



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:06 PM UTC

PDB ID : 1P6H / pdb_00001p6h
Title : Rat neuronal NOS 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 : 1.98 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

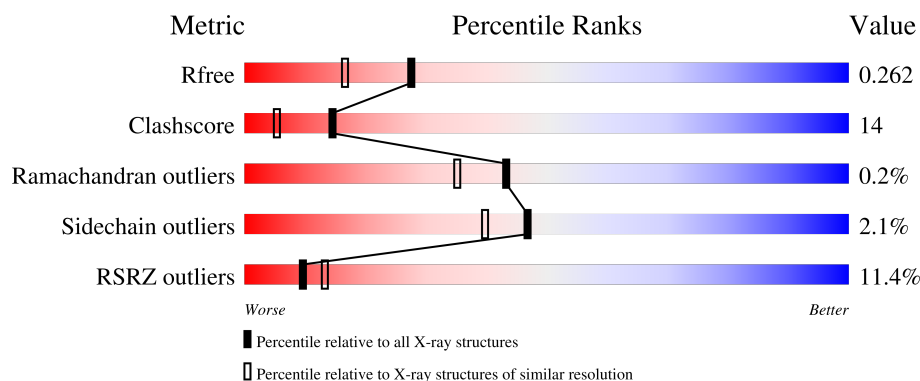
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	16% 63% 31% • •
1	B	421	6% 71% 24% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	860	-	-	X	-

2 Entry composition [i](#)

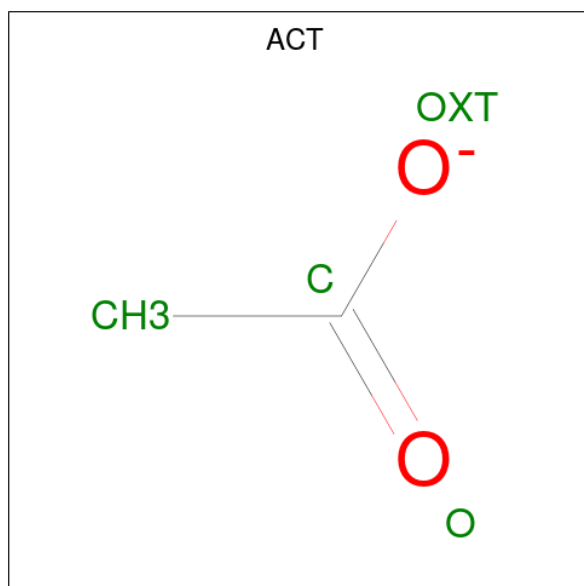
There are 7 unique types of molecules in this entry. The entry contains 7314 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_2H_3O_2^-$).

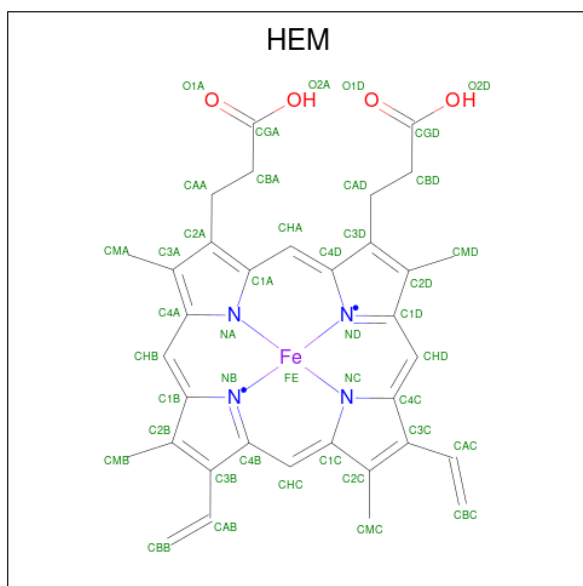


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

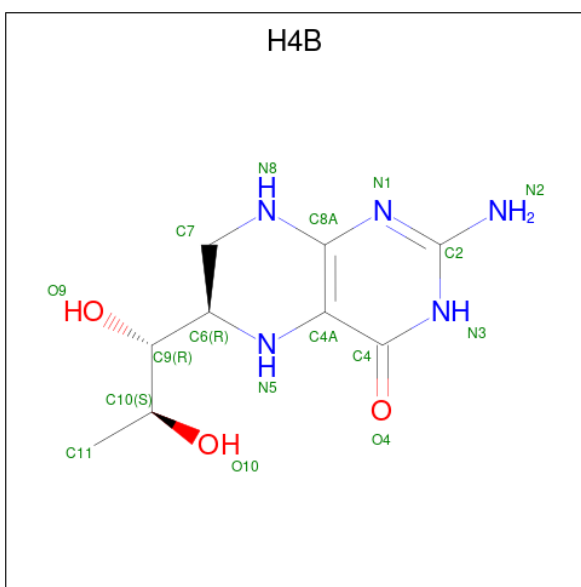
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



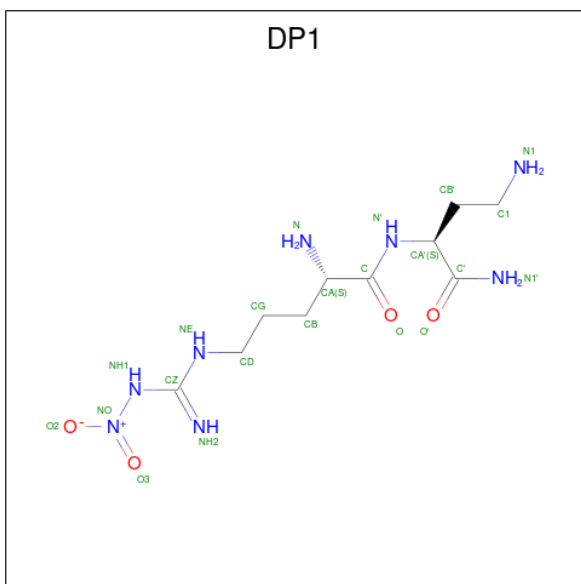
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



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

- Molecule 6 is L-N(OMEGA)-NITROARGININE-2,4-L-DIAMINOBTYRIC AMIDE (CCD ID: DP1) (formula: $C_{10}H_{22}N_8O_4$).



