



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:51 AM UTC

PDB ID : 1RS6 / pdb_00001rs6
Title : Rat neuronal NOS heme domain with D-lysine-D-nitroarginine amide bound
Authors : Flinspach, M.; Li, H.; Jamal, J.; Yang, W.; Huang, H.; Silverman, R.B.; Poulos, T.L.
Deposited on : 2003-12-09
Resolution : 1.95 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

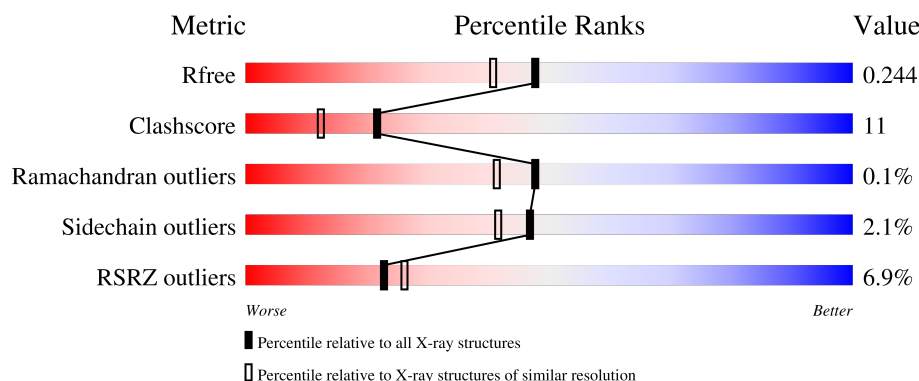
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	421	9% 67% 27% • •
1	B	421	4% 75% 20% • •

2 Entry composition [i](#)

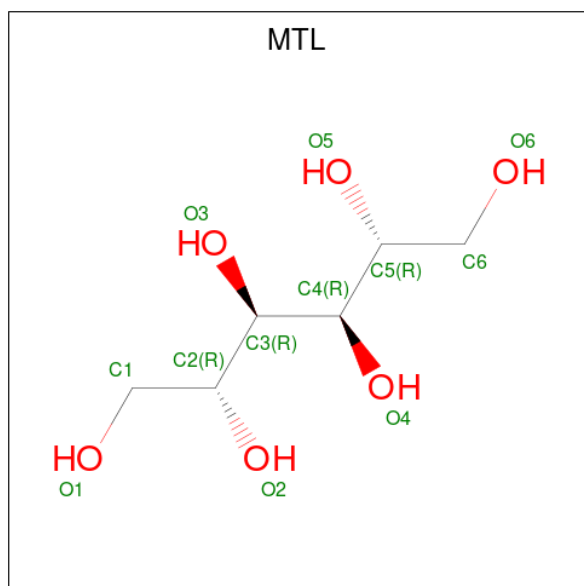
There are 8 unique types of molecules in this entry. The entry contains 7401 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

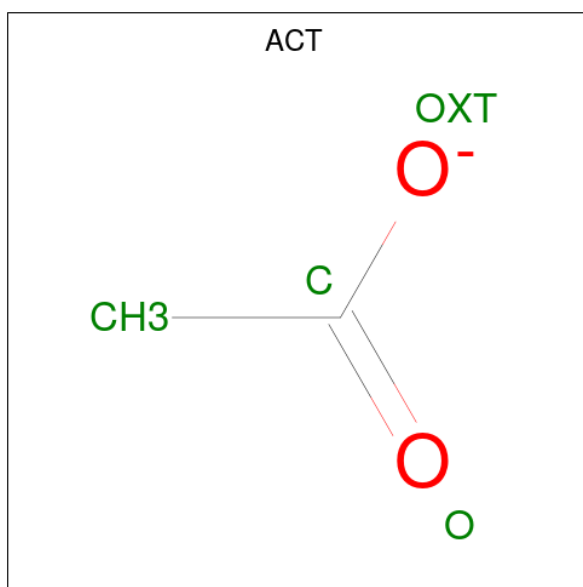
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	2	0
			3315	2121	566	606	22			
1	B	410	Total	C	N	O	S	0	2	0
			3343	2138	573	611	21			

- Molecule 2 is D-MANNITOL (CCD ID: MTL) (formula: C₆H₁₄O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

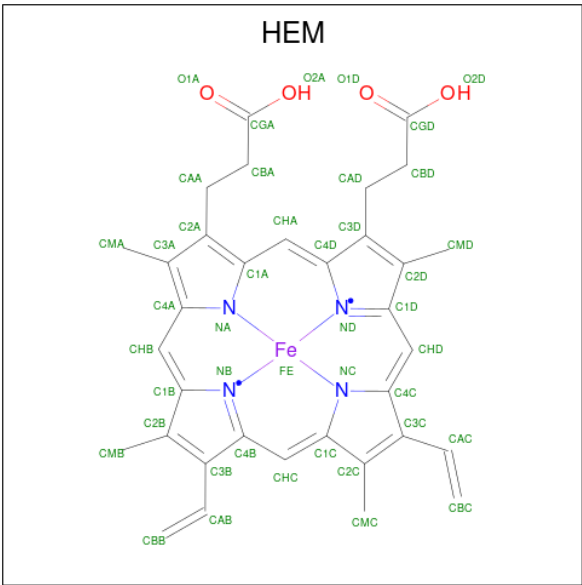


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

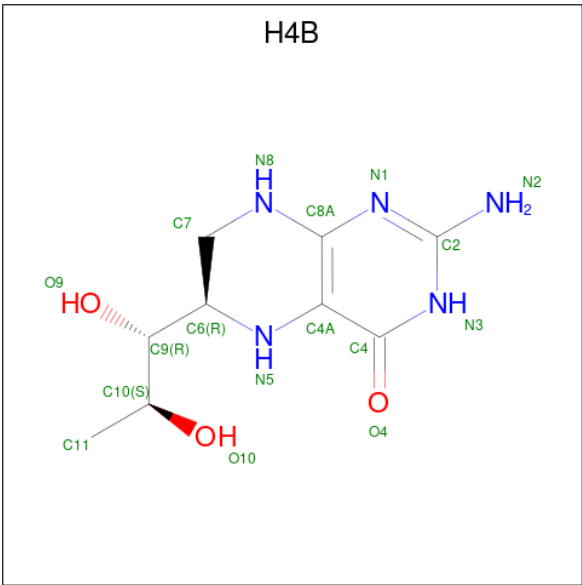
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C₉H₁₅N₅O₃).

