



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 10:17 AM BST

PDB ID : 6YJV
Title : Crystal structure of unliganded MGAT5 (alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase V) luminal domain with a Lys329-Ile345 loop truncation, in complex with UDP-2-deoxy-2-fluoroglucose and biantennary pentasaccharide M592
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Deposited on : 2020-04-04
Resolution : 1.70 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 : 2.13.1
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) : 2.13.1

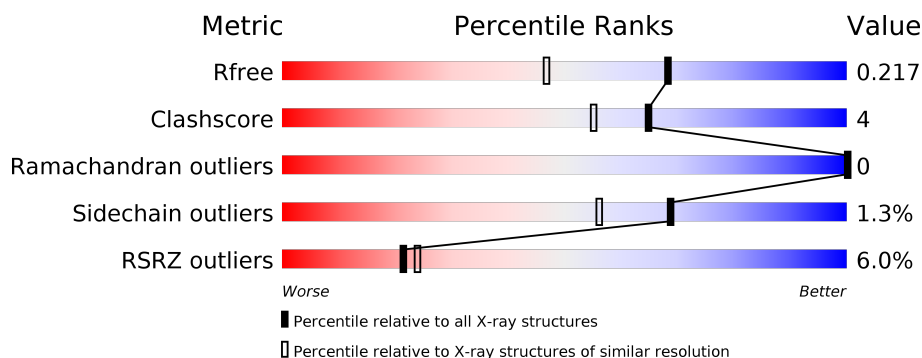
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	AAA	515	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>••</div> </div> </div>
1	BBB	515	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div> </div>
2	A	4	<div> <div></div> <div> <div>75%</div> <div>25%</div> </div> </div>
3	B	2	<div> <div></div> <div>100%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17115 atoms, of which 8281 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 Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyl transferase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	504	Total	C	H	N	O	S	202	2	0
			8183	2633	4096	700	727	27			
1	BBB	502	Total	C	H	N	O	S	202	0	0
			8114	2612	4060	696	720	26			

There are 32 discrepancies between the modelled and reference sequences:

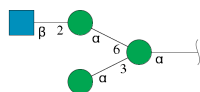
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	LYS	deletion	UNP Q09328
AAA	?	-	LYS	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	?	-	GLY	deletion	UNP Q09328
AAA	?	-	ASN	deletion	UNP Q09328
AAA	?	-	ARG	deletion	UNP Q09328
AAA	?	-	SER	deletion	UNP Q09328
AAA	?	-	GLY	deletion	UNP Q09328
AAA	?	-	CYS	deletion	UNP Q09328
AAA	?	-	PRO	deletion	UNP Q09328
AAA	?	-	THR	deletion	UNP Q09328
AAA	?	-	VAL	deletion	UNP Q09328
AAA	330	GLY	ASP	conflict	UNP Q09328
AAA	331	GLY	ARG	conflict	UNP Q09328
AAA	332	GLY	ILE	conflict	UNP Q09328
BBB	?	-	LYS	deletion	UNP Q09328
BBB	?	-	LYS	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	?	-	GLY	deletion	UNP Q09328
BBB	?	-	ASN	deletion	UNP Q09328
BBB	?	-	ARG	deletion	UNP Q09328
BBB	?	-	SER	deletion	UNP Q09328

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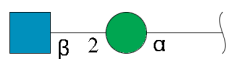
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	?	-	GLY	deletion	UNP Q09328
BBB	?	-	CYS	deletion	UNP Q09328
BBB	?	-	PRO	deletion	UNP Q09328
BBB	?	-	THR	deletion	UNP Q09328
BBB	?	-	VAL	deletion	UNP Q09328
BBB	330	GLY	ASP	conflict	UNP Q09328
BBB	331	GLY	ARG	conflict	UNP Q09328
BBB	332	GLY	ILE	conflict	UNP Q09328

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose.



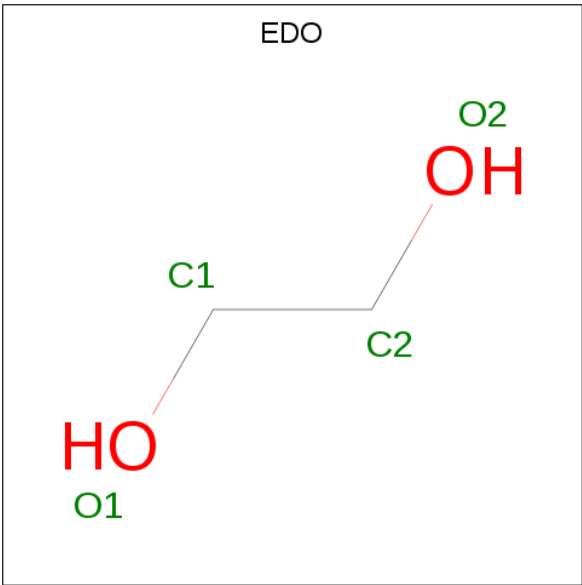
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	4	Total	C	H	N	O	13	0	0
			93	26	45	1	21			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose.



