



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:18 AM UTC

PDB ID : 1ZZQ / pdb_00001zzq
Title : Rat nNOS D597N mutant with L-N(omega)-Nitroarginine-(4R)-amino-L-proline amide bound
Authors : Li, H.; Flinspach, M.L.; Igarashi, J.; Jamal, J.; Yang, W.; Gomez-Vidal, J.A.; Litzinger, E.A.; Silverman, R.B.; Poulos, T.L.
Deposited on : 2005-06-14
Resolution : 1.90 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

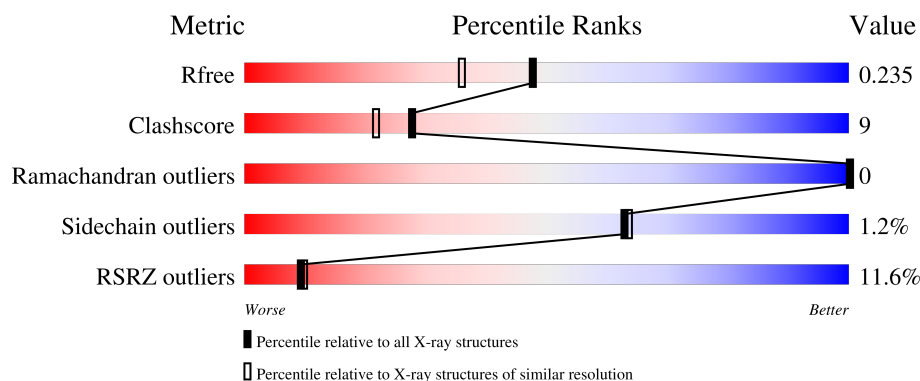
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	420	18% 73% 23% ..
1	B	420	4% 79% 18% ..

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7441 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.

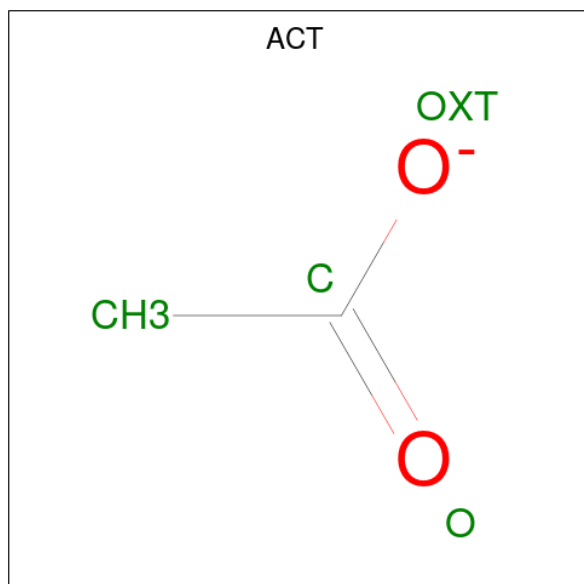
- Molecule 1 is a protein called Nitric-oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	6	0
			3327	2126	570	609	22			
1	B	410	Total	C	N	O	S	0	6	0
			3354	2143	577	613	21			

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 ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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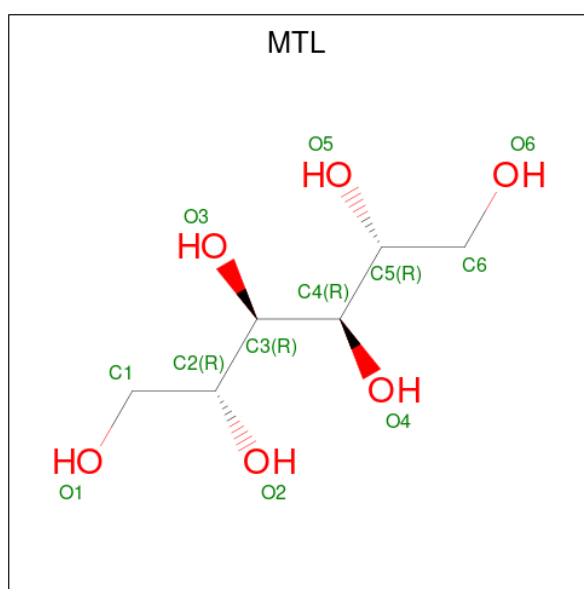
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

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

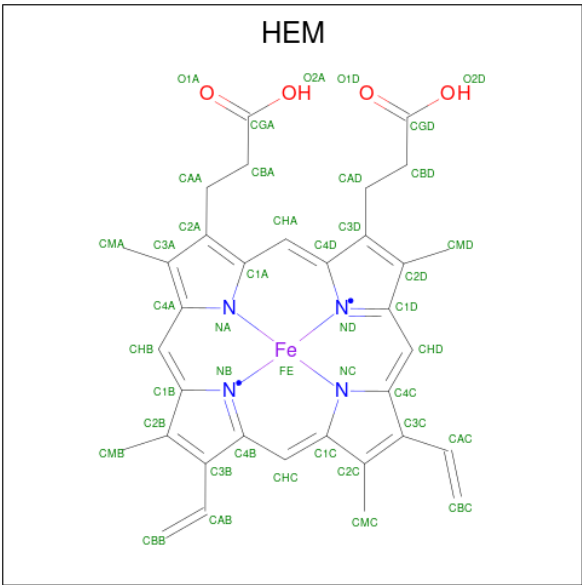
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is D-MANNITOL (CCD ID: MTL) (formula: C₆H₁₄O₆).



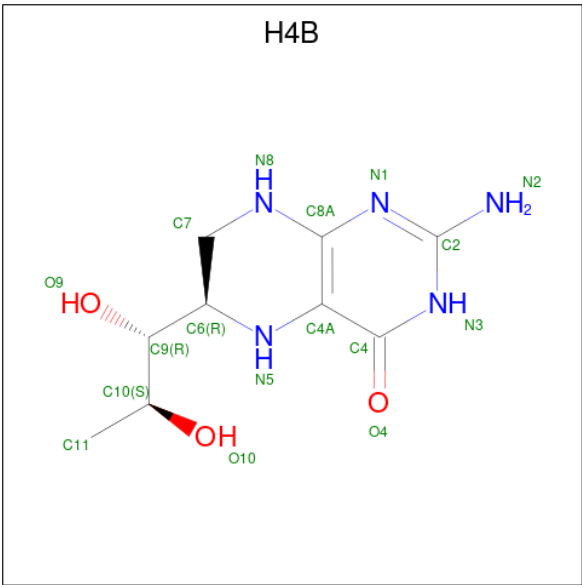
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		

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



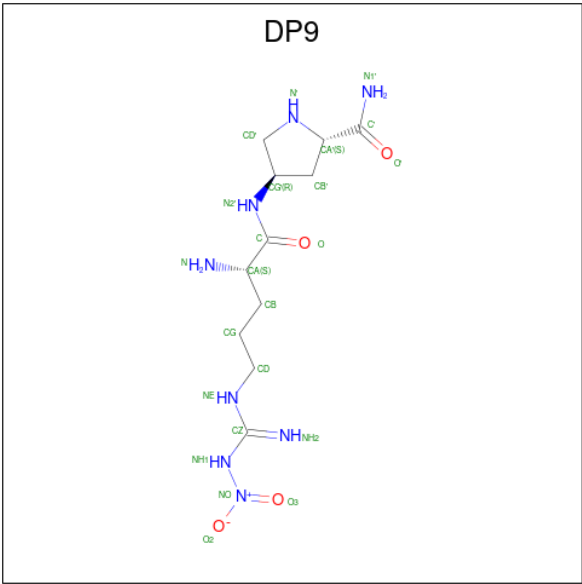
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 7 is L-N(OMEGA)-NITROARGININE-(4R)-AMINO-L-PROLINE AMIDE (CCD ID: DP9) (formula: C₁₁H₂₂N₈O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	1
			46	22	16	8		
7	B	1	Total	C	N	O	0	1
			45	22	15	8		

