wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2021 – 05:03 am GMT

PDB ID	:	7AK8
Title	:	Structure of Salmonella TacT1 toxin bound to TacA1 antitoxin C-terminal peptide
Authors	:	Grabe, G.J.; Morgan, R.M.L.; Helaine, S.; Hare, S.A.
Deposited on	:	2020-09-30
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

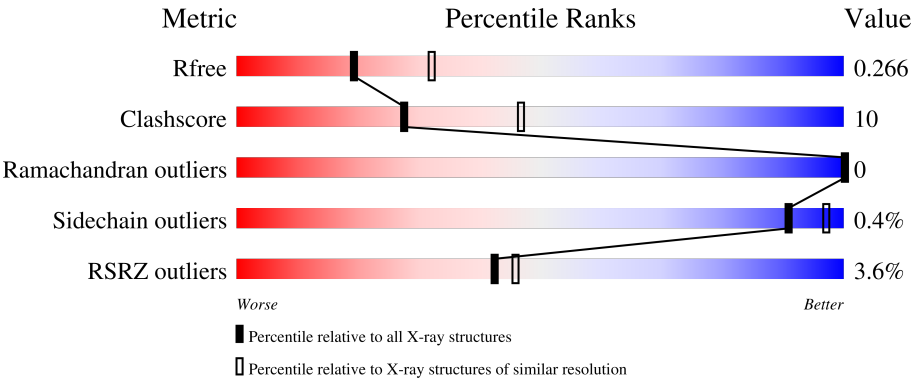
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	164	80% 10% 9%
1	B	164	5% 76% 15% 8%
1	C	164	2% 69% 22% 9%
1	D	164	2% 73% 18% 9%
1	E	164	4% 74% 17% 9%

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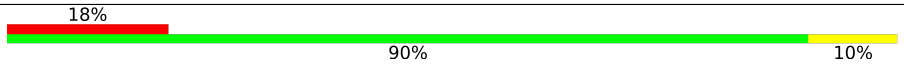
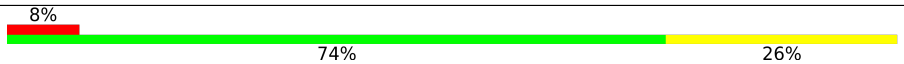
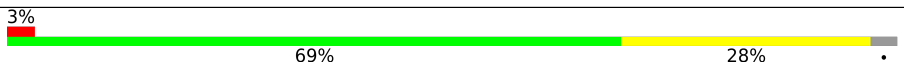
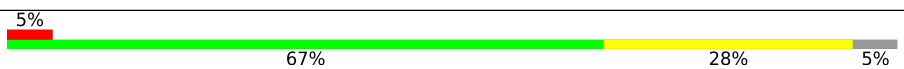
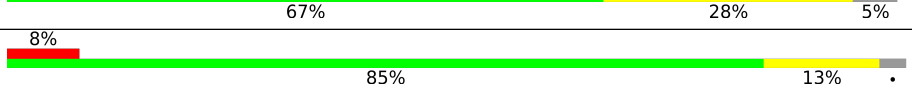
Mol	Chain	Length	Quality of chain
1	F	164	
2	G	39	
2	H	39	
2	I	39	
2	J	39	
2	K	39	
2	L	39	

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
4	GOL	B	202	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9384 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 GCN5 family acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1158	741	209	205	3			
1	B	151	Total	C	N	O	S	0	0	0
			1167	746	211	207	3			
1	C	150	Total	C	N	O	S	0	0	0
			1162	743	210	206	3			
1	D	150	Total	C	N	O	S	0	0	0
			1162	743	210	206	3			
1	E	149	Total	C	N	O	S	0	0	0
			1158	741	209	205	3			
1	F	149	Total	C	N	O	S	0	0	0
			1152	737	208	204	3			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP A0A0D6I609
A	-1	GLY	-	expression tag	UNP A0A0D6I609
A	0	SER	-	expression tag	UNP A0A0D6I609
A	1	VAL	-	expression tag	UNP A0A0D6I609
A	140	PHE	TYR	engineered mutation	UNP A0A0D6I609
B	-2	MET	-	initiating methionine	UNP A0A0D6I609
B	-1	GLY	-	expression tag	UNP A0A0D6I609
B	0	SER	-	expression tag	UNP A0A0D6I609
B	1	VAL	-	expression tag	UNP A0A0D6I609
B	140	PHE	TYR	engineered mutation	UNP A0A0D6I609
C	-2	MET	-	initiating methionine	UNP A0A0D6I609
C	-1	GLY	-	expression tag	UNP A0A0D6I609
C	0	SER	-	expression tag	UNP A0A0D6I609
C	1	VAL	-	expression tag	UNP A0A0D6I609
C	140	PHE	TYR	engineered mutation	UNP A0A0D6I609
D	-2	MET	-	initiating methionine	UNP A0A0D6I609
D	-1	GLY	-	expression tag	UNP A0A0D6I609

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP A0A0D6I609
D	1	VAL	-	expression tag	UNP A0A0D6I609
D	140	PHE	TYR	engineered mutation	UNP A0A0D6I609
E	-2	MET	-	initiating methionine	UNP A0A0D6I609
E	-1	GLY	-	expression tag	UNP A0A0D6I609
E	0	SER	-	expression tag	UNP A0A0D6I609
E	1	VAL	-	expression tag	UNP A0A0D6I609
E	140	PHE	TYR	engineered mutation	UNP A0A0D6I609
F	-2	MET	-	initiating methionine	UNP A0A0D6I609
F	-1	GLY	-	expression tag	UNP A0A0D6I609
F	0	SER	-	expression tag	UNP A0A0D6I609
F	1	VAL	-	expression tag	UNP A0A0D6I609
F	140	PHE	TYR	engineered mutation	UNP A0A0D6I609

- Molecule 2 is a protein called TacA1 antitoxin peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	38	Total	C	N	O	0	0	0
			318	205	49	64			
2	H	39	Total	C	N	O	0	0	0
			322	207	50	65			
2	I	39	Total	C	N	O	0	0	0
			322	207	50	65			
2	J	38	Total	C	N	O	0	0	0
			314	202	49	63			
2	K	37	Total	C	N	O	0	0	0
			310	200	48	62			
2	L	38	Total	C	N	O	0	0	0
			314	202	49	63			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	50	GLY	-	expression tag	UNP A0A2J0RDY6
G	51	SER	-	expression tag	UNP A0A2J0RDY6
H	50	GLY	-	expression tag	UNP A0A2J0RDY6
H	51	SER	-	expression tag	UNP A0A2J0RDY6
I	50	GLY	-	expression tag	UNP A0A2J0RDY6
I	51	SER	-	expression tag	UNP A0A2J0RDY6
J	50	GLY	-	expression tag	UNP A0A2J0RDY6
J	51	SER	-	expression tag	UNP A0A2J0RDY6
K	50	GLY	-	expression tag	UNP A0A2J0RDY6

