



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2022 – 04:12 pm BST

PDB ID : 7OCQ
Title : NADH bound to the dehydrogenase domain of the bifunctional mannitol-1-phosphate dehydrogenase/phosphatase MtlD from *Acinetobacter baumannii*
Authors : Tam, H.K.; Mueller, V.; Pos, K.M.
Deposited on : 2021-04-28
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

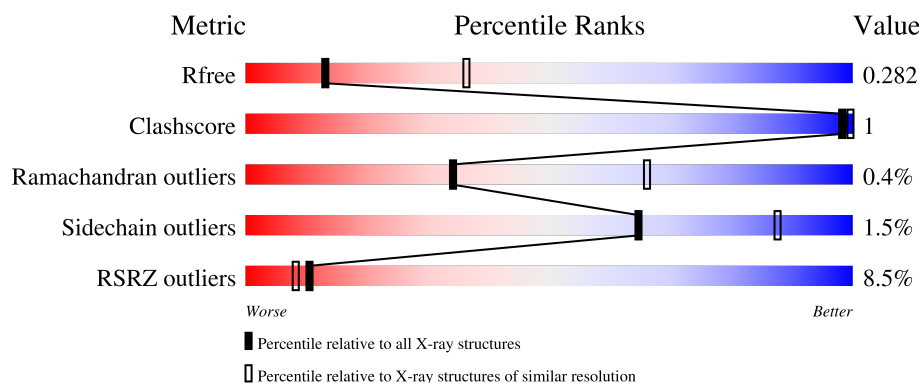
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

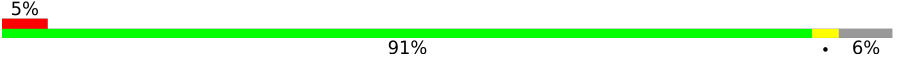

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	
1	B	727	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	EPE	B	801	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11214 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 HAD hydrolase, family IA, variant 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5533	3515	946	1039	33			
1	B	679	Total	C	N	O	S	0	0	0
			5486	3485	939	1030	32			

There are 26 discrepancies between the modelled and reference sequences:

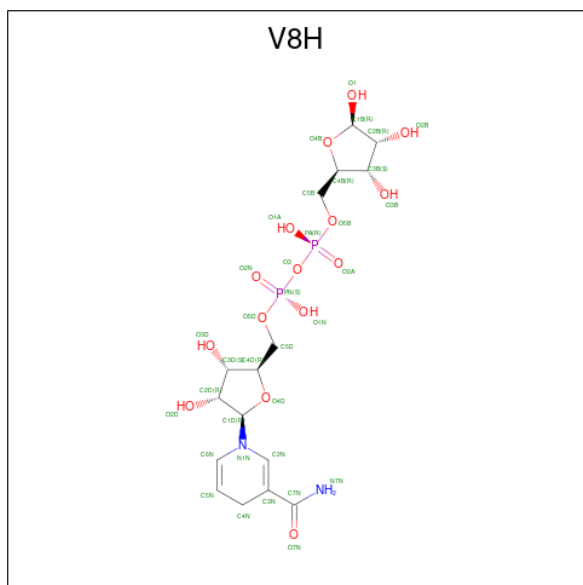
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP D0C7J2
A	2	VAL	-	expression tag	UNP D0C7J2
A	717	ALA	-	expression tag	UNP D0C7J2
A	718	ALA	-	expression tag	UNP D0C7J2
A	719	ALA	-	expression tag	UNP D0C7J2
A	720	LEU	-	expression tag	UNP D0C7J2
A	721	GLU	-	expression tag	UNP D0C7J2
A	722	HIS	-	expression tag	UNP D0C7J2
A	723	HIS	-	expression tag	UNP D0C7J2
A	724	HIS	-	expression tag	UNP D0C7J2
A	725	HIS	-	expression tag	UNP D0C7J2
A	726	HIS	-	expression tag	UNP D0C7J2
A	727	HIS	-	expression tag	UNP D0C7J2
B	1	MET	-	initiating methionine	UNP D0C7J2
B	2	VAL	-	expression tag	UNP D0C7J2
B	717	ALA	-	expression tag	UNP D0C7J2
B	718	ALA	-	expression tag	UNP D0C7J2
B	719	ALA	-	expression tag	UNP D0C7J2
B	720	LEU	-	expression tag	UNP D0C7J2
B	721	GLU	-	expression tag	UNP D0C7J2
B	722	HIS	-	expression tag	UNP D0C7J2
B	723	HIS	-	expression tag	UNP D0C7J2
B	724	HIS	-	expression tag	UNP D0C7J2
B	725	HIS	-	expression tag	UNP D0C7J2
B	726	HIS	-	expression tag	UNP D0C7J2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	727	HIS	-	expression tag	UNP D0C7J2