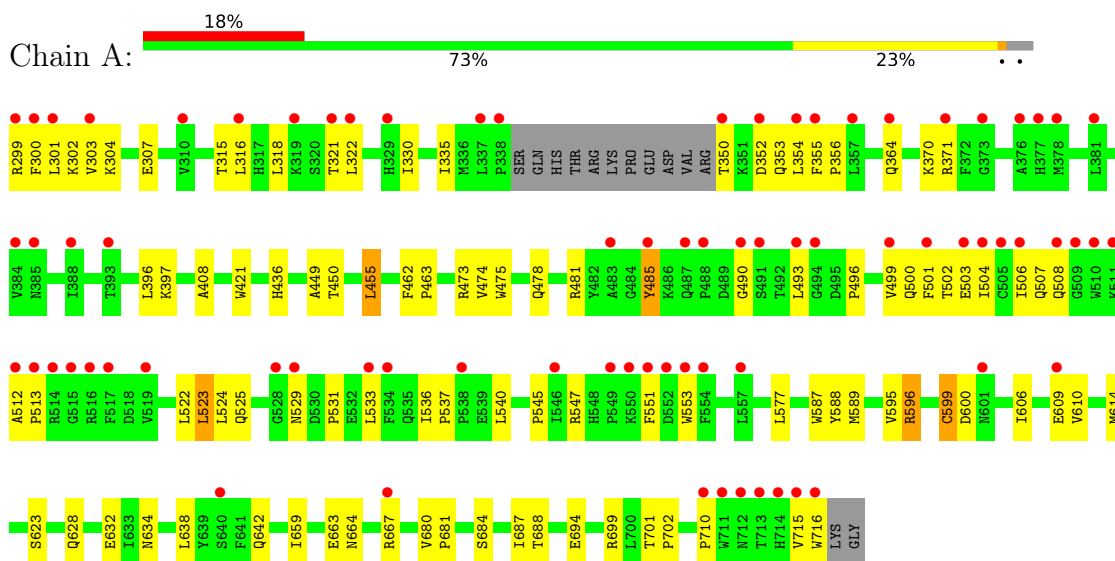
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	225	Total	O	0	3
			225	225		
8	B	291	Total	O	0	4
			291	291		

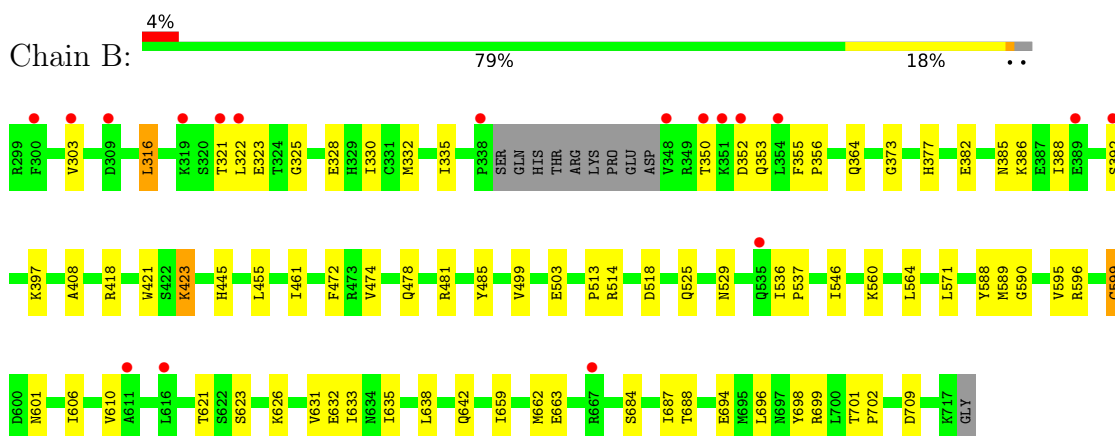
3 Residue-property plots [i](#)

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	51.86Å 110.32Å 164.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.89 – 1.90 35.89 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.8 (35.89-1.90) 99.0 (35.89-1.91)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.244 0.212 , 0.235	Depositor DCC
R_{free} test set	3705 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.8	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	0.95	EDS
Total number of atoms	7441	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 4.70% 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, DP9, H4B, HEM

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	0/3450	0.94	13/4679 (0.3%)
1	B	0.53	0/3477	0.98	19/4714 (0.4%)
All	All	0.50	0/6927	0.96	32/9393 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	MET	N-CA-C	-8.06	96.10	109.24
1	A	589	MET	N-CA-C	-7.76	97.03	109.76
1	A	354	LEU	N-CA-C	7.76	119.52	111.14
1	A	421	TRP	N-CA-C	7.32	120.19	111.33
1	A	490	GLY	N-CA-C	-7.25	106.06	114.69
1	B	474	VAL	N-CA-C	-6.88	97.95	107.99
1	B	421	TRP	N-CA-C	6.78	119.54	111.33
1	B	596	ARG	N-CA-C	6.70	118.46	111.03
1	A	623	SER	N-CA-C	-6.32	105.54	113.18
1	B	590	GLY	N-CA-C	6.08	120.25	112.83
1	A	688	THR	N-CA-C	-5.90	101.41	110.32
1	A	599	CYS	N-CA-C	5.85	120.58	113.38
1	A	588	TYR	N-CA-C	5.83	119.11	110.48
1	B	623	SER	N-CA-C	-5.80	106.16	113.18
1	B	635	ILE	N-CA-C	-5.78	104.88	110.72
1	A	606	ILE	N-CA-C	5.77	117.72	112.29
1	B	588	TYR	N-CA-C	5.72	118.94	110.48
1	B	599	CYS	N-CA-C	5.58	120.97	113.72
1	B	418	ARG	N-CA-C	5.56	119.54	112.87
1	A	596	ARG	N-CA-C	5.52	118.36	111.24
1	B	688	THR	N-CA-C	-5.48	102.57	110.40
1	B	461	ILE	N-CA-C	5.43	115.40	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	397	LYS	N-CA-C	-5.39	103.27	110.55
1	B	709	ASP	CA-C-N	5.37	125.44	119.32
1	B	709	ASP	C-N-CA	5.37	125.44	119.32
1	B	564	LEU	N-CA-C	5.37	118.35	108.69
1	A	474	VAL	N-CA-C	-5.34	99.47	107.37
1	A	408	ALA	N-CA-C	-5.22	105.59	111.28
1	B	455	LEU	N-CA-C	5.21	117.59	110.24
1	B	408	ALA	N-CA-C	-5.18	105.63	111.28
1	B	472	PHE	N-CA-C	-5.17	100.82	109.24
1	A	455	LEU	N-CA-C	5.14	117.49	110.24

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	3327	0	3238	77	0
1	B	3354	0	3273	50	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
4	A	12	0	14	1	0
4	B	12	0	14	0	0
5	A	43	0	30	2	0
5	B	43	0	30	0	0
6	A	17	0	15	0	0
6	B	17	0	15	0	0
7	A	46	0	42	0	0
7	B	45	0	39	1	0
8	A	225	0	0	9	0
8	B	291	0	0	8	0
All	All	7441	0	6716	123	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 9.

