



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:27 AM UTC

PDB ID : 1ZZR / pdb_00001zzr
Title : Rat nNOS D597N/M336V double mutant with L-N(omega)-Nitroarginine-(4 R)-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 : 2.05 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

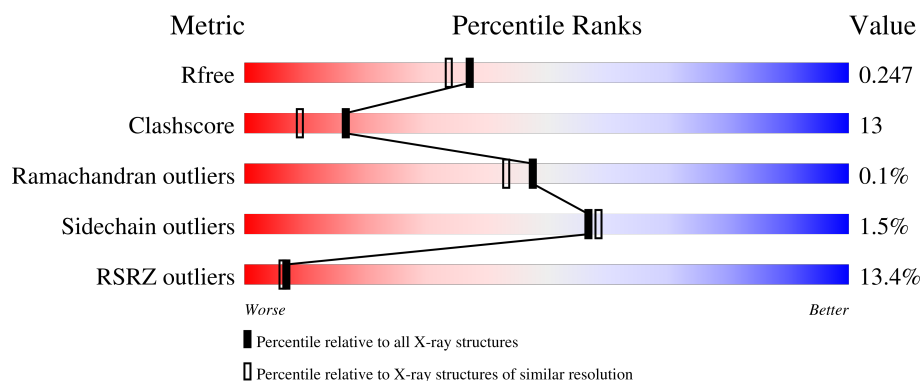
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	22% 66% 29% ..
1	B	420	4% 77% 20% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7256 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
			3312	2121	567	604	20			
1	B	411	Total	C	N	O	S	0	0	0
			3344	2140	575	609	20			

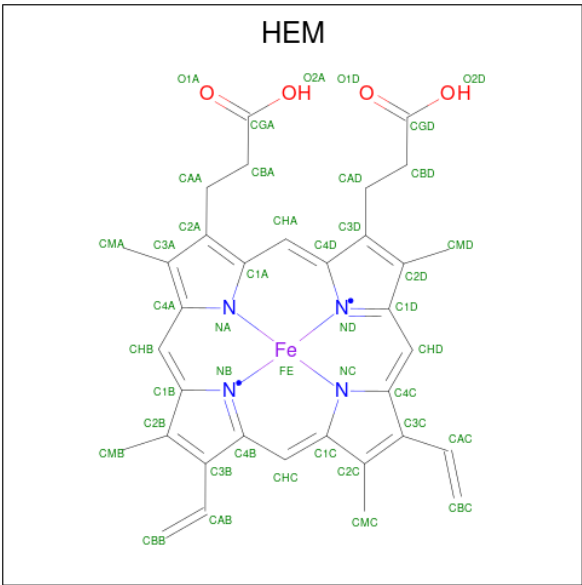
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	engineered mutation	UNP P29476
A	597	ASN	ASP	engineered mutation	UNP P29476
B	336	VAL	MET	engineered mutation	UNP P29476
B	597	ASN	ASP	engineered mutation	UNP P29476

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

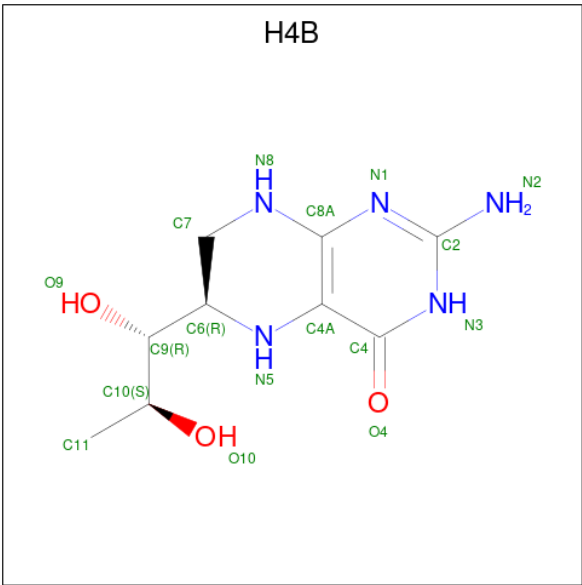
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



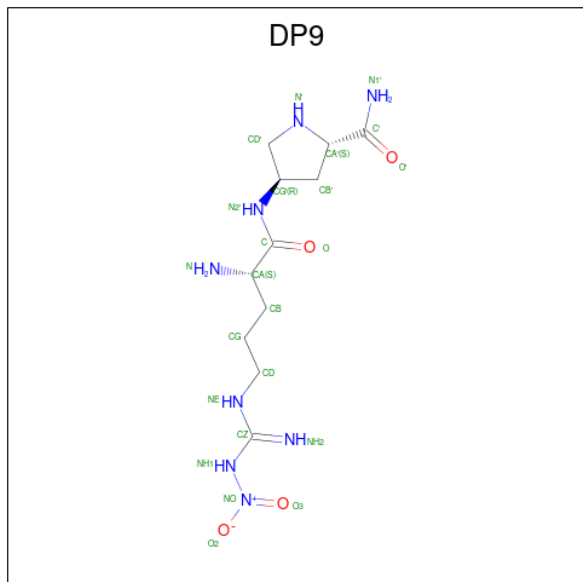
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C₉H₁₅N₅O₃).



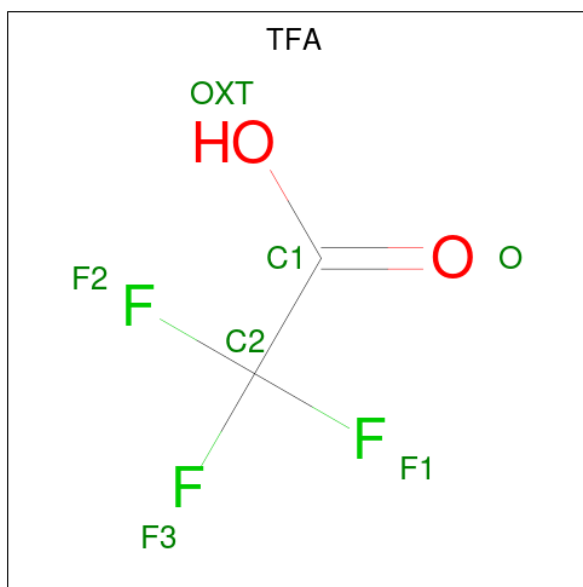
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		
4	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is L-N(OMEGA)-NITROARGININE-(4R)-AMINO-L-PROLINE AMIDE (CCD ID: DP9) (formula: $C_{11}H_{22}N_8O_4$).



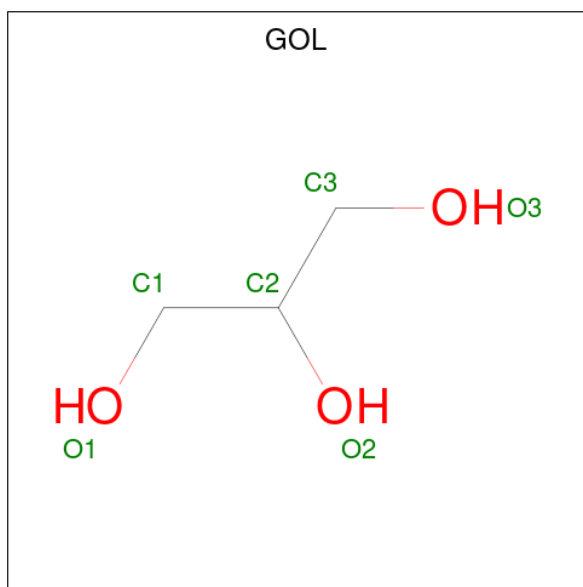
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			23	11	8	4		
5	B	1	Total	C	N	O	0	0
			23	11	8	4		

