



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:47 pm BST

PDB ID : 6FKU
Title : Structure and function of aldehyde dehydrogenase from *Thermus thermophilus*: An enzyme with an evolutionarily-distinct C-terminal arm (Recombinant protein with shortened C-terminal, in complex with NADP)
Authors : Hayes, K.A.; Noor, M.R.; Djeghader, A.; Soulimane, T.
Deposited on : 2018-01-24
Resolution : 2.40 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

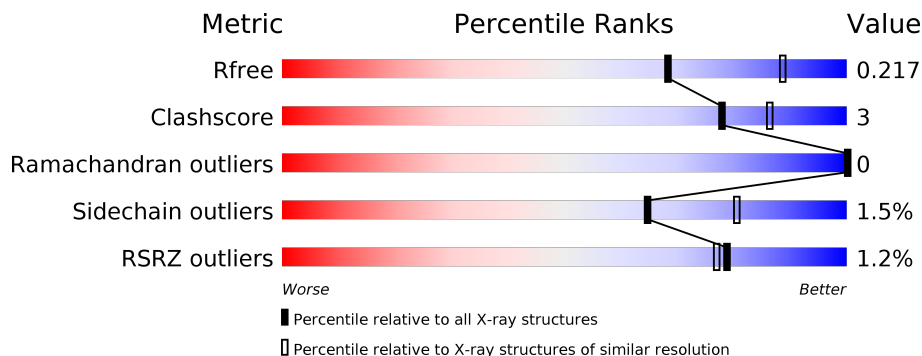
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	521	 2% 90% 7%
1	B	521	 2% 90% 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8407 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	511	Total	C	N	O	S	0	0	0
			4006	2567	706	725	8			
1	B	507	Total	C	N	O	S	0	0	0
			3968	2544	696	721	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP Q72KD3
A	-4	HIS	-	expression tag	UNP Q72KD3
A	-3	HIS	-	expression tag	UNP Q72KD3
A	-2	HIS	-	expression tag	UNP Q72KD3
A	-1	HIS	-	expression tag	UNP Q72KD3
A	0	HIS	-	expression tag	UNP Q72KD3
A	1	HIS	-	expression tag	UNP Q72KD3
B	-5	MET	-	initiating methionine	UNP Q72KD3
B	-4	HIS	-	expression tag	UNP Q72KD3
B	-3	HIS	-	expression tag	UNP Q72KD3
B	-2	HIS	-	expression tag	UNP Q72KD3
B	-1	HIS	-	expression tag	UNP Q72KD3
B	0	HIS	-	expression tag	UNP Q72KD3
B	1	HIS	-	expression tag	UNP Q72KD3

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



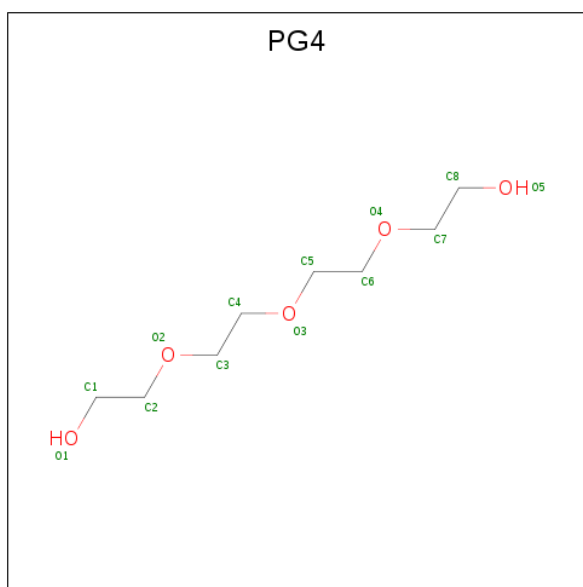
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



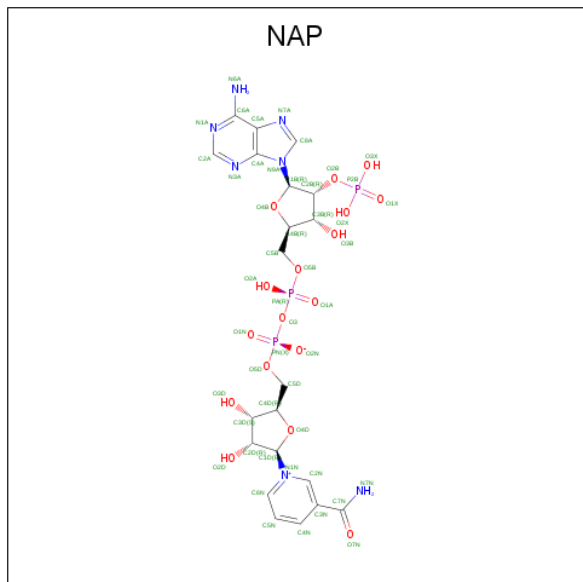
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