- Molecule 2 is [[(2 {R},3 {S},4 {R},5 {R})-5-(3-aminocarbonyl-4 {H}-pyridin-1-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {S},4 {R},5 {R})-3,4,5-tris(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (three-letter code: V8H) (formula:).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	16	2	15	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

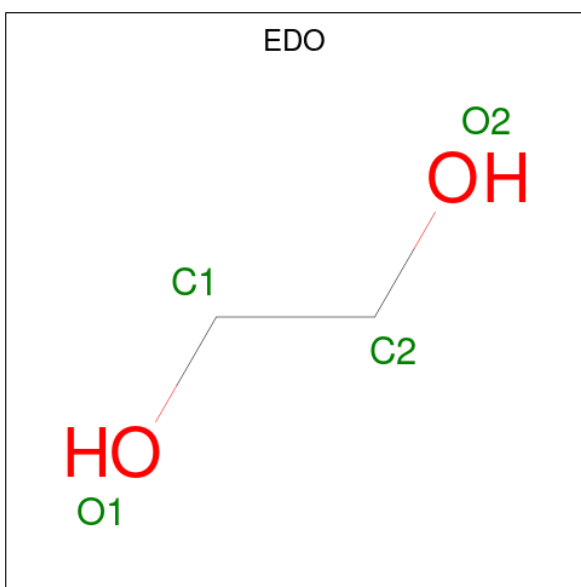
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



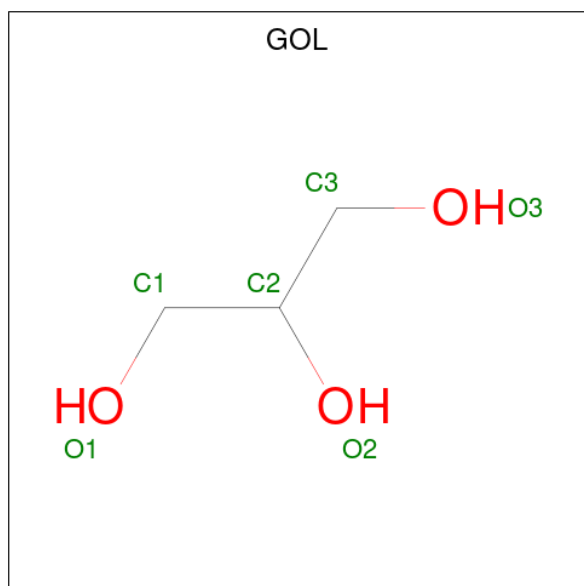
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