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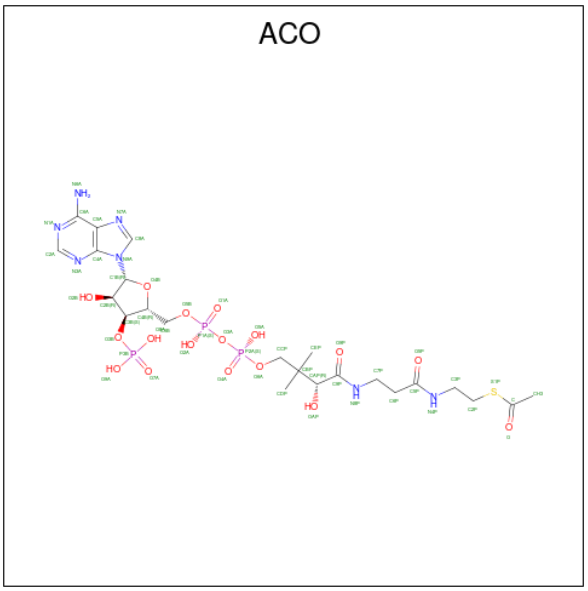
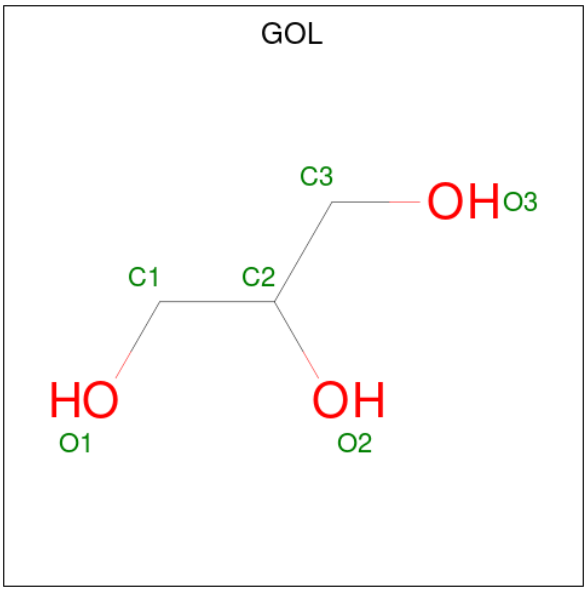
Chain	Residue	Modelled	Actual	Comment	Reference
K	51	SER	-	expression tag	UNP A0A2J0RDY6
L	50	GLY	-	expression tag	UNP A0A2J0RDY6
L	51	SER	-	expression tag	UNP A0A2J0RDY6

- Molecule 3 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	F	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	36	Total O 36 36	0	0
5	B	26	Total O 26 26	0	0
5	C	35	Total O 35 35	0	0
5	D	21	Total O 21 21	0	0
5	E	25	Total O 25 25	0	0
5	F	28	Total O 28 28	0	0
5	G	11	Total O 11 11	0	0
5	H	5	Total O 5 5	0	0
5	I	7	Total O 7 7	0	0
5	J	4	Total O 4 4	0	0
5	K	9	Total O 9 9	0	0

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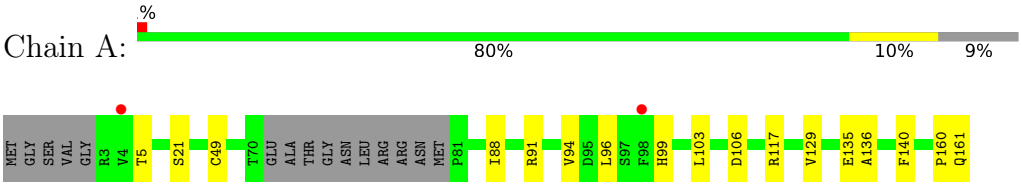
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	6	Total O 6 6	0	0

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.

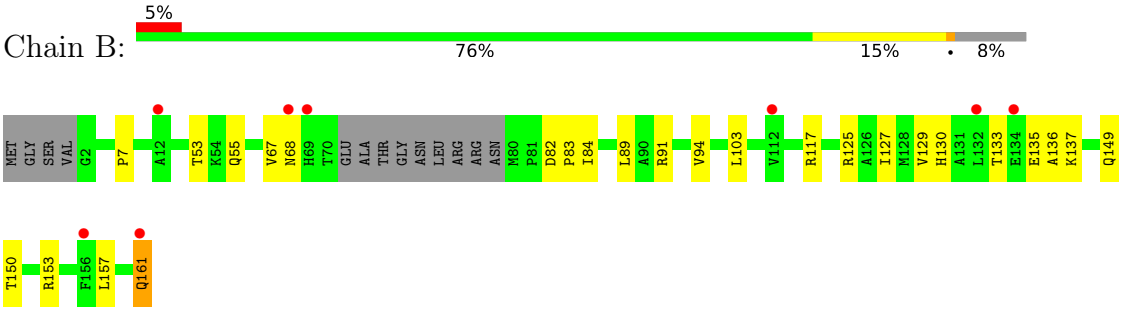
• Molecule 1: GCN5 family acetyltransferase

Chain A:



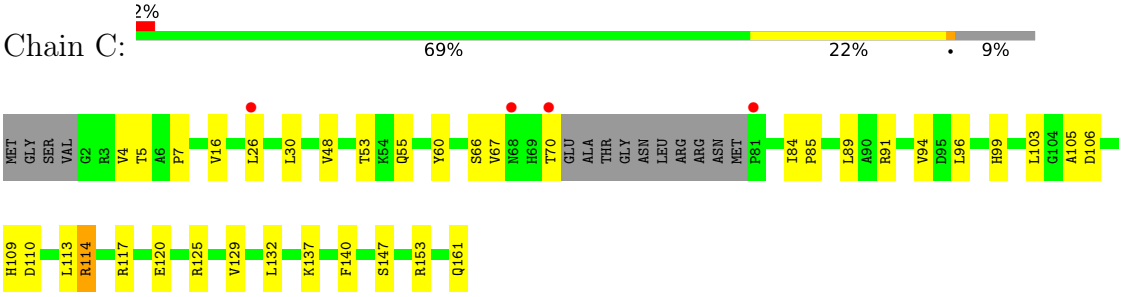
• Molecule 1: GCN5 family acetyltransferase