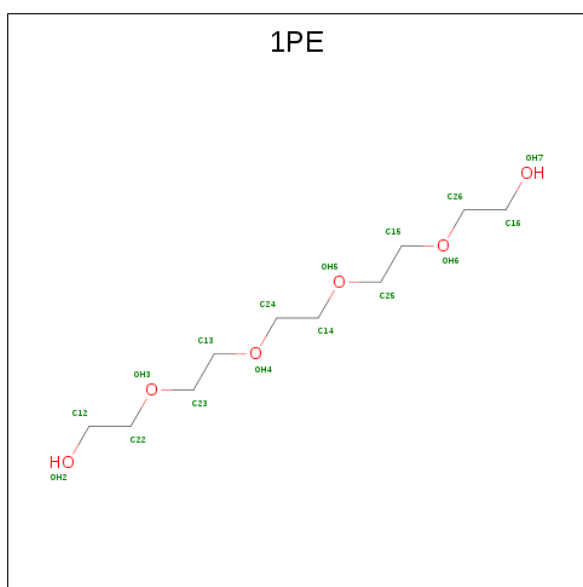
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

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



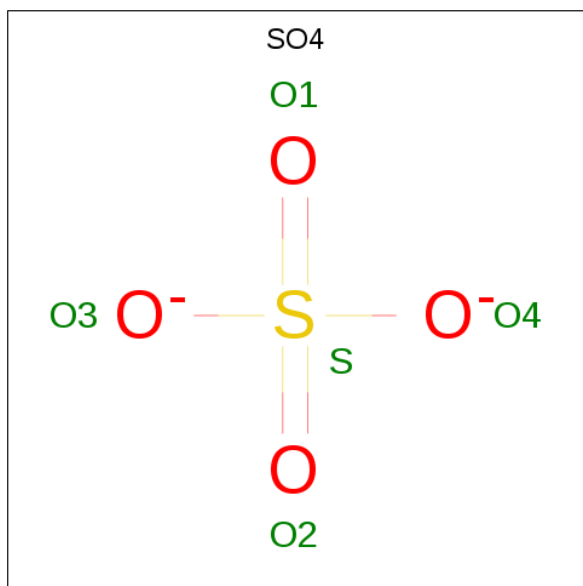
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			
5	A	1	Total	48	21	7	17	3	0	0
5	B	1	Total	48	21	7	17	3	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	B	1	Total	C	O	0	0
			16	10	6		
6	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

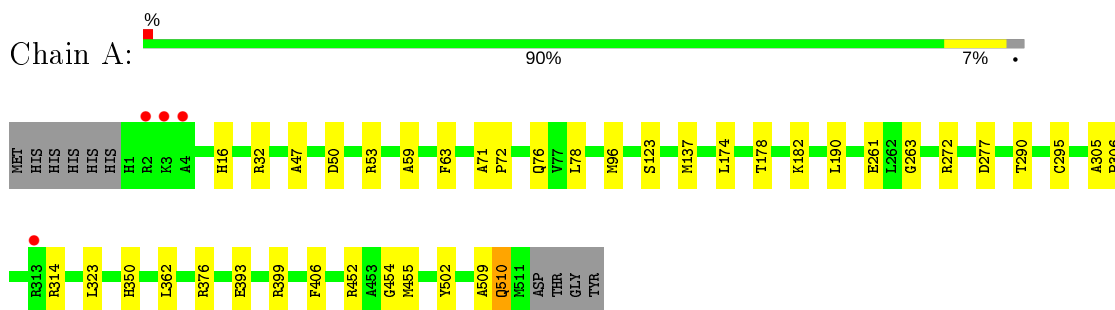
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	90	Total	O	0	0
			90	90		
8	B	90	Total	O	0	0
			90	90		

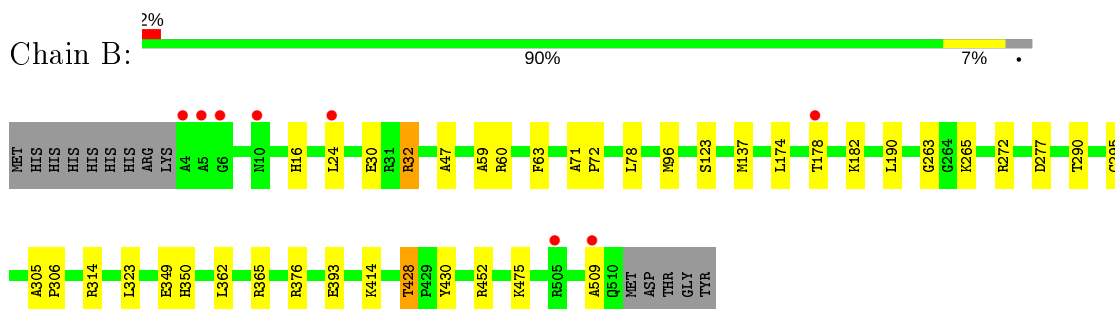
3 Residue-property plots [i](#)