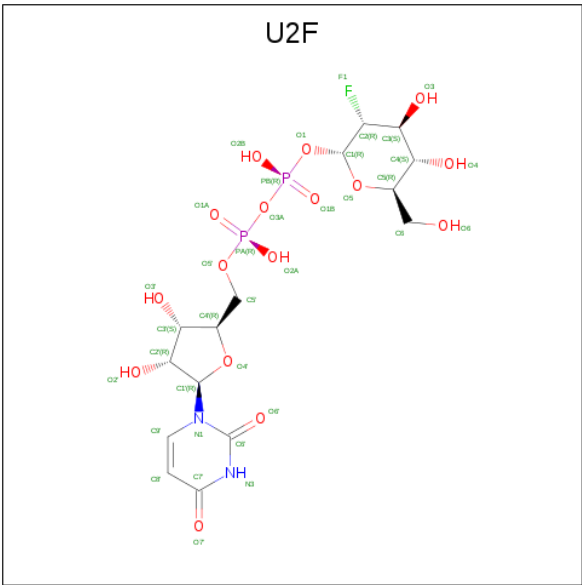
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	2	Total	C	H	N	O	6	0	0
			52	14	26	1	11			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
4	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 5 is URIDINE-5'-DIPHOSPHATE-2-DEOXY-2-FLUORO-ALPHA-D-GLUCOSE (three-letter code: U2F) (formula: C₁₅H₂₃FN₂O₁₆P₂) (labeled as "Ligand of Interest" by author).



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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	BBB	1	Total	C	F	H	N	O	P	5	0
			57	15	1	21	2	16	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	BBB	1	Total	O	S	0	0
			5	4	1		
6	BBB	1	Total	O	S	0	0
			5	4	1		
6	BBB	1	Total	O	S	0	0
			5	4	1		

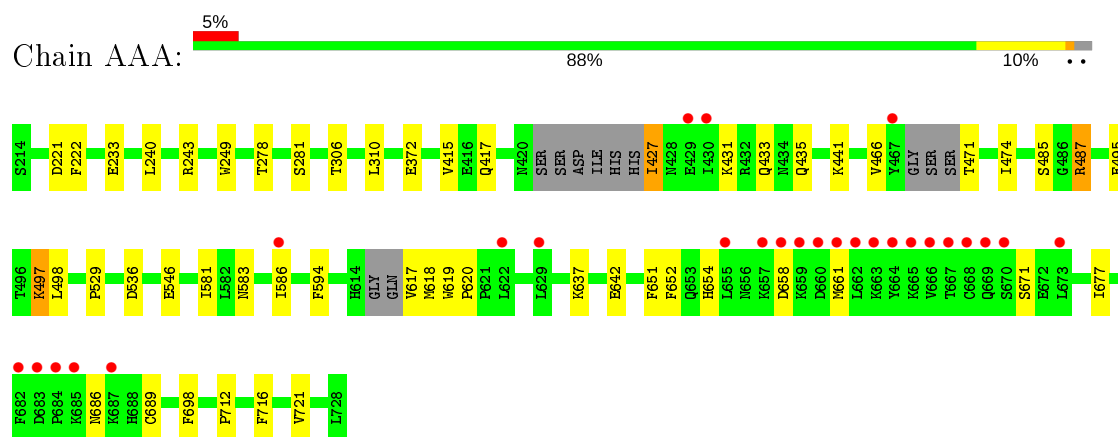
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	252	Total	O	0	0
			252	252		
7	BBB	257	Total	O	0	0
			257	257		

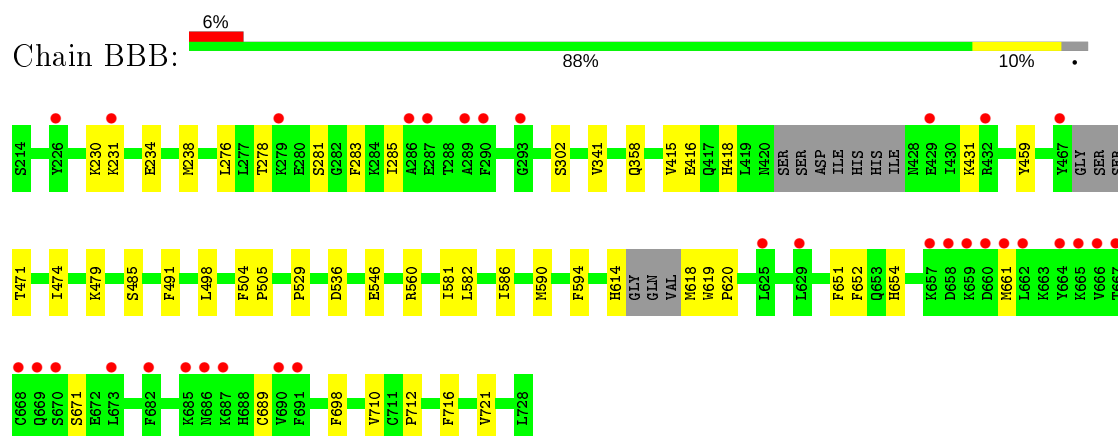
3 Residue-property plots [i](#)

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.

