Full wwPDB X-ray Structure Validation Report (i)

Apr 12, 2022 – 02:55 pm BST

PDB ID	:	7OCP
Title	:	NADPH 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	:	2.75 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 (i) symbol.

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

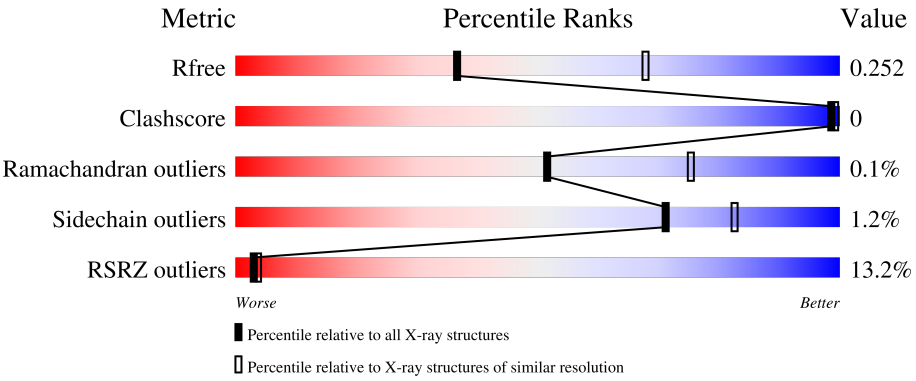
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 <=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	9% 92% · 5%
1	B	727	16% 91% · 6%

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
7	EPE	B	1001	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11216 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	688	Total	C	N	O	S	0	0	0
			5552	3526	949	1045	32			
1	B	680	Total	C	N	O	S	0	0	0
			5494	3491	940	1031	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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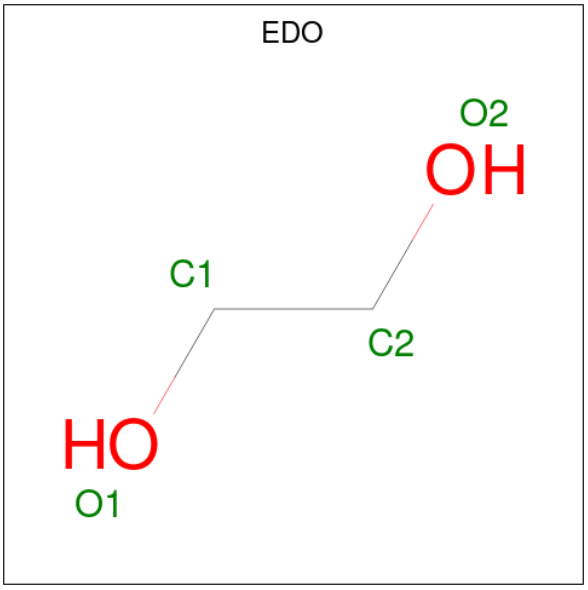
Chain	Residue	Modelled	Actual	Comment	Reference
B	727	HIS	-	expression tag	UNP D0C7J2

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

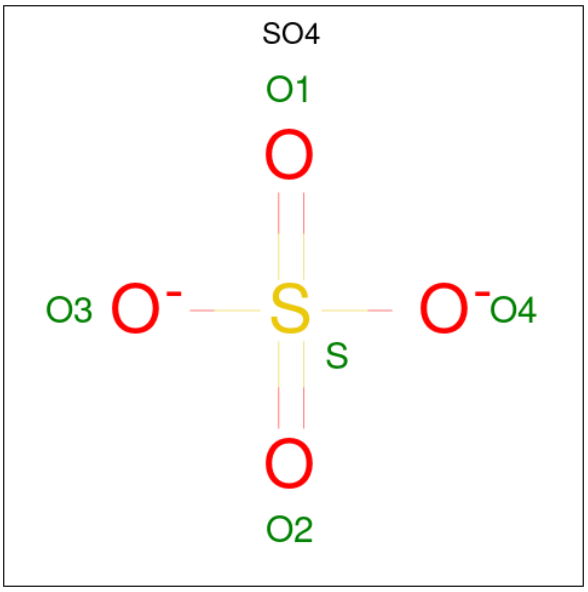


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0

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

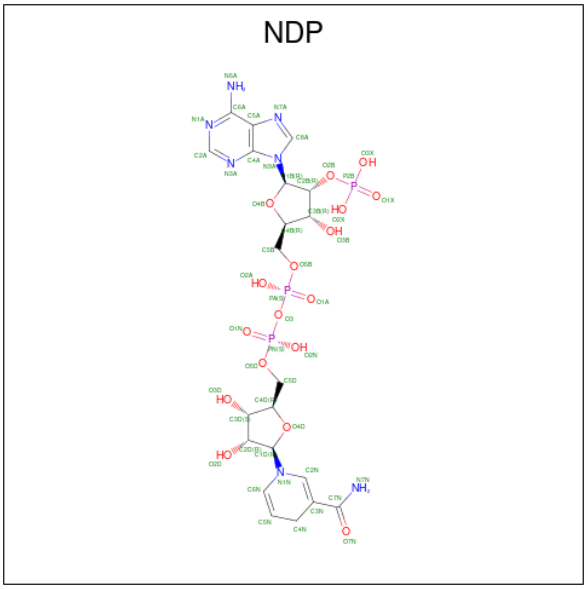
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

