



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:44 PM UTC

PDB ID : 7OCT / pdb_00007oct
Title : NADPH bound to the dehydrogenase domain of the bifunctional mannitol-1-phosphate dehydrogenase/phosphatase MtlD-N374A from *Acinetobacter baumannii*
Authors : Tam, H.K.; Mueller, V.; Pos, K.M.
Deposited on : 2021-04-28
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

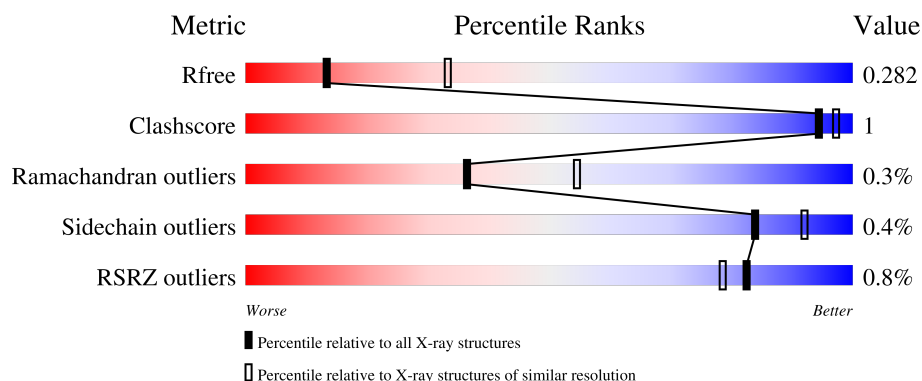
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	91% 6%
1	B	727	90% 7%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11275 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	2	0
			5546	3523	950	1040	33			
1	B	678	Total	C	N	O	S	0	0	0
			5473	3480	935	1026	32			

There are 28 discrepancies between the modelled and reference sequences:

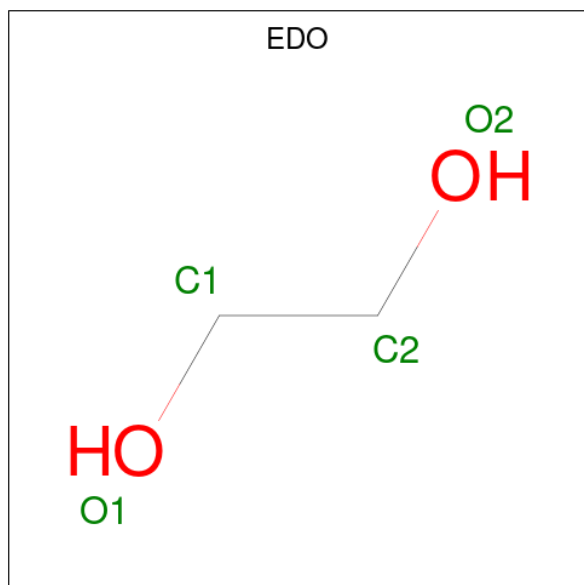
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP D0C7J2
A	2	VAL	-	expression tag	UNP D0C7J2
A	374	ALA	ASN	engineered mutation	UNP D0C7J2
A	717	ALA	-	expression tag	UNP D0C7J2
A	718	ALA	-	expression tag	UNP D0C7J2
A	719	ALA	-	expression tag	UNP D0C7J2
A	720	LEU	-	expression 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	374	ALA	ASN	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	725	HIS	-	expression tag	UNP D0C7J2
B	726	HIS	-	expression tag	UNP D0C7J2
B	727	HIS	-	expression tag	UNP D0C7J2