- Molecule 6 is trifluoroacetic acid (CCD ID: TFA) (formula: $C_2HF_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	F	O	0	0
			7	2	3	2		
6	B	1	Total	C	F	O	0	0
			7	2	3	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

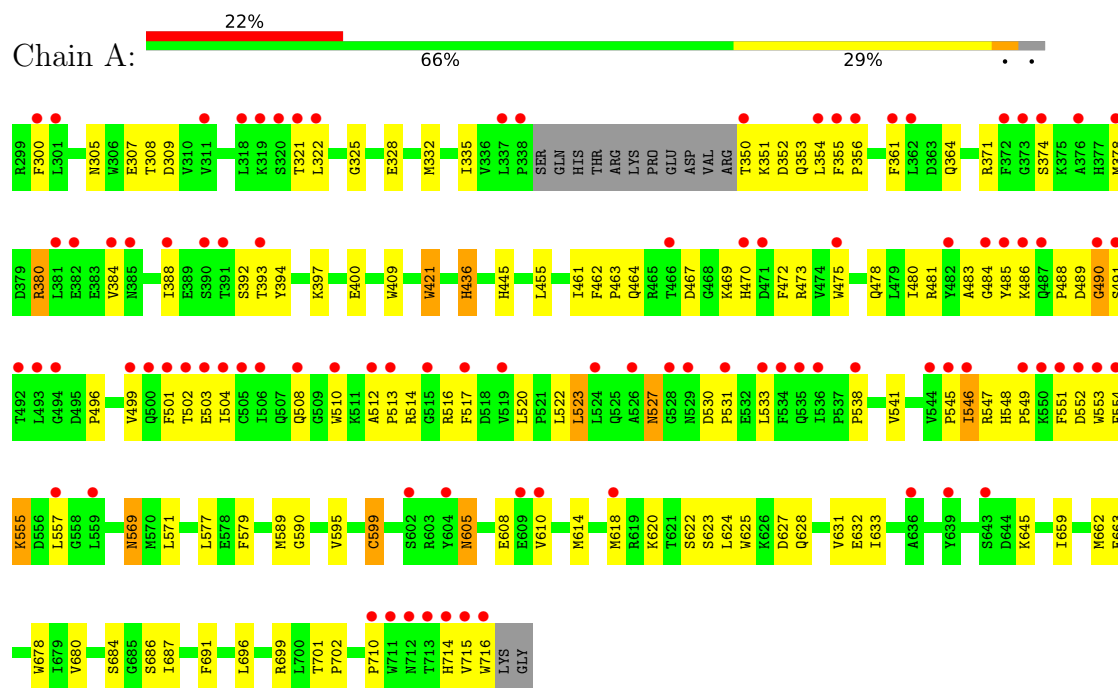
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	162	Total	O	0	0
			162	162		
8	B	245	Total	O	0	0
			245	245		

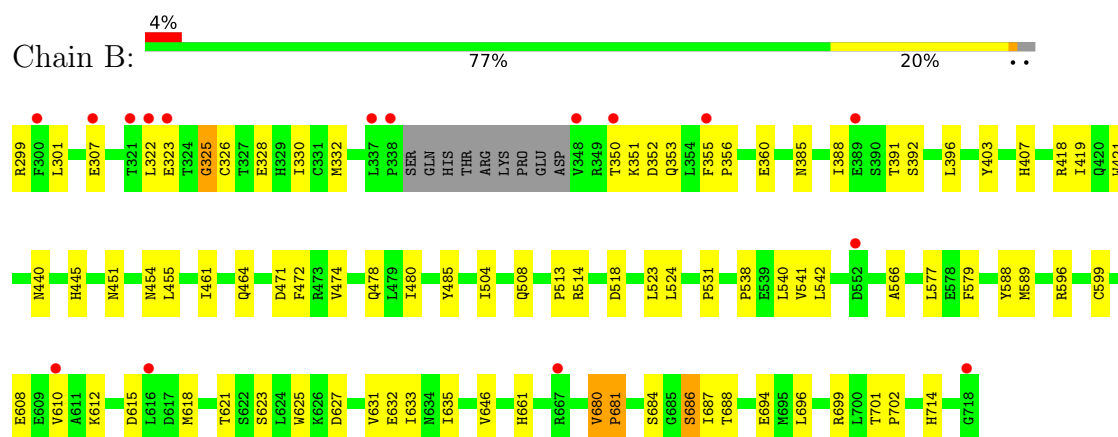
3 Residue-property plots [i](#)

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	52.43Å 111.95Å 164.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 2.05 49.32 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.32-2.05) 98.8 (49.32-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.260 0.218 , 0.247	Depositor DCC
R_{free} test set	3036 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.822	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	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	0.95	EDS
Total number of atoms	7256	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: DP9, TFA, GOL, HEM, ZN, H4B

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	0.51	0/3405	0.97	16/4621 (0.3%)
1	B	0.57	1/3437 (0.0%)	1.01	20/4661 (0.4%)
All	All	0.54	1/6842 (0.0%)	0.99	36/9282 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	681	PRO	CA-C	6.19	1.55	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	MET	N-CA-C	-9.48	94.22	109.76
1	B	589	MET	N-CA-C	-9.02	94.98	109.76
1	B	421	TRP	N-CA-C	8.15	121.19	111.33
1	A	397	LYS	N-CA-C	-6.92	101.39	110.53
1	A	421	TRP	N-CA-C	6.64	119.08	111.11
1	B	474	VAL	N-CA-C	-6.58	98.26	107.80
1	B	326	CYS	CA-CB-SG	6.32	128.93	114.40
1	A	680	VAL	CA-C-N	6.06	126.62	120.38
1	A	680	VAL	C-N-CA	6.06	126.62	120.38
1	B	680	VAL	CA-C-N	5.96	124.01	119.66
1	B	680	VAL	C-N-CA	5.96	124.01	119.66
1	A	455	LEU	N-CA-C	5.95	118.62	110.24
1	A	490	GLY	N-CA-C	-5.89	106.37	114.67
1	B	714	HIS	N-CA-C	5.87	118.84	110.10
1	B	596	ARG	N-CA-C	5.82	117.50	111.03
1	B	623	SER	N-CA-C	-5.81	106.20	113.28
1	B	455	LEU	N-CA-C	5.69	118.48	110.23
1	B	688	THR	N-CA-C	-5.66	102.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	CYS	N-CA-C	5.60	121.00	113.72
1	A	546	ILE	N-CA-C	5.54	116.37	107.73
1	B	599	CYS	N-CA-C	5.53	120.91	113.72
1	B	471	ASP	N-CA-C	5.49	117.82	110.35
1	A	623	SER	N-CA-C	-5.48	106.55	113.18
1	B	325	GLY	N-CA-C	-5.46	107.82	114.92
1	B	461	ILE	N-CA-C	5.46	115.45	107.37
1	B	588	TYR	N-CA-C	5.42	118.50	110.48
1	A	436	HIS	N-CA-C	-5.39	105.49	111.36
1	B	418	ARG	N-CA-C	5.35	119.29	112.87
1	B	472	PHE	N-CA-C	-5.26	100.66	109.24
1	A	461	ILE	N-CA-C	5.25	115.15	107.37
1	A	714	HIS	N-CA-C	5.24	117.82	109.96
1	A	354	LEU	N-CA-C	5.16	117.70	111.40
1	B	524	LEU	N-CA-C	5.08	117.25	109.07
1	A	325	GLY	N-CA-C	-5.07	107.99	114.37
1	A	305	ASN	N-CA-C	-5.01	100.36	108.52
1	B	686	SER	N-CA-C	5.01	119.02	113.01

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	3312	0	3223	126	0
1	B	3344	0	3261	53	0
2	A	1	0	0	0	0
3	A	43	0	30	1	0
3	B	43	0	30	2	0
4	A	17	0	15	1	0
4	B	17	0	15	0	0
5	A	23	0	21	0	0
5	B	23	0	21	0	0
6	A	7	0	0	0	0
6	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	162	0	0	10	0
8	B	245	0	0	4	0
All	All	7256	0	6632	173	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 13.

