



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 08:15 AM EDT

PDB ID : 1ZZR
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

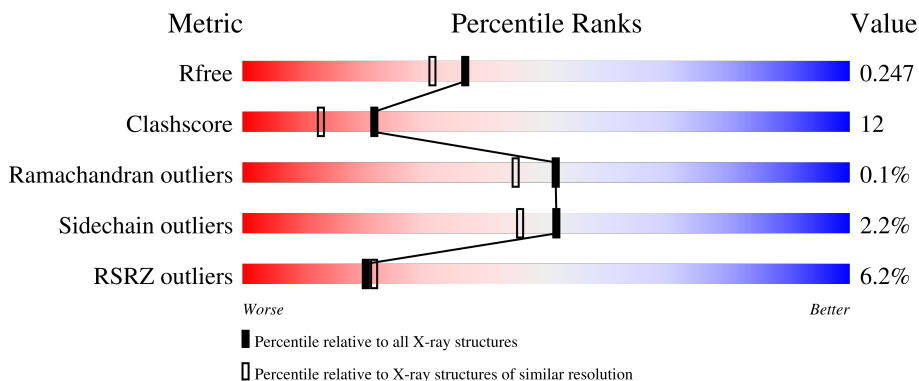
1 Overall quality at a glance

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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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	 10% 68% 27% . .
1	B	420	 2% 81% 16% .

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
			Total	C	N	O	S			
1	A	407	3312	2121	567	604	20	0	0	0
1	B	411	3344	2140	575	609	20	0	0	0

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 (three-letter code: ZN) (formula: Zn).

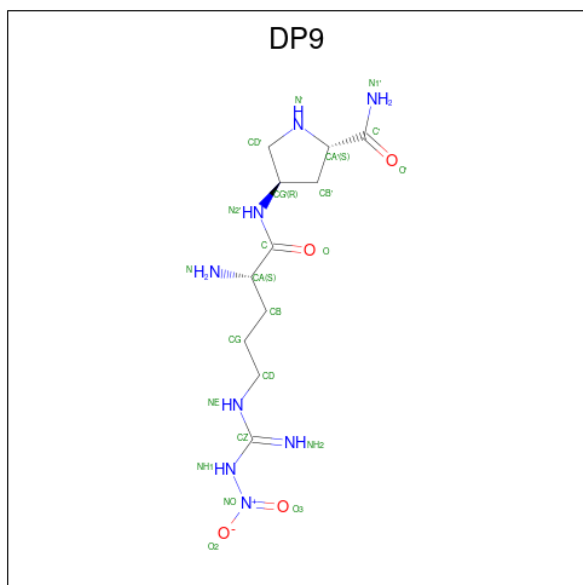
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).

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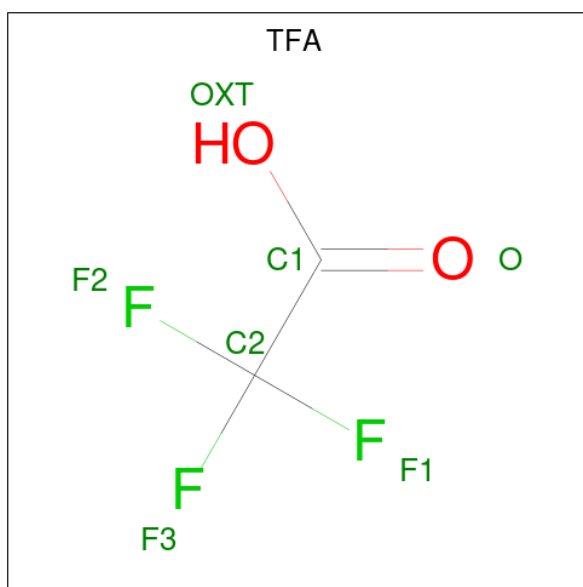
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	17	9	5	3	0	0

- Molecule 5 is L-N(OMEGA)-NITROARGININE-(4R)-AMINO-L-PROLINE AMIDE (three-letter code: DP9) (formula: C₁₁H₂₂N₈O₄).



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

- Molecule 6 is trifluoroacetic acid (three-letter code: TFA) (formula: C₂HF₃O₂).



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 (three-letter code: 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		

