



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:07 PM UTC

PDB ID : 6FKU / pdb_00006fku
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 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

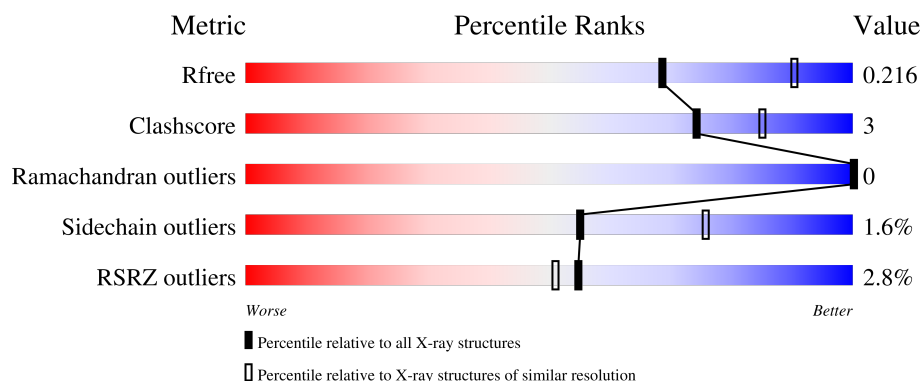
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	521	2% 90% 8% .
1	B	521	3% 89% 8% .

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
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 (CCD ID: PGE) (formula: C₆H₁₄O₄).



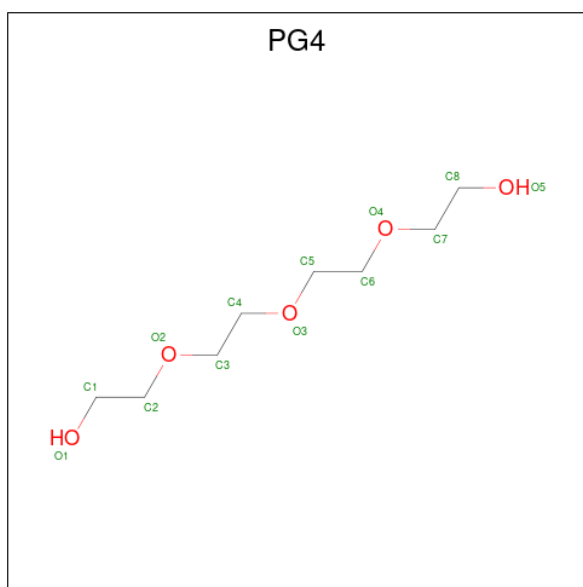
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: 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 (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

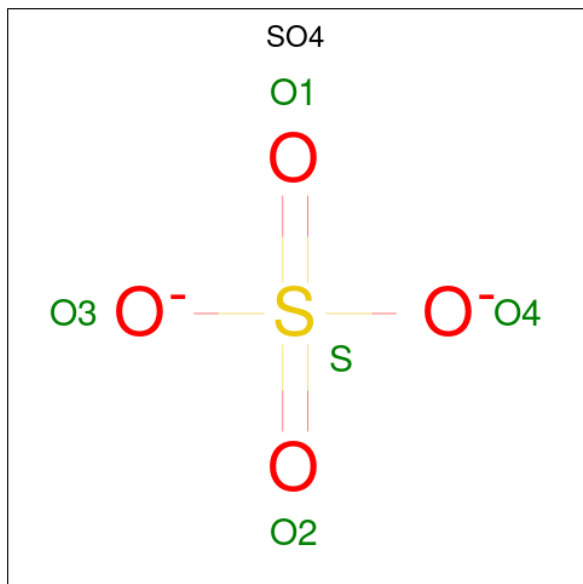
- # NAP

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

- 1PE
-
- The diagram shows the chemical structure of 1PE, a diacylglycerol. It consists of a glycerol backbone with two fatty acid chains. The first fatty acid chain is attached to the first carbon of the glycerol backbone and is labeled with C12, C22, and C23. The second fatty acid chain is attached to the second carbon of the glycerol backbone and is labeled with C13, C24, C14, C25, C15, C26, and C16. The structure is shown in a zig-zag conformation, with the glycerol backbone at the bottom and the fatty acid chains extending upwards. The terminal groups of the fatty acid chains are labeled OH2 and OH7, respectively.

