



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:09 pm BST

PDB ID : 4CJX
Title : The crystal structure of Trypanosoma brucei N5, N10- methylenetetrahydrofolate dehydrogenase-cyclohydrolase (FolD) complexed with NADP cofactor and inhibitor
Authors : Eadsforth, T.C.; Hunter, W.N.
Deposited on : 2013-12-23
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 : 2.11
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) : 2.11

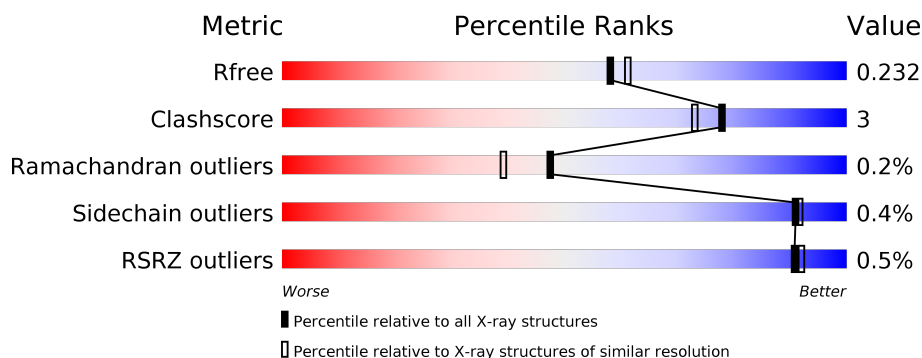
1 Overall quality at a glance

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 on 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	319	
1	B	319	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4961 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 C-1-TETRAHYDROFOLATE SYNTHASE, CYTOPLASMIC, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	41	6	0
			2266	1430	417	406	13			
1	B	297	Total	C	N	O	S	50	4	0
			2250	1417	411	408	14			

There are 44 discrepancies between the modelled and reference sequences:

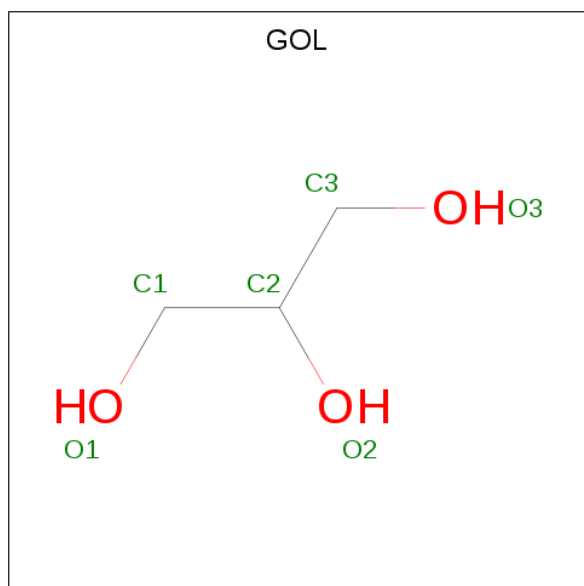
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q57WP0
A	-19	GLY	-	expression tag	UNP Q57WP0
A	-18	SER	-	expression tag	UNP Q57WP0
A	-17	SER	-	expression tag	UNP Q57WP0
A	-16	HIS	-	expression tag	UNP Q57WP0
A	-15	HIS	-	expression tag	UNP Q57WP0
A	-14	HIS	-	expression tag	UNP Q57WP0
A	-13	HIS	-	expression tag	UNP Q57WP0
A	-12	HIS	-	expression tag	UNP Q57WP0
A	-11	HIS	-	expression tag	UNP Q57WP0
A	-10	SER	-	expression tag	UNP Q57WP0
A	-9	SER	-	expression tag	UNP Q57WP0
A	-8	GLY	-	expression tag	UNP Q57WP0
A	-7	GLU	-	expression tag	UNP Q57WP0
A	-6	ASN	-	expression tag	UNP Q57WP0
A	-5	LEU	-	expression tag	UNP Q57WP0
A	-4	TYR	-	expression tag	UNP Q57WP0
A	-3	PHE	-	expression tag	UNP Q57WP0
A	-2	GLN	-	expression tag	UNP Q57WP0
A	-1	GLY	-	expression tag	UNP Q57WP0
A	0	HIS	-	expression tag	UNP Q57WP0
A	80	ALA	THR	conflict	UNP Q57WP0
B	-20	MET	-	expression tag	UNP Q57WP0
B	-19	GLY	-	expression tag	UNP Q57WP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	expression tag	UNP Q57WP0
B	-17	SER	-	expression tag	UNP Q57WP0
B	-16	HIS	-	expression tag	UNP Q57WP0
B	-15	HIS	-	expression tag	UNP Q57WP0
B	-14	HIS	-	expression tag	UNP Q57WP0
B	-13	HIS	-	expression tag	UNP Q57WP0
B	-12	HIS	-	expression tag	UNP Q57WP0
B	-11	HIS	-	expression tag	UNP Q57WP0
B	-10	SER	-	expression tag	UNP Q57WP0
B	-9	SER	-	expression tag	UNP Q57WP0
B	-8	GLY	-	expression tag	UNP Q57WP0
B	-7	GLU	-	expression tag	UNP Q57WP0
B	-6	ASN	-	expression tag	UNP Q57WP0
B	-5	LEU	-	expression tag	UNP Q57WP0
B	-4	TYR	-	expression tag	UNP Q57WP0
B	-3	PHE	-	expression tag	UNP Q57WP0
B	-2	GLN	-	expression tag	UNP Q57WP0
B	-1	GLY	-	expression tag	UNP Q57WP0
B	0	HIS	-	expression tag	UNP Q57WP0
B	80	ALA	THR	conflict	UNP Q57WP0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



