



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 01:14 AM UTC

PDB ID : 1RS7 / pdb_00001rs7
Title : Rat neuronal NOS heme domain with D-phenylalanine-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

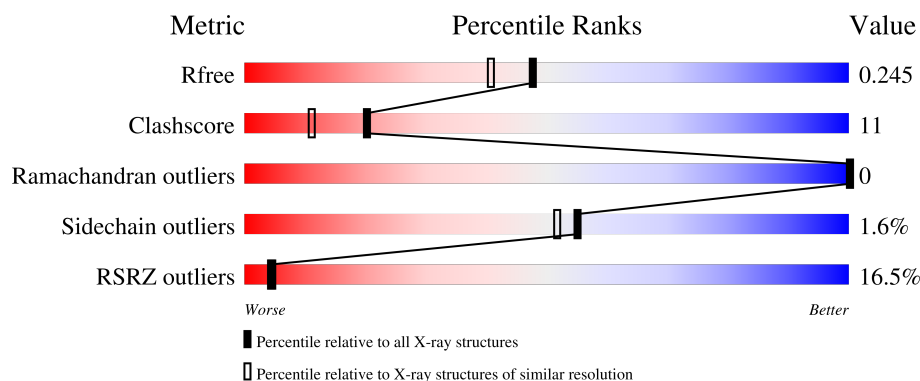
1 Overall quality at a glance

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	24% 67% 27% • •
1	B	421	8% 80% 16% • •

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7408 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
			3313	2121	566	605	21			
1	B	410	Total	C	N	O	S	0	0	0
			3341	2138	573	609	21			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).

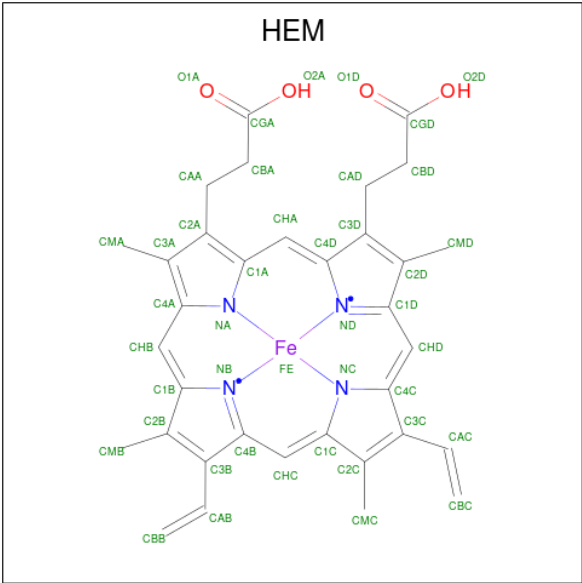


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

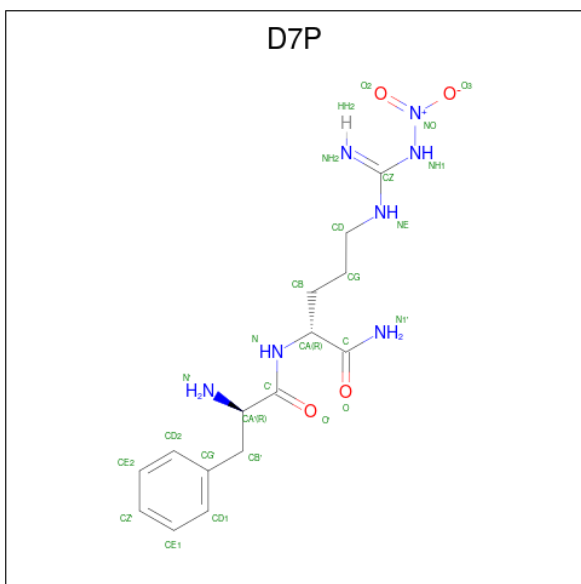
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).





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

- Molecule 6 is D-phenylalanyl-N 5 -(N-nitrocarbamimidoyl)-D-ornithinamide (CCD ID: D7P) (formula: $C_{15}H_{23}N_7O_4$).



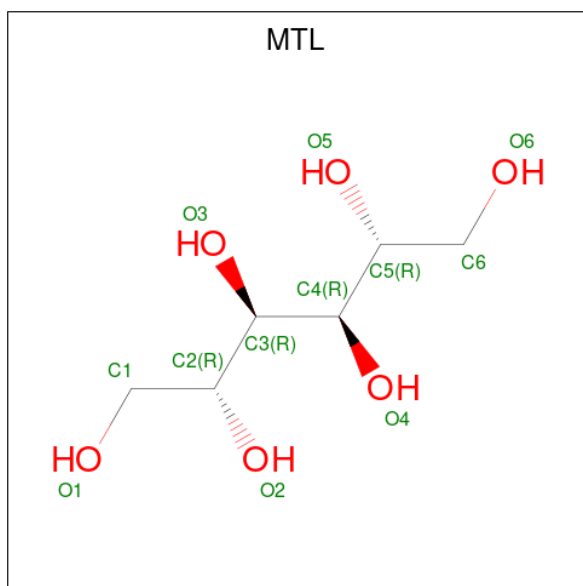
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			26	15	7	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			26	15	7	4		

- Molecule 7 is D-MANNITOL (CCD ID: MTL) (formula: $C_6H_{14}O_6$).



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

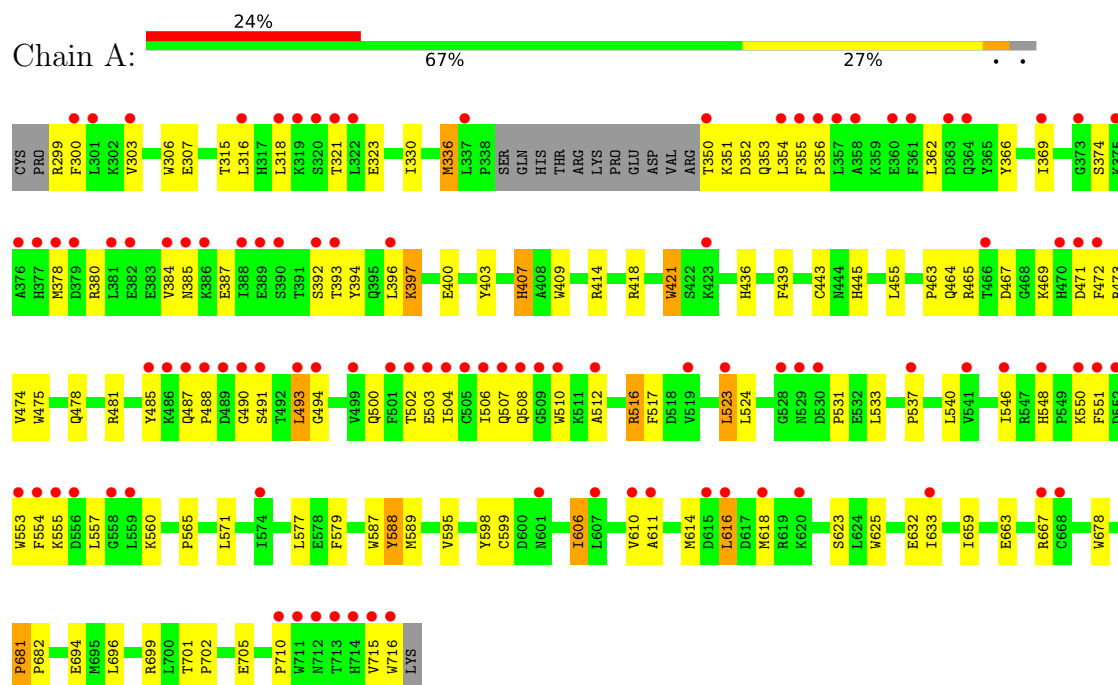
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	257	Total	O	0	0
			257	257		
8	B	304	Total	O	0	0
			304	304		

