455:LEU:HA	2.06	0.55
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.89	0.55
1:A:384:VAL:O	1:A:388:ILE:HG13	2.06	0.55
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.88	0.55
1:B:353:GLN:O	1:B:356:PRO:HG2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.89	0.54
1:B:350:THR:HG22	1:B:352:ASP:H	1.72	0.54
1:B:337:LEU:HD21	4:B:800:JRS:H15	1.88	0.54
1:A:496:PRO:O	1:A:499:VAL:HG23	2.08	0.54
1:B:317:HIS:O	1:B:320:SER:HB3	2.07	0.54
1:A:525:GLN:HG3	1:A:529:ASN:O	2.07	0.54
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.41	0.54
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.43	0.54
1:A:546:ILE:HG13	1:A:598:TYR:OH	2.08	0.54
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.22	0.54
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.43	0.53
1:A:604:TYR:HB2	7:A:82:HOH:O	2.06	0.53
1:A:316:LEU:HD12	1:A:319:LYS:HD2	1.90	0.53
1:A:350:THR:HG22	1:A:352:ASP:H	1.73	0.53
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.92	0.52
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.40	0.51
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.76	0.51
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.75	0.51
1:A:610:VAL:O	1:A:614:MET:HG3	2.09	0.51
1:B:610:VAL:O	1:B:614:MET:HG3	2.11	0.51
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.24	0.51
1:A:366:TYR:CD2	1:A:369:ILE:HD11	2.45	0.51
1:A:467:ASP:CG	1:A:469:LYS:H	2.19	0.50
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.77	0.49
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.94	0.49
1:B:542:LEU:HD21	1:B:646:VAL:HG22	1.94	0.49
1:B:373:GLY:HA2	1:B:378:MET:HE3	1.95	0.48
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.95	0.48
1:A:604:TYR:CB	7:A:82:HOH:O	2.60	0.48
1:B:504:ILE:O	1:B:508:GLN:HG2	2.14	0.48
2:A:750:HEM:O1A	7:A:141:HOH:O	2.20	0.48
1:A:675:ASP:O	1:A:679:ILE:HG12	2.14	0.48
1:A:701:THR:HA	1:A:702:PRO:C	2.39	0.48
1:B:448:TYR:CD2	1:B:448:TYR:C	2.92	0.48
1:A:553:TRP:CZ3	1:A:613:LYS:HB3	2.49	0.47
2:A:750:HEM:HBB2	2:A:750:HEM:CHC	2.36	0.47
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.97	0.47
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.44	0.47
1:A:550:LYS:HE3	1:A:550:LYS:HB2	1.48	0.47
2:A:750:HEM:HHC	2:A:750:HEM:CBB	2.41	0.47
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:CYS:O	1:B:583:PRO:C	2.57	0.47
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.49	0.46
1:A:355:PHE:N	1:A:356:PRO:CD	2.78	0.46
1:A:469:LYS:C	1:A:470:HIS:HD1	2.24	0.46
1:B:658:PHE:HE2	1:B:662:MET:HE3	1.80	0.46
1:A:478:GLN:HA	1:A:566:ALA:O	2.17	0.46
1:B:548:HIS:ND1	1:B:549:PRO:HD2	2.31	0.46
1:B:445:HIS:C	1:B:445:HIS:CD2	2.95	0.45
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.98	0.45
1:A:321:THR:HG23	1:A:322:LEU:H	1.82	0.45
1:B:523:LEU:CD1	1:B:531:PRO:HB2	2.47	0.45
1:B:391:THR:O	1:B:392:SER:CB	2.63	0.45
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.42	0.45
1:A:373:GLY:O	1:A:374:SER:O	2.34	0.45
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.52	0.45
1:A:625:TRP:CH2	1:A:626:LYS:HE3	2.52	0.45
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.99	0.44
1:A:686:SER:HA	1:A:691:PHE:CG	2.51	0.44
1:A:524:LEU:O	1:A:531:PRO:HA	2.17	0.44
1:B:300:PHE:N	1:B:300:PHE:CD1	2.84	0.44
1:B:557:LEU:HD22	1:B:609:GLU:CD	2.43	0.44
1:B:554:PHE:HB3	7:B:190:HOH:O	2.17	0.44
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.47	0.44
1:A:393:THR:OG1	1:A:394:TYR:N	2.51	0.44
1:A:445:HIS:C	1:A:445:HIS:CD2	2.95	0.44
1:A:517:PHE:CB	1:A:560:LYS:HE3	2.48	0.44
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.53	0.43
1:A:631:VAL:HG11	1:B:628:GLN:HG3	2.01	0.43
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.46	0.43
2:B:750:HEM:HBC2	2:B:750:HEM:HMC1	1.98	0.43
1:A:321:THR:HG23	1:A:322:LEU:N	2.32	0.43
1:B:322:LEU:HB3	1:B:699:ARG:CZ	2.49	0.43
1:A:331:CYS:HB3	1:B:697:ASN:HB3	2.01	0.43
1:A:546:ILE:HB	1:A:559:LEU:HB2	2.01	0.43
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.88	0.43
1:B:316:LEU:HB3	1:B:671:GLY:HA3	2.01	0.43
1:B:566:ALA:HB2	1:B:585:SER:HB3	2.00	0.43
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.54	0.43
2:B:750:HEM:HMC1	2:B:750:HEM:CBC	2.48	0.43
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.51	0.42
1:A:553:TRP:HE3	1:A:613:LYS:HZ2	1.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.55	0.42
1:A:667:ARG:NH1	1:A:667:ARG:HG3	2.34	0.42
1:B:403:TYR:CD2	1:B:403:TYR:C	2.96	0.42
1:B:409:TRP:CH2	2:B:750:HEM:HMC3	2.55	0.42
1:A:353:GLN:O	1:A:356:PRO:HD2	2.19	0.42
1:A:553:TRP:CZ3	1:A:613:LYS:CB	3.02	0.42
1:B:449:ALA:HB1	7:B:17:HOH:O	2.20	0.42
1:B:662:MET:HE1	1:B:695:MET:HG2	2.01	0.42
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.35	0.42
1:B:353:GLN:H	1:B:353:GLN:HG2	1.51	0.42
1:B:606:ILE:O	1:B:610:VAL:HG23	2.20	0.42
1:A:299:ARG:O	1:A:317:HIS:CE1	2.73	0.42
1:A:462:PHE:HB2	1:A:581:ALA:HB3	2.01	0.42
2:B:750:HEM:CMC	2:B:750:HEM:CBC	2.94	0.42
1:B:474:VAL:HG11	1:B:568:SER:HB2	2.02	0.41
1:A:706:TYR:OH	2:A:750:HEM:CGD	2.68	0.41
1:B:706:TYR:CZ	4:B:800:JRS:H16	2.55	0.41
1:A:546:ILE:HG12	1:A:560:LYS:HA	2.02	0.41
1:A:686:SER:OG	1:B:682:PRO:HB2	2.21	0.41
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.79	0.41
2:B:750:HEM:HHC	2:B:750:HEM:CBB	2.50	0.41
1:A:320:SER:HA	1:A:700:LEU:HD23	2.03	0.41
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.56	0.41
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.56	0.41
1:A:373:GLY:HA2	1:A:378:MET:HE3	2.03	0.41
1:A:537:PRO:HA	1:A:538:PRO:HD2	1.98	0.41
1:B:332:MET:HE3	1:B:338:PRO:HB3	2.01	0.41
1:B:589:MET:HA	1:B:649:VAL:O	2.20	0.41
1:A:322:LEU:HB2	1:A:699:ARG:HB2	2.03	0.41
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.56	0.41
1:A:469:LYS:C	1:A:470:HIS:ND1	2.79	0.41
1:B:299:ARG:CZ	1:B:299:ARG:CB	2.96	0.41
1:A:684:SER:HB3	1:A:687:ILE:HD11	2.03	0.41
2:A:750:HEM:HBA2	4:A:800:JRS:H7AA	2.03	0.41
1:B:473:ARG:HD3	1:B:580:SER:HB2	2.02	0.41
1:A:555:LYS:N	7:A:8:HOH:O	2.54	0.40
1:B:323:GLU:O	1:B:699:ARG:HD3	2.21	0.40
1:B:566:ALA:HA	1:B:584:PHE:O	2.21	0.40
1:A:650:ASP:OD2	1:A:652:HIS:HB2	2.21	0.40
1:B:355:PHE:N	1:B:356:PRO:CD	2.84	0.40
1:A:472:PHE:C	1:A:473:ARG:HG2	2.47	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.10	0.40
1:B:595:VAL:O	1:B:599:CYS:HB2	2.21	0.40
1:B:366:TYR:HA	1:B:369:ILE:HG12	2.03	0.40
1:B:590:GLY:HA2	1:B:648:ILE:HD11	2.02	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%)	382 (95%)	20 (5%)	1 (0%)	43	44
1	B	407/422 (96%)	391 (96%)	16 (4%)	0	100	100
All	All	810/844 (96%)	773 (95%)	36 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	SER