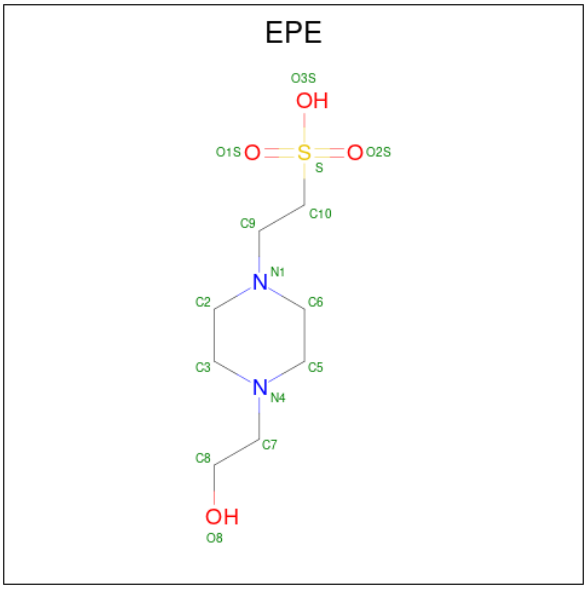


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 48 21 7 17 3	0	0
5	B	1	Total C N O P 48 21 7 17 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	1	Total Cl 1 1	0	0

- Molecule 7 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
7	B	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 8 is water.

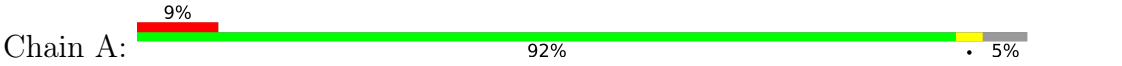
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	26	Total O 26 26	0	0
8	B	10	Total O 10 10	0	0

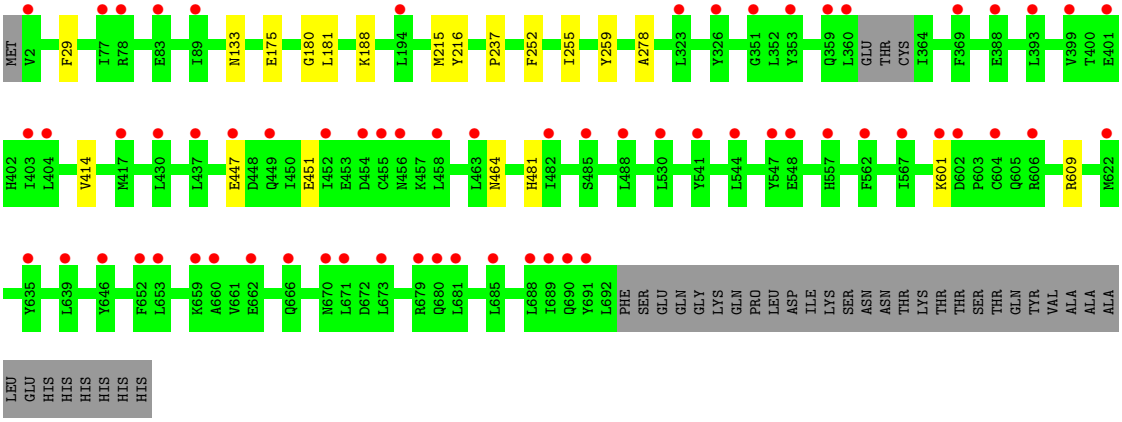
3 Residue-property plots (i)

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: HAD hydrolase, family IA, variant 3

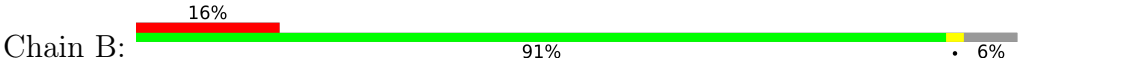
Chain A:

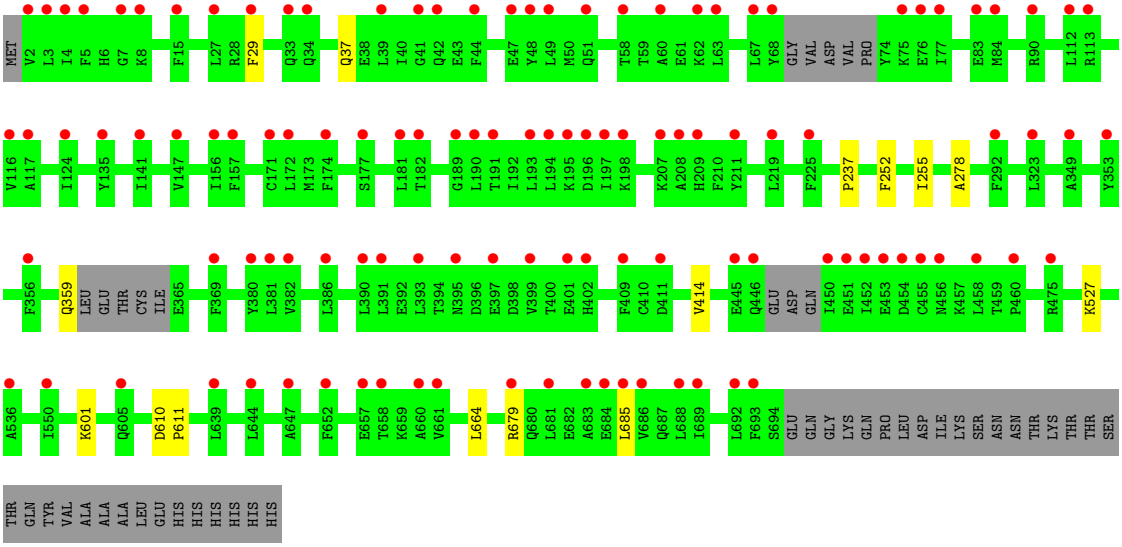




• Molecule 1: HAD hydrolase, family IA, variant 3

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	99.66Å 157.69Å 219.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.75 48.59 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.59-2.75) 100.0 (48.59-2.75)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.220 , 0.255 0.220 , 0.252	Depositor DCC
R_{free} test set	2262 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	71.0	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11216	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, SO4, EDO, EPE, NDP, CL

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	0/5656	0.69	0/7636
1	B	0.66	0/5596	0.69	0/7549
All	All	0.65	0/11252	0.69	0/15185

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

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	5552	0	5527	6	0
1	B	5494	0	5467	5	0
2	A	4	0	6	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	48	0	26	0	0
5	B	48	0	26	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	15	0	18	0	0
8	A	26	0	0	0	0
8	B	10	0	0	0	0
All	All	11216	0	11070	10	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 0.

All (10) 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:252:PHE:HB2	1:A:278:ALA:HB1	1.96	0.47
1:A:259:TYR:CE2	1:A:414:VAL:HG13	2.50	0.46
1:B:664:LEU:HD11	1:B:685:LEU:HD23	1.99	0.45
1:B:252:PHE:HB2	1:B:278:ALA:HB1	1.99	0.44
1:A:175:GLU:HG2	1:A:180:GLY:C	2.39	0.43
1:B:255:ILE:HD11	1:B:414:VAL:HG11	2.00	0.42
1:A:237:PRO:HG3	1:B:237:PRO:HG3	2.02	0.41
1:A:175:GLU:HG2	1:A:181:LEU:N	2.35	0.41
1:A:255:ILE:HD11	1:A:414:VAL:HG11	2.03	0.40
1:B:610:ASP:N	1:B:611:PRO:HD3	2.36	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	684/727 (94%)	646 (94%)	36 (5%)	2 (0%)	41 60
1	B	672/727 (92%)	637 (95%)	35 (5%)	0	100 100
All	All	1356/1454 (93%)	1283 (95%)	71 (5%)	2 (0%)	51 75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	447	GLU

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	607/642 (94%)	598 (98%)	9 (2%)	65	78
1	B	600/642 (94%)	594 (99%)	6 (1%)	76	85
All	All	1207/1284 (94%)	1192 (99%)	15 (1%)	71	82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PHE
1	A	133	ASN
1	A	215	MET
1	A	216	TYR
1	A	451	GLU
1	A	464	ASN
1	A	481	HIS
1	A	601	LYS
1	A	609	ARG
1	B	29	PHE
1	B	37	GLN
1	B	359	GLN
1	B	527	LYS
1	B	601	LYS
1	B	679	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	SO4	B	1003	-	4,4,4	0.39	0	6,6,6	0.04	0
4	SO4	A	805	-	4,4,4	0.39	0	6,6,6	0.05	0
2	EDO	A	801	-	3,3,3	0.05	0	2,2,2	0.18	0
5	NDP	B	1002	-	45,52,52	2.41	7 (15%)	53,80,80	1.71	11 (20%)
7	EPE	B	1001	-	15,15,15	1.05	2 (13%)	18,20,20	2.32	4 (22%)
4	SO4	A	803	-	4,4,4	0.39	0	6,6,6	0.05	0
5	NDP	A	804	-	45,52,52	2.42	7 (15%)	53,80,80	1.59	9 (16%)