All (173) 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	1.28	1.14
1:A:523:LEU:CD2	1:A:531:PRO:HB2	2.14	0.75
3:A:750:HEM:HMC2	3:A:750:HEM:HBC2	1.70	0.72
1:A:699:ARG:HD2	8:A:1050:HOH:O	1.90	0.72
1:A:350:THR:HB	1:A:353:GLN:HG3	1.71	0.72
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.06	0.71
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.56	0.71
1:A:350:THR:HG22	1:A:352:ASP:H	1.58	0.69
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.76	0.67
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.10	0.67
1:A:620:LYS:HE3	1:A:622:SER:OG	1.95	0.66
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.11	0.66
1:A:436:HIS:HB2	8:A:995:HOH:O	1.96	0.65
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.78	0.65
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.80	0.64
8:A:979:HOH:O	1:B:307:GLU:HG3	1.98	0.64
1:B:325:GLY:O	1:B:332:MET:HG3	1.98	0.63
1:A:332:MET:HE2	1:B:696:LEU:HD21	1.80	0.63
1:B:350:THR:HG22	1:B:352:ASP:H	1.64	0.63
1:A:350:THR:HB	1:A:353:GLN:CG	2.30	0.62
1:A:350:THR:HB	1:A:353:GLN:CD	2.26	0.61
1:B:504:ILE:O	1:B:508:GLN:HG2	2.00	0.61
1:A:374:SER:O	1:A:378:MET:HG2	2.00	0.61
1:A:378:MET:HA	1:A:378:MET:HE2	1.81	0.61
1:B:323:GLU:O	1:B:699:ARG:HD3	2.01	0.60
1:A:555:LYS:NZ	1:A:555:LYS:HB3	2.15	0.60
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.34	0.57
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.87	0.57
1:B:356:PRO:O	1:B:360:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:621:THR:HG22	8:B:1025:HOH:O	2.06	0.56
1:A:523:LEU:HD22	1:A:531:PRO:CB	2.20	0.56
1:B:388:ILE:O	1:B:392:SER:N	2.36	0.56
1:A:610:VAL:O	1:A:614:MET:HG3	2.06	0.56
1:A:545:PRO:HG2	1:A:547:ARG:NH2	2.21	0.55
1:A:322:LEU:HB2	1:A:699:ARG:HB2	1.87	0.55
1:A:684:SER:HB3	1:A:687:ILE:CG1	2.36	0.55
1:A:322:LEU:HB2	1:A:699:ARG:HE	1.72	0.55
1:A:351:LYS:HE2	1:A:392:SER:CB	2.38	0.54
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.33	0.53
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.91	0.53
1:B:299:ARG:HD2	8:B:1076:HOH:O	2.08	0.53
1:B:391:THR:O	1:B:392:SER:HB2	2.09	0.53
1:A:322:LEU:CB	1:A:699:ARG:HE	2.23	0.52
1:A:467:ASP:C	1:A:469:LYS:H	2.17	0.52
1:A:462:PHE:HB3	1:A:463:PRO:CD	2.39	0.52
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.25	0.52
1:A:488:PRO:HD2	8:A:972:HOH:O	2.10	0.52
1:B:328:GLU:OE1	1:B:328:GLU:N	2.43	0.52
1:A:355:PHE:N	1:A:356:PRO:HD2	2.25	0.52
1:A:485:TYR:CE1	1:A:514:ARG:HA	2.45	0.51
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.46	0.51
1:A:684:SER:HB3	1:A:687:ILE:HG12	1.92	0.51
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.75	0.51
1:A:361:PHE:O	1:A:364:GLN:HG2	2.10	0.51
1:A:380:ARG:O	1:A:384:VAL:HG23	2.11	0.51
1:A:701:THR:HA	1:A:702:PRO:C	2.36	0.50
1:A:716:TRP:H	1:A:716:TRP:CD1	2.29	0.50
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.46	0.50
1:A:618:MET:HE3	1:A:625:TRP:CH2	2.46	0.50
1:A:475:TRP:CE3	1:A:523:LEU:HD13	2.47	0.50
1:B:440:ASN:ND2	8:B:1091:HOH:O	2.39	0.50
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.93	0.50
1:A:307:GLU:HG3	8:B:939:HOH:O	2.11	0.50
1:A:510:TRP:HB2	1:A:533:LEU:CD1	2.41	0.50
1:A:659:ILE:O	1:A:663:GLU:HG3	2.12	0.50
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.47	0.50
1:A:551:PHE:HE1	1:A:614:MET:HE3	1.77	0.49
1:B:351:LYS:HE2	1:B:392:SER:HA	1.94	0.49
1:A:470:HIS:HB3	1:A:527:ASN:ND2	2.26	0.49
1:A:627:ASP:O	1:A:631:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.95	0.49
1:A:516:ARG:HD3	1:A:517:PHE:HE1	1.78	0.49
1:A:516:ARG:HD3	1:A:517:PHE:CE1	2.48	0.48
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.01	0.48
1:B:684:SER:HB3	1:B:687:ILE:HD11	1.95	0.48
1:A:371:ARG:HG3	1:A:371:ARG:NH2	2.27	0.48
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.13	0.48
1:A:489:ASP:OD2	1:A:489:ASP:O	2.31	0.48
1:A:504:ILE:O	1:A:508:GLN:HG2	2.13	0.47
1:A:715:VAL:O	1:A:715:VAL:HG23	2.14	0.47
1:A:332:MET:HE3	1:B:301:LEU:HD13	1.96	0.47
1:B:542:LEU:HD21	1:B:646:VAL:HG22	1.95	0.47
1:A:555:LYS:HB3	1:A:555:LYS:HZ3	1.78	0.47
1:A:569:ASN:HD22	1:A:569:ASN:H	1.61	0.47
1:A:351:LYS:HE2	1:A:392:SER:CA	2.45	0.47
1:A:522:LEU:O	1:A:533:LEU:HA	2.15	0.47
1:B:322:LEU:HB3	1:B:699:ARG:CZ	2.44	0.47
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.50	0.47
1:A:321:THR:HG23	1:A:322:LEU:HG	1.96	0.47
1:A:328:GLU:H	1:A:328:GLU:CD	2.21	0.47
1:A:696:LEU:HD22	1:B:330:ILE:HD11	1.97	0.47
1:A:499:VAL:O	1:A:503:GLU:HG3	2.15	0.46
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.97	0.46
1:A:483:ALA:HB3	8:A:1041:HOH:O	2.14	0.46
1:A:548:HIS:ND1	1:A:549:PRO:HD2	2.30	0.46
3:B:750:HEM:HMC1	3:B:750:HEM:HBC2	1.98	0.46
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.81	0.46
1:A:489:ASP:C	1:A:491:SER:H	2.23	0.46
1:A:483:ALA:HB1	1:A:502:THR:CG2	2.45	0.46
1:A:484:GLY:O	1:A:499:VAL:HA	2.16	0.46
1:A:514:ARG:HH21	1:A:514:ARG:HG3	1.80	0.46
1:B:478:GLN:HA	1:B:566:ALA:O	2.16	0.46
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.81	0.45
1:A:595:VAL:O	1:A:599:CYS:HB2	2.16	0.45
1:A:445:HIS:C	1:A:445:HIS:CD2	2.94	0.45
1:A:485:TYR:CE2	1:A:512:ALA:HB1	2.50	0.45
1:A:488:PRO:C	1:A:490:GLY:H	2.24	0.45
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.81	0.45
1:A:351:LYS:HE2	1:A:392:SER:HA	1.97	0.45
1:A:686:SER:HA	1:A:691:PHE:CG	2.51	0.45
1:A:464:GLN:NE2	1:A:577:LEU:HD22	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:MET:CE	1:A:632:GLU:HG3	2.47	0.45
1:B:627:ASP:O	1:B:631:VAL:HG23	2.17	0.45
1:B:355:PHE:N	1:B:356:PRO:HD2	2.32	0.45
3:B:750:HEM:HBC2	3:B:750:HEM:CMC	2.47	0.45
1:B:618:MET:HG2	1:B:625:TRP:CD2	2.52	0.45
1:A:388:ILE:O	1:A:392:SER:N	2.50	0.44
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.82	0.44
1:B:610:VAL:HG21	1:B:633:ILE:HD11	1.98	0.44
1:B:701:THR:HA	1:B:702:PRO:C	2.42	0.44
1:B:523:LEU:HG	1:B:531:PRO:HB2	1.99	0.44
1:A:463:PRO:HB2	1:A:472:PHE:CE1	2.52	0.44
1:A:618:MET:HG2	1:A:625:TRP:CD2	2.53	0.43
1:B:480:ILE:HD13	1:B:541:VAL:HG13	1.99	0.43
1:A:308:THR:O	1:A:309:ASP:HB2	2.19	0.43
1:A:478:GLN:HB2	1:A:481:ARG:CG	2.48	0.43
1:A:530:ASP:CG	8:A:959:HOH:O	2.61	0.43
1:A:610:VAL:HG21	1:A:633:ILE:HD11	2.00	0.43
1:A:488:PRO:C	1:A:490:GLY:N	2.76	0.43
1:A:332:MET:HE2	1:B:696:LEU:CD2	2.47	0.43
1:B:350:THR:HG22	1:B:351:LYS:N	2.34	0.43
1:B:445:HIS:C	1:B:445:HIS:CD2	2.97	0.43
1:A:569:ASN:HD22	1:A:569:ASN:N	2.15	0.43
1:A:335:ILE:HD13	1:B:694:GLU:HB3	1.99	0.43
1:A:501:PHE:CD2	1:A:520:LEU:HD13	2.54	0.43
1:A:501:PHE:HD2	1:A:520:LEU:HD13	1.84	0.43
1:A:551:PHE:CD2	1:A:551:PHE:N	2.86	0.43
1:A:552:ASP:O	1:A:555:LYS:HG2	2.19	0.43
1:A:571:LEU:C	1:A:571:LEU:HD23	2.43	0.43
1:A:684:SER:O	1:A:687:ILE:HG12	2.19	0.42
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.54	0.42
1:B:684:SER:HB3	1:B:687:ILE:CG1	2.49	0.42
1:A:678:TRP:HA	4:A:760:H4B:N1	2.34	0.42
1:A:321:THR:HG23	1:A:322:LEU:N	2.35	0.42
1:A:701:THR:HB	8:A:980:HOH:O	2.18	0.42
1:A:393:THR:OG1	1:A:394:TYR:N	2.52	0.42
1:A:595:VAL:CG1	1:B:686:SER:OG	2.68	0.42
1:B:513:PRO:HG2	1:B:518:ASP:OD2	2.19	0.42
1:A:523:LEU:HG	1:A:533:LEU:CD2	2.49	0.42
1:A:614:MET:HE3	1:A:632:GLU:HG3	2.00	0.42
1:B:391:THR:O	1:B:392:SER:CB	2.67	0.42
1:A:554:PHE:HB3	8:A:1056:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:LEU:HD12	1:B:635:ILE:HG13	2.00	0.42
1:B:396:LEU:HG	1:B:577:LEU:HD12	2.02	0.42
1:A:553:TRP:HZ3	1:A:557:LEU:HD11	1.85	0.42
1:B:451:ASN:HB3	1:B:454:ASN:O	2.18	0.42
1:A:545:PRO:HG2	1:A:547:ARG:HH21	1.85	0.41
1:A:590:GLY:HA3	8:A:962:HOH:O	2.19	0.41
1:B:419:ILE:HG13	1:B:661:HIS:HB2	2.02	0.41
1:B:608:GLU:O	1:B:612:LYS:HG3	2.21	0.41
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.56	0.41
1:A:605:ASN:ND2	8:A:1058:HOH:O	2.41	0.41
1:A:686:SER:HA	1:A:691:PHE:CB	2.50	0.41
1:B:612:LYS:O	1:B:615:ASP:N	2.48	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.91	0.41
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.54	0.41
1:A:332:MET:HB3	1:A:335:ILE:HG13	2.03	0.40
1:A:486:LYS:HE2	1:A:499:VAL:HG11	2.03	0.40
1:A:300:PHE:N	1:A:300:PHE:CD1	2.89	0.40
1:A:467:ASP:C	1:A:469:LYS:N	2.77	0.40
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.56	0.40
1:A:569:ASN:H	1:A:569:ASN:ND2	2.19	0.40
1:A:608:GLU:HG2	1:A:618:MET:HE1	2.03	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	403/420 (96%)	375 (93%)	27 (7%)	1 (0%)	43	37
1	B	407/420 (97%)	391 (96%)	16 (4%)	0	100	100
All	All	810/840 (96%)	766 (95%)	43 (5%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	605	ASN