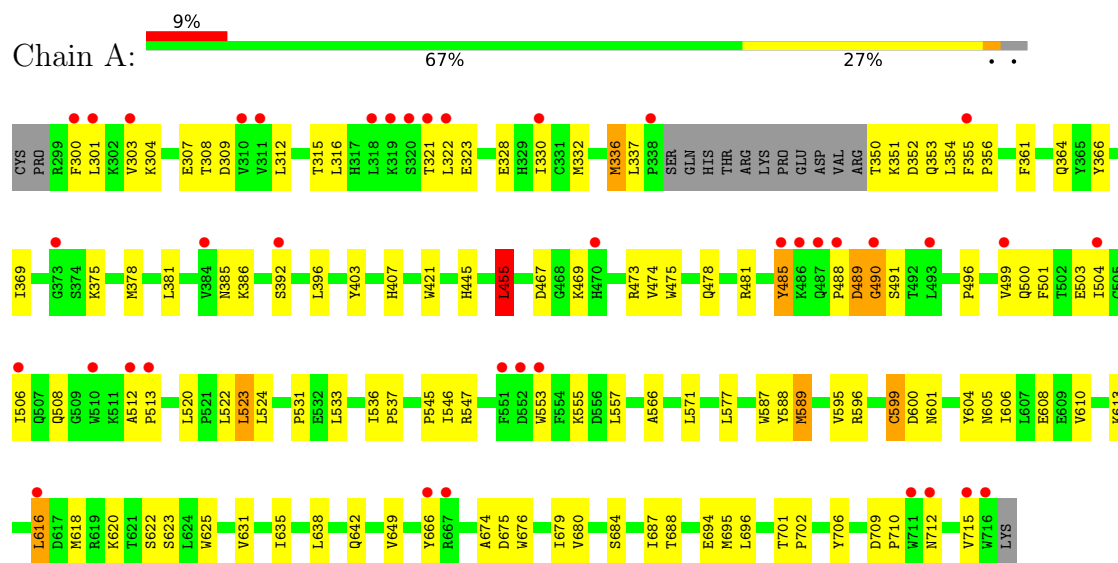


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			17	9	5	3		
6	B	1	Total	C	N	O	0	0
			17	9	5	3		

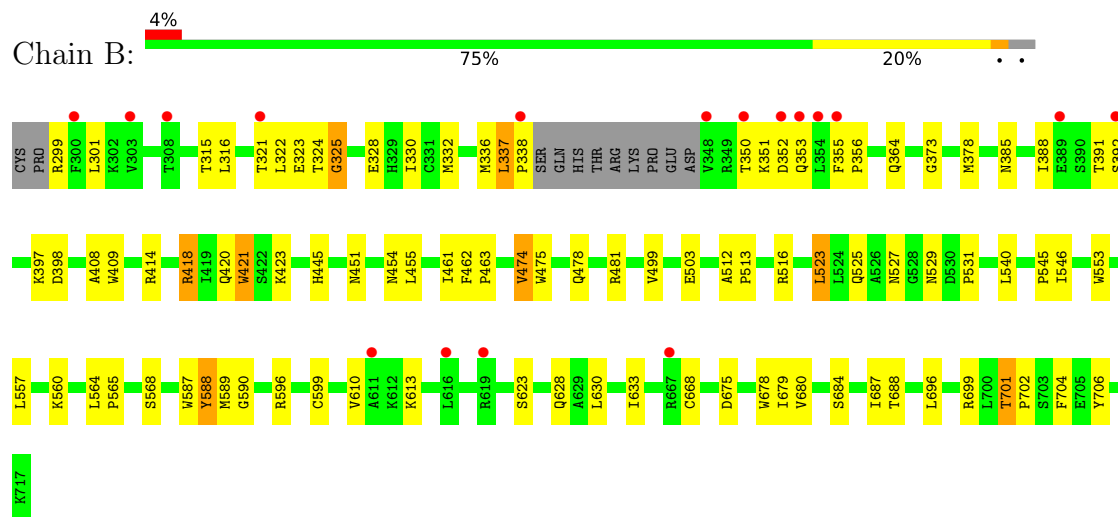
3 Residue-property plots [i](#)

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	51.59Å 109.81Å 164.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.08 – 1.95 27.08 – 1.95	Depositor EDS
% Data completeness (in resolution range)	92.4 (27.08-1.95) 92.0 (27.08-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.254 0.209 , 0.244	Depositor DCC
R_{free} test set	3434 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7401	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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, H4B, MTL, ZN, ACT, DP2

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	0.52	0/3418	0.99	13/4637 (0.3%)
1	B	0.56	0/3446	1.01	24/4672 (0.5%)
All	All	0.54	0/6864	1.00	37/9309 (0.4%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-8.71	95.04	109.24
1	A	354	LEU	N-CA-C	8.18	119.83	111.07
1	A	490	GLY	N-CA-C	-8.15	104.62	115.21
1	A	589	MET	N-CA-C	-7.96	96.26	109.24
1	B	421	TRP	N-CA-C	7.44	120.33	111.33
1	A	421	TRP	N-CA-C	6.87	119.64	111.33
1	A	474	VAL	N-CA-C	-6.72	98.06	107.80
1	B	623	SER	N-CA-C	-6.66	105.16	113.28
1	A	623	SER	N-CA-C	-6.42	105.45	113.28
1	A	688	THR	N-CA-C	-6.41	102.06	110.39
1	A	588	TYR	N-CA-C	6.38	119.92	110.48
1	B	688	THR	N-CA-C	-6.27	101.44	110.40
1	B	474	VAL	N-CA-C	-6.08	98.37	107.37
1	B	680	VAL	CA-C-N	6.03	124.06	119.66
1	B	680	VAL	C-N-CA	6.03	124.06	119.66
1	B	599	CYS	N-CA-C	5.88	121.36	113.72
1	B	590	GLY	N-CA-C	5.81	119.92	112.83
1	B	455	LEU	N-CA-C	5.67	118.44	110.23
1	B	588	TYR	N-CA-C	5.62	118.79	110.48
1	A	599	CYS	N-CA-C	5.56	120.34	113.50
1	A	375	LYS	N-CA-C	-5.37	105.51	111.36
1	B	704	PHE	N-CA-C	-5.32	100.51	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	THR	N-CA-C	-5.31	107.47	114.31
1	B	545	PRO	N-CA-C	-5.29	102.89	111.19
1	B	418	ARG	N-CA-C	5.27	119.34	113.01
1	A	546	ILE	N-CA-C	5.22	115.61	107.99
1	B	397	LYS	N-CA-C	-5.18	103.69	110.53
1	B	596	ARG	N-CA-C	5.17	117.91	111.24
1	B	706	TYR	N-CA-C	-5.17	103.58	110.55
1	B	461	ILE	N-CA-C	5.13	114.96	107.37
1	B	564	LEU	N-CA-C	5.13	117.93	108.69
1	B	408	ALA	N-CA-C	-5.12	105.70	111.28
1	A	455	LEU	N-CA-C	5.11	117.64	110.23
1	B	701	THR	N-CA-C	-5.06	103.16	110.40
1	B	557	LEU	N-CA-C	-5.06	106.94	113.01
1	B	325	GLY	N-CA-C	-5.04	107.58	114.64
1	A	566	ALA	N-CA-C	5.02	116.78	107.60