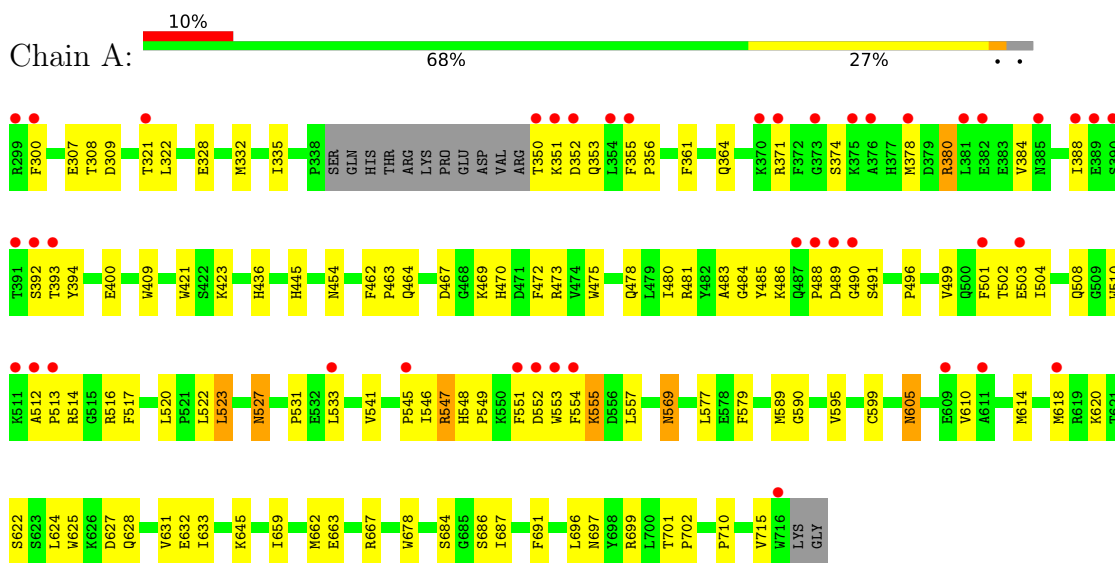
- Molecule 8 is water.

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

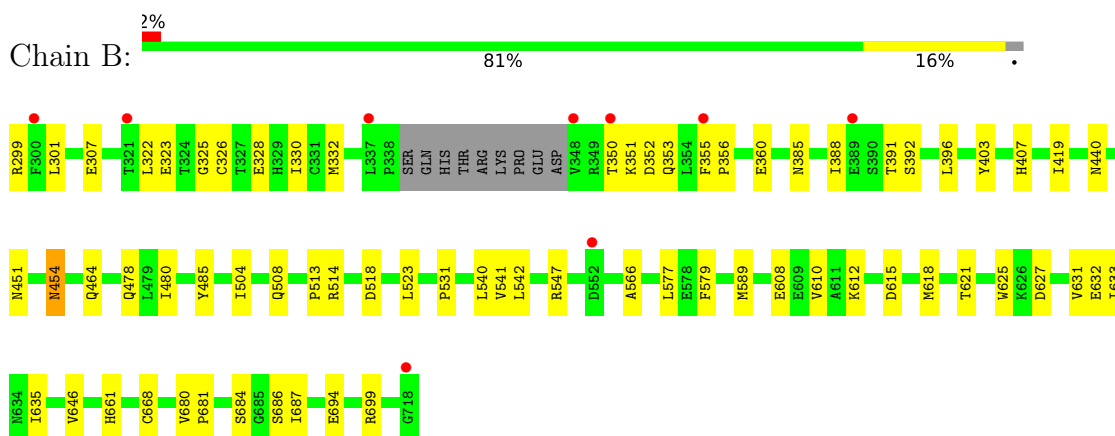
3 Residue-property plots i

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) 98.9 (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)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.260 0.217 , 0.247	Depositor DCC
R_{free} test set	3036 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtrriage
Anisotropy	0.822	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DP9, HEM, H4B, ZN, TFA

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	0.43	0/3405	0.64	1/4621 (0.0%)
1	B	0.46	0/3437	0.67	2/4661 (0.0%)
All	All	0.44	0/6842	0.66	3/9282 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	CYS	CA-CB-SG	8.30	128.93	114.00
1	A	589	MET	N-CA-C	-6.22	94.22	111.00
1	B	589	MET	N-CA-C	-5.93	94.98	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	115	0
1	B	3344	0	3261	48	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	160	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 12.

All (160) 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: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: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: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:332:MET:HE1	1:B:301:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:SER:HB3	1:A:687:ILE:CD1	2.34	0.57
1:A:350:THR:HB	1:A:353:GLN:CD	2.26	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
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: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: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:464:GLN:HB3	1:A:579:PHE:CE2	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
1:A:516:ARG:HD3	1:A:517:PHE:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.33	0.48
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:467:ASP:C	1:A:469:LYS:H	2.17	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: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: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:483:ALA:HB1	1:A:502:THR:CG2	2.45	0.46
1:A:701:THR:HA	1:A:702:PRO:C	2.36	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:485:TYR:CE2	1:A:512:ALA:HB1	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:610:VAL:HG21	1:A:633:ILE:HD11	2.00	0.43
1:B:350:THR:HG22	1:B:351:LYS:N	2.34	0.43
1:A:328:GLU:H	1:A:328:GLU:CD	2.21	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: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: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
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:A:489:ASP:C	1:A:491:SER:H	2.23	0.41
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ASN:ND2	8:A:1058:HOH:O	2.41	0.41
1:A:423:LYS:NZ	8:A:1014:HOH:O	2.53	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:488:PRO:C	1:A:490:GLY:H	2.24	0.41
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.54	0.41
1:A:445:HIS:C	1:A:445:HIS:CD2	2.94	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: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

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	403/420 (96%)	375 (93%)	27 (7%)	1 (0%)	47	39
1	B	407/420 (97%)	391 (96%)	16 (4%)	0	100	100
All	All	810/840 (96%)	766 (95%)	43 (5%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	605	ASN