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: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.23Å 105.23Å 315.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 2.40 48.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.11-2.40) 100.0 (48.11-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.183 , 0.209 0.193 , 0.217	Depositor DCC
R_{free} test set	2000 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtrriage
Anisotropy	0.005	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8407	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: PGE, NAP, 1PE, PG4, SO4, PEG

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	0.38	0/4110	0.58	0/5580
1	B	0.38	0/4071	0.57	0/5530
All	All	0.38	0/8181	0.58	0/11110

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	A	0	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	ARG	Sidechain
1	A	32	ARG	Sidechain
1	B	272	ARG	Sidechain
1	B	32	ARG	Sidechain
1	B	365	ARG	Sidechain

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	4006	0	3965	24	1
1	B	3968	0	3920	24	1
2	A	50	0	70	1	0
2	B	10	0	14	5	0
3	A	7	0	10	1	0
3	B	14	0	20	0	0
4	A	13	0	18	1	0
5	A	48	0	25	4	0
5	B	48	0	25	4	0
6	A	16	0	22	0	0
6	B	32	0	44	1	0
7	A	10	0	0	0	0
7	B	5	0	0	0	0
8	A	90	0	0	2	0
8	B	90	0	0	1	0
All	All	8407	0	8133	48	1

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 (48) 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:B:428:THR:HG22	1:B:430:TYR:H	1.37	0.90
1:A:50:ASP:OD1	1:A:53:ARG:NH1	2.13	0.81
1:B:30:GLU:OE2	1:B:32:ARG:NH1	2.18	0.76
1:B:59:ALA:O	1:B:178:THR:HG21	1.90	0.71
1:B:265:LYS:HB3	1:B:428:THR:HG21	1.73	0.71
1:A:59:ALA:O	1:A:178:THR:HG21	1.91	0.70
1:A:452:ARG:HH22	2:B:603:PGE:C5	2.09	0.66
1:B:295:CYS:SG	5:B:605:NAP:C4N	2.89	0.60
1:A:452:ARG:HH22	2:B:603:PGE:H52	1.66	0.59
1:A:295:CYS:SG	5:A:708:NAP:C4N	2.93	0.57
1:A:510:GLN:NE2	8:A:802:HOH:O	2.42	0.53
1:B:60:ARG:HG3	2:B:603:PGE:H32	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ASP:OD1	1:B:314:ARG:NH1	2.41	0.51
1:B:305:ALA:HB3	1:B:306:PRO:HD3	1.92	0.51
1:B:414:LYS:HE2	6:B:604:1PE:H221	1.92	0.51
1:A:16:HIS:CE1	1:A:47:ALA:HB2	2.48	0.49
1:B:428:THR:HB	8:B:751:HOH:O	2.11	0.48
1:B:96:MET:HA	1:B:190:LEU:HD11	1.96	0.48
1:A:277:ASP:OD1	1:A:314:ARG:NH1	2.40	0.47
1:B:16:HIS:CE1	1:B:47:ALA:HB2	2.49	0.47
1:A:96:MET:HA	1:A:190:LEU:HD11	1.97	0.47
1:B:263:GLY:HA2	5:B:605:NAP:O2D	2.15	0.47
1:B:295:CYS:HB3	5:B:605:NAP:C2N	2.46	0.46
1:B:323:LEU:HD23	1:B:376:ARG:HB3	1.99	0.45
1:A:63:PHE:HB2	1:A:178:THR:CG2	2.46	0.45
1:A:362:LEU:HD11	1:A:393:GLU:HG3	1.98	0.45
1:A:502:TYR:OH	8:A:801:HOH:O	2.15	0.45
1:A:323:LEU:HD23	1:A:376:ARG:HB3	1.99	0.45
1:A:305:ALA:HB3	1:A:306:PRO:HD3	1.98	0.44
4:A:706:PG4:H41	1:B:475:LYS:HG3	1.99	0.44
1:A:137:MET:CE	1:A:509:ALA:HA	2.46	0.44
1:A:263:GLY:HA2	5:A:708:NAP:O2D	2.17	0.44
1:B:78:LEU:HD11	1:B:174:LEU:HB2	2.00	0.44
1:B:362:LEU:HD11	1:B:393:GLU:HG3	1.99	0.43
1:A:452:ARG:NH2	2:B:603:PGE:C5	2.78	0.43
1:B:428:THR:HG22	1:B:430:TYR:N	2.19	0.43
1:A:78:LEU:HD11	1:A:174:LEU:HB2	2.01	0.43
1:B:137:MET:CE	1:B:509:ALA:HA	2.49	0.43
1:B:63:PHE:HB2	1:B:178:THR:CG2	2.49	0.43
1:B:295:CYS:SG	5:B:605:NAP:C3N	3.07	0.42
1:A:452:ARG:NH2	2:B:603:PGE:H52	2.33	0.42
1:A:399:ARG:NH2	3:A:702:PEG:H21	2.35	0.42
1:A:261:GLU:HB3	5:A:708:NAP:C7N	2.50	0.42
2:A:707:PGE:H4	1:B:452:ARG:HG2	2.02	0.41
1:A:295:CYS:HB3	5:A:708:NAP:C2N	2.51	0.41
1:B:71:ALA:N	1:B:72:PRO:CD	2.84	0.41
1:A:71:ALA:N	1:A:72:PRO:CD	2.85	0.40
1:A:454:GLY:C	1:A:455:MET:HG3	2.42	0.40