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	3315	0	3223	93	0
1	B	3343	0	3258	59	0
2	A	12	0	14	1	0
2	B	12	0	14	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0
5	B	43	0	30	3	0
6	A	17	0	15	0	0
6	B	17	0	15	2	0
7	A	24	0	28	1	0
7	B	24	0	27	0	0
8	A	230	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	312	0	0	8	0
All	All	7401	0	6660	146	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 (146) 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:523:LEU:HD22	1:B:531:PRO:HB2	1.43	1.00
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.55	0.89
1:B:350:THR:HB	1:B:353:GLN:OE1	1.79	0.82
1:A:350:THR:HB	1:A:353:GLN:HG3	1.64	0.78
1:B:350:THR:HG22	1:B:352:ASP:H	1.47	0.78
5:A:750:HEM:HMC2	5:A:750:HEM:HBC2	1.67	0.76
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.68	0.74
1:A:350:THR:HG22	1:A:352:ASP:H	1.53	0.73
1:B:699:ARG:HB3	8:B:1090:HOH:O	1.90	0.71
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.77	0.67
1:A:332:MET:HE2	1:B:696:LEU:HD21	1.77	0.66
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.78	0.65
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.80	0.64
1:A:350:THR:HB	1:A:353:GLN:CG	2.30	0.62
1:B:299:ARG:HB3	1:B:299:ARG:NH1	2.14	0.62
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.83	0.61
1:A:503:GLU:HG3	8:A:1013:HOH:O	2.00	0.60
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.16	0.60
1:A:467:ASP:OD1	1:A:469:LYS:HB2	2.02	0.60
1:B:355:PHE:N	1:B:356:PRO:HD2	2.17	0.59
1:B:668:CYS:HB3	8:B:998:HOH:O	2.02	0.59
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.84	0.59
1:B:351:LYS:HE2	1:B:392:SER:OG	2.03	0.59
1:B:299:ARG:HB3	1:B:299:ARG:HH11	1.68	0.59
1:B:325:GLY:O	1:B:332:MET:HE2	2.02	0.58
1:A:308:THR:O	1:A:309:ASP:HB2	2.04	0.57
8:A:941:HOH:O	1:B:337:LEU:HD23	2.05	0.57
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.40	0.57
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.87	0.56
1:B:337:LEU:HD23	1:B:337:LEU:N	2.21	0.56
1:A:307:GLU:HG3	8:B:951:HOH:O	2.03	0.56
1:A:553:TRP:CE3	1:A:613:LYS:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:ARG:HG2	8:B:1160:HOH:O	2.05	0.55
1:A:489:ASP:HB2	1:A:491:SER:OG	2.07	0.55
1:A:353:GLN:O	1:A:356:PRO:HD2	2.07	0.55
1:B:336:MET:HG2	1:B:337:LEU:HD22	1.89	0.55
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.89	0.55
1:A:396:LEU:HG	1:A:577:LEU:HD12	1.88	0.55
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.89	0.54
1:A:488:PRO:C	1:A:490:GLY:H	2.16	0.54
1:B:336:MET:HE3	6:B:761:H4B:H9	1.90	0.53
1:B:565:PRO:HB3	1:B:588:TYR:CZ	2.44	0.53
1:A:328:GLU:O	1:B:324:THR:HG23	2.08	0.52
1:B:322:LEU:HD12	8:B:1090:HOH:O	2.09	0.52
1:A:485:TYR:HA	8:A:1099:HOH:O	2.10	0.51
1:A:488:PRO:C	1:A:490:GLY:N	2.66	0.51
1:A:606:ILE:O	1:A:610:VAL:HG23	2.09	0.51
1:A:571:LEU:C	1:A:571:LEU:HD23	2.36	0.51
1:A:555:LYS:HZ2	1:A:555:LYS:HB3	1.76	0.51
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.92	0.50
1:A:675:ASP:O	1:A:679:ILE:HG12	2.12	0.50
1:A:378:MET:HA	1:A:378:MET:HE2	1.92	0.50
1:A:321:THR:HG21	8:A:1107:HOH:O	2.10	0.49
1:A:321:THR:HG23	1:A:322:LEU:HG	1.94	0.49
1:A:638:LEU:O	1:A:642:GLN:HG3	2.11	0.49
1:A:620:LYS:HE3	1:A:622:SER:OG	2.13	0.49
1:A:715:VAL:O	1:A:715:VAL:HG23	2.12	0.49
1:B:391:THR:O	1:B:392:SER:HB2	2.12	0.49
1:A:351:LYS:HE2	1:A:392:SER:HA	1.94	0.49
1:A:350:THR:HB	1:A:353:GLN:CD	2.38	0.49
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.78	0.49
1:A:522:LEU:O	1:A:533:LEU:HA	2.13	0.48
1:A:608:GLU:HG3	1:A:618:MET:HE1	1.94	0.48
1:A:491:SER:HB2	8:A:1100:HOH:O	2.14	0.47
5:B:750:HEM:CMC	5:B:750:HEM:HBC2	2.44	0.47
1:A:304:LYS:O	1:A:694:GLU:HG3	2.15	0.47
1:A:701:THR:HA	1:A:702:PRO:C	2.39	0.47
1:B:675:ASP:O	1:B:679:ILE:HG12	2.15	0.47
1:A:706:TYR:CE2	7:A:792:DP2:HD'2	2.50	0.47
1:A:303:VAL:CG1	1:A:694:GLU:O	2.63	0.47
1:A:496:PRO:O	1:A:499:VAL:HG23	2.14	0.46
1:B:332:MET:HE3	1:B:338:PRO:HB2	1.96	0.46
1:A:524:LEU:O	1:A:531:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PHE:CD2	1:A:315:THR:HG22	2.51	0.46
1:A:553:TRP:HZ3	1:A:557:LEU:HD11	1.81	0.46
1:A:601:ASN:HB2	8:A:970:HOH:O	2.15	0.46
1:B:373:GLY:HA2	1:B:378:MET:HE3	1.97	0.46
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.50	0.46
1:A:488:PRO:O	1:A:490:GLY:N	2.49	0.46
1:B:587:TRP:H	5:B:750:HEM:HAB	1.80	0.46
1:A:506:ILE:C	1:A:508:GLN:H	2.24	0.46
1:A:545:PRO:HG2	1:A:547:ARG:HH11	1.81	0.45
1:B:388:ILE:O	1:B:392:SER:N	2.43	0.45
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.45
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.05	0.45
1:A:445:HIS:C	1:A:445:HIS:CD2	2.94	0.45
1:A:366:TYR:CD2	1:A:369:ILE:HD11	2.52	0.45
1:B:525:GLN:HG3	1:B:529:ASN:O	2.17	0.45
1:A:336:MET:HE1	8:A:989:HOH:O	2.16	0.45
5:A:750:HEM:HBC2	5:A:750:HEM:CMC	2.44	0.44
1:A:351:LYS:HE2	1:A:392:SER:CA	2.46	0.44
1:A:555:LYS:HB3	1:A:555:LYS:NZ	2.32	0.44
1:B:462:PHE:HB3	1:B:463:PRO:HD2	1.99	0.44
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.99	0.44
1:A:332:MET:HE1	1:B:301:LEU:HD22	2.00	0.44
1:A:536:ILE:O	1:A:537:PRO:C	2.60	0.44
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.52	0.44
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.88	0.44
5:B:750:HEM:HBC2	5:B:750:HEM:HMC1	2.00	0.44
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.99	0.43
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.00	0.43
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.99	0.43
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.54	0.43
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.54	0.43
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.48	0.43
1:A:500:GLN:O	1:A:504:ILE:HG13	2.19	0.43
1:B:364:GLN:NE2	8:B:1119:HOH:O	2.52	0.43
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.49	0.43
1:A:321:THR:HG23	1:A:322:LEU:N	2.34	0.43
1:A:366:TYR:HA	1:A:369:ILE:HG12	2.01	0.43
1:B:553:TRP:CH2	1:B:613:LYS:HB2	2.54	0.43
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.49	0.43
1:B:398:ASP:HB2	8:B:1080:HOH:O	2.19	0.42
1:B:337:LEU:N	1:B:337:LEU:CD2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ARG:O	1:A:600:ASP:HB2	2.19	0.42
1:A:323:GLU:HA	1:B:328:GLU:O	2.19	0.42
1:A:595:VAL:O	1:A:599:CYS:HB2	2.19	0.42
1:B:299:ARG:NH1	1:B:299:ARG:CB	2.83	0.42
1:B:516:ARG:HG3	8:B:1033:HOH:O	2.19	0.42
1:A:687:ILE:HD13	1:B:630:LEU:HD22	2.01	0.42
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.55	0.42
1:B:445:HIS:CD2	1:B:445:HIS:C	2.98	0.42
1:A:361:PHE:O	1:A:364:GLN:HG2	2.19	0.42
1:A:506:ILE:C	1:A:508:GLN:N	2.76	0.42
1:B:323:GLU:O	1:B:699:ARG:HD3	2.20	0.42
1:A:501:PHE:HB2	2:A:870:MTL:H61	2.01	0.41
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.84	0.41
1:B:451:ASN:HB3	1:B:454:ASN:O	2.20	0.41
1:B:499:VAL:O	1:B:503:GLU:HG3	2.19	0.41
1:A:303:VAL:HG11	1:A:694:GLU:O	2.19	0.41
1:B:678:TRP:HA	6:B:761:H4B:N1	2.35	0.41
1:A:489:ASP:C	1:A:491:SER:H	2.27	0.41
1:A:709:ASP:HB2	1:A:712:ASN:ND2	2.35	0.41
1:A:300:PHE:CD1	1:A:300:PHE:N	2.89	0.41
1:A:312:LEU:HB3	1:A:666:TYR:CD2	2.56	0.41
1:A:355:PHE:CZ	1:A:385:ASN:ND2	2.89	0.41
1:A:473:ARG:CZ	1:A:710:PRO:HG3	2.50	0.41
1:B:512:ALA:HA	1:B:513:PRO:HD3	1.92	0.41
1:A:381:LEU:HD12	1:A:381:LEU:HA	1.95	0.41
1:B:418:ARG:C	1:B:420:GLN:N	2.79	0.41
1:B:474:VAL:HG11	1:B:568:SER:HB2	2.03	0.41
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.02	0.40
1:A:604:TYR:O	1:A:605:ASN:C	2.64	0.40
1:A:589:MET:HA	1:A:649:VAL:O	2.20	0.40
1:A:386:LYS:HD3	1:A:386:LYS:HA	1.92	0.40
1:B:332:MET:HE3	1:B:338:PRO:CB	2.51	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	405/421 (96%)	384 (95%)	20 (5%)	1 (0%)	43	36
1	B	408/421 (97%)	394 (97%)	14 (3%)	0	100	100
All	All	813/842 (97%)	778 (96%)	34 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP

