Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 11:13 pm GMT

PDB ID	:	6TJJ
Title	:	Structure of Cerezyme at pH 4.6
Authors	:	Rowland, R.J.; Davies, G.J.
Deposited on	:	2019-11-26
Resolution	:	1.59 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 (i) 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 (i)) were used in the production of this report:

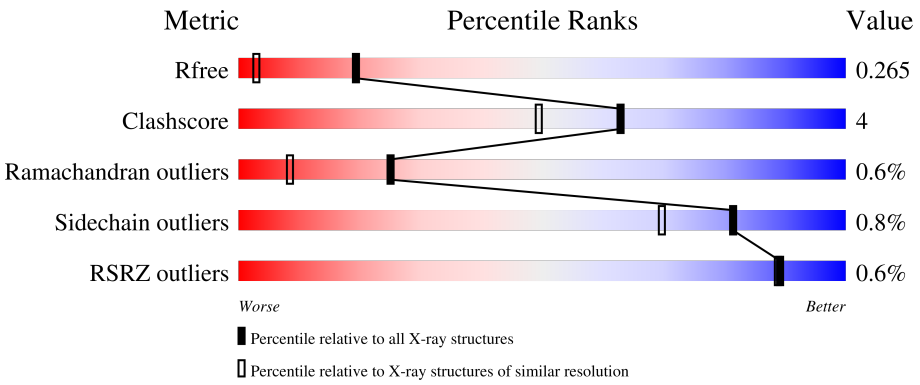
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.59 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	AAA	497	93% 7%
1	BBB	497	% 92% 8%
2	A	2	100%
2	B	2	100%

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	ACT	AAA	510	-	-	X	-
4	ACT	AAA	517	-	-	X	-
4	ACT	BBB	506	-	-	X	-
4	ACT	BBB	517	-	-	X	-
5	NAG	AAA	521	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16970 atoms, of which 7997 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	497	7963	2579	3949	692	726	17	211	10	0
1	BBB	497	7907	2575	3913	681	721	17	213	9	0

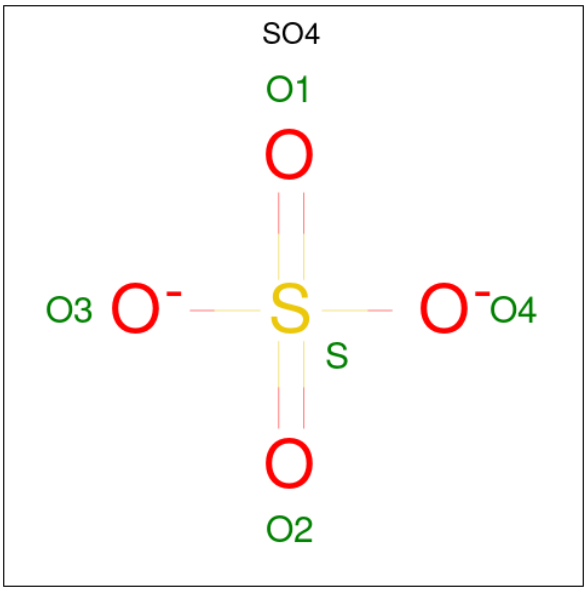
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	495	HIS	ARG	conflict	UNP P04062
BBB	495	HIS	ARG	conflict	UNP P04062