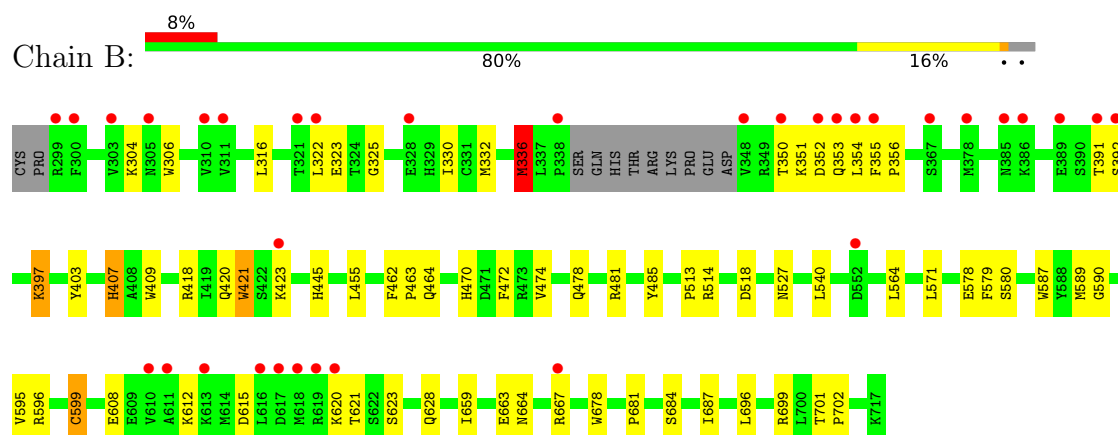
3 Residue-property plots [i](#)

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	52.09Å 110.91Å 165.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.06 – 1.95 39.06 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.2 (39.06-1.95) 91.4 (39.06-1.95)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.50 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.251 0.209 , 0.245	Depositor DCC
R_{free} test set	3221 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7408	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: MTL, ACT, H4B, HEM, D7P, ZN

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	0.55	0/3406	0.98	15/4621 (0.3%)
1	B	0.62	1/3434 (0.0%)	0.99	15/4656 (0.3%)
All	All	0.59	1/6840 (0.0%)	0.98	30/9277 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	MET	SD-CE	-5.17	1.66	1.79

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	421	TRP	N-CA-C	7.94	120.94	111.33
1	B	589	MET	N-CA-C	-7.82	96.50	109.24
1	A	589	MET	N-CA-C	-7.42	97.14	109.24
1	A	681	PRO	CA-C-N	7.29	127.45	119.87
1	A	681	PRO	C-N-CA	7.29	127.45	119.87
1	A	354	LEU	N-CA-C	7.03	118.73	111.14
1	B	407	HIS	CA-CB-CG	-6.98	106.82	113.80
1	A	421	TRP	N-CA-C	6.92	119.70	111.33
1	B	354	LEU	N-CA-C	6.79	118.47	111.14
1	A	407	HIS	CA-CB-CG	-6.31	107.49	113.80
1	A	397	LYS	N-CA-C	-6.13	101.40	110.48
1	B	418	ARG	N-CA-C	6.07	120.29	113.01
1	A	599	CYS	N-CA-C	5.97	121.48	113.72
1	A	418	ARG	N-CA-C	5.95	120.15	113.01
1	A	557	LEU	N-CA-C	-5.86	105.39	112.54
1	B	599	CYS	N-CA-C	5.82	121.29	113.72
1	B	474	VAL	N-CA-C	-5.76	99.57	107.99
1	B	623	SER	N-CA-C	-5.64	105.89	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	VAL	N-CA-C	-5.57	99.86	107.99
1	B	681	PRO	CA-C-N	5.43	126.15	120.12
1	B	681	PRO	C-N-CA	5.43	126.15	120.12
1	A	623	SER	N-CA-C	-5.37	106.72	113.28
1	B	472	PHE	N-CA-C	-5.31	101.05	109.76
1	A	588	TYR	N-CA-C	5.30	118.33	110.48
1	B	564	LEU	N-CA-C	5.30	118.23	108.69
1	B	397	LYS	N-CA-C	-5.27	103.43	110.55
1	A	490	GLY	N-CA-C	-5.21	107.80	114.37
1	B	590	GLY	N-CA-C	5.18	119.15	112.83
1	B	596	ARG	N-CA-C	5.17	117.70	111.40
1	A	606	ILE	N-CA-C	5.12	117.90	112.83