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

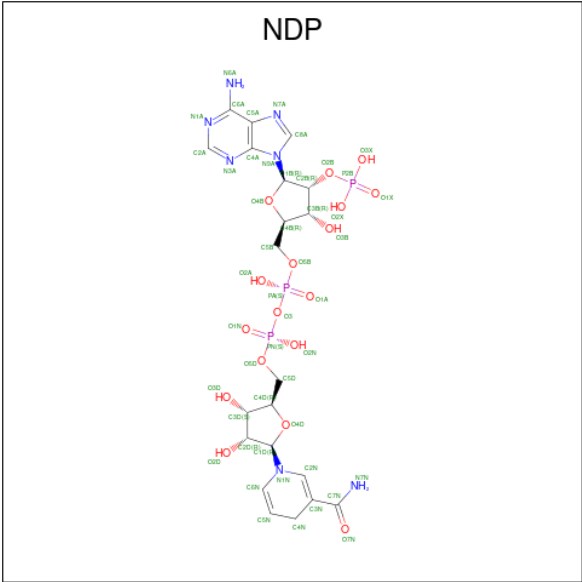


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

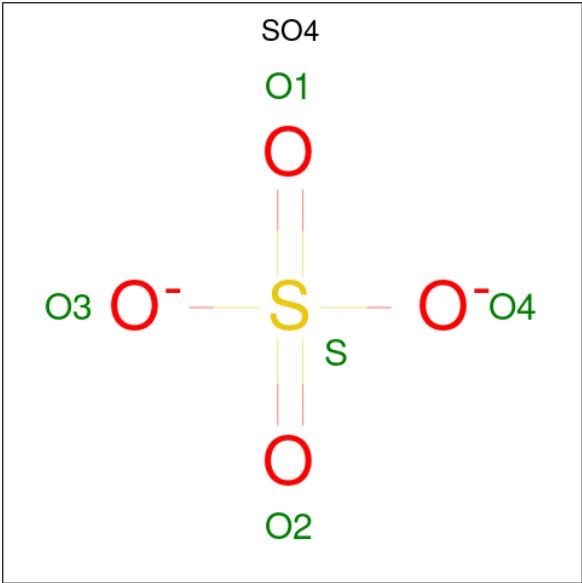
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

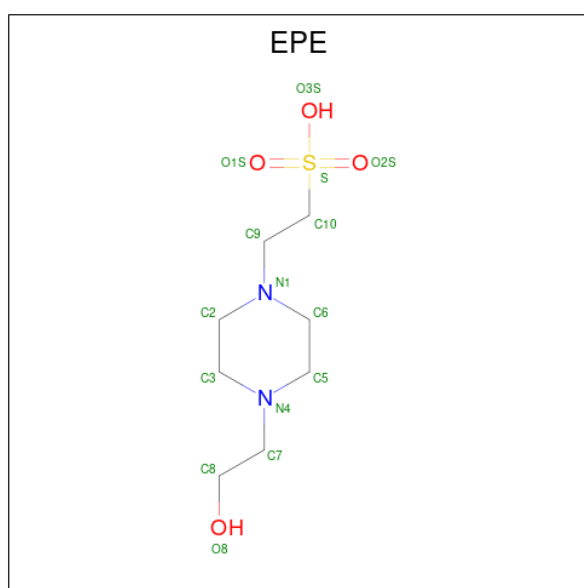
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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 POTASSIUM ION (CCD ID: K) (formula: K).

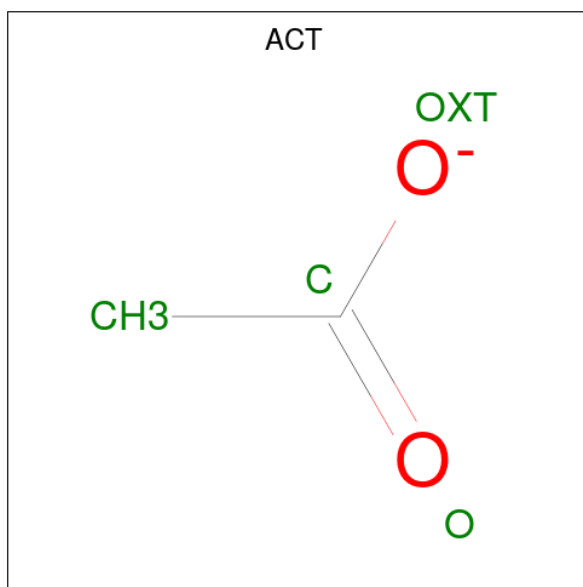
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

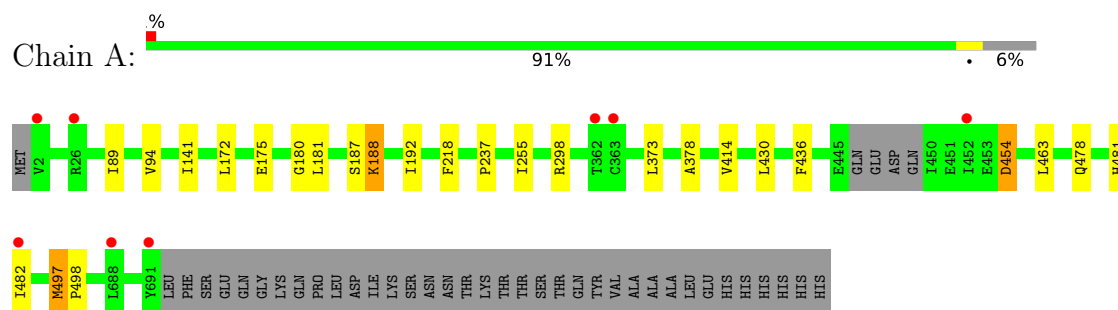
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	51	Total	O	0	0
			51	51		
10	B	24	Total	O	0	0
			24	24		