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	363/375 (97%)	355 (98%)	8 (2%)	45	44
1	B	366/375 (98%)	363 (99%)	3 (1%)	73	77
All	All	729/750 (97%)	718 (98%)	11 (2%)	57	58

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	ARG
1	A	523	LEU
1	A	527	ASN
1	A	538	PRO
1	A	555	LYS
1	A	569	ASN
1	A	645	LYS
1	A	662	MET
1	B	353	GLN
1	B	538	PRO
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	HIS
1	A	436	HIS
1	A	454	ASN
1	A	464	GLN
1	A	507	GLN

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Mol	Chain	Res	Type
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN
1	A	642	GLN
1	A	697	ASN
1	A	712	ASN
1	A	714	HIS
1	B	364	GLN
1	B	385	ASN
1	B	407	HIS
1	B	425	GLN
1	B	454	ASN
1	B	508	GLN
1	B	527	ASN
1	B	535	GLN
1	B	601	ASN
1	B	697	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DP9	A	799	-	17,23,23	1.03	2 (11%)	20,30,30	1.86	4 (20%)
6	TFA	A	865	-	6,6,6	1.29	1 (16%)	9,9,9	0.72	0
5	DP9	B	800	-	17,23,23	1.00	1 (5%)	20,30,30	1.87	4 (20%)
7	GOL	A	880	-	5,5,5	0.34	0	5,5,5	0.30	0
3	HEM	A	750	1	50,50,50	1.43	9 (18%)	67,82,82	1.21	6 (8%)
6	TFA	B	866	-	6,6,6	2.00	2 (33%)	9,9,9	1.21	1 (11%)
4	H4B	B	761	-	17,18,18	1.78	3 (17%)	14,26,26	1.80	4 (28%)
3	HEM	B	750	1	50,50,50	1.35	8 (16%)	67,82,82	1.16	4 (5%)
7	GOL	B	881	-	5,5,5	0.33	0	5,5,5	0.34	0
4	H4B	A	760	-	17,18,18	1.54	3 (17%)	14,26,26	2.01	4 (28%)