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	363/375 (97%)	352 (97%)	11 (3%)	41	34
1	B	366/375 (98%)	361 (99%)	5 (1%)	67	65
All	All	729/750 (97%)	713 (98%)	16 (2%)	52	46

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	ARG
1	A	454	ASN
1	A	523	LEU
1	A	527	ASN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	645	LYS
1	A	662	MET
1	A	667	ARG
1	A	697	ASN
1	B	353	GLN
1	B	454	ASN
1	B	540	LEU
1	B	547	ARG
1	B	668	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	GLN
1	A	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	605	ASN

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Mol	Chain	Res	Type
1	A	642	GLN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN
1	B	454	ASN
1	B	527	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	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 monosaccharides 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
4	H4B	A	760	-	16,18,18	2.15	3 (18%)	11,26,26	4.23	9 (81%)
3	HEM	B	750	1	27,50,50	1.70	7 (25%)	17,82,82	1.68	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TFA	A	865	-	3,6,6	0.41	0	3,9,9	1.11	0
3	HEM	A	750	1	27,50,50	1.78	8 (29%)	17,82,82	1.70	4 (23%)
7	GOL	B	881	-	5,5,5	0.32	0	5,5,5	0.32	0
7	GOL	A	880	-	5,5,5	0.33	0	5,5,5	0.29	0
6	TFA	B	866	-	3,6,6	1.27	1 (33%)	3,9,9	1.33	0
5	DP9	A	799	-	18,23,23	0.96	1 (5%)	21,30,30	1.88	5 (23%)
5	DP9	B	800	-	18,23,23	1.02	1 (5%)	21,30,30	1.91	4 (19%)
4	H4B	B	761	-	16,18,18	2.27	5 (31%)	11,26,26	4.46	9 (81%)

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	761	H4B	C4-N3	5.27	1.42	1.33
4	A	760	H4B	C4-N3	5.20	1.42	1.33
4	A	760	H4B	C4A-N5	4.72	1.47	1.38
4	B	761	H4B	C4A-N5	4.19	1.46	1.38
3	B	750	HEM	C3B-CAB	-4.13	1.39	1.47
4	B	761	H4B	C6-N5	4.07	1.53	1.45
3	A	750	HEM	C3C-CAC	-3.73	1.40	1.47
4	A	760	H4B	C6-N5	3.68	1.53	1.45
3	B	750	HEM	C3C-C2C	-3.58	1.35	1.40
3	A	750	HEM	C3B-C2B	-3.42	1.35	1.40
3	A	750	HEM	C3B-CAB	-3.33	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	800	DP9	CG'-N2'	2.95	1.52	1.46
3	B	750	HEM	C3C-CAC	-2.88	1.41	1.47
4	B	761	H4B	C7-C6	2.87	1.55	1.52
5	A	799	DP9	CG'-N2'	2.78	1.52	1.46
3	A	750	HEM	C4A-NA	2.56	1.41	1.36
3	A	750	HEM	C1D-ND	2.54	1.41	1.36
3	A	750	HEM	CMD-C2D	2.48	1.56	1.51
3	B	750	HEM	C4B-NB	2.32	1.40	1.36
3	B	750	HEM	C1A-NA	2.31	1.40	1.36
3	A	750	HEM	CMB-C2B	2.25	1.56	1.51
3	B	750	HEM	CMC-C2C	2.15	1.56	1.51
3	A	750	HEM	C4B-NB	2.09	1.40	1.36
6	B	866	TFA	F2-C2	2.08	1.40	1.32
4	B	761	H4B	C8A-N1	2.07	1.38	1.34
3	B	750	HEM	CMB-C2B	2.01	1.56	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	761	H4B	C4-C4A-C8A	9.71	123.19	114.57
4	A	760	H4B	C4-C4A-C8A	8.81	122.39	114.57
4	A	760	H4B	C4-N3-C2	5.75	125.07	115.93
4	B	761	H4B	C4-N3-C2	5.54	124.74	115.93
4	A	760	H4B	N3-C2-N1	-4.85	117.81	125.42
5	A	799	DP9	CD-NE-CZ	4.50	131.72	123.50
4	B	761	H4B	C4-C4A-N5	-4.42	115.42	119.12
5	B	800	DP9	CD-NE-CZ	4.40	131.54	123.50
4	B	761	H4B	N3-C2-N1	-4.40	118.51	125.42
3	A	750	HEM	CBA-CAA-C2A	-4.26	104.62	112.49
3	B	750	HEM	CBD-CAD-C3D	-3.91	105.28	112.48
5	B	800	DP9	C'-CA'-N'	-3.84	104.70	111.88
4	A	760	H4B	C2-N1-C8A	3.70	122.84	114.54
4	A	760	H4B	C4A-C4-N3	-3.69	113.52	124.01
5	A	799	DP9	O'-C'-N1'	-3.64	116.67	123.00
3	A	750	HEM	CBD-CAD-C3D	-3.60	105.85	112.48
4	B	761	H4B	C4A-C4-N3	-3.59	113.80	124.01
5	B	800	DP9	O'-C'-N1'	-3.40	117.08	123.00
4	B	761	H4B	N2-C2-N1	3.39	122.52	117.25
4	A	760	H4B	N2-C2-N1	3.35	122.46	117.25
4	B	761	H4B	C4A-N5-C6	-3.31	112.15	121.16
5	A	799	DP9	C'-CA'-N'	-3.27	105.77	111.88
4	B	761	H4B	C2-N1-C8A	3.27	121.86	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	750	HEM	C1D-C2D-C3D	-3.13	104.82	107.00
4	A	760	H4B	C4A-N5-C6	-3.01	112.96	121.16
4	B	761	H4B	O9-C9-C6	2.70	115.45	108.98
3	B	750	HEM	CBA-CAA-C2A	-2.69	107.53	112.49
5	B	800	DP9	CA'-C'-N1'	2.62	121.18	116.69
4	A	760	H4B	O9-C9-C6	2.48	114.90	108.98
4	A	760	H4B	C4-C4A-N5	-2.44	117.08	119.12
5	A	799	DP9	CA'-C'-N1'	2.43	120.85	116.69
3	A	750	HEM	C1D-C2D-C3D	-2.25	105.43	107.00
3	B	750	HEM	CMD-C2D-C3D	2.09	128.88	124.94
3	A	750	HEM	CMC-C2C-C3C	2.06	128.53	124.68
5	A	799	DP9	CB'-CA'-C'	2.01	114.41	111.19