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	A	2	56	16	28	2	10	5	0	0
2	B	2	56	16	28	2	10	5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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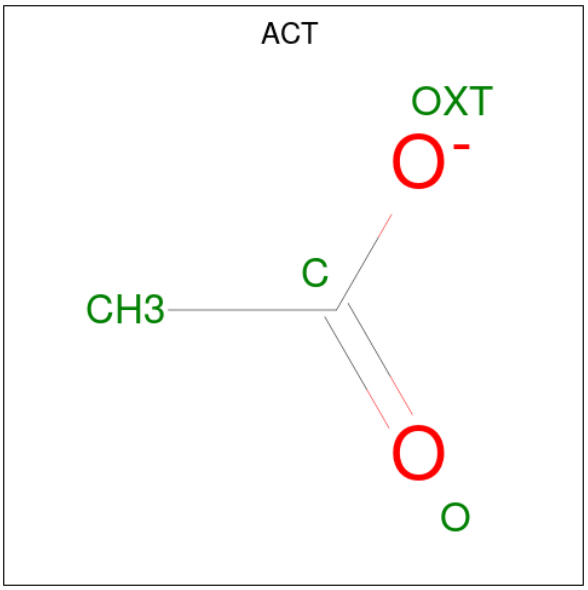
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	BBB	1	5	4	1		0	0
			Total	O	S			
3	BBB	1	5	4	1		0	0
			Total	O	S			
3	BBB	1	5	4	1		0	0
			Total	O	S			
3	BBB	1	5	4	1		0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	AAA	1	7	2	3	2	0	0
			Total	C	H	O		
4	AAA	1	7	2	3	2	0	0
			Total	C	H	O		
4	AAA	1	7	2	3	2	0	0
			Total	C	H	O		
4	AAA	1	7	2	3	2	0	0
			Total	C	H	O		
4	AAA	1	7	2	3	2	0	0
			Total	C	H	O		
4	AAA	1	7	2	3	2	0	0
			Total	C	H	O		
4	AAA	1	7	2	3	2	0	0

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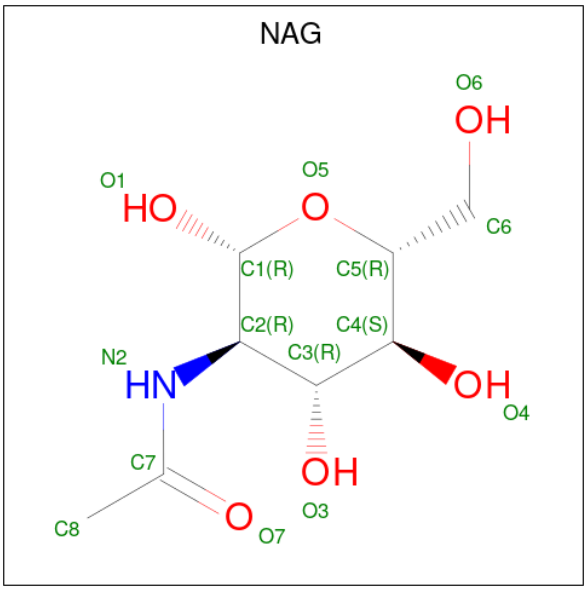
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	BBB	1	7	2	3	2	0	0
			Total	C	H	O		
4	BBB	1	7	2	3	2	0	0
			Total	C	H	O		
4	BBB	1	7	2	3	2	0	0
			Total	C	H	O		
4	BBB	1	14	4	6	4	0	1
			Total	C	H	O		
4	BBB	1	7	2	3	2	0	0
			Total	C	H	O		
4	BBB	1	7	2	3	2	0	0
			Total	C	H	O		
4	BBB	1	7	2	3	2	0	0
			Total	C	H	O		
4	BBB	1	7	2	3	2	0	0
			Total	C	H	O		
4	BBB	1	7	2	3	2	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	AAA	1	28	8	14	1	5	3	0
			Total	C	H	N	O		
5	BBB	1	28	8	14	1	5	3	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
6	BBB	1	1	1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
7	BBB	1	1	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	AAA	357	363	363	0	6
			Total	O		
8	BBB	358	358	358	0	0

3 Residue-property plots (i)

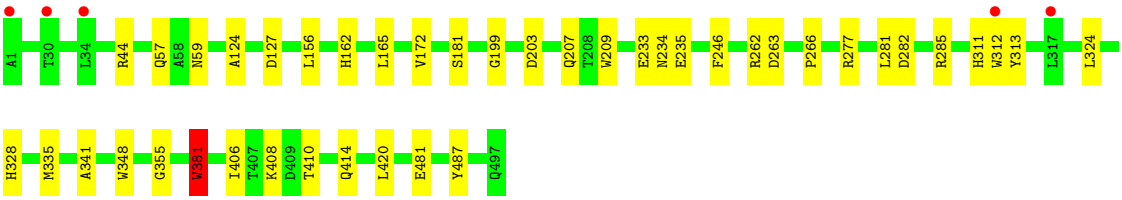
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glucosylceramidase