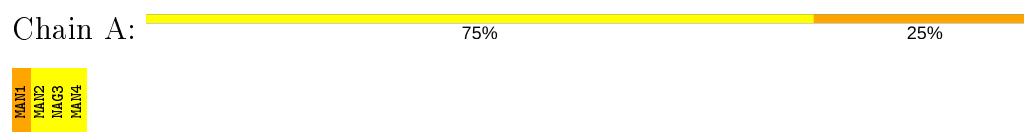
- Molecule 1: Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A



- Molecule 1: Alpha-1,6-mannosylglycoprotein 6-beta-N-acetylglucosaminyltransferase A



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose

Chain B:

100%

HAH1
HAH2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.52Å 69.21Å 90.65Å 108.42° 92.25° 106.54°	Depositor
Resolution (Å)	44.14 – 1.70 44.14 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.7 (44.14-1.70) 94.7 (44.14-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.175 , 0.211 0.184 , 0.217	Depositor DCC
R_{free} test set	3663 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	17115	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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: SO4, U2F, MAN, NAG, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AAA	0.69	0/4191	0.81	0/5658
1	BBB	0.69	0/4158	0.81	0/5613
All	All	0.69	0/8349	0.81	0/11271

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	4087	4096	4071	35	0
1	BBB	4054	4060	4034	33	0
2	A	48	45	42	2	0
3	B	26	26	24	0	0
4	AAA	4	6	6	2	0
4	BBB	4	6	6	0	0
5	AAA	36	21	21	0	0
5	BBB	36	21	21	0	0
6	AAA	15	0	0	1	0
6	BBB	15	0	0	0	0
7	AAA	252	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BBB	257	0	0	5	0
All	All	8834	8281	8225	67	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 4.