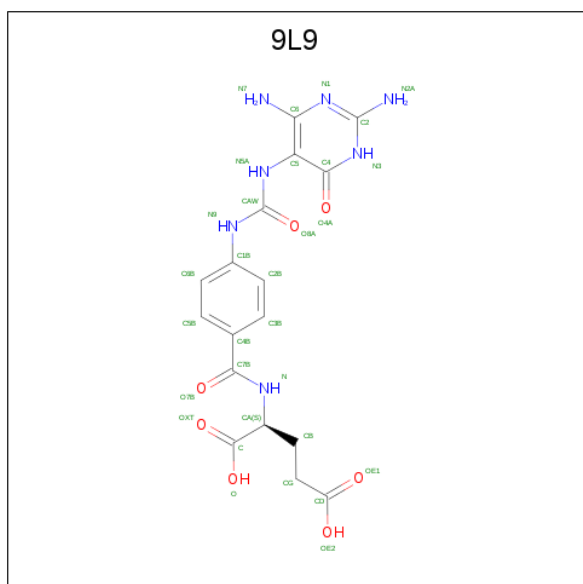
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is (2S)-2-[[4-[[2,4-bis(azanyl)-6-oxidanylidene-1H-pyrimidin-5-yl]carbamoylaminophenyl]carbonylamino]pentanedioic acid (three-letter code: 9L9) (formula: $C_{17}H_{19}N_7O_7$).



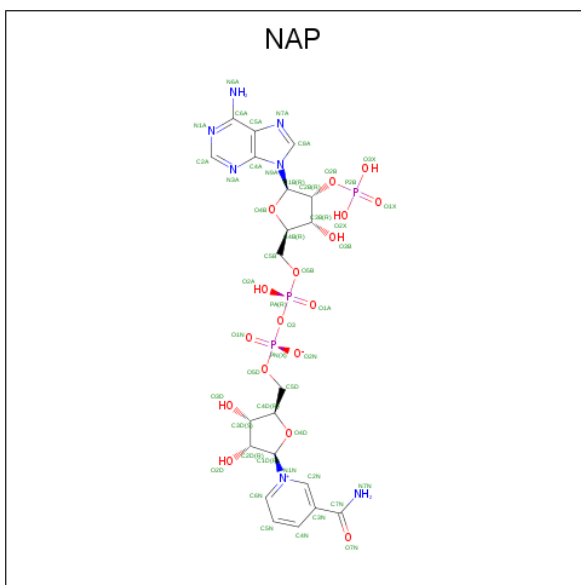
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			31	17	7	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			31	17	7	7		

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 17	P 3	0	0


- Molecule 6 is water.