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%)	351 (97%)	12 (3%)	33	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	366/377 (97%)	358 (98%)	8 (2%)	45 53
All	All	729/754 (97%)	709 (97%)	20 (3%)	39 45

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

Mol	Chain	Res	Type
1	A	370	LYS
1	A	371	ARG
1	A	381	LEU
1	A	389	GLU
1	A	390	SER
1	A	393	THR
1	A	523	LEU
1	A	555	LYS
1	A	609	GLU
1	A	615	ASP
1	A	620	LYS
1	A	645	LYS
1	B	299	ARG
1	B	300	PHE
1	B	353	GLN
1	B	419	ILE
1	B	423	LYS
1	B	540	LEU
1	B	667	ARG
1	B	707	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	A	436	HIS
1	A	454	ASN
1	A	527	ASN
1	A	642	GLN
1	A	697	ASN
1	A	707	GLN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN
1	B	436	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	628	GLN
1	B	642	GLN
1	B	697	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	H4B	A	760	-	17,18,18	1.08	1 (5%)	14,26,26	2.16	6 (42%)
5	ACT	A	860	-	3,3,3	0.73	0	3,3,3	0.99	0
2	HEM	A	750	1	50,50,50	2.02	13 (26%)	67,82,82	1.78	12 (17%)
4	JRS	A	800	-	28,29,29	0.68	0	29,38,38	1.59	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	JRS	B	800	-	28,29,29	0.75	0	29,38,38	1.64	5 (17%)
5	ACT	B	860	-	3,3,3	0.63	0	3,3,3	1.46	0
3	H4B	B	760	-	17,18,18	0.95	2 (11%)	14,26,26	2.02	5 (35%)
2	HEM	B	750	1	50,50,50	1.66	10 (20%)	67,82,82	1.57	11 (16%)

