



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:23 PM UTC

PDB ID : 1P6K / pdb_00001p6k
Title : Rat neuronal NOS D597N mutant heme domain with L-N(omega)-nitroarginine-2,4-L-diaminobutyric amide bound
Authors : Flinspach, M.L.; Li, H.; Jamal, J.; Yang, W.; Huang, H.; Hah, J.-M.; Gomez-Vidal, J.A.; Litzinger, E.A.; Silverman, R.B.; Poulos, T.L.
Deposited on : 2003-04-29
Resolution : 1.78 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

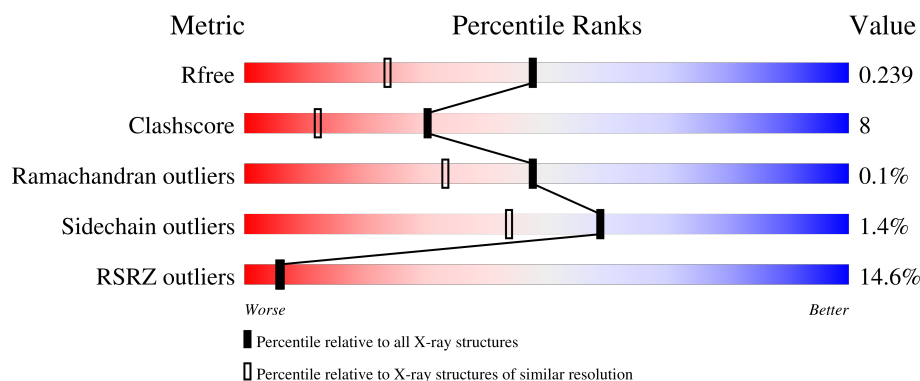
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	21% 73% 22% ..
1	B	421	7% 81% 16% ..

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7451 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.

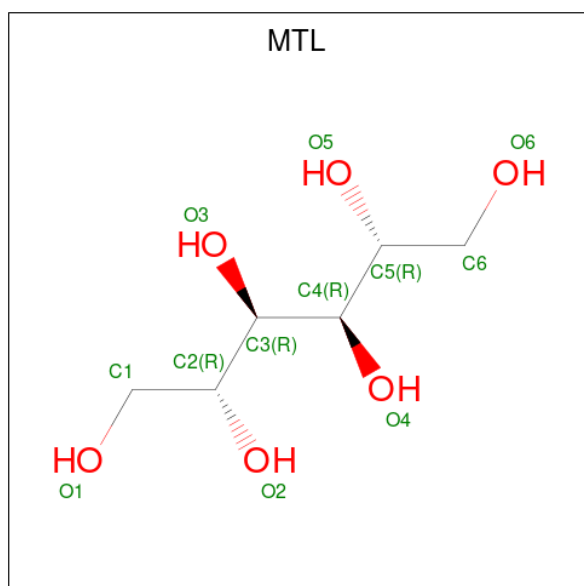
- Molecule 1 is a protein called Nitric-oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	6	0
			3324	2124	570	608	22			
1	B	410	Total	C	N	O	S	0	9	0
			3357	2143	577	614	23			

There are 2 discrepancies between the modelled and reference sequences:

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

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



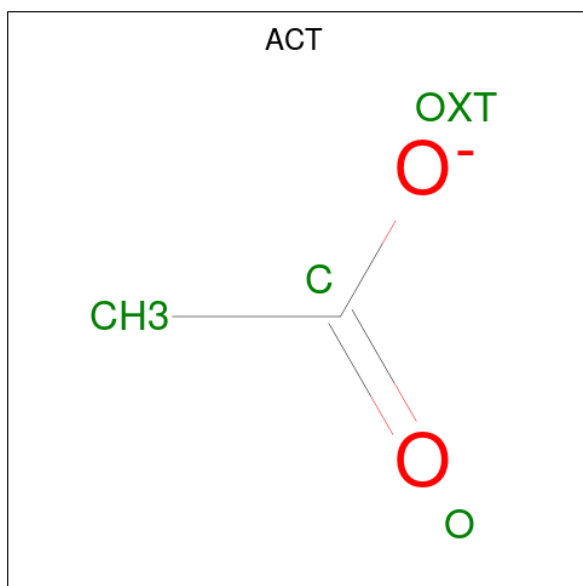
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).

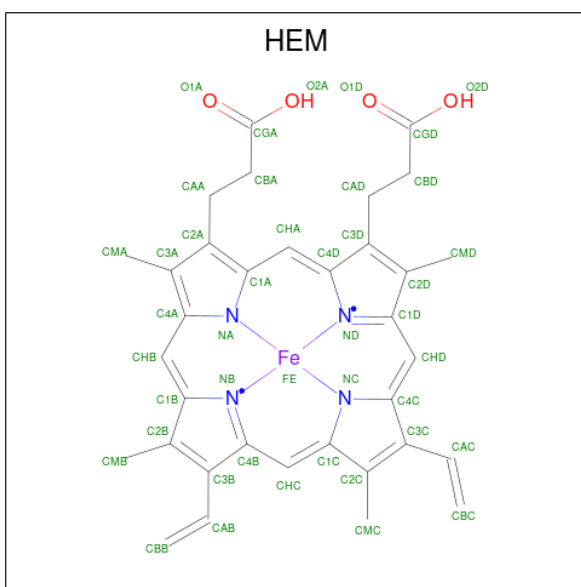


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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

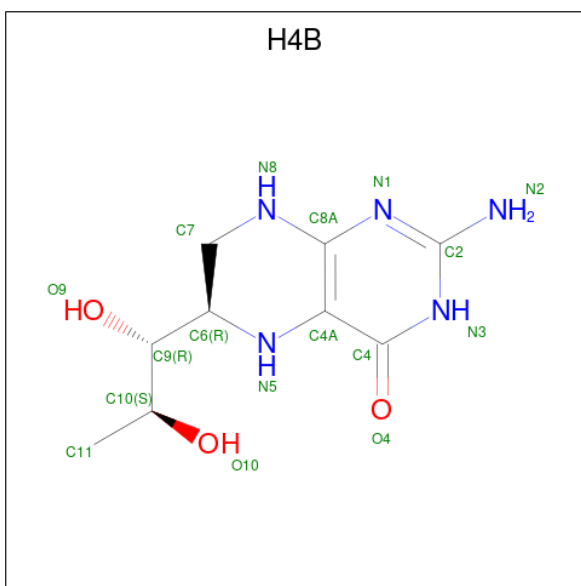
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