Chain B:



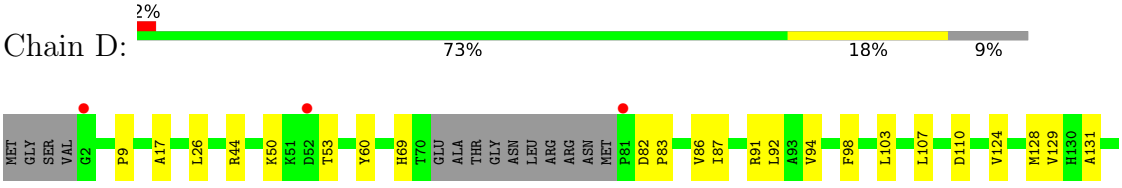
• Molecule 1: GCN5 family acetyltransferase

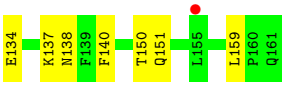
Chain C:



• Molecule 1: GCN5 family acetyltransferase

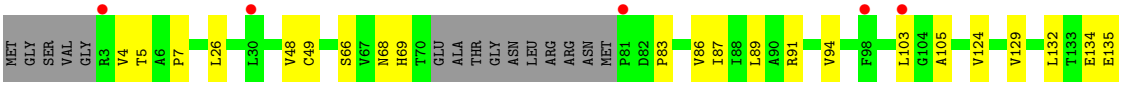
Chain D:





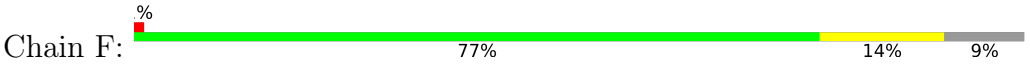
• Molecule 1: GCN5 family acetyltransferase

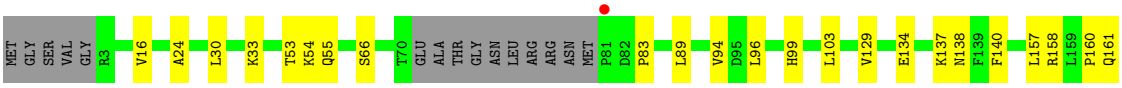
Chain E:



• Molecule 1: GCN5 family acetyltransferase

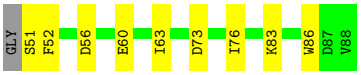
Chain F:





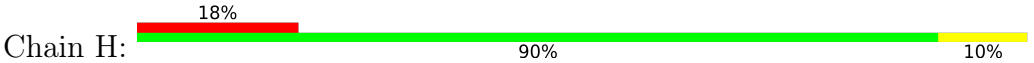
• Molecule 2: TacA1 antitoxin peptide

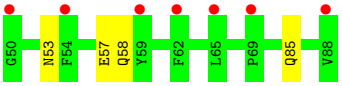
Chain G:



• Molecule 2: TacA1 antitoxin peptide

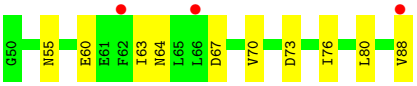
Chain H:





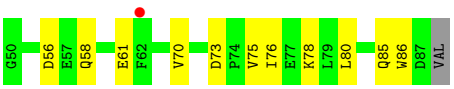
• Molecule 2: TacA1 antitoxin peptide

Chain I:



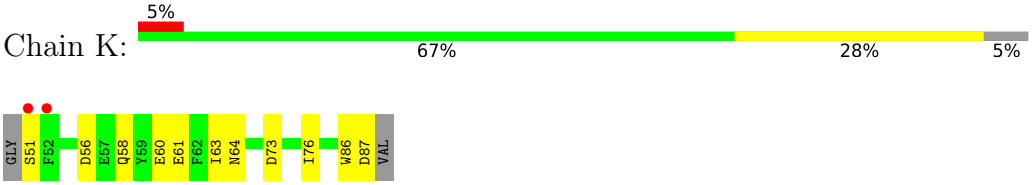
• Molecule 2: TacA1 antitoxin peptide

Chain J:



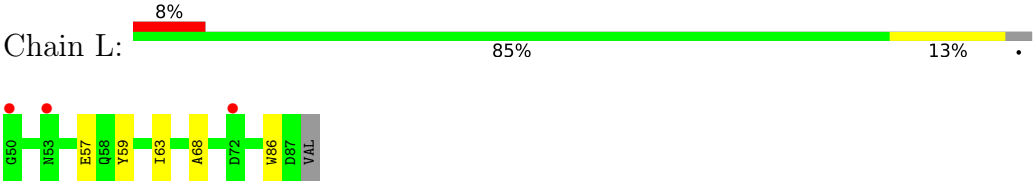
• Molecule 2: TacA1 antitoxin peptide

Chain K:



• Molecule 2: TacA1 antitoxin peptide

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	96.14Å 96.14Å 120.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.85 – 2.50 48.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.85-2.50) 100.0 (48.85-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.214 , 0.268 0.215 , 0.266	Depositor DCC
R_{free} test set	2094 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l 0.178 for h,-h-k,-l 0.054 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9384	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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: ACO, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.64	0/1182	0.77	0/1597
1	B	1.62	1/1191 (0.1%)	0.88	2/1610 (0.1%)
1	C	0.64	0/1186	0.81	1/1602 (0.1%)
1	D	0.66	0/1186	0.78	0/1602
1	E	0.64	0/1182	0.77	0/1597
1	F	0.63	0/1176	0.77	0/1590
2	G	0.65	0/326	0.76	0/443
2	H	0.63	0/330	0.78	0/448
2	I	0.67	0/330	0.83	0/448
2	J	0.71	0/322	0.75	0/438
2	K	0.67	0/318	0.77	0/433
2	L	0.67	0/322	0.81	0/438
All	All	0.84	1/9051 (0.0%)	0.79	3/12246 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	GLN	CA-CB	50.69	2.65	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	161	GLN	CA-CB-CG	-11.26	88.63	113.40
1	B	91	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	C	114	ARG	CG-CD-NE	-5.14	101.00	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1158	0	1176	18	0
1	B	1167	0	1180	27	0
1	C	1162	0	1179	34	0
1	D	1162	0	1179	30	0
1	E	1158	0	1176	23	0
1	F	1152	0	1160	24	0
2	G	318	0	296	7	0
2	H	322	0	299	4	0
2	I	322	0	299	8	0
2	J	314	0	290	14	0
2	K	310	0	287	10	0
2	L	314	0	290	5	0
3	A	51	0	34	1	0
3	B	51	0	34	3	0
3	C	51	0	34	3	0
3	D	51	0	34	3	0
3	E	51	0	34	4	0
3	F	51	0	34	1	0
4	B	6	0	8	4	0
5	A	36	0	0	4	0
5	B	26	0	0	1	0
5	C	35	0	0	1	0
5	D	21	0	0	3	0
5	E	25	0	0	1	0
5	F	28	0	0	3	0
5	G	11	0	0	1	0
5	H	5	0	0	0	0
5	I	7	0	0	0	0
5	J	4	0	0	0	0
5	K	9	0	0	0	0
5	L	6	0	0	1	0
All	All	9384	0	9023	181	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 10.