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	NDP	B	1002	-	-	10/30/77/77	0/5/5/5
7	EPE	B	1001	-	-	3/9/19/19	0/1/1/1
2	EDO	A	801	-	-	0/1/1/1	-
5	NDP	A	804	-	-	9/30/77/77	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804	NDP	P2B-O2B	13.28	1.84	1.59
5	B	1002	NDP	P2B-O2B	13.20	1.84	1.59
5	A	804	NDP	PN-O5D	4.46	1.77	1.59
5	B	1002	NDP	PN-O5D	4.06	1.75	1.59
7	B	1001	EPE	C10-S	3.15	1.82	1.77
5	B	1002	NDP	O2B-C2B	-2.96	1.33	1.44
5	A	804	NDP	C4A-N3A	2.91	1.39	1.35
5	A	804	NDP	C2A-N1A	2.82	1.39	1.33
5	A	804	NDP	O2B-C2B	-2.78	1.34	1.44
5	B	1002	NDP	C2A-N1A	2.73	1.39	1.33
5	B	1002	NDP	C4A-N3A	2.54	1.39	1.35
5	B	1002	NDP	C7N-N7N	2.34	1.39	1.33
5	A	804	NDP	C7N-N7N	2.26	1.39	1.33
7	B	1001	EPE	O3S-S	2.15	1.55	1.47
5	A	804	NDP	C2A-N3A	2.06	1.35	1.32
5	B	1002	NDP	O5D-C5D	-2.05	1.36	1.44

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1001	EPE	O1S-S-C10	8.08	116.64	106.92
5	B	1002	NDP	PN-O3-PA	-7.00	108.79	132.83
5	A	804	NDP	PN-O3-PA	-6.33	111.11	132.83
5	B	1002	NDP	O2B-P2B-O1X	-3.33	96.55	109.39
5	A	804	NDP	O2B-P2B-O1X	-3.16	97.18	109.39
5	B	1002	NDP	PA-O5B-C5B	-2.92	104.54	121.68
5	B	1002	NDP	C3N-C2N-N1N	-2.88	118.98	123.10
5	A	804	NDP	PA-O5B-C5B	-2.75	105.56	121.68
5	A	804	NDP	O4B-C4B-C3B	2.64	110.34	105.11
5	B	1002	NDP	O5D-PN-O1N	-2.63	98.81	109.07
7	B	1001	EPE	O3S-S-C10	-2.55	101.64	105.77
5	A	804	NDP	O3X-P2B-O2X	2.49	117.16	107.64
5	B	1002	NDP	O3X-P2B-O2X	2.45	117.00	107.64
5	B	1002	NDP	O2N-PN-O1N	2.38	124.00	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1002	NDP	O7N-C7N-N7N	-2.32	117.45	122.88
5	A	804	NDP	PN-O5D-C5D	-2.32	108.09	121.68
5	A	804	NDP	O5D-PN-O1N	-2.29	100.11	109.07
7	B	1001	EPE	C7-N4-C5	2.28	117.06	111.23
5	B	1002	NDP	C2A-N1A-C6A	-2.26	114.88	118.75
5	A	804	NDP	C2A-N1A-C6A	-2.24	114.93	118.75
5	A	804	NDP	O2N-PN-O1N	2.23	123.27	112.24
5	B	1002	NDP	PN-O5D-C5D	-2.15	109.05	121.68
5	B	1002	NDP	O4B-C4B-C3B	2.04	109.16	105.11
7	B	1001	EPE	C3-C2-N1	2.01	114.76	110.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	804	NDP	C2N-C3N-C7N-N7N
5	B	1002	NDP	C5D-O5D-PN-O3
5	B	1002	NDP	C5D-O5D-PN-O1N
5	B	1002	NDP	C5D-O5D-PN-O2N
5	B	1002	NDP	O4D-C4D-C5D-O5D
5	B	1002	NDP	C3D-C4D-C5D-O5D
7	B	1001	EPE	C8-C7-N4-C5
7	B	1001	EPE	S-C10-C9-N1
5	A	804	NDP	C1B-C2B-O2B-P2B
5	A	804	NDP	C3B-C2B-O2B-P2B
5	B	1002	NDP	O4B-C4B-C5B-O5B
5	A	804	NDP	PN-O3-PA-O2A
5	A	804	NDP	O4D-C1D-N1N-C6N
5	B	1002	NDP	O4D-C1D-N1N-C6N
7	B	1001	EPE	C8-C7-N4-C3
5	A	804	NDP	O4D-C4D-C5D-O5D
5	A	804	NDP	C5B-O5B-PA-O3
5	B	1002	NDP	C2B-O2B-P2B-O2X
5	B	1002	NDP	C3B-C4B-C5B-O5B
5	A	804	NDP	PN-O3-PA-O1A
5	A	804	NDP	C5B-O5B-PA-O1A
5	B	1002	NDP	C2D-C1D-N1N-C6N