All (67) 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:BBB:283:PHE:CZ	1:BBB:341:VAL:HG21	1.95	1.02
1:BBB:614:HIS:O	7:BBB:901:HOH:O	2.02	0.78
1:BBB:654:HIS:HE1	7:BBB:1117:HOH:O	1.76	0.68
1:AAA:617:VAL:HG11	7:AAA:1033:HOH:O	1.94	0.67
1:BBB:416:GLU:OE1	1:BBB:418:HIS:HE1	1.80	0.65
1:AAA:471:THR:O	1:AAA:471:THR:HG22	1.98	0.63
1:BBB:283:PHE:CE2	1:BBB:341:VAL:HG21	2.33	0.62
1:AAA:435:GLN:NE2	1:AAA:495:GLU:HG3	2.18	0.59
1:AAA:415:VAL:O	4:AAA:805:EDO:O2	2.21	0.58
1:AAA:671:SER:HA	1:AAA:689:CYS:O	2.04	0.57
1:AAA:637:LYS:NZ	7:AAA:904:HOH:O	2.37	0.57
1:BBB:661:MET:HE3	1:BBB:710:VAL:HG21	1.86	0.57
1:BBB:671:SER:HA	1:BBB:689:CYS:O	2.04	0.57
1:BBB:230:LYS:HB2	1:BBB:231:LYS:HE3	1.86	0.56
7:AAA:923:HOH:O	2:A:1:MAN:H1	2.05	0.56
1:BBB:560:ARG:HD2	7:BBB:1049:HOH:O	2.07	0.55
1:AAA:661:MET:HA	1:AAA:661:MET:CE	2.37	0.54
1:BBB:498:LEU:HD13	1:BBB:581:ILE:HD13	1.91	0.53
1:BBB:661:MET:CE	1:BBB:710:VAL:HG21	2.40	0.51
1:AAA:240:LEU:HD21	1:BBB:491:PHE:CE2	2.44	0.51
1:BBB:618:MET:HG2	7:BBB:1103:HOH:O	2.09	0.51
1:AAA:661:MET:HA	1:AAA:661:MET:HE2	1.91	0.51
1:AAA:487:ARG:NE	6:AAA:809:SO4:O2	2.33	0.51
1:AAA:498:LEU:HD13	1:AAA:581:ILE:HD13	1.92	0.50
1:AAA:529:PRO:HB2	1:AAA:546:GLU:HB3	1.94	0.50
1:BBB:341:VAL:HG23	7:BBB:979:HOH:O	2.11	0.49
1:BBB:238:MET:HG2	1:BBB:302:SER:OG	2.14	0.48
1:BBB:471:THR:HB	1:BBB:474:ILE:HD12	1.96	0.48
1:AAA:471:THR:O	1:AAA:471:THR:CG2	2.61	0.48
1:BBB:529:PRO:HB2	1:BBB:546:GLU:HB3	1.96	0.48
1:BBB:431:LYS:HG3	1:BBB:586:ILE:HD13	1.96	0.48
1:BBB:283:PHE:CZ	1:BBB:341:VAL:CG2	2.84	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:435:GLN:HE22	1:AAA:495:GLU:CG	2.27	0.47
1:BBB:234:GLU:O	1:BBB:238:MET:HG3	2.15	0.47
1:BBB:651:PHE:HB2	1:BBB:712:PRO:HB2	1.97	0.47
1:BBB:230:LYS:HB2	1:BBB:231:LYS:CE	2.45	0.47
1:AAA:278:THR:OG1	1:AAA:281:SER:HB3	2.15	0.46
1:AAA:686:ASN:N	1:AAA:686:ASN:HD22	2.13	0.46
1:BBB:278:THR:OG1	1:BBB:281:SER:HB3	2.16	0.46
1:AAA:618:MET:CE	1:AAA:654:HIS:HE1	2.27	0.46
1:BBB:283:PHE:HZ	1:BBB:341:VAL:HG21	1.68	0.46
1:AAA:435:GLN:HE22	1:AAA:495:GLU:HG3	1.81	0.46
1:BBB:459:TYR:HB3	1:BBB:582:LEU:HD11	1.99	0.45
1:AAA:233:GLU:HG2	1:BBB:479:LYS:HD3	1.99	0.45
1:BBB:619:TRP:HA	1:BBB:620:PRO:C	2.37	0.45
1:BBB:716:PHE:HB2	1:BBB:721:VAL:HA	1.99	0.44
1:AAA:417:GLN:HE21	4:AAA:805:EDO:H21	1.82	0.44
1:AAA:716:PHE:HB2	1:AAA:721:VAL:HA	1.99	0.44
1:BBB:652:PHE:HB3	1:BBB:698:PHE:CD1	2.51	0.44
1:AAA:652:PHE:HB3	1:AAA:698:PHE:CD1	2.52	0.43
1:BBB:504:PHE:CG	1:BBB:505:PRO:HA	2.53	0.43
1:AAA:372:GLU:HB3	1:AAA:677:ILE:HG21	2.00	0.43
1:AAA:619:TRP:HA	1:AAA:620:PRO:C	2.39	0.43
1:AAA:485:SER:HB3	1:BBB:485:SER:OG	2.18	0.43
1:AAA:427:ILE:HD11	1:AAA:586:ILE:HG22	2.00	0.42
7:AAA:923:HOH:O	2:A:1:MAN:C1	2.65	0.42
1:AAA:433:GLN:HA	1:AAA:497:LYS:HG3	2.02	0.42
1:AAA:583:ASN:ND2	7:AAA:915:HOH:O	2.49	0.42
1:AAA:222:PHE:HE1	1:AAA:306:THR:HG23	1.84	0.42
1:AAA:651:PHE:HB2	1:AAA:712:PRO:HB2	2.03	0.41
1:AAA:249:TRP:HB3	1:AAA:310:LEU:HD11	2.02	0.41
1:BBB:276:LEU:HD12	1:BBB:285:ILE:HD13	2.03	0.41
1:AAA:466:VAL:HG11	1:AAA:474:ILE:HD11	2.03	0.41
1:BBB:415:VAL:HG23	1:BBB:594:PHE:HB3	2.02	0.41
1:AAA:686:ASN:N	1:AAA:686:ASN:ND2	2.69	0.40
1:AAA:415:VAL:HG23	1:AAA:594:PHE:HB3	2.02	0.40
1:AAA:243:ARG:NH1	7:AAA:924:HOH:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	AAA	498/515 (97%)	491 (99%)	7 (1%)	0	100	100
1	BBB	494/515 (96%)	485 (98%)	9 (2%)	0	100	100
All	All	992/1030 (96%)	976 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	AAA	449/456 (98%)	440 (98%)	9 (2%)	55	38
1	BBB	444/456 (97%)	441 (99%)	3 (1%)	84	77
All	All	893/912 (98%)	881 (99%)	12 (1%)	69	56

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

Mol	Chain	Res	Type
1	AAA	221	ASP
1	AAA	427	ILE
1	AAA	431	LYS
1	AAA	441	LYS
1	AAA	487	ARG
1	AAA	497	LYS
1	AAA	536	ASP
1	AAA	642	GLU

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Mol	Chain	Res	Type
1	AAA	658	ASP
1	BBB	358	GLN
1	BBB	536	ASP
1	BBB	590	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

6 monosaccharides 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	MAN	A	1	2	12,12,12	0.72	0	17,17,17	1.09	1 (5%)
2	MAN	A	2	2	11,11,12	0.77	0	15,15,17	1.08	1 (6%)
2	NAG	A	3	2	14,14,15	1.01	1 (7%)	17,19,21	0.94	0
2	MAN	A	4	2	11,11,12	0.70	0	15,15,17	1.74	4 (26%)
3	MAN	B	1	3	12,12,12	1.00	0	17,17,17	1.23	2 (11%)
3	NAG	B	2	3	14,14,15	0.54	0	17,19,21	1.27	2 (11%)