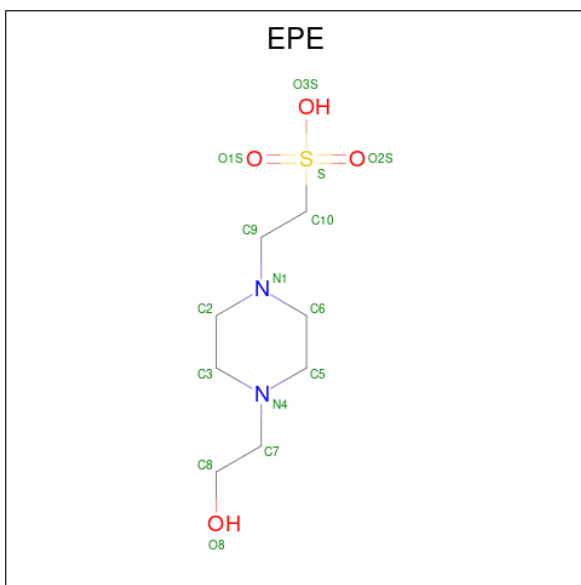


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

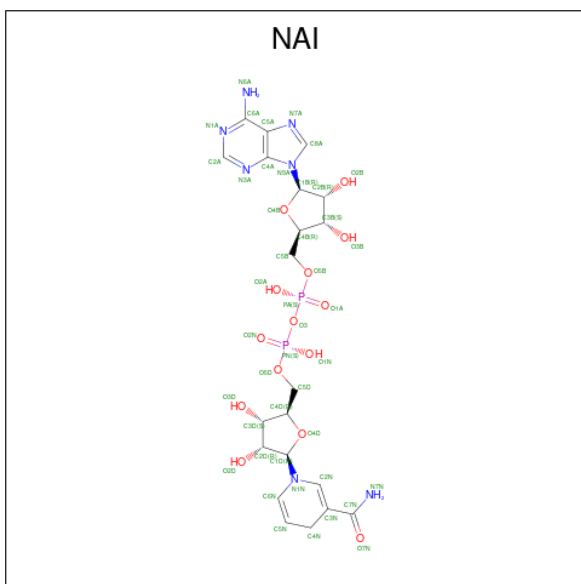
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Cl	0	0
			4	4		
7	B	3	Total	Cl	0	0
			3	3		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 15	C 8	N 2	O 4	S 1	0	0
8	B	1	Total 15	C 8	N 2	O 4	S 1	0	0

- Molecule 9 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	27	Total 27	O 27	0	0
10	B	15	Total 15	O 15	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.30Å 157.34Å 219.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.42 – 2.90 48.42 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.42-2.90) 100.0 (48.42-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.232 , 0.288 0.231 , 0.282	Depositor DCC
R_{free} test set	1881 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	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	0.94	EDS
Total number of atoms	11214	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: V8H, CL, MG, SO4, EPE, EDO, NAI, GOL

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	0.65	0/5637	0.68	0/7608
1	B	0.66	0/5588	0.69	0/7538
All	All	0.65	0/11225	0.69	0/15146

There are no bond length outliers.

There are no bond angle outliers.

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	5533	0	5505	8	0
1	B	5486	0	5456	6	0
2	A	35	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
5	A	8	0	12	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	3	0	0	0	0
8	B	30	0	36	1	0
9	B	44	0	27	0	0
10	A	27	0	0	0	0
10	B	15	0	0	0	0
All	All	11214	0	11052	13	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 1.

All (13) 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:255:ILE:HD11	1:A:414:VAL:HG11	1.86	0.57
1:B:255:ILE:HG21	1:B:372:ILE:HG21	1.92	0.52
1:B:252:PHE:HB3	1:B:280:THR:HB	1.95	0.47
1:A:187:SER:O	1:A:188:LYS:HB2	2.15	0.46
1:A:259:TYR:CE2	1:A:414:VAL:HG13	2.52	0.45
1:A:462:GLN:HB2	1:B:427:TYR:CZ	2.54	0.43
1:A:497:MET:HB2	1:A:498:PRO:HD3	2.01	0.43
1:B:234:MET:HE3	1:B:234:MET:O	2.19	0.42
1:B:28:ARG:HA	1:B:31:THR:OG1	2.20	0.42
1:B:255:ILE:HD12	1:B:414:VAL:HG11	2.03	0.41
1:A:298:ARG:NH2	8:B:802:EPE:O1S	2.39	0.40
1:A:175:GLU:HG2	1:A:181:LEU:N	2.36	0.40
1:A:252:PHE:HB2	1:A:278:ALA:HB1	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	680/727 (94%)	650 (96%)	28 (4%)	2 (0%)	41	71
1	B	671/727 (92%)	632 (94%)	36 (5%)	3 (0%)	34	66
All	All	1351/1454 (93%)	1282 (95%)	64 (5%)	5 (0%)	34	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	454	ASP
1	B	445	GLU
1	B	454	ASP
1	B	656	GLU

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	605/642 (94%)	596 (98%)	9 (2%)	65	87
1	B	599/642 (93%)	590 (98%)	9 (2%)	65	87
All	All	1204/1284 (94%)	1186 (98%)	18 (2%)	65	87

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	29	PHE
1	A	133	ASN
1	A	202	ASP
1	A	215	MET
1	A	216	TYR
1	A	375	LYS
1	A	518	ASP
1	A	584	ASP
1	B	133	ASN
1	B	139	ASP

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Mol	Chain	Res	Type
1	B	317	ASP
1	B	421	LEU
1	B	456	ASN
1	B	510	LYS
1	B	601	LYS
1	B	610	ASP
1	B	679	ARG