Chain AAA: 93% 7%

• Molecule 1: Glucosylceramidase

Chain BBB: % 92% 8%



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 100%

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.07Å 285.87Å 91.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.44 – 1.59 77.32 – 1.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.44-1.59) 100.0 (77.32-1.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.215 , 0.245 0.234 , 0.265	Depositor DCC
R_{free} test set	9698 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16970	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NAG, K, SO4, ACT

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	0/4134	0.83	0/5634
1	BBB	0.71	0/4118	0.83	0/5618
All	All	0.70	0/8252	0.83	0/11252

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 (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	AAA	4014	3949	3917	27	0
1	BBB	3994	3913	3873	35	0
2	A	28	28	25	0	0
2	B	28	28	25	0	0
3	AAA	55	0	0	1	0
3	BBB	35	0	0	2	0
4	AAA	28	21	21	5	0
4	BBB	40	30	30	4	0
5	AAA	14	14	13	0	0
5	BBB	14	14	13	0	0
6	BBB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BBB	1	0	0	0	0
8	AAA	363	0	0	9	0
8	BBB	358	0	0	13	0
All	All	8973	7997	7917	69	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 (69) 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:207:GLN:NE2	1:BBB:263:ASP:OD1	2.11	0.83
1:BBB:156[A]:LEU:CD1	8:BBB:715:HOH:O	2.36	0.73
1:AAA:235:GLU:OE2	8:AAA:601:HOH:O	2.06	0.72
1:AAA:270:ASN:ND2	8:AAA:603:HOH:O	2.23	0.72
1:BBB:57:GLN:HE21	1:BBB:481:GLU:HG3	1.60	0.67
1:BBB:355:GLY:H	1:BBB:414:GLN:HE21	1.46	0.64
1:BBB:165:LEU:HD22	1:BBB:172:VAL:HB	1.81	0.60
4:AAA:512:ACT:H1	8:AAA:813:HOH:O	2.02	0.60
1:BBB:235:GLU:OE2	1:BBB:313:TYR:OH	2.16	0.59
1:BBB:328:HIS:HD2	8:BBB:854:HOH:O	1.84	0.59
1:BBB:156[A]:LEU:HD13	8:BBB:715:HOH:O	2.00	0.58
1:AAA:328:HIS:HD2	8:AAA:838:HOH:O	1.87	0.57
1:AAA:207:GLN:OE1	1:AAA:263:ASP:OD1	2.23	0.57
1:BBB:156[A]:LEU:HD12	8:BBB:715:HOH:O	2.01	0.56
1:BBB:355:GLY:H	1:BBB:414:GLN:NE2	2.03	0.56
1:BBB:57:GLN:NE2	1:BBB:481:GLU:HG3	2.23	0.53
1:BBB:312:TRP:CZ2	1:BBB:324:LEU:HD11	2.44	0.52
4:BBB:506:ACT:H2	8:BBB:840:HOH:O	2.10	0.52
1:BBB:203:ASP:OD1	1:BBB:203:ASP:C	2.48	0.51
1:BBB:312:TRP:HZ2	1:BBB:324:LEU:HD11	1.75	0.51
4:AAA:510:ACT:H3	8:AAA:868:HOH:O	2.10	0.50
1:AAA:312:TRP:CZ2	1:AAA:318:ALA:HB2	2.46	0.50