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

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

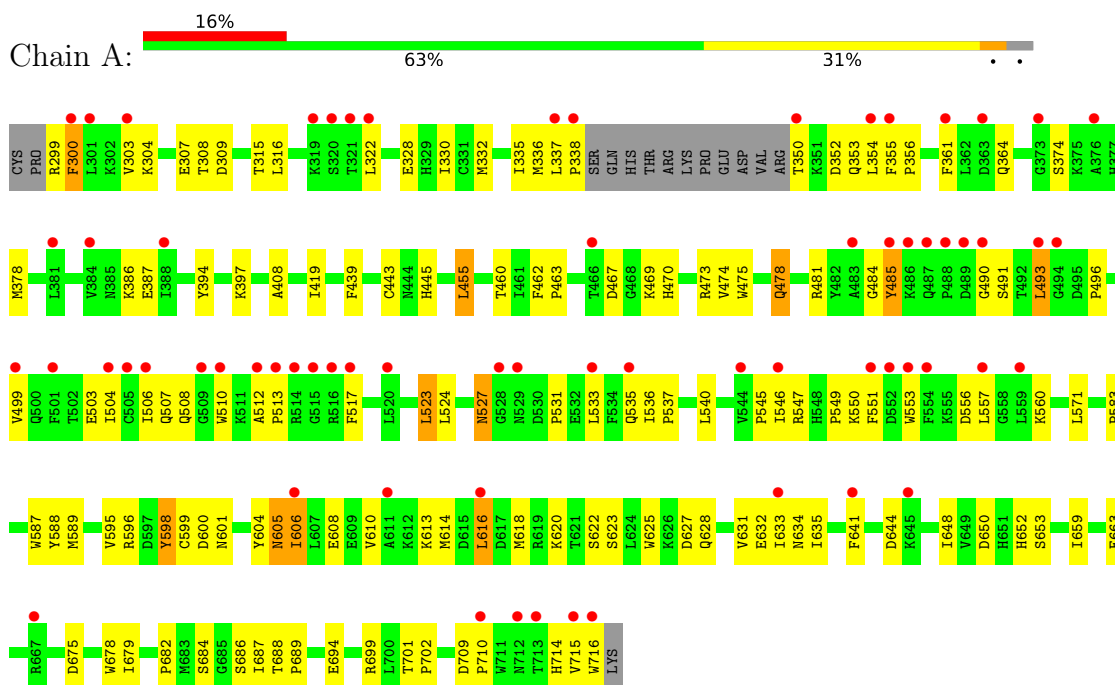
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	214	Total	O	0	0
			214	214		
7	B	273	Total	O	0	0
			273	273		

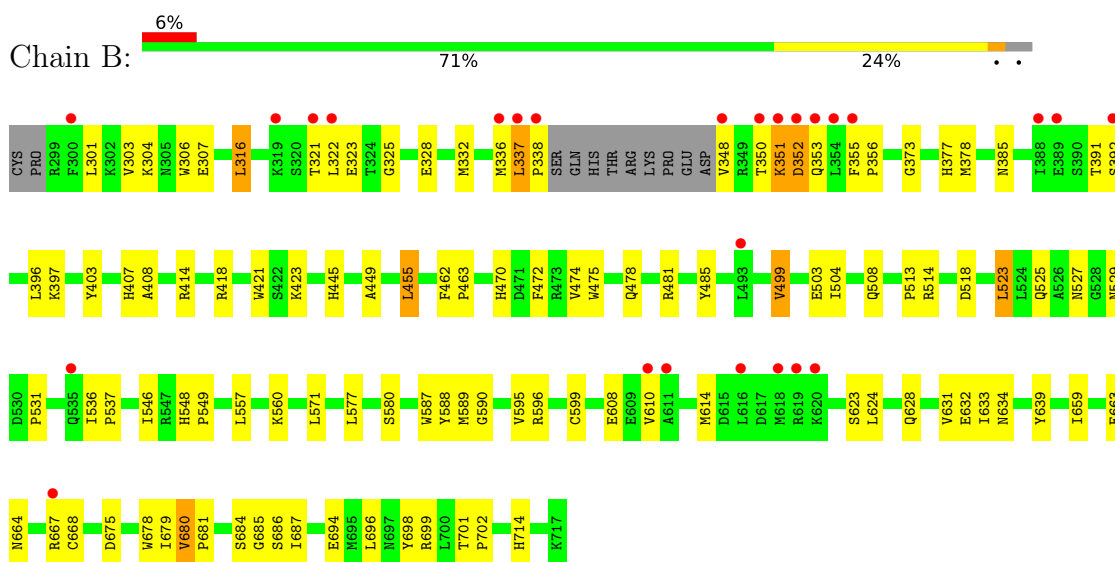
3 Residue-property plots

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

- Molecule 1: Nitric-oxide synthase, brain



- Molecule 1: Nitric-oxide synthase, brain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.94Å 110.22Å 164.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.94 – 1.98 43.94 – 1.98	Depositor EDS
% Data completeness (in resolution range)	94.9 (43.94-1.98) 94.9 (43.94-1.98)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.273 0.223 , 0.262	Depositor DCC
R_{free} test set	3322 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7314	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: H4B, HEM, DP1, ACT, 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	0.47	0/3406	0.97	19/4621 (0.4%)
1	B	0.55	0/3434	1.00	19/4656 (0.4%)
All	All	0.51	0/6840	0.99	38/9277 (0.4%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-8.65	95.15	109.24
1	A	354	LEU	N-CA-C	8.51	120.17	111.07
1	A	589	MET	N-CA-C	-8.15	95.96	109.24
1	A	490	GLY	N-CA-C	-7.49	105.18	114.92
1	B	351	LYS	N-CA-C	-7.43	103.17	111.71
1	B	472	PHE	N-CA-C	-6.93	98.39	109.76
1	B	421	TRP	N-CA-C	6.58	119.29	111.33
1	A	588	TYR	N-CA-C	6.56	119.75	110.50
1	A	606	ILE	N-CA-C	6.47	119.23	112.83
1	B	599	CYS	N-CA-C	6.30	121.10	113.17
1	A	688	THR	N-CA-C	-6.26	102.25	110.39
1	B	623	SER	N-CA-C	-6.20	105.20	112.89
1	A	623	SER	N-CA-C	-6.13	105.76	113.18
1	A	546	ILE	N-CA-C	5.82	117.13	108.23
1	A	474	VAL	N-CA-C	-5.81	99.38	107.80
1	A	557	LEU	N-CA-C	-5.79	105.31	112.38
1	B	590	GLY	N-CA-C	5.61	119.68	112.83
1	B	474	VAL	N-CA-C	-5.59	99.10	107.37
1	B	596	ARG	N-CA-C	5.57	118.42	111.24
1	B	408	ALA	N-CA-C	-5.56	105.22	111.28
1	A	408	ALA	N-CA-C	-5.54	105.33	111.71
1	A	455	LEU	N-CA-C	5.47	117.95	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	686	SER	N-CA-C	5.44	119.54	113.01
1	A	478	GLN	N-CA-C	-5.39	100.87	109.23
1	B	499	VAL	N-CA-C	5.34	115.55	110.42
1	A	598	TYR	N-CA-C	5.32	118.23	111.69
1	B	418	ARG	N-CA-C	5.30	119.37	113.01
1	A	709	ASP	N-CA-C	-5.30	101.85	109.48
1	A	686	SER	N-CA-C	5.30	119.37	113.01
1	B	714	HIS	N-CA-C	5.26	117.94	110.10
1	A	599	CYS	N-CA-C	5.25	120.54	113.72
1	A	689	PRO	N-CA-C	5.18	120.64	113.65
1	B	557	LEU	N-CA-C	-5.09	106.58	112.89
1	B	397	LYS	N-CA-C	-5.07	103.71	110.55
1	B	680	VAL	CA-C-N	5.05	123.35	119.66
1	B	680	VAL	C-N-CA	5.05	123.35	119.66
1	A	397	LYS	N-CA-C	-5.05	103.01	110.48
1	B	588	TYR	N-CA-C	5.03	117.92	110.48

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	111	0
1	B	3341	0	3256	82	0
2	A	4	0	3	2	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	43	0	30	4	0
4	B	43	0	30	3	0
5	A	17	0	15	1	0
5	B	17	0	15	0	0
6	A	22	0	21	1	0
6	B	22	0	21	1	0
7	A	214	0	0	13	0
7	B	273	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7314	0	6615	188	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 14.