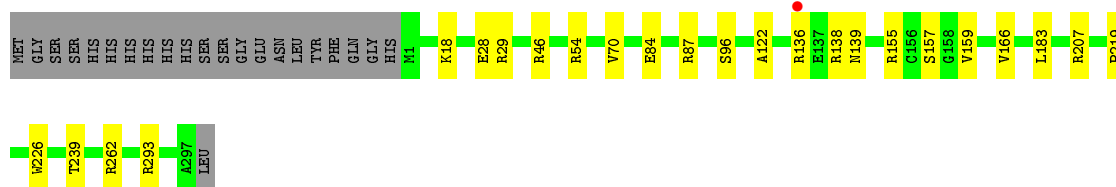
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	180	Total O 180 180	0	0
6	B	142	Total O 142 142	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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.

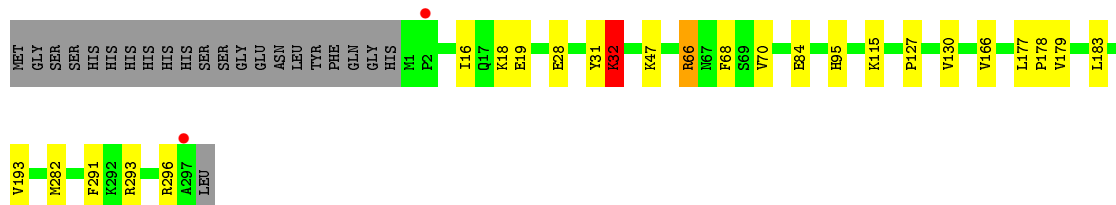
- Molecule 1: C-1-TETRAHYDROFOLATE SYNTHASE, CYTOPLASMIC, PUTATIVE

Chain A: 



- Molecule 1: C-1-TETRAHYDROFOLATE SYNTHASE, CYTOPLASMIC, PUTATIVE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.22Å 77.33Å 128.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.45 – 2.05 53.06 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.45-2.05) 99.9 (53.06-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.180 , 0.228 0.188 , 0.232	Depositor DCC
R_{free} test set	1862 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4961	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1719e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, NAP, PEG, 9L9

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	1.19	5/2316 (0.2%)	1.01	17/3144 (0.5%)
1	B	0.99	8/2294 (0.3%)	0.93	7/3114 (0.2%)
All	All	1.10	13/4610 (0.3%)	0.97	24/6258 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	GLU	CG-CD	-37.72	0.95	1.51
1	A	29	ARG	CD-NE	-28.39	0.98	1.46
1	B	115	LYS	CD-CE	-27.87	0.81	1.51
1	B	47	LYS	CD-CE	-20.26	1.00	1.51
1	A	18	LYS	CD-CE	-12.61	1.19	1.51
1	B	32	LYS	CA-CB	-12.32	1.26	1.53
1	B	19	GLU	CB-CG	-10.10	1.32	1.52
1	A	155	ARG	CD-NE	-8.88	1.31	1.46
1	A	136	ARG	CA-CB	7.78	1.71	1.53
1	B	18	LYS	CG-CD	-6.75	1.29	1.52
1	B	296	ARG	CB-CG	-6.60	1.34	1.52
1	B	293	ARG	CB-CG	-5.95	1.36	1.52
1	B	28	GLU	CG-CD	-5.37	1.44	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	LYS	CG-CD-CE	19.59	170.68	111.90
1	A	155	ARG	CG-CD-NE	17.46	148.46	111.80
1	A	155	ARG	CD-NE-CZ	17.12	147.57	123.60
1	B	115	LYS	CD-CE-NZ	12.51	140.46	111.70
1	A	29	ARG	CG-CD-NE	12.38	137.79	111.80
1	B	19	GLU	CA-CB-CG	12.16	140.14	113.40
1	A	139	ASN	N-CA-C	-11.57	79.75	111.00
1	A	28	GLU	CB-CG-CD	10.21	141.78	114.20
1	B	32	LYS	CB-CA-C	9.63	129.65	110.40
1	A	139	ASN	N-CA-CB	9.24	127.23	110.60
1	B	47	LYS	CG-CD-CE	9.16	139.37	111.90
1	A	139	ASN	C-N-CD	9.12	147.55	128.40
1	A	136	ARG	N-CA-CB	-8.98	94.44	110.60
1	B	47	LYS	CD-CE-NZ	8.16	130.46	111.70
1	A	18	LYS	CG-CD-CE	7.89	135.58	111.90
1	A	138	ARG	C-N-CA	-7.76	102.30	121.70
1	B	296	ARG	CA-CB-CG	-7.60	96.69	113.40
1	A	293	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	136	ARG	CB-CA-C	-7.39	95.61	110.40
1	A	293	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	28	GLU	CG-CD-OE2	-5.28	107.73	118.30
1	A	28	GLU	CG-CD-OE1	5.28	128.86	118.30
1	A	139	ASN	C-N-CA	-5.20	100.17	122.00
1	A	54	ARG	NE-CZ-NH1	5.06	122.83	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	32	LYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	66	ARG	Sidechain