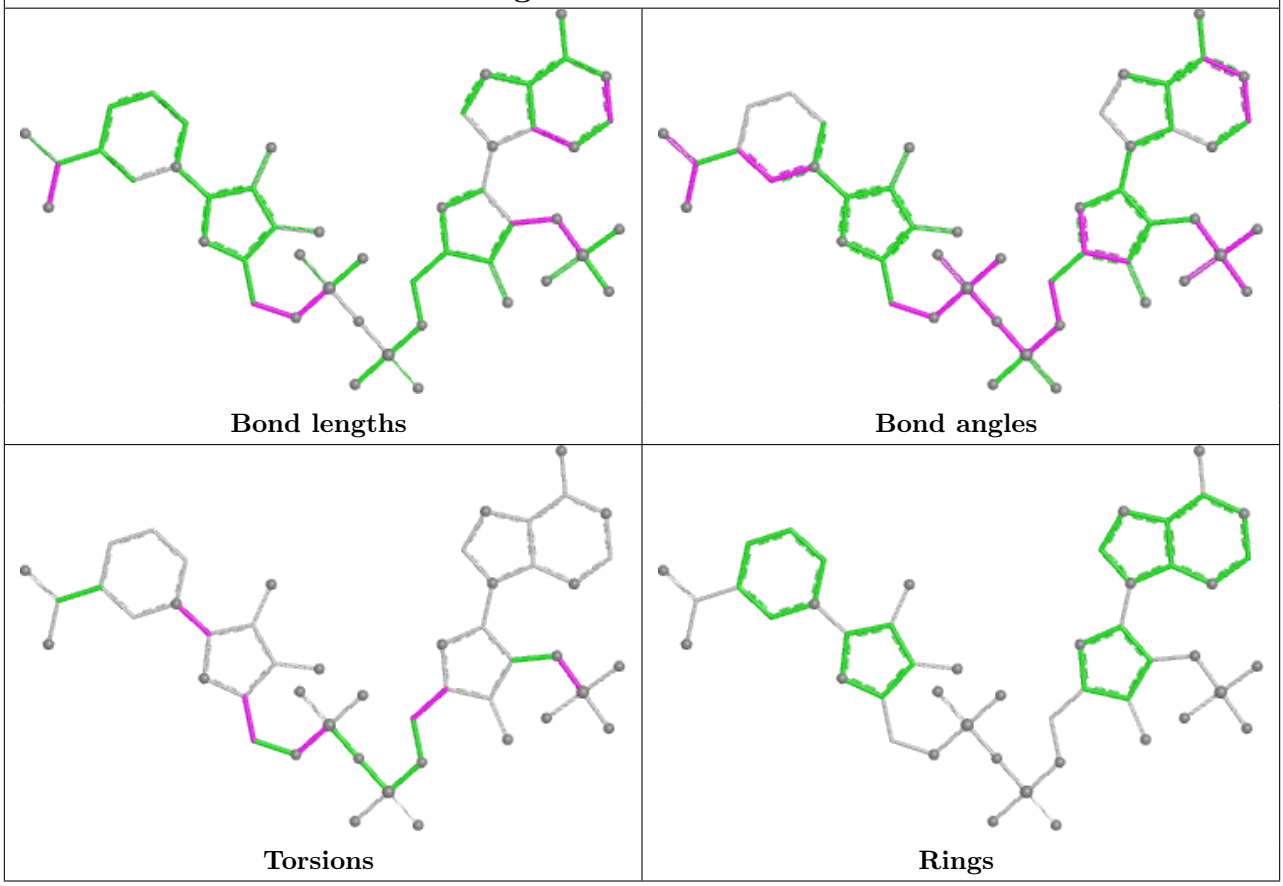
There are no ring outliers.

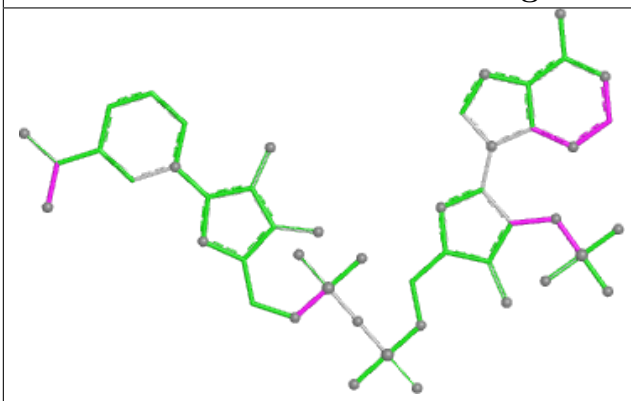
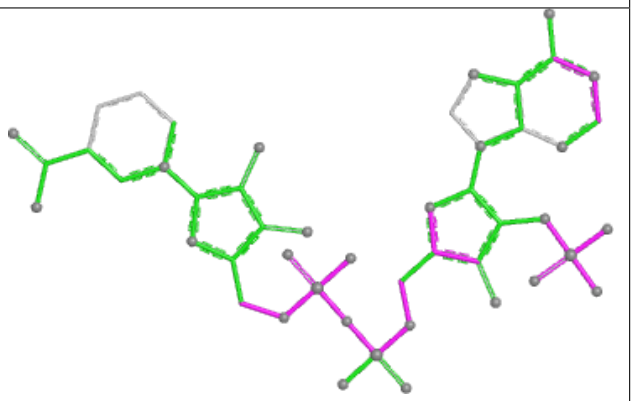
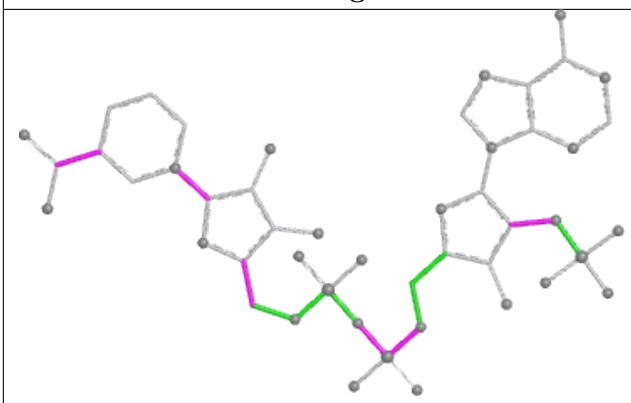
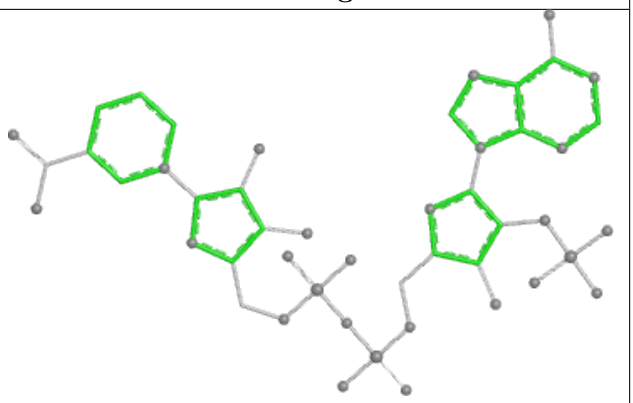
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NDP B 1002