All (188) 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	1.09	0.96
1:B:523:LEU:HD22	1:B:531:PRO:HB2	1.50	0.91
1:A:350:THR:HB	1:A:353:GLN:HG3	1.58	0.85
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.60	0.83
1:B:373:GLY:H	1:B:377:HIS:CD2	1.98	0.81
1:A:613:LYS:HE2	7:A:977:HOH:O	1.82	0.78
1:B:668:CYS:HB3	7:B:1012:HOH:O	1.87	0.73
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.05	0.72
1:A:616:LEU:HD13	1:A:625:TRP:HB2	1.72	0.71
1:A:353:GLN:O	1:A:356:PRO:HD2	1.94	0.68
1:B:350:THR:HB	1:B:353:GLN:OE1	1.95	0.66
1:A:608:GLU:HG2	1:A:618:MET:HE1	1.78	0.66
1:A:350:THR:HG22	1:A:352:ASP:H	1.60	0.66
1:A:307:GLU:HG3	7:B:904:HOH:O	1.95	0.65
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.79	0.65
1:A:545:PRO:HD3	7:A:1050:HOH:O	1.96	0.64
1:B:337:LEU:N	1:B:337:LEU:HD23	2.13	0.64
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.79	0.63
1:A:304:LYS:O	1:A:694:GLU:HG3	1.99	0.62
4:B:750:HEM:HMC1	4:B:750:HEM:HBC2	1.81	0.62
1:A:508:GLN:HG3	7:A:1025:HOH:O	2.00	0.61
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.36	0.61
1:A:336:MET:HE2	1:B:306:TRP:CD2	2.35	0.60
1:A:517:PHE:HB2	1:A:560:LYS:HE2	1.84	0.60
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.67	0.60
1:B:571:LEU:HD12	1:B:580:SER:HA	1.83	0.59
1:A:507:GLN:O	1:A:507:GLN:HG2	2.03	0.59
1:A:598:TYR:O	1:A:606:ILE:HG12	2.02	0.58
1:B:350:THR:HG22	1:B:352:ASP:H	1.68	0.58
1:A:682:PRO:HG3	7:A:903:HOH:O	2.02	0.58
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.85	0.58
1:A:610:VAL:O	1:A:614:MET:HG3	2.03	0.58
1:A:595:VAL:HG23	1:A:634:ASN:HD21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.29	0.57
1:A:571:LEU:C	1:A:571:LEU:HD23	2.30	0.57
1:B:391:THR:O	1:B:392:SER:HB2	2.05	0.57
1:A:595:VAL:HG11	1:A:682:PRO:HB2	1.85	0.57
7:A:1001:HOH:O	1:B:307:GLU:HG3	2.05	0.56
1:B:455:LEU:HD23	1:B:455:LEU:N	2.19	0.56
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.86	0.56
1:A:491:SER:HB2	7:A:1102:HOH:O	2.05	0.56
1:A:300:PHE:CD2	1:A:315:THR:HG22	2.41	0.56
1:A:493:LEU:HA	7:A:950:HOH:O	2.05	0.55
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.37	0.55
1:A:556:ASP:HB2	7:A:977:HOH:O	2.05	0.55
4:B:750:HEM:HBC2	4:B:750:HEM:CMC	2.37	0.55
1:B:352:ASP:HB3	1:B:353:GLN:OE1	2.07	0.55
4:A:750:HEM:HMC2	4:A:750:HEM:HBC2	1.87	0.55
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.38	0.54
1:B:373:GLY:HA2	1:B:378:MET:HE3	1.90	0.54
1:B:355:PHE:N	1:B:356:PRO:HD2	2.22	0.54
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.90	0.54
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.38	0.54
1:B:316:LEU:HB3	1:B:698:TYR:OH	2.06	0.54
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.90	0.53
1:A:620:LYS:HE3	1:A:622:SER:OG	2.07	0.53
1:A:499:VAL:O	1:A:503:GLU:HG2	2.09	0.53
1:A:524:LEU:O	1:A:531:PRO:HA	2.08	0.53
1:B:350:THR:HB	1:B:352:ASP:HB3	1.91	0.53
1:A:332:MET:HE2	1:B:696:LEU:HD21	1.90	0.53
1:A:350:THR:HB	1:A:353:GLN:CG	2.36	0.52
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.45	0.52
1:B:481:ARG:HG2	7:B:984:HOH:O	2.09	0.52
1:A:478:GLN:HG3	6:A:790:DP1:O'	2.09	0.52
1:B:470:HIS:HB3	1:B:527:ASN:ND2	2.24	0.52
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.92	0.52
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.92	0.52
1:A:361:PHE:O	1:A:364:GLN:HG2	2.10	0.52
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.25	0.52
1:B:549:PRO:HG3	1:B:639:TYR:CG	2.45	0.51
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.92	0.51
1:A:336:MET:HE2	1:B:306:TRP:CG	2.46	0.51
1:B:323:GLU:O	1:B:699:ARG:HD3	2.11	0.51
1:B:373:GLY:N	1:B:377:HIS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:MET:HE3	1:A:625:TRP:CH2	2.46	0.50
1:A:631:VAL:HG11	1:B:628:GLN:HG2	1.94	0.50
1:A:714:HIS:ND1	7:A:1114:HOH:O	2.34	0.50
1:B:608:GLU:HB2	7:B:1062:HOH:O	2.12	0.50
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.94	0.49
1:A:535:GLN:NE2	7:A:956:HOH:O	2.46	0.49
2:A:860:ACT:H3	4:A:750:HEM:HMB3	1.95	0.49
1:B:321:THR:HG23	1:B:322:LEU:N	2.27	0.49
1:B:659:ILE:O	1:B:663:GLU:HG3	2.12	0.49
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.47	0.49
1:A:659:ILE:O	1:A:663:GLU:HG3	2.13	0.49
1:A:715:VAL:O	1:A:715:VAL:HG23	2.12	0.49
1:A:300:PHE:CD1	1:A:300:PHE:N	2.80	0.49
1:A:387:GLU:OE2	1:A:394:TYR:HA	2.13	0.48
1:B:445:HIS:C	1:B:445:HIS:CD2	2.91	0.48
1:B:350:THR:C	1:B:352:ASP:N	2.70	0.48
1:B:403:TYR:O	1:B:407:HIS:HD2	1.96	0.48
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.39	0.48
1:B:462:PHE:HB3	1:B:463:PRO:CD	2.43	0.48
1:B:595:VAL:HG23	1:B:634:ASN:HD21	1.79	0.48
1:B:684:SER:HB3	1:B:687:ILE:CD1	2.42	0.48
1:B:664:ASN:O	1:B:667:ARG:HG2	2.14	0.48