All (1) 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:123:SER:OG	1:B:123:SER:OG[7_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	509/521 (98%)	492 (97%)	17 (3%)	0	100	100
1	B	505/521 (97%)	489 (97%)	16 (3%)	0	100	100
All	All	1014/1042 (97%)	981 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	408/417 (98%)	402 (98%)	6 (2%)	65	80
1	B	404/417 (97%)	398 (98%)	6 (2%)	65	80
All	All	812/834 (97%)	800 (98%)	12 (2%)	65	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	182	LYS
1	A	290	THR

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Mol	Chain	Res	Type
1	A	350	HIS
1	A	406	PHE
1	A	510	GLN
1	B	24	LEU
1	B	182	LYS
1	B	290	THR
1	B	349	GLU
1	B	350	HIS
1	B	428	THR

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

Mol	Chain	Res	Type
1	A	510	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](#)

18 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
2	PGE	B	603	-	9,9,9	0.51	0	8,8,8	0.52	0
2	PGE	A	707	-	9,9,9	0.70	0	8,8,8	0.63	0
6	1PE	B	602	-	15,15,15	0.63	0	14,14,14	0.46	0
7	SO4	A	710	-	4,4,4	0.29	0	6,6,6	0.18	0
3	PEG	A	702	-	6,6,6	0.56	0	5,5,5	0.30	0
5	NAP	A	708	-	45,52,52	0.94	2 (4%)	56,80,80	1.28	7 (12%)
7	SO4	A	711	-	4,4,4	0.35	0	6,6,6	0.41	0
6	1PE	B	604	-	15,15,15	0.68	0	14,14,14	0.60	0
7	SO4	B	607	-	4,4,4	0.43	0	6,6,6	0.45	0
2	PGE	A	701	-	9,9,9	0.53	0	8,8,8	0.42	0
3	PEG	B	606	-	6,6,6	0.63	0	5,5,5	0.49	0
2	PGE	A	705	-	9,9,9	0.57	0	8,8,8	0.45	0
3	PEG	B	601	-	6,6,6	0.57	0	5,5,5	0.46	0
5	NAP	B	605	-	45,52,52	1.04	4 (8%)	56,80,80	1.22	5 (8%)
4	PG4	A	706	-	12,12,12	0.63	0	11,11,11	0.91	0
6	1PE	A	709	-	15,15,15	0.57	0	14,14,14	0.43	0
2	PGE	A	704	-	9,9,9	0.64	0	8,8,8	0.37	0
2	PGE	A	703	-	9,9,9	0.58	0	8,8,8	0.32	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
2	PGE	B	603	-	-	3/7/7/7	-
2	PGE	A	707	-	-	4/7/7/7	-
6	1PE	B	602	-	-	9/13/13/13	-
3	PEG	A	702	-	-	2/4/4/4	-
5	NAP	A	708	-	-	3/31/67/67	0/5/5/5
6	1PE	B	604	-	-	6/13/13/13	-
2	PGE	A	701	-	-	4/7/7/7	-
3	PEG	B	606	-	-	1/4/4/4	-
2	PGE	A	705	-	-	7/7/7/7	-
3	PEG	B	601	-	-	3/4/4/4	-
5	NAP	B	605	-	-	2/31/67/67	0/5/5/5
4	PG4	A	706	-	-	5/10/10/10	-
6	1PE	A	709	-	-	6/13/13/13	-
2	PGE	A	704	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	A	703	-	-	2/7/7/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	708	NAP	P2B-O2B	3.16	1.65	1.59
5	B	605	NAP	P2B-O2B	2.99	1.65	1.59
5	B	605	NAP	C2A-N3A	2.91	1.36	1.32
5	B	605	NAP	O4B-C1B	2.42	1.44	1.41
5	B	605	NAP	C5A-C4A	2.33	1.47	1.40
5	A	708	NAP	O4B-C1B	2.06	1.43	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	708	NAP	N3A-C2A-N1A	-3.69	122.92	128.68
5	A	708	NAP	PN-O3-PA	-3.61	120.45	132.83
5	B	605	NAP	N3A-C2A-N1A	-3.20	123.68	128.68
5	B	605	NAP	PN-O3-PA	-3.20	121.86	132.83
5	A	708	NAP	C1B-N9A-C4A	-3.13	121.14	126.64
5	B	605	NAP	O4D-C1D-C2D	-2.59	103.14	106.93
5	A	708	NAP	O4D-C1D-C2D	-2.58	103.15	106.93
5	A	708	NAP	O2B-P2B-O1X	-2.58	99.44	109.39
5	B	605	NAP	C1B-N9A-C4A	-2.36	122.49	126.64
5	A	708	NAP	C4A-C5A-N7A	-2.30	107.00	109.40
5	B	605	NAP	C4A-C5A-N7A	-2.17	107.14	109.40
5	A	708	NAP	O2A-PA-O1A	2.11	122.68	112.24