All (123) 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	1.16	0.92
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.50	0.91
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.03	0.74
1:B:373:GLY:H	1:B:377:HIS:CD2	2.07	0.70
1:B:350:THR:HG22	1:B:352:ASP:H	1.58	0.69
1:A:350:THR:HG22	1:A:352:ASP:H	1.58	0.69
1:B:325:GLY:O	1:B:332:MET:HE2	1.95	0.67
5:A:750:HEM:HMC2	5:A:750:HEM:HBC2	1.77	0.64
1:A:350:THR:HB	1:A:353:GLN:HG3	1.79	0.64
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.21	0.64
1:B:350:THR:HB	1:B:353:GLN:HG2	1.79	0.64
1:A:436:HIS:HB2	8:A:998:HOH:O	1.98	0.62
1:A:506:ILE:HD11	1:A:512:ALA:HB2	1.81	0.62
1:A:303:VAL:HG13	1:A:694:GLU:HB2	1.81	0.62
1:A:503:GLU:HG3	8:A:1001:HOH:O	2.00	0.61
1:A:307:GLU:HG3	8:B:914:HOH:O	2.01	0.60
1:A:664:ASN:HA	1:A:667:ARG:NH1	2.15	0.60
1:A:502:THR:O	1:A:506:ILE:HG12	2.01	0.60
1:A:364:GLN:HG2	8:A:1088:HOH:O	2.01	0.60
1:A:299:ARG:HA	8:A:1077:HOH:O	2.01	0.59
1:A:614:MET:CE	1:A:632:GLU:HG3	2.33	0.59
1:B:382[A]:GLU:OE2	1:B:386:LYS:HE3	2.02	0.59
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.83	0.58
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.85	0.58
1:A:397:LYS:NZ	8:A:1093:HOH:O	2.38	0.57
1:A:545:PRO:HG2	1:A:547:ARG:HH11	1.71	0.56
1:A:370:LYS:C	1:A:371:ARG:HG2	2.31	0.55
1:B:499:VAL:O	1:B:503:GLU:HG3	2.06	0.55
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.31	0.55
1:A:524:LEU:O	1:A:531:PRO:HA	2.06	0.55
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.23	0.53
1:A:304:LYS:O	1:A:694:GLU:HG3	2.09	0.53
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.39	0.53
1:A:609:GLU:HG3	8:A:986:HOH:O	2.08	0.53
1:A:595:VAL:HG23	1:A:634:ASN:HD21	1.75	0.52
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.90	0.52
1:A:667:ARG:HD3	8:A:1024:HOH:O	2.11	0.51
1:A:504:ILE:O	1:A:508:GLN:HB2	2.10	0.51
1:B:546:ILE:HG12	1:B:560:LYS:HA	1.93	0.50
1:A:350:THR:HB	1:A:353:GLN:CG	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:PHE:HB2	4:A:870:MTL:H61	1.93	0.50
1:A:614:MET:HE3	1:A:632:GLU:HG3	1.93	0.50
1:B:478:GLN:HB2	1:B:481[B]:ARG:CG	2.42	0.50
1:B:626:LYS:NZ	8:B:1141:HOH:O	2.45	0.50
1:B:638:LEU:O	1:B:642:GLN:HG3	2.11	0.49
1:A:299:ARG:HE	1:A:318:LEU:HD13	1.77	0.49
1:A:300:PHE:CD2	1:A:315:THR:HG22	2.47	0.49
1:B:659:ILE:O	1:B:663:GLU:HG3	2.12	0.49
1:B:323:GLU:O	1:B:699:ARG:HD3	2.13	0.49
1:A:715:VAL:O	1:A:715:VAL:HG23	2.12	0.48
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.94	0.48
1:A:364:GLN:HG3	8:A:1031:HOH:O	2.14	0.48
1:B:445:HIS:C	1:B:445:HIS:CD2	2.92	0.48
1:B:478:GLN:HB2	1:B:481[A]:ARG:HG3	1.95	0.48
1:A:303:VAL:CG1	1:A:694:GLU:O	2.62	0.48
1:A:536:ILE:O	1:A:537:PRO:C	2.55	0.47
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.49	0.47
1:B:595:VAL:O	1:B:599:CYS:HB2	2.14	0.47
1:A:449:ALA:O	1:A:455:LEU:HA	2.15	0.47
1:A:659:ILE:O	1:A:663:GLU:HG3	2.15	0.47
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.49	0.47
1:A:701:THR:HA	1:A:702:PRO:C	2.40	0.47
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.44	0.47
1:B:701:THR:HA	1:B:702:PRO:C	2.40	0.47
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.97	0.46
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.49	0.46
1:B:321:THR:HG23	1:B:322:LEU:N	2.31	0.46
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.98	0.46
1:A:610:VAL:O	1:A:614:MET:HG3	2.16	0.46
1:B:662:MET:HE3	8:B:922:HOH:O	2.15	0.46
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.97	0.46
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.98	0.46
1:B:684:SER:HB3	1:B:687:ILE:HG12	1.98	0.46
1:B:321:THR:HG23	1:B:322:LEU:H	1.80	0.45
7:B:800[B]:DP9:HG1	8:B:926[B]:HOH:O	2.16	0.45
1:B:606:ILE:HD11	1:B:633:ILE:HD13	1.97	0.45
1:B:621:THR:HG22	8:B:1140:HOH:O	2.16	0.45
1:A:303:VAL:HG11	1:A:694:GLU:O	2.17	0.45
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.98	0.45
1:B:525:GLN:HG3	1:B:529:ASN:O	2.16	0.45
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:GLN:CD	1:B:481[A]:ARG:HE	2.25	0.44
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.99	0.44
1:B:355:PHE:N	1:B:356:PRO:HD2	2.31	0.44
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.82	0.44
1:A:478:GLN:HB2	1:A:481[A]:ARG:HG3	1.99	0.44
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.86	0.44
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.53	0.43
1:B:478:GLN:HB2	1:B:481[B]:ARG:HG3	2.00	0.43
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.98	0.43
1:A:396:LEU:HG	1:A:577:LEU:HD12	2.00	0.43
1:A:525:GLN:HG3	1:A:529:ASN:O	2.19	0.43
1:B:364:GLN:NE2	8:B:1109:HOH:O	2.52	0.43
1:A:355:PHE:N	1:A:356:PRO:HD2	2.33	0.43
1:B:316:LEU:HB3	1:B:698:TYR:OH	2.19	0.43
1:B:571:LEU:C	1:B:571:LEU:HD23	2.43	0.42
1:B:423:LYS:NZ	8:B:1152:HOH:O	2.28	0.42
1:A:450:THR:HA	1:A:455:LEU:HD22	2.01	0.42
1:A:522:LEU:O	1:A:533:LEU:HA	2.20	0.42
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.50	0.42
1:A:302:LYS:NZ	8:A:1084:HOH:O	2.52	0.42
1:A:500:GLN:O	1:A:504:ILE:HG13	2.19	0.42
1:A:322:LEU:HB2	1:A:699:ARG:HB2	2.01	0.42
1:A:350:THR:HB	1:A:353:GLN:CD	2.45	0.42
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.50	0.42
1:A:475:TRP:CE3	1:A:523:LEU:HD13	2.54	0.42
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.87	0.42
1:A:370:LYS:O	1:A:371:ARG:HG2	2.20	0.41
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.55	0.41
1:B:321:THR:HG23	1:B:322:LEU:HG	2.02	0.41
1:A:595:VAL:O	1:A:599:CYS:HB2	2.20	0.41
1:A:716:TRP:H	1:A:716:TRP:CD1	2.38	0.41
1:A:596:ARG:O	1:A:600:ASP:HB2	2.20	0.41
5:A:750:HEM:HHC	5:A:750:HEM:HBB2	2.02	0.41
1:B:601:ASN:HB3	8:B:1090:HOH:O	2.20	0.41
1:A:628:GLN:CG	1:B:631:VAL:HG11	2.51	0.41
1:A:638:LEU:O	1:A:642:GLN:HG3	2.20	0.41
1:B:388:ILE:O	1:B:392:SER:N	2.49	0.41
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.02	0.40
1:B:536:ILE:O	1:B:537:PRO:C	2.62	0.40
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.54	0.40
1:A:503:GLU:O	1:A:507:GLN:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/420 (97%)	391 (96%)	18 (4%)	0	100	100
1	B	412/420 (98%)	403 (98%)	9 (2%)	0	100	100
All	All	821/840 (98%)	794 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/375 (98%)	364 (99%)	5 (1%)	59	59
1	B	372/375 (99%)	368 (99%)	4 (1%)	65	67
All	All	741/750 (99%)	732 (99%)	9 (1%)	63	63