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	2266	0	2421	11	2
1	B	2250	0	2386	11	2
2	A	6	0	8	0	0
3	A	7	0	10	0	0
4	A	31	0	17	4	0
4	B	31	0	17	1	0
5	A	48	0	25	4	0
6	A	180	0	0	1	0
6	B	142	0	0	0	0
All	All	4961	0	4884	27	2

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 3.

All (27) 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:262[B]:ARG:CG	1:A:262[B]:ARG:HH11	1.63	1.10
1:A:262[B]:ARG:HG2	1:A:262[B]:ARG:NH1	1.49	1.07
4:A:1300:9L9:H72N	5:A:1301:NAP:H4N	1.38	0.88
1:A:262[B]:ARG:HG2	1:A:262[B]:ARG:HH11	0.70	0.76
1:A:96:SER:HB3	1:A:122:ALA:HB2	1.76	0.68
1:B:166:VAL:HG11	1:B:183:LEU:HD13	1.82	0.61
1:A:262[B]:ARG:CG	1:A:262[B]:ARG:NH1	2.34	0.56
1:B:16:ILE:HD13	1:B:282:MET:HE3	1.87	0.55
1:A:87[B]:ARG:HD3	6:A:2065:HOH:O	2.08	0.54
4:A:1300:9L9:H5A	5:A:1301:NAP:H5N	1.74	0.52
4:A:1300:9L9:N7	5:A:1301:NAP:H4N	2.18	0.49
1:A:166:VAL:HG11	1:A:183:LEU:HD13	1.95	0.48
1:A:70:VAL:HG11	1:A:84:GLU:HG2	1.95	0.48
1:B:70:VAL:HG11	1:B:84:GLU:HG2	1.96	0.47
4:A:1300:9L9:H72N	5:A:1301:NAP:C4N	2.20	0.46
1:B:177:LEU:HB3	1:B:178:PRO:CD	2.46	0.46
1:B:16:ILE:HD13	1:B:282:MET:CE	2.45	0.45
1:B:177:LEU:HB3	1:B:178:PRO:HD3	1.99	0.44
1:B:66:ARG:HD3	1:B:68:PHE:CZ	2.53	0.44
1:B:66:ARG:HD3	1:B:68:PHE:CE1	2.53	0.44
1:A:219:PRO:HG3	1:A:239:THR:HB	2.00	0.44
1:B:31:TYR:O	1:B:32:LYS:C	2.57	0.42
4:B:1298:9L9:O8A	4:B:1298:9L9:H6B	2.20	0.42
1:A:157:SER:HB2	1:A:159:VAL:HG23	2.01	0.42
1:A:207:ARG:HA	1:A:226:TRP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:HIS:CE1	1:B:291:PHE:HD1	2.39	0.40
1:B:127:PRO:HA	1:B:130:VAL:HG12	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:NH1	1:B:32:LYS:CE[4_555]	1.78	0.42
1:A:46:ARG:NH1	1:B:32:LYS:NZ[4_555]	1.85	0.35

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	301/319 (94%)	292 (97%)	9 (3%)	0	100	100
1	B	299/319 (94%)	290 (97%)	8 (3%)	1 (0%)	41	31
All	All	600/638 (94%)	582 (97%)	17 (3%)	1 (0%)	47	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	32	LYS

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	248/261 (95%)	248 (100%)	0	100	100
1	B	246/261 (94%)	244 (99%)	2 (1%)	81	82
All	All	494/522 (95%)	492 (100%)	2 (0%)	91	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	179	VAL
1	B	193	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	B	17	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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	9L9	A	1300	-	26,32,32	1.90	4 (15%)	32,44,44	1.04	2 (6%)
3	PEG	A	1299	-	6,6,6	0.61	0	5,5,5	0.30	0
2	GOL	A	1298	-	5,5,5	0.73	0	5,5,5	0.54	0
5	NAP	A	1301	-	45,52,52	1.00	3 (6%)	56,80,80	1.28	5 (8%)
4	9L9	B	1298	-	26,32,32	2.15	6 (23%)	32,44,44	1.65	8 (25%)