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	MAN	A	1	2	-	0/2/22/22	0/1/1/1
2	MAN	A	2	2	-	2/2/19/22	0/1/1/1
2	NAG	A	3	2	-	1/6/23/26	0/1/1/1
2	MAN	A	4	2	-	0/2/19/22	0/1/1/1
3	MAN	B	1	3	-	2/2/22/22	0/1/1/1
3	NAG	B	2	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	NAG	O5-C1	-2.25	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4	MAN	C1-C2-C3	4.35	115.01	109.67
3	B	2	NAG	O5-C1-C2	-2.96	106.61	111.29
2	A	2	MAN	C1-O5-C5	2.74	115.91	112.19
2	A	4	MAN	C3-C4-C5	2.46	114.63	110.24
2	A	1	MAN	C6-C5-C4	-2.37	107.46	113.00
2	A	4	MAN	C2-C3-C4	2.24	114.78	110.89
3	B	1	MAN	O1-C1-C2	2.21	115.26	109.03
3	B	1	MAN	O5-C5-C4	2.15	113.60	109.69
2	A	4	MAN	O4-C4-C3	-2.03	105.66	110.35
3	B	2	NAG	C2-N2-C7	2.01	125.76	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	MAN	O5-C5-C6-O6
2	A	2	MAN	C4-C5-C6-O6
3	B	1	MAN	O5-C5-C6-O6
3	B	1	MAN	C4-C5-C6-O6
3	B	2	NAG	C3-C2-N2-C7
2	A	3	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	MAN	2	0

5.6 Ligand geometry

10 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	$\# Z > 2$
6	SO4	BBB	806	-	4,4,4	0.30	0	6,6,6	0.12	0
6	SO4	BBB	807	-	4,4,4	0.35	0	6,6,6	0.06	0
6	SO4	BBB	805	-	4,4,4	0.33	0	6,6,6	0.15	0
6	SO4	AAA	809	-	4,4,4	0.41	0	6,6,6	0.15	0
5	U2F	BBB	804	-	31,38,38	1.23	4 (12%)	39,58,58	1.90	8 (20%)
4	EDO	BBB	803	-	3,3,3	0.16	0	2,2,2	0.26	0
6	SO4	AAA	807	-	4,4,4	0.37	0	6,6,6	0.14	0
6	SO4	AAA	808	-	4,4,4	0.34	0	6,6,6	0.13	0
4	EDO	AAA	805	-	3,3,3	0.13	0	2,2,2	0.15	0
5	U2F	AAA	806	-	31,38,38	0.99	1 (3%)	39,58,58	1.56	3 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	U2F	AAA	806	-	-	4/20/59/59	0/3/3/3
5	U2F	BBB	804	-	-	5/20/59/59	0/3/3/3
4	EDO	AAA	805	-	-	0/1/1/1	-
4	EDO	BBB	803	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AAA	806	U2F	C2-C1	-4.02	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	BBB	804	U2F	C2-C3	3.18	1.55	1.52
5	BBB	804	U2F	C2-C1	2.99	1.55	1.52
5	BBB	804	U2F	O4'-C1'	2.54	1.44	1.41
5	BBB	804	U2F	C9'-C8'	2.14	1.42	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	BBB	804	U2F	F1-C2-C1	6.00	114.30	107.57
5	AAA	806	U2F	F1-C2-C3	5.82	114.02	108.85
5	BBB	804	U2F	O4'-C1'-C2'	-5.40	99.03	106.93
5	AAA	806	U2F	O5-C1-O1	4.36	117.07	111.36
5	BBB	804	U2F	F1-C2-C3	3.81	112.23	108.85
5	BBB	804	U2F	O5-C1-O1	3.69	116.19	111.36
5	BBB	804	U2F	O5-C5-C6	3.00	113.91	106.44
5	BBB	804	U2F	O6-C6-C5	2.43	119.62	111.29
5	AAA	806	U2F	C1-C2-C3	-2.37	107.12	110.60
5	BBB	804	U2F	C3-C4-C5	2.05	113.90	110.24
5	BBB	804	U2F	C9'-N1-C6'	-2.04	117.95	121.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