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	LEU
1	A	321	THR
1	A	485	TYR
1	A	493	LEU
1	A	523	LEU
1	B	303	VAL
1	B	316	LEU
1	B	328	GLU
1	B	423	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	A	425	GLN
1	A	451	ASN
1	A	454	ASN
1	A	500	GLN
1	A	507	GLN
1	A	628	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	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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	1.24	7 (14%)	67,82,82	1.22	5 (7%)
2	ACT	A	860	-	3,3,3	0.89	0	3,3,3	0.80	0
7	DP9	A	799[A]	-	17,23,23	1.05	1 (5%)	20,30,30	1.88	6 (30%)
7	DP9	A	799[B]	-	17,23,23	0.94	1 (5%)	20,30,30	1.95	5 (25%)
2	ACT	B	861	-	3,3,3	0.92	0	3,3,3	0.73	0
4	MTL	A	870	-	11,11,11	1.07	0	14,14,14	0.72	0
5	HEM	B	750	1	50,50,50	1.12	3 (6%)	67,82,82	1.22	7 (10%)
6	H4B	A	760	-	17,18,18	1.46	3 (17%)	14,26,26	2.08	4 (28%)
7	DP9	B	800[B]	-	16,22,23	66.53	3 (18%)	18,28,30	2.02	5 (27%)
6	H4B	B	761	-	17,18,18	1.70	3 (17%)	14,26,26	1.85	3 (21%)
4	MTL	B	871	-	11,11,11	0.94	0	14,14,14	0.75	0
7	DP9	B	800[A]	-	17,23,23	0.99	1 (5%)	20,30,30	1.99	6 (30%)

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	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DP9	A	799[A]	-	-	1/20/32/32	0/1/1/1
7	DP9	A	799[B]	-	-	8/20/32/32	0/1/1/1
4	MTL	A	870	-	-	0/16/16/16	-
5	HEM	B	750	1	-	1/14/54/54	-
6	H4B	A	760	-	-	0/8/17/17	0/2/2/2
7	DP9	B	800[B]	-	-	6/17/29/32	0/1/1/1
6	H4B	B	761	-	-	0/8/17/17	0/2/2/2
4	MTL	B	871	-	-	0/16/16/16	-
7	DP9	B	800[A]	-	-	2/20/32/32	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	800[B]	DP9	O3-NO	266.10	8.17	1.24
6	A	760	H4B	C4A-N5	3.90	1.47	1.37
6	B	761	H4B	C4A-N5	3.82	1.46	1.37
6	B	761	H4B	C6-N5	3.60	1.53	1.47
6	A	760	H4B	C6-N5	3.12	1.53	1.47
5	A	750	HEM	CHD-C4C	3.08	1.44	1.38
5	B	750	HEM	CMD-C2D	2.98	1.56	1.50
7	A	799[A]	DP9	CG'-N2'	2.88	1.52	1.46
7	B	800[A]	DP9	CG'-N2'	2.73	1.52	1.46
5	A	750	HEM	FE-NB	2.49	2.02	1.94
7	B	800[B]	DP9	CG'-N2'	2.46	1.51	1.46
7	A	799[B]	DP9	CG'-N2'	2.41	1.51	1.46
5	B	750	HEM	CAB-C3B	-2.33	1.41	1.47
5	A	750	HEM	CAC-C3C	-2.25	1.41	1.47
7	B	800[B]	DP9	CA-C	2.25	1.55	1.51
5	A	750	HEM	CAB-C3B	-2.18	1.41	1.47
6	B	761	H4B	C7-N8	2.12	1.48	1.46
5	B	750	HEM	CMB-C2B	2.11	1.55	1.50
5	A	750	HEM	CMA-C3A	2.09	1.55	1.50
6	A	760	H4B	C4-N3	2.07	1.42	1.38
5	A	750	HEM	CMC-C2C	2.04	1.55	1.50
5	A	750	HEM	CHC-C1C	2.01	1.42	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	760	H4B	C2-N1-C8A	5.72	123.46	113.36
6	B	761	H4B	C2-N1-C8A	5.24	122.60	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	800[A]	DP9	CD-NE-CZ	4.76	132.18	123.46
7	A	799[B]	DP9	CD-NE-CZ	4.60	131.90	123.46
7	A	799[A]	DP9	CD-NE-CZ	4.57	131.84	123.46
7	B	800[B]	DP9	CD-NE-CZ	4.48	131.68	123.46
7	A	799[B]	DP9	C'-CA'-N'	-4.08	102.75	111.16
7	B	800[B]	DP9	C'-CA'-N'	-3.84	103.24	111.16
7	B	800[B]	DP9	O'-C'-N1'	-3.78	116.37	123.04
7	A	799[B]	DP9	O'-C'-N1'	-3.63	116.63	123.04
7	A	799[A]	DP9	O'-C'-N1'	-3.53	116.81	123.04
7	B	800[A]	DP9	O'-C'-N1'	-3.49	116.87	123.04
7	B	800[A]	DP9	C'-CA'-N'	-3.33	104.30	111.16
6	A	760	H4B	N3-C2-N1	-2.97	117.89	123.32
5	A	750	HEM	C3B-C4B-NB	2.91	111.56	109.47
7	A	799[A]	DP9	C'-CA'-N'	-2.89	105.21	111.16
5	B	750	HEM	CBA-CAA-C2A	-2.88	104.57	112.53
6	A	760	H4B	O10-C10-C9	-2.82	105.11	109.77
7	A	799[B]	DP9	CA'-C'-N1'	2.74	121.42	116.76
7	B	800[B]	DP9	CA'-C'-N1'	2.73	121.41	116.76
6	B	761	H4B	N3-C2-N1	-2.71	118.35	123.32
7	B	800[A]	DP9	CA'-C'-N1'	2.70	121.35	116.76
7	A	799[A]	DP9	CA'-C'-N1'	2.61	121.20	116.76
5	A	750	HEM	CAB-C3B-C2B	-2.57	120.06	128.43
5	B	750	HEM	C2B-C1B-NB	2.50	112.72	109.84
7	B	800[A]	DP9	CG'-N2'-C	2.43	127.20	123.29
5	A	750	HEM	CHC-C4B-NB	-2.34	121.90	124.42
6	B	761	H4B	O10-C10-C9	-2.34	105.90	109.77
7	A	799[A]	DP9	CG'-N2'-C	2.27	126.95	123.29
7	B	800[A]	DP9	NE-CZ-NH2	-2.27	116.08	120.26
5	B	750	HEM	CAB-C3B-C2B	-2.23	121.17	128.43
7	A	799[B]	DP9	NE-CZ-NH2	-2.23	116.15	120.26
5	A	750	HEM	CAB-C3B-C4B	2.20	134.09	124.39
7	B	800[B]	DP9	NE-CZ-NH2	-2.19	116.21	120.26
5	B	750	HEM	C2D-C1D-ND	2.19	112.44	109.90
6	A	760	H4B	O9-C9-C6	2.14	114.40	109.28
7	A	799[A]	DP9	NE-CZ-NH2	-2.10	116.39	120.26
5	B	750	HEM	C4C-NC-C1C	-2.09	102.41	105.82
5	A	750	HEM	C1B-NB-C4B	-2.07	102.75	105.21
5	B	750	HEM	C4A-NA-C1A	-2.06	102.47	105.82
5	B	750	HEM	C3A-C4A-NA	2.05	113.43	110.14

There are no chirality outliers.