The worst 5 of 181 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:D:50:LYS:O	1:D:53:THR:HG22	1.28	1.27
1:E:150:THR:HG21	2:K:58:GLN:HA	1.44	0.99
1:C:60:TYR:OH	1:C:114:ARG:NH1	1.96	0.98
1:D:50:LYS:HB2	1:D:53:THR:HG21	1.62	0.81
1:A:21:SER:O	1:A:99:HIS:HE1	1.65	0.80

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	145/164 (88%)	144 (99%)	1 (1%)	0	100	100
1	B	147/164 (90%)	142 (97%)	5 (3%)	0	100	100
1	C	146/164 (89%)	144 (99%)	2 (1%)	0	100	100
1	D	146/164 (89%)	144 (99%)	2 (1%)	0	100	100
1	E	145/164 (88%)	144 (99%)	1 (1%)	0	100	100
1	F	145/164 (88%)	144 (99%)	1 (1%)	0	100	100
2	G	36/39 (92%)	36 (100%)	0	0	100	100
2	H	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
2	I	37/39 (95%)	37 (100%)	0	0	100	100
2	J	36/39 (92%)	36 (100%)	0	0	100	100
2	K	35/39 (90%)	34 (97%)	1 (3%)	0	100	100
2	L	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
All	All	1091/1218 (90%)	1076 (99%)	15 (1%)	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	122/133 (92%)	122 (100%)	0	100 100
1	B	122/133 (92%)	122 (100%)	0	100 100
1	C	122/133 (92%)	121 (99%)	1 (1%)	81 93
1	D	122/133 (92%)	122 (100%)	0	100 100
1	E	122/133 (92%)	121 (99%)	1 (1%)	81 93
1	F	120/133 (90%)	120 (100%)	0	100 100
2	G	35/35 (100%)	33 (94%)	2 (6%)	20 39
2	H	35/35 (100%)	35 (100%)	0	100 100
2	I	35/35 (100%)	35 (100%)	0	100 100
2	J	34/35 (97%)	34 (100%)	0	100 100
2	K	34/35 (97%)	34 (100%)	0	100 100
2	L	34/35 (97%)	34 (100%)	0	100 100
All	All	937/1008 (93%)	933 (100%)	4 (0%)	91 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	66	SER
1	E	134	GLU
2	G	56	ASP
2	G	83	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	69	HIS
1	E	151	GLN
2	G	53	ASN
2	H	53	ASN
2	K	53	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

7 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

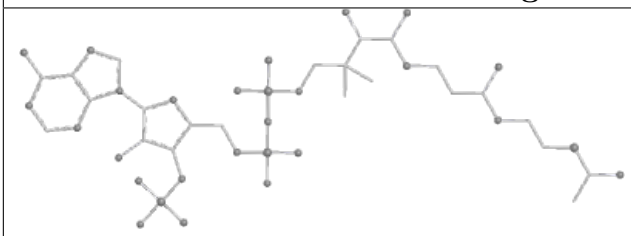
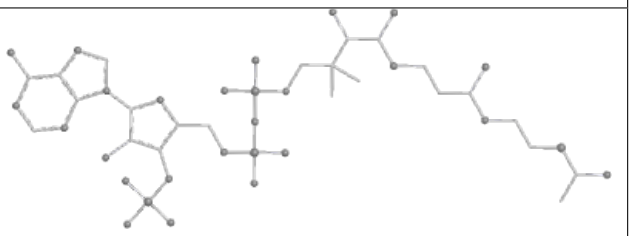
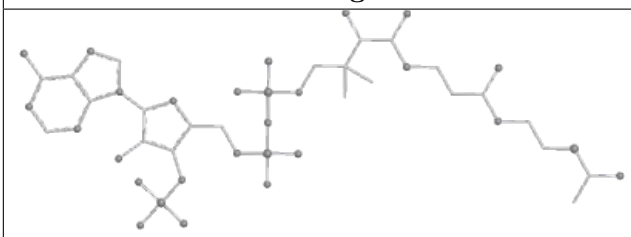
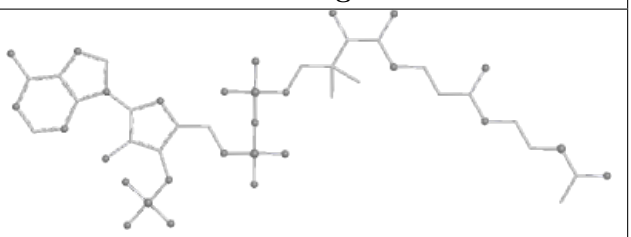
There are no chirality outliers.