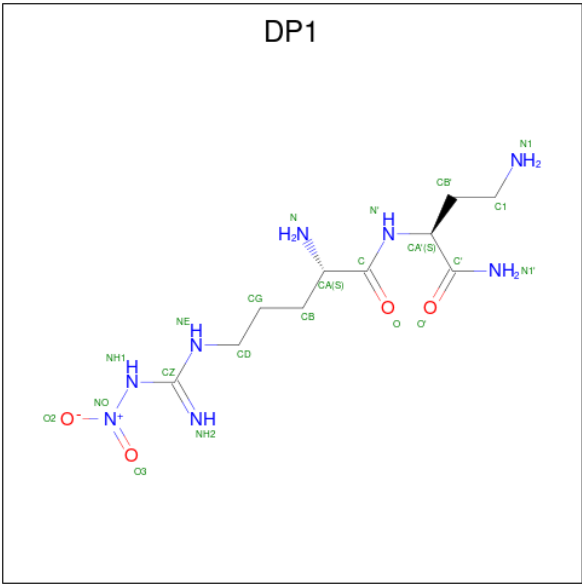
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



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

- Molecule 7 is L-N(OMEGA)-NITROARGININE-2,4-L-DIAMINO BUTYRIC AMIDE (CCD ID: DP1) (formula: C₁₀H₂₂N₈O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			22	10	8	4		
7	B	1	Total	C	N	O	0	0
			22	10	8	4		

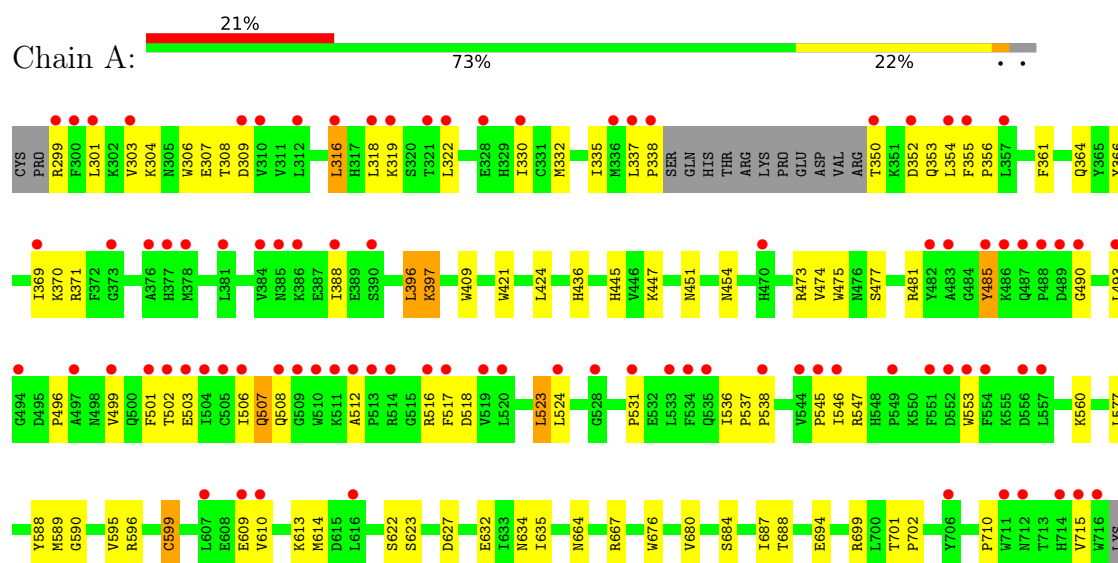
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	259	Total	O	0	0
			259	259		
8	B	314	Total	O	0	0
			314	314		

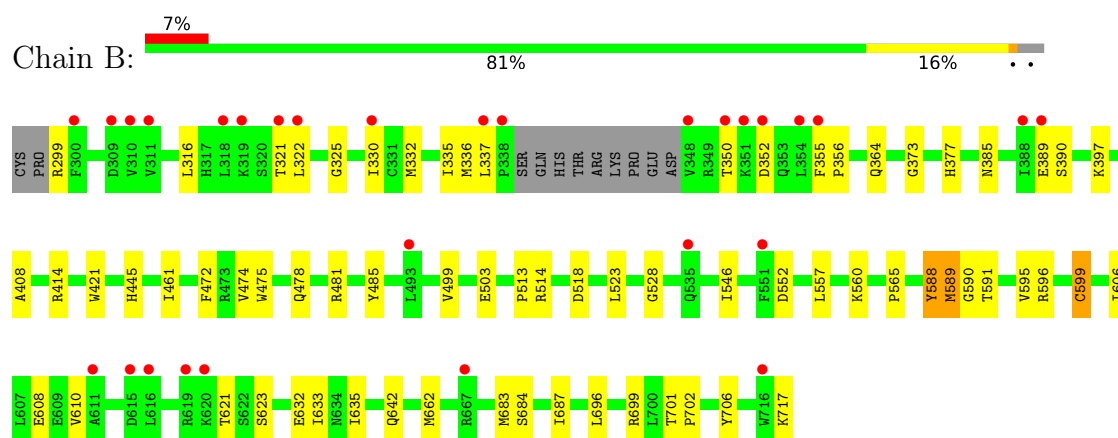
3 Residue-property plots [i](#)

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	51.77Å 109.74Å 164.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 1.78 49.38 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.38-1.78) 99.0 (49.38-1.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.250 0.214 , 0.239	Depositor DCC
R_{free} test set	5019 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.9	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	0.96	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% 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, ZN, MTL, HEM, H4B, DP1

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	0.46	0/3447	0.95	14/4675 (0.3%)
1	B	0.51	0/3495	0.98	14/4736 (0.3%)
All	All	0.49	0/6942	0.96	28/9411 (0.3%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-8.16	95.93	109.24
1	A	589	MET	N-CA-C	-8.01	96.18	109.24
1	A	354	LEU	N-CA-C	7.64	119.39	111.14
1	B	408	ALA	N-CA-C	-6.68	104.00	111.28
1	B	474	VAL	N-CA-C	-6.61	98.34	107.99
1	A	596	ARG	N-CA-C	6.59	118.35	111.03
1	B	421	TRP	N-CA-C	6.59	119.31	111.33
1	B	623	SER	N-CA-C	-6.56	105.25	113.18
1	A	588	TYR	N-CA-C	6.22	119.69	110.48
1	B	596	ARG	N-CA-C	6.02	119.01	111.24
1	A	474	VAL	N-CA-C	-5.92	98.61	107.37
1	A	623	SER	N-CA-C	-5.90	106.04	113.18
1	B	588	TYR	N-CA-C	5.89	119.20	110.48
1	A	599	CYS	N-CA-C	5.77	120.48	113.38
1	B	461	ILE	N-CA-C	5.72	115.84	107.37
1	B	590	GLY	N-CA-C	5.72	119.81	112.83
1	A	490	GLY	N-CA-C	-5.68	106.69	114.64
1	B	557	LEU	N-CA-C	-5.65	106.23	113.01
1	A	688	THR	N-CA-C	-5.54	102.48	110.40
1	A	397	LYS	N-CA-C	-5.51	103.12	110.55
1	B	390	SER	N-CA-C	5.48	117.34	111.36
1	A	590	GLY	N-CA-C	5.42	119.19	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	B	397	LYS	N-CA-C	-5.33	102.58	110.48
1	A	635	ILE	N-CA-C	-5.12	105.55	110.72
1	A	424	LEU	N-CA-C	5.10	117.69	110.10
1	A	546	ILE	N-CA-C	5.09	116.01	108.23
1	B	472	PHE	N-CA-C	-5.08	100.95	109.24
1	B	599	CYS	N-CA-C	5.03	120.25	113.72