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 (CCD ID: 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		

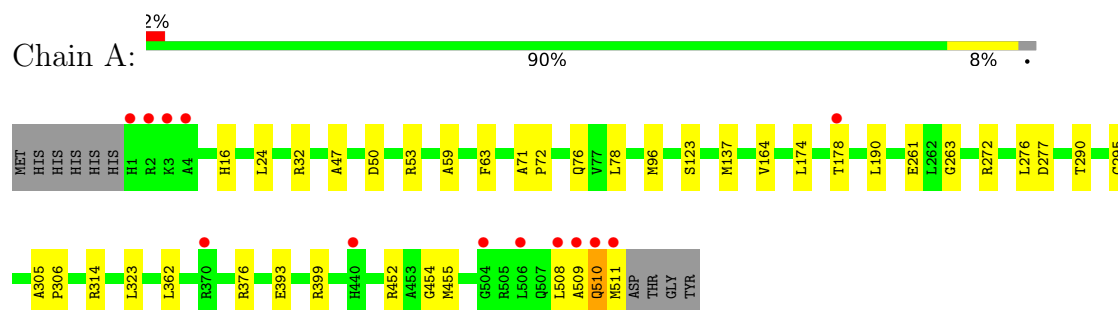
- Molecule 8 is water.

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

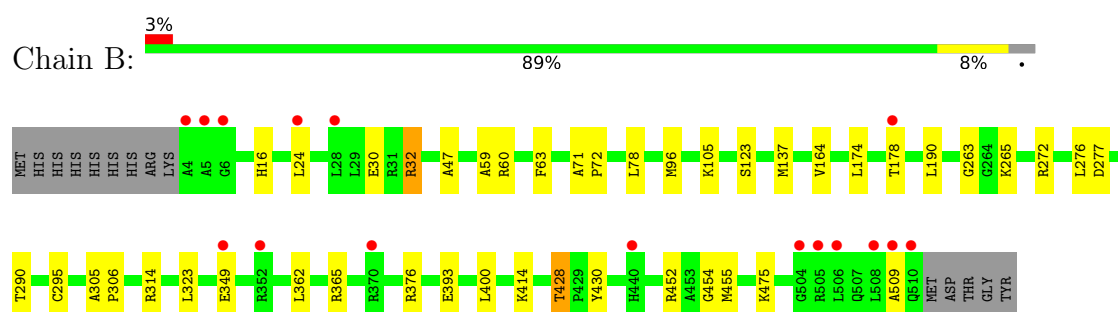
3 Residue-property plots

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: 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)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.183 , 0.209 0.193 , 0.216	Depositor DCC
R_{free} test set	2000 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8407	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage'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: PEG, NAP, PGE, SO4, 1PE, PG4

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	0.61	0/4110	0.82	0/5580
1	B	0.61	0/4071	0.81	0/5530
All	All	0.61	0/8181	0.81	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

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	25	1
1	B	3968	0	3920	26	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	1	0
8	B	90	0	0	1	0
All	All	8407	0	8133	50	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 (50) 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:323:LEU:HD23	1:A:376:ARG:HB3	1.99	0.45
1:A:454:GLY:C	1:A:455:MET:HG3	2.42	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:A:452:ARG:NH2	2:B:603:PGE:C5	2.78	0.43
1:B:362:LEU:HD11	1:B:393:GLU:HG3	1.99	0.43
1:B:428:THR:HG22	1:B:430:TYR:N	2.19	0.43
1:B:454:GLY:C	1:B:455:MET:HG3	2.43	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
1:A:508:LEU:HD23	1:A:511:MET:HE2	2.01	0.41
2:A:707:PGE:H4	1:B:452:ARG:HG2	2.02	0.41
1:A:511:MET:HE3	1:B:105:LYS:HG2	2.01	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

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%)	57	77
1	B	404/417 (97%)	397 (98%)	7 (2%)	53	74
All	All	812/834 (97%)	799 (98%)	13 (2%)	55	76

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	76	GLN
1	A	164	VAL

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Mol	Chain	Res	Type
1	A	276	LEU
1	A	290	THR
1	A	510	GLN
1	B	24	LEU
1	B	164	VAL
1	B	276	LEU
1	B	290	THR
1	B	349	GLU
1	B	400	LEU
1	B	428	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	HIS
1	A	510	GLN
1	B	440	HIS