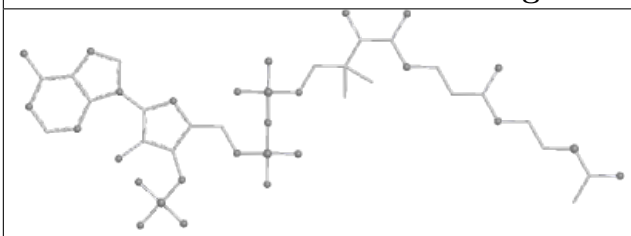
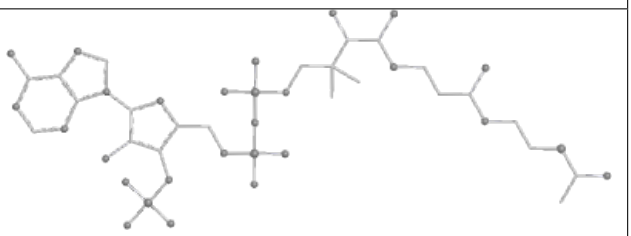
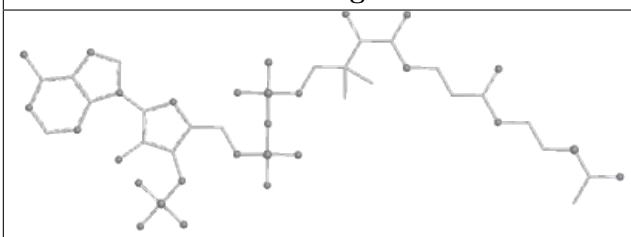
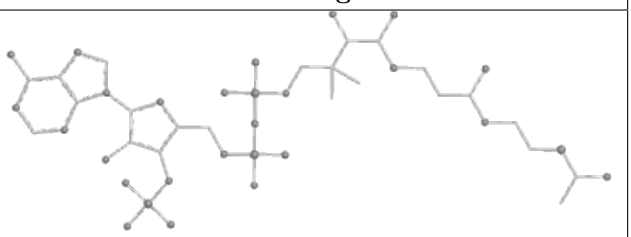
There are no torsion outliers.

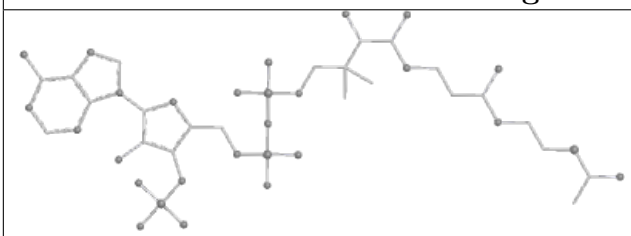
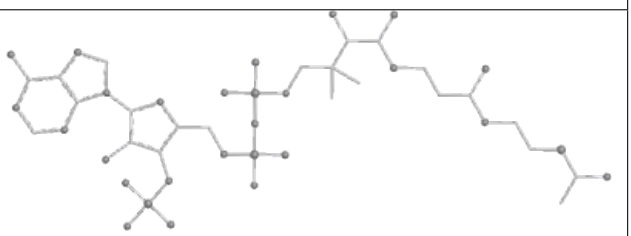
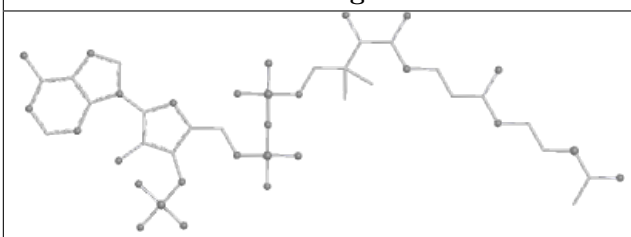
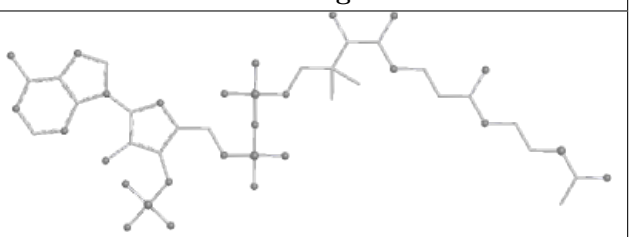
There are no ring outliers.

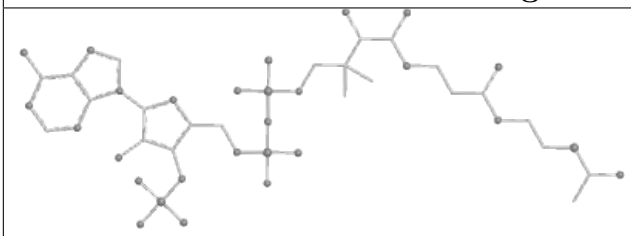
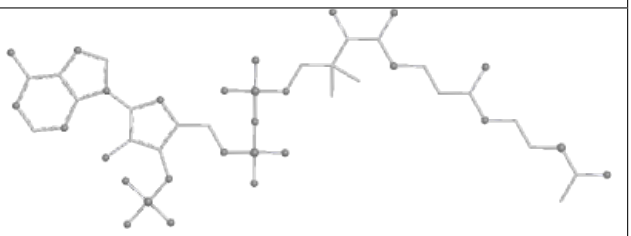
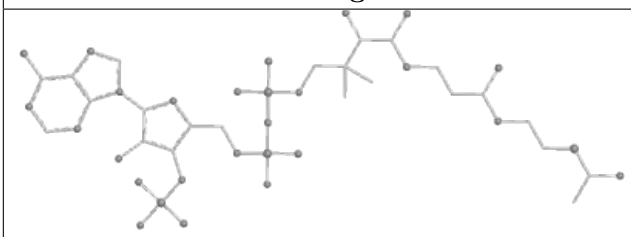
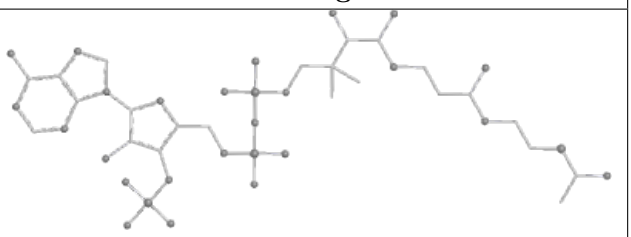
No monomer is involved in short contacts.