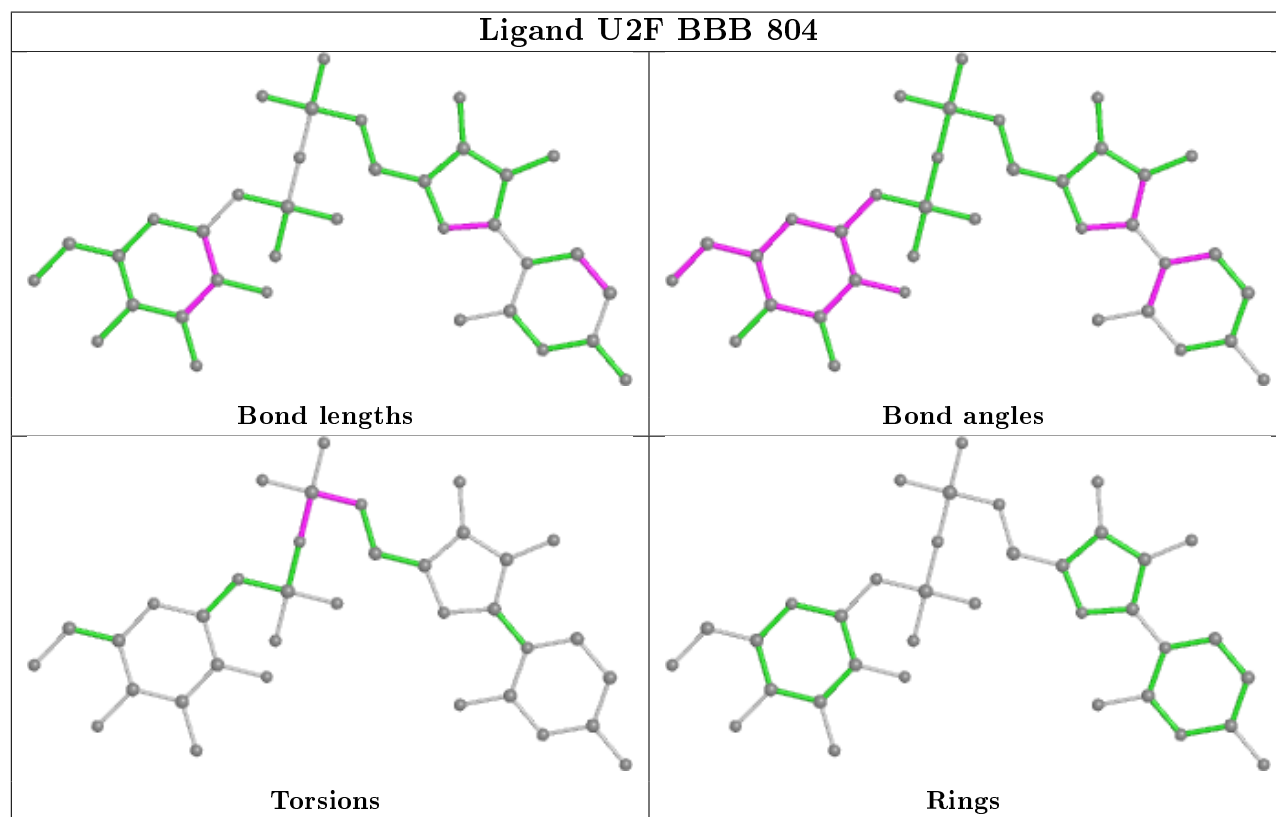
Mol	Chain	Res	Type	Atoms
5	BBB	804	U2F	C5'-O5'-PA-O3A
5	BBB	804	U2F	C5'-O5'-PA-O2A
5	AAA	806	U2F	PA-O3A-PB-O1B
5	AAA	806	U2F	O4'-C4'-C5'-O5'
5	BBB	804	U2F	PB-O3A-PA-O2A
5	BBB	804	U2F	C5'-O5'-PA-O1A
5	AAA	806	U2F	PA-O3A-PB-O2B
5	AAA	806	U2F	C3'-C4'-C5'-O5'
4	BBB	803	EDO	O1-C1-C2-O2
5	BBB	804	U2F	PB-O3A-PA-O1A