All (21) torsion outliers are listed below:

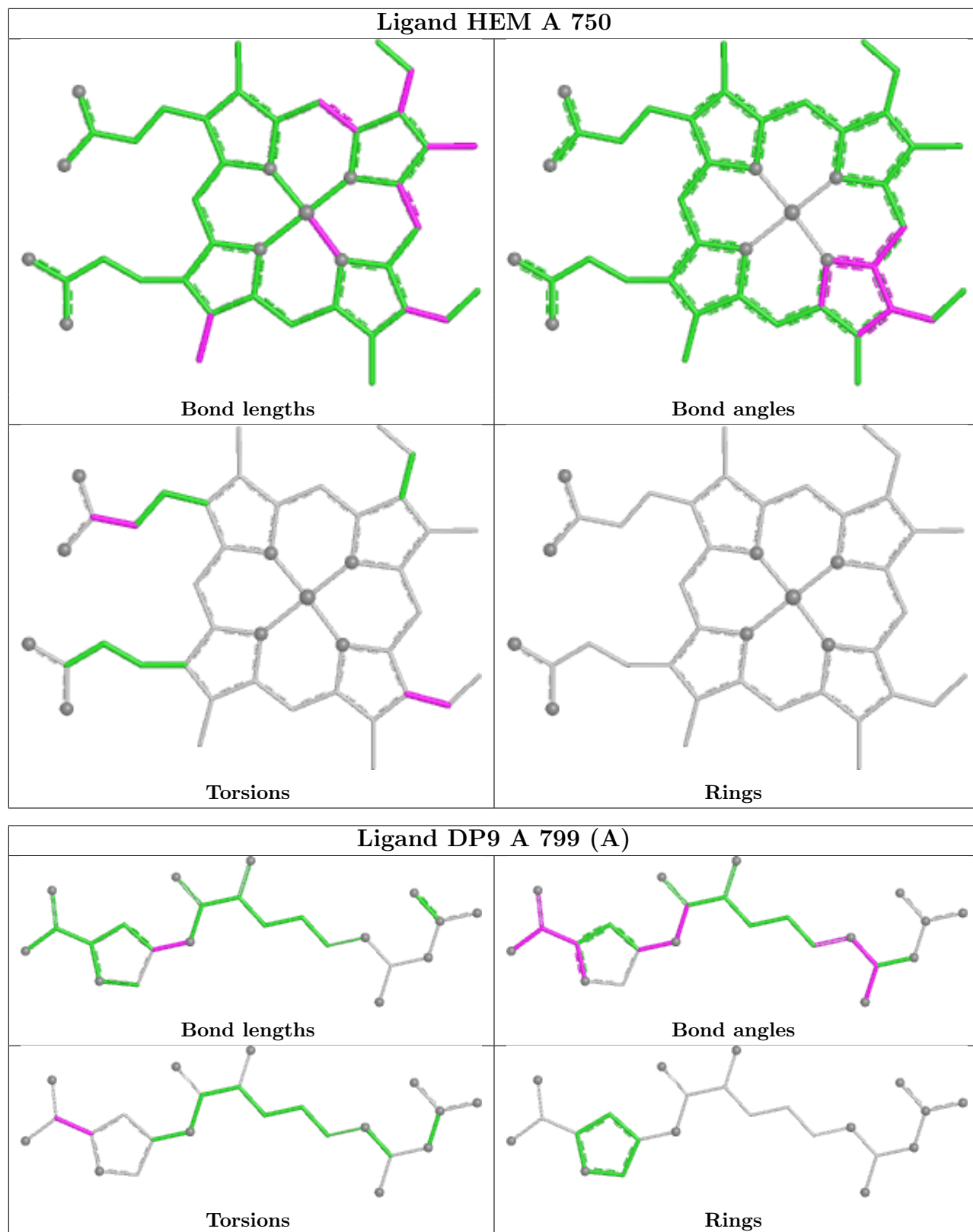
Mol	Chain	Res	Type	Atoms
7	A	799[B]	DP9	O-C-CA-CB
7	A	799[B]	DP9	N2'-C-CA-CB
7	B	800[A]	DP9	N-CA-CB-CG
7	B	800[B]	DP9	CZ-NH1-NO-O3
7	B	800[B]	DP9	N2'-C-CA-CB
7	B	800[B]	DP9	O-C-CA-CB
7	B	800[A]	DP9	C-CA-CB-CG
5	B	750	HEM	C4B-C3B-CAB-CBB
5	A	750	HEM	C4B-C3B-CAB-CBB
7	A	799[A]	DP9	O'-C'-CA'-CB'
7	A	799[B]	DP9	O'-C'-CA'-CB'
7	A	799[B]	DP9	N1'-C'-CA'-CB'
7	B	800[B]	DP9	CA-CB-CG-CD
7	A	799[B]	DP9	CA-CB-CG-CD
7	A	799[B]	DP9	CD'-CG'-N2'-C
7	B	800[B]	DP9	CD'-CG'-N2'-C
7	B	800[B]	DP9	CG-CD-NE-CZ
7	A	799[B]	DP9	CG-CD-NE-CZ
5	A	750	HEM	CAD-CBD-CGD-O2D
7	A	799[B]	DP9	O'-C'-CA'-N'
5	A	750	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

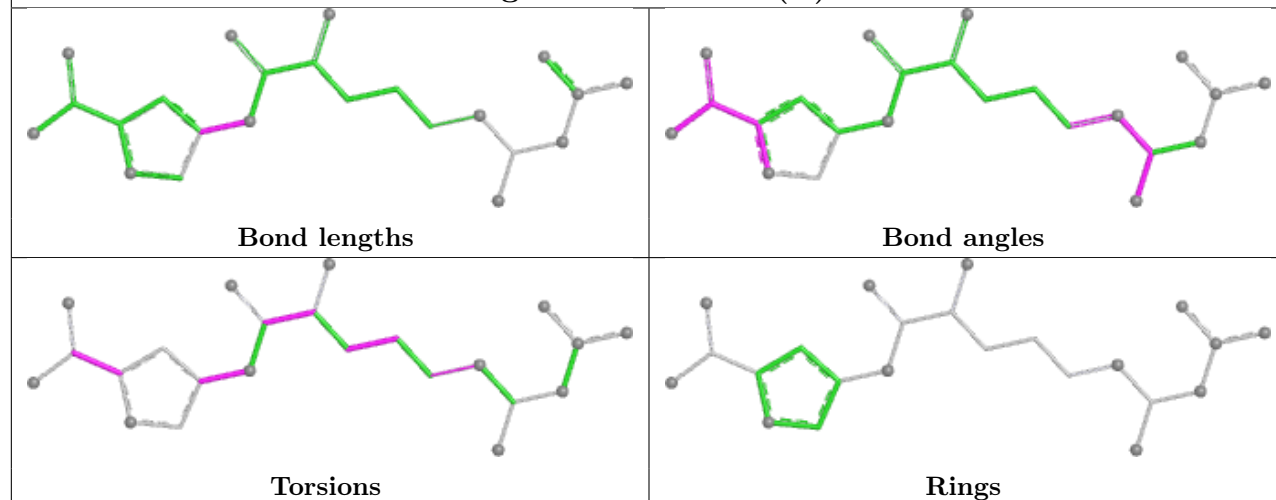
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	750	HEM	2	0
4	A	870	MTL	1	0
7	B	800[B]	DP9	1	0