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	3324	0	3237	72	0
1	B	3357	0	3279	44	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	4	0
5	B	43	0	30	0	0
6	A	17	0	15	0	0
6	B	17	0	15	0	0
7	A	22	0	21	2	0
7	B	22	0	21	1	0
8	A	259	0	0	8	0
8	B	314	0	0	6	0
All	All	7451	0	6682	114	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 8.

All (114) 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:373:GLY:H	1:B:377:HIS:HD2	1.11	0.92
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.51	0.91
1:A:396:LEU:HD22	1:A:577:LEU:HD12	1.54	0.86
1:A:350:THR:HB	1:A:353:GLN:HG3	1.62	0.82
1:B:373:GLY:H	1:B:377:HIS:CD2	2.01	0.74
1:A:307:GLU:HG3	8:B:941:HOH:O	1.88	0.74
1:A:396:LEU:CD2	1:A:577:LEU:HD12	2.21	0.70
1:A:503:GLU:HG3	8:A:1043:HOH:O	1.90	0.70
1:B:350:THR:HG22	1:B:352:ASP:H	1.55	0.70
1:A:350:THR:HG22	1:A:352:ASP:H	1.57	0.69
1:A:506:ILE:C	1:A:508:GLN:H	2.02	0.68
1:A:506:ILE:O	1:A:508:GLN:N	2.27	0.67
1:A:609:GLU:HG3	8:A:995:HOH:O	1.95	0.66
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.22	0.65
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.79	0.65
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.81	0.61
1:A:299:ARG:HA	8:A:1045:HOH:O	2.00	0.61
1:A:502:THR:O	1:A:506:ILE:HG12	2.02	0.60
1:A:361:PHE:O	1:A:364:GLN:HG2	2.02	0.59
1:B:355:PHE:N	1:B:356:PRO:HD2	2.18	0.59
1:B:621:THR:HG22	8:B:1165:HOH:O	2.03	0.59
1:A:545:PRO:HD3	8:A:1080:HOH:O	2.03	0.59
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.85	0.59
1:A:304:LYS:O	1:A:694:GLU:HG3	2.03	0.58
1:A:506:ILE:C	1:A:508:GLN:N	2.60	0.58
1:A:350:THR:HB	1:A:353:GLN:CG	2.33	0.57
1:A:614:MET:CE	1:A:632:GLU:HG3	2.34	0.57
1:A:664:ASN:OD1	1:A:667:ARG:NH2	2.38	0.56
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.89	0.55
1:A:481[A]:ARG:NH2	7:A:790:DP1:O	2.40	0.55
1:A:306:TRP:NE1	1:B:336[B]:MET:HG3	2.22	0.55
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.23	0.54
5:A:750:HEM:HMC1	5:A:750:HEM:HBC2	1.89	0.54
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.38	0.54
1:B:336[A]:MET:HG3	1:B:337:LEU:CD2	2.38	0.54
1:B:478:GLN:HB2	1:B:481[A]:ARG:HG3	1.90	0.53
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.24	0.52
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.91	0.52
1:A:370:LYS:C	1:A:371:ARG:HG2	2.34	0.52
1:A:332:MET:HE3	1:A:338:PRO:HB3	1.91	0.52
1:A:536:ILE:O	1:A:537:PRO:C	2.51	0.51
1:B:481[A]:ARG:NH2	7:B:791:DP1:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.45	0.51
1:A:477[B]:SER:OG	1:A:481[B]:ARG:HD2	2.10	0.50
1:B:325:GLY:O	1:B:332:MET:HE2	2.11	0.50
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.27	0.50
1:A:396:LEU:HD22	1:A:577:LEU:CD1	2.36	0.50
1:A:701:THR:HA	1:A:702:PRO:C	2.37	0.50
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.94	0.49
1:B:608:GLU:HG3	8:B:989:HOH:O	2.11	0.49
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.94	0.49
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.94	0.49
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.94	0.49
1:A:303:VAL:CG1	1:A:694:GLU:O	2.61	0.49
1:B:364:GLN:NE2	8:B:1140:HOH:O	2.46	0.48
1:A:355:PHE:N	1:A:356:PRO:HD2	2.28	0.48
1:A:501:PHE:HB2	2:A:870:MTL:H61	1.95	0.48
1:A:595:VAL:HG23	1:A:634:ASN:HD21	1.79	0.48
1:A:701:THR:HG23	8:A:994:HOH:O	2.13	0.48
1:A:516:ARG:HG2	1:A:517:PHE:CE1	2.48	0.48
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.43	0.48
1:A:299:ARG:HE	1:A:318:LEU:HD22	1.79	0.47
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.43	0.47
1:A:303:VAL:HG11	1:A:694:GLU:O	2.14	0.47
1:A:451:ASN:HB3	1:A:454:ASN:O	2.15	0.47
1:B:336[A]:MET:HG3	1:B:337:LEU:HD23	1.97	0.47
1:B:595:VAL:O	1:B:599:CYS:HB2	2.15	0.47
1:B:701:THR:HA	1:B:702:PRO:C	2.40	0.47
1:A:553:TRP:CE3	1:A:613:LYS:HD3	2.50	0.47
1:B:499:VAL:O	1:B:503:GLU:HG3	2.16	0.46
1:A:335:ILE:HB	1:A:338:PRO:HG3	1.97	0.46
1:A:316:LEU:HD23	1:A:319:LYS:HD2	1.97	0.46
1:A:485:TYR:OH	1:A:518:ASP:OD2	2.34	0.46
1:A:436:HIS:HB2	8:A:1007:HOH:O	2.15	0.45
1:A:507:GLN:O	1:A:507:GLN:HG2	2.17	0.45
1:B:589:MET:HE3	1:B:591:THR:OG1	2.17	0.45
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.52	0.45
1:A:715:VAL:O	1:A:715:VAL:HG23	2.16	0.45
1:B:445:HIS:C	1:B:445:HIS:CD2	2.95	0.45
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.99	0.45
1:A:447:LYS:HD2	8:A:1145:HOH:O	2.17	0.45
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.47	0.44
1:B:606:ILE:HD11	1:B:633:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.47	0.44
1:A:445:HIS:CD2	1:A:445:HIS:C	2.96	0.44
1:A:524:LEU:O	1:A:531:PRO:HA	2.18	0.44
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.52	0.44
1:B:478:GLN:HB2	1:B:481[B]:ARG:CG	2.47	0.43
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.54	0.43
1:B:528:GLY:O	1:B:717:LYS:HE2	2.19	0.43
1:B:565:PRO:HB3	1:B:588:TYR:CZ	2.54	0.42
1:B:321:THR:HG21	8:B:1063:HOH:O	2.19	0.42
1:A:308:THR:O	1:A:309:ASP:HB2	2.19	0.42
5:A:750:HEM:HBC2	5:A:750:HEM:CMC	2.49	0.42
1:A:684:SER:HB3	1:A:687:ILE:HG12	2.00	0.42
1:A:366:TYR:HA	1:A:369:ILE:HG12	2.02	0.42
1:B:299:ARG:HB3	1:B:299:ARG:HH11	1.85	0.42
1:A:622:SER:CB	1:B:642:GLN:HE22	2.33	0.42
5:A:750:HEM:HBB2	5:A:750:HEM:HHC	2.00	0.42
1:A:517:PHE:HB2	1:A:560:LYS:HE2	2.01	0.42
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.01	0.42
5:A:750:HEM:O2A	7:A:790:DP1:HA	2.19	0.42
1:B:632:GLU:HA	1:B:635:ILE:HD12	2.01	0.41
1:A:595:VAL:O	1:A:599:CYS:HB2	2.20	0.41
1:A:397:LYS:NZ	8:A:1109:HOH:O	2.52	0.41
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.56	0.41
1:A:330:ILE:HD11	1:B:696:LEU:HB3	2.02	0.41
1:A:627:ASP:OD2	1:B:683:MET:HE2	2.21	0.41
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.86	0.41
1:A:610:VAL:O	1:A:614:MET:HG3	2.21	0.40
1:B:355:PHE:N	1:B:356:PRO:CD	2.84	0.40
1:B:414:ARG:NH1	1:B:706:TYR:OH	2.53	0.40
1:B:662:MET:HE3	8:B:924:HOH:O	2.21	0.40
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.56	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	409/421 (97%)	388 (95%)	20 (5%)	1 (0%)	43	29
1	B	415/421 (99%)	404 (97%)	11 (3%)	0	100	100
All	All	824/842 (98%)	792 (96%)	31 (4%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	GLN