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	PEG	O1-C1-C2-O2
2	A	705	PGE	O1-C1-C2-O2
2	A	701	PGE	O2-C3-C4-O3
6	A	709	1PE	OH6-C15-C25-OH5
6	A	709	1PE	OH5-C14-C24-OH4
2	A	707	PGE	O1-C1-C2-O2
2	B	603	PGE	O2-C3-C4-O3
3	A	702	PEG	O2-C3-C4-O4
4	A	706	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
2	A	703	PGE	O3-C5-C6-O4
6	B	602	1PE	OH5-C14-C24-OH4
6	B	604	1PE	OH2-C12-C22-OH3
3	B	601	PEG	O1-C1-C2-O2
2	A	705	PGE	O3-C5-C6-O4
4	A	706	PG4	C4-C3-O2-C2
6	A	709	1PE	C24-C14-OH5-C25
2	B	603	PGE	O3-C5-C6-O4
3	B	606	PEG	O2-C3-C4-O4
3	B	601	PEG	O2-C3-C4-O4
5	B	605	NAP	C4D-C5D-O5D-PN
2	A	707	PGE	O3-C5-C6-O4
5	B	605	NAP	C2B-O2B-P2B-O1X
6	B	602	1PE	C25-C15-OH6-C26
6	B	602	1PE	C16-C26-OH6-C15
6	A	709	1PE	C12-C22-OH3-C23
2	A	707	PGE	C1-C2-O2-C3
6	B	602	1PE	C15-C25-OH5-C14
2	A	705	PGE	C1-C2-O2-C3
5	A	708	NAP	C2B-O2B-P2B-O2X
2	A	701	PGE	O3-C5-C6-O4
6	B	604	1PE	OH4-C13-C23-OH3
5	A	708	NAP	C4D-C5D-O5D-PN
2	B	603	PGE	O1-C1-C2-O2
6	A	709	1PE	OH7-C16-C26-OH6
2	A	705	PGE	C3-C4-O3-C5
4	A	706	PG4	C1-C2-O2-C3
2	A	704	PGE	C6-C5-O3-C4
6	B	604	1PE	C23-C13-OH4-C24
2	A	705	PGE	C4-C3-O2-C2
2	A	701	PGE	C1-C2-O2-C3
2	A	703	PGE	C6-C5-O3-C4
6	B	604	1PE	C12-C22-OH3-C23
3	B	601	PEG	C4-C3-O2-C2
6	A	709	1PE	C15-C25-OH5-C14
6	B	604	1PE	C15-C25-OH5-C14
4	A	706	PG4	O3-C5-C6-O4
6	B	602	1PE	C23-C13-OH4-C24
2	A	705	PGE	O2-C3-C4-O3
2	A	705	PGE	C6-C5-O3-C4
2	A	704	PGE	O2-C3-C4-O3
2	A	707	PGE	O2-C3-C4-O3