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%)	357 (98%)	8 (2%)	45	40
1	B	368/377 (98%)	361 (98%)	7 (2%)	50	45
All	All	733/754 (97%)	718 (98%)	15 (2%)	47	43

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	336	MET
1	A	337	LEU
1	A	455	LEU
1	A	485	TYR
1	A	523	LEU
1	A	616	LEU
1	A	635	ILE
1	B	316	LEU
1	B	321	THR
1	B	337	LEU

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Mol	Chain	Res	Type
1	B	423	LYS
1	B	523	LEU
1	B	527	ASN
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	A	454	ASN
1	A	487	GLN
1	A	628	GLN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN
1	B	425	GLN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	664	ASN
1	B	697	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z > 2$
6	H4B	B	761	-	17,18,18	1.82	3 (17%)	14,26,26	1.78	3 (21%)
3	ACT	A	860	-	3,3,3	0.95	0	3,3,3	0.85	0
7	DP2	B	793	-	18,23,23	1.11	2 (11%)	23,28,28	1.47	3 (13%)
2	MTL	A	870	-	11,11,11	1.19	0	14,14,14	0.65	0
5	HEM	B	750	1	50,50,50	1.34	6 (12%)	67,82,82	1.17	5 (7%)
3	ACT	B	861	-	3,3,3	0.99	0	3,3,3	0.71	0
2	MTL	B	871	-	11,11,11	1.18	0	14,14,14	0.60	0
5	HEM	A	750	1	50,50,50	1.25	4 (8%)	67,82,82	1.11	6 (8%)
7	DP2	A	792	-	18,23,23	0.94	0	23,28,28	1.22	2 (8%)
6	H4B	A	760	-	17,18,18	1.94	4 (23%)	14,26,26	2.03	3 (21%)

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
6	H4B	B	761	-	-	0/8/17/17	0/2/2/2
7	DP2	B	793	-	-	6/25/28/28	-
2	MTL	A	870	-	-	0/16/16/16	-
5	HEM	B	750	1	-	2/14/54/54	-
2	MTL	B	871	-	-	0/16/16/16	-
5	HEM	A	750	1	-	1/14/54/54	-
7	DP2	A	792	-	-	6/25/28/28	-
6	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	760	H4B	C4A-N5	4.80	1.49	1.37
6	A	760	H4B	C6-N5	4.08	1.54	1.47
6	B	761	H4B	C6-N5	4.06	1.54	1.47
6	B	761	H4B	C4A-N5	4.00	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	760	H4B	C4-N3	3.05	1.44	1.38
5	B	750	HEM	CHB-C1B	3.04	1.44	1.38
5	B	750	HEM	CMD-C2D	2.97	1.56	1.50
5	A	750	HEM	CAB-C3B	-2.97	1.39	1.47
5	B	750	HEM	CAB-C3B	-2.92	1.39	1.47
5	A	750	HEM	FE-NB	2.55	2.02	1.94
5	B	750	HEM	C3C-C4C	-2.50	1.41	1.46
6	A	760	H4B	C8A-N1	2.45	1.39	1.36
5	B	750	HEM	CHD-C4C	2.37	1.43	1.38
5	A	750	HEM	CMC-C2C	2.35	1.55	1.50
7	B	793	DP2	O-C	-2.34	1.19	1.23
5	B	750	HEM	FE-NA	2.29	2.02	1.95
7	B	793	DP2	C'-N	2.21	1.38	1.34
6	B	761	H4B	C4-N3	2.10	1.42	1.38
5	A	750	HEM	CMD-C2D	2.00	1.54	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	760	H4B	C2-N1-C8A	5.49	123.05	113.36
6	B	761	H4B	C2-N1-C8A	4.95	122.09	113.36
7	B	793	DP2	O-C-N2	-4.02	115.94	123.04
6	A	760	H4B	N3-C2-N1	-3.29	117.30	123.32
7	A	792	DP2	O-C-N2	-3.25	117.31	123.04
7	B	793	DP2	CA-C-N2	3.24	122.28	116.76
6	B	761	H4B	N3-C2-N1	-2.65	118.47	123.32
6	A	760	H4B	O10-C10-C9	-2.64	105.41	109.77
5	A	750	HEM	CBD-CAD-C3D	-2.58	105.39	112.53
5	A	750	HEM	CBA-CAA-C2A	-2.58	105.41	112.53
5	A	750	HEM	CAA-C2A-C1A	2.56	129.94	124.94
5	B	750	HEM	C2D-C1D-ND	2.55	112.86	109.90
5	B	750	HEM	C4C-NC-C1C	-2.49	101.76	105.82
5	A	750	HEM	C2B-C1B-NB	2.32	112.50	109.84
7	A	792	DP2	CA-C-N2	2.32	120.70	116.76
7	B	793	DP2	CD-NE-CZ	2.28	127.64	123.46
6	B	761	H4B	O10-C10-C9	-2.16	106.20	109.77
5	B	750	HEM	C4A-NA-C1A	-2.12	102.36	105.82
5	B	750	HEM	CMA-C3A-C4A	2.11	128.63	125.42
5	A	750	HEM	C2A-C1A-NA	2.09	112.47	110.15
5	A	750	HEM	CMA-C3A-C4A	2.04	128.52	125.42
5	B	750	HEM	CBA-CAA-C2A	-2.01	106.97	112.53