There are no chirality outliers.

All (6) 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
5	A	799	DP9	N-CA-CB-CG

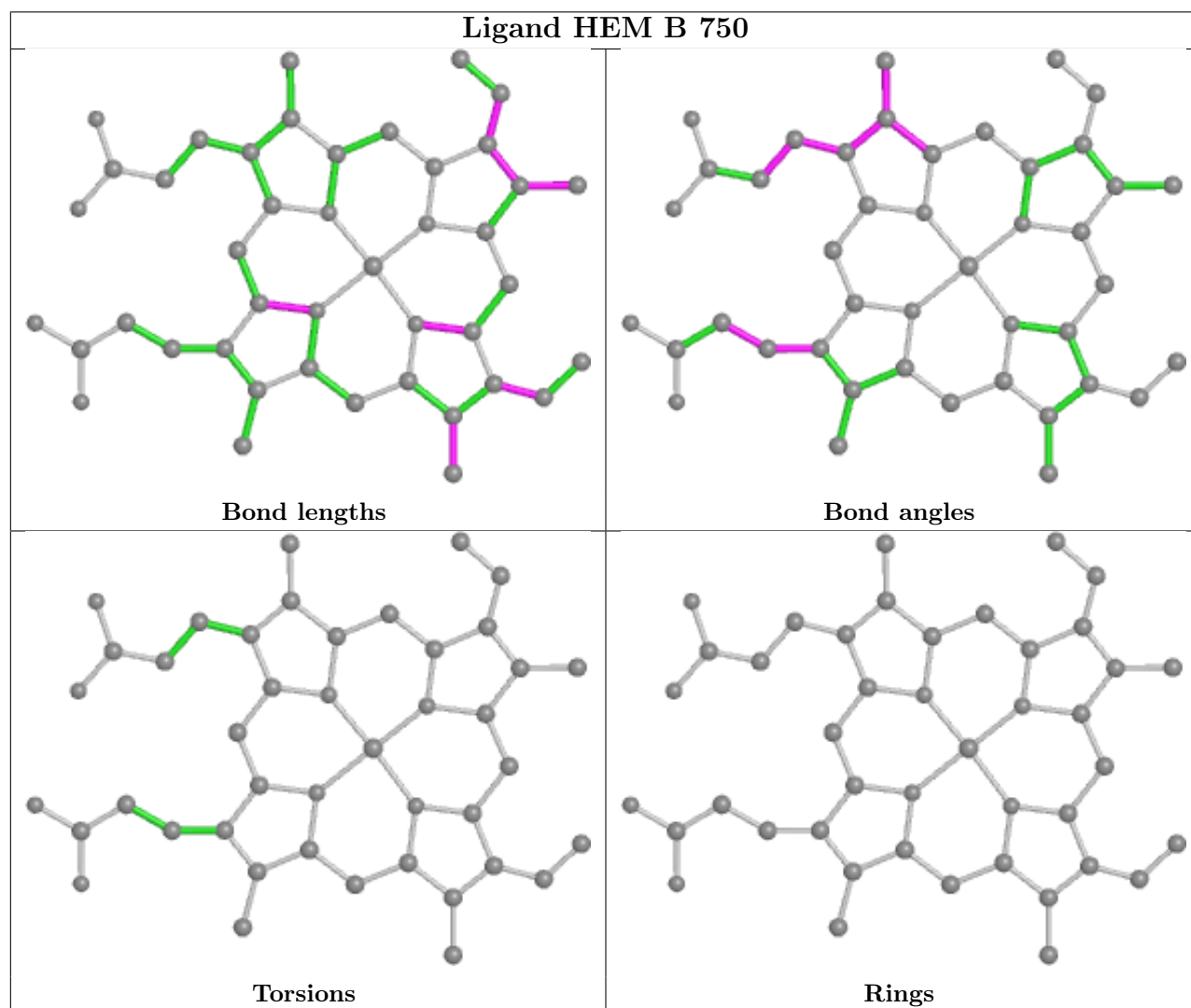
There are no ring outliers.