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	3313	0	3221	106	0
1	B	3341	0	3256	51	0
2	A	4	0	3	1	0
2	B	4	0	3	1	0
3	A	1	0	0	0	0
4	A	43	0	30	2	0
4	B	43	0	30	1	0
5	A	17	0	15	1	0
5	B	17	0	15	1	0
6	A	26	0	24	0	0
6	B	26	0	24	0	0
7	B	12	0	14	0	0
8	A	257	0	0	10	0
8	B	304	0	0	8	0
All	All	7408	0	6635	152	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 (152) 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	1.50	0.94
1:B:699:ARG:HG2	8:B:1175:HOH:O	1.73	0.88
1:A:396:LEU:CD2	1:A:577:LEU:HD12	2.10	0.81
1:A:611:ALA:HB1	1:A:616:LEU:HD11	1.65	0.77
1:B:336:MET:HE1	1:B:678:TRP:CZ2	2.19	0.77
1:A:595:VAL:HG11	1:A:682:PRO:HB2	1.67	0.76
1:A:667:ARG:HD3	8:A:1155:HOH:O	1.87	0.74
1:A:350:THR:HG22	1:A:352:ASP:H	1.52	0.74
1:B:350:THR:HG22	1:B:352:ASP:H	1.53	0.73
1:A:321:THR:HG21	8:A:1014:HOH:O	1.89	0.73
1:B:351:LYS:HE2	1:B:392:SER:OG	1.89	0.72
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.05	0.71
1:B:336:MET:HE1	1:B:678:TRP:HZ2	1.54	0.71
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.75	0.69
1:A:502:THR:O	1:A:506:ILE:HG12	1.93	0.69
1:A:504:ILE:HA	1:A:507:GLN:HG2	1.76	0.67
1:A:350:THR:HB	1:A:353:GLN:HG3	1.77	0.67
1:A:306:TRP:NE1	1:B:336:MET:HG3	2.13	0.64
1:B:391:THR:O	1:B:392:SER:HB2	1.98	0.63
1:A:659:ILE:O	1:A:663:GLU:HG3	1.99	0.62
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.23	0.62
1:A:396:LEU:HD23	1:A:577:LEU:HD12	1.81	0.61
1:B:455:LEU:HD12	1:B:587:TRP:HB3	1.83	0.61
1:B:664:ASN:O	1:B:667:ARG:HG2	2.00	0.61
1:B:323:GLU:O	1:B:699:ARG:HD3	2.01	0.60
1:A:396:LEU:HD21	1:A:577:LEU:HD12	1.84	0.59
1:B:325:GLY:O	1:B:332:MET:HE2	2.03	0.59
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.85	0.58
1:A:350:THR:HB	1:A:353:GLN:CG	2.34	0.57
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.19	0.57
1:A:350:THR:HG22	1:A:352:ASP:N	2.19	0.57
1:A:500:GLN:NE2	8:A:1116:HOH:O	2.38	0.56
1:B:659:ILE:O	1:B:663:GLU:HG3	2.05	0.56
1:A:374:SER:O	1:A:378:MET:HG2	2.06	0.56
1:A:467:ASP:OD1	1:A:469:LYS:HB2	2.06	0.55
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.21	0.55
1:A:611:ALA:CB	1:A:616:LEU:HD11	2.36	0.55
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.88	0.55
1:A:611:ALA:HB1	1:A:616:LEU:CD1	2.36	0.55
1:A:504:ILE:HA	1:A:507:GLN:CG	2.36	0.54
1:A:715:VAL:HG22	8:A:1142:HOH:O	2.08	0.53
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.90	0.53
1:A:351:LYS:HE2	1:A:392:SER:HA	1.90	0.53
1:A:436:HIS:HB2	8:A:994:HOH:O	2.08	0.53
1:A:560:LYS:NZ	8:A:1129:HOH:O	2.41	0.53
1:B:455:LEU:HD12	1:B:587:TRP:CB	2.39	0.53
2:A:860:ACT:H1	4:A:750:HEM:HMB2	1.90	0.52
1:B:608:GLU:HG3	8:B:1052:HOH:O	2.09	0.52
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.91	0.52
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.45	0.52
1:A:396:LEU:HD12	1:A:400:GLU:HB3	1.92	0.52
1:A:614:MET:CE	1:A:632:GLU:HG3	2.41	0.51
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.91	0.51
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.41	0.51
1:A:351:LYS:HE2	1:A:392:SER:CB	2.41	0.50
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.47	0.50
1:A:565:PRO:HB3	1:A:588:TYR:CZ	2.47	0.50
1:A:504:ILE:O	1:A:508:GLN:HB2	2.11	0.50
1:A:336:MET:HE1	1:A:678:TRP:CZ2	2.47	0.50
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.93	0.50
1:A:715:VAL:O	1:A:715:VAL:HG23	2.12	0.49
1:A:516:ARG:HG2	1:A:517:PHE:CE1	2.48	0.49
1:B:571:LEU:HD11	1:B:578:GLU:HB3	1.95	0.49
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.06	0.49
1:A:336:MET:HE1	1:A:678:TRP:HZ2	1.78	0.49
1:A:300:PHE:CD2	1:A:315:THR:HG22	2.48	0.49
1:A:696:LEU:HB3	1:B:330:ILE:HD11	1.93	0.49
1:A:504:ILE:CA	1:A:507:GLN:HG2	2.42	0.49
1:B:336:MET:HE3	8:B:878:HOH:O	2.13	0.49
1:A:362:LEU:HD11	1:A:384:VAL:HG21	1.95	0.48
1:A:351:LYS:HE2	1:A:392:SER:CA	2.44	0.48
1:A:546:ILE:HG12	1:A:560:LYS:HA	1.95	0.48
1:B:355:PHE:N	1:B:356:PRO:HD2	2.27	0.48
1:B:445:HIS:C	1:B:445:HIS:CD2	2.91	0.48
1:B:304:LYS:NZ	8:B:1072:HOH:O	2.46	0.48
1:A:523:LEU:HG	1:A:533:LEU:HD23	1.94	0.48
1:B:621:THR:HG22	8:B:1035:HOH:O	2.13	0.48
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LEU:O	1:A:531:PRO:HA	2.14	0.48
1:A:699:ARG:HH21	1:A:705:GLU:CD	2.22	0.48
1:B:350:THR:O	1:B:353:GLN:HG2	2.14	0.48
1:A:307:GLU:HG3	8:B:965:HOH:O	2.14	0.47
1:A:503:GLU:O	1:A:507:GLN:HG2	2.14	0.47
1:A:506:ILE:HD11	1:A:512:ALA:HB2	1.96	0.47
1:A:491:SER:HB2	8:A:1045:HOH:O	2.14	0.47
1:B:595:VAL:O	1:B:599:CYS:HB2	2.14	0.47
1:A:465:ARG:NE	1:A:471:ASP:OD2	2.47	0.47
1:A:355:PHE:N	1:A:356:PRO:HD2	2.30	0.47
1:A:300:PHE:HD2	1:A:315:THR:HG22	1.80	0.47
1:A:336:MET:HG3	1:B:306:TRP:CD1	2.50	0.47
1:A:523:LEU:HG	1:A:533:LEU:CD2	2.45	0.47
1:B:701:THR:HA	1:B:702:PRO:C	2.40	0.47
1:B:612:LYS:O	1:B:615:ASP:N	2.42	0.46
1:B:684:SER:HB3	1:B:687:ILE:HG12	1.97	0.46
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.15	0.46
1:B:391:THR:O	1:B:392:SER:CB	2.63	0.46
1:A:555:LYS:HZ2	1:A:555:LYS:HB3	1.81	0.46
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.04	0.45
1:B:620:LYS:NZ	8:B:1163:HOH:O	2.48	0.45
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.33	0.45
1:A:350:THR:HB	1:A:353:GLN:OE1	2.16	0.45
1:A:701:THR:HA	1:A:702:PRO:C	2.42	0.45
1:A:445:HIS:C	1:A:445:HIS:CD2	2.95	0.45
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.51	0.45
1:A:306:TRP:CD1	1:B:336:MET:HG3	2.52	0.45
1:A:366:TYR:HA	1:A:369:ILE:HG12	1.99	0.44
1:A:560:LYS:NZ	8:A:1128:HOH:O	2.47	0.44
1:A:350:THR:HG23	8:A:1078:HOH:O	2.17	0.44
1:A:681:PRO:HA	1:A:682:PRO:HD3	1.77	0.44
1:A:716:TRP:H	1:A:716:TRP:CD1	2.33	0.44
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.98	0.44
1:A:396:LEU:HD12	1:A:400:GLU:CB	2.47	0.44
1:A:598:TYR:O	1:A:606:ILE:HG12	2.18	0.44
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.48	0.43
1:B:420:GLN:HG2	2:B:861:ACT:H2	2.01	0.43
1:A:350:THR:HB	1:A:353:GLN:CD	2.44	0.43
1:B:678:TRP:HA	5:B:761:H4B:N1	2.33	0.43
1:A:299:ARG:HG3	1:A:318:LEU:CD2	2.48	0.43
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LEU:HD23	1:A:494:GLY:N	2.33	0.43
1:A:548:HIS:C	1:A:550:LYS:H	2.26	0.43
1:A:618:MET:HA	1:A:625:TRP:CD1	2.54	0.43
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.54	0.43
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.53	0.43
1:B:608:GLU:O	1:B:612:LYS:HG3	2.19	0.43
1:A:487:GLN:HB3	1:A:488:PRO:CD	2.49	0.43
1:A:487:GLN:HB3	1:A:488:PRO:HD2	2.01	0.42
1:A:571:LEU:C	1:A:571:LEU:HD23	2.45	0.42
1:A:610:VAL:HG21	1:A:633:ILE:HD11	2.02	0.42
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.54	0.42
1:A:414:ARG:HD3	1:A:678:TRP:CD2	2.55	0.42
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.55	0.42
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.85	0.41
1:A:682:PRO:HG3	8:A:902:HOH:O	2.19	0.41
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.50	0.41
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.36	0.41
1:B:571:LEU:HD13	1:B:580:SER:HA	2.03	0.41
1:A:393:THR:OG1	1:A:394:TYR:N	2.52	0.41
1:B:397:LYS:HD3	8:B:1043:HOH:O	2.19	0.41
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.03	0.41
4:B:750:HEM:CMC	4:B:750:HEM:HBC2	2.50	0.41
1:A:323:GLU:O	1:A:699:ARG:HD3	2.21	0.41
1:A:510:TRP:HB2	1:A:533:LEU:HD13	2.02	0.41
1:A:678:TRP:HA	5:A:760:H4B:N1	2.35	0.41
1:A:504:ILE:HA	1:A:507:GLN:CD	2.45	0.40
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.36	0.40
1:A:306:TRP:CE2	1:B:336:MET:HG3	2.55	0.40
1:A:380:ARG:NH1	1:A:397:LYS:HE2	2.37	0.40
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.37	0.40
1:A:303:VAL:CG1	1:A:694:GLU:O	2.70	0.40
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	403/421 (96%)	383 (95%)	20 (5%)	0	100	100
1	B	406/421 (96%)	394 (97%)	12 (3%)	0	100	100
All	All	809/842 (96%)	777 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	363/377 (96%)	355 (98%)	8 (2%)	45	40
1	B	366/377 (97%)	362 (99%)	4 (1%)	65	64
All	All	729/754 (97%)	717 (98%)	12 (2%)	55	52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	336	MET
1	A	385	ASN
1	A	485	TYR
1	A	493	LEU
1	A	516	ARG
1	A	523	LEU
1	A	616	LEU
1	B	316	LEU
1	B	336	MET
1	B	423	LYS
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	385	ASN
1	A	395	GLN
1	A	425	GLN
1	A	454	ASN
1	A	487	GLN
1	A	500	GLN
1	A	529	ASN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN
1	B	454	ASN
1	B	527	ASN
1	B	535	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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	B	861	-	3,3,3	0.93	0	3,3,3	0.76	0
2	ACT	A	860	-	3,3,3	0.89	0	3,3,3	0.85	0
6	D7P	A	797	-	21,26,26	1.32	1 (4%)	28,33,33	1.25	3 (10%)
6	D7P	B	798	-	21,26,26	1.34	4 (19%)	28,33,33	1.36	4 (14%)
4	HEM	A	750	1	50,50,50	1.33	5 (10%)	67,82,82	1.22	6 (8%)
5	H4B	B	761	-	17,18,18	2.23	7 (41%)	14,26,26	1.93	4 (28%)
7	MTL	B	871	-	11,11,11	1.15	0	14,14,14	0.92	0
5	H4B	A	760	-	17,18,18	1.83	4 (23%)	14,26,26	2.02	3 (21%)
4	HEM	B	750	1	50,50,50	1.47	7 (14%)	67,82,82	1.14	4 (5%)