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 oligosaccharides 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	$\# Z > 2$
3	PEG	B	601	-	6,6,6	0.58	0	5,5,5	0.46	0
6	1PE	B	604	-	15,15,15	0.69	0	14,14,14	0.60	0
2	PGE	A	703	-	9,9,9	0.59	0	8,8,8	0.32	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	0.48	0
6	1PE	B	602	-	15,15,15	0.63	0	14,14,14	0.46	0
4	PG4	A	706	-	12,12,12	0.63	0	11,11,11	0.90	0
2	PGE	A	705	-	9,9,9	0.58	0	8,8,8	0.45	0
5	NAP	B	605	-	50,52,52	1.35	7 (14%)	71,80,80	1.55	8 (11%)
3	PEG	A	702	-	6,6,6	0.56	0	5,5,5	0.29	0
7	SO4	A	711	-	4,4,4	0.43	0	6,6,6	0.41	0
2	PGE	B	603	-	9,9,9	0.52	0	8,8,8	0.51	0
5	NAP	A	708	-	50,52,52	1.35	7 (14%)	71,80,80	1.58	13 (18%)
7	SO4	B	607	-	4,4,4	0.52	0	6,6,6	0.44	0
2	PGE	A	707	-	9,9,9	0.70	0	8,8,8	0.62	0
2	PGE	A	704	-	9,9,9	0.64	0	8,8,8	0.37	0
6	1PE	A	709	-	15,15,15	0.57	0	14,14,14	0.43	0
7	SO4	A	710	-	4,4,4	0.40	0	6,6,6	0.16	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
3	PEG	B	601	-	-	3/4/4/4	-
6	1PE	B	604	-	-	6/13/13/13	-
2	PGE	A	703	-	-	2/7/7/7	-
2	PGE	A	701	-	-	4/7/7/7	-
3	PEG	B	606	-	-	1/4/4/4	-
6	1PE	B	602	-	-	9/13/13/13	-
4	PG4	A	706	-	-	5/10/10/10	-
2	PGE	A	705	-	-	7/7/7/7	-
5	NAP	B	605	-	-	5/35/67/67	0/5/5/5
3	PEG	A	702	-	-	2/4/4/4	-
2	PGE	B	603	-	-	3/7/7/7	-
5	NAP	A	708	-	-	6/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	A	707	-	-	4/7/7/7	-
2	PGE	A	704	-	-	3/7/7/7	-
6	1PE	A	709	-	-	6/13/13/13	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	NAP	C5A-C4A	4.49	1.47	1.39
5	A	708	NAP	PA-O3	3.85	1.63	1.59
5	A	708	NAP	C5A-C4A	3.76	1.45	1.39
5	A	708	NAP	PN-O3	3.54	1.63	1.59
5	B	605	NAP	PN-O3	3.47	1.63	1.59
5	A	708	NAP	P2B-O2B	3.28	1.65	1.59
5	B	605	NAP	P2B-O2B	3.09	1.65	1.59
5	B	605	NAP	C5A-N7A	-2.57	1.34	1.39
5	A	708	NAP	C5A-C6A	2.40	1.47	1.41
5	A	708	NAP	C5A-N7A	-2.38	1.34	1.39
5	B	605	NAP	C5A-C6A	2.34	1.47	1.41
5	B	605	NAP	C8A-N7A	2.30	1.36	1.31
5	A	708	NAP	C4A-N9A	-2.07	1.33	1.37
5	B	605	NAP	PA-O3	2.04	1.61	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	605	NAP	C5A-C4A-N3A	-5.31	119.40	126.72
5	A	708	NAP	C5A-C4A-N3A	-4.92	119.94	126.72
5	B	605	NAP	N3A-C4A-N9A	4.64	135.06	127.17
5	A	708	NAP	N3A-C4A-N9A	4.16	134.24	127.17
5	A	708	NAP	N3A-C2A-N1A	-3.74	122.92	128.58
5	A	708	NAP	C2A-N3A-C4A	3.53	120.46	111.83
5	B	605	NAP	C4A-N9A-C8A	3.47	109.38	105.74
5	A	708	NAP	C4A-N9A-C8A	3.44	109.35	105.74
5	B	605	NAP	N3A-C2A-N1A	-3.24	123.68	128.58
5	B	605	NAP	C2A-N3A-C4A	3.13	119.48	111.83
5	A	708	NAP	C4A-C5A-N7A	-3.13	107.00	110.58
5	B	605	NAP	C4A-C5A-N7A	-3.01	107.14	110.58
5	A	708	NAP	N9A-C8A-N7A	-2.95	109.75	113.94
5	A	708	NAP	C5A-N7A-C8A	2.94	108.07	103.45
5	B	605	NAP	C5A-N7A-C8A	2.84	107.91	103.45
5	A	708	NAP	O2B-P2B-O1X	-2.78	99.44	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	605	NAP	N9A-C8A-N7A	-2.75	110.03	113.94
5	A	708	NAP	C6A-C5A-N7A	2.44	136.79	132.09
5	A	708	NAP	C4A-N9A-C1B	-2.35	121.14	126.63
5	A	708	NAP	O2A-PA-O1A	2.20	122.68	112.44
5	A	708	NAP	O3-PN-O1N	-2.14	104.28	110.70