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	FE-NA	6.65	2.17	1.95
2	A	750	HEM	C3D-C2D	6.30	1.50	1.36
2	B	750	HEM	C3D-C2D	6.19	1.50	1.36
2	A	750	HEM	FE-NB	4.23	2.07	1.94
2	A	750	HEM	CMC-C2C	3.72	1.58	1.50
2	A	750	HEM	FE-NC	3.64	2.07	1.95
2	B	750	HEM	FE-NA	3.63	2.07	1.95
2	B	750	HEM	CMD-C2D	3.05	1.57	1.50
2	A	750	HEM	CAB-C3B	3.01	1.55	1.47
2	A	750	HEM	CMB-C2B	2.76	1.56	1.50
2	A	750	HEM	CMD-C2D	2.71	1.56	1.50
2	B	750	HEM	CMC-C2C	2.71	1.56	1.50
3	A	760	H4B	O4-C4	2.62	1.28	1.23
2	B	750	HEM	CMB-C2B	2.59	1.56	1.50
2	B	750	HEM	FE-NC	2.37	2.03	1.95
2	A	750	HEM	FE-ND	2.34	2.02	1.94
2	A	750	HEM	C2A-C3A	-2.32	1.32	1.38
2	A	750	HEM	O1D-CGD	2.30	1.29	1.22
3	B	760	H4B	O4-C4	2.26	1.27	1.23
2	A	750	HEM	CAC-C3C	2.23	1.53	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	CAC-C3C	2.18	1.53	1.47
2	B	750	HEM	C3C-C4C	-2.17	1.42	1.46
2	A	750	HEM	CMA-C3A	2.11	1.55	1.50
3	B	760	H4B	C7-C6	2.08	1.54	1.52
2	B	750	HEM	C3B-C2B	-2.04	1.33	1.37
2	B	750	HEM	CAB-C3B	2.00	1.52	1.47

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CBA-CAA-C2A	-5.77	96.57	112.53
4	B	800	JRS	C6A-N1A-C2A	5.72	122.35	118.07
3	A	760	H4B	C2-N1-C8A	4.75	121.75	113.36
2	B	750	HEM	CBD-CAD-C3D	-4.30	100.64	112.53
2	A	750	HEM	CHA-C4D-ND	4.20	129.56	124.37
2	A	750	HEM	C4D-ND-C1D	3.88	109.80	105.21
2	B	750	HEM	CHA-C4D-ND	3.82	129.09	124.37
2	A	750	HEM	CBD-CAD-C3D	-3.80	102.03	112.53
3	B	760	H4B	C2-N1-C8A	3.75	119.98	113.36
2	B	750	HEM	CMD-C2D-C1D	3.39	130.33	125.03
2	A	750	HEM	CMD-C2D-C1D	3.37	130.30	125.03
3	B	760	H4B	C2-N3-C4	-3.06	119.57	125.11
2	A	750	HEM	C4C-C3C-C2C	2.98	109.40	106.81
3	A	760	H4B	C11-C10-C9	-2.94	108.51	112.11
2	A	750	HEM	CHD-C4C-NC	2.92	127.64	124.45
2	B	750	HEM	C2A-C1A-NA	-2.92	106.92	110.15
2	B	750	HEM	C1A-CHA-C4D	-2.89	119.44	126.25
4	A	800	JRS	C6A-N1A-C2A	2.88	120.22	118.07
2	A	750	HEM	CBC-CAC-C3C	-2.85	113.28	127.53
4	B	800	JRS	C3A-C2A-N1A	-2.80	119.53	122.73
4	A	800	JRS	C4-C11-C12	-2.79	115.85	120.54
2	A	750	HEM	C2A-C1A-NA	-2.75	107.10	110.15
2	A	750	HEM	CHD-C1D-ND	2.71	127.34	124.42
2	B	750	HEM	O1D-CGD-CBD	-2.70	114.52	123.09
3	B	760	H4B	C4-C4A-N5	2.69	123.61	116.27
3	B	760	H4B	O9-C9-C10	-2.68	104.04	109.14
2	B	750	HEM	C4C-C3C-C2C	2.66	109.12	106.81
2	B	750	HEM	C1D-C2D-C3D	-2.58	104.26	106.98
3	A	760	H4B	N2-C2-N3	2.58	122.21	116.76
3	B	760	H4B	C4A-C4-N3	2.57	119.18	112.13
3	A	760	H4B	C4-C4A-N5	2.56	123.25	116.27
2	B	750	HEM	CAD-C3D-C4D	2.55	129.14	124.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	N3-C2-N1	-2.53	118.70	123.32
4	A	800	JRS	C7A-C2A-N1A	2.52	119.65	116.57
4	A	800	JRS	O1-C1-C2	-2.42	101.42	109.44
4	A	800	JRS	F13-C13-C14	2.42	122.42	118.55
2	A	750	HEM	C1D-C2D-C3D	-2.38	104.48	106.98
4	B	800	JRS	C4-C11-C12	-2.37	116.55	120.54
3	A	760	H4B	C4A-C4-N3	2.34	118.55	112.13
4	B	800	JRS	O1-C1-C2	-2.33	101.72	109.44
4	A	800	JRS	C1-C2-N2	2.33	117.07	111.43
2	B	750	HEM	CHA-C4D-C3D	-2.14	121.29	125.23
4	A	800	JRS	C3-N2-C2	2.09	123.31	113.40
4	B	800	JRS	O1-C3'-C2'	-2.05	105.41	111.23
2	B	750	HEM	CBC-CAC-C3C	-2.05	117.26	127.53
2	A	750	HEM	O1D-CGD-CBD	-2.03	116.67	123.09

There are no chirality outliers.