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	792	DP2	O-C-CA-N
7	B	793	DP2	CE'-CD'-CG'-CB'
7	A	792	DP2	CA'-CB'-CG'-CD'
5	B	750	HEM	C4B-C3B-CAB-CBB
7	A	792	DP2	N2-C-CA-N
7	A	792	DP2	O-C-CA-CB
7	A	792	DP2	CG-CD-NE-CZ
7	B	793	DP2	CG-CD-NE-CZ
7	B	793	DP2	N-CA-CB-CG
5	B	750	HEM	C2B-C3B-CAB-CBB
5	A	750	HEM	C4B-C3B-CAB-CBB
7	A	792	DP2	O2-N1-NH1-CZ
7	B	793	DP2	O2-N1-NH1-CZ
7	B	793	DP2	O-C-CA-N
7	B	793	DP2	C-CA-CB-CG

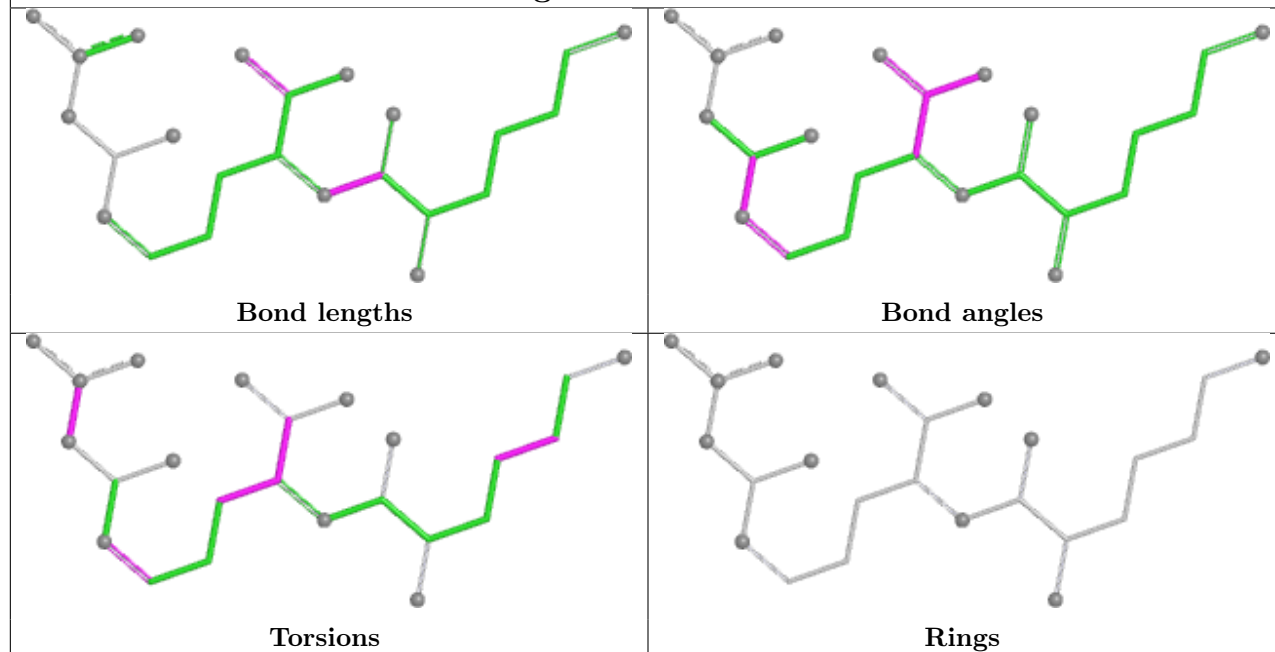
There are no ring outliers.

5 monomers are involved in 9 short contacts:

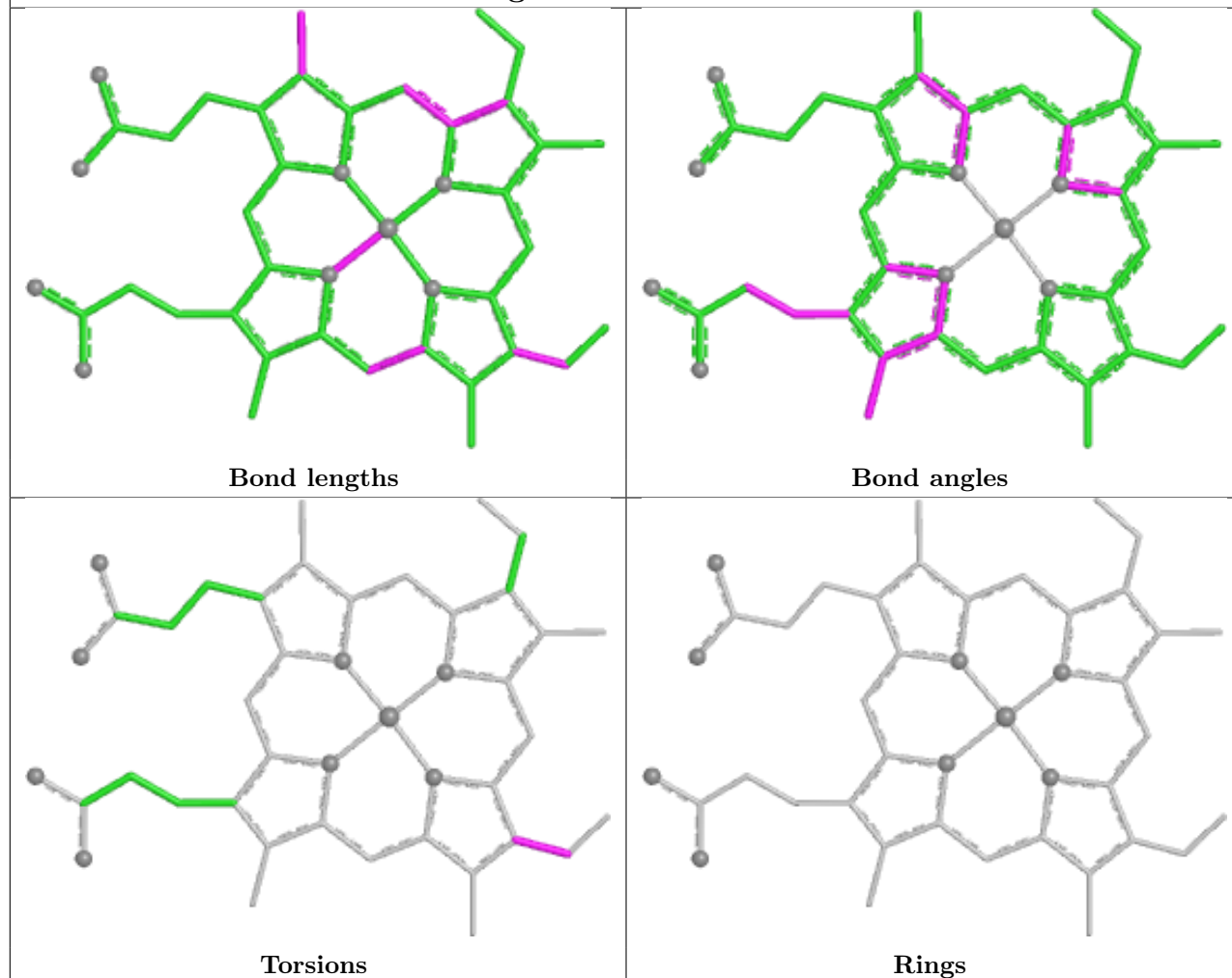
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	761	H4B	2	0
2	A	870	MTL	1	0
5	B	750	HEM	3	0
5	A	750	HEM	2	0
7	A	792	DP2	1	0

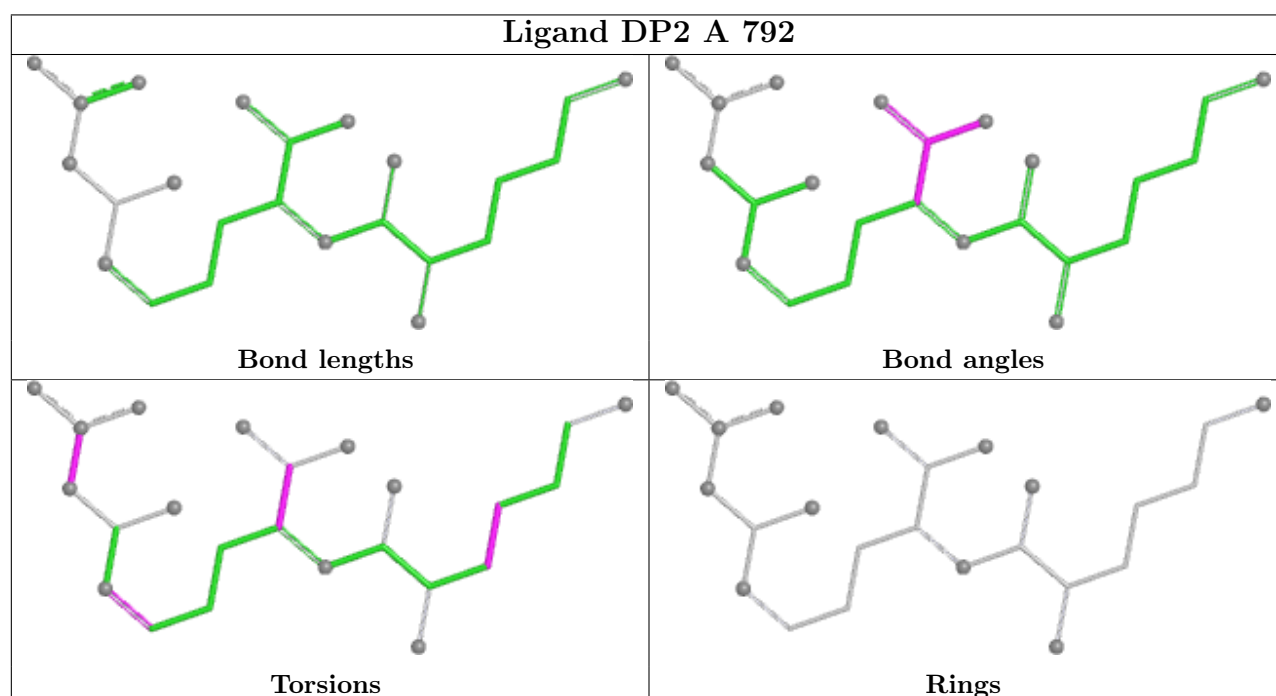
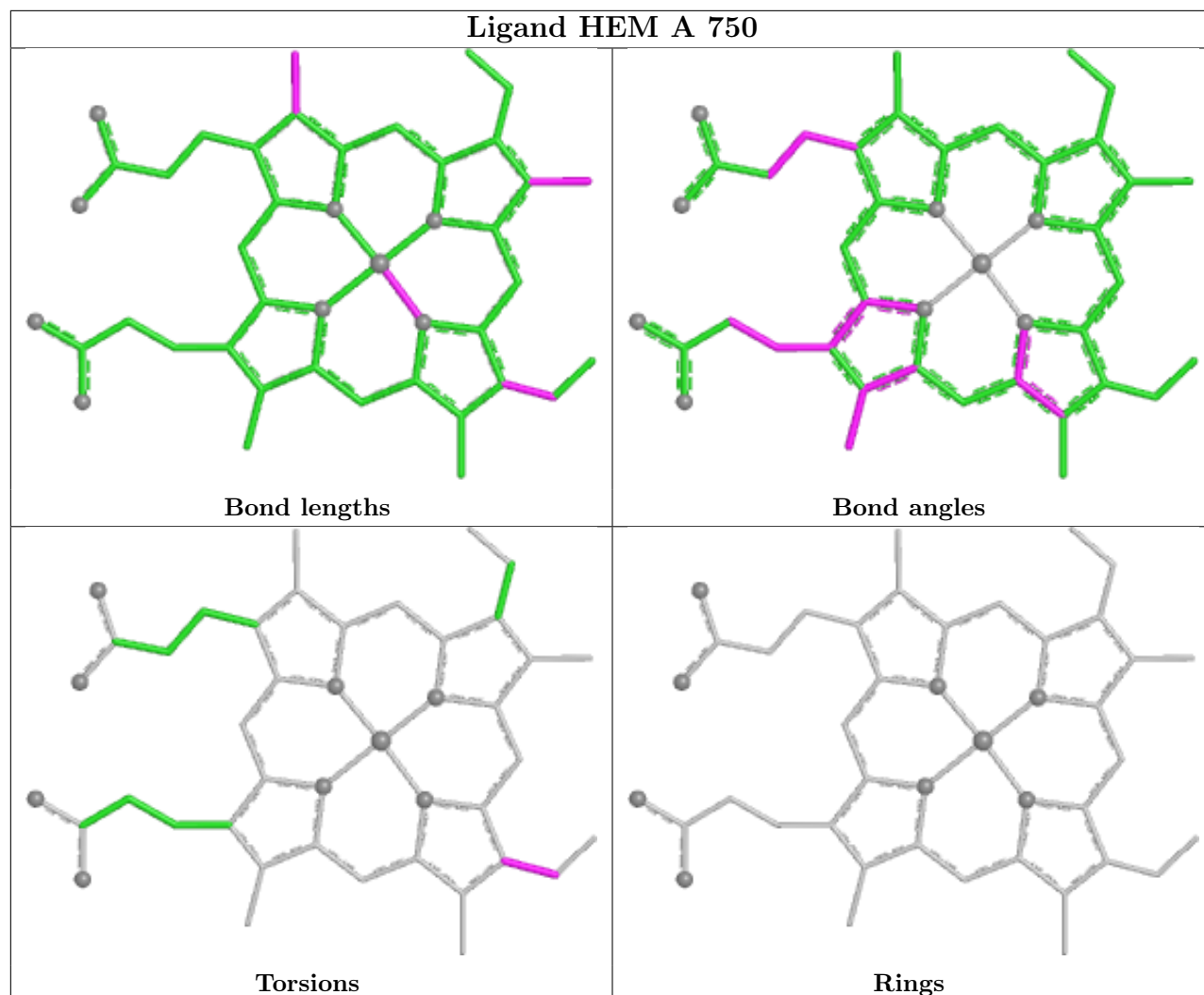
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 DP2 B 793