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.79	0.47
1:A:620:LYS:HB3	7:A:1020:HOH:O	2.14	0.47
1:B:701:THR:HA	1:B:702:PRO:C	2.39	0.47
1:A:716:TRP:H	1:A:716:TRP:CD1	2.32	0.47
1:A:601:ASN:HB3	7:A:1023:HOH:O	2.13	0.47
1:B:351:LYS:HE2	1:B:392:SER:OG	2.15	0.47
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.50	0.47
1:A:308:THR:O	1:A:309:ASP:HB2	2.15	0.47
1:A:653:SER:HB2	7:B:1073:HOH:O	2.14	0.47
1:A:439:PHE:CZ	1:A:443:CYS:SG	3.08	0.47
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.96	0.46
1:A:545:PRO:HD2	1:A:644:ASP:OD2	2.15	0.46
1:A:701:THR:HA	1:A:702:PRO:C	2.40	0.46
1:A:336:MET:HE2	1:B:306:TRP:CE2	2.50	0.46
1:A:299:ARG:CG	1:A:300:PHE:N	2.78	0.46
1:B:614:MET:CE	1:B:632:GLU:HG3	2.45	0.46
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.96	0.46
1:B:667:ARG:HG3	7:B:1012:HOH:O	2.15	0.46
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.46	0.45
1:B:328:GLU:H	1:B:328:GLU:CD	2.25	0.45
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.97	0.45
1:A:523:LEU:HG	1:A:533:LEU:HD23	1.97	0.45
1:A:445:HIS:CD2	1:A:445:HIS:C	2.95	0.45
1:A:460:THR:O	1:A:583:PRO:HD2	2.16	0.45
1:B:675:ASP:O	1:B:679:ILE:HG12	2.16	0.45
1:A:338:PRO:HB3	7:A:1051:HOH:O	2.17	0.45
2:A:860:ACT:H1	4:A:750:HEM:HAB	1.98	0.45
1:B:332:MET:HE3	1:B:338:PRO:HB2	1.98	0.45
1:B:610:VAL:O	1:B:614:MET:HG3	2.17	0.45
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.99	0.44
1:A:504:ILE:O	1:A:508:GLN:HB2	2.17	0.44
1:A:506:ILE:C	1:A:508:GLN:H	2.26	0.44
1:A:374:SER:O	1:A:378:MET:HG2	2.17	0.44
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.97	0.44
1:B:504:ILE:O	1:B:508:GLN:HG2	2.18	0.44
1:A:353:GLN:C	1:A:356:PRO:HD2	2.42	0.44
1:A:675:ASP:O	1:A:679:ILE:HG12	2.17	0.44
1:B:325:GLY:O	1:B:332:MET:HE2	2.17	0.44
1:A:604:TYR:O	1:A:605:ASN:C	2.61	0.44
1:B:337:LEU:N	1:B:337:LEU:CD2	2.80	0.44
1:B:396:LEU:HG	1:B:577:LEU:HD12	2.00	0.44
1:A:537:PRO:HB2	1:A:540:LEU:HG	2.00	0.44
1:B:336:MET:HB3	1:B:337:LEU:HD23	1.99	0.44
1:B:548:HIS:ND1	1:B:549:PRO:HD2	2.32	0.44
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.99	0.44
4:A:750:HEM:HBC2	4:A:750:HEM:CMC	2.47	0.44
1:B:336:MET:HB3	1:B:337:LEU:CD2	2.47	0.44
1:B:462:PHE:HB3	1:B:463:PRO:HD2	1.99	0.44
1:A:303:VAL:CG1	1:A:694:GLU:O	2.66	0.44
1:B:587:TRP:H	4:B:750:HEM:HAB	1.83	0.44
1:A:484:GLY:O	1:A:499:VAL:HA	2.18	0.43
1:A:322:LEU:HB2	1:A:699:ARG:HB2	2.00	0.43
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.34	0.43
1:A:536:ILE:O	1:A:537:PRO:C	2.60	0.43
1:A:549:PRO:O	1:A:550:LYS:HG3	2.18	0.43
1:A:618:MET:HA	1:A:625:TRP:CD1	2.53	0.43
1:A:627:ASP:O	1:A:631:VAL:HG23	2.19	0.43
1:B:321:THR:HG23	1:B:322:LEU:H	1.83	0.43
1:A:678:TRP:HA	5:A:760:H4B:N1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:HIS:HB3	1:A:527:ASN:OD1	2.19	0.43
1:A:596:ARG:O	1:A:600:ASP:HB2	2.19	0.43
1:B:499:VAL:O	1:B:503:GLU:HG3	2.19	0.43
1:A:510:TRP:HB2	1:A:533:LEU:HD13	2.01	0.43
1:B:304:LYS:NZ	7:B:1081:HOH:O	2.50	0.43
1:B:348:VAL:HG22	1:B:348:VAL:O	2.19	0.42
1:A:467:ASP:C	1:A:469:LYS:H	2.27	0.42
1:A:496:PRO:O	1:A:499:VAL:HG23	2.19	0.42
1:B:525:GLN:HG3	1:B:529:ASN:O	2.19	0.42
1:A:635:ILE:HG13	1:B:624:LEU:HD12	2.01	0.42
1:B:478:GLN:HG3	6:B:791:DP1:O'	2.20	0.42
1:B:536:ILE:O	1:B:537:PRO:C	2.61	0.42
1:A:355:PHE:N	1:A:356:PRO:CD	2.83	0.42
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.50	0.42
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.85	0.41
1:A:551:PHE:CD2	1:A:551:PHE:N	2.86	0.41
1:A:614:MET:HE3	1:A:632:GLU:HG3	2.01	0.41
1:A:328:GLU:H	1:A:328:GLU:CD	2.29	0.41
1:A:485:TYR:HE2	1:A:512:ALA:HB1	1.84	0.41
1:A:595:VAL:HG23	1:A:634:ASN:ND2	2.34	0.41
1:B:449:ALA:O	1:B:455:LEU:HA	2.21	0.41
1:A:386:LYS:HD3	1:A:386:LYS:HA	1.75	0.41
1:A:299:ARG:HG2	1:A:300:PHE:N	2.35	0.41
1:A:523:LEU:HG	1:A:533:LEU:CD2	2.50	0.41
1:A:628:GLN:CG	1:B:631:VAL:HG11	2.51	0.41
1:A:614:MET:CE	1:A:632:GLU:HG3	2.50	0.41
1:A:641:PHE:CG	1:A:648:ILE:HD12	2.55	0.40
1:B:548:HIS:HA	1:B:549:PRO:HD3	1.93	0.40
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.94	0.40
1:A:650:ASP:OD2	1:A:652:HIS:HB2	2.21	0.40
1:A:684:SER:HB3	1:A:687:ILE:HG12	2.03	0.40
1:B:684:SER:O	1:B:685:GLY:C	2.64	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%)	371 (92%)	31 (8%)	1 (0%)	43	35
1	B	406/421 (96%)	393 (97%)	12 (3%)	1 (0%)	43	35
All	All	809/842 (96%)	764 (94%)	43 (5%)	2 (0%)	43	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	605	ASN
1	B	352	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	363/377 (96%)	354 (98%)	9 (2%)	42	33
1	B	366/377 (97%)	360 (98%)	6 (2%)	55	50
All	All	729/754 (97%)	714 (98%)	15 (2%)	47	40