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	D7P	A	797	-	-	5/24/27/27	0/1/1/1
4	HEM	B	750	1	-	1/14/54/54	-
6	D7P	B	798	-	-	5/24/27/27	0/1/1/1
4	HEM	A	750	1	-	0/14/54/54	-
7	MTL	B	871	-	-	0/16/16/16	-
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	H4B	B	761	-	-	0/8/17/17	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	761	H4B	C6-N5	5.10	1.56	1.47
5	A	760	H4B	C4A-N5	4.87	1.49	1.37
5	B	761	H4B	C4A-N5	4.73	1.48	1.37
4	B	750	HEM	CMD-C2D	3.89	1.58	1.50
5	A	760	H4B	C6-N5	3.63	1.54	1.47
4	B	750	HEM	CHB-C1B	3.39	1.45	1.38
5	B	761	H4B	C7-N8	3.03	1.49	1.46
4	A	750	HEM	CMA-C3A	2.93	1.56	1.50
4	A	750	HEM	FE-NA	2.89	2.04	1.95
4	B	750	HEM	FE-ND	2.84	2.03	1.94
4	B	750	HEM	CAB-C3B	-2.75	1.40	1.47
6	A	797	D7P	CA-N	2.67	1.51	1.45
5	B	761	H4B	C4-N3	2.63	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	750	HEM	CAB-C3B	-2.56	1.40	1.47
4	B	750	HEM	CMC-C2C	2.53	1.56	1.50
5	A	760	H4B	C4-N3	2.48	1.43	1.38
5	B	761	H4B	C9-C10	2.46	1.57	1.53
4	A	750	HEM	CMC-C2C	2.46	1.55	1.50
6	B	798	D7P	CD2-CG'	2.44	1.43	1.38
4	B	750	HEM	CAA-C2A	2.40	1.57	1.51
6	B	798	D7P	CZ'-CE1	2.34	1.43	1.38
4	A	750	HEM	CMB-C2B	2.26	1.55	1.50
6	B	798	D7P	CA-N	2.25	1.50	1.45
4	B	750	HEM	FE-NA	2.23	2.02	1.95
5	A	760	H4B	C9-C10	2.11	1.56	1.53
5	B	761	H4B	C7-C6	2.07	1.54	1.52
5	B	761	H4B	C8A-N1	2.06	1.39	1.36
6	B	798	D7P	O-C	-2.05	1.20	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	760	H4B	C2-N1-C8A	5.54	123.14	113.36
5	B	761	H4B	C2-N1-C8A	4.98	122.15	113.36
6	B	798	D7P	CD-NE-CZ	3.48	129.84	123.46
5	B	761	H4B	N3-C2-N1	-3.29	117.30	123.32
5	A	760	H4B	N3-C2-N1	-3.28	117.32	123.32
4	B	750	HEM	CMB-C2B-C1B	3.22	130.07	125.03
6	A	797	D7P	CD-NE-CZ	3.06	129.06	123.46
6	B	798	D7P	O-C-N1'	-2.99	117.76	123.04
6	B	798	D7P	CB-CA-N	-2.84	105.28	110.91
4	A	750	HEM	CBD-CAD-C3D	-2.84	104.67	112.53
4	A	750	HEM	CMB-C2B-C1B	2.83	129.46	125.03
6	A	797	D7P	O-C-N1'	-2.83	118.05	123.04
4	A	750	HEM	CAB-C3B-C2B	-2.72	119.60	128.43
5	A	760	H4B	O10-C10-C9	-2.51	105.61	109.77
6	A	797	D7P	CB-CA-N	-2.46	106.03	110.91
5	B	761	H4B	O9-C9-C6	2.46	115.16	109.28
4	A	750	HEM	C2A-C1A-NA	2.40	112.82	110.15
4	A	750	HEM	C2B-C1B-NB	2.33	112.52	109.84
4	A	750	HEM	CBA-CAA-C2A	-2.33	106.10	112.53
6	B	798	D7P	CA-C-N1'	2.23	120.56	116.76
4	B	750	HEM	CAB-C3B-C2B	-2.23	121.19	128.43
5	B	761	H4B	O10-C10-C9	-2.15	106.21	109.77
4	B	750	HEM	C4A-NA-C1A	-2.14	102.32	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	750	HEM	CMB-C2B-C3B	-2.01	123.56	128.43