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	DP9	A	799	-	-	2/20/32/32	0/1/1/1
6	TFA	A	865	-	-	0/6/6/6	-
5	DP9	B	800	-	-	0/20/32/32	0/1/1/1
7	GOL	A	880	-	-	2/4/4/4	-
3	HEM	A	750	1	-	2/14/54/54	-
6	TFA	B	866	-	-	0/6/6/6	-
4	H4B	B	761	-	-	0/8/17/17	0/2/2/2
3	HEM	B	750	1	-	1/14/54/54	-
7	GOL	B	881	-	-	2/4/4/4	-
4	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	760	H4B	C4A-N5	4.19	1.47	1.37
6	B	866	TFA	C2-C1	-3.88	1.36	1.52
4	B	761	H4B	C4A-N5	3.73	1.46	1.37
4	B	761	H4B	C6-N5	3.60	1.53	1.47
4	A	760	H4B	C6-N5	3.20	1.53	1.47
3	A	750	HEM	FE-NB	3.06	2.04	1.94
3	B	750	HEM	CHD-C4C	3.04	1.44	1.38
3	A	750	HEM	CMB-C2B	3.00	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	800	DP9	CG'-N2'	2.98	1.52	1.46
3	B	750	HEM	CAB-C3B	-2.95	1.39	1.47
3	A	750	HEM	CMD-C2D	2.94	1.56	1.50
4	B	761	H4B	C7-C6	2.93	1.55	1.52
6	A	865	TFA	C2-C1	-2.89	1.40	1.52
3	B	750	HEM	CMC-C2C	2.89	1.56	1.50
5	A	799	DP9	CG'-N2'	2.81	1.52	1.46
3	B	750	HEM	CMB-C2B	2.72	1.56	1.50
3	A	750	HEM	CAC-C3C	-2.71	1.40	1.47
3	A	750	HEM	FE-NA	2.69	2.04	1.95
3	B	750	HEM	FE-ND	2.61	2.02	1.94
3	A	750	HEM	FE-ND	2.39	2.02	1.94
3	A	750	HEM	CAB-C3B	-2.34	1.41	1.47
3	A	750	HEM	CMC-C2C	2.30	1.55	1.50
3	B	750	HEM	C3B-C4B	2.21	1.49	1.44
5	A	799	DP9	O3-NO	2.18	1.30	1.24
6	B	866	TFA	OXT-C1	-2.09	1.22	1.30
3	A	750	HEM	CMA-C3A	2.08	1.55	1.50
3	B	750	HEM	CAC-C3C	-2.05	1.41	1.47
4	A	760	H4B	C7-C6	2.05	1.54	1.52
3	B	750	HEM	C2A-C3A	-2.02	1.33	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	760	H4B	C2-N1-C8A	5.37	122.84	113.36
4	B	761	H4B	C2-N1-C8A	4.82	121.86	113.36
5	A	799	DP9	CD-NE-CZ	4.51	131.72	123.46
5	B	800	DP9	CD-NE-CZ	4.41	131.54	123.46
5	A	799	DP9	O'-C'-N1'	-3.61	116.67	123.04
5	B	800	DP9	O'-C'-N1'	-3.37	117.08	123.04
3	A	750	HEM	CMB-C2B-C1B	3.20	130.03	125.03
5	B	800	DP9	C'-CA'-N'	-3.13	104.70	111.16
3	B	750	HEM	C2B-C1B-NB	3.11	113.41	109.84
4	A	760	H4B	N3-C2-N1	-3.01	117.81	123.32
6	B	866	TFA	F1-C2-C1	-2.93	101.43	111.90
3	A	750	HEM	CBA-CAA-C2A	-2.86	104.62	112.53
4	A	760	H4B	O10-C10-C9	-2.73	105.25	109.77
4	B	761	H4B	N3-C2-N1	-2.63	118.51	123.32
3	B	750	HEM	CBD-CAD-C3D	-2.62	105.28	112.53
5	A	799	DP9	C'-CA'-N'	-2.61	105.77	111.16
5	B	800	DP9	CA'-C'-N1'	2.60	121.18	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	761	H4B	O9-C9-C6	2.57	115.45	109.28
3	A	750	HEM	C3B-C4B-NB	2.50	111.27	109.47
3	A	750	HEM	CAB-C3B-C2B	-2.46	120.43	128.43
3	A	750	HEM	CBD-CAD-C3D	-2.42	105.85	112.53
5	A	799	DP9	CA'-C'-N1'	2.40	120.85	116.76
4	A	760	H4B	O9-C9-C6	2.35	114.90	109.28
3	B	750	HEM	C2D-C1D-ND	2.20	112.44	109.90
3	A	750	HEM	C2B-C1B-NB	2.15	112.31	109.84
4	B	761	H4B	O10-C10-C9	-2.10	106.30	109.77
3	B	750	HEM	C1D-C2D-C3D	-2.06	104.82	106.98

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	881	GOL	O1-C1-C2-C3
7	A	880	GOL	O1-C1-C2-C3
7	B	881	GOL	O1-C1-C2-O2
5	A	799	DP9	C-CA-CB-CG
7	A	880	GOL	O1-C1-C2-O2
3	B	750	HEM	C4B-C3B-CAB-CBB
5	A	799	DP9	N-CA-CB-CG
3	A	750	HEM	CAD-CBD-CGD-O2D
3	A	750	HEM	CAD-CBD-CGD-O1D

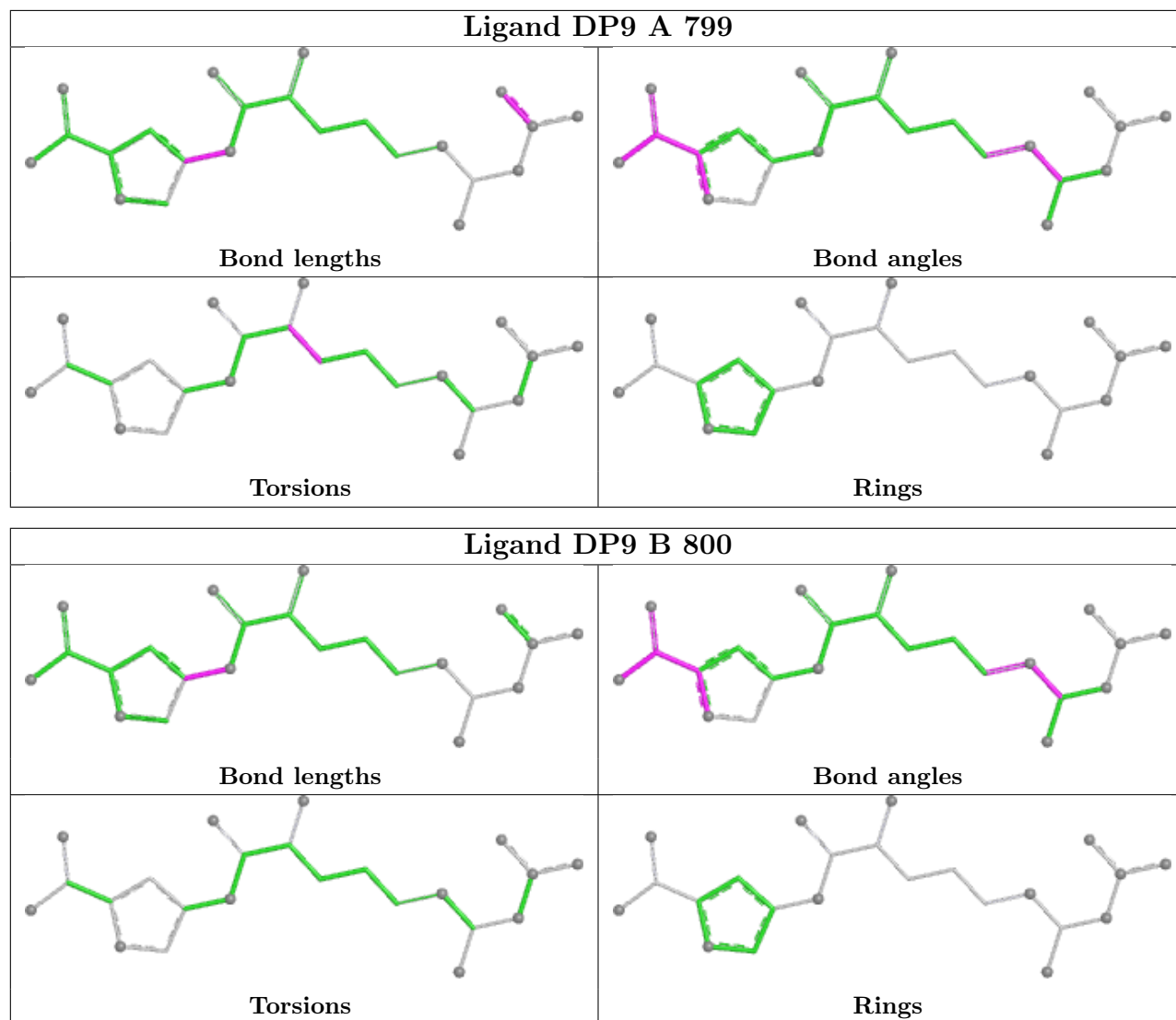
There are no ring outliers.