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

Mol	Chain	Res	Type
1	A	133	ASN
1	B	133	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 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 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
6	GOL	A	806	-	5,5,5	0.10	0	5,5,5	0.30	0
8	EPE	B	802	-	15,15,15	1.22	3 (20%)	18,20,20	2.32	5 (27%)
5	EDO	A	804	-	3,3,3	0.08	0	2,2,2	0.24	0
5	EDO	A	805	-	3,3,3	0.07	0	2,2,2	0.23	0
9	NAI	B	803	-	42,48,48	0.59	0	47,73,73	0.68	1 (2%)
4	SO4	A	803	-	4,4,4	0.39	0	6,6,6	0.05	0
6	GOL	B	807	-	5,5,5	0.11	0	5,5,5	0.29	0
4	SO4	B	805	-	4,4,4	0.39	0	6,6,6	0.05	0
2	V8H	A	801	-	34,37,37	0.87	1 (2%)	42,56,56	1.06	4 (9%)
8	EPE	B	801	-	15,15,15	1.28	3 (20%)	18,20,20	1.44	3 (16%)
4	SO4	B	806	-	4,4,4	0.39	0	6,6,6	0.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	806	-	-	2/4/4/4	-
8	EPE	B	802	-	-	4/9/19/19	0/1/1/1
5	EDO	A	804	-	-	1/1/1/1	-
5	EDO	A	805	-	-	0/1/1/1	-
9	NAI	B	803	-	-	8/25/72/72	0/5/5/5
6	GOL	B	807	-	-	2/4/4/4	-
2	V8H	A	801	-	-	6/25/68/68	0/3/3/3
8	EPE	B	801	-	-	4/9/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	801	EPE	C10-S	3.66	1.82	1.77
2	A	801	V8H	C6N-C5N	3.53	1.39	1.33
8	B	802	EPE	C10-S	3.20	1.82	1.77
8	B	802	EPE	O2S-S	2.23	1.51	1.45
8	B	801	EPE	O3S-S	2.15	1.55	1.47
8	B	801	EPE	O1S-S	2.07	1.51	1.45
8	B	802	EPE	O1S-S	2.04	1.51	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	802	EPE	C6-N1-C2	4.92	119.91	108.83
8	B	802	EPE	O1S-S-C10	4.83	112.73	106.92
8	B	802	EPE	O2S-S-C10	4.38	112.19	106.92
8	B	802	EPE	O2S-S-O1S	-3.77	100.89	113.95
8	B	801	EPE	O1S-S-C10	3.38	110.98	106.92
2	A	801	V8H	C1B-C2B-C3B	3.14	106.23	102.30
2	A	801	V8H	PA-O3-PN	-3.04	122.40	132.83
8	B	801	EPE	O3S-S-C10	-2.63	101.52	105.77
2	A	801	V8H	O4B-C1B-C2B	2.54	107.59	104.46
8	B	801	EPE	C9-N1-C2	2.30	117.11	111.23
9	B	803	NAI	C5A-C6A-N6A	2.29	123.83	120.35
8	B	802	EPE	C3-C2-N1	2.26	115.27	110.64
2	A	801	V8H	C3D-C2D-C1D	2.07	105.36	101.43

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	V8H	C2N-C3N-C7N-N7N
2	A	801	V8H	C5D-O5D-PN-O2N
6	A	806	GOL	C1-C2-C3-O3
8	B	801	EPE	C10-C9-N1-C2
8	B	801	EPE	S-C10-C9-N1
9	B	803	NAI	C5D-O5D-PN-O3
9	B	803	NAI	C5D-O5D-PN-O1N
8	B	801	EPE	N4-C7-C8-O8
6	B	807	GOL	C1-C2-C3-O3
6	A	806	GOL	O2-C2-C3-O3
6	B	807	GOL	O2-C2-C3-O3
5	A	804	EDO	O1-C1-C2-O2
9	B	803	NAI	O4D-C4D-C5D-O5D
8	B	802	EPE	C9-C10-S-O3S
8	B	802	EPE	N4-C7-C8-O8
8	B	801	EPE	C10-C9-N1-C6
9	B	803	NAI	PN-O3-PA-O5B
2	A	801	V8H	C5D-O5D-PN-O3
9	B	803	NAI	C3D-C4D-C5D-O5D
9	B	803	NAI	PA-O3-PN-O2N
2	A	801	V8H	O4D-C1D-N1N-C6N
8	B	802	EPE	C9-C10-S-O1S
8	B	802	EPE	C9-C10-S-O2S
9	B	803	NAI	O4D-C1D-N1N-C6N
2	A	801	V8H	PN-O3-PA-O1A