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	709	1PE	OH6-C15-C25-OH5
2	A	701	PGE	O2-C3-C4-O3
2	A	705	PGE	O1-C1-C2-O2
3	A	702	PEG	O1-C1-C2-O2
6	A	709	1PE	OH5-C14-C24-OH4
2	B	603	PGE	O2-C3-C4-O3
2	A	707	PGE	O1-C1-C2-O2
3	A	702	PEG	O2-C3-C4-O4
4	A	706	PG4	O4-C7-C8-O5
6	B	602	1PE	OH5-C14-C24-OH4
2	A	703	PGE	O3-C5-C6-O4
6	B	604	1PE	OH2-C12-C22-OH3
2	A	705	PGE	O3-C5-C6-O4
3	B	601	PEG	O1-C1-C2-O2
2	B	603	PGE	O3-C5-C6-O4
4	A	706	PG4	C4-C3-O2-C2
6	A	709	1PE	C24-C14-OH5-C25
3	B	601	PEG	O2-C3-C4-O4
3	B	606	PEG	O2-C3-C4-O4
2	A	707	PGE	O3-C5-C6-O4
2	A	707	PGE	C1-C2-O2-C3
6	B	602	1PE	C25-C15-OH6-C26
6	B	602	1PE	C16-C26-OH6-C15
6	A	709	1PE	C12-C22-OH3-C23
6	B	602	1PE	C15-C25-OH5-C14
2	A	701	PGE	O3-C5-C6-O4
2	A	705	PGE	C1-C2-O2-C3
5	A	708	NAP	C2B-C1B-N9A-C8A
5	B	605	NAP	C2B-C1B-N9A-C8A
6	B	604	1PE	OH4-C13-C23-OH3
6	B	604	1PE	C23-C13-OH4-C24
2	B	603	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	709	1PE	OH7-C16-C26-OH6
2	A	705	PGE	C3-C4-O3-C5
5	A	708	NAP	C4D-C5D-O5D-PN
5	B	605	NAP	C4D-C5D-O5D-PN
2	A	704	PGE	C6-C5-O3-C4
4	A	706	PG4	C1-C2-O2-C3
5	B	605	NAP	C2B-O2B-P2B-O1X
2	A	705	PGE	C4-C3-O2-C2
2	A	701	PGE	C1-C2-O2-C3
6	B	604	1PE	C12-C22-OH3-C23
2	A	703	PGE	C6-C5-O3-C4
3	B	601	PEG	C4-C3-O2-C2
6	A	709	1PE	C15-C25-OH5-C14
5	A	708	NAP	O4B-C1B-N9A-C8A
6	B	604	1PE	C15-C25-OH5-C14
6	B	602	1PE	C23-C13-OH4-C24
2	A	705	PGE	C6-C5-O3-C4
4	A	706	PG4	O3-C5-C6-O4
2	A	705	PGE	O2-C3-C4-O3
6	B	602	1PE	OH2-C12-C22-OH3
2	A	704	PGE	O2-C3-C4-O3
5	B	605	NAP	O4B-C1B-N9A-C8A
2	A	707	PGE	O2-C3-C4-O3
6	B	602	1PE	OH7-C16-C26-OH6
6	B	604	1PE	OH7-C16-C26-OH6
5	A	708	NAP	C2B-O2B-P2B-O2X
2	A	701	PGE	C4-C3-O2-C2
6	B	602	1PE	C13-C23-OH3-C22
5	A	708	NAP	C2B-C1B-N9A-C4A
5	B	605	NAP	C2B-C1B-N9A-C4A
2	A	704	PGE	C4-C3-O2-C2
4	A	706	PG4	C3-C4-O3-C5
5	A	708	NAP	C3B-C2B-O2B-P2B
6	B	602	1PE	OH6-C15-C25-OH5