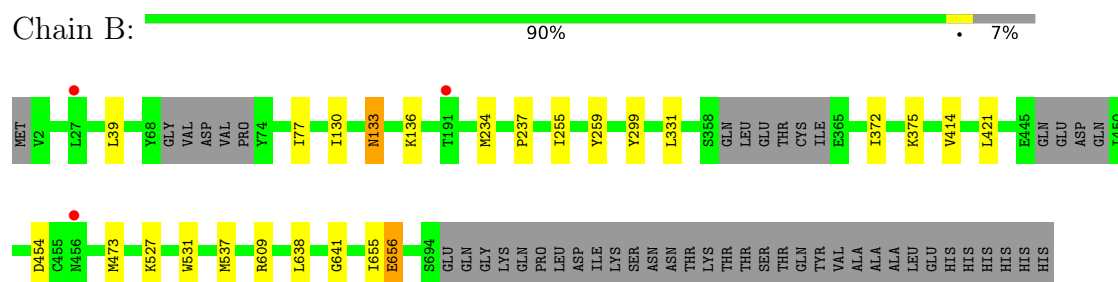
3 Residue-property plots

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



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



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 156.96Å 220.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 2.85 48.43 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.43-2.85) 100.0 (48.43-2.85)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.227 , 0.278 0.228 , 0.282	Depositor DCC
R_{free} test set	2054 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11275	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, EPE, SO4, CL, NDP, ACT, EDO

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	1.01	0/5654	1.54	0/7633
1	B	1.01	0/5575	1.53	0/7521
All	All	1.01	0/11229	1.54	0/15154

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	5546	0	5526	15	0
1	B	5473	0	5450	16	0
2	A	12	0	18	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	48	0	26	0	0
4	B	48	0	26	0	0
5	A	10	0	0	0	0
5	B	20	0	0	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	A	1	0	0	0	0
8	B	30	0	36	2	0
9	B	8	0	6	0	0
10	A	51	0	0	0	0
10	B	24	0	0	0	0
All	All	11275	0	11088	28	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 (28) 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:172:LEU:HD22	1:A:192:ILE:HD11	1.90	0.52
1:B:255:ILE:HG21	1:B:372:ILE:HG21	1.91	0.51
1:A:454:ASP:HA	1:A:463:LEU:HD21	1.93	0.50
1:A:255:ILE:HD11	1:A:414:VAL:HG11	1.94	0.49
1:A:175:GLU:HG2	1:A:180:GLY:C	2.38	0.48
1:A:436:PHE:HB3	1:A:482:ILE:HD11	1.95	0.47
1:B:421:LEU:HD11	8:B:1201:EPE:H71	1.97	0.46
1:A:497:MET:HB2	1:A:498:PRO:HD3	1.99	0.44
1:A:430:LEU:HD22	1:B:473:MET:HE1	2.00	0.44
1:B:39:LEU:HD22	1:B:77:ILE:HD13	1.99	0.44
1:B:537:MET:HE2	1:B:641:GLY:HA3	1.99	0.44
1:B:130:ILE:HD12	8:B:1209:EPE:H22	2.00	0.44
1:A:298:ARG:CZ	1:B:136:LYS:HB3	2.48	0.43
1:B:259:TYR:CE2	1:B:414:VAL:HG13	2.54	0.43
1:A:187:SER:O	1:A:188:LYS:HB2	2.17	0.43
1:A:192:ILE:HD13	1:A:218:PHE:CE1	2.54	0.43
1:A:89:ILE:HG23	1:A:94:VAL:HG22	2.00	0.42
1:A:175:GLU:HG2	1:A:181:LEU:N	2.34	0.42
1:B:234:MET:HE3	1:B:234:MET:O	2.19	0.42
1:B:331:LEU:C	1:B:331:LEU:HD23	2.45	0.42
1:B:537:MET:HE1	1:B:638:LEU:HD23	2.00	0.42
1:A:373:LEU:HD23	1:A:378:ALA:HB1	2.01	0.42
1:B:527:LYS:O	1:B:531:TRP:HB3	2.20	0.41
1:B:655:ILE:O	1:B:656:GLU:HB2	2.20	0.41
1:A:478:GLN:HA	1:A:481:HIS:CE1	2.56	0.41
1:B:133:ASN:C	1:B:133:ASN:HD22	2.29	0.41
1:B:234:MET:HE1	1:B:299:TYR:CZ	2.56	0.41
1:A:237:PRO:HG3	1:B:237:PRO:HG3	2.03	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%)	657 (96%)	25 (4%)	2 (0%)	36	54
1	B	670/727 (92%)	635 (95%)	33 (5%)	2 (0%)	36	54
All	All	1354/1454 (93%)	1292 (95%)	58 (4%)	4 (0%)	36	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	B	656	GLU
1	B	454	ASP
1	A	497	MET