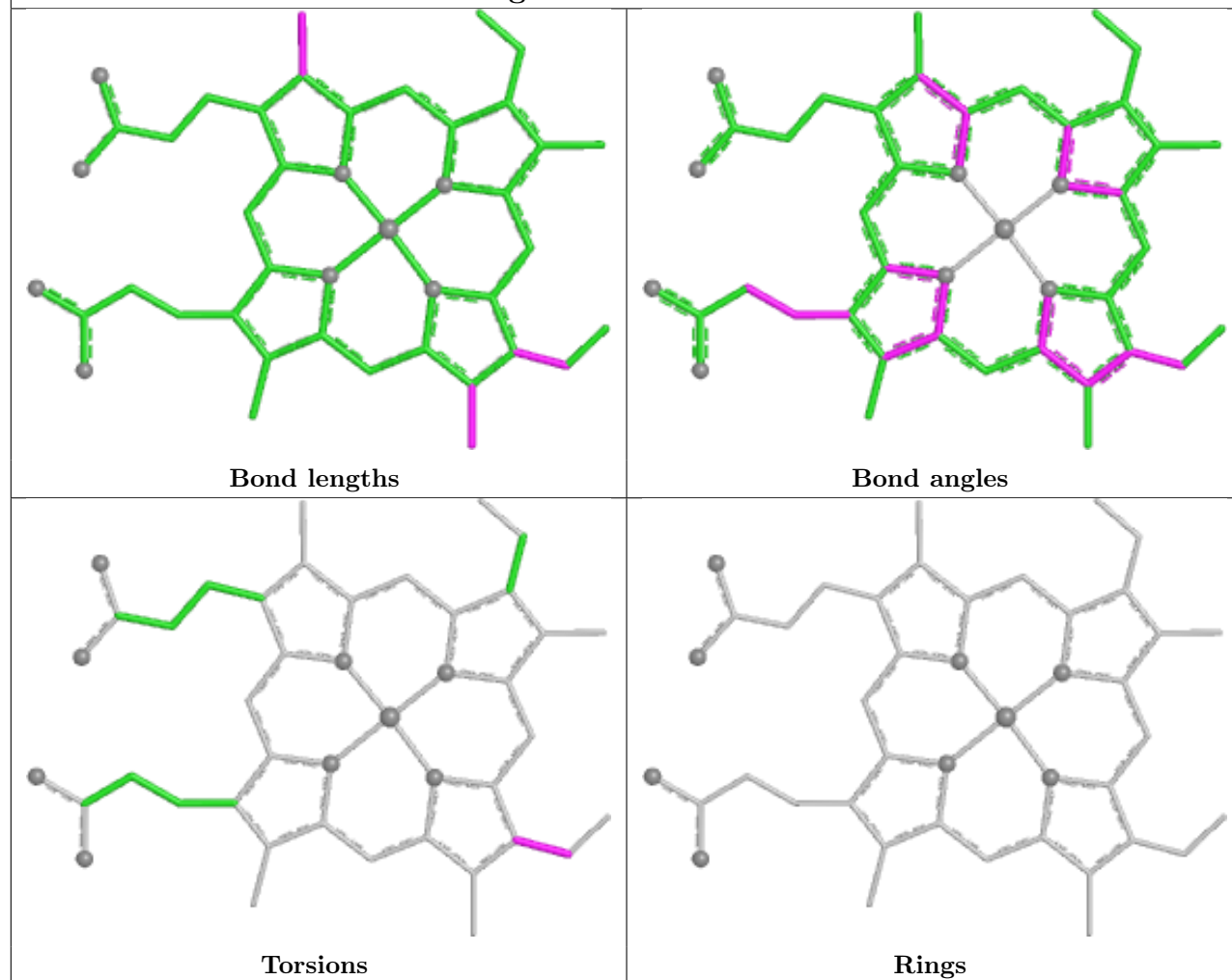
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

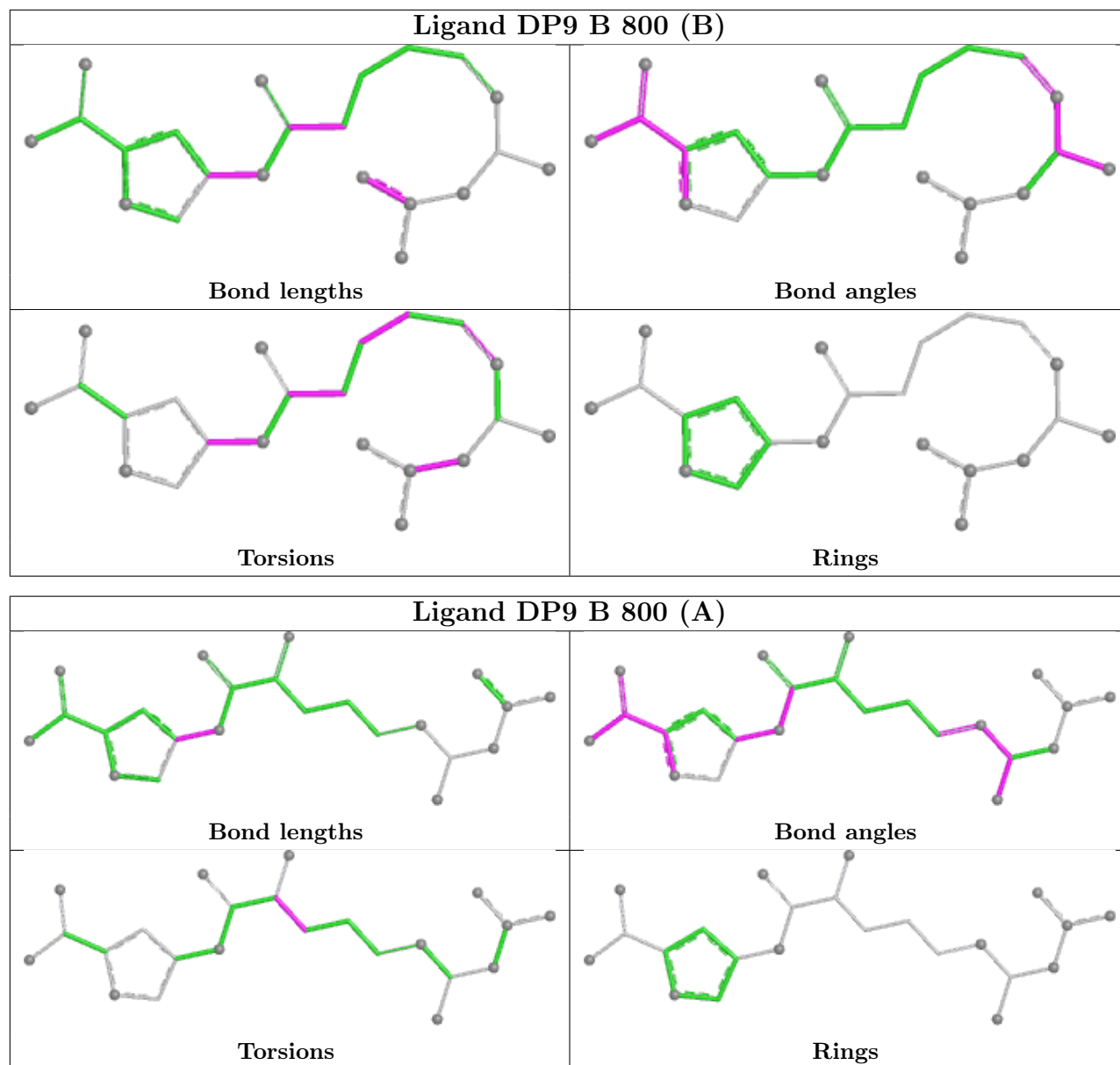


Ligand DP9 A 799 (B)