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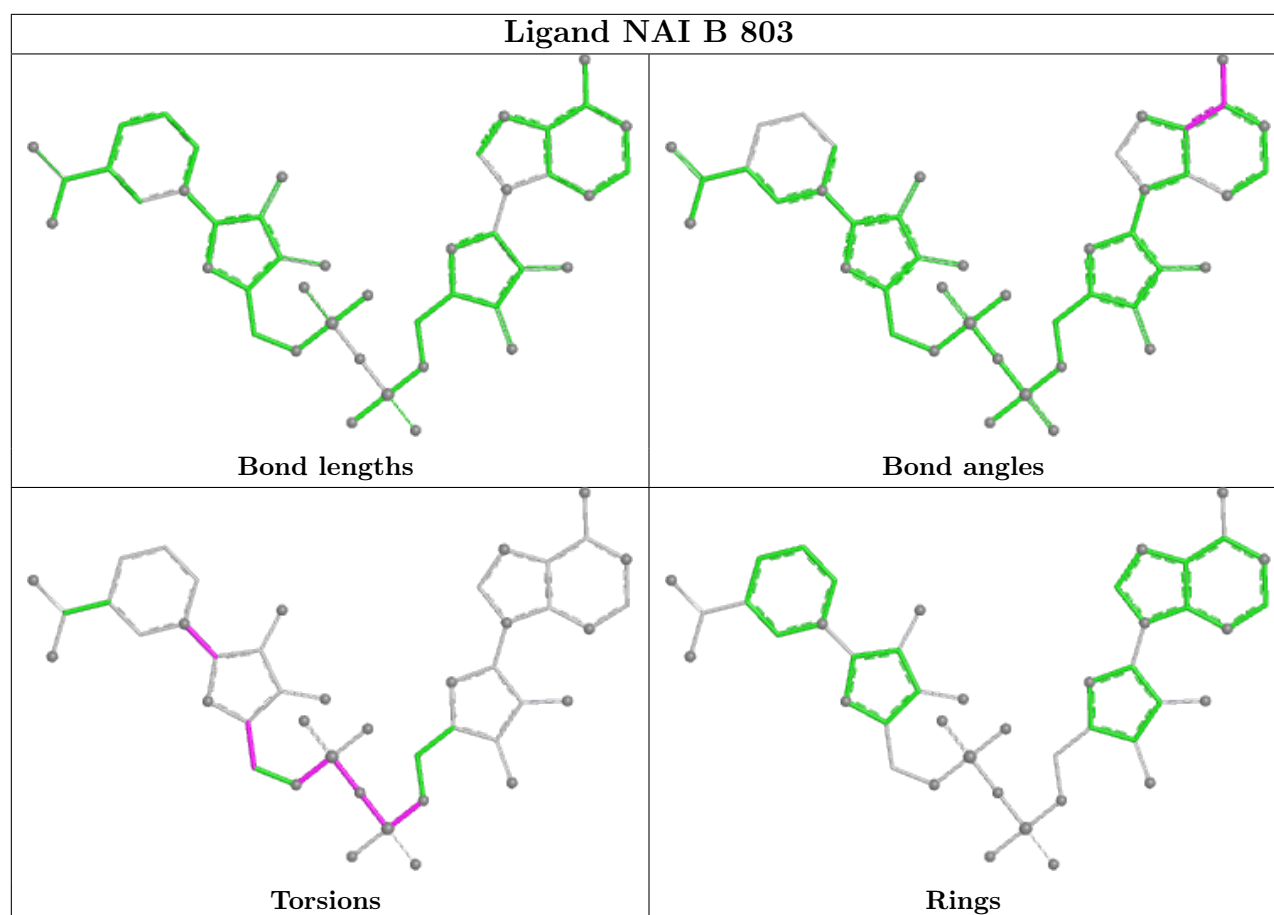
Mol	Chain	Res	Type	Atoms
9	B	803	NAI	C5B-O5B-PA-O1A
2	A	801	V8H	O4B-C4B-C5B-O5B