Ligand NDP A 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

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

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, 95^{th} 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	688/727 (94%)	0.87	66 (9%) 8 9	50, 87, 147, 165	0
1	B	680/727 (93%)	1.07	115 (16%) 1 1	64, 99, 157, 201	0
All	All	1368/1454 (94%)	0.97	181 (13%) 3 4	50, 93, 151, 201	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	GLN	7.2
1	B	83	GLU	6.7
1	A	447	GLU	6.5
1	B	208	ALA	6.4
1	A	353	TYR	6.1
1	B	197	ILE	5.8
1	B	353	TYR	5.5
1	A	659	LYS	5.0
1	A	660	ALA	4.6
1	A	454	ASP	4.6
1	A	455	CYS	4.6
1	A	456	ASN	4.6
1	A	452	ILE	4.5
1	A	679	ARG	4.5
1	B	458	LEU	4.5
1	B	116	VAL	4.5
1	B	68	TYR	4.4
1	B	39	LEU	4.4
1	B	191	THR	4.4
1	B	156	ILE	4.3
1	B	456	ASN	4.3
1	B	190	LEU	4.2
1	B	77	ILE	4.1
1	B	5	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	29	PHE	4.1
1	B	182	THR	4.0
1	B	401	GLU	4.0
1	B	41	GLY	3.9
1	B	8	LYS	3.9
1	B	409	PHE	3.8
1	B	391	LEU	3.8
1	B	693	PHE	3.8
1	B	117	ALA	3.8
1	A	359	GLN	3.7
1	A	393	LEU	3.6
1	B	658	THR	3.6
1	B	451	GLU	3.5
1	B	67	LEU	3.5
1	A	635	TYR	3.5
1	A	673	LEU	3.5
1	B	113	ARG	3.5
1	A	671	LEU	3.5
1	A	666	GLN	3.4
1	A	601	LYS	3.4
1	B	386	LEU	3.4
1	B	684	GLU	3.4
1	A	652	PHE	3.4
1	B	196	ASP	3.4
1	B	4	ILE	3.3
1	B	2	VAL	3.3
1	A	689	ILE	3.3
1	B	453	GLU	3.3
1	A	691	TYR	3.3
1	B	51	GLN	3.3
1	A	639	LEU	3.3
1	A	399	VAL	3.3
1	B	657	GLU	3.3
1	B	209	HIS	3.3
1	B	454	ASP	3.3
1	A	688	LEU	3.2
1	B	112	LEU	3.2
1	A	360	LEU	3.2
1	A	622	MET	3.1
1	B	174	PHE	3.1
1	B	63	LEU	3.1
1	B	660	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	171	CYS	3.1
1	B	47	GLU	3.1
1	B	225	PHE	3.1
1	A	670	ASN	3.0
1	B	42	GLN	3.0
1	B	455	CYS	3.0
1	A	690	GLN	2.9
1	B	411	ASP	2.9
1	A	430	LEU	2.9
1	B	356	PHE	2.9
1	A	547	TYR	2.9
1	B	198	LYS	2.9
1	B	390	LEU	2.9
1	A	83	GLU	2.9
1	B	84	MET	2.9
1	B	661	VAL	2.9
1	B	60	ALA	2.9
1	B	48	TYR	2.9
1	A	662	GLU	2.9
1	B	679	ARG	2.8
1	A	544	LEU	2.8
1	B	207	LYS	2.8
1	B	382	VAL	2.8
1	B	49	LEU	2.8
1	B	685	LEU	2.7
1	A	485	SER	2.7
1	B	75	LYS	2.7
1	B	692	LEU	2.7
1	B	33	GLN	2.7
1	A	323	LEU	2.6
1	B	219	LEU	2.6
1	B	652	PHE	2.6
1	B	195	LYS	2.6
1	A	685	LEU	2.6
1	B	124	ILE	2.6
1	A	417	MET	2.6
1	A	530	LEU	2.6
1	B	450	ILE	2.5
1	A	388	GLU	2.5
1	A	646	TYR	2.5
1	B	44	PHE	2.5
1	B	58	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	452	ILE	2.5
1	A	681	LEU	2.5
1	A	326	TYR	2.5
1	B	27	LEU	2.5
1	B	460	PRO	2.5
1	A	680	GLN	2.5
1	B	550	ILE	2.5
1	B	683	ALA	2.4
1	A	77	ILE	2.4
1	A	653	LEU	2.4
1	A	557	HIS	2.4
1	B	181	LEU	2.4
1	B	380	TYR	2.4
1	A	401	GLU	2.4
1	B	62	LYS	2.4
1	A	351	GLY	2.4
1	A	606	ARG	2.4
1	B	90	ARG	2.4
1	A	602	ASP	2.4
1	B	323	LEU	2.4
1	B	381	LEU	2.4
1	A	369	PHE	2.4
1	B	172	LEU	2.3
1	A	548	GLU	2.3
1	B	76	GLU	2.3
1	B	189	GLY	2.3
1	B	349	ALA	2.3
1	A	463	LEU	2.3
1	B	475	ARG	2.3
1	A	604	CYS	2.3
1	A	403	ILE	2.3
1	B	397	GLU	2.2
1	B	647	ALA	2.2
1	B	644	LEU	2.2
1	B	211	TYR	2.2
1	B	147	VAL	2.2
1	B	639	LEU	2.2
1	B	15	PHE	2.2
1	B	157	PHE	2.2
1	A	482	ILE	2.2
1	A	488	LEU	2.2
1	B	395	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	688	LEU	2.2
1	A	194	LEU	2.2
1	B	681	LEU	2.2
1	A	562	PHE	2.2
1	B	445	GLU	2.1
1	B	446	GLN	2.1
1	B	536	ALA	2.1
1	A	567	ILE	2.1
1	B	393	LEU	2.1
1	B	689	ILE	2.1
1	B	34	GLN	2.1
1	B	292	PHE	2.1
1	A	437	LEU	2.1
1	A	541	TYR	2.1
1	A	89	ILE	2.1
1	B	399	VAL	2.1
1	B	686	VAL	2.1
1	A	78	ARG	2.1
1	B	7	GLY	2.1
1	A	2	VAL	2.1
1	B	177	SER	2.1
1	A	404	LEU	2.1
1	B	141	ILE	2.1
1	B	605	GLN	2.1
1	B	193	LEU	2.0
1	B	135	TYR	2.0
1	B	369	PHE	2.0
1	A	458	LEU	2.0
1	B	3	LEU	2.0
1	B	194	LEU	2.0
1	B	402	HIS	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