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

Mol	Chain	Res	Type
1	A	300	PHE
1	A	316	LEU
1	A	337	LEU
1	A	419	ILE
1	A	485	TYR
1	A	493	LEU
1	A	523	LEU
1	A	527	ASN
1	A	616	LEU
1	B	303	VAL

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Mol	Chain	Res	Type
1	B	316	LEU
1	B	337	LEU
1	B	423	LYS
1	B	455	LEU
1	B	523	LEU

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

Mol	Chain	Res	Type
1	A	451	ASN
1	A	454	ASN
1	A	500	GLN
1	A	535	GLN
1	A	634	ASN
1	A	697	ASN
1	B	364	GLN
1	B	377	HIS
1	B	407	HIS
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	664	ASN
1	B	697	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	A	750	1	50,50,50	1.19	3 (6%)	67,82,82	1.21	7 (10%)
4	HEM	B	750	1	50,50,50	1.20	4 (8%)	67,82,82	1.13	4 (5%)
2	ACT	A	860	-	3,3,3	0.92	0	3,3,3	0.83	0
5	H4B	A	760	-	17,18,18	1.64	3 (17%)	14,26,26	2.09	4 (28%)
5	H4B	B	761	-	17,18,18	1.92	5 (29%)	14,26,26	1.86	4 (28%)
6	DP1	A	790	-	16,21,21	0.86	0	20,26,26	0.86	0
2	ACT	B	861	-	3,3,3	0.96	0	3,3,3	0.71	0
6	DP1	B	791	-	16,21,21	0.85	0	20,26,26	0.97	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
4	HEM	A	750	1	-	0/14/54/54	-
4	HEM	B	750	1	-	2/14/54/54	-
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
5	H4B	B	761	-	-	0/8/17/17	0/2/2/2
6	DP1	A	790	-	-	7/23/26/26	-
6	DP1	B	791	-	-	6/23/26/26	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	761	H4B	C6-N5	4.41	1.55	1.47
5	B	761	H4B	C4A-N5	3.96	1.47	1.37
5	A	760	H4B	C6-N5	3.95	1.54	1.47
5	A	760	H4B	C4A-N5	3.86	1.46	1.37
4	B	750	HEM	CAB-C3B	-3.04	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	750	HEM	CMD-C2D	2.63	1.56	1.50
5	B	761	H4B	C7-N8	2.56	1.49	1.46
4	A	750	HEM	FE-NA	2.40	2.03	1.95
4	B	750	HEM	CHB-C1B	2.39	1.43	1.38
5	A	760	H4B	C4-N3	2.36	1.43	1.38
4	A	750	HEM	CHD-C4C	2.33	1.42	1.38
4	B	750	HEM	CAC-C3C	-2.29	1.41	1.47
5	B	761	H4B	C8A-N1	2.25	1.39	1.36
5	B	761	H4B	C9-C10	2.13	1.56	1.53
4	A	750	HEM	CMA-C3A	2.01	1.54	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	760	H4B	C2-N1-C8A	5.71	123.44	113.36
5	B	761	H4B	C2-N1-C8A	4.82	121.86	113.36
5	A	760	H4B	N3-C2-N1	-3.23	117.42	123.32
5	B	761	H4B	N3-C2-N1	-2.87	118.06	123.32
4	A	750	HEM	C3B-C4B-NB	2.75	111.44	109.47
4	A	750	HEM	C4B-C3B-C2B	-2.72	104.78	107.28
5	A	760	H4B	O10-C10-C9	-2.70	105.31	109.77
4	A	750	HEM	CMA-C3A-C4A	2.64	129.44	125.42
5	B	761	H4B	O9-C9-C6	2.54	115.37	109.28
4	A	750	HEM	C3B-C2B-C1B	2.38	108.20	106.41
5	B	761	H4B	O10-C10-C9	-2.29	105.98	109.77
4	A	750	HEM	CAB-C3B-C2B	-2.23	121.19	128.43
4	B	750	HEM	C3B-C4B-NB	2.21	111.06	109.47
4	B	750	HEM	C4C-NC-C1C	-2.13	102.36	105.82
4	B	750	HEM	C4A-CHB-C1B	-2.08	121.35	126.25
5	A	760	H4B	O9-C9-C6	2.08	114.25	109.28
4	A	750	HEM	CHC-C4B-NB	-2.07	122.20	124.42
4	A	750	HEM	CAB-C3B-C4B	2.06	133.51	124.39
4	B	750	HEM	C4A-NA-C1A	-2.05	102.48	105.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	790	DP1	O'-C'-CA'-CB'
6	A	790	DP1	N1'-C'-CA'-CB'
6	B	791	DP1	N-CA-CB-CG
6	B	791	DP1	N1'-C'-CA'-CB'

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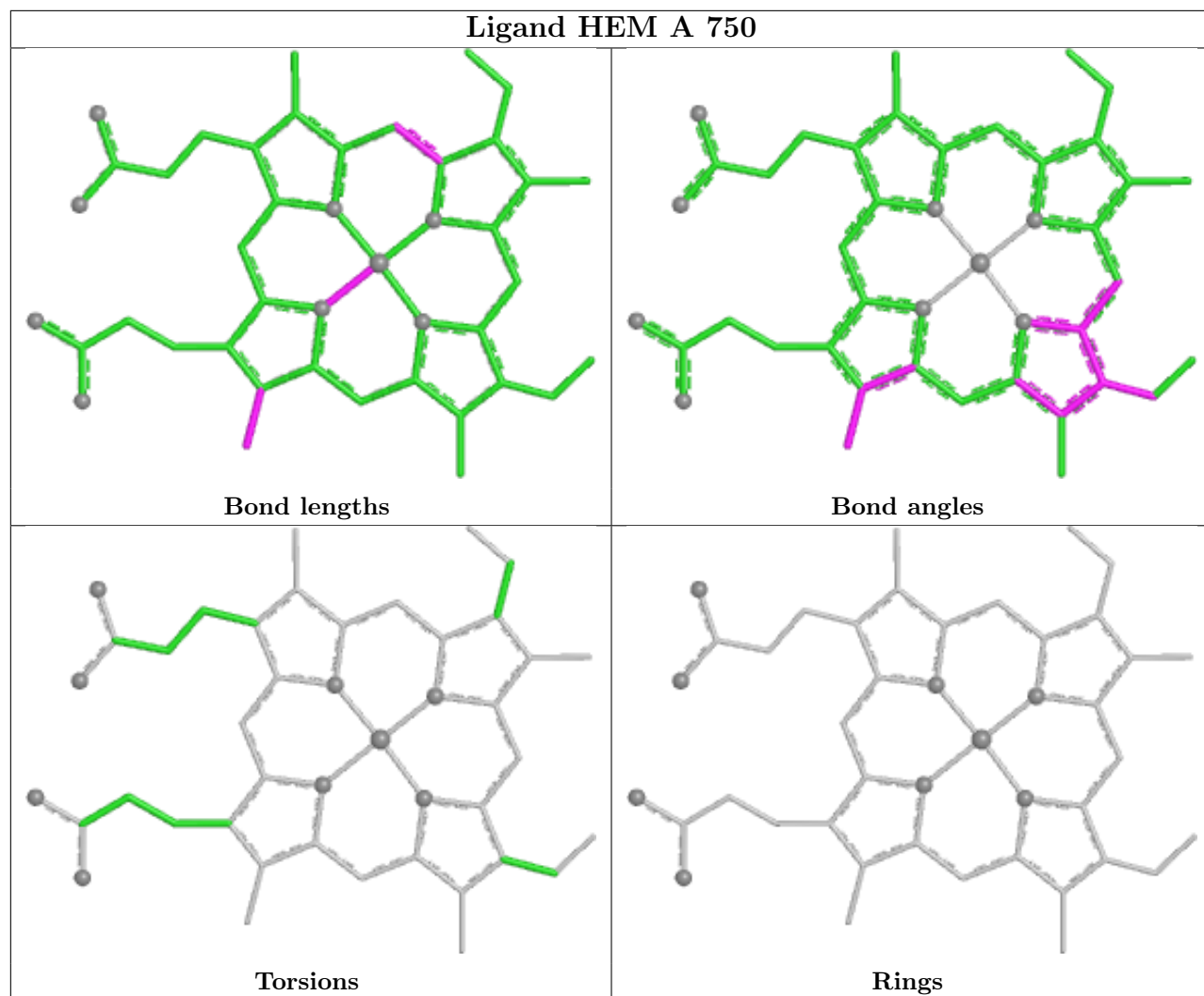
Mol	Chain	Res	Type	Atoms
6	B	791	DP1	C-CA-CB-CG
6	B	791	DP1	O'-C'-CA'-CB'
4	B	750	HEM	C2B-C3B-CAB-CBB
6	A	790	DP1	O'-C'-CA'-N'
6	A	790	DP1	N1'-C'-CA'-N'
6	B	791	DP1	O'-C'-CA'-N'
6	B	791	DP1	N1'-C'-CA'-N'
6	A	790	DP1	C-CA-CB-CG
4	B	750	HEM	C4B-C3B-CAB-CBB
6	A	790	DP1	N-CA-CB-CG
6	A	790	DP1	N1-C1-CB'-CA'