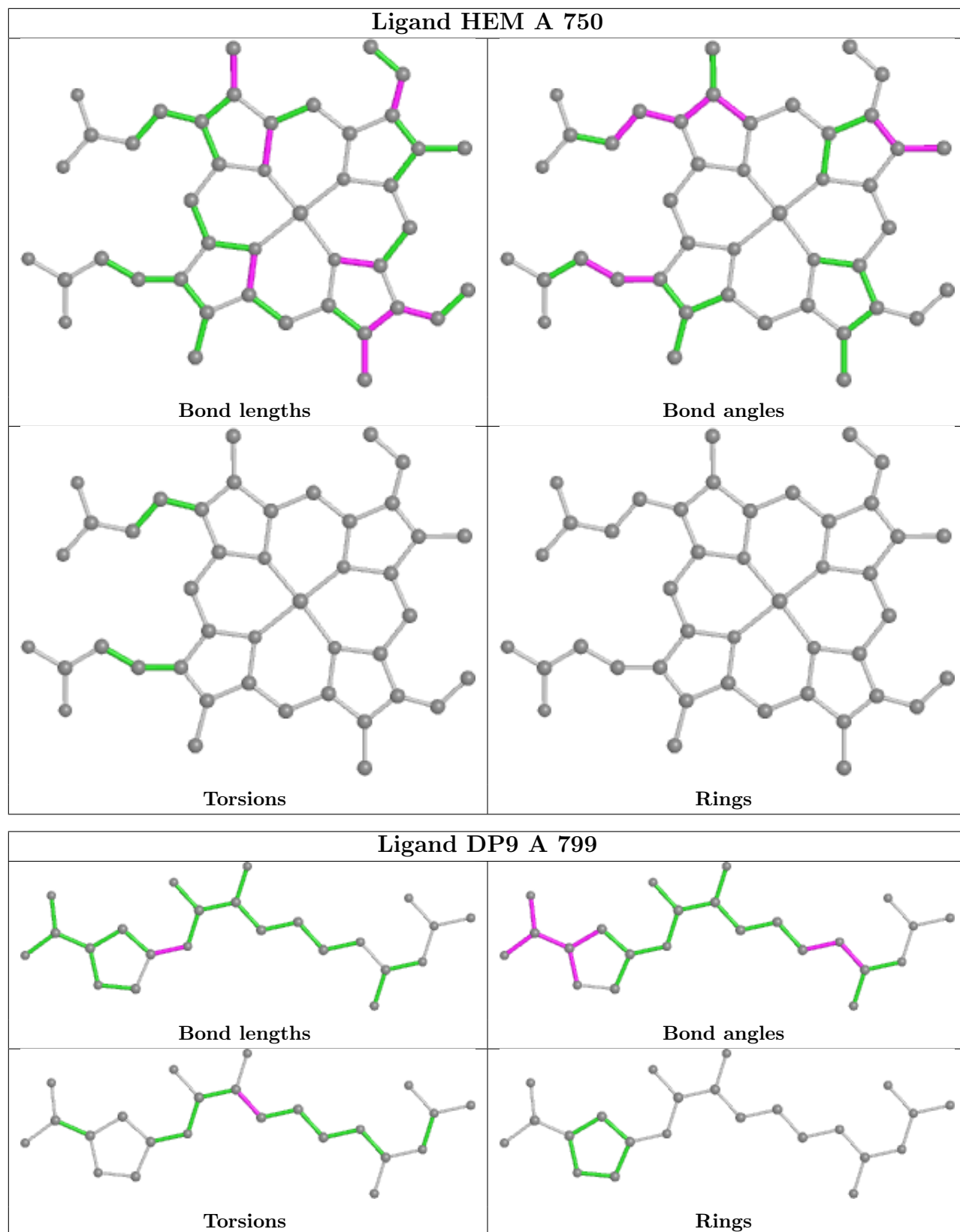
3 monomers are involved in 4 short contacts:

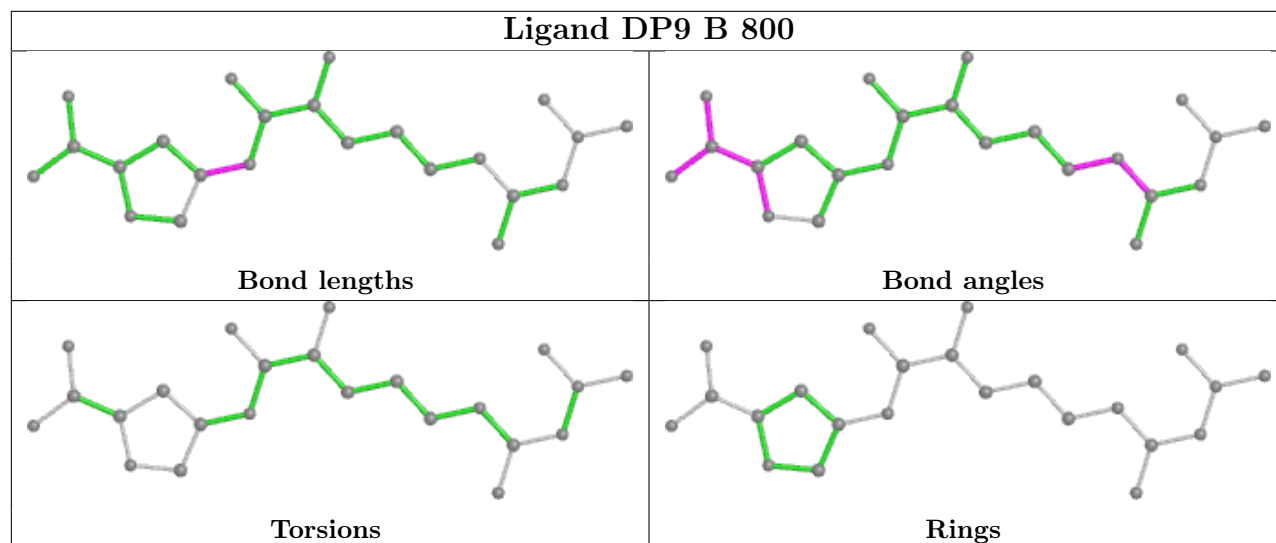
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	760	H4B	1	0
3	B	750	HEM	2	0
3	A	750	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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%)	0.66	42 (10%) 6 6	22, 45, 75, 86	0
1	B	411/420 (97%)	0.21	9 (2%) 62 66	21, 35, 59, 83	0
All	All	818/840 (97%)	0.44	51 (6%) 20 22	21, 39, 71, 86	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	6.0
1	A	355	PHE	5.5
1	A	352	ASP	4.4
1	A	488	PRO	4.3
1	B	300	PHE	4.1
1	A	321	THR	3.9
1	A	388	ILE	3.7
1	B	718	GLY	3.7
1	A	551	PHE	3.7
1	A	554	PHE	3.5
1	A	393	THR	3.5
1	B	321	THR	3.5
1	A	373	GLY	3.3
1	B	350	THR	3.3
1	B	337	LEU	3.2
1	A	300	PHE	3.2
1	A	299	ARG	3.1
1	A	553	TRP	3.1
1	A	351	LYS	3.1
1	A	511	LYS	3.0
1	A	391	THR	3.0
1	A	716	TRP	2.9
1	A	371	ARG	2.9
1	A	390	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	375	LYS	2.8
1	A	381	LEU	2.8
1	A	490	GLY	2.7
1	A	392	SER	2.7
1	A	501	PHE	2.6
1	A	609	GLU	2.6
1	A	385	ASN	2.6
1	B	389	GLU	2.5
1	A	533	LEU	2.5
1	B	355	PHE	2.5
1	A	389	GLU	2.4
1	A	611	ALA	2.4
1	A	378	MET	2.3
1	A	376	ALA	2.3
1	A	503	GLU	2.3
1	A	512	ALA	2.3
1	A	487	GLN	2.3
1	A	489	ASP	2.2
1	A	382	GLU	2.2
1	A	552	ASP	2.2
1	A	354	LEU	2.1
1	B	552	ASP	2.1
1	A	545	PRO	2.1
1	A	618	MET	2.1
1	A	370	LYS	2.1
1	A	513	PRO	2.0
1	A	350	THR	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 monosaccharides in this entry.