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	606/641 (94%)	604 (100%)	2 (0%)	86	93
1	B	597/641 (93%)	594 (100%)	3 (0%)	81	90
All	All	1203/1282 (94%)	1198 (100%)	5 (0%)	84	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ILE
1	A	454	ASP
1	B	133	ASN
1	B	375	LYS
1	B	609	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	133	ASN
1	A	149	GLN
1	A	282	ASN
1	A	395	ASN
1	A	476	ASN
1	A	519	GLN
1	A	535	HIS
1	A	617	HIS
1	B	37	GLN
1	B	133	ASN
1	B	395	ASN
1	B	402	HIS
1	B	439	GLN
1	B	476	ASN
1	B	492	HIS
1	B	666	GLN
1	B	670	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	1210	-	4,4,4	0.35	0	6,6,6	0.07	0
4	NDP	B	1206	-	51,52,52	2.54	11 (21%)	71,80,80	1.50	15 (21%)
4	NDP	A	805	-	51,52,52	2.58	10 (19%)	71,80,80	1.41	13 (18%)
8	EPE	B	1209	-	15,15,15	1.29	2 (13%)	19,20,20	1.78	5 (26%)
5	SO4	B	1203	3	4,4,4	0.35	0	6,6,6	0.06	0
5	SO4	A	806	-	4,4,4	0.35	0	6,6,6	0.10	0
5	SO4	B	1208	-	4,4,4	0.36	0	6,6,6	0.07	0
8	EPE	B	1201	-	15,15,15	1.32	3 (20%)	19,20,20	1.96	7 (36%)
9	ACT	B	1204	-	3,3,3	1.02	0	3,3,3	0.82	0
2	EDO	A	804	-	3,3,3	0.06	0	2,2,2	0.12	0
9	ACT	B	1205	-	3,3,3	1.01	0	3,3,3	0.80	0
5	SO4	B	1207	-	4,4,4	0.34	0	6,6,6	0.07	0
2	EDO	A	803	-	3,3,3	0.07	0	2,2,2	0.16	0
5	SO4	A	807	-	4,4,4	0.34	0	6,6,6	0.08	0
2	EDO	A	801	-	3,3,3	0.07	0	2,2,2	0.10	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
4	NDP	B	1206	-	-	8/34/77/77	0/5/5/5
4	NDP	A	805	-	-	12/34/77/77	0/5/5/5
8	EPE	B	1209	-	-	6/9/19/19	0/1/1/1
8	EPE	B	1201	-	-	4/9/19/19	0/1/1/1
2	EDO	A	804	-	-	1/1/1/1	-
2	EDO	A	803	-	-	0/1/1/1	-
2	EDO	A	801	-	-	1/1/1/1	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1206	NDP	P2B-O2B	14.20	1.84	1.59
4	A	805	NDP	P2B-O2B	13.85	1.83	1.59
4	A	805	NDP	PA-O3	6.41	1.66	1.59
4	B	1206	NDP	PA-O3	4.66	1.64	1.59
4	A	805	NDP	PN-O5D	4.47	1.76	1.59
4	B	1206	NDP	PN-O5D	4.46	1.76	1.59
8	B	1209	EPE	O1S-S	3.59	1.55	1.45
8	B	1201	EPE	C10-S	3.49	1.82	1.77
4	A	805	NDP	C5A-C4A	3.05	1.44	1.39
4	B	1206	NDP	C5A-C4A	3.03	1.44	1.39
4	A	805	NDP	O2B-C2B	-2.93	1.34	1.44
4	A	805	NDP	C2A-N1A	2.93	1.39	1.33
4	B	1206	NDP	O2B-C2B	-2.90	1.34	1.44
8	B	1209	EPE	C10-S	2.88	1.81	1.77
4	B	1206	NDP	C2A-N1A	2.83	1.39	1.33
4	A	805	NDP	C4A-N3A	2.79	1.39	1.34
4	A	805	NDP	C8A-N9A	2.45	1.41	1.37
4	B	1206	NDP	C4A-N3A	2.43	1.39	1.34
4	B	1206	NDP	C8A-N9A	2.36	1.41	1.37
8	B	1201	EPE	O1S-S	2.32	1.51	1.45
8	B	1201	EPE	O2S-S	2.27	1.51	1.45
4	B	1206	NDP	C2B-C1B	2.16	1.58	1.53
4	B	1206	NDP	C7N-N7N	2.14	1.39	1.33
4	A	805	NDP	C7N-N7N	2.10	1.39	1.33
4	A	805	NDP	C2B-C1B	2.07	1.58	1.53
4	B	1206	NDP	O5D-C5D	-2.02	1.36	1.44