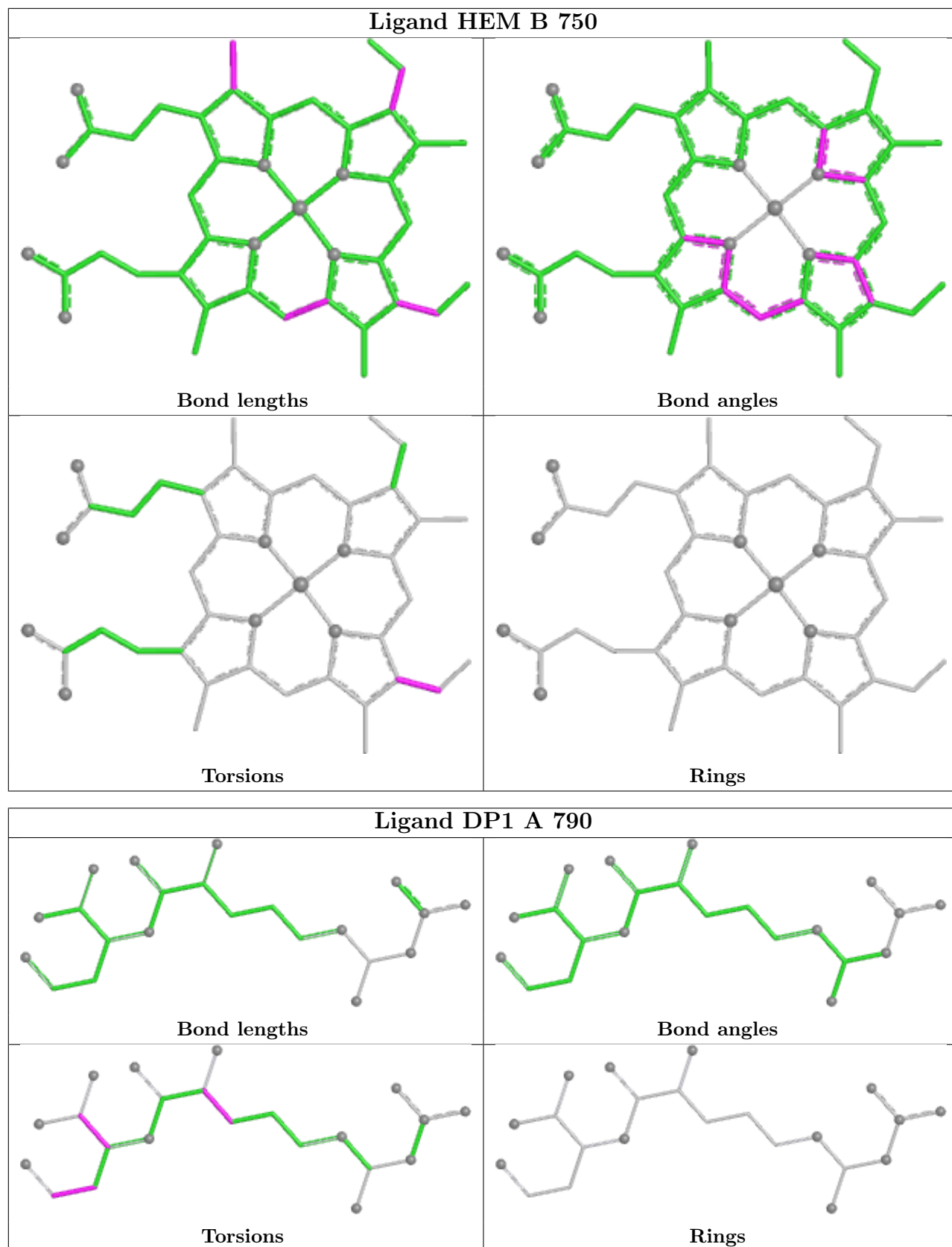
There are no ring outliers.

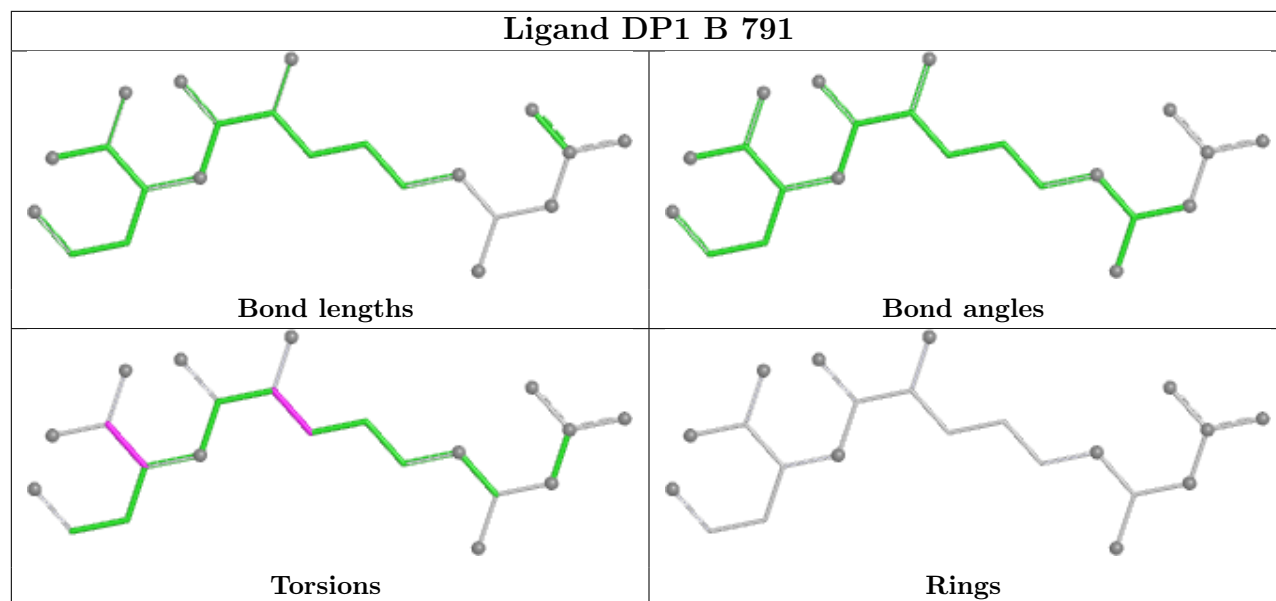
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	750	HEM	4	0
4	B	750	HEM	3	0
2	A	860	ACT	2	0
5	A	760	H4B	1	0
6	A	790	DP1	1	0
6	B	791	DP1	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.