Ligand HEM B 750





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	407/420 (96%)	0.98	77 (18%) 3 3	20, 38, 60, 73	6 (1%)
1	B	410/420 (97%)	0.35	18 (4%) 39 41	16, 29, 49, 66	6 (1%)
All	All	817/840 (97%)	0.67	95 (11%) 9 10	16, 33, 57, 73	12 (1%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	THR	5.3
1	A	715	VAL	4.8
1	A	716	TRP	4.8
1	B	350	THR	4.2
1	A	300	PHE	4.2
1	A	505	CYS	4.1
1	A	506	ILE	4.0
1	A	504	ILE	3.9
1	A	552	ASP	3.8
1	A	510	TRP	3.8
1	A	355	PHE	3.6
1	A	488	PRO	3.6
1	B	338	PRO	3.6
1	A	384	VAL	3.6
1	B	352	ASP	3.6
1	A	493	LEU	3.5
1	A	321	THR	3.4
1	A	303	VAL	3.2
1	B	616	LEU	3.2
1	A	373	GLY	3.2
1	A	381	LEU	3.2
1	A	517	PHE	3.2
1	A	554	PHE	3.2
1	A	553	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	512	ALA	3.2
1	B	348	VAL	3.2
1	A	322	LEU	3.2
1	B	300	PHE	3.2
1	A	501	PHE	3.1
1	A	711	TRP	3.1
1	A	533	LEU	3.1
1	B	611	ALA	3.1
1	B	354	LEU	3.1
1	A	551	PHE	3.1
1	A	513	PRO	3.0
1	A	549	PRO	3.0
1	B	392	SER	2.9
1	A	509	GLY	2.9
1	B	303	VAL	2.8
1	A	319	LYS	2.8
1	A	364	GLN	2.7
1	A	376	ALA	2.7
1	A	385	ASN	2.7
1	B	322	LEU	2.7
1	A	299	ARG	2.7
1	A	557	LEU	2.7
1	A	714	HIS	2.6
1	A	487	GLN	2.6
1	A	503	GLU	2.6
1	A	494	GLY	2.6
1	A	519	VAL	2.5
1	A	316	LEU	2.5
1	A	667	ARG	2.5
1	B	319	LYS	2.5
1	A	515	GLY	2.4
1	A	301	LEU	2.4
1	A	354	LEU	2.4
1	A	508	GLN	2.4
1	A	514	ARG	2.3
1	A	534	PHE	2.3
1	B	389	GLU	2.3
1	A	546	ILE	2.3
1	A	538	PRO	2.3
1	B	535	GLN	2.3
1	A	350	THR	2.3
1	A	485	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	528	GLY	2.3
1	B	309	ASP	2.3
1	A	712	ASN	2.3
1	A	338	PRO	2.3
1	A	710	PRO	2.3
1	A	377	HIS	2.2
1	A	393	THR	2.2
1	A	337	LEU	2.2
1	A	371	ARG	2.2
1	A	609	GLU	2.2
1	A	352	ASP	2.2
1	A	490	GLY	2.2
1	B	667	ARG	2.1
1	A	491	SER	2.1
1	A	640	SER	2.1
1	A	499	VAL	2.1
1	A	511	LYS	2.1
1	A	550	LYS	2.1
1	A	357	LEU	2.1
1	A	601	ASN	2.1
1	A	516	ARG	2.1
1	A	310	VAL	2.1
1	A	388	ILE	2.0
1	B	351	LYS	2.0
1	A	378	MET	2.0
1	A	713	THR	2.0
1	A	529	ASN	2.0
1	A	483	ALA	2.0
1	A	329	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

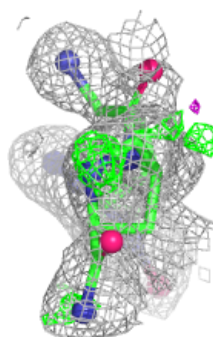
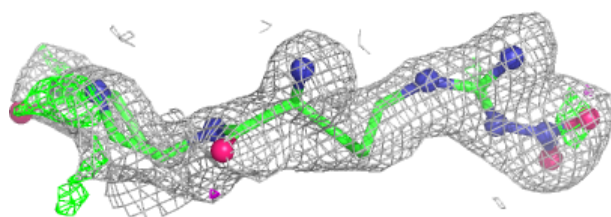
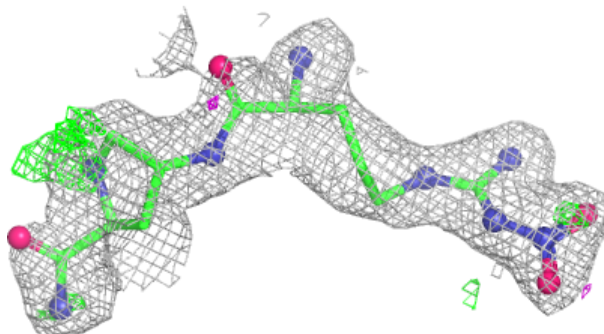
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MTL	A	870	12/12	0.69	0.15	54,55,56,56	0
7	DP9	B	800[A]	23/23	0.77	0.18	33,35,36,36	23
7	DP9	B	800[B]	22/23	0.77	0.18	35,38,38,38	22
7	DP9	A	799[A]	23/23	0.79	0.16	34,37,38,39	23
7	DP9	A	799[B]	23/23	0.79	0.16	34,38,40,40	23
4	MTL	B	871	12/12	0.88	0.11	46,47,48,48	0
2	ACT	A	860	4/4	0.91	0.16	57,57,57,57	0
2	ACT	B	861	4/4	0.93	0.11	39,39,39,39	0
6	H4B	A	760	17/17	0.95	0.06	22,22,24,24	0
6	H4B	B	761	17/17	0.97	0.05	22,22,24,24	0
5	HEM	A	750	43/43	0.98	0.06	22,23,25,26	0
5	HEM	B	750	43/43	0.98	0.06	20,21,24,27	0
3	ZN	A	900	1/1	0.99	0.02	30,30,30,30	0

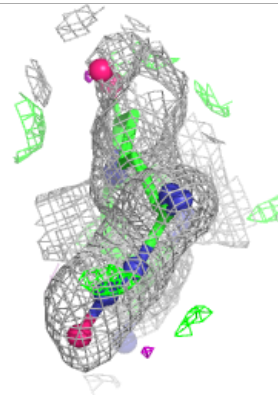
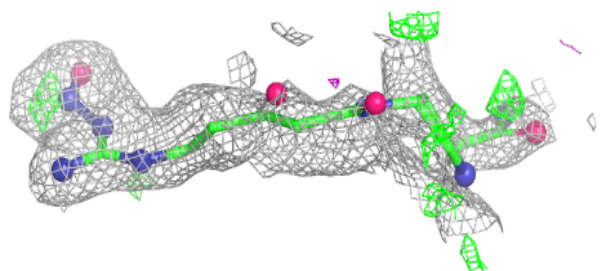
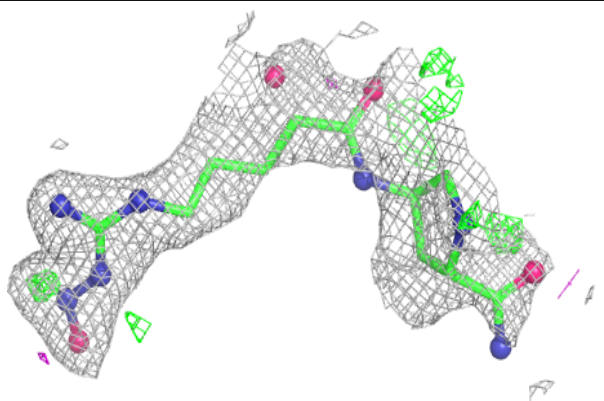
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DP9 B 800 (A):

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

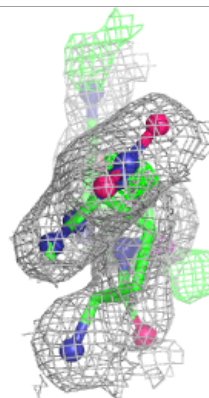
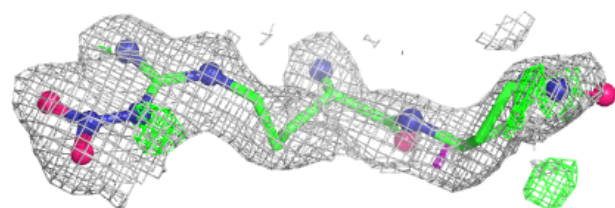
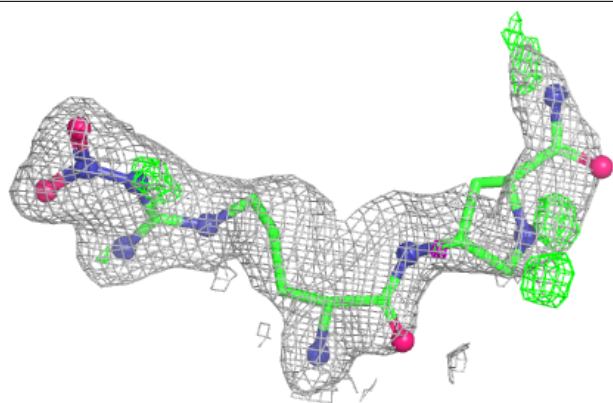
**Electron density around DP9 B 800 (B):**