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1201	EPE	O1S-S-C10	4.79	113.96	106.73
8	B	1209	EPE	C6-N1-C2	4.42	118.36	108.84
8	B	1201	EPE	O2S-S-O1S	-4.22	100.08	113.82
4	B	1206	NDP	C3N-C2N-N1N	-4.19	117.05	123.20
4	B	1206	NDP	O3-PA-O1A	-3.62	99.81	110.70
4	B	1206	NDP	O2B-P2B-O1X	-3.60	96.50	109.33
4	A	805	NDP	O3-PA-O1A	-3.58	99.95	110.70
4	A	805	NDP	O2B-P2B-O1X	-3.46	96.98	109.33
4	A	805	NDP	P2B-O2B-C2B	-3.39	114.38	123.43
4	B	1206	NDP	P2B-O2B-C2B	-3.29	114.63	123.43
8	B	1209	EPE	C3-C2-N1	2.99	116.69	110.65
8	B	1209	EPE	O1S-S-C10	-2.83	102.46	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	805	NDP	PA-O5B-C5B	-2.75	105.57	121.35
4	B	1206	NDP	PA-O5B-C5B	-2.67	106.03	121.35
8	B	1209	EPE	O3S-S-C10	2.51	110.91	106.00
4	A	805	NDP	O3X-P2B-O2X	2.49	117.15	107.80
4	B	1206	NDP	O3X-P2B-O2X	2.48	117.10	107.80
8	B	1209	EPE	O3S-S-O2S	2.42	117.46	111.40
4	B	1206	NDP	C2A-N1A-C6A	-2.42	114.76	118.73
4	B	1206	NDP	O4B-C4B-C3B	2.39	109.89	105.15
8	B	1201	EPE	O2S-S-C10	2.38	110.33	106.73
4	A	805	NDP	N3A-C4A-N9A	2.36	131.18	127.17
4	B	1206	NDP	N3A-C4A-N9A	2.36	131.18	127.17
4	B	1206	NDP	O2N-PN-O3	2.35	113.61	107.27
4	A	805	NDP	O2N-PN-O3	2.34	113.59	107.27
4	B	1206	NDP	O2N-PN-O1N	2.33	123.28	112.44
4	A	805	NDP	O2N-PN-O1N	2.31	123.20	112.44
4	A	805	NDP	C2A-N1A-C6A	-2.31	114.93	118.73
4	B	1206	NDP	O7N-C7N-N7N	-2.30	117.75	122.89
8	B	1201	EPE	C6-N1-C2	2.29	113.78	108.84
4	A	805	NDP	O7N-C7N-N7N	-2.28	117.79	122.89
8	B	1201	EPE	C3-C2-N1	2.21	115.10	110.65
8	B	1201	EPE	O3S-S-C10	2.14	110.19	106.00
4	A	805	NDP	PN-O5D-C5D	-2.14	109.10	121.35
4	A	805	NDP	C5A-C4A-N3A	-2.13	123.78	126.72
4	B	1206	NDP	C5A-C4A-N3A	-2.10	123.83	126.72
4	A	805	NDP	O5D-PN-O1N	-2.06	100.77	108.94
4	B	1206	NDP	O5D-PN-O1N	-2.06	100.77	108.94
4	B	1206	NDP	PN-O5D-C5D	-2.02	109.77	121.35
8	B	1201	EPE	C9-N1-C6	2.01	116.58	111.24

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	805	NDP	C5B-O5B-PA-O1A
4	A	805	NDP	C5B-O5B-PA-O3
4	A	805	NDP	C2N-C3N-C7N-N7N
4	B	1206	NDP	C2D-C1D-N1N-C2N
8	B	1201	EPE	C10-C9-N1-C6
8	B	1201	EPE	N4-C7-C8-O8
8	B	1201	EPE	S-C10-C9-N1
8	B	1209	EPE	C10-C9-N1-C6
8	B	1209	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
4	B	1206	NDP	C2D-C1D-N1N-C6N
4	A	805	NDP	O4B-C4B-C5B-O5B
4	A	805	NDP	C3B-C4B-C5B-O5B
4	B	1206	NDP	O4D-C4D-C5D-O5D
8	B	1209	EPE	C10-C9-N1-C2
4	B	1206	NDP	C3D-C4D-C5D-O5D
8	B	1209	EPE	C9-C10-S-O3S
4	A	805	NDP	C1B-C2B-O2B-P2B
8	B	1209	EPE	C9-C10-S-O1S
8	B	1209	EPE	C9-C10-S-O2S
4	A	805	NDP	C5D-O5D-PN-O1N
8	B	1201	EPE	C10-C9-N1-C2
4	A	805	NDP	C3B-C2B-O2B-P2B
4	A	805	NDP	PN-O3-PA-O1A
4	B	1206	NDP	O4D-C1D-N1N-C2N
4	A	805	NDP	O4D-C1D-N1N-C6N
4	B	1206	NDP	O4D-C1D-N1N-C6N
4	A	805	NDP	PN-O3-PA-O2A
2	A	801	EDO	O1-C1-C2-O2
4	A	805	NDP	C2D-C1D-N1N-C6N
4	B	1206	NDP	PA-O3-PN-O2N
4	B	1206	NDP	C2B-O2B-P2B-O3X
2	A	804	EDO	O1-C1-C2-O2