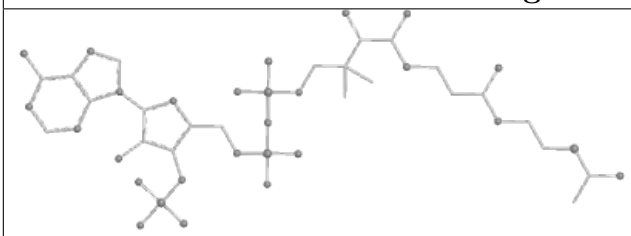
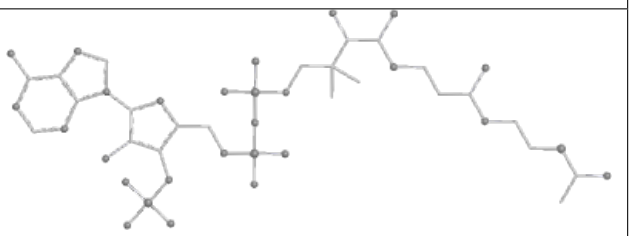
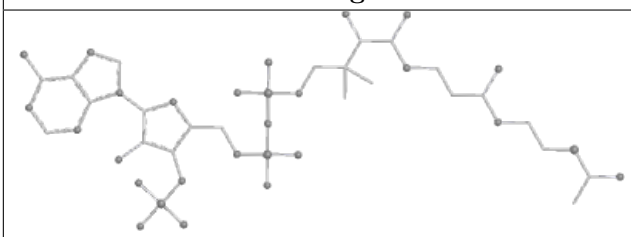
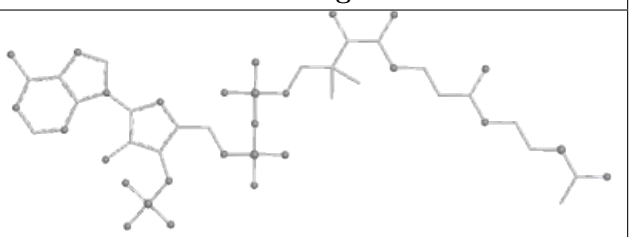
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

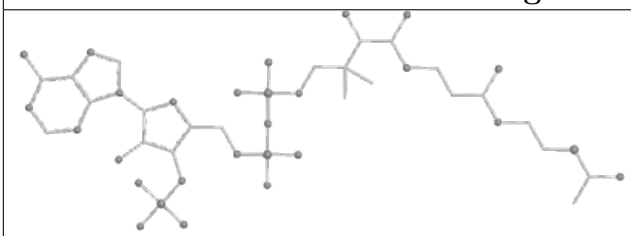
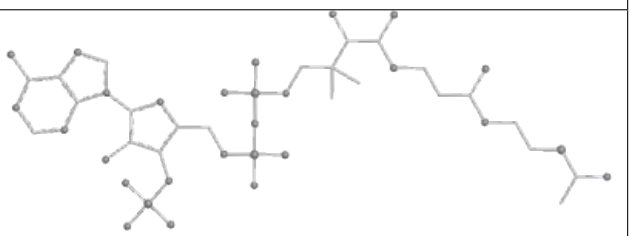
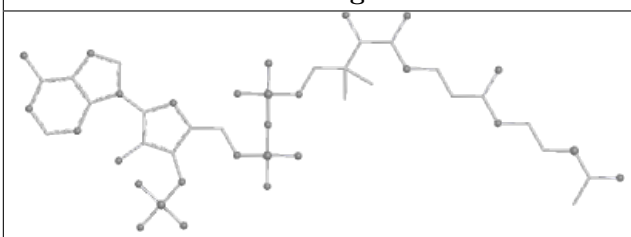
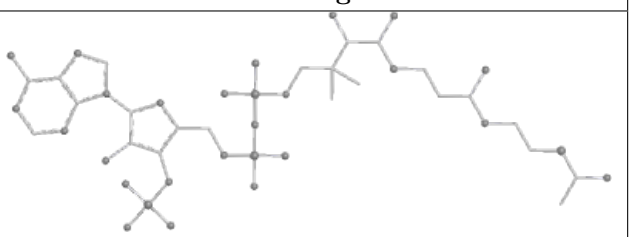
Ligand ACO A 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACO B 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACO C 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACO D 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACO E 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACO F 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 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	149/164 (90%)	0.25	2 (1%) 77 79	47, 65, 99, 120	0
1	B	151/164 (92%)	0.46	8 (5%) 26 28	46, 74, 126, 161	0
1	C	150/164 (91%)	0.35	4 (2%) 54 58	47, 70, 124, 160	0
1	D	150/164 (91%)	0.42	4 (2%) 54 58	51, 75, 113, 147	0
1	E	149/164 (90%)	0.38	6 (4%) 38 41	51, 72, 107, 128	0
1	F	149/164 (90%)	0.27	1 (0%) 87 89	52, 70, 108, 151	0
2	G	38/39 (97%)	0.10	0 100 100	56, 78, 92, 97	0
2	H	39/39 (100%)	0.78	7 (17%) 1 1	67, 106, 128, 133	0
2	I	39/39 (100%)	0.66	3 (7%) 13 13	75, 99, 129, 141	0
2	J	38/39 (97%)	0.33	1 (2%) 56 59	60, 91, 106, 106	0
2	K	37/39 (94%)	0.28	2 (5%) 25 27	65, 81, 94, 107	0
2	L	38/39 (97%)	0.67	3 (7%) 12 12	70, 94, 115, 122	0
All	All	1127/1218 (92%)	0.38	41 (3%) 42 46	46, 76, 118, 161	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	81	PRO	9.6
2	I	88	VAL	7.3
1	D	2	GLY	5.8
1	D	81	PRO	5.4
1	F	81	PRO	4.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

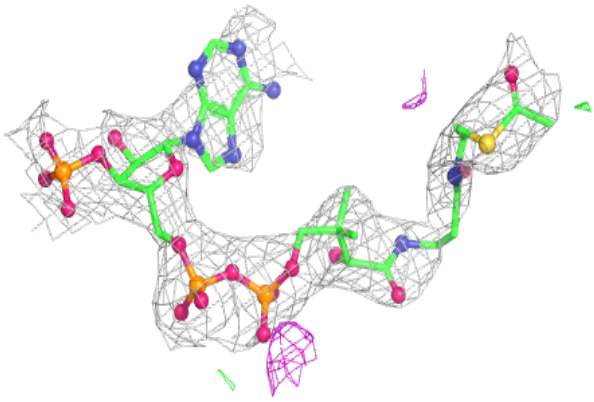
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

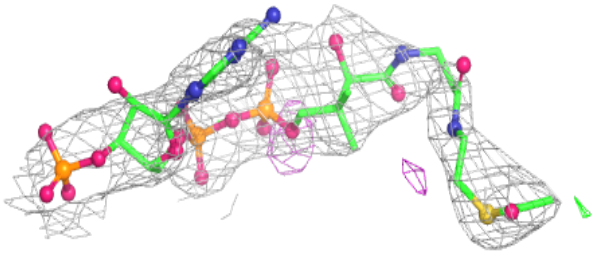
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACO	B	201	51/51	0.86	0.26	96,121,152,156	0
3	ACO	C	201	51/51	0.88	0.18	96,112,128,131	0
4	GOL	B	202	6/6	0.92	0.21	60,65,66,68	0
3	ACO	D	201	51/51	0.93	0.15	78,94,109,122	0
3	ACO	A	201	51/51	0.95	0.12	71,86,94,103	0
3	ACO	F	201	51/51	0.96	0.15	59,74,90,102	0
3	ACO	E	201	51/51	0.96	0.13	67,85,104,110	0