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	369/377 (98%)	362 (98%)	7 (2%)	50	32
1	B	375/377 (100%)	372 (99%)	3 (1%)	73	63
All	All	744/754 (99%)	734 (99%)	10 (1%)	59	46

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	337	LEU
1	A	396	LEU
1	A	485	TYR
1	A	493	LEU
1	A	523	LEU
1	A	538	PRO
1	B	316	LEU
1	B	389	GLU
1	B	552	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	451	ASN
1	A	454	ASN
1	A	500	GLN
1	A	508	GLN
1	A	634	ASN
1	A	697	ASN
1	B	364	GLN
1	B	377	HIS
1	B	385	ASN
1	B	425	GLN
1	B	451	ASN
1	B	454	ASN
1	B	507	GLN
1	B	527	ASN
1	B	535	GLN
1	B	634	ASN
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 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	$\# Z > 2$
5	HEM	A	750	1	50,50,50	1.34	7 (14%)	67,82,82	1.25	8 (11%)
3	ACT	A	860	-	3,3,3	0.90	0	3,3,3	0.81	0
2	MTL	B	871	-	11,11,11	0.92	0	14,14,14	0.77	1 (7%)
3	ACT	B	861	-	3,3,3	0.93	0	3,3,3	0.75	0
2	MTL	A	870	-	11,11,11	1.18	1 (9%)	14,14,14	0.74	0
5	HEM	B	750	1	50,50,50	1.10	2 (4%)	67,82,82	1.53	11 (16%)
7	DP1	B	791	-	16,21,21	0.72	0	20,26,26	0.99	0
6	H4B	B	761	-	17,18,18	1.59	2 (11%)	14,26,26	1.82	3 (21%)
6	H4B	A	760	-	17,18,18	1.65	3 (17%)	14,26,26	2.04	4 (28%)
7	DP1	A	790	-	16,21,21	0.71	0	20,26,26	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	750	1	-	0/14/54/54	-
2	MTL	B	871	-	-	0/16/16/16	-
2	MTL	A	870	-	-	1/16/16/16	-
5	HEM	B	750	1	-	1/14/54/54	-
7	DP1	B	791	-	-	5/23/26/26	-
6	H4B	B	761	-	-	0/8/17/17	0/2/2/2
6	H4B	A	760	-	-	0/8/17/17	0/2/2/2
7	DP1	A	790	-	-	4/23/26/26	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	760	H4B	C4A-N5	4.22	1.47	1.37
5	A	750	HEM	FE-NB	3.85	2.06	1.94
6	B	761	H4B	C6-N5	3.83	1.54	1.47
6	A	760	H4B	C6-N5	3.45	1.53	1.47
6	B	761	H4B	C4A-N5	3.28	1.45	1.37
5	A	750	HEM	CAC-C3C	-2.73	1.40	1.47
5	A	750	HEM	CMC-C2C	2.35	1.55	1.50
5	A	750	HEM	C4A-C3A	2.24	1.48	1.43
5	A	750	HEM	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	750	HEM	CMD-C2D	2.14	1.55	1.50
6	A	760	H4B	C4-N3	2.12	1.42	1.38
5	A	750	HEM	C3C-C2C	2.09	1.41	1.37
5	B	750	HEM	O2A-CGA	-2.06	1.24	1.30
5	A	750	HEM	C3B-C4B	2.05	1.48	1.44
2	A	870	MTL	C1-C2	2.05	1.57	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	760	H4B	C2-N1-C8A	5.51	123.08	113.36
6	B	761	H4B	C2-N1-C8A	4.89	121.99	113.36
5	B	750	HEM	C3B-C4B-NB	4.67	112.82	109.47
5	A	750	HEM	CHC-C4B-NB	-3.58	120.57	124.42
5	B	750	HEM	C4B-C3B-C2B	-3.45	104.11	107.28
5	B	750	HEM	C4C-NC-C1C	-3.39	100.29	105.82
5	A	750	HEM	C3B-C4B-NB	3.33	111.86	109.47
5	A	750	HEM	CHD-C4C-NC	-2.96	121.23	124.45
6	A	760	H4B	N3-C2-N1	-2.78	118.23	123.32
6	A	760	H4B	O10-C10-C9	-2.78	105.17	109.77
6	B	761	H4B	N3-C2-N1	-2.77	118.25	123.32
6	B	761	H4B	O10-C10-C9	-2.62	105.43	109.77
5	B	750	HEM	CMC-C2C-C1C	2.57	129.25	124.73
5	B	750	HEM	C2D-C1D-ND	2.52	112.82	109.90
5	A	750	HEM	CAB-C3B-C2B	-2.46	120.42	128.43
5	B	750	HEM	C3B-C2B-C1B	2.36	108.18	106.41
5	B	750	HEM	CAB-C3B-C2B	-2.28	121.03	128.43
6	A	760	H4B	O9-C9-C6	2.25	114.66	109.28
5	B	750	HEM	CAB-C3B-C4B	2.19	134.08	124.39
5	B	750	HEM	CBA-CAA-C2A	-2.19	106.47	112.53
5	B	750	HEM	CHD-C4C-NC	-2.19	122.07	124.45
5	A	750	HEM	C3C-C2C-C1C	-2.16	105.00	107.05
5	B	750	HEM	C4A-CHB-C1B	-2.11	121.27	126.25
5	A	750	HEM	C2A-C1A-NA	2.09	112.47	110.15
2	B	871	MTL	C5-C4-C3	-2.08	109.28	112.48
5	A	750	HEM	CBD-CAD-C3D	-2.03	106.91	112.53
5	A	750	HEM	CAB-C3B-C4B	2.02	133.34	124.39