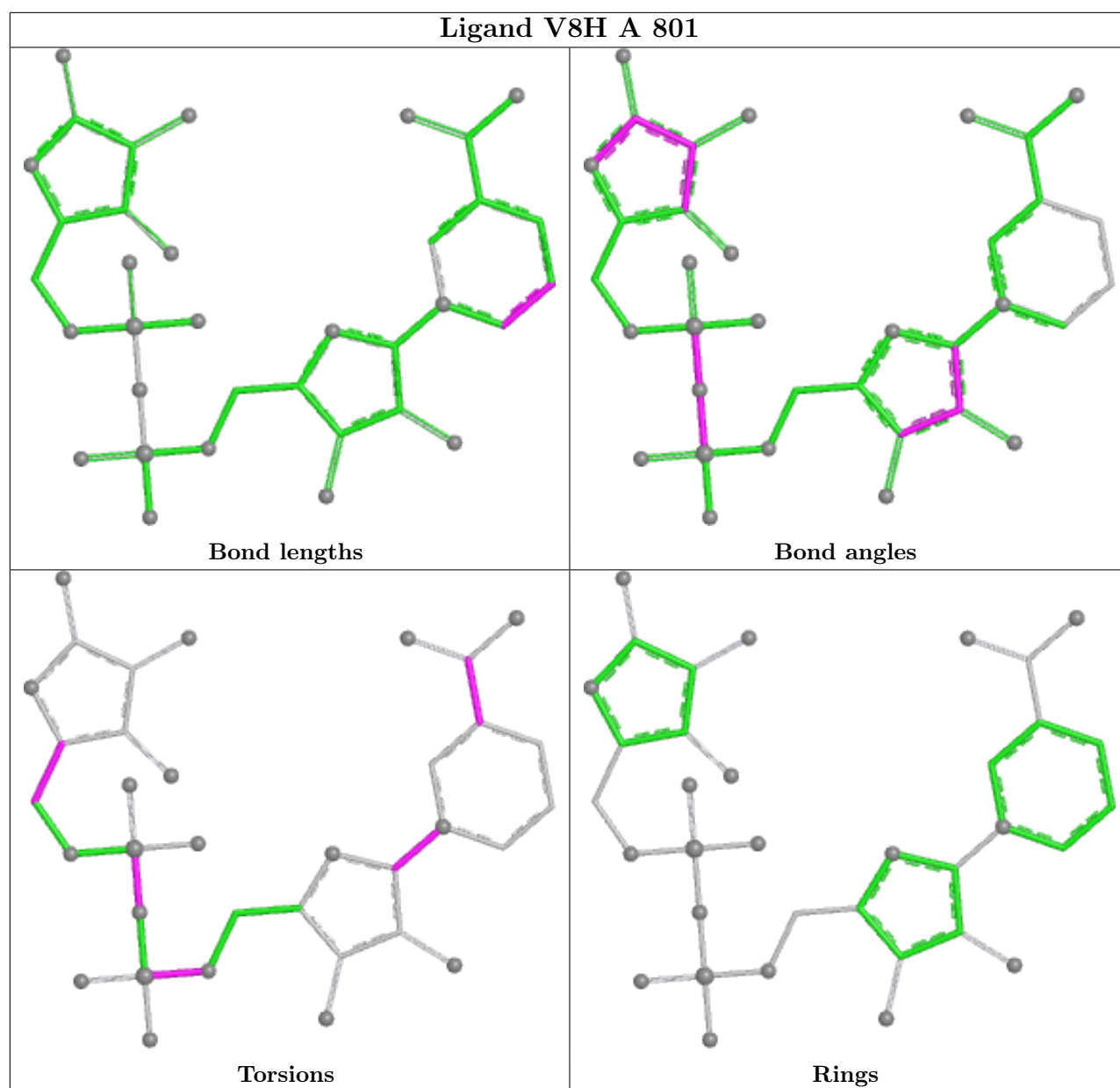
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	802	EPE	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	686/727 (94%)	0.66	38 (5%) 25 21	62, 96, 144, 167	0
1	B	679/727 (93%)	0.82	78 (11%) 4 3	74, 101, 153, 189	0
All	All	1365/1454 (93%)	0.74	116 (8%) 10 8	62, 99, 148, 189	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	ILE	6.5
1	B	5	PHE	5.2
1	B	191	THR	5.0
1	B	68	TYR	4.8
1	A	454	ASP	4.8
1	B	208	ALA	4.5
1	A	363	CYS	4.5
1	B	190	LEU	4.4
1	B	386	LEU	4.3
1	A	689	ILE	4.2
1	B	33	GLN	4.2
1	B	174	PHE	4.1
1	A	456	ASN	4.1
1	B	454	ASP	4.1
1	B	48	TYR	4.0
1	A	601	LYS	3.8
1	B	2	VAL	3.8
1	B	453	GLU	3.8
1	B	83	GLU	3.6
1	A	660	ALA	3.6
1	B	51	GLN	3.5
1	A	399	VAL	3.5
1	A	393	LEU	3.3
1	B	49	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	67	LEU	3.3
1	B	29	PHE	3.2
1	B	76	GLU	3.2
1	B	209	HIS	3.2
1	A	353	TYR	3.1
1	B	196	ASP	3.1
1	B	8	LYS	3.1
1	B	458	LEU	3.0
1	B	39	LEU	3.0
1	A	604	CYS	3.0
1	B	124	ILE	3.0
1	B	455	CYS	2.9
1	B	9	PRO	2.9
1	B	461	ASP	2.9
1	A	391	LEU	2.9
1	A	688	LEU	2.9
1	A	602	ASP	2.9
1	B	3	LEU	2.9
1	B	211	TYR	2.9
1	B	157	PHE	2.9
1	A	671	LEU	2.8
1	A	646	TYR	2.8
1	A	659	LYS	2.8
1	B	647	ALA	2.8
1	A	430	LEU	2.8
1	B	116	VAL	2.8
1	A	685	LEU	2.8
1	B	393	LEU	2.8
1	A	455	CYS	2.7
1	B	117	ALA	2.7
1	B	660	ALA	2.6
1	A	639	LEU	2.6
1	B	193	LEU	2.6
1	B	684	GLU	2.6
1	B	198	LYS	2.6
1	A	323	LEU	2.6
1	B	60	ALA	2.5
1	B	172	LEU	2.5
1	B	219	LEU	2.5
1	A	635	TYR	2.5
1	A	380	TYR	2.5
1	A	463	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	404	LEU	2.5
1	B	456	ASN	2.4
1	A	369	PHE	2.4
1	B	460	PRO	2.4
1	B	452	ILE	2.4
1	B	212	TYR	2.4
1	B	84	MET	2.4
1	A	547	TYR	2.4
1	A	684	GLU	2.3
1	A	398	ASP	2.3
1	A	452	ILE	2.3
1	B	55	LEU	2.3
1	B	156	ILE	2.3
1	B	66	ARG	2.3
1	B	468	ILE	2.3
1	B	15	PHE	2.3
1	B	369	PHE	2.3
1	B	657	GLU	2.3
1	A	679	ARG	2.3
1	B	10	VAL	2.2
1	B	207	LYS	2.2
1	B	692	LEU	2.2
1	A	403	ILE	2.2
1	A	682	GLU	2.2
1	A	334	LEU	2.2
1	B	451	GLU	2.2
1	B	646	TYR	2.2
1	B	75	LYS	2.2
1	B	142	THR	2.2
1	A	285	PHE	2.2
1	B	655	ILE	2.2
1	B	42	GLN	2.2
1	B	658	THR	2.2
1	A	148	GLU	2.2
1	B	27	LEU	2.1
1	B	544	LEU	2.1
1	B	146	GLU	2.1
1	B	112	LEU	2.1
1	A	675	THR	2.1
1	B	74	TYR	2.1
1	B	388	GLU	2.1
1	B	58	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	681	LEU	2.1
1	A	653	LEU	2.1
1	B	192	ILE	2.1
1	B	7	GLY	2.1
1	B	34	GLN	2.0
1	B	40	ILE	2.0
1	B	46	HIS	2.0
1	B	654	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	804	4/4	0.66	0.23	94,94,94,96	0
8	EPE	B	801	15/15	0.72	0.45	78,80,83,83	15
6	GOL	B	807	6/6	0.73	0.28	88,89,90,90	0
6	GOL	A	806	6/6	0.73	0.34	106,107,108,110	0
5	EDO	A	805	4/4	0.78	0.33	86,87,88,88	0
2	V8H	A	801	35/35	0.81	0.28	93,100,108,109	35
7	CL	A	810	1/1	0.83	0.18	93,93,93,93	0
4	SO4	B	806	5/5	0.84	0.18	138,138,139,139	0
8	EPE	B	802	15/15	0.86	0.33	110,113,118,120	0
7	CL	B	809	1/1	0.89	0.15	75,75,75,75	0
4	SO4	A	803	5/5	0.91	0.16	106,106,107,107	0
7	CL	A	808	1/1	0.92	0.24	87,87,87,87	0
9	NAI	B	803	44/44	0.92	0.18	83,90,104,105	0
7	CL	A	809	1/1	0.93	0.19	79,79,79,79	0
7	CL	A	807	1/1	0.93	0.26	85,85,85,85	0