1:BBB:408:LYS:O	1:BBB:410:THR:HG23	2.12	0.50
4:BBB:517:ACT:H2	8:BBB:772:HOH:O	2.12	0.49
1:AAA:200[A]:GLN:HE21	1:AAA:201:PRO:HD2	1.77	0.49
1:AAA:434:VAL:HG11	1:AAA:450[B]:MET:HG3	1.94	0.49
1:BBB:207:GLN:HE22	1:BBB:263:ASP:HA	1.78	0.49
1:AAA:176:ALA:HB3	1:AAA:230:VAL:HG12	1.96	0.48
1:BBB:162:HIS:HD2	4:BBB:506:ACT:H1	1.78	0.48
1:BBB:381:TRP:HA	1:BBB:381:TRP:CE3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:406:ILE:HD12	8:BBB:904:HOH:O	2.14	0.47
1:BBB:487[B]:TYR:OH	3:BBB:505:SO4:O4	2.28	0.47
4:AAA:517:ACT:H3	8:AAA:804:HOH:O	2.14	0.47
3:AAA:503:SO4:O3	8:AAA:602:HOH:O	2.19	0.46
1:BBB:199:GLY:HA3	1:BBB:203:ASP:OD2	2.15	0.46
1:BBB:277:ARG:NH1	3:BBB:507:SO4:O2	2.49	0.46
1:AAA:150:PRO:HB3	4:AAA:510:ACT:H1	1.97	0.46
1:AAA:95:ALA:HB3	1:AAA:406[B]:ILE:CD1	2.46	0.46
1:AAA:293:LYS:HE2	1:AAA:330:LEU:HD13	1.98	0.45
1:BBB:285:ARG:CD	1:BBB:312:TRP:CZ3	3.00	0.45
1:BBB:44:ARG:HD3	8:BBB:678:HOH:O	2.15	0.45
1:AAA:82:GLY:HA3	1:AAA:118[A]:ILE:O	2.16	0.45
4:AAA:517:ACT:H2	8:AAA:779:HOH:O	2.17	0.45
1:BBB:312:TRP:CE3	8:BBB:746:HOH:O	2.56	0.45
1:BBB:381:TRP:HA	1:BBB:381:TRP:HE3	1.82	0.44
1:BBB:312:TRP:O	1:BBB:341:ALA:HA	2.18	0.44
1:AAA:381:TRP:HA	1:AAA:381:TRP:CE3	2.53	0.44
1:AAA:397:PHE:HZ	8:AAA:688:HOH:O	1.99	0.43
1:AAA:312:TRP:HA	1:AAA:312:TRP:CE3	2.53	0.43
1:BBB:181:SER:HA	1:BBB:209:TRP:CZ3	2.53	0.43
1:AAA:206:HIS:NE2	1:AAA:255:HIS:NE2	2.52	0.43
4:BBB:517:ACT:CH3	8:BBB:772:HOH:O	2.66	0.43
1:BBB:408:LYS:NZ	8:BBB:625:HOH:O	2.51	0.43
1:AAA:483:ILE:O	1:AAA:485:PRO:HD3	2.20	0.42
1:BBB:127:ASP:HB3	1:BBB:246:PHE:CG	2.54	0.42
1:BBB:59:ASN:CB	8:BBB:857:HOH:O	2.67	0.41
1:AAA:309:ALA:HA	1:AAA:337:PHE:O	2.19	0.41
1:AAA:82:GLY:HA3	1:AAA:118[B]:ILE:O	2.18	0.41
1:BBB:234:ASN:OD1	1:BBB:311:HIS:HE1	2.04	0.41
1:BBB:262[A]:ARG:O	1:BBB:266:PRO:HG2	2.20	0.41
1:AAA:151:GLU:CD	1:AAA:155:LYS:HE3	2.40	0.41
1:AAA:347:PHE:HB3	8:BBB:819:HOH:O	2.20	0.41
1:AAA:381:TRP:HA	1:AAA:381:TRP:HE3	1.86	0.40
1:BBB:282:ASP:OD1	1:BBB:311:HIS:NE2	2.45	0.40
1:AAA:245:PRO:HG3	1:BBB:348:TRP:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AAA	505/497 (102%)	488 (97%)	15 (3%)	2 (0%)	34 15
1	BBB	504/497 (101%)	481 (95%)	19 (4%)	4 (1%)	19 6
All	All	1009/994 (102%)	969 (96%)	34 (3%)	6 (1%)	25 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	233	GLU
1	AAA	281	LEU
1	BBB	281	LEU
1	BBB	381	TRP
1	AAA	381	TRP
1	BBB	124	ALA