Ligand HEM B 750





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/421 (96%)	0.75	39 (9%) 13 15	23, 38, 62, 77	2 (0%)
1	B	410/421 (97%)	0.30	17 (4%) 41 48	22, 33, 54, 70	2 (0%)
All	All	817/842 (97%)	0.52	56 (6%) 23 26	22, 36, 59, 77	4 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	PHE	5.1
1	A	715	VAL	4.4
1	A	716	TRP	4.2
1	A	486	LYS	4.1
1	B	352	ASP	4.1
1	A	355	PHE	4.0
1	B	350	THR	3.8
1	A	338	PRO	3.6
1	B	321	THR	3.4
1	A	321	THR	3.4
1	A	504	ILE	3.4
1	A	551	PHE	3.4
1	A	303	VAL	3.3
1	B	348	VAL	3.3
1	A	506	ILE	3.2
1	B	354	LEU	3.1
1	A	493	LEU	3.0
1	A	330	ILE	2.9
1	A	552	ASP	2.9
1	B	392	SER	2.9
1	A	310	VAL	2.8
1	A	373	GLY	2.8
1	B	338	PRO	2.8
1	A	490	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	320	SER	2.7
1	A	553	TRP	2.6
1	A	512	ALA	2.6
1	B	389	GLU	2.6
1	B	611	ALA	2.6
1	B	355	PHE	2.6
1	A	301	LEU	2.6
1	A	485	TYR	2.5
1	A	616	LEU	2.5
1	B	353	GLN	2.5
1	A	513	PRO	2.5
1	A	510	TRP	2.5
1	A	311	VAL	2.5
1	B	300	PHE	2.5
1	A	319	LYS	2.5
1	A	470	HIS	2.4
1	A	667	ARG	2.4
1	A	488	PRO	2.3
1	B	619	ARG	2.3
1	A	711	TRP	2.3
1	B	667	ARG	2.2
1	A	318	LEU	2.2
1	A	322	LEU	2.2
1	B	616	LEU	2.2
1	B	308	THR	2.1
1	A	712	ASN	2.1
1	A	392	SER	2.1
1	A	384	VAL	2.1
1	A	666	TYR	2.0
1	B	303	VAL	2.0
1	A	487	GLN	2.0
1	A	499	VAL	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 ⓘ

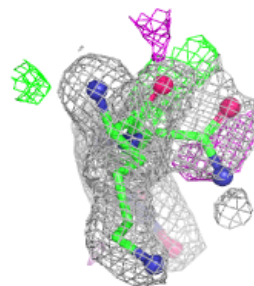
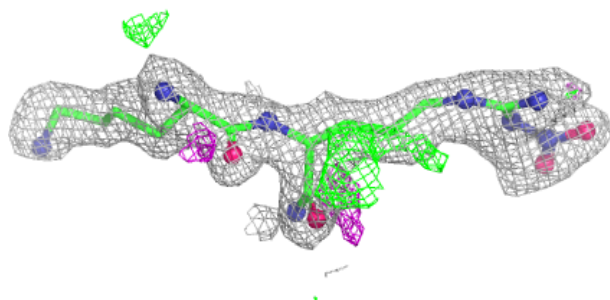
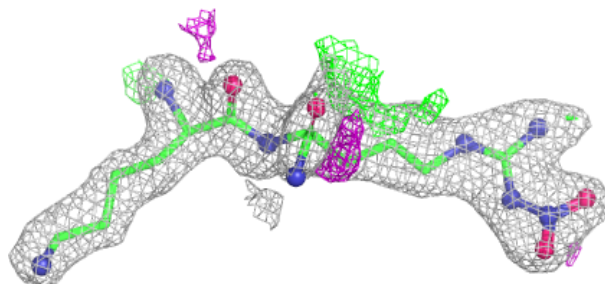
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MTL	A	870	12/12	0.78	0.12	46,50,52,52	0
2	MTL	B	871	12/12	0.81	0.12	45,49,50,50	0
7	DP2	A	792	24/24	0.84	0.12	33,39,42,43	0
7	DP2	B	793	24/24	0.88	0.10	29,39,42,43	0
3	ACT	A	860	4/4	0.89	0.15	57,58,58,58	0
3	ACT	B	861	4/4	0.95	0.09	38,38,39,39	0
6	H4B	B	761	17/17	0.95	0.06	24,25,27,28	0
6	H4B	A	760	17/17	0.97	0.05	23,25,27,28	0
5	HEM	A	750	43/43	0.97	0.07	23,26,27,28	0
5	HEM	B	750	43/43	0.98	0.06	22,23,26,28	0
4	ZN	A	900	1/1	0.99	0.02	33,33,33,33	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.