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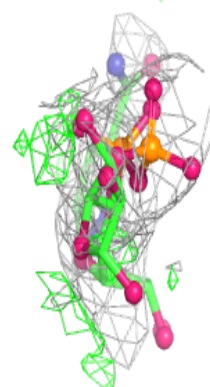
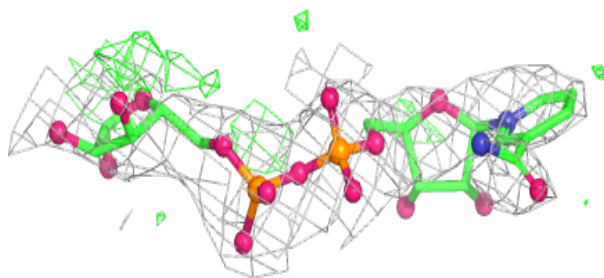
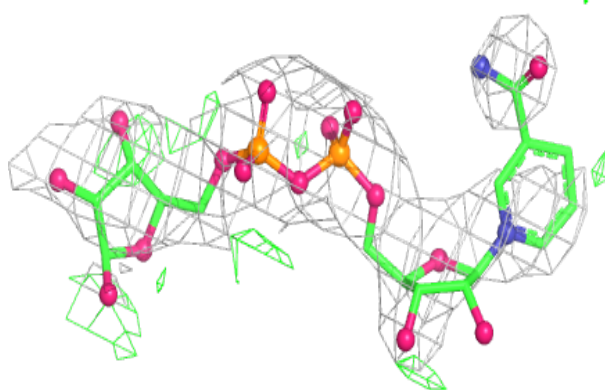
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	804	1/1	0.94	0.14	92,92,92,92	0
7	CL	B	810	1/1	0.95	0.11	68,68,68,68	0
7	CL	B	808	1/1	0.95	0.18	81,81,81,81	0
3	MG	A	802	1/1	0.96	0.23	55,55,55,55	0
4	SO4	B	805	5/5	0.97	0.16	95,95,95,96	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.