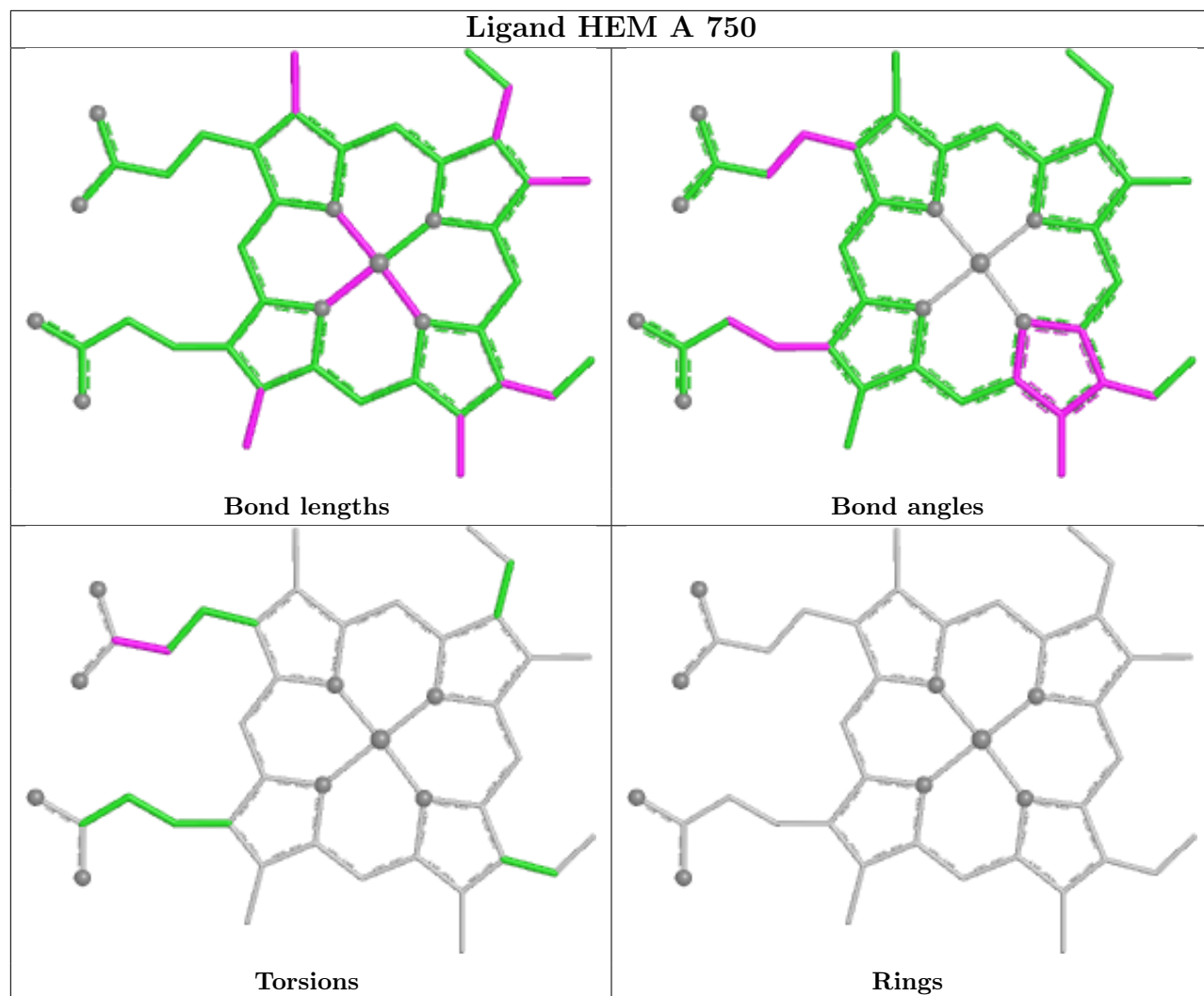
3 monomers are involved in 4 short contacts:

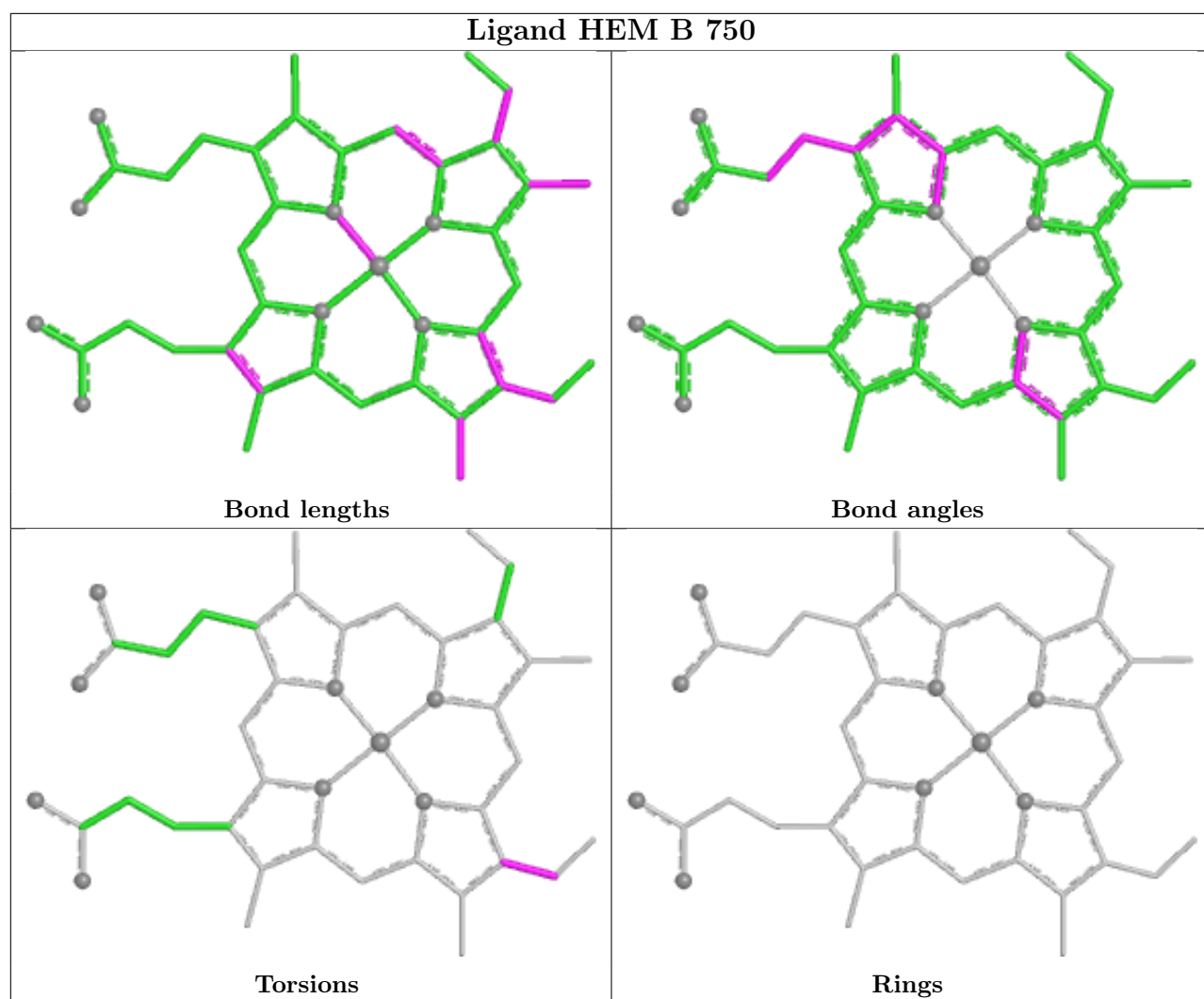
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	750	HEM	1	0
3	B	750	HEM	2	0
4	A	760	H4B	1	0