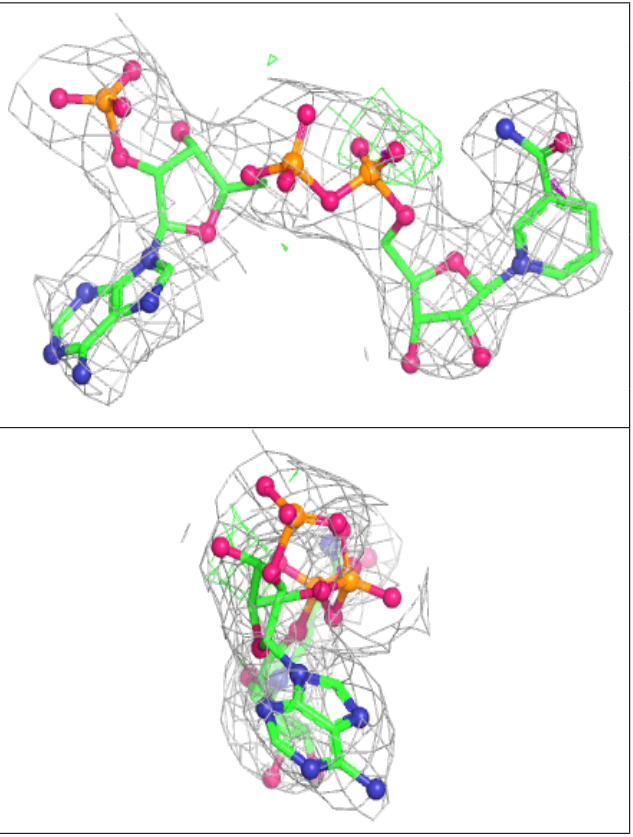
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