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	797	D7P	N-CA-CB-CG
6	A	797	D7P	C-CA-CB-CG
6	B	798	D7P	N-CA-CB-CG
6	A	797	D7P	CG-CD-NE-CZ
6	A	797	D7P	N1'-C-CA-N
6	A	797	D7P	O-C-CA-N
6	B	798	D7P	N1'-C-CA-N
6	B	798	D7P	O-C-CA-N
6	B	798	D7P	CG-CD-NE-CZ
4	B	750	HEM	C4B-C3B-CAB-CBB
6	B	798	D7P	C-CA-CB-CG

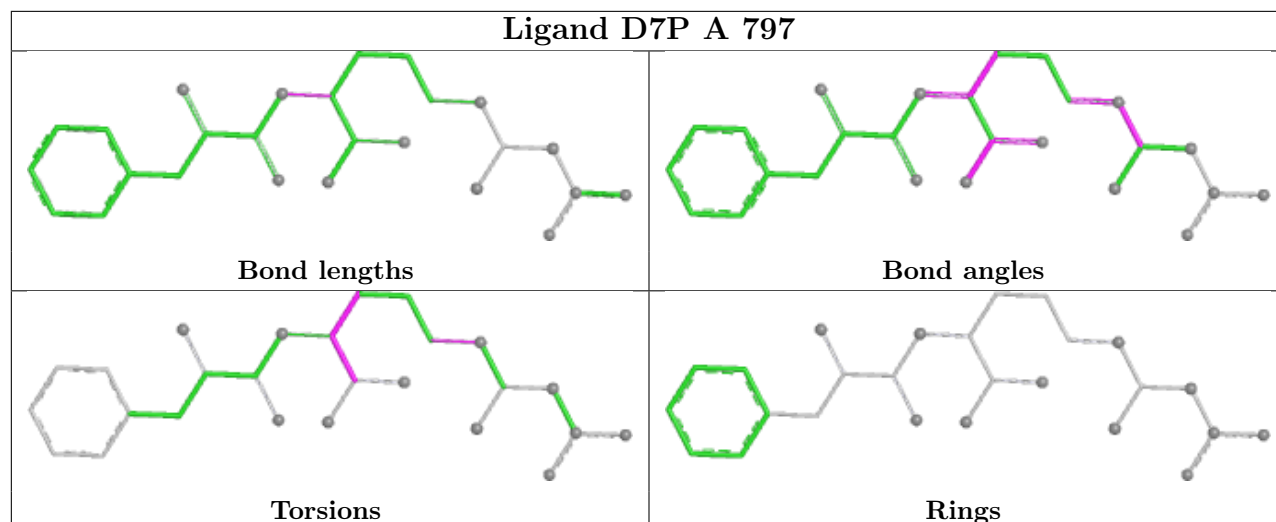
There are no ring outliers.

6 monomers are involved in 6 short contacts:

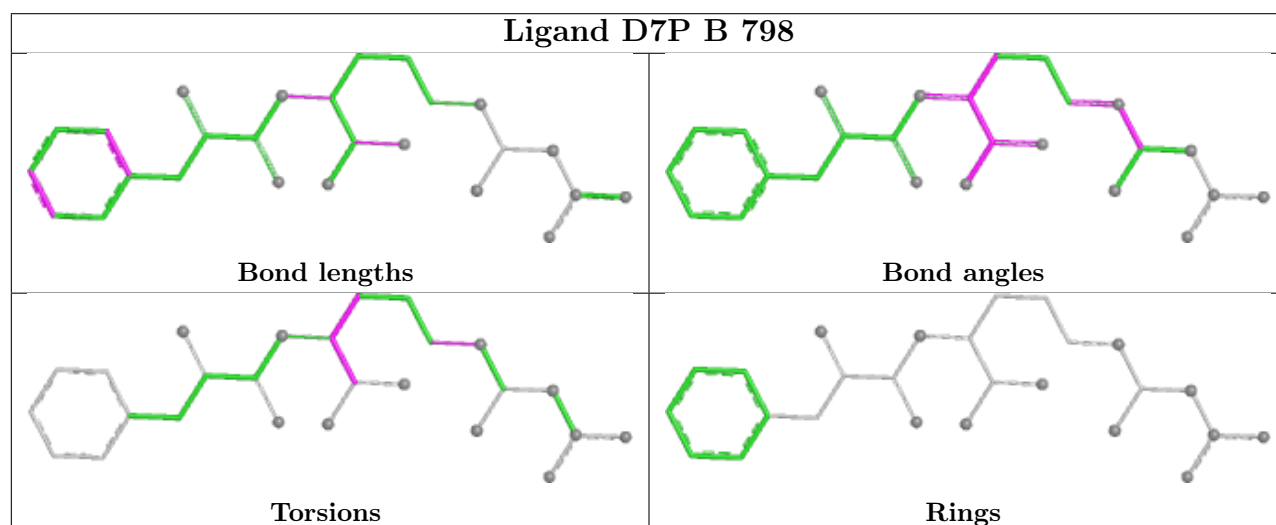
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	861	ACT	1	0
2	A	860	ACT	1	0
4	A	750	HEM	2	0
5	B	761	H4B	1	0
5	A	760	H4B	1	0
4	B	750	HEM	1	0