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%)	1.05	67 (16%) 4 5	22, 41, 66, 78	0
1	B	410/421 (97%)	0.48	26 (6%) 26 34	21, 33, 56, 71	0
All	All	817/842 (97%)	0.76	93 (11%) 10 13	21, 37, 63, 78	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	5.2
1	A	715	VAL	4.8
1	B	348	VAL	4.4
1	A	322	LEU	3.9
1	A	300	PHE	3.9
1	B	322	LEU	3.9
1	A	488	PRO	3.8
1	A	513	PRO	3.8
1	A	554	PHE	3.7
1	A	355	PHE	3.7
1	A	493	LEU	3.7
1	A	350	THR	3.5
1	A	486	LYS	3.5
1	B	300	PHE	3.5
1	A	321	THR	3.5
1	A	303	VAL	3.4
1	A	485	TYR	3.4
1	A	551	PHE	3.3
1	B	321	THR	3.3
1	B	350	THR	3.2
1	A	504	ILE	3.2
1	A	512	ALA	3.1
1	A	373	GLY	3.1
1	A	510	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	301	LEU	3.0
1	B	392	SER	3.0
1	A	499	VAL	2.9
1	B	611	ALA	2.9
1	A	506	ILE	2.9
1	A	553	TRP	2.9
1	A	501	PHE	2.8
1	A	552	ASP	2.8
1	A	557	LEU	2.8
1	A	517	PHE	2.8
1	A	381	LEU	2.8
1	B	620	LYS	2.7
1	A	384	VAL	2.7
1	A	337	LEU	2.7
1	A	533	LEU	2.7
1	B	354	LEU	2.7
1	A	338	PRO	2.7
1	B	353	GLN	2.7
1	B	388	ILE	2.6
1	A	645	LYS	2.6
1	A	616	LEU	2.6
1	A	528	GLY	2.6
1	A	710	PRO	2.5
1	B	610	VAL	2.5
1	B	355	PHE	2.5
1	A	535	GLN	2.5
1	A	713	THR	2.5
1	A	712	ASN	2.4
1	A	361	PHE	2.4
1	A	319	LYS	2.4
1	A	376	ALA	2.4
1	A	514	ARG	2.4
1	B	667	ARG	2.4
1	A	611	ALA	2.4
1	B	389	GLU	2.4
1	A	490	GLY	2.4
1	A	509	GLY	2.4
1	A	544	VAL	2.4
1	A	505	CYS	2.4
1	A	667	ARG	2.3
1	B	338	PRO	2.3
1	B	351	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	483	ALA	2.3
1	A	515	GLY	2.3
1	B	618	MET	2.3
1	B	493	LEU	2.3
1	A	520	LEU	2.2
1	A	487	GLN	2.2
1	A	633	ILE	2.2
1	A	489	ASP	2.2
1	A	516	ARG	2.2
1	B	619	ARG	2.2
1	B	535	GLN	2.2
1	A	466	THR	2.2
1	A	363	ASP	2.2
1	A	320	SER	2.2
1	B	337	LEU	2.2
1	B	319	LYS	2.2
1	A	354	LEU	2.1
1	A	559	LEU	2.1
1	A	494	GLY	2.1
1	A	641	PHE	2.1
1	B	352	ASP	2.1
1	A	606	ILE	2.0
1	B	336	MET	2.0
1	B	616	LEU	2.0
1	A	388	ILE	2.0
1	A	546	ILE	2.0
1	A	529	ASN	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,

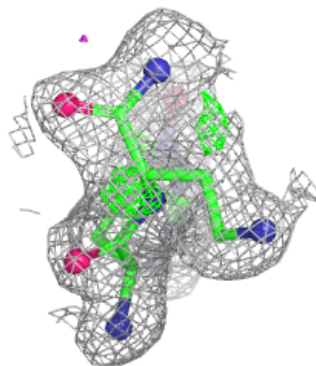
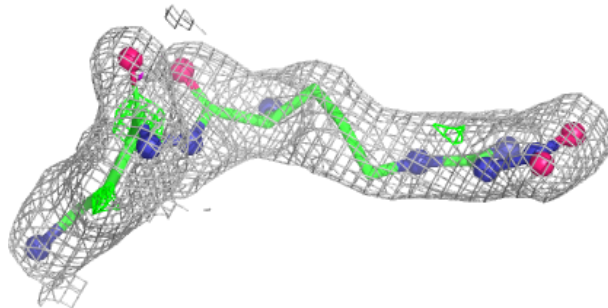
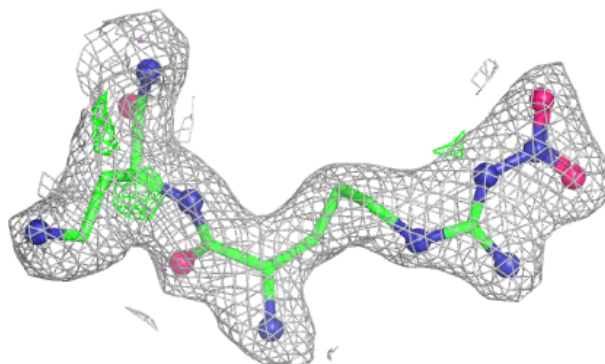
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DP1	B	791	22/22	0.85	0.12	28,34,37,38	0
6	DP1	A	790	22/22	0.87	0.12	31,37,43,44	0
2	ACT	A	860	4/4	0.91	0.15	64,64,64,64	0
2	ACT	B	861	4/4	0.92	0.12	42,43,43,44	0
5	H4B	B	761	17/17	0.95	0.06	22,24,29,30	0
5	H4B	A	760	17/17	0.96	0.07	24,25,30,31	0
4	HEM	A	750	43/43	0.97	0.07	24,27,28,28	0
4	HEM	B	750	43/43	0.98	0.07	22,24,27,29	0
3	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.