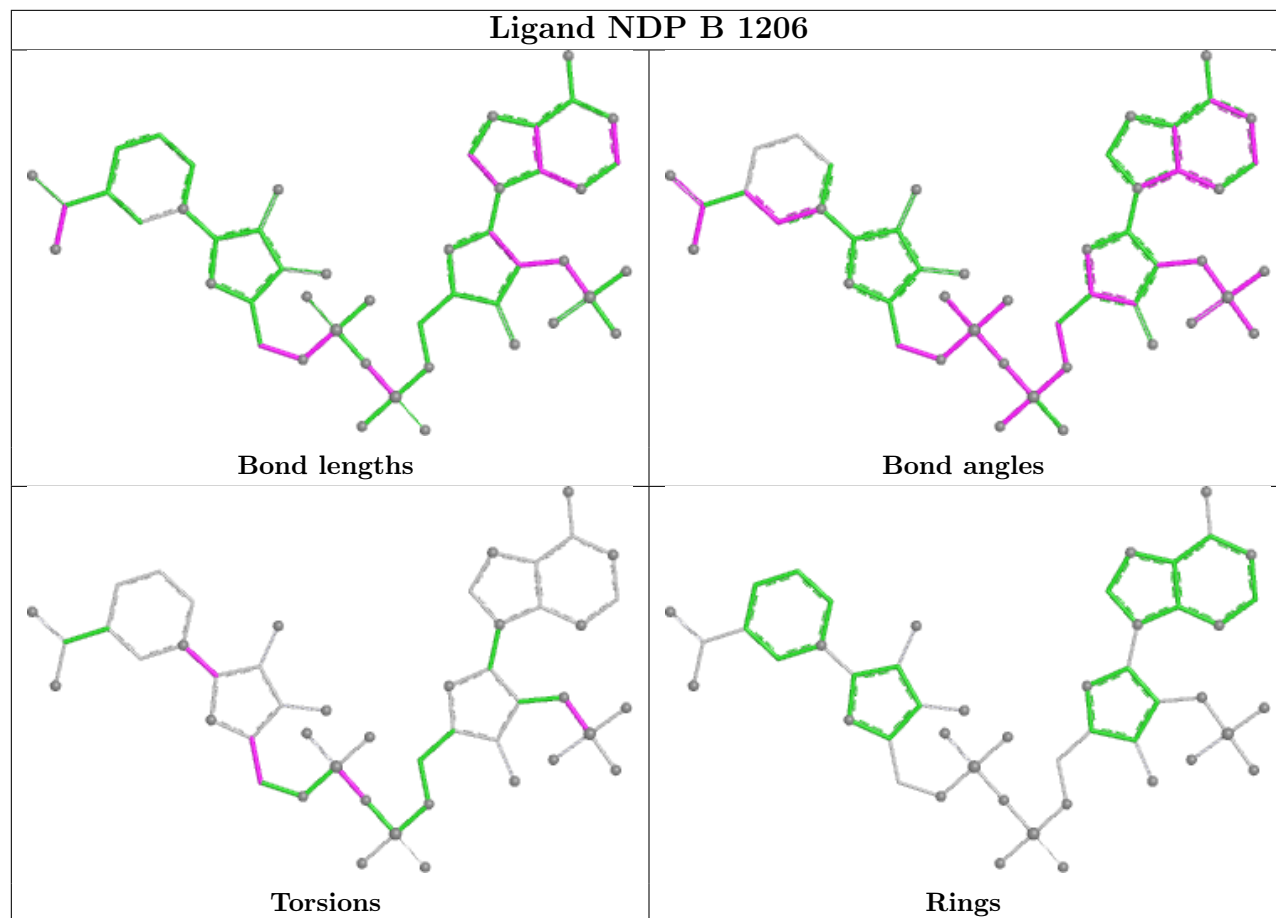
There are no ring outliers.