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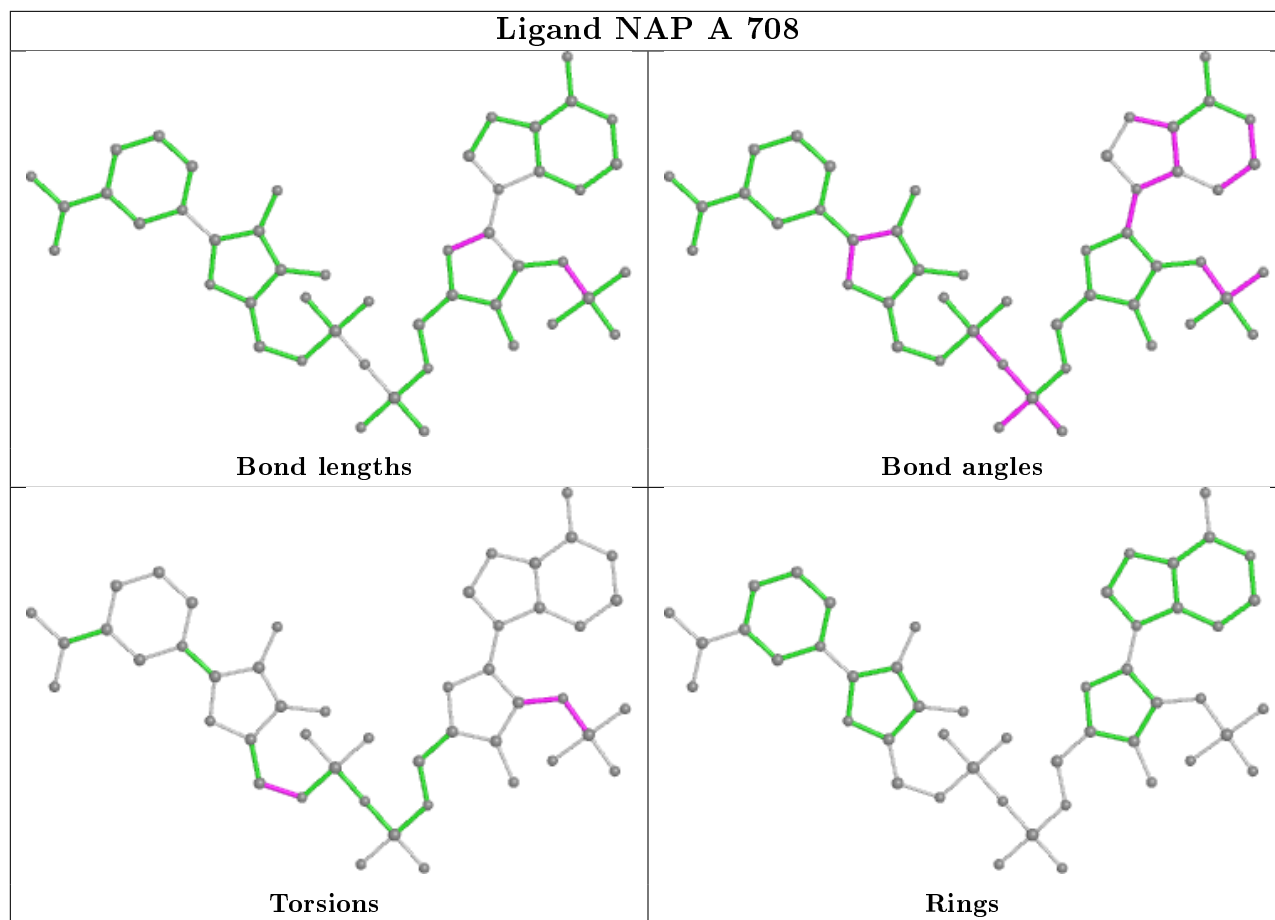
Mol	Chain	Res	Type	Atoms
6	B	602	1PE	OH2-C12-C22-OH3
6	B	602	1PE	C13-C23-OH3-C22
2	A	704	PGE	C4-C3-O2-C2
4	A	706	PG4	C3-C4-O3-C5
6	B	604	1PE	OH7-C16-C26-OH6
6	B	602	1PE	OH7-C16-C26-OH6
2	A	701	PGE	C4-C3-O2-C2
6	B	602	1PE	OH6-C15-C25-OH5
5	A	708	NAP	C3B-C2B-O2B-P2B