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

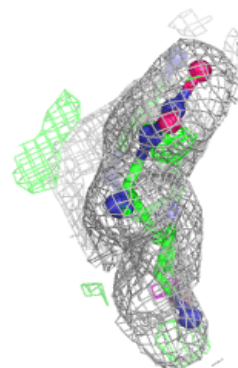
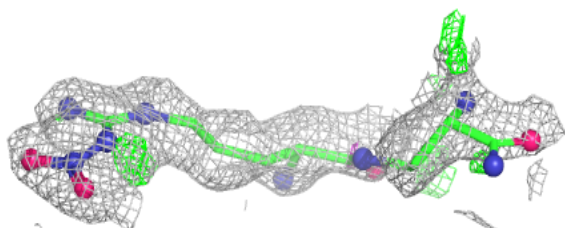
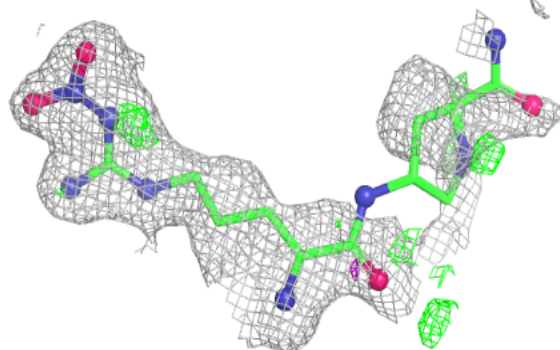


Electron density around DP9 A 799 (A):

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

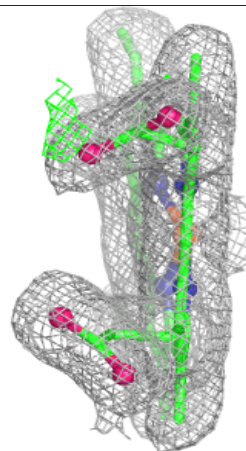
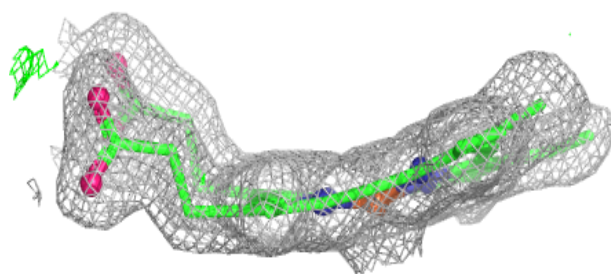
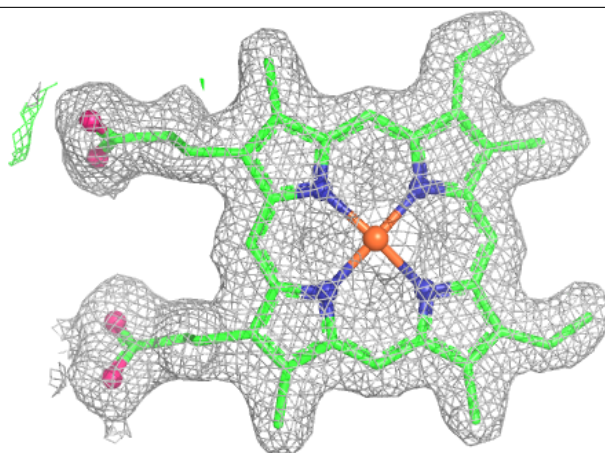
**Electron density around DP9 A 799 (B):**

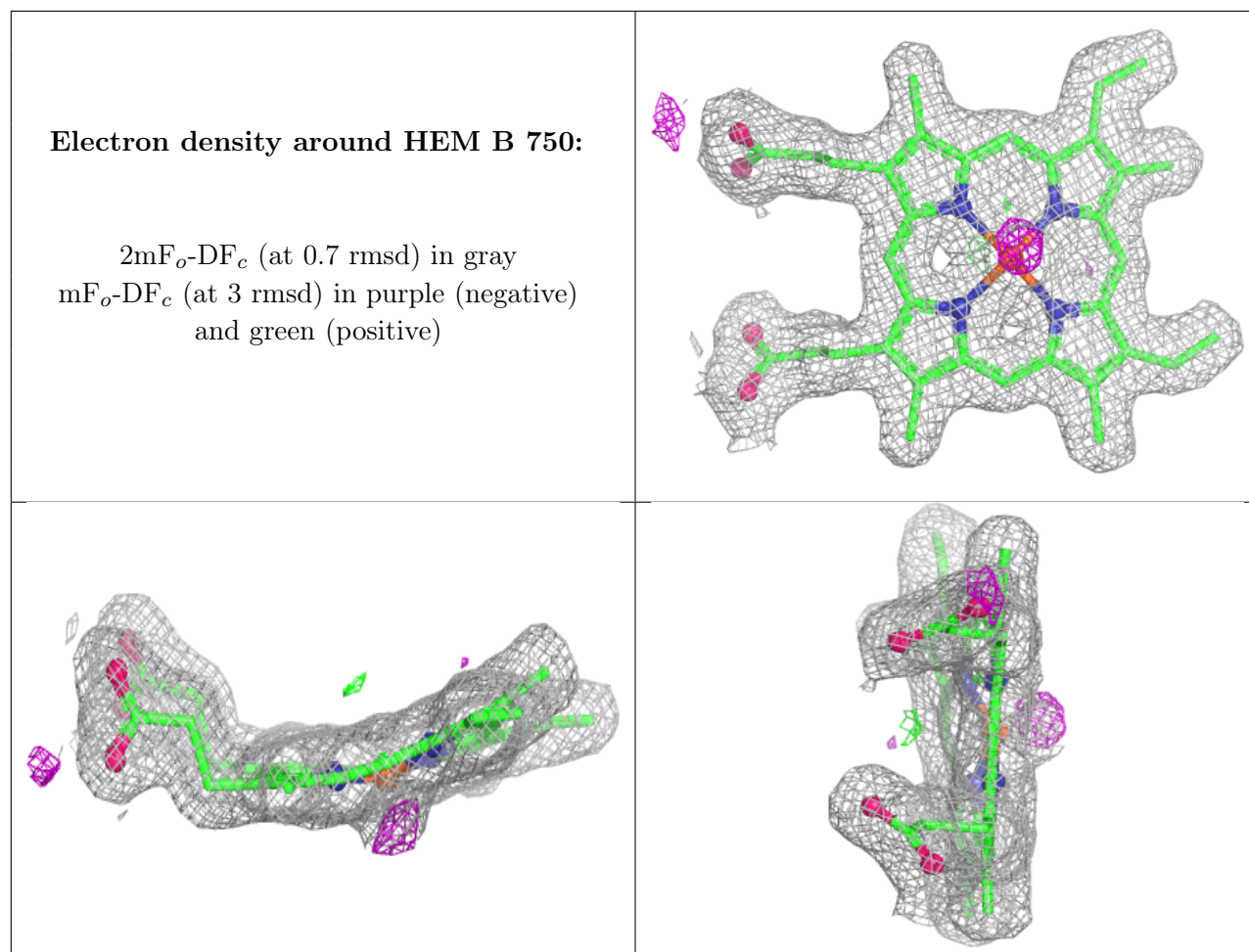
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.