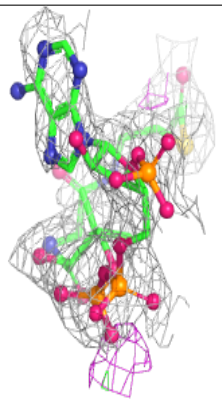
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO B 201:

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

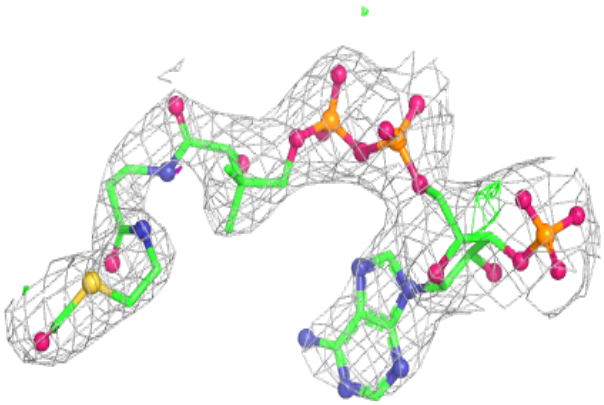


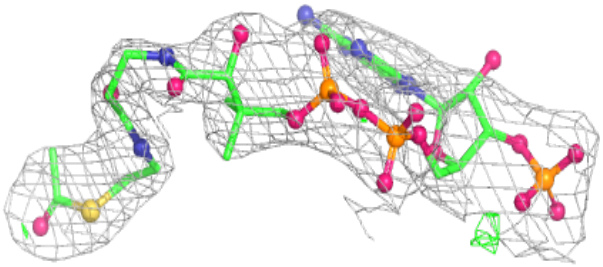


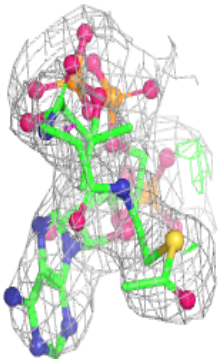


Electron density around ACO C 201:

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

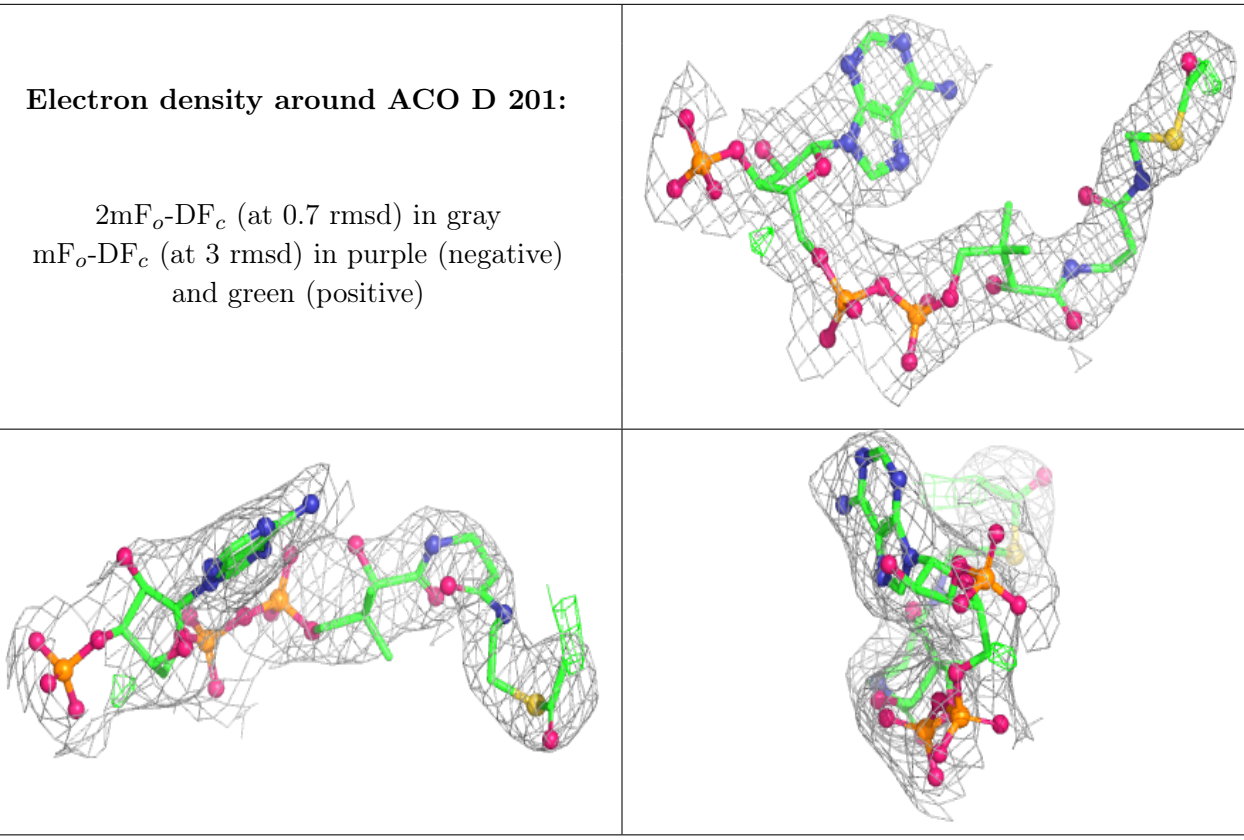






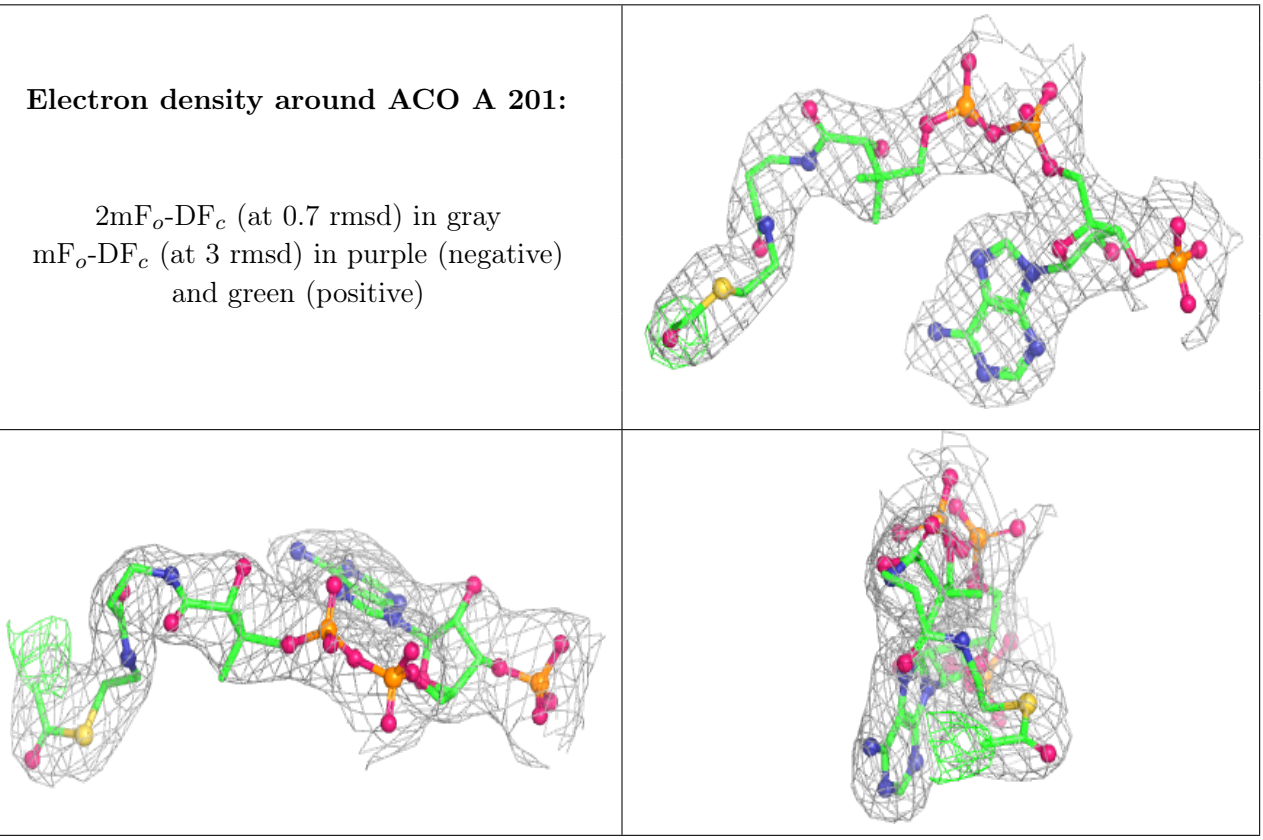
Electron density around ACO D 201:

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



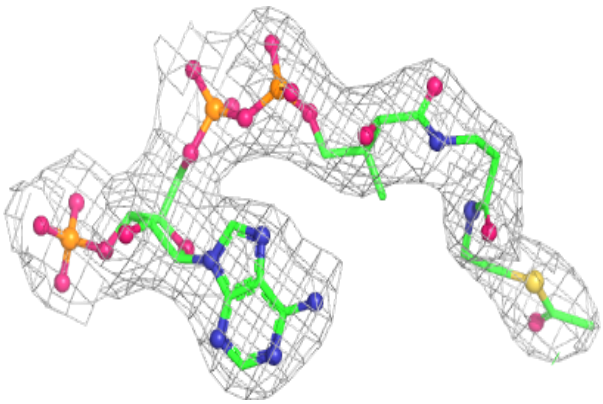
Electron density around ACO A 201:

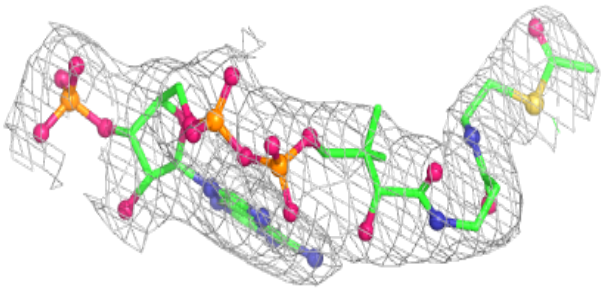
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

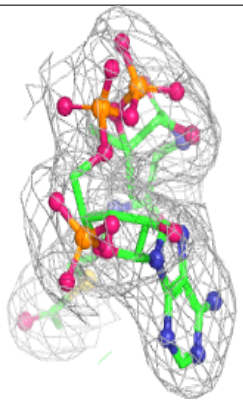


Electron density around ACO F 201:

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

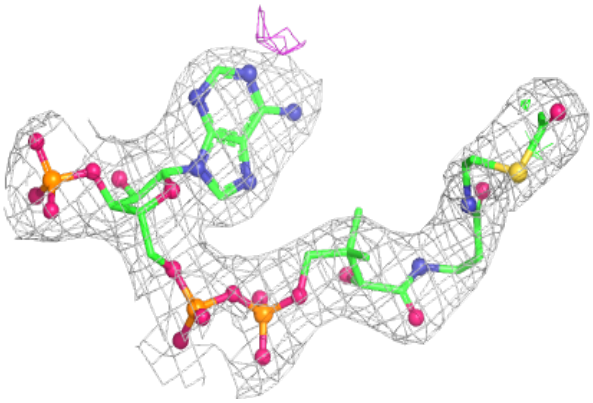


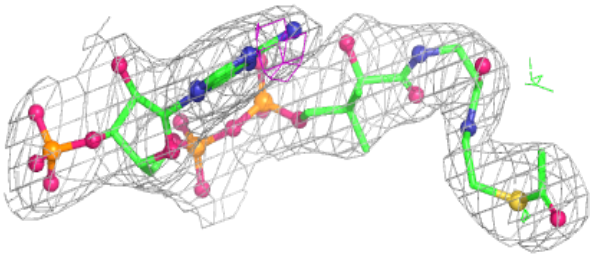


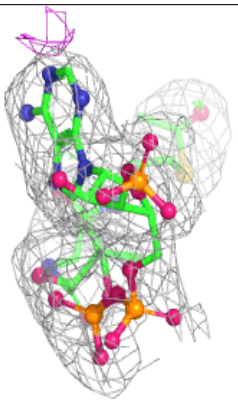


Electron density around ACO E 201:

$2mF_o$-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.