There are no ring outliers.

7 monomers are involved in 17 short contacts:

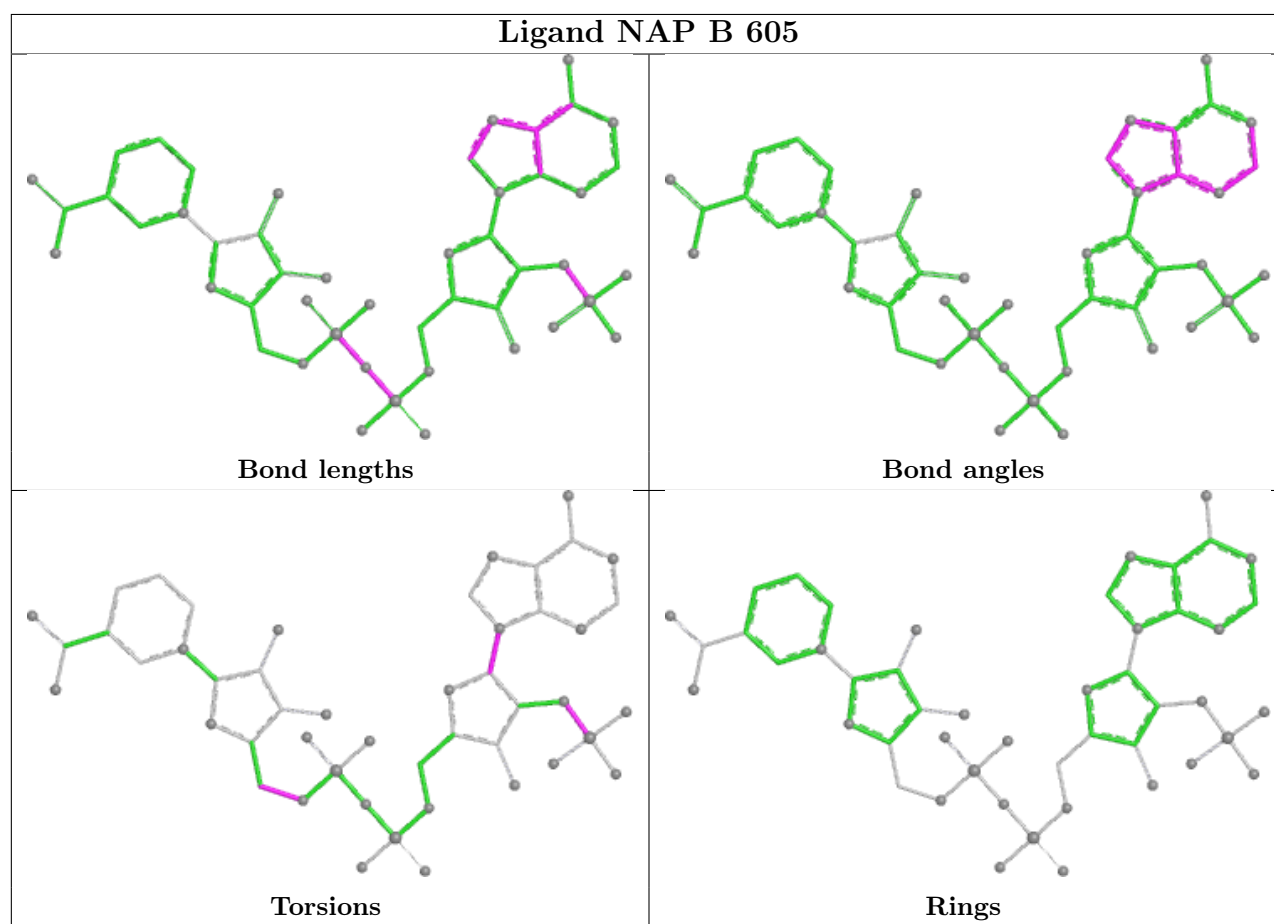
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	604	1PE	1	0
4	A	706	PG4	1	0
5	B	605	NAP	4	0