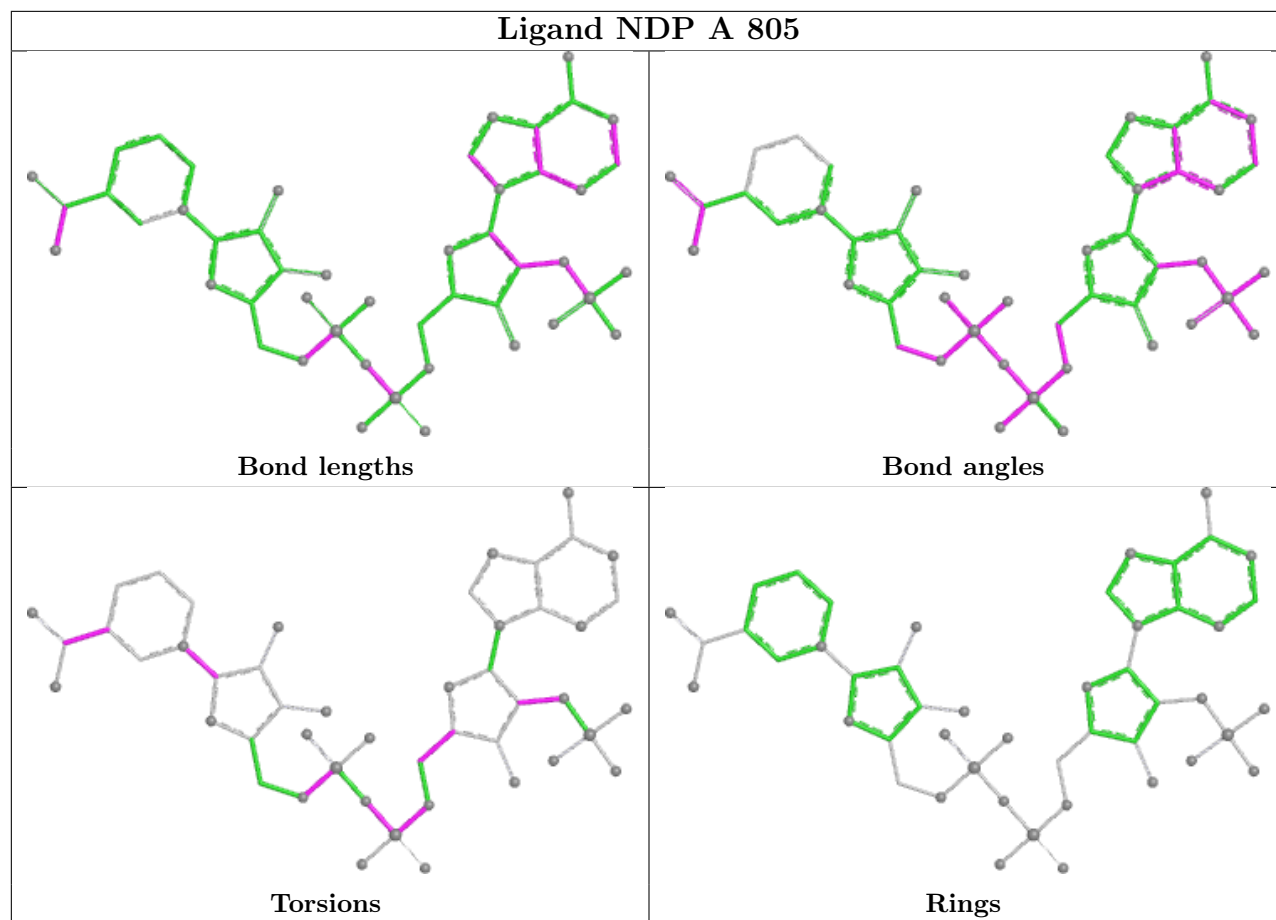
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1209	EPE	1	0
8	B	1201	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 [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	686/727 (94%)	0.19	8 (1%) 76 71	27, 75, 120, 137	2 (0%)
1	B	678/727 (93%)	0.30	3 (0%) 88 87	50, 82, 138, 172	0
All	All	1364/1454 (93%)	0.24	11 (0%) 82 78	27, 79, 128, 172	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	691	TYR	4.5
1	A	2	VAL	3.5
1	A	362	THR	2.9
1	A	452	ILE	2.8
1	B	27	LEU	2.7
1	A	482	ILE	2.6
1	B	456	ASN	2.3
1	A	26[A]	ARG	2.2
1	A	363	CYS	2.2
1	A	688	LEU	2.1
1	B	191	THR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