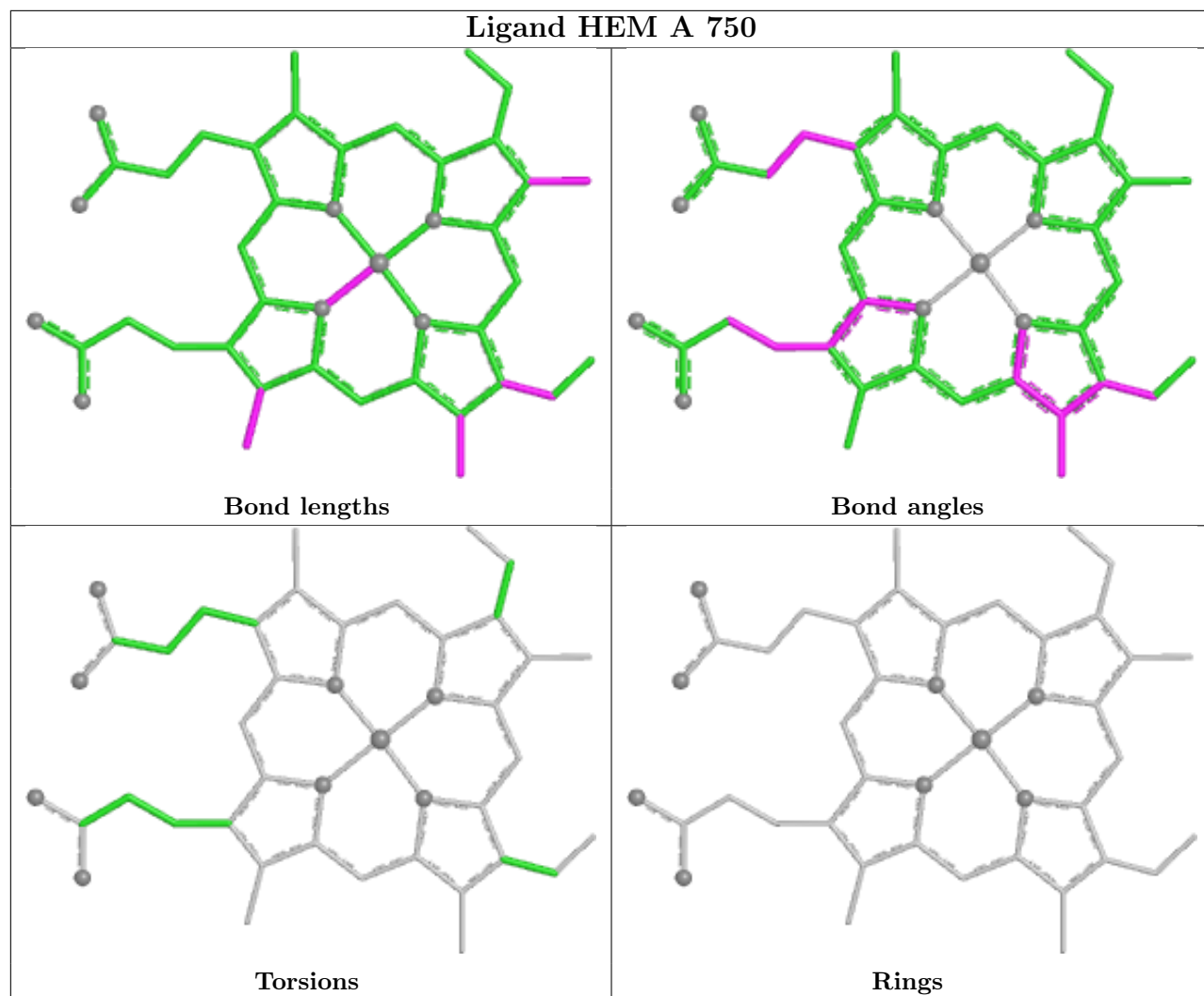
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