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	9L9	A	1300	-	-	0/19/25/25	0/2/2/2
3	PEG	A	1299	-	-	3/4/4/4	-
2	GOL	A	1298	-	-	4/4/4/4	-
5	NAP	A	1301	-	-	18/31/67/67	0/5/5/5
4	9L9	B	1298	-	-	2/19/25/25	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1298	9L9	C2-N2A	6.72	1.47	1.33
4	A	1300	9L9	C2-N2A	6.44	1.46	1.33
4	B	1298	9L9	C6-N7	5.02	1.46	1.34
4	B	1298	9L9	C4-N3	4.36	1.40	1.33
4	A	1300	9L9	C6-N7	4.28	1.44	1.34
4	A	1300	9L9	C4-N3	3.95	1.39	1.33
5	A	1301	NAP	C2N-N1N	2.97	1.38	1.35
5	A	1301	NAP	O4D-C1D	2.93	1.45	1.41
4	B	1298	9L9	C5-C6	-2.67	1.36	1.41
5	A	1301	NAP	C5A-C4A	2.49	1.47	1.40
4	B	1298	9L9	C2-N3	2.48	1.39	1.35
4	A	1300	9L9	C1B-N9	-2.36	1.36	1.41
4	B	1298	9L9	C1B-N9	-2.23	1.37	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1298	9L9	C2-N1-C6	4.43	121.88	116.99
5	A	1301	NAP	N3A-C2A-N1A	-3.49	123.22	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1301	NAP	O7N-C7N-C3N	3.19	123.45	119.63
4	B	1298	9L9	CB-CA-N	3.14	114.77	110.19
4	B	1298	9L9	C4B-C7B-N	2.87	122.56	117.06
4	A	1300	9L9	N2A-C2-N1	2.59	121.27	117.25
4	A	1300	9L9	C5-C6-N1	2.41	122.44	117.66
4	B	1298	9L9	CB-CG-CD	-2.34	108.56	113.59
5	A	1301	NAP	C6N-N1N-C2N	-2.25	119.92	121.97
4	B	1298	9L9	CA-N-C7B	2.24	125.22	122.34
4	B	1298	9L9	C4-C5-N5A	2.22	121.99	117.67
4	B	1298	9L9	O7B-C7B-C4B	-2.18	117.05	120.94
5	A	1301	NAP	O2B-P2B-O1X	-2.11	101.26	109.39
4	B	1298	9L9	C4-N3-C2	-2.08	112.61	115.93
5	A	1301	NAP	C4A-C5A-N7A	-2.06	107.25	109.40

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1298	GOL	O1-C1-C2-C3
5	A	1301	NAP	C2B-O2B-P2B-O3X
5	A	1301	NAP	C2D-C1D-N1N-C2N
5	A	1301	NAP	C2D-C1D-N1N-C6N
4	B	1298	9L9	N-CA-CB-CG
5	A	1301	NAP	C2N-C3N-C7N-N7N
5	A	1301	NAP	C4N-C3N-C7N-N7N
5	A	1301	NAP	O4D-C4D-C5D-O5D
5	A	1301	NAP	C4N-C3N-C7N-O7N
5	A	1301	NAP	C2N-C3N-C7N-O7N
5	A	1301	NAP	C3B-C2B-O2B-P2B
3	A	1299	PEG	O2-C3-C4-O4
3	A	1299	PEG	O1-C1-C2-O2
2	A	1298	GOL	C1-C2-C3-O3
5	A	1301	NAP	C1B-C2B-O2B-P2B
2	A	1298	GOL	O1-C1-C2-O2
5	A	1301	NAP	C3D-C4D-C5D-O5D
2	A	1298	GOL	O2-C2-C3-O3
5	A	1301	NAP	O4B-C4B-C5B-O5B
5	A	1301	NAP	PA-O3-PN-O5D
5	A	1301	NAP	C5B-O5B-PA-O2A
4	B	1298	9L9	C-CA-CB-CG
3	A	1299	PEG	C1-C2-O2-C3
5	A	1301	NAP	C5B-O5B-PA-O3