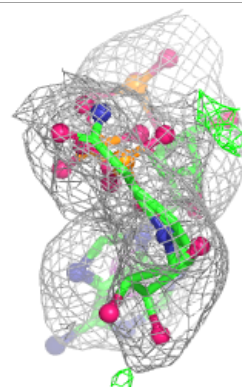
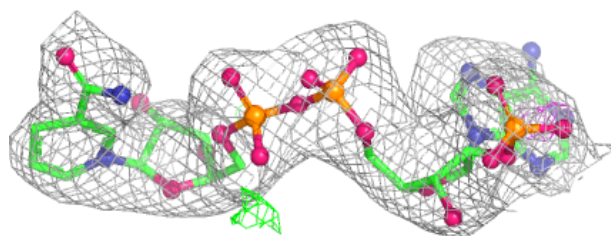
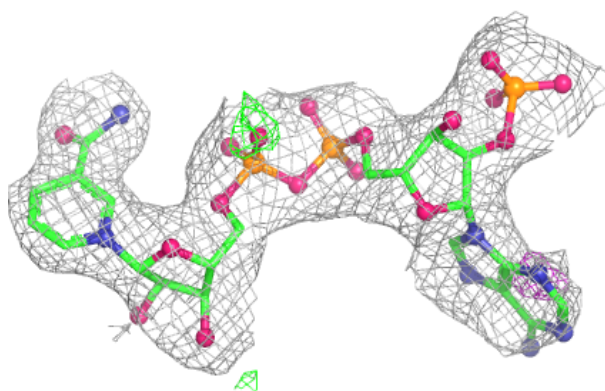
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	801	4/4	0.59	0.27	86,86,89,89	0
2	EDO	A	804	4/4	0.68	0.27	97,98,99,101	0
8	EPE	B	1201	15/15	0.74	0.33	62,64,66,66	15
9	ACT	B	1205	4/4	0.74	0.22	91,92,92,93	0
8	EPE	B	1209	15/15	0.79	0.29	83,86,91,91	15
5	SO4	B	1203	5/5	0.81	0.11	133,134,134,135	0
9	ACT	B	1204	4/4	0.83	0.13	54,55,55,56	0
5	SO4	A	807	5/5	0.83	0.14	108,109,109,110	0
7	K	A	809	1/1	0.84	0.13	73,73,73,73	0
5	SO4	B	1207	5/5	0.91	0.10	65,66,66,66	0
5	SO4	B	1210	5/5	0.91	0.18	72,72,73,73	0
6	CL	A	808	1/1	0.91	0.10	64,64,64,64	0
4	NDP	A	805	48/48	0.91	0.09	72,80,90,93	0
3	MG	A	802	1/1	0.92	0.17	53,53,53,53	0
2	EDO	A	803	4/4	0.93	0.12	73,73,74,74	0
5	SO4	B	1208	5/5	0.94	0.10	46,46,47,47	0
4	NDP	B	1206	48/48	0.94	0.08	56,64,76,78	0
5	SO4	A	806	5/5	0.95	0.09	64,65,65,65	0
3	MG	B	1202	1/1	0.96	0.07	78,78,78,78	0
6	CL	B	1211	1/1	0.97	0.05	55,55,55,55	0

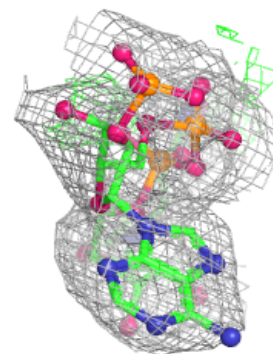
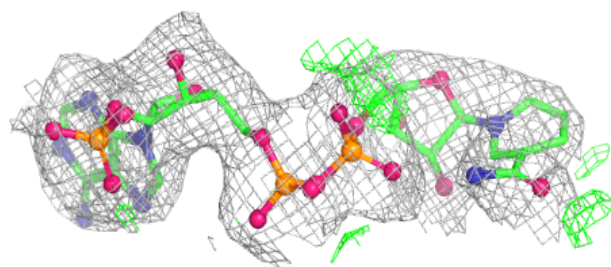
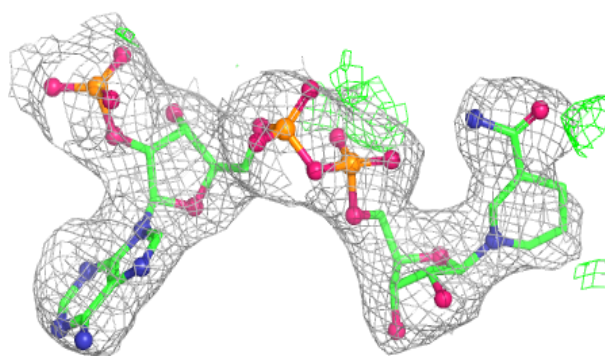
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP A 805:

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

**Electron density around NDP B 1206:**

$2mF_o-DF_c$ (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.