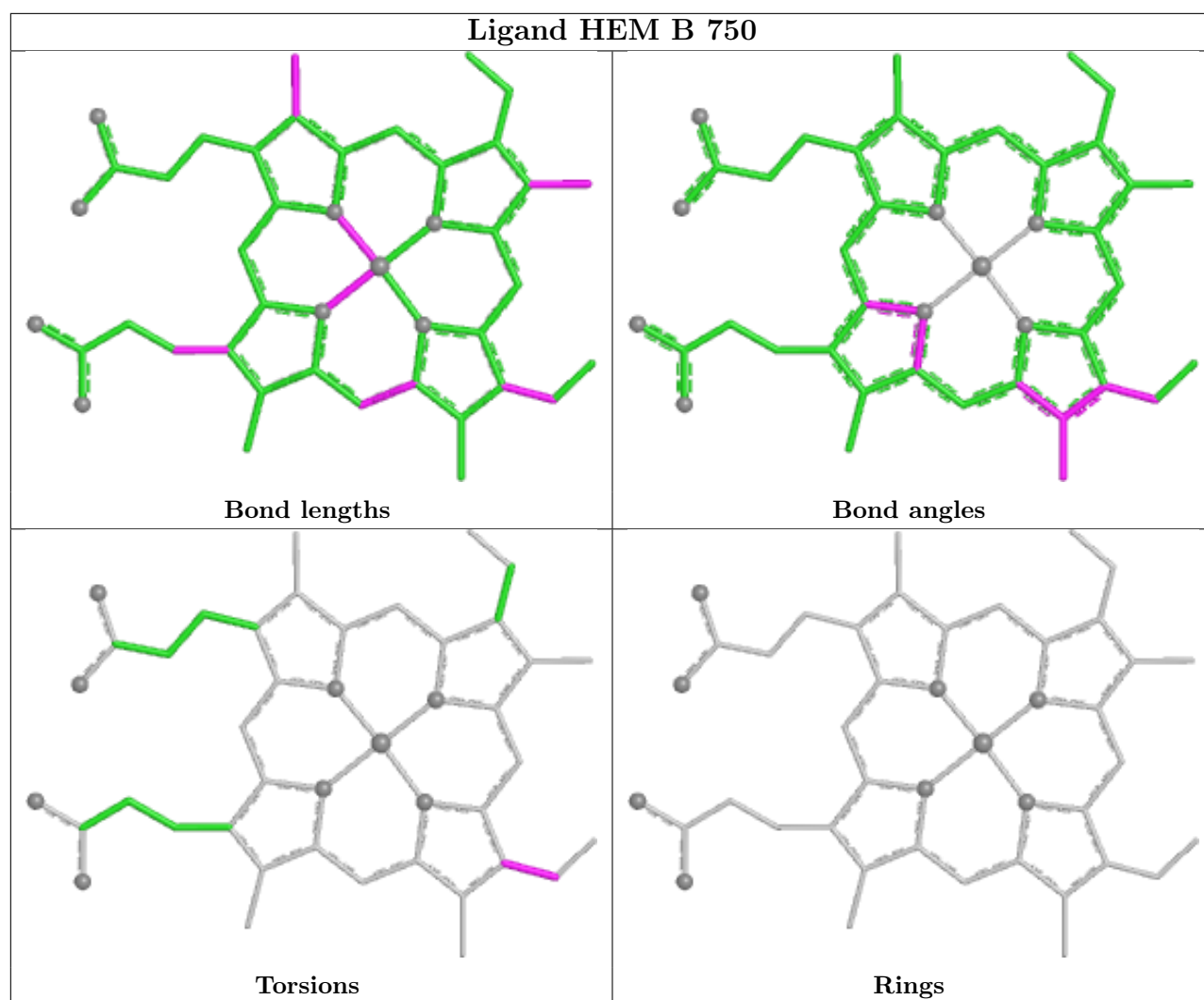
Ligand D7P A 797



Ligand D7P B 798







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%)	1.22	101 (24%) 2 1	18, 38, 61, 75	0
1	B	410/421 (97%)	0.56	34 (8%) 17 20	18, 29, 51, 65	0
All	All	817/842 (97%)	0.89	135 (16%) 4 4	18, 32, 58, 75	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	4.9
1	A	355	PHE	4.7
1	A	373	GLY	4.6
1	A	303	VAL	4.5
1	A	504	ILE	4.5
1	A	715	VAL	4.4
1	B	322	LEU	4.4
1	B	300	PHE	4.4
1	B	321	THR	4.2
1	A	301	LEU	4.2
1	A	300	PHE	4.0
1	A	551	PHE	3.9
1	A	506	ILE	3.9
1	A	470	HIS	3.8
1	A	378	MET	3.8
1	B	355	PHE	3.8
1	A	510	TRP	3.7
1	A	552	ASP	3.7
1	A	528	GLY	3.7
1	A	556	ASP	3.7
1	A	601	ASN	3.7
1	B	350	THR	3.6
1	A	711	TRP	3.5
1	B	348	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	376	ALA	3.5
1	B	389	GLU	3.4
1	B	338	PRO	3.4
1	A	358	ALA	3.3
1	A	493	LEU	3.3
1	B	352	ASP	3.3
1	A	553	TRP	3.2
1	A	485	TYR	3.2
1	A	384	VAL	3.2
1	B	611	ALA	3.1
1	A	491	SER	3.1
1	A	490	GLY	3.1
1	A	471	ASP	3.1
1	A	548	HIS	3.1
1	A	382	GLU	3.1
1	A	494	GLY	3.0
1	A	555	LYS	3.0
1	A	357	LEU	3.0
1	A	350	THR	3.0
1	A	501	PHE	2.9
1	A	388	ILE	2.9
1	A	607	LEU	2.9
1	A	616	LEU	2.9
1	A	390	SER	2.9
1	B	299	ARG	2.9
1	A	507	GLN	2.8
1	B	667	ARG	2.8
1	A	361	PHE	2.8
1	A	321	THR	2.8
1	A	319	LYS	2.8
1	A	611	ALA	2.8
1	B	616	LEU	2.8
1	A	488	PRO	2.8
1	A	668	CYS	2.7
1	B	354	LEU	2.7
1	B	353	GLN	2.7
1	A	385	ASN	2.7
1	A	512	ALA	2.7
1	A	714	HIS	2.7
1	A	356	PRO	2.7
1	A	381	LEU	2.7
1	B	392	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	369	ILE	2.7
1	B	303	VAL	2.7
1	A	354	LEU	2.6
1	A	487	GLN	2.6
1	A	529	ASN	2.6
1	A	360	GLU	2.6
1	A	499	VAL	2.6
1	A	386	LYS	2.6
1	A	392	SER	2.6
1	A	505	CYS	2.6
1	A	322	LEU	2.5
1	B	386	LYS	2.5
1	B	367	SER	2.5
1	A	554	PHE	2.5
1	A	316	LEU	2.5
1	B	619	ARG	2.5
1	A	489	ASP	2.5
1	A	546	ILE	2.4
1	A	396	LEU	2.4
1	A	713	THR	2.4
1	A	519	VAL	2.4
1	A	318	LEU	2.4
1	A	550	LYS	2.4
1	B	391	THR	2.4
1	B	423	LYS	2.4
1	B	552	ASP	2.3
1	B	328	GLU	2.3
1	A	509	GLY	2.3
1	A	541	VAL	2.3
1	B	310	VAL	2.3
1	A	375	LYS	2.3
1	A	530	ASP	2.2
1	A	712	ASN	2.2
1	A	618	MET	2.2
1	A	466	THR	2.2
1	A	559	LEU	2.2
1	A	363	ASP	2.2
1	A	379	ASP	2.2
1	A	633	ILE	2.2
1	A	486	LYS	2.2
1	A	389	GLU	2.2
1	A	337	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	423	LYS	2.2
1	B	305	ASN	2.2
1	B	378	MET	2.2
1	B	385	ASN	2.2
1	A	364	GLN	2.1
1	A	320	SER	2.1
1	A	667	ARG	2.1
1	A	472	PHE	2.1
1	A	393	THR	2.1
1	A	558	GLY	2.1
1	B	610	VAL	2.1
1	A	523	LEU	2.1
1	B	617	ASP	2.1
1	A	377	HIS	2.1
1	A	508	GLN	2.1
1	A	615	ASP	2.1
1	B	613	LYS	2.0
1	A	502	THR	2.0
1	A	503	GLU	2.0
1	A	620	LYS	2.0
1	B	620	LYS	2.0
1	B	618	MET	2.0
1	A	574	ILE	2.0
1	A	537	PRO	2.0
1	A	710	PRO	2.0
1	A	610	VAL	2.0
1	B	311	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 [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,

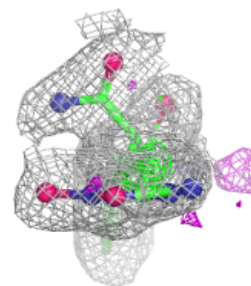
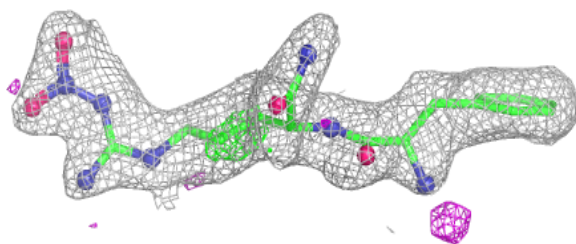
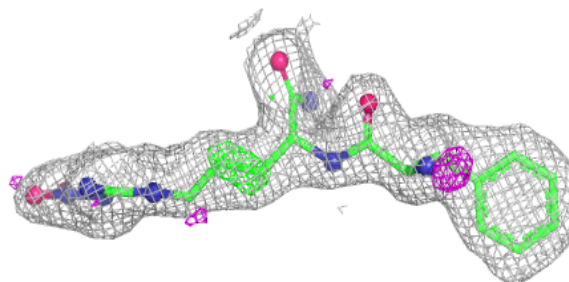
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACT	A	860	4/4	0.83	0.16	54,54,54,54	0
6	D7P	A	797	26/26	0.88	0.12	31,35,39,40	0
6	D7P	B	798	26/26	0.90	0.11	30,32,35,35	0
7	MTL	B	871	12/12	0.92	0.09	29,32,34,34	0
2	ACT	B	861	4/4	0.93	0.10	40,40,40,40	0
5	H4B	B	761	17/17	0.96	0.05	16,18,21,21	0
5	H4B	A	760	17/17	0.96	0.06	19,21,24,24	0
4	HEM	B	750	43/43	0.98	0.06	17,18,21,21	0
4	HEM	A	750	43/43	0.98	0.06	19,20,21,22	0
3	ZN	A	900	1/1	1.00	0.02	31,31,31,31	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.