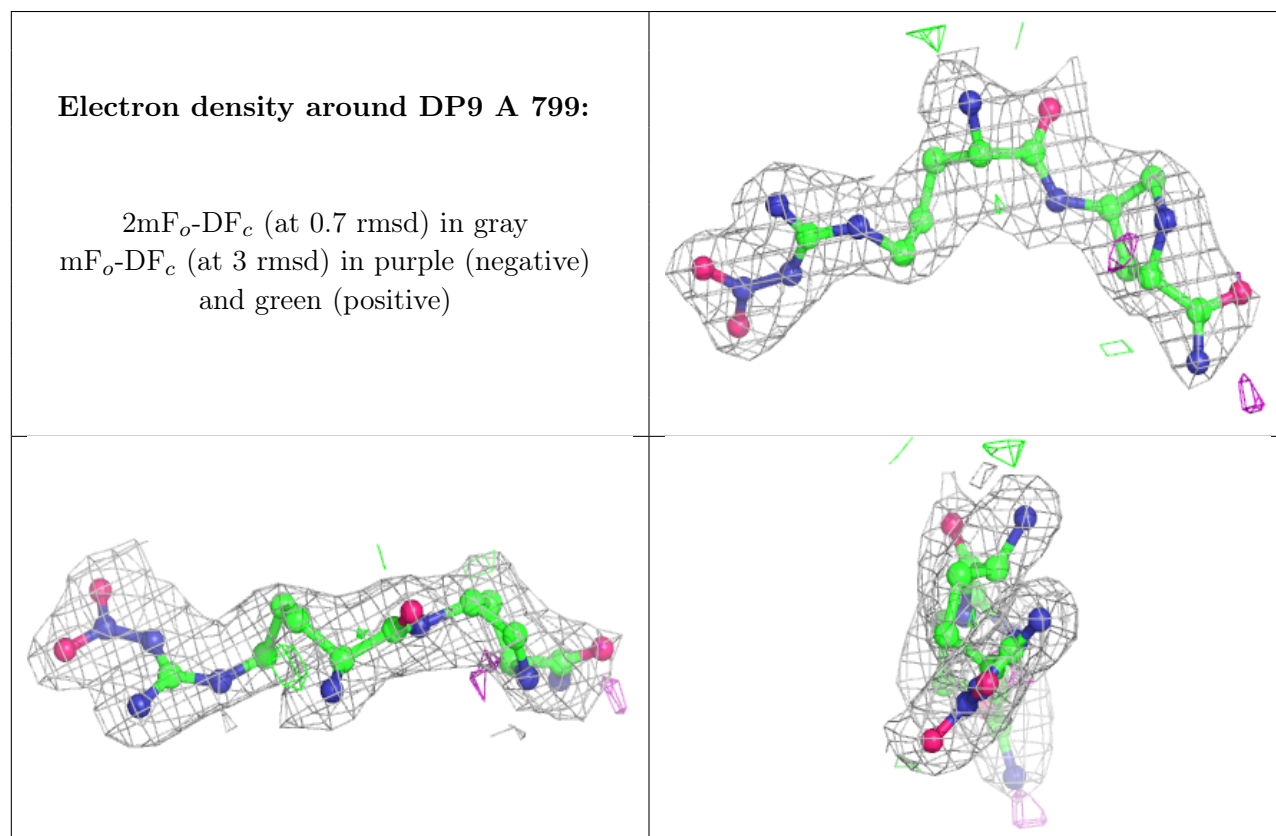
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

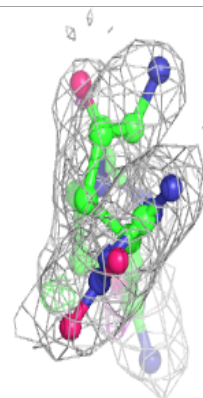
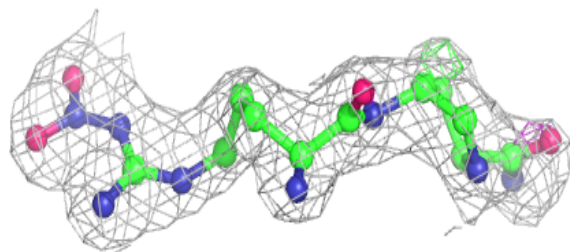
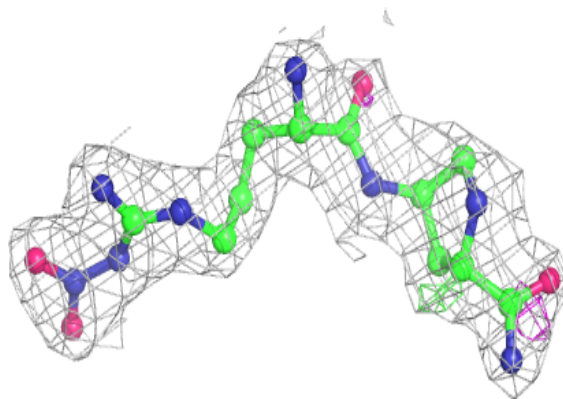
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	B	881	6/6	0.73	0.26	55,59,59,60	0
6	TFA	B	866	7/7	0.88	0.27	42,45,48,48	0
7	GOL	A	880	6/6	0.89	0.16	49,49,51,52	0
5	DP9	A	799	23/23	0.90	0.17	31,44,52,55	0
5	DP9	B	800	23/23	0.92	0.17	29,40,50,52	0
6	TFA	A	865	7/7	0.95	0.20	47,48,49,49	0
4	H4B	B	761	17/17	0.96	0.15	20,23,27,29	0
4	H4B	A	760	17/17	0.97	0.11	26,29,30,32	0
3	HEM	A	750	43/43	0.98	0.11	25,28,30,32	0
3	HEM	B	750	43/43	0.98	0.14	22,26,29,31	0
2	ZN	A	900	1/1	0.99	0.11	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.