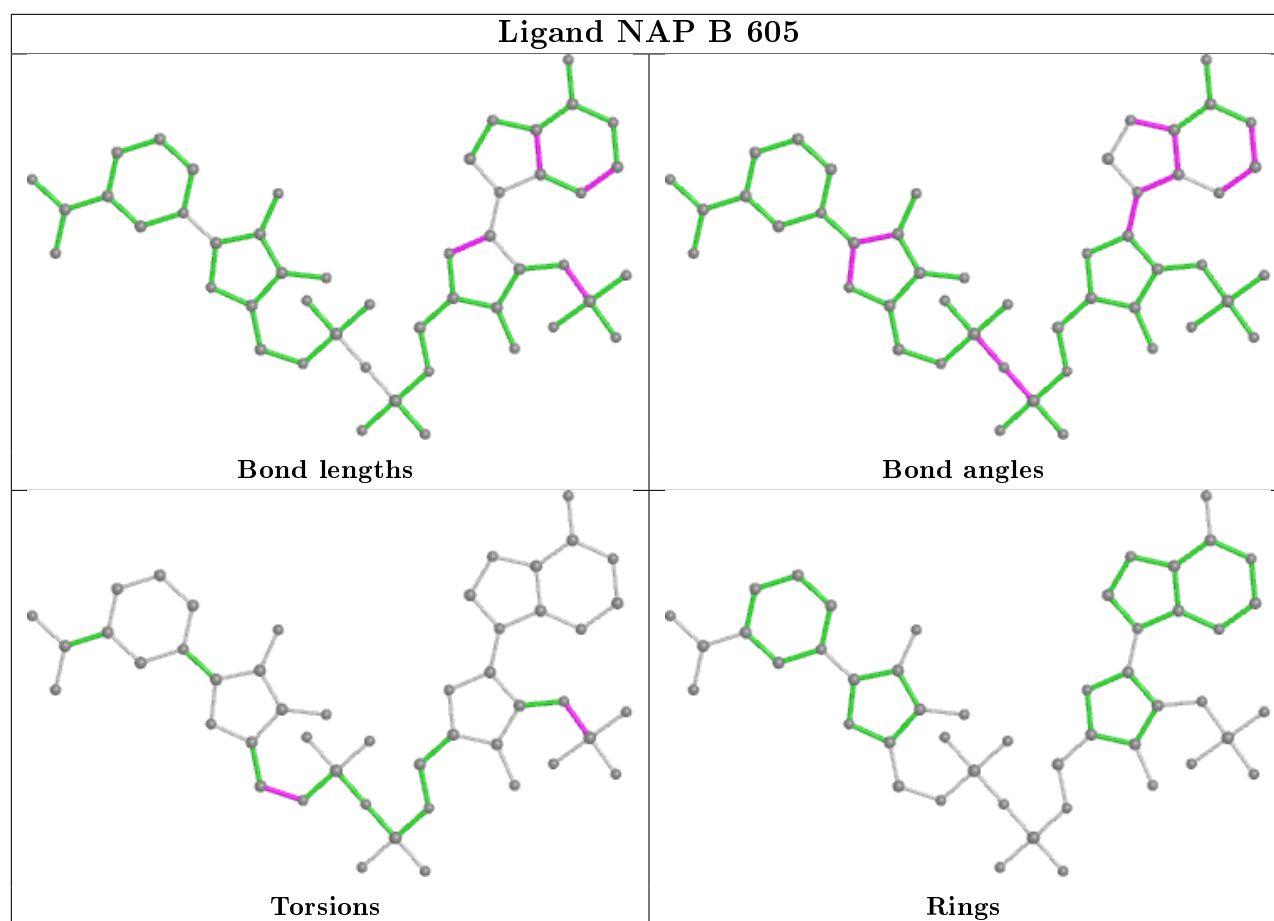
There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	603	PGE	5	0
2	A	707	PGE	1	0
3	A	702	PEG	1	0
5	A	708	NAP	4	0
6	B	604	1PE	1	0
5	B	605	NAP	4	0
4	A	706	PG4	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	511/521 (98%)	-0.43	4 (0%) 86 84	31, 41, 66, 105	0
1	B	507/521 (97%)	-0.35	8 (1%) 72 70	31, 40, 62, 100	0
All	All	1018/1042 (97%)	-0.39	12 (1%) 79 77	31, 40, 64, 105	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	ALA	4.3
1	A	3	LYS	3.8
1	B	4	ALA	3.7
1	B	6	GLY	3.1
1	B	509	ALA	3.1
1	B	505	ARG	2.7
1	B	10	ASN	2.5
1	A	4	ALA	2.5
1	A	2	ARG	2.4
1	B	178	THR	2.1
1	A	313	ARG	2.1
1	B	24	LEU	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 carbohydrates in this entry.