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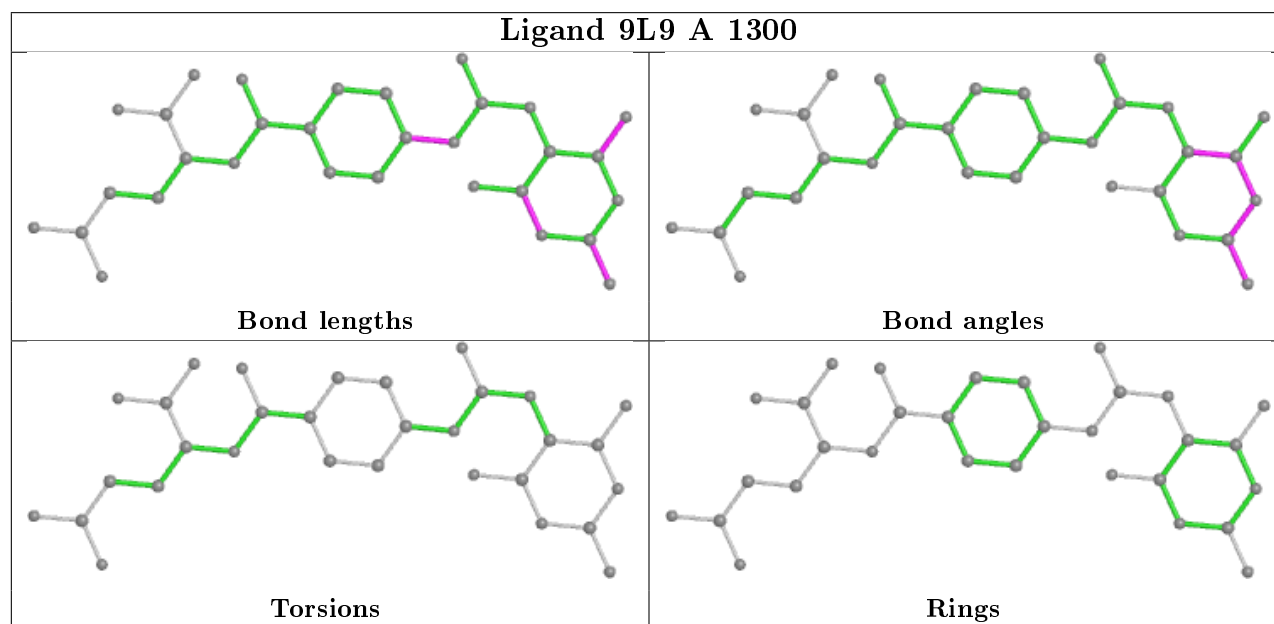
Mol	Chain	Res	Type	Atoms
5	A	1301	NAP	C3B-C4B-C5B-O5B
5	A	1301	NAP	PA-O3-PN-O2N
5	A	1301	NAP	C5D-O5D-PN-O1N