There are no chirality outliers.

All (11) torsion outliers are listed below:

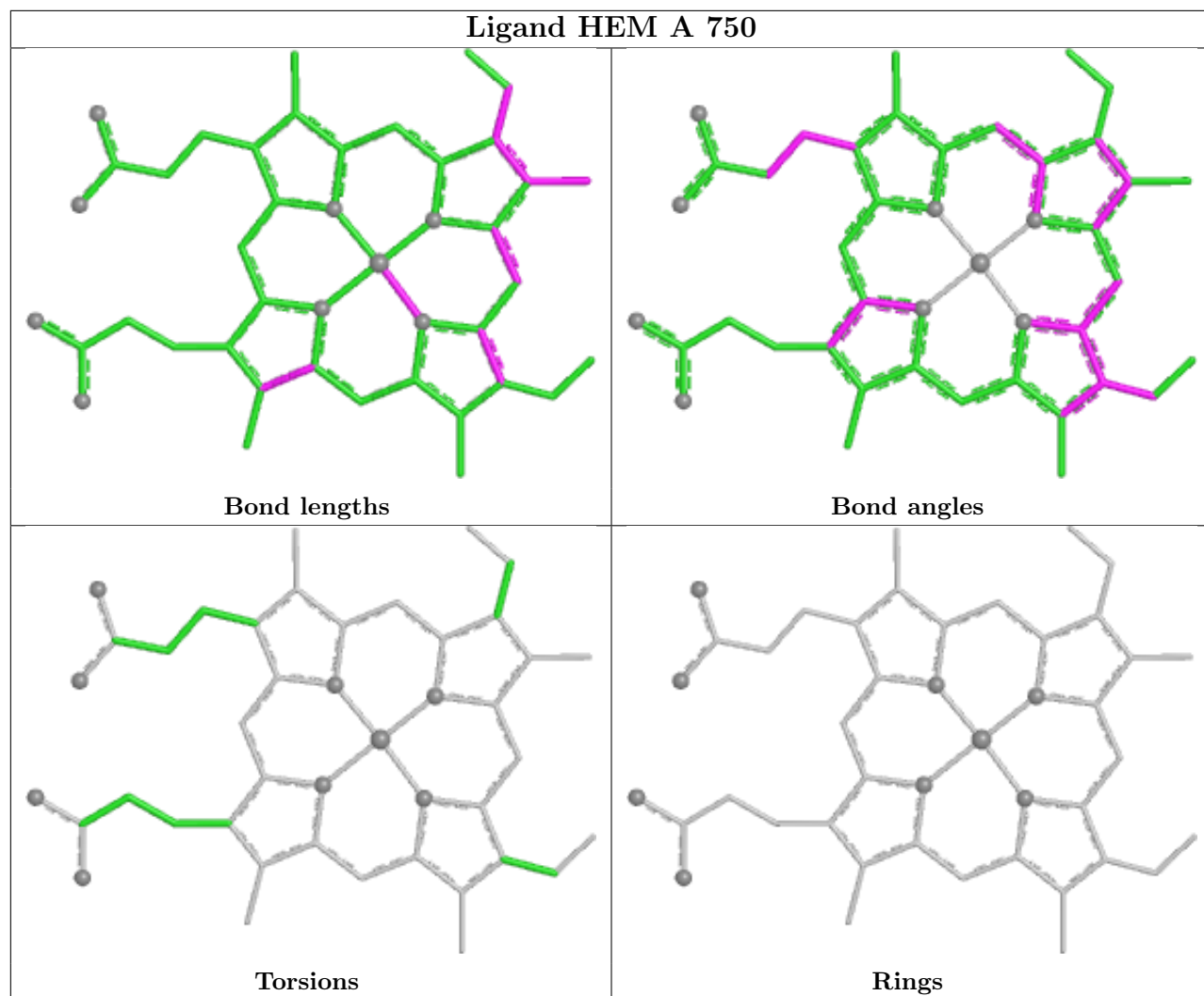
Mol	Chain	Res	Type	Atoms
7	B	791	DP1	O-C-CA-N
7	A	790	DP1	O-C-CA-CB
7	A	790	DP1	N'-C-CA-CB
7	B	791	DP1	N'-C-CA-CB
5	B	750	HEM	C4B-C3B-CAB-CBB
7	B	791	DP1	O-C-CA-CB
7	B	791	DP1	N'-C-CA-N
7	B	791	DP1	CA-CB-CG-CD
7	A	790	DP1	O-C-CA-N
7	A	790	DP1	N'-C-CA-N
2	A	870	MTL	O1-C1-C2-C3