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	AAA	432/424 (102%)	428 (99%)	4 (1%)	78 65
1	BBB	428/424 (101%)	425 (99%)	3 (1%)	84 73
All	All	860/848 (101%)	853 (99%)	7 (1%)	81 70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	112	GLU
1	AAA	335	MET
1	AAA	350	GLN
1	AAA	381	TRP
1	BBB	335	MET
1	BBB	381	TRP
1	BBB	420	LEU

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

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)

4 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	NAG	A	1	1,2	14,14,15	0.60	0	17,19,21	1.47	2 (11%)
2	NAG	A	2	2	14,14,15	0.50	0	17,19,21	1.47	3 (17%)
2	NAG	B	1	1,2	14,14,15	0.59	0	17,19,21	1.22	3 (17%)
2	NAG	B	2	2	14,14,15	0.48	0	17,19,21	1.00	1 (5%)

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	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	2/6/23/26	0/1/1/1
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	NAG	O5-C1-C2	-3.93	105.08	111.29
2	A	2	NAG	O5-C5-C6	3.20	112.22	107.20
2	B	1	NAG	C2-N2-C7	-2.98	118.66	122.90
2	A	1	NAG	O3-C3-C2	-2.98	103.31	109.47
2	A	2	NAG	O4-C4-C5	2.81	116.28	109.30
2	A	2	NAG	C3-C4-C5	-2.79	105.25	110.24
2	B	1	NAG	O5-C5-C6	2.63	111.33	107.20
2	B	2	NAG	C1-O5-C5	2.32	115.33	112.19
2	B	1	NAG	O3-C3-C2	-2.17	104.97	109.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

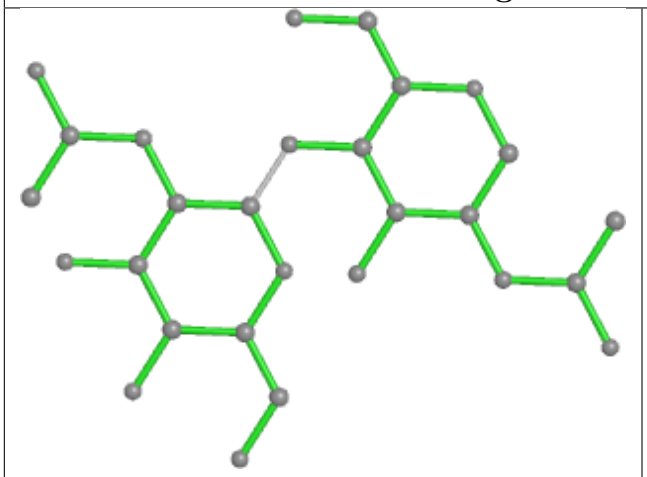
Mol	Chain	Res	Type	Atoms
2	A	2	NAG	O5-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

There are no ring outliers.

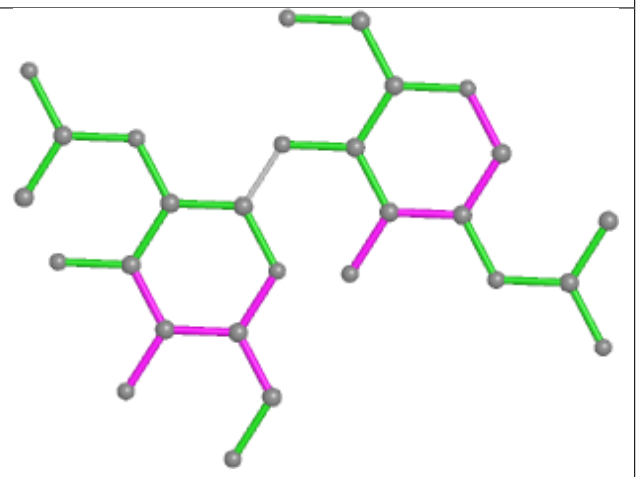
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