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	407/420 (96%)	1.08	94 (23%) 2 1	22, 45, 75, 86	0
1	B	411/420 (97%)	0.25	16 (3%) 43 44	21, 35, 59, 83	0
All	All	818/840 (97%)	0.66	110 (13%) 7 6	21, 39, 71, 86	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	PHE	5.5
1	A	321	THR	5.0
1	A	355	PHE	4.7
1	A	533	LEU	4.5
1	A	711	TRP	4.3
1	A	554	PHE	4.3
1	A	716	TRP	4.1
1	A	322	LEU	4.0
1	A	528	GLY	4.0
1	B	348	VAL	3.9
1	A	715	VAL	3.9
1	A	501	PHE	3.9
1	B	337	LEU	3.8
1	B	321	THR	3.7
1	A	512	ALA	3.7
1	A	553	TRP	3.6
1	A	551	PHE	3.6
1	B	350	THR	3.5
1	A	338	PRO	3.5
1	A	485	TYR	3.5
1	A	504	ILE	3.4
1	A	381	LEU	3.4
1	A	505	CYS	3.4
1	B	322	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	376	ALA	3.3
1	A	493	LEU	3.3
1	A	535	GLN	3.1
1	B	300	PHE	3.1
1	A	712	ASN	3.1
1	A	384	VAL	3.1
1	A	531	PRO	3.0
1	A	486	LYS	3.0
1	A	487	GLN	2.9
1	A	506	ILE	2.9
1	A	513	PRO	2.9
1	B	338	PRO	2.9
1	A	320	SER	2.8
1	A	502	THR	2.8
1	A	508	GLN	2.8
1	A	350	THR	2.8
1	A	510	TRP	2.8
1	A	643	SER	2.7
1	A	517	PHE	2.7
1	A	319	LYS	2.7
1	A	354	LEU	2.7
1	A	559	LEU	2.6
1	A	499	VAL	2.6
1	A	388	ILE	2.6
1	A	475	TRP	2.6
1	A	618	MET	2.6
1	A	529	ASN	2.6
1	A	356	PRO	2.6
1	A	550	LYS	2.5
1	A	526	ALA	2.5
1	A	361	PHE	2.5
1	A	311	VAL	2.5
1	A	466	THR	2.5
1	A	378	MET	2.5
1	A	373	GLY	2.5
1	A	710	PRO	2.5
1	A	610	VAL	2.4
1	A	471	ASP	2.4
1	A	374	SER	2.4
1	A	491	SER	2.4
1	A	544	VAL	2.4
1	A	492	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	616	LEU	2.4
1	A	490	GLY	2.4
1	A	545	PRO	2.4
1	A	503	GLU	2.3
1	B	355	PHE	2.3
1	A	337	LEU	2.3
1	A	390	SER	2.3
1	A	536	ILE	2.3
1	A	546	ILE	2.3
1	A	391	THR	2.3
1	A	301	LEU	2.3
1	A	557	LEU	2.3
1	A	519	VAL	2.2
1	A	482	TYR	2.2
1	A	393	THR	2.2
1	A	494	GLY	2.2
1	A	604	TYR	2.2
1	B	667	ARG	2.2
1	B	307	GLU	2.2
1	A	500	GLN	2.2
1	A	636	ALA	2.2
1	A	549	PRO	2.1
1	A	382	GLU	2.1
1	B	610	VAL	2.1
1	A	484	GLY	2.1
1	B	718	GLY	2.1
1	A	362	LEU	2.1
1	A	602	SER	2.1
1	A	639	TYR	2.1
1	A	609	GLU	2.1
1	A	372	PHE	2.1
1	A	714	HIS	2.1
1	B	552	ASP	2.1
1	A	515	GLY	2.1
1	A	385	ASN	2.1
1	A	470	HIS	2.1
1	A	713	THR	2.1
1	A	534	PHE	2.1
1	A	524	LEU	2.0
1	A	552	ASP	2.0
1	A	538	PRO	2.0
1	B	323	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	389	GLU	2.0
1	A	318	LEU	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](#)

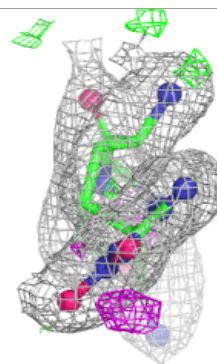
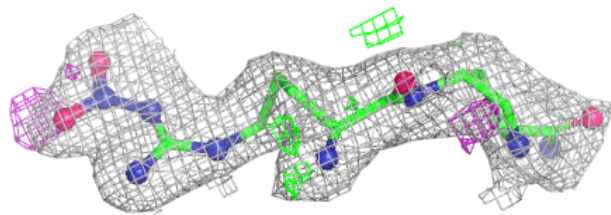
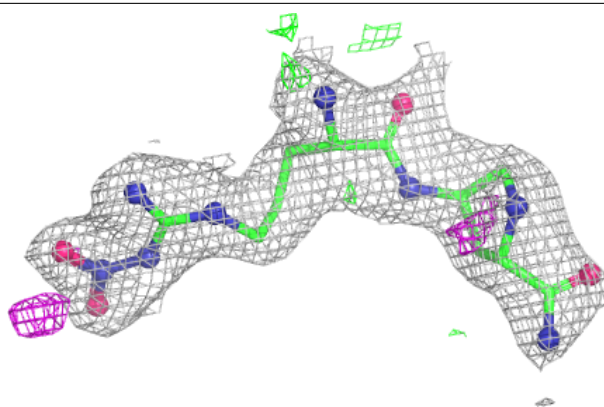
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TFA	B	866	7/7	0.81	0.21	42,45,48,48	0
7	GOL	B	881	6/6	0.84	0.16	55,59,59,60	0
5	DP9	A	799	23/23	0.87	0.13	31,44,52,55	0
7	GOL	A	880	6/6	0.89	0.11	49,49,51,52	0
5	DP9	B	800	23/23	0.90	0.11	29,40,50,52	0
6	TFA	A	865	7/7	0.91	0.14	47,48,49,49	0
4	H4B	A	760	17/17	0.96	0.06	26,29,30,32	0
4	H4B	B	761	17/17	0.96	0.05	20,23,27,29	0
3	HEM	A	750	43/43	0.98	0.06	25,28,30,32	0
3	HEM	B	750	43/43	0.98	0.06	22,26,29,31	0
2	ZN	A	900	1/1	0.99	0.02	32,32,32,32	0