6.4 Ligands

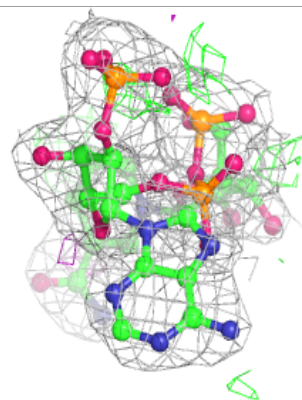
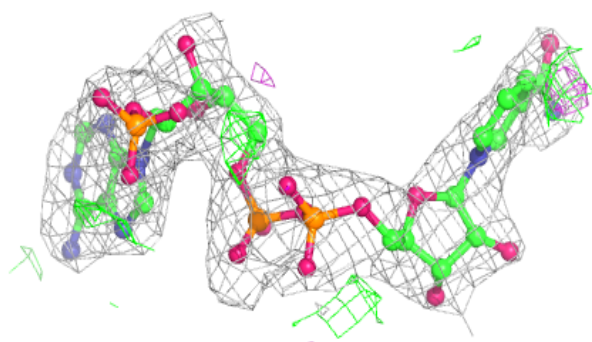
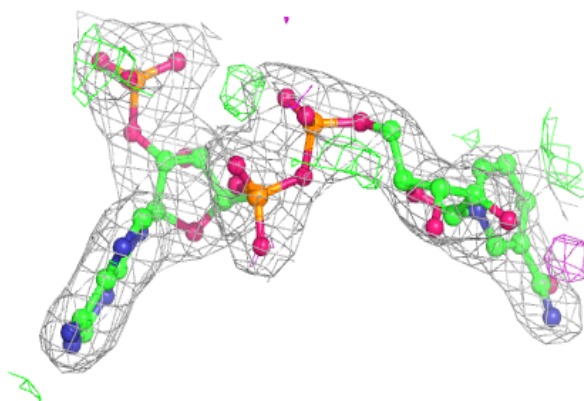
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PGE	B	603	10/10	0.70	0.28	82,89,93,95	0
2	PGE	A	707	10/10	0.73	0.21	66,79,86,87	0
6	1PE	B	602	16/16	0.80	0.24	69,80,89,92	0
3	PEG	B	606	7/7	0.80	0.27	64,67,75,78	0
2	PGE	A	701	10/10	0.83	0.25	57,65,68,68	0
6	1PE	A	709	16/16	0.84	0.43	58,75,79,81	0
6	1PE	B	604	16/16	0.87	0.34	63,71,75,76	0
4	PG4	A	706	13/13	0.88	0.21	52,65,74,75	0
3	PEG	A	702	7/7	0.89	0.15	55,61,69,71	0
2	PGE	A	703	10/10	0.89	0.22	61,66,69,69	0
2	PGE	A	705	10/10	0.90	0.14	57,63,74,76	0
2	PGE	A	704	10/10	0.91	0.24	65,67,68,69	0
3	PEG	B	601	7/7	0.91	0.17	57,58,61,62	0
5	NAP	A	708	48/48	0.97	0.11	34,47,65,69	0
7	SO4	A	711	5/5	0.97	0.11	46,49,53,59	0
5	NAP	B	605	48/48	0.97	0.12	35,48,76,80	0
7	SO4	B	607	5/5	0.99	0.08	46,49,56,59	0
7	SO4	A	710	5/5	0.99	0.08	44,47,48,50	0

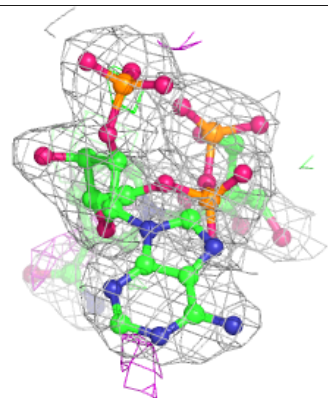
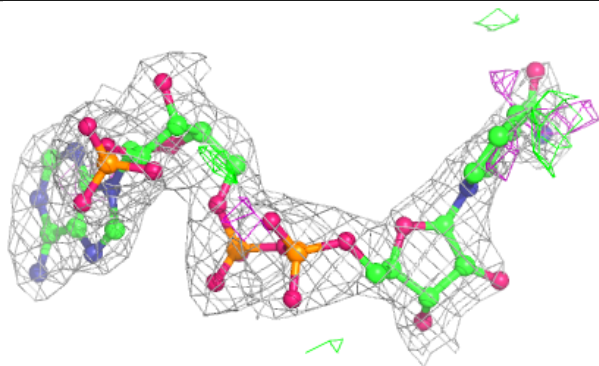
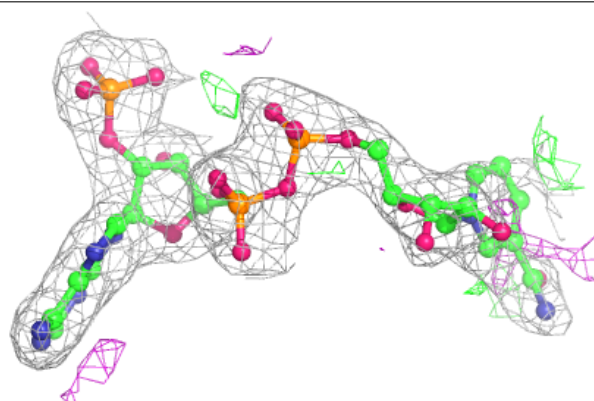
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 708:

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

**Electron density around NAP B 605:**

$2mF_o-DF_c$ (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.