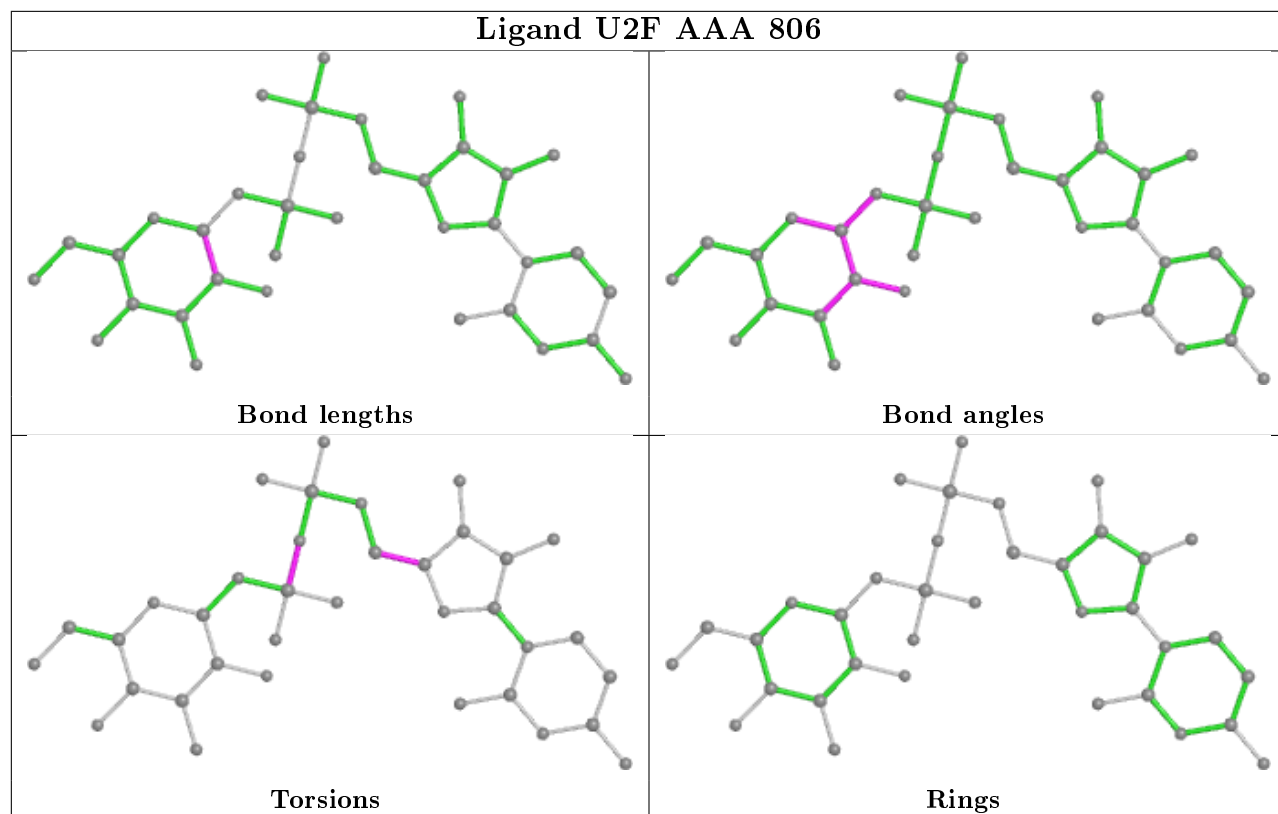
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	809	SO4	1	0
4	AAA	805	EDO	2	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	AAA	504/515 (97%)	0.12	27 (5%)	25 28	28, 42, 74, 110	0
1	BBB	502/515 (97%)	0.18	33 (6%)	18 20	27, 42, 81, 102	0
All	All	1006/1030 (97%)	0.15	60 (5%)	21 24	27, 42, 77, 110	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	666	VAL	8.1
1	AAA	662	LEU	8.0
1	BBB	662	LEU	7.2
1	BBB	666	VAL	5.8
1	BBB	685	LYS	5.3
1	BBB	669	GLN	5.2
1	BBB	667	THR	5.2
1	BBB	665	LYS	5.1
1	BBB	659	LYS	5.0
1	BBB	290	PHE	4.9
1	BBB	668	CYS	4.7
1	AAA	660	ASP	4.6
1	BBB	658	ASP	4.5
1	AAA	665	LYS	4.5
1	AAA	669	GLN	4.5
1	BBB	286	ALA	4.4
1	AAA	668	CYS	4.4
1	BBB	691	PHE	4.3
1	BBB	682	PHE	4.3
1	AAA	467	TYR	4.3
1	AAA	659	LYS	4.1
1	BBB	661	MET	3.9
1	BBB	226	TYR	3.9
1	BBB	293	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	AAA	664	TYR	3.7
1	BBB	670	SER	3.6
1	BBB	664	TYR	3.6
1	AAA	658	ASP	3.5
1	BBB	686	ASN	3.0
1	AAA	661	MET	3.0
1	AAA	670	SER	3.0
1	AAA	673	LEU	3.0
1	AAA	667	THR	2.9
1	AAA	682	PHE	2.8
1	BBB	429	GLU	2.8
1	AAA	657	LYS	2.8
1	AAA	655	LEU	2.7
1	BBB	289	ALA	2.7
1	BBB	657	LYS	2.7
1	BBB	231	LYS	2.7
1	AAA	430	ILE	2.6
1	AAA	586	ILE	2.6
1	AAA	685	LYS	2.6
1	AAA	683	ASP	2.6
1	BBB	673	LEU	2.6
1	BBB	432	ARG	2.5
1	AAA	622	LEU	2.5
1	BBB	467	TYR	2.5
1	BBB	687	LYS	2.5
1	AAA	687	LYS	2.5
1	AAA	429	GLU	2.4
1	BBB	287	GLU	2.4
1	AAA	629	LEU	2.3
1	BBB	629	LEU	2.2
1	BBB	279	LYS	2.2
1	BBB	690	VAL	2.1
1	AAA	684	PRO	2.1
1	BBB	625	LEU	2.1
1	AAA	663	LYS	2.1
1	BBB	660	ASP	2.1