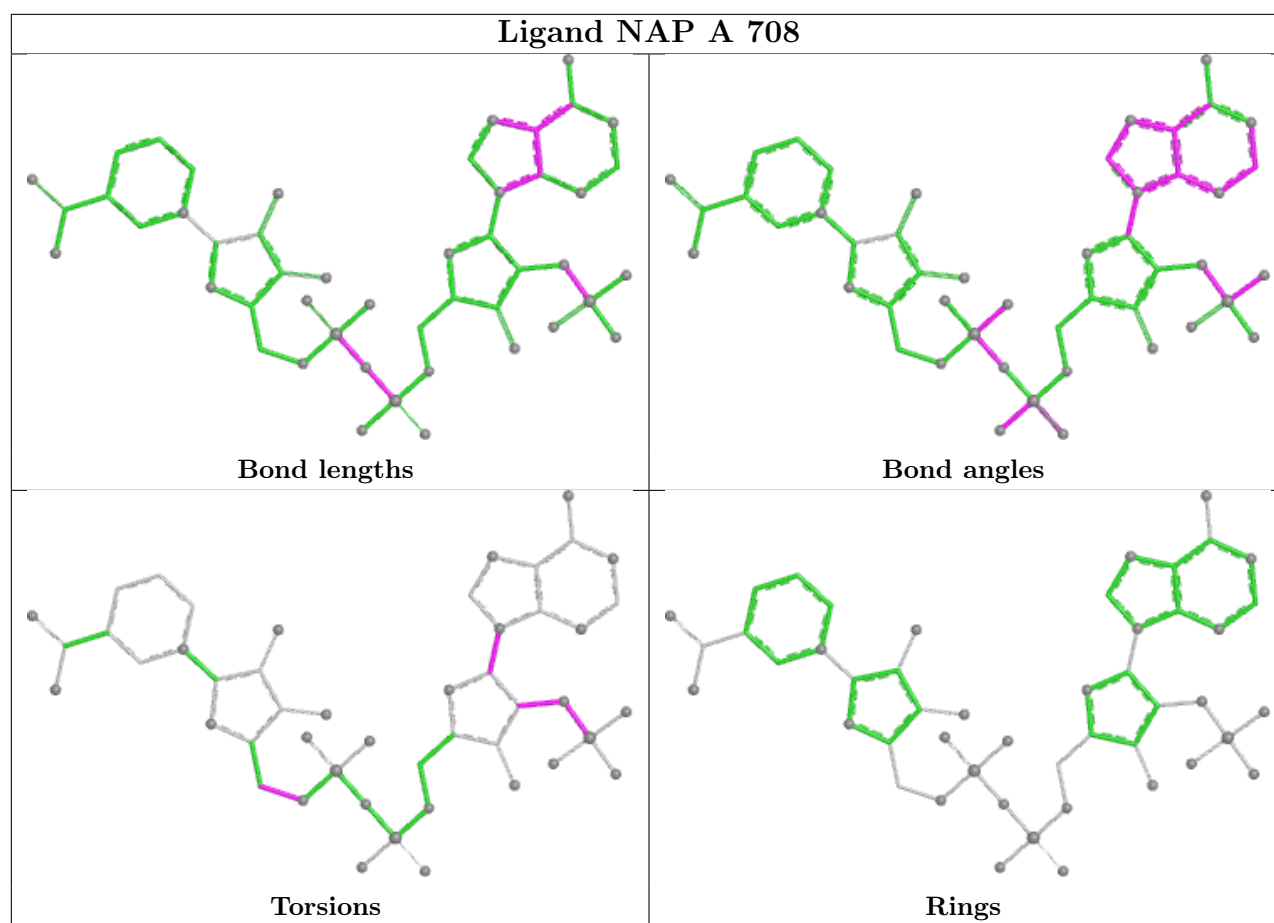
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	PEG	1	0
2	B	603	PGE	5	0
5	A	708	NAP	4	0
2	A	707	PGE	1	0