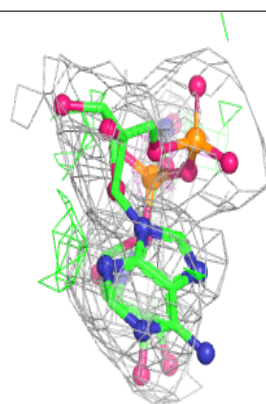
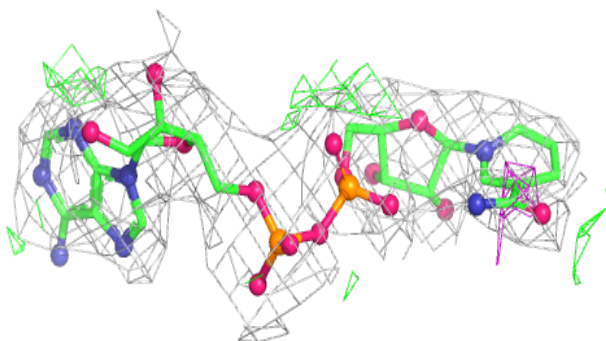
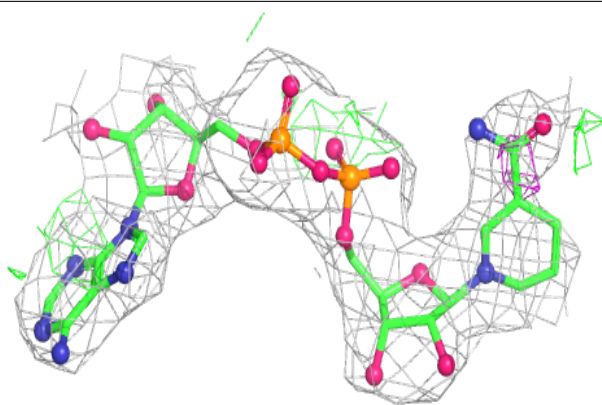
Electron density around V8H A 801:

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 NAI B 803:

$2mF_o-DF_c$ (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.