All (17) torsion outliers are listed below:

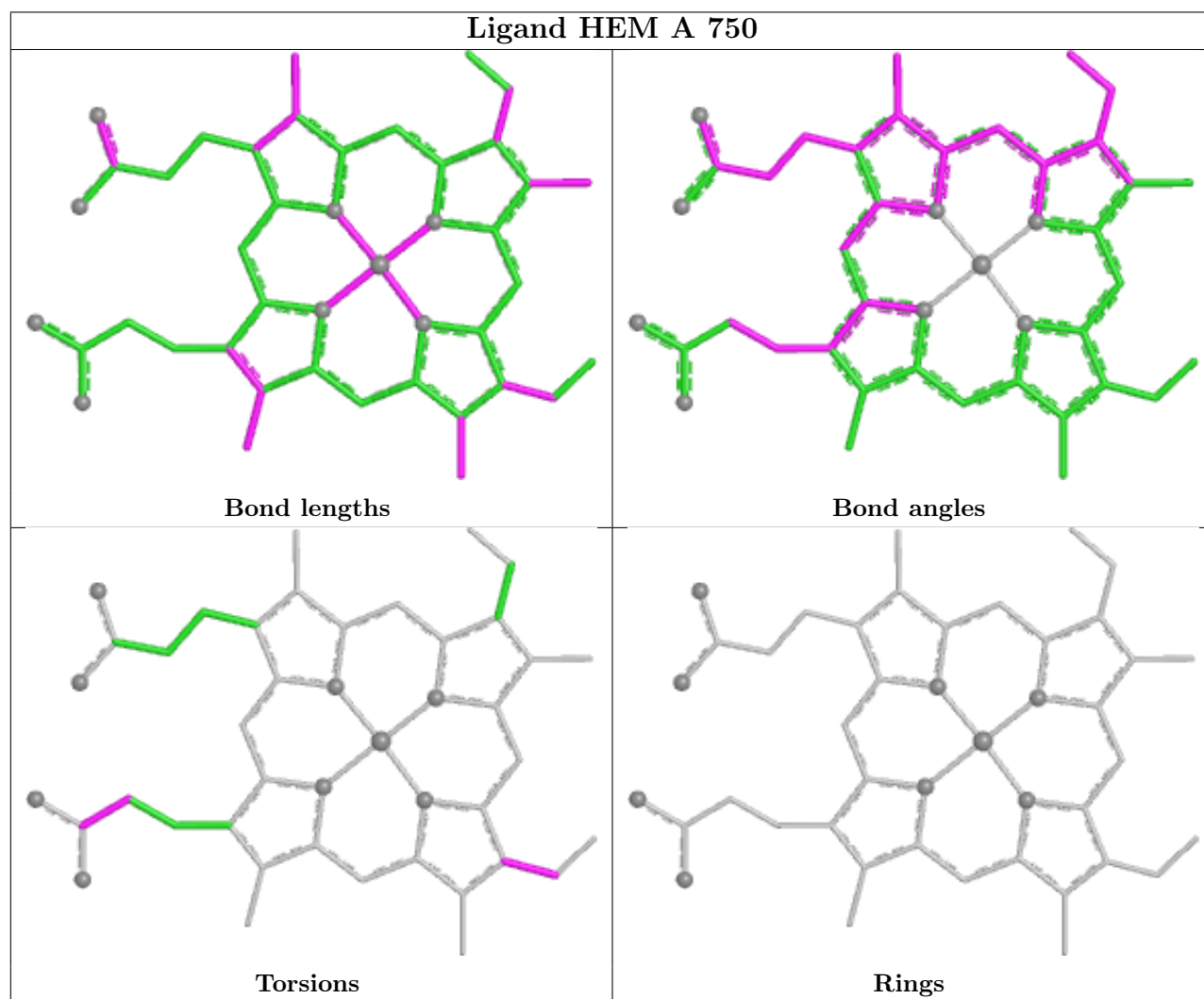
Mol	Chain	Res	Type	Atoms
4	A	800	JRS	C4'-C3'-O1-C1
4	A	800	JRS	C1-C2-N2-C3
4	B	800	JRS	C2'-C3'-O1-C1
4	B	800	JRS	C4'-C3'-O1-C1
4	B	800	JRS	N2-C3-C4-C11
2	B	750	HEM	C2A-CAA-CBA-CGA
4	A	800	JRS	C4-C3-N2-C2
4	A	800	JRS	C2'-C3'-O1-C1
2	A	750	HEM	C4B-C3B-CAB-CBB
4	A	800	JRS	C2-C1-O1-C3'
2	A	750	HEM	CAA-CBA-CGA-O1A
2	A	750	HEM	CAA-CBA-CGA-O2A
4	B	800	JRS	C1-C2-N2-C3
4	B	800	JRS	C4-C3-N2-C2
4	A	800	JRS	N2-C3-C4-C11
3	B	760	H4B	N5-C6-C9-O9
4	B	800	JRS	C2-C1-O1-C3'

There are no ring outliers.