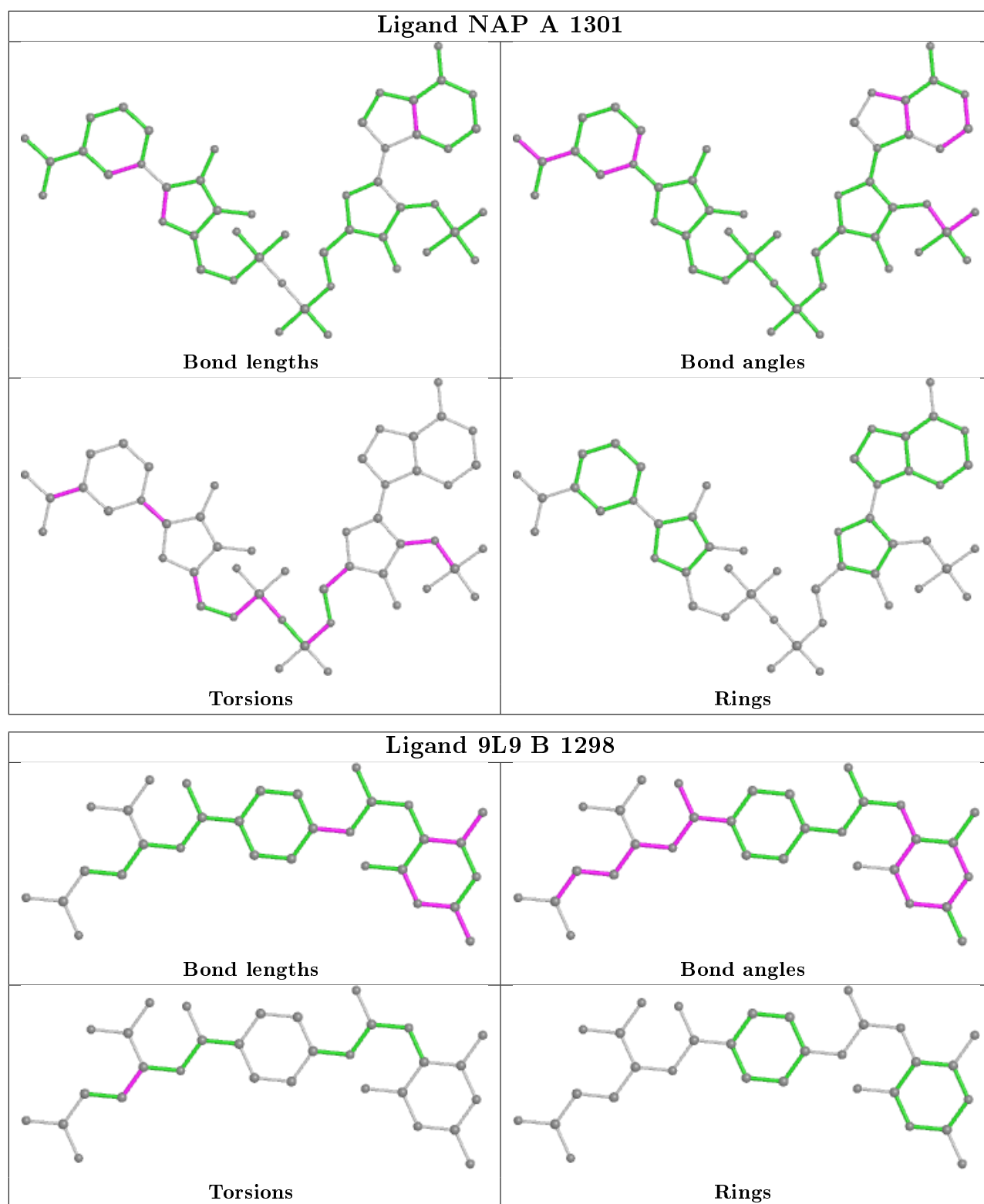
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1300	9L9	4	0
5	A	1301	NAP	4	0
4	B	1298	9L9	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	297/319 (93%)	-0.53	1 (0%) 94 94	12, 19, 33, 67	9 (3%)
1	B	297/319 (93%)	-0.40	2 (0%) 87 89	12, 24, 47, 68	12 (4%)
All	All	594/638 (93%)	-0.46	3 (0%) 91 92	12, 21, 46, 68	21 (3%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	ALA	4.6
1	A	136	ARG	3.7
1	B	2	PRO	2.2

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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	1298	6/6	0.68	0.19	43,44,46,47	0
3	PEG	A	1299	7/7	0.81	0.17	36,40,42,44	0

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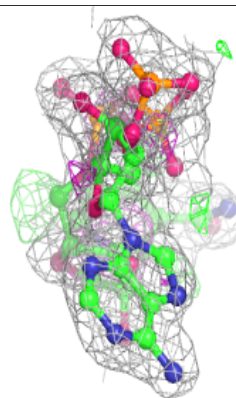
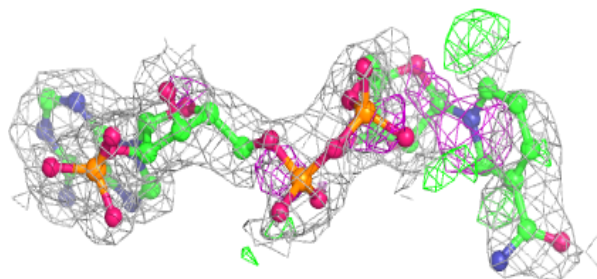
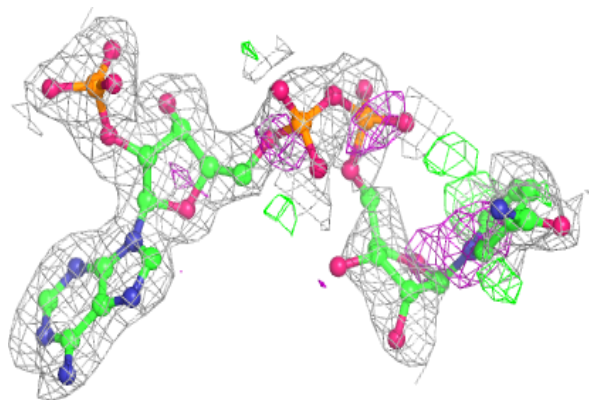
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAP	A	1301	48/48	0.84	0.20	29,46,74,84	0
4	9L9	B	1298	31/31	0.94	0.10	16,20,31,35	0
4	9L9	A	1300	31/31	0.95	0.10	13,17,28,30	0