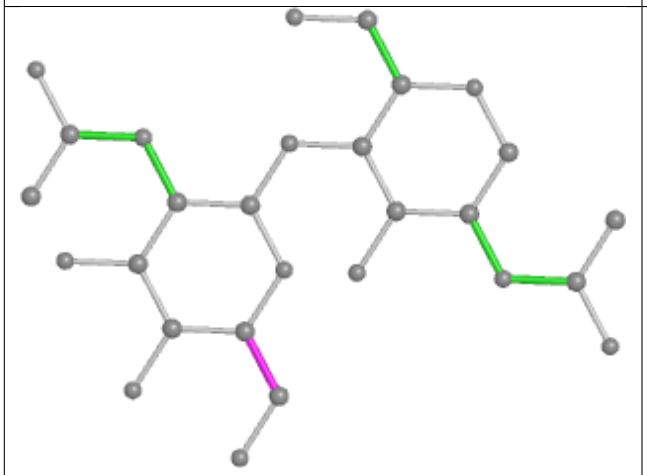
Oligosaccharide Chain A



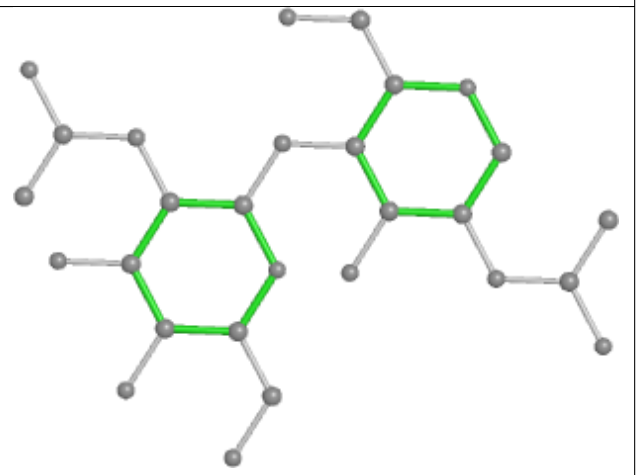
Bond lengths



Bond angles

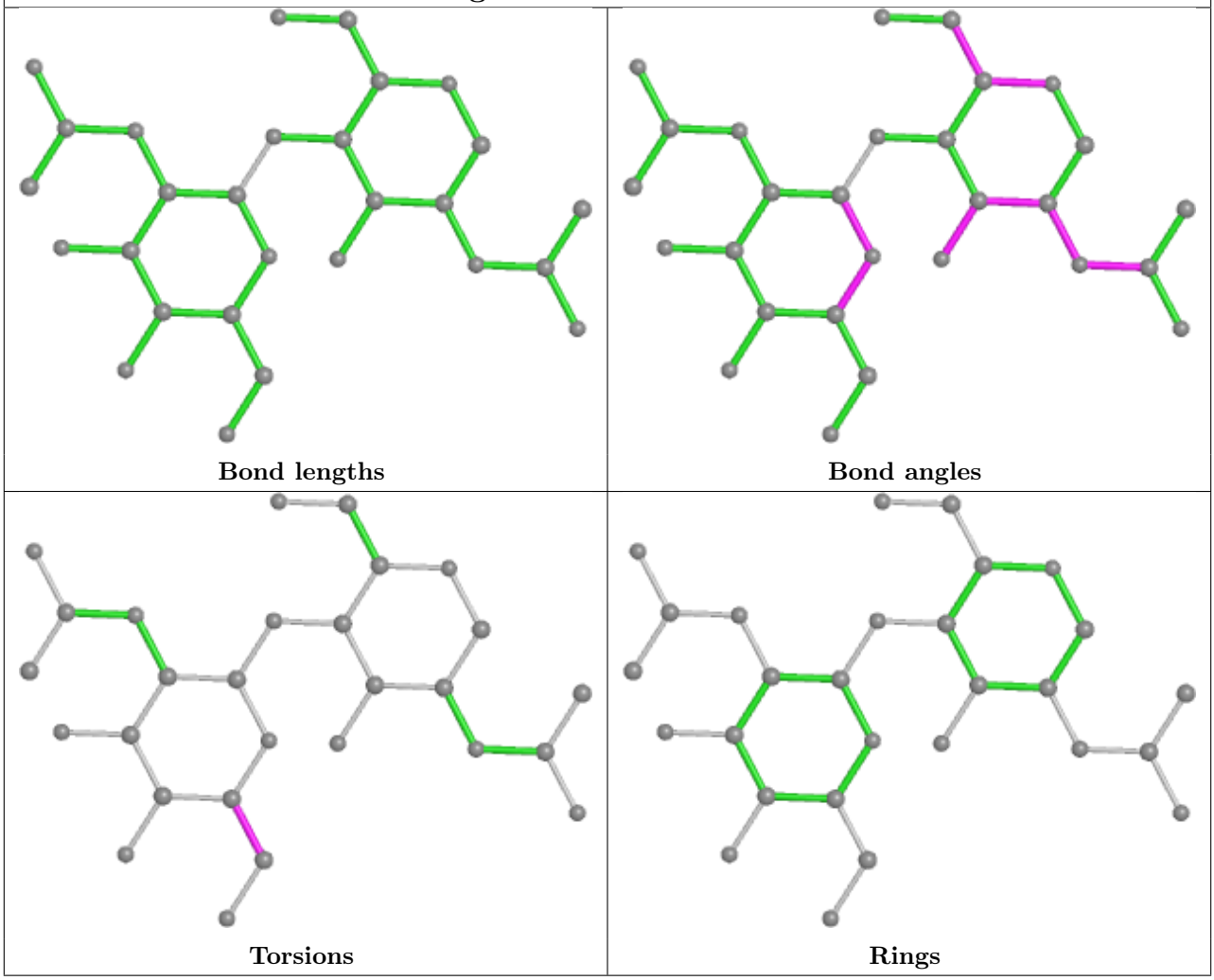


Torsions



Rings

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	AAA	517	-	3,3,3	1.03	0	3,3,3	0.74	0
3	SO4	AAA	502	-	4,4,4	0.46	0	6,6,6	0.22	0
3	SO4	AAA	507	-	4,4,4	0.36	0	6,6,6	0.17	0
4	ACT	BBB	508	-	3,3,3	1.15	0	3,3,3	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	AAA	512	-	3,3,3	1.05	0	3,3,3	1.10	0
3	SO4	BBB	505	-	4,4,4	0.33	0	6,6,6	0.10	0
3	SO4	BBB	502	-	4,4,4	0.35	0	6,6,6	0.24	0
4	ACT	BBB	506	-	3,3,3	0.85	0	3,3,3	0.84	0
3	SO4	AAA	506	-	4,4,4	0.35	0	6,6,6	0.13	0
4	ACT	AAA	510	-	3,3,3	0.94	0	3,3,3	0.98	0
4	ACT	BBB	513[B]	-	3,3,3	0.97	0	3,3,3	0.72	0
3	SO4	BBB	504	-	4,4,4	0.38	0	6,6,6	0.28	0
4	ACT	BBB	517	-	3,3,3	1.15	0	3,3,3	0.67	0
3	SO4	BBB	518	-	4,4,4	0.37	0	6,6,6	0.05	0
3	SO4	AAA	508	-	4,4,4	0.34	0	6,6,6	0.13	0
4	ACT	AAA	514	-	3,3,3	1.16	0	3,3,3	0.65	0
5	NAG	AAA	521	1	14,14,15	0.45	0	17,19,21	1.40	2 (11%)
3	SO4	AAA	501	-	4,4,4	0.52	0	6,6,6	0.16	0
3	SO4	AAA	511	-	4,4,4	0.36	0	6,6,6	0.11	0
4	ACT	BBB	519	-	3,3,3	1.16