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	511/521 (98%)	-0.11	13 (2%) 58 54	31, 41, 66, 105	0
1	B	507/521 (97%)	-0.16	16 (3%) 50 46	31, 40, 62, 100	0
All	All	1018/1042 (97%)	-0.13	29 (2%) 55 51	31, 40, 64, 105	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ALA	6.9
1	A	3	LYS	5.7
1	B	5	ALA	5.3
1	B	509	ALA	5.1
1	B	178	THR	4.6
1	B	508	LEU	4.0
1	A	510	GLN	3.8
1	A	2	ARG	3.7
1	B	506	LEU	3.7
1	B	504	GLY	3.5
1	A	509	ALA	3.5
1	B	505	ARG	3.1
1	A	440	HIS	3.1
1	B	352	ARG	3.1
1	B	510	GLN	2.9
1	B	24	LEU	2.9
1	B	28	LEU	2.9
1	A	511	MET	2.8
1	A	4	ALA	2.7
1	A	178	THR	2.7
1	B	370	ARG	2.7
1	A	508	LEU	2.7
1	B	440	HIS	2.6
1	B	349	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	370	ARG	2.5
1	A	504	GLY	2.3
1	A	506	LEU	2.3
1	A	1	HIS	2.2
1	B	6	GLY	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](#)

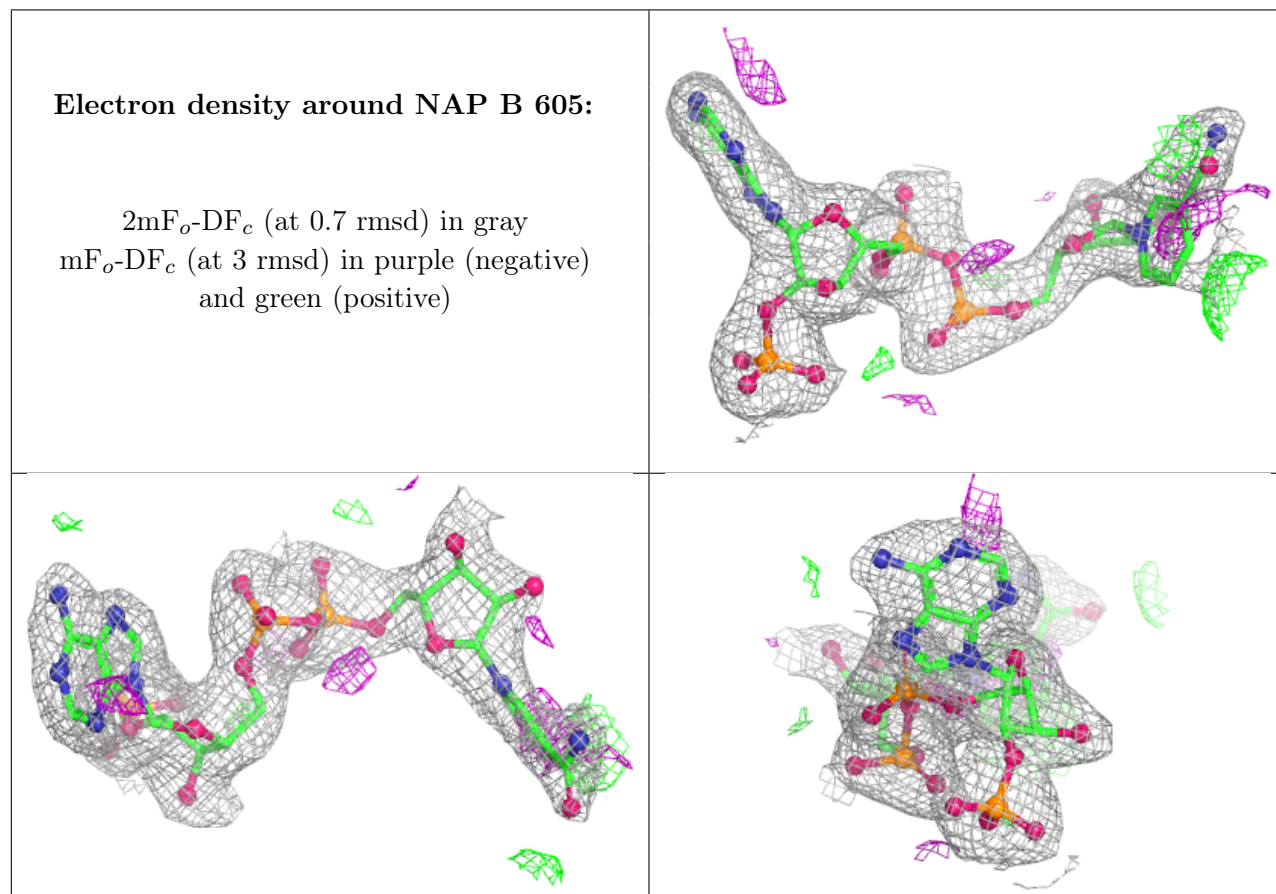
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