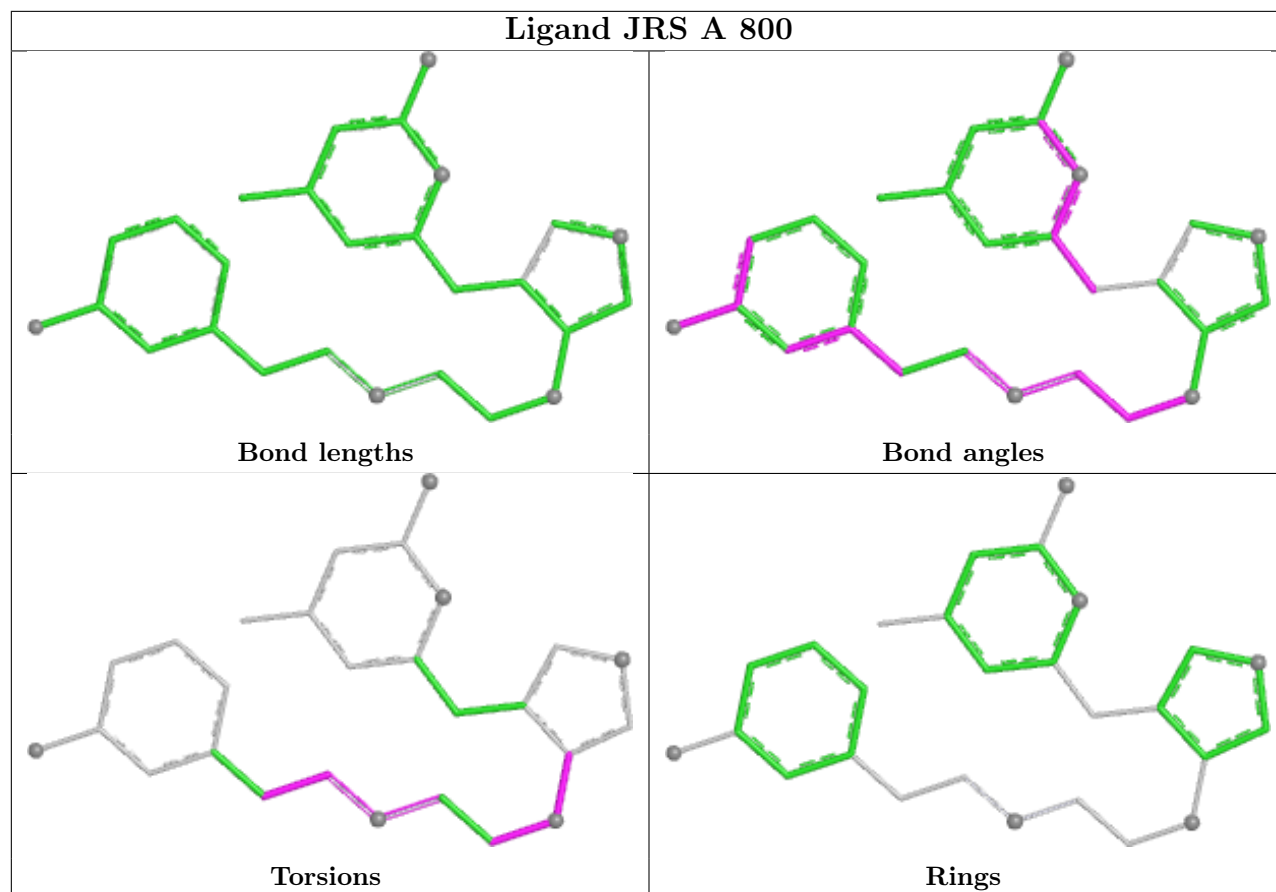
4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	10	0
4	A	800	JRS	3	0
4	B	800	JRS	3	0
2	B	750	HEM	9	0