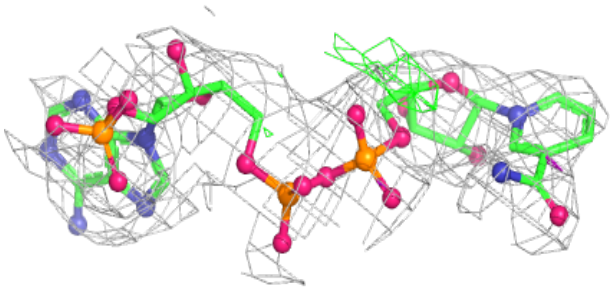
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EPE	B	1001	15/15	0.69	0.46	91,93,94,95	15
2	EDO	A	801	4/4	0.76	0.19	102,103,103,104	0
4	SO4	A	805	5/5	0.81	0.18	118,118,118,119	0
6	CL	B	1005	1/1	0.82	0.16	97,97,97,97	0
3	MG	B	1004	1/1	0.86	0.17	89,89,89,89	0
6	CL	A	806	1/1	0.88	0.20	73,73,73,73	0
4	SO4	B	1003	5/5	0.90	0.13	99,99,100,100	0
3	MG	A	802	1/1	0.90	0.26	57,57,57,57	0
5	NDP	A	804	48/48	0.91	0.16	97,101,106,111	0
5	NDP	B	1002	48/48	0.94	0.16	75,85,100,102	0
4	SO4	A	803	5/5	0.96	0.17	96,97,98,98	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 NDP A 804:

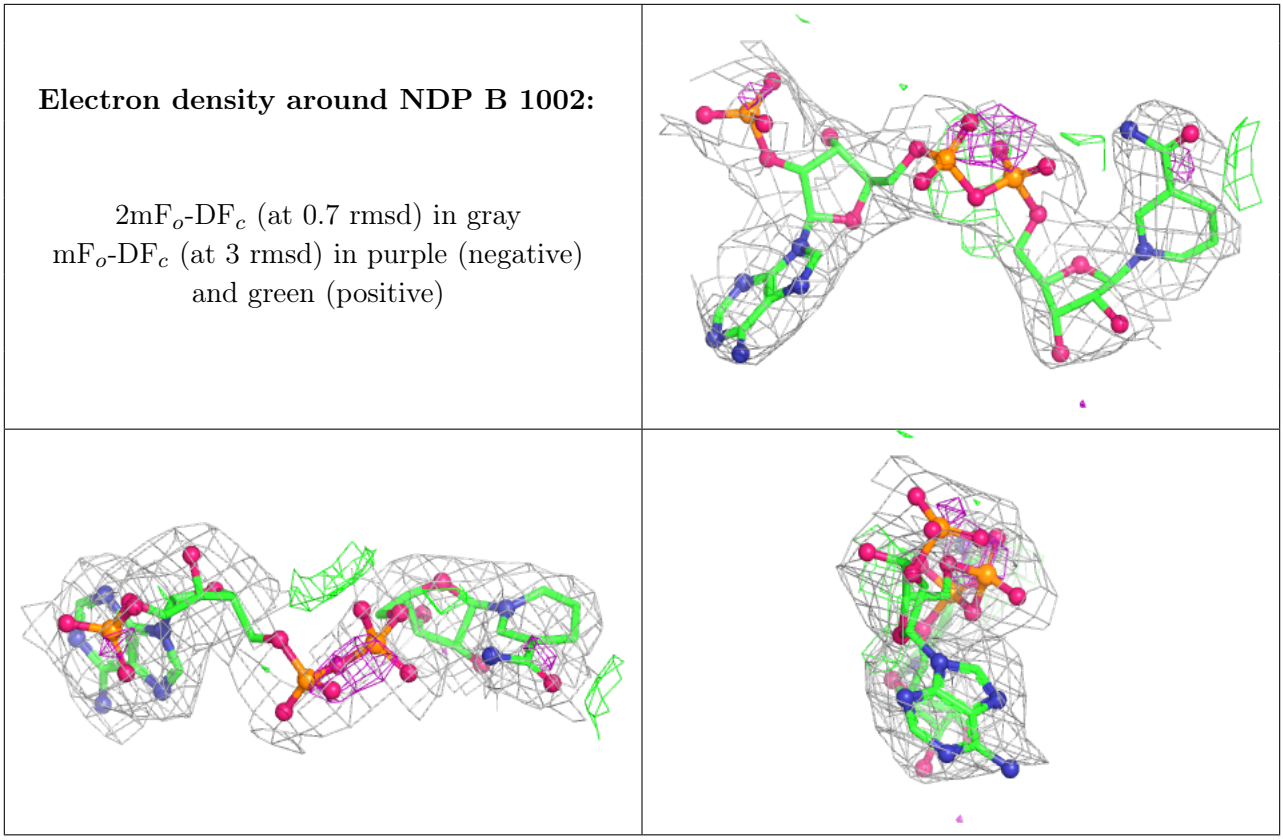
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around NDP B 1002:

$2mF_o$-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.