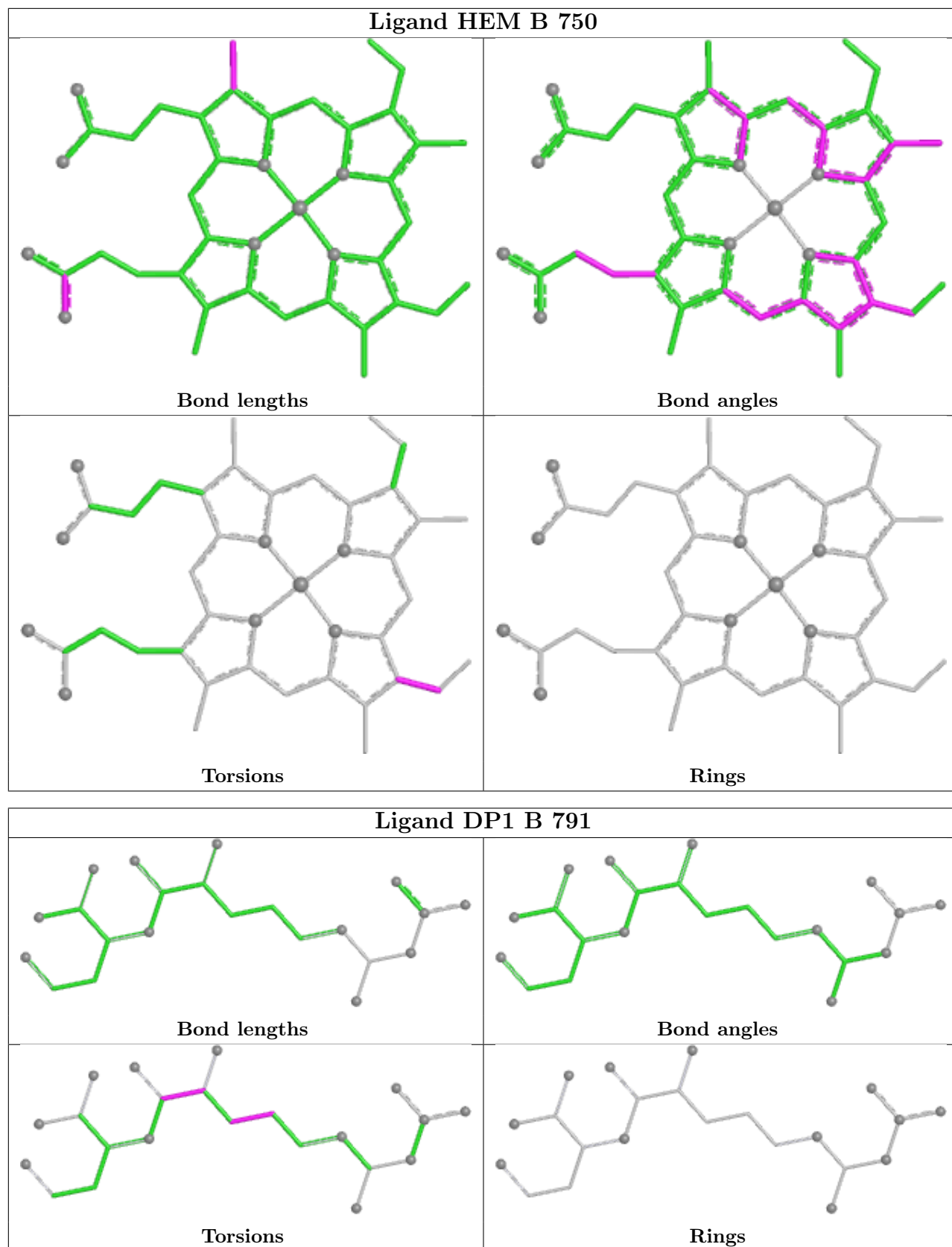
There are no ring outliers.

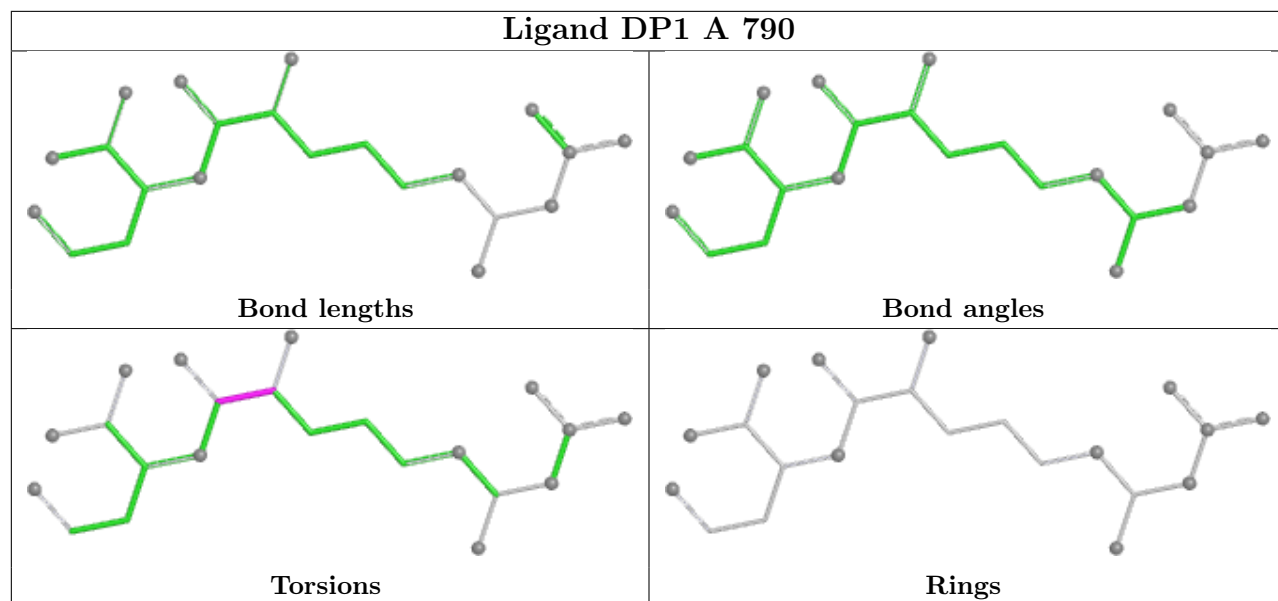
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	750	HEM	4	0
2	A	870	MTL	1	0
7	B	791	DP1	1	0
7	A	790	DP1	2	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