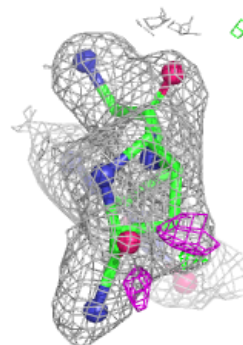
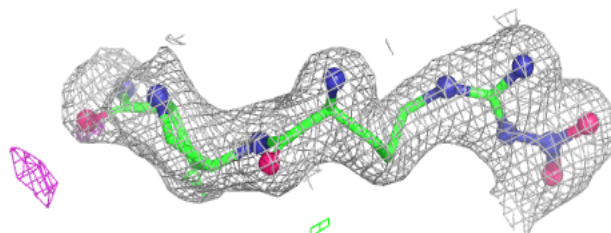
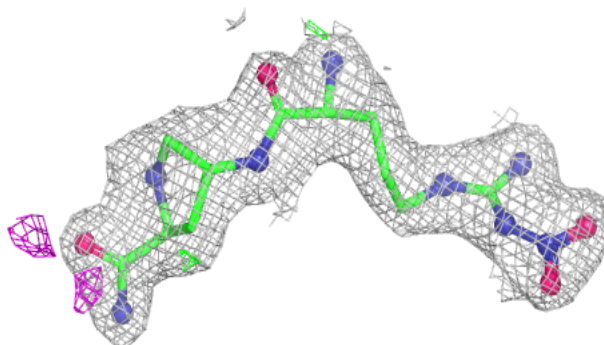
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DP9 A 799:

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

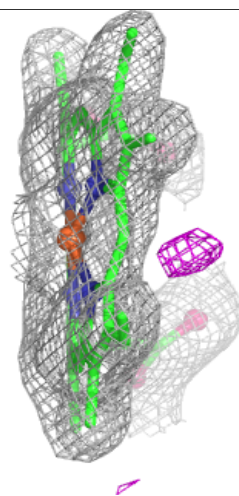
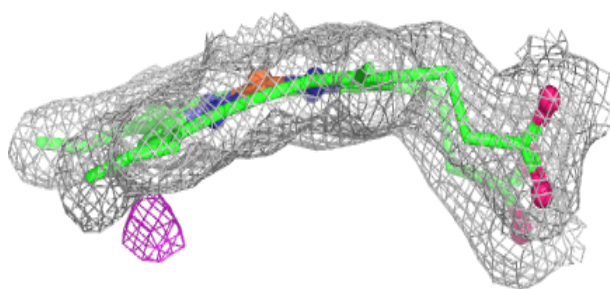
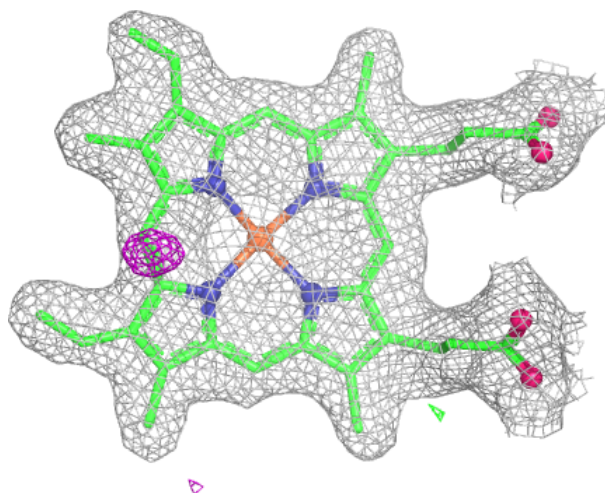
**Electron density around DP9 B 800:**

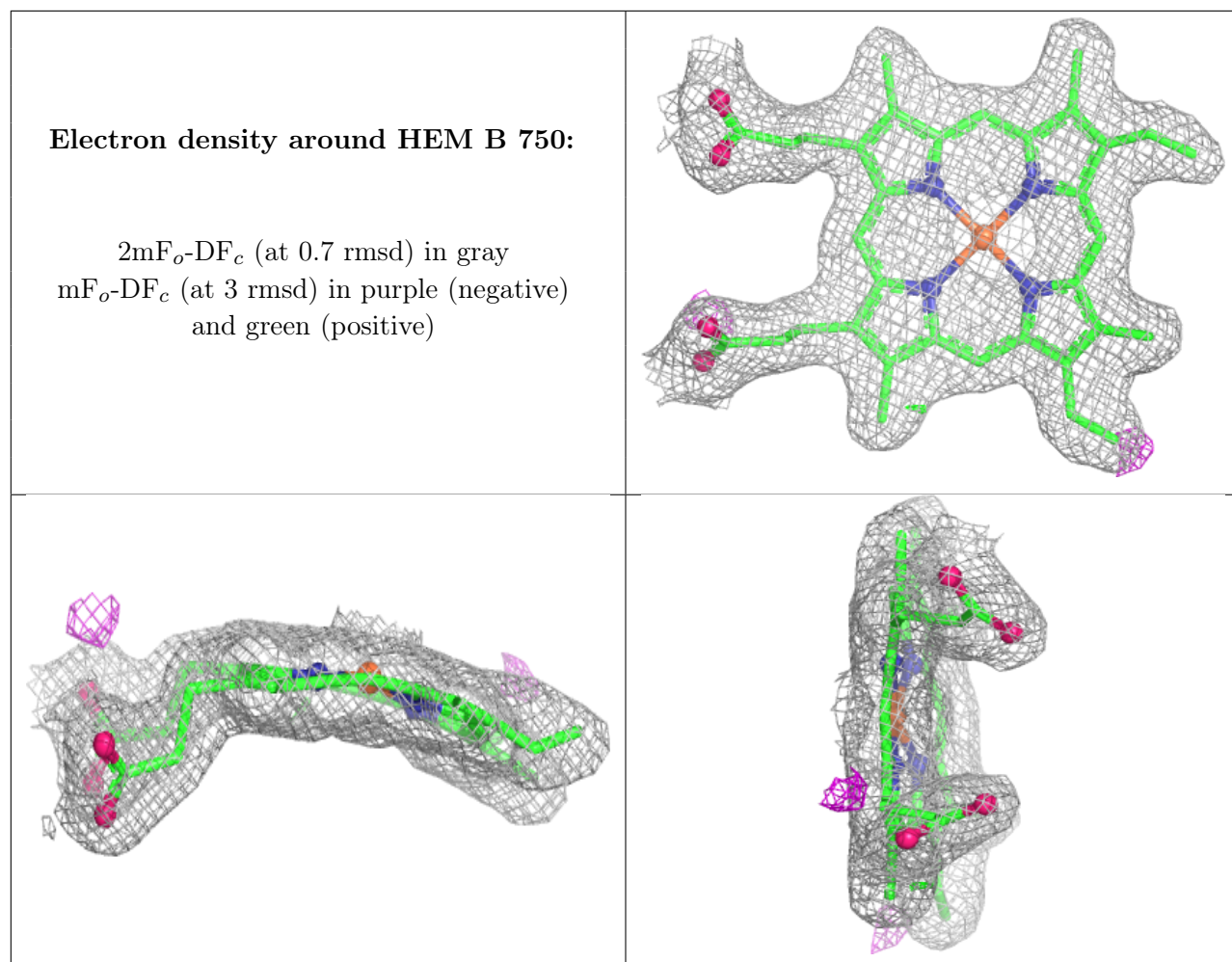
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.