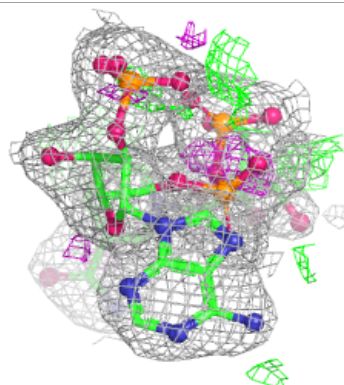
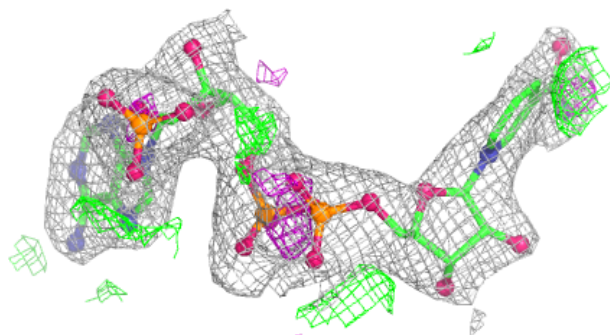
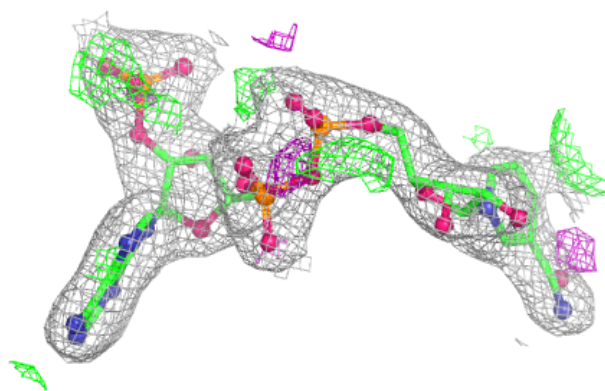
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	1PE	B	602	16/16	0.83	0.27	69,80,89,92	0
3	PEG	B	606	7/7	0.84	0.23	64,67,75,78	0
2	PGE	B	603	10/10	0.84	0.23	82,89,93,95	0
6	1PE	B	604	16/16	0.86	0.20	63,71,75,76	0
2	PGE	A	701	10/10	0.87	0.16	57,65,68,68	0
4	PG4	A	706	13/13	0.87	0.19	52,65,74,75	0
2	PGE	A	704	10/10	0.88	0.18	65,67,68,69	0
3	PEG	B	601	7/7	0.88	0.18	57,58,61,62	0
2	PGE	A	707	10/10	0.88	0.21	66,79,86,87	0
2	PGE	A	705	10/10	0.90	0.17	57,63,74,76	0
6	1PE	A	709	16/16	0.90	0.20	58,75,79,81	0
2	PGE	A	703	10/10	0.91	0.17	61,66,69,69	0
3	PEG	A	702	7/7	0.94	0.15	55,61,69,71	0
5	NAP	B	605	48/48	0.96	0.09	35,48,76,80	0
5	NAP	A	708	48/48	0.96	0.09	34,47,65,69	0
7	SO4	B	607	5/5	0.96	0.11	46,49,56,59	0
7	SO4	A	711	5/5	0.97	0.11	46,49,53,59	0
7	SO4	A	710	5/5	0.98	0.07	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)



6.5 Other polymers [i](#)

There are no such residues in this entry.