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%)	1.21	90 (22%) 2 2	23, 39, 59, 70	6 (1%)
1	B	410/421 (97%)	0.64	29 (7%) 22 26	18, 32, 50, 66	9 (2%)
All	All	817/842 (97%)	0.92	119 (14%) 6 6	18, 35, 56, 70	15 (1%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	510	TRP	5.1
1	A	300	PHE	5.1
1	A	716	TRP	4.8
1	A	321	THR	4.6
1	A	715	VAL	4.6
1	A	355	PHE	4.5
1	A	503	GLU	4.4
1	B	338	PRO	4.3
1	A	504	ILE	4.1
1	A	509	GLY	4.0
1	A	299	ARG	4.0
1	A	711	TRP	3.9
1	A	506	ILE	3.8
1	A	533	LEU	3.8
1	A	488	PRO	3.8
1	A	505	CYS	3.7
1	A	303	VAL	3.7
1	B	348	VAL	3.6
1	A	508	GLN	3.6
1	A	554	PHE	3.6
1	A	384	VAL	3.6
1	A	501	PHE	3.5
1	A	551	PHE	3.5
1	A	493	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	381	LEU	3.4
1	B	352	ASP	3.4
1	A	352	ASP	3.3
1	A	557	LEU	3.3
1	B	321	THR	3.3
1	A	549	PRO	3.3
1	B	337	LEU	3.2
1	A	534	PHE	3.2
1	B	350	THR	3.2
1	A	316	LEU	3.2
1	A	322	LEU	3.1
1	A	338	PRO	3.0
1	A	553	TRP	3.0
1	B	354	LEU	3.0
1	A	512	ALA	3.0
1	A	337	LEU	3.0
1	B	300	PHE	3.0
1	A	330	ILE	2.9
1	A	609	GLU	2.9
1	A	310	VAL	2.9
1	A	499	VAL	2.9
1	A	517	PHE	2.8
1	A	538	PRO	2.8
1	B	322	LEU	2.8
1	A	552	ASP	2.8
1	A	485	TYR	2.7
1	B	667	ARG	2.7
1	A	487	GLN	2.7
1	A	336	MET	2.7
1	A	385	ASN	2.6
1	A	712	ASN	2.6
1	A	357	LEU	2.6
1	A	350	THR	2.6
1	A	319	LYS	2.6
1	A	513	PRO	2.6
1	A	328	GLU	2.6
1	B	389	GLU	2.5
1	A	312	LEU	2.5
1	A	519	VAL	2.5
1	B	611	ALA	2.5
1	B	355	PHE	2.5
1	B	616	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	388	ILE	2.5
1	A	546	ILE	2.5
1	A	514	ARG	2.5
1	A	301	LEU	2.4
1	B	309	ASP	2.4
1	A	386	LYS	2.4
1	B	493	LEU	2.4
1	A	706	TYR	2.4
1	B	330	ILE	2.4
1	B	318	LEU	2.4
1	A	483	ALA	2.4
1	A	610	VAL	2.4
1	B	535	GLN	2.3
1	A	373	GLY	2.3
1	A	494	GLY	2.3
1	A	376	ALA	2.3
1	A	490	GLY	2.3
1	A	556	ASP	2.3
1	A	502	THR	2.2
1	A	489	ASP	2.2
1	B	310	VAL	2.2
1	B	311	VAL	2.2
1	A	545	PRO	2.2
1	A	486	LYS	2.2
1	A	616	LEU	2.2
1	B	388	ILE	2.2
1	A	318	LEU	2.2
1	A	524	LEU	2.2
1	B	619	ARG	2.2
1	B	551	PHE	2.2
1	A	511	LYS	2.2
1	A	531	PRO	2.2
1	A	354	LEU	2.1
1	A	607	LEU	2.1
1	B	319	LYS	2.1
1	B	351	LYS	2.1
1	B	620	LYS	2.1
1	A	378	MET	2.1
1	A	482	TYR	2.1
1	A	497	ALA	2.1
1	A	544	VAL	2.1
1	A	309	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	535	GLN	2.1
1	B	716	TRP	2.1
1	A	369	ILE	2.1
1	A	377	HIS	2.1
1	A	714	HIS	2.1
1	A	390	SER	2.1
1	A	520	LEU	2.1
1	A	528	GLY	2.0
1	B	615	ASP	2.0
1	A	470	HIS	2.0
1	A	516	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

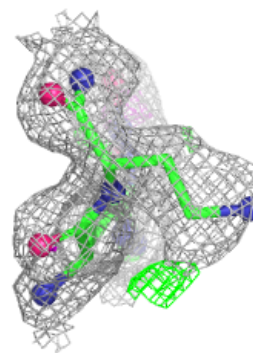
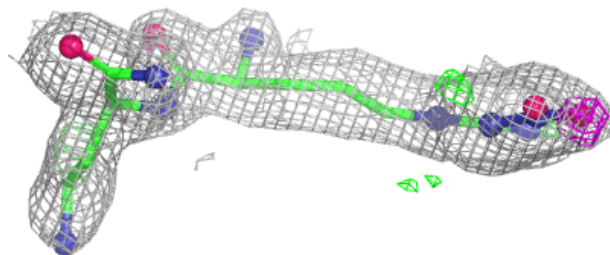
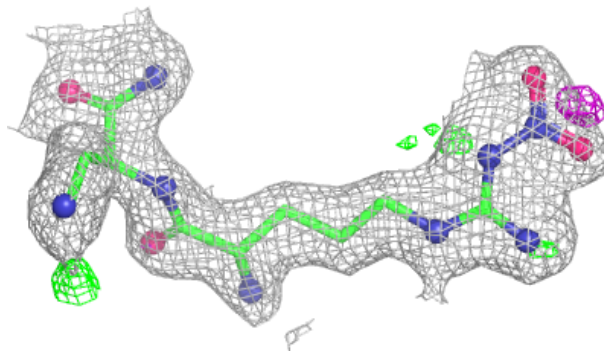
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MTL	A	870	12/12	0.78	0.13	51,51,52,52	0
7	DP1	A	790	22/22	0.84	0.13	39,43,45,45	0
7	DP1	B	791	22/22	0.84	0.14	41,43,44,44	0
2	MTL	B	871	12/12	0.90	0.10	45,46,47,47	0
3	ACT	A	860	4/4	0.91	0.16	60,60,60,60	0
3	ACT	B	861	4/4	0.93	0.12	45,45,45,45	0
6	H4B	A	760	17/17	0.95	0.06	24,25,26,26	0
6	H4B	B	761	17/17	0.96	0.06	24,25,27,27	0
5	HEM	A	750	43/43	0.98	0.06	25,26,27,27	0
5	HEM	B	750	43/43	0.98	0.06	23,23,26,28	0
4	ZN	A	900	1/1	0.99	0.03	34,34,34,34	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.