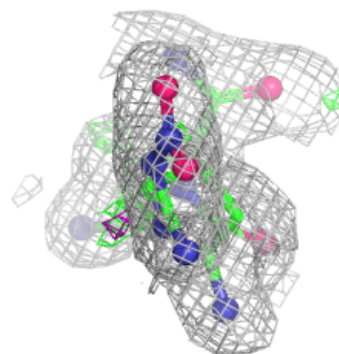
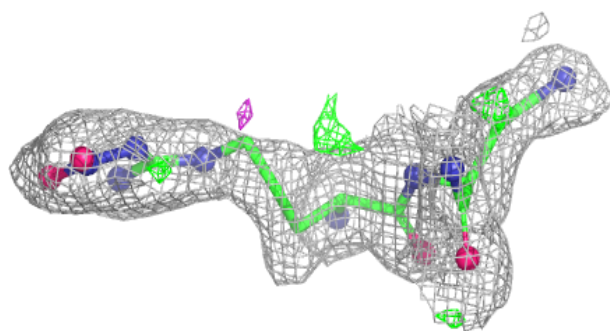
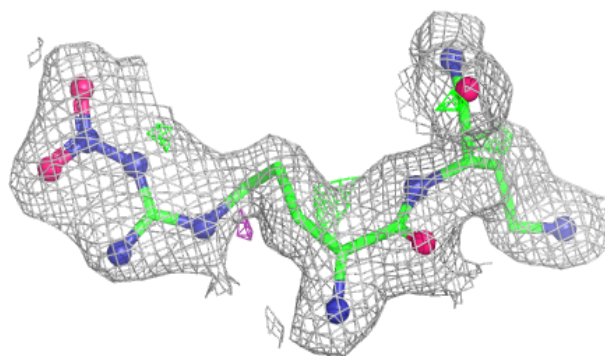
Electron density around DP1 B 791:

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



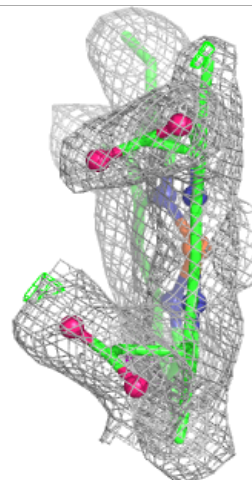
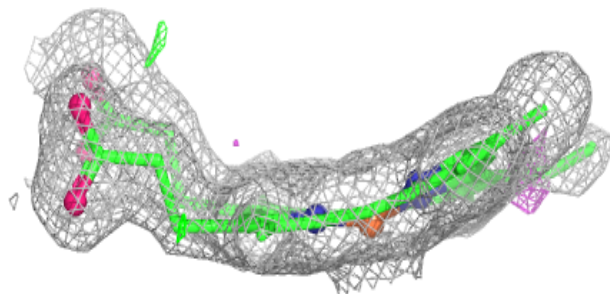
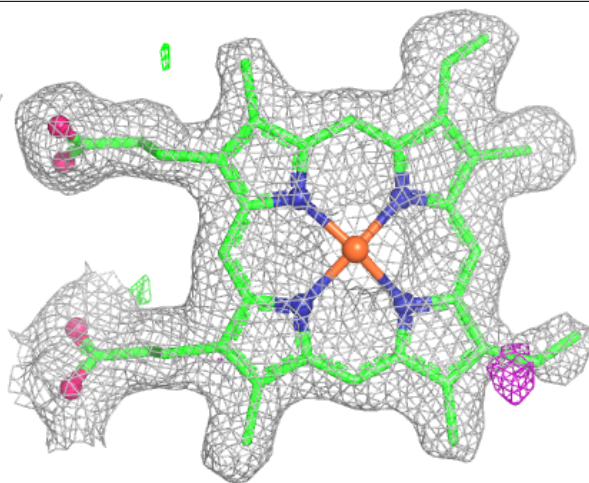
Electron density around DP1 A 790:

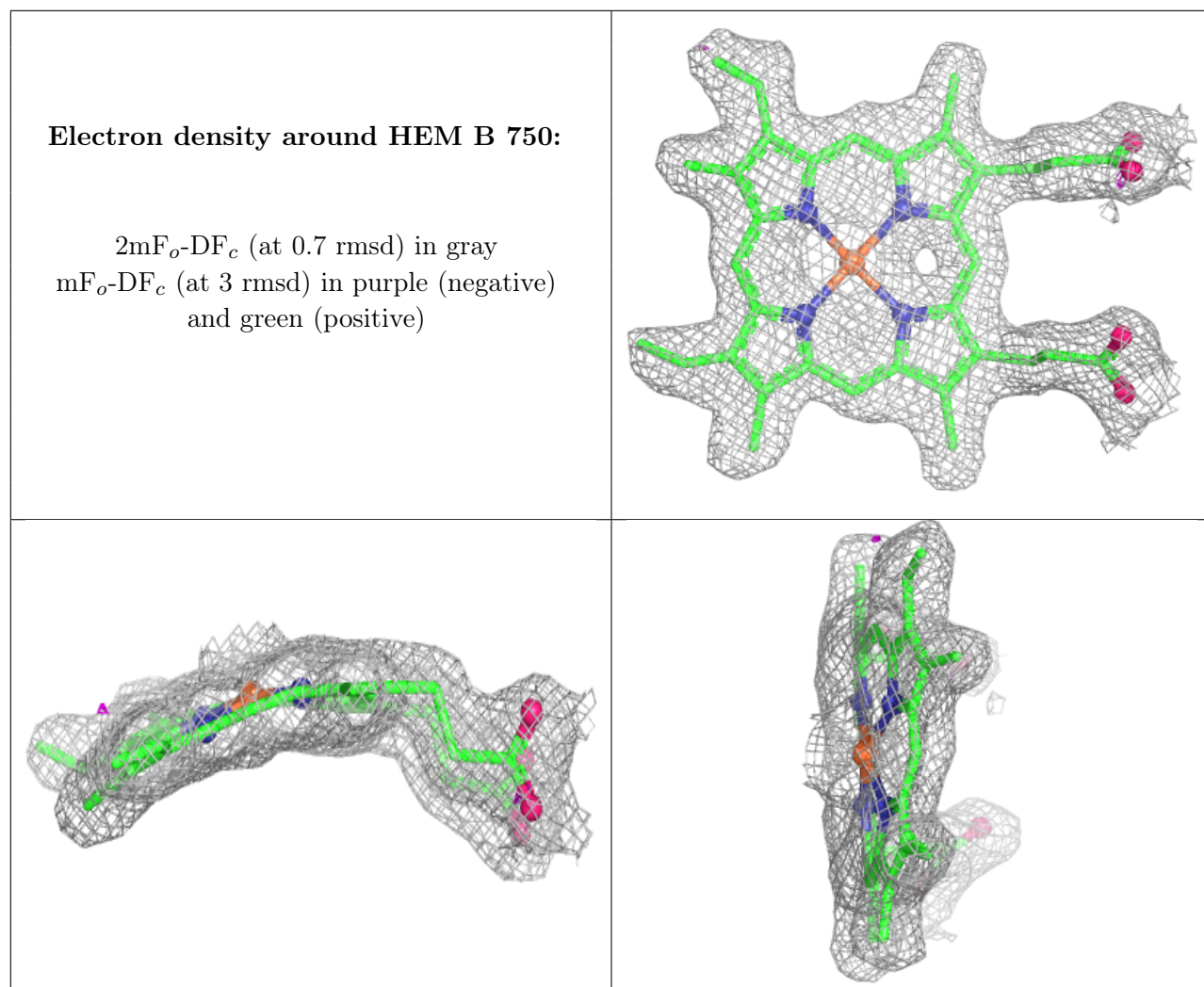
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 750:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.