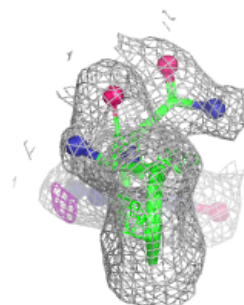
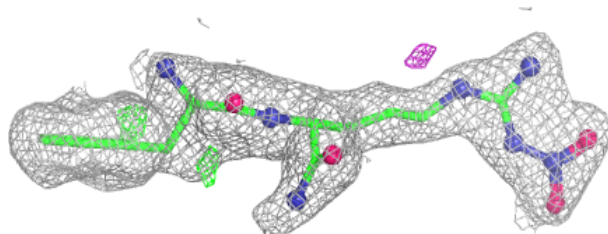
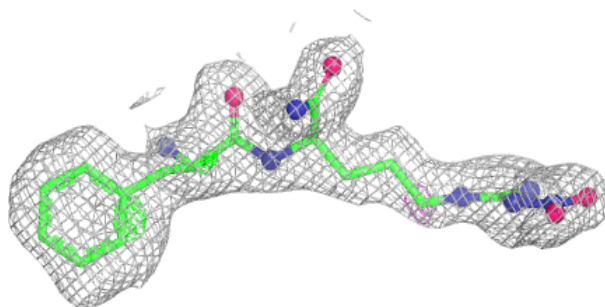
Electron density around D7P A 797:

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



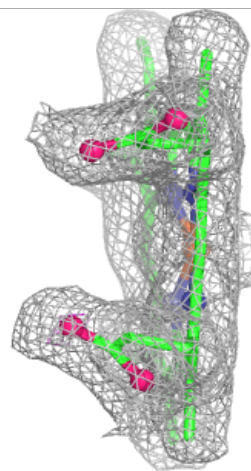
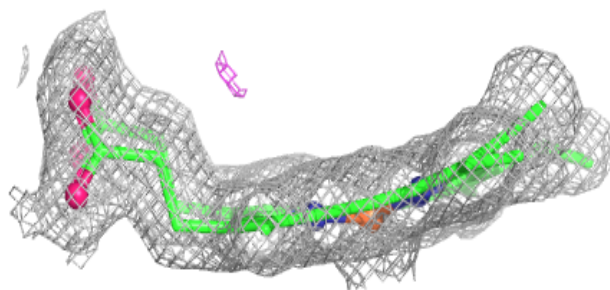
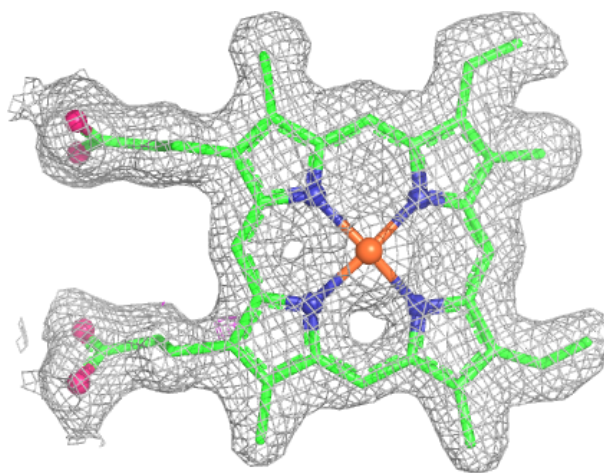
Electron density around D7P B 798:

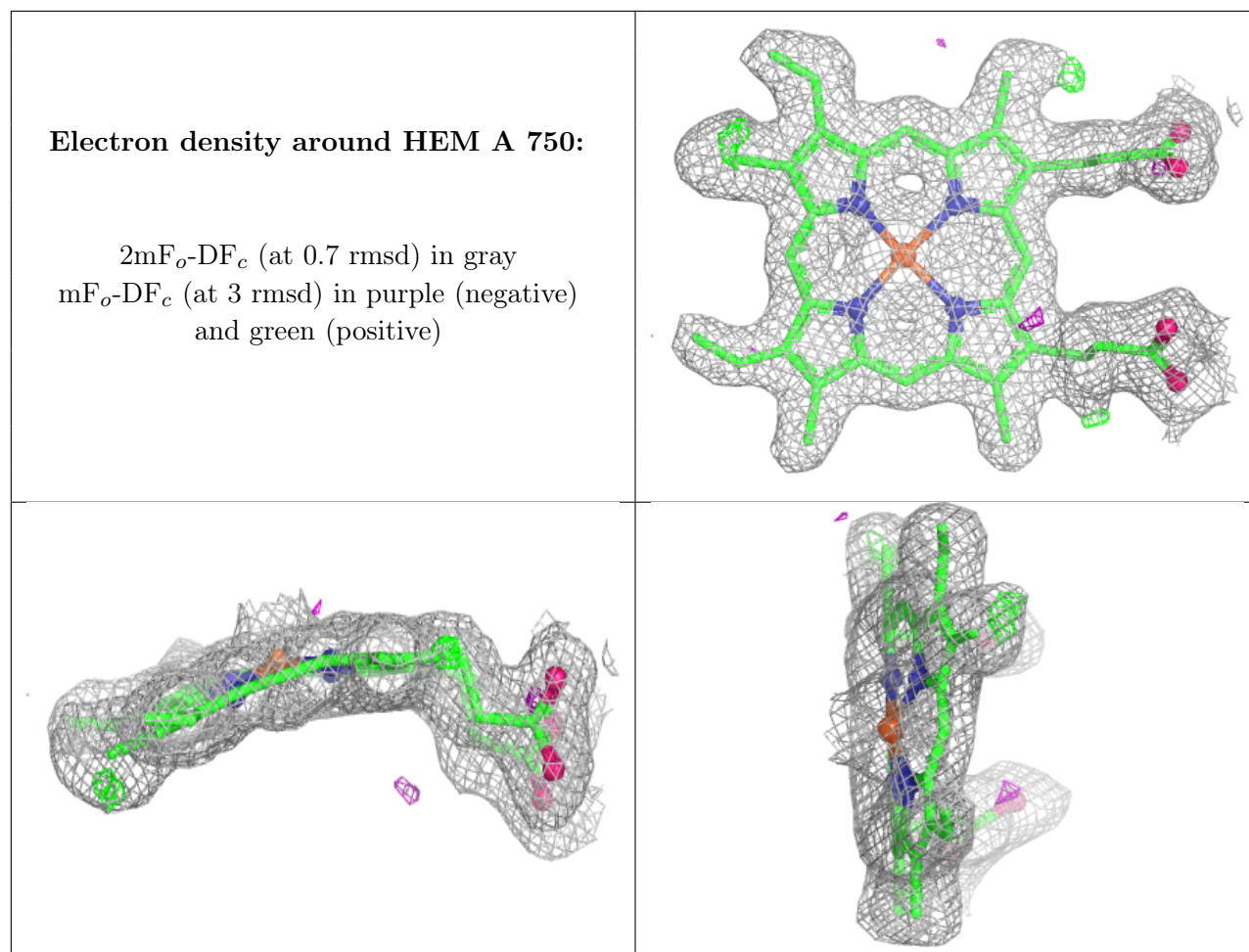
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 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.