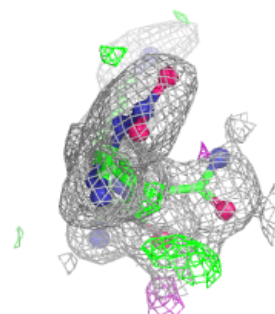
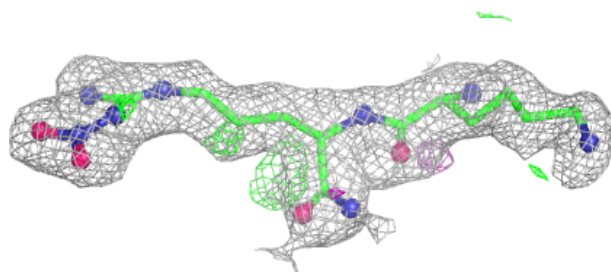
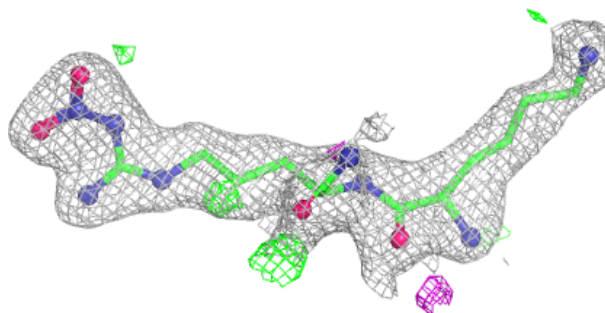
Electron density around DP2 A 792:

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



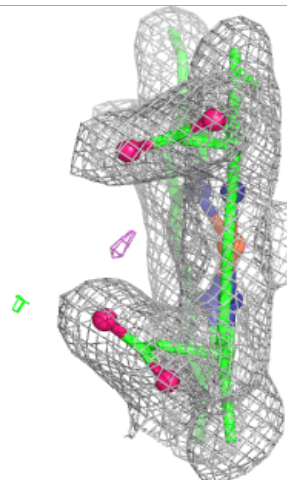
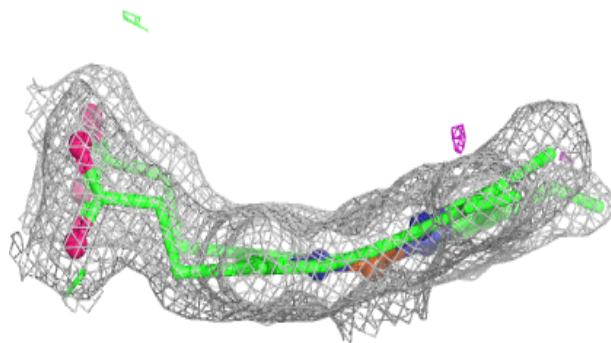
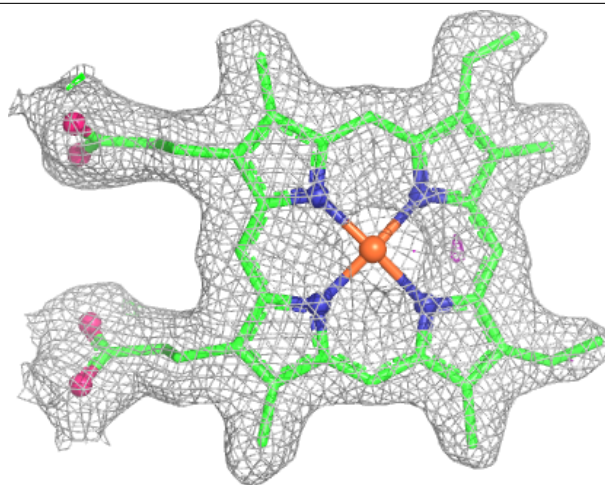
Electron density around DP2 B 793:

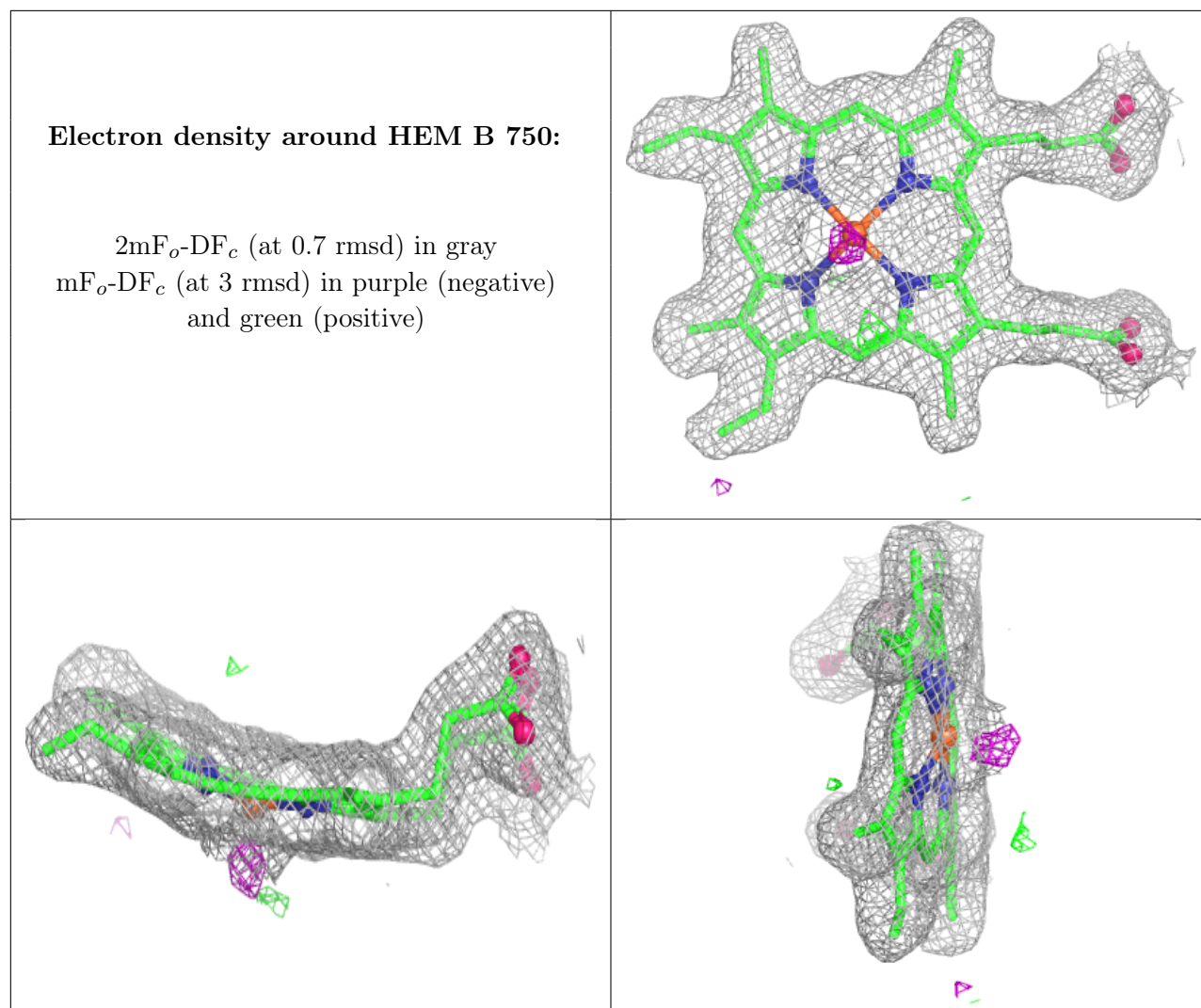
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 750:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.