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

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	MAN	A	4	11/12	0.84	0.17	85,92,95,100	4
3	MAN	B	1	12/12	0.94	0.08	34,41,48,49	3
2	MAN	A	1	12/12	0.94	0.11	38,72,91,98	3
2	MAN	A	2	11/12	0.97	0.07	33,37,46,46	3
3	NAG	B	2	14/15	0.97	0.06	28,30,36,38	3
2	NAG	A	3	14/15	0.98	0.09	29,32,34,34	3

6.4 Ligands

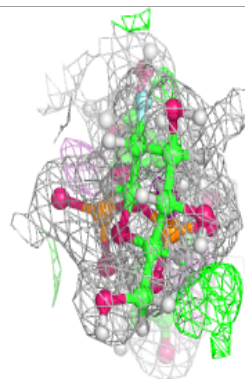
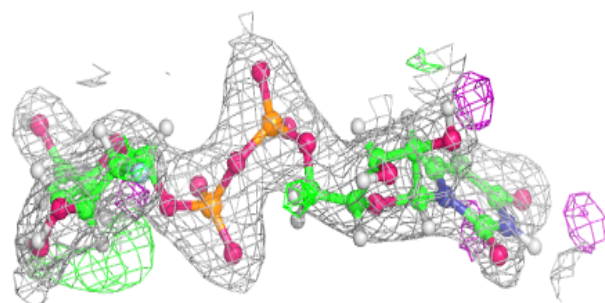
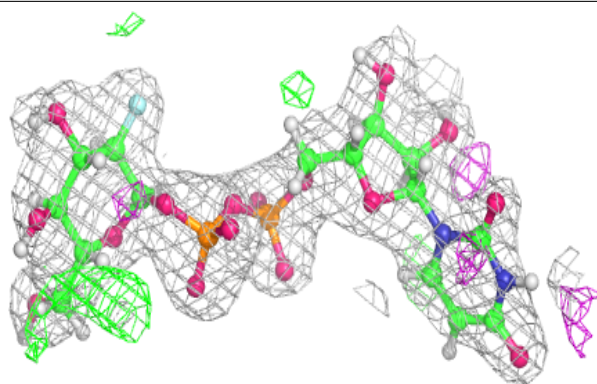
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	BBB	807	5/5	0.81	0.18	127,131,139,142	0
6	SO4	BBB	805	5/5	0.85	0.13	72,74,81,82	5
6	SO4	AAA	807	5/5	0.88	0.13	55,59,65,67	5
4	EDO	BBB	803	4/4	0.91	0.36	50,69,73,73	1
6	SO4	AAA	808	5/5	0.93	0.10	53,57,60,65	5
6	SO4	AAA	809	5/5	0.95	0.09	64,65,67,70	5
6	SO4	BBB	806	5/5	0.95	0.17	62,62,63,66	5
4	EDO	AAA	805	4/4	0.95	0.09	59,65,67,67	1
5	U2F	BBB	804	36/36	0.96	0.10	36,48,55,60	5
5	U2F	AAA	806	36/36	0.98	0.08	33,47,59,60	5

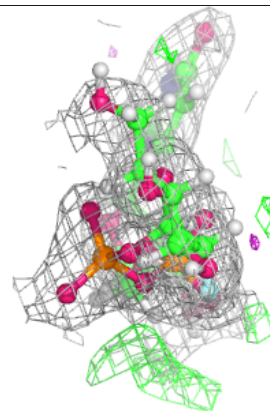
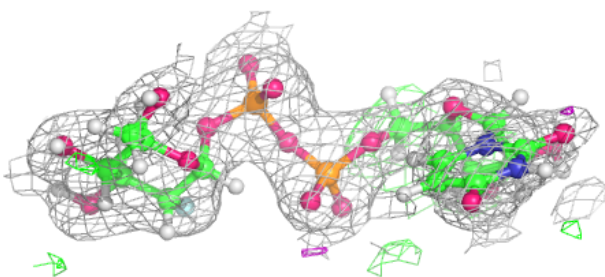
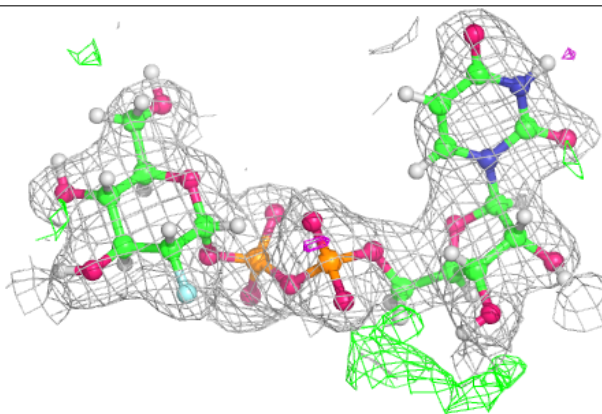
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U2F BBB 804:

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

**Electron density around U2F AAA 806:**

$2mF_o - DF_c$ (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.