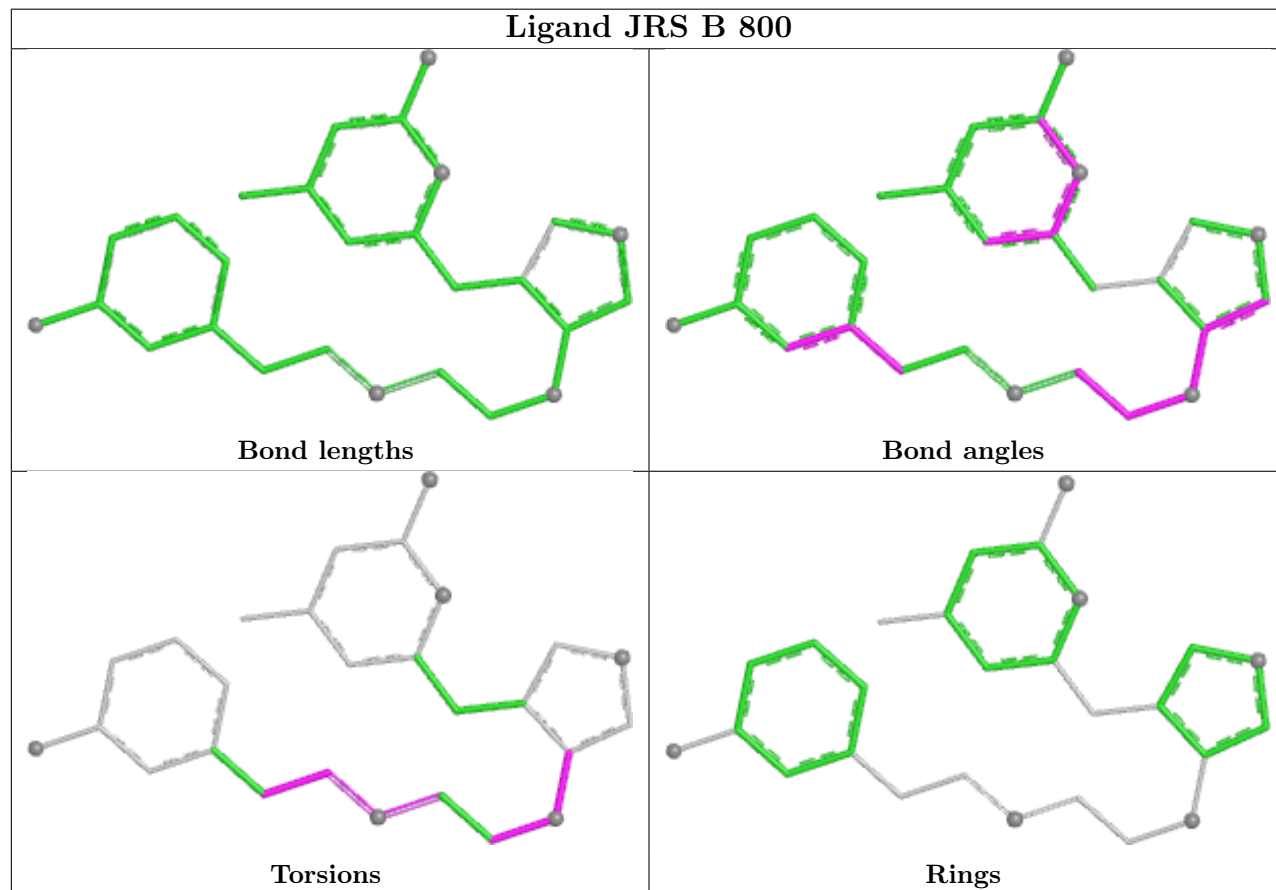
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