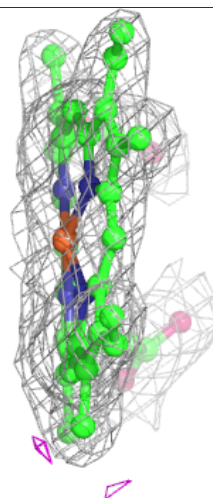
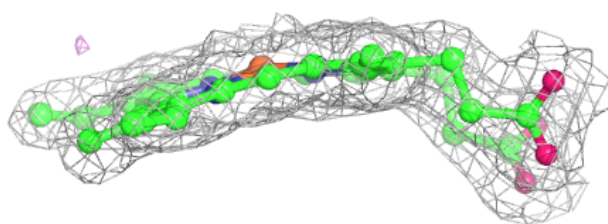
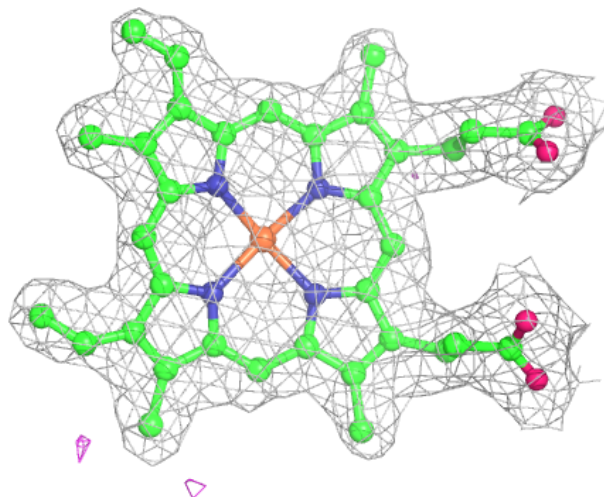
Electron density around DP9 B 800:

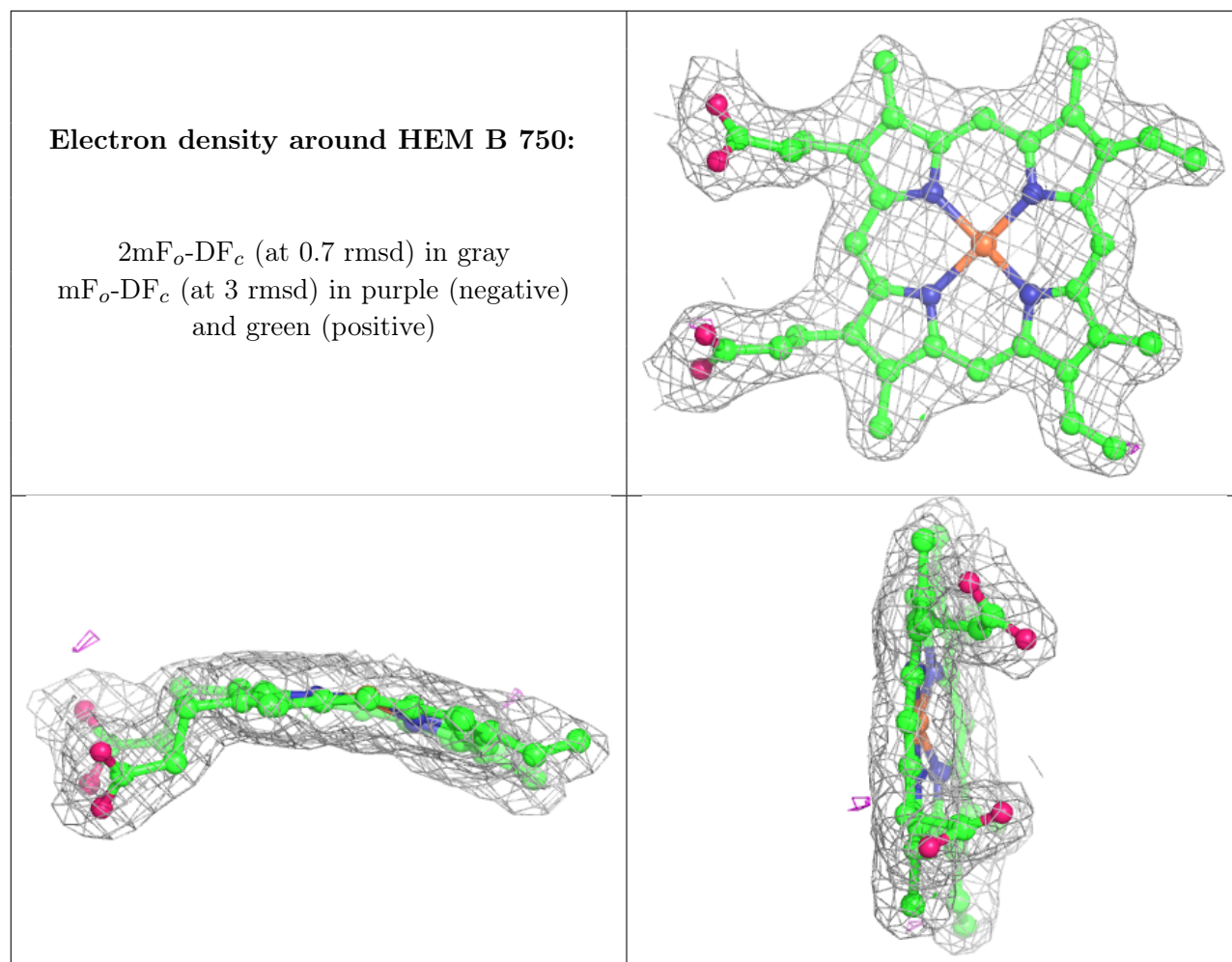
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [i](#)

There are no such residues in this entry.