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.

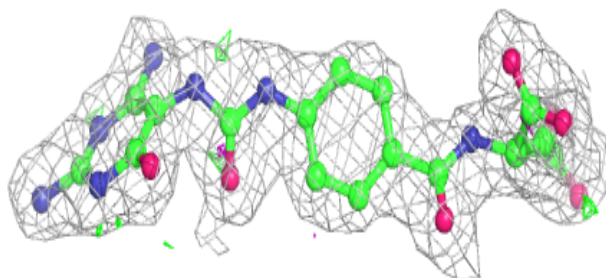
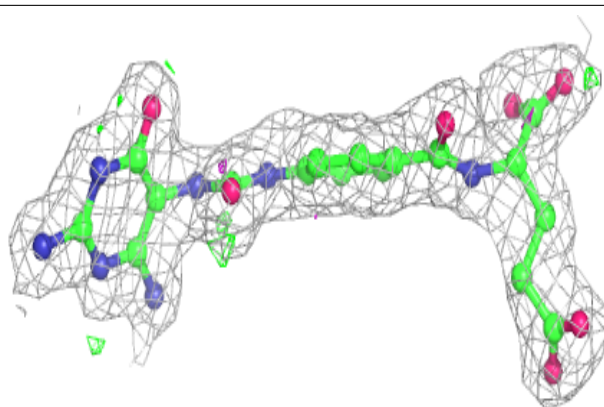
Electron density around NAP A 1301:

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

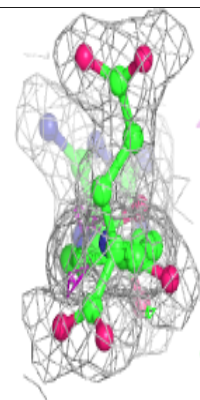
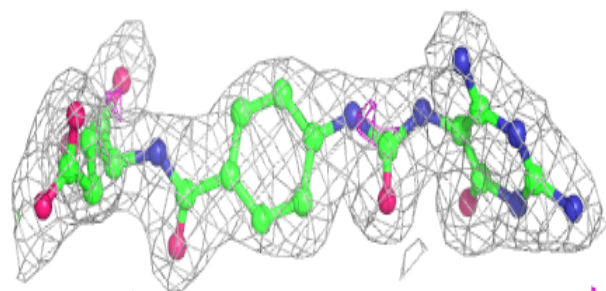
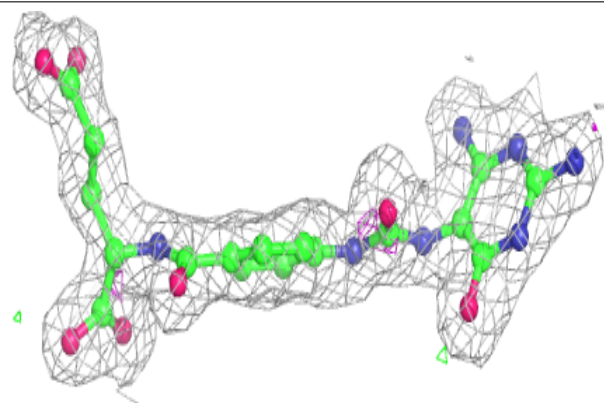


Electron density around 9L9 B 1298:

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

**Electron density around 9L9 A 1300:**

$2mF_o-DF_c$ (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.