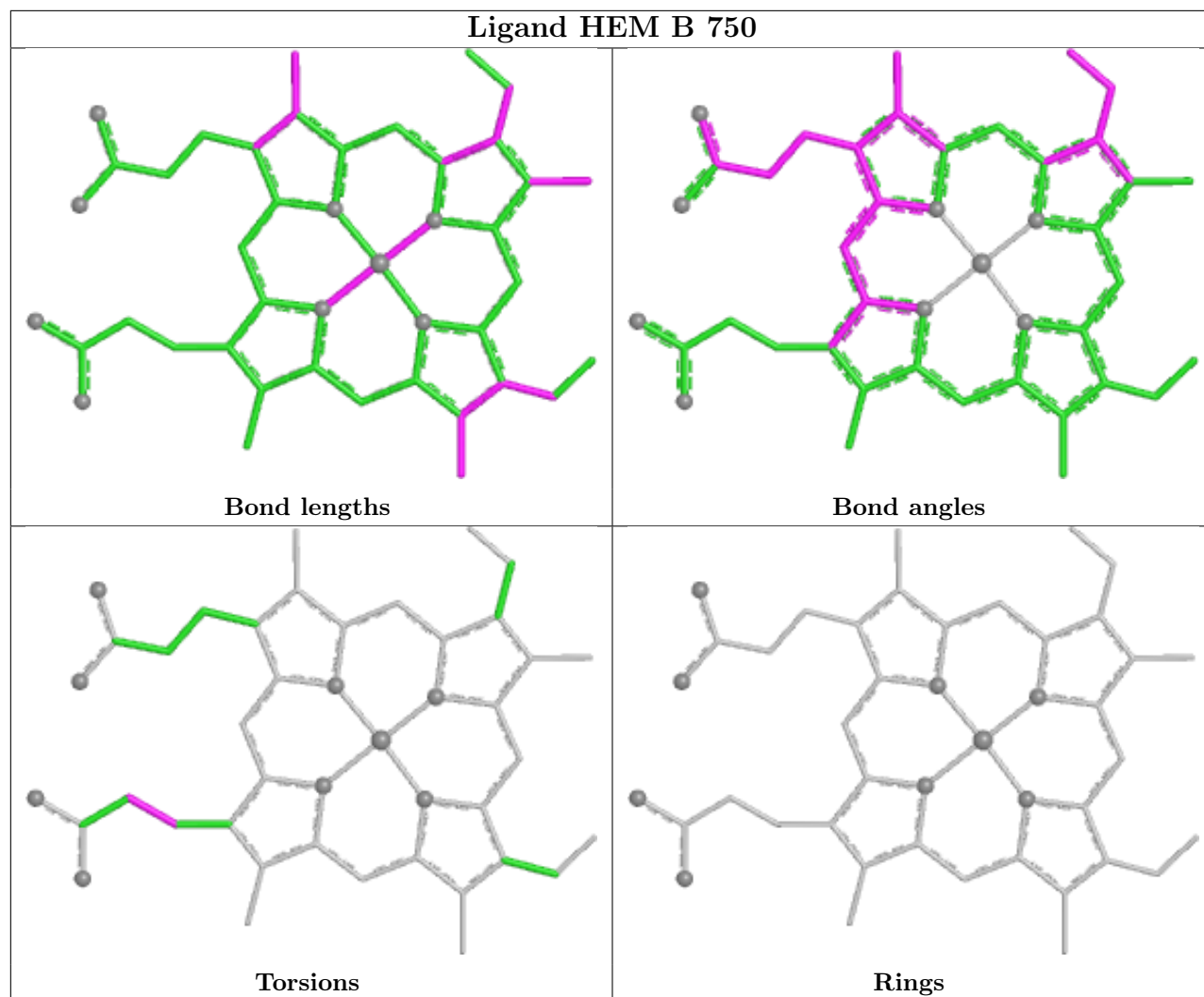


Ligand JRS A 800



Ligand JRS 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%)	-0.06	4 (0%) 79 81	28, 64, 116, 149	1 (0%)
1	B	411/422 (97%)	-0.27	4 (0%) 79 81	24, 54, 87, 113	1 (0%)
All	All	818/844 (96%)	-0.16	8 (0%) 79 81	24, 59, 110, 149	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	3.7
1	A	338	PRO	2.8
1	B	338	PRO	2.4
1	B	352	ASP	2.3
1	B	350	THR	2.2
1	A	706	TYR	2.2
1	A	321	THR	2.1
1	A	373	GLY	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,

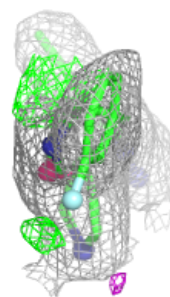
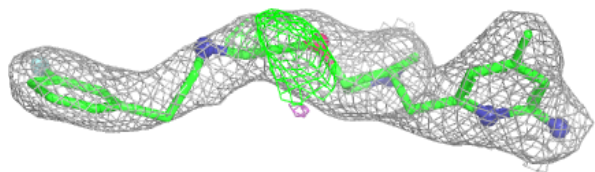
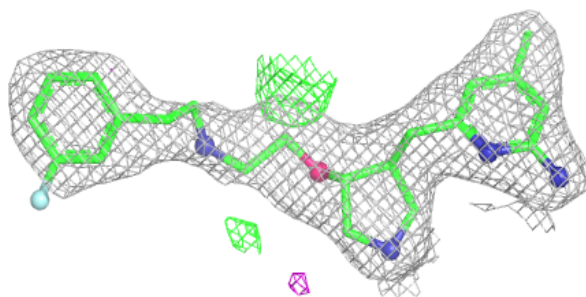
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	860	4/4	0.85	0.17	82,84,84,84	0
4	JRS	B	800	27/27	0.90	0.11	44,56,85,92	0
5	ACT	B	860	4/4	0.90	0.14	63,66,66,67	0
4	JRS	A	800	27/27	0.91	0.10	34,60,87,92	0
3	H4B	B	760	17/17	0.94	0.08	39,45,52,55	0
3	H4B	A	760	17/17	0.95	0.07	39,45,52,52	0
2	HEM	A	750	43/43	0.98	0.06	37,44,64,68	0
2	HEM	B	750	43/43	0.98	0.07	35,42,60,65	0
6	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.

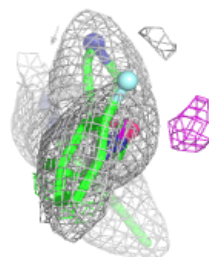
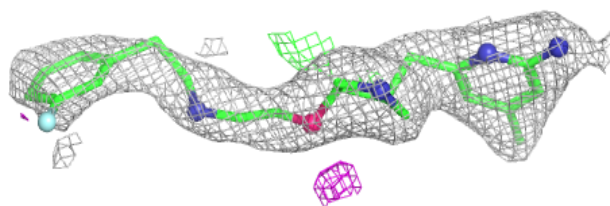
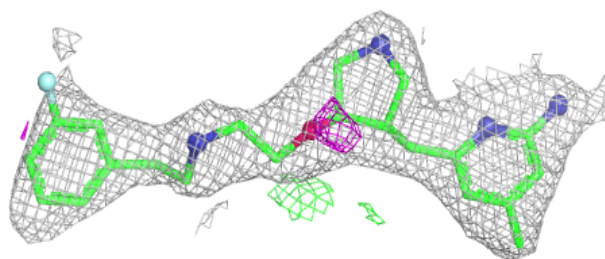
Electron density around JRS B 800:

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



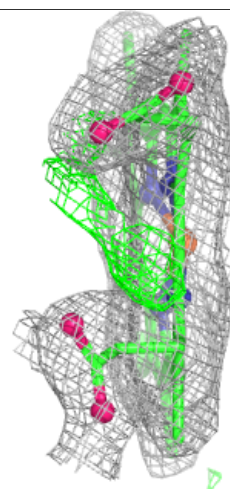
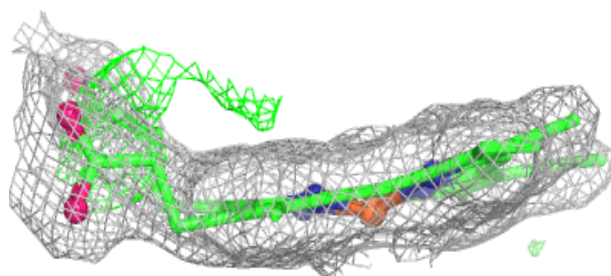
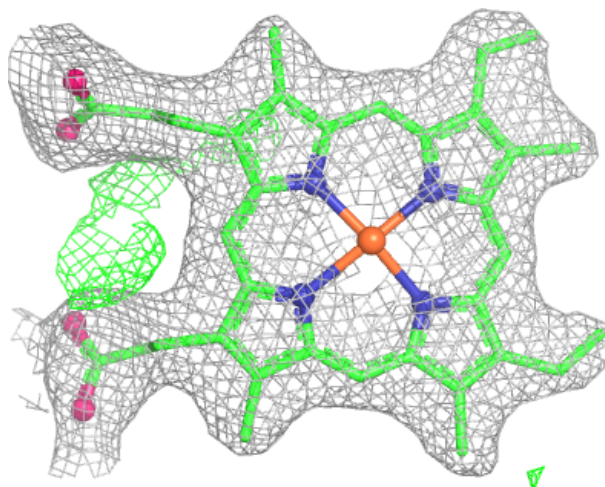
Electron density around JRS A 800:

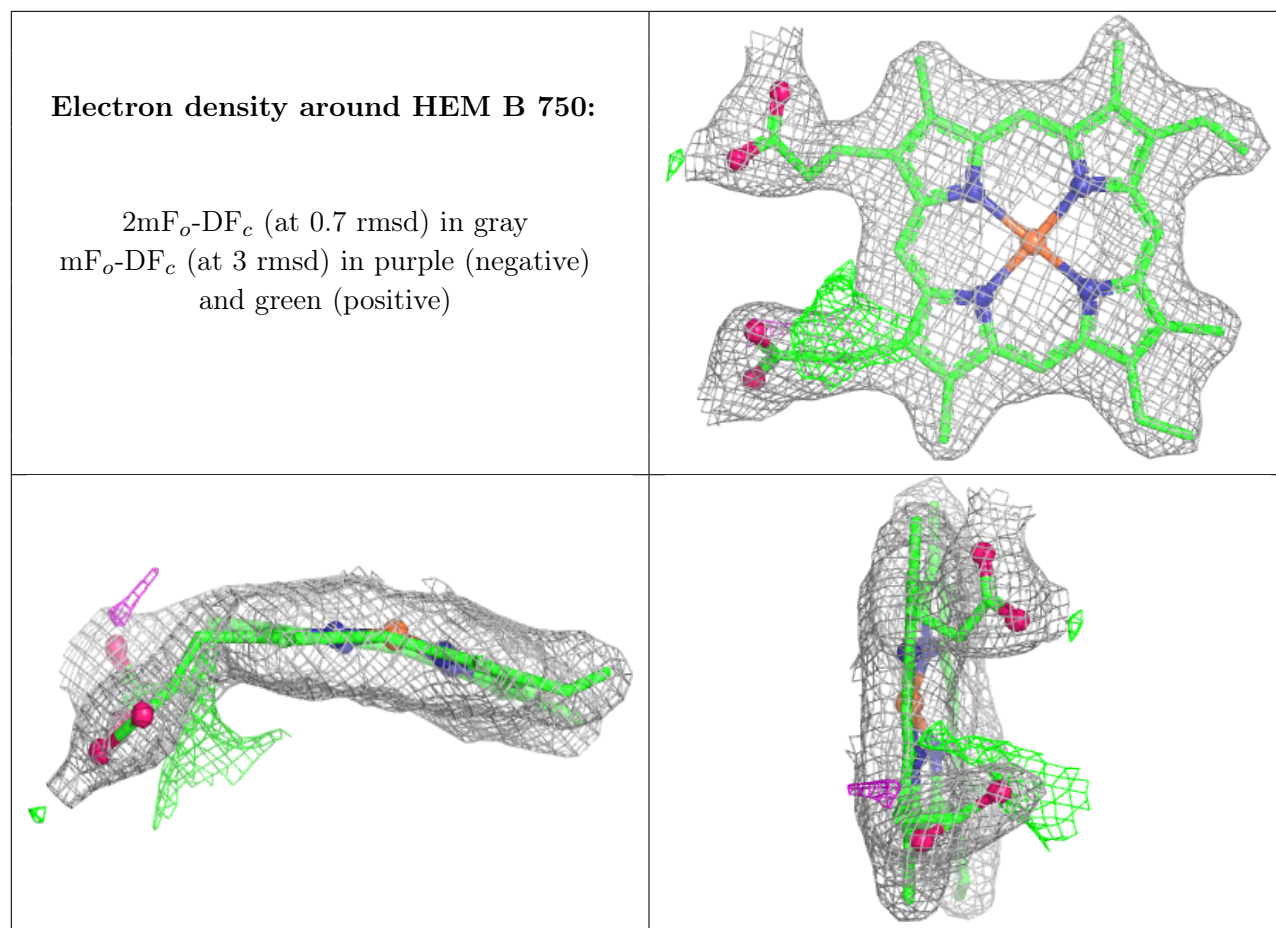
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.