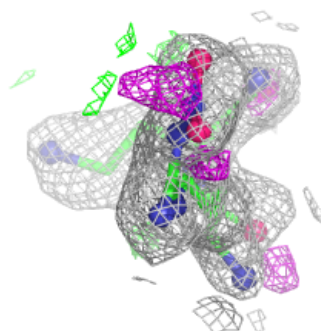
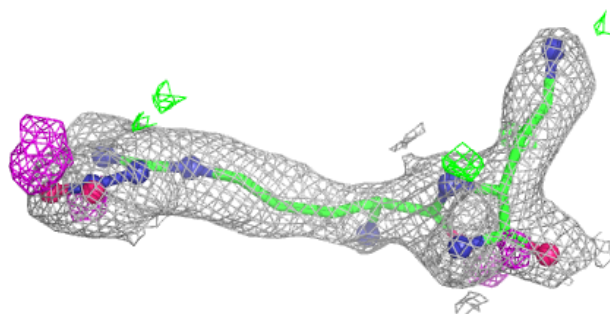
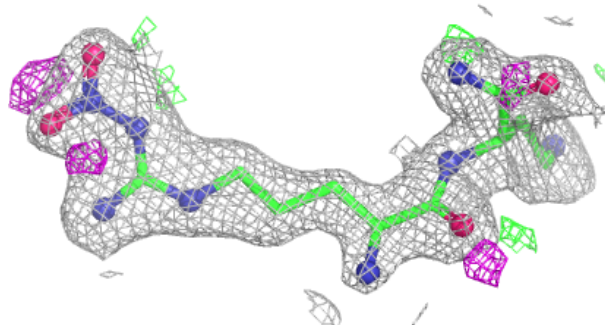
Electron density around DP1 A 790:

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

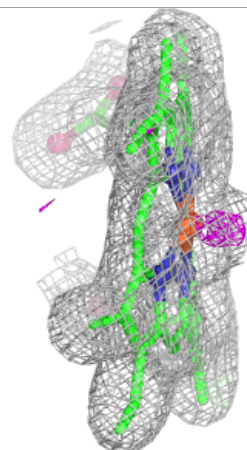
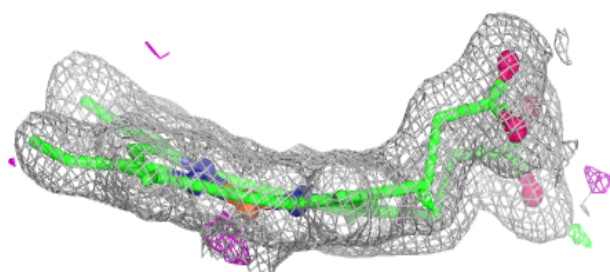
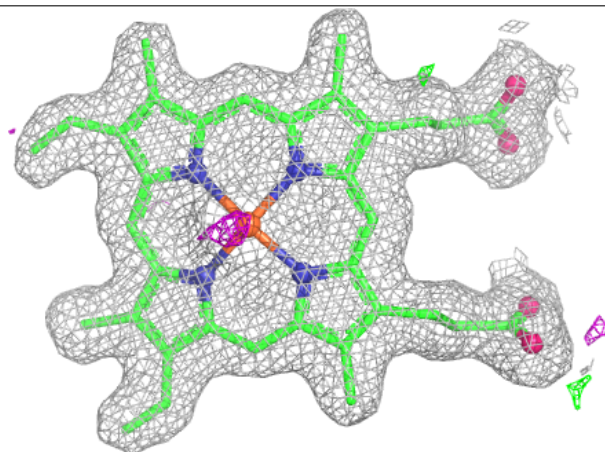


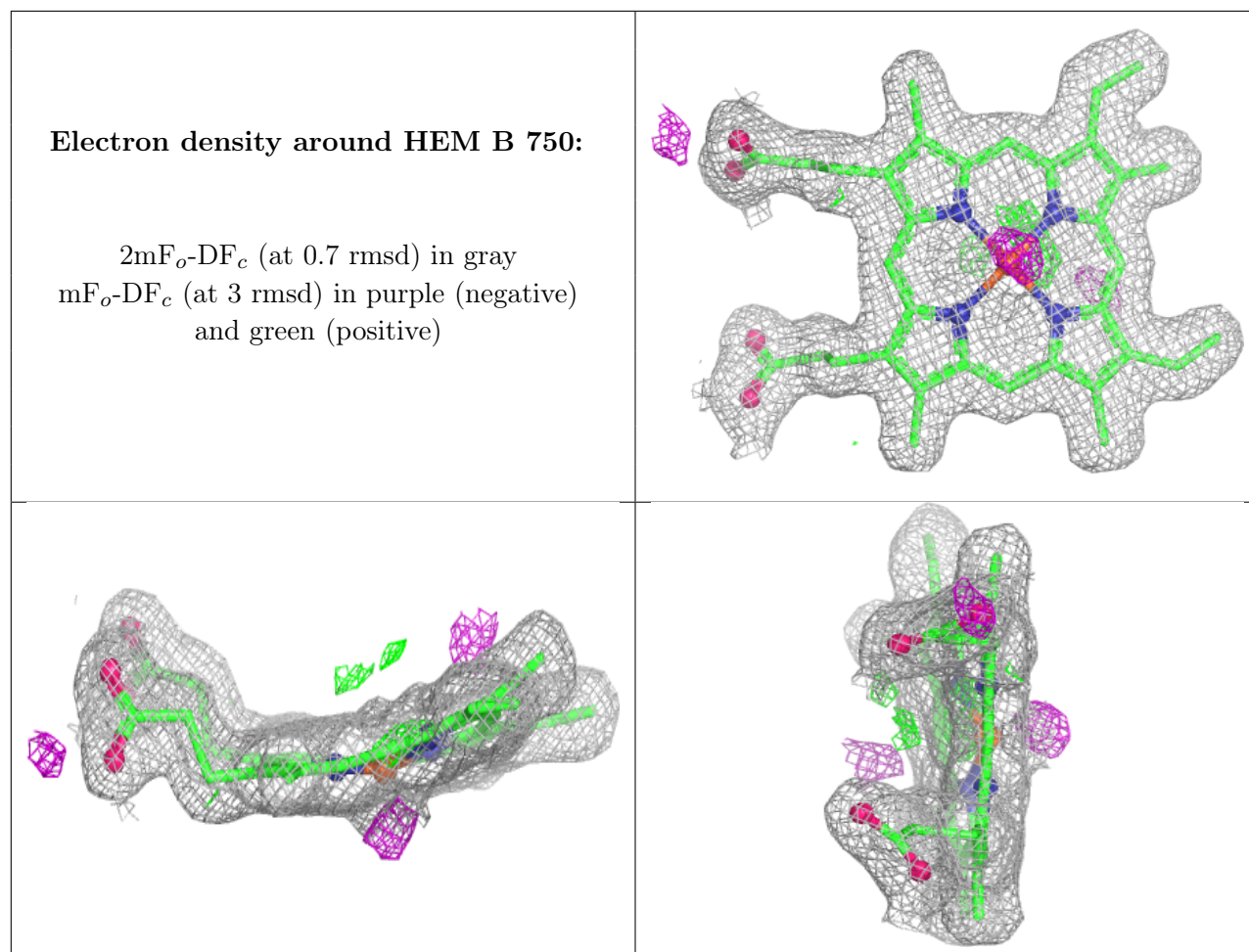
Electron density around DP1 B 791:

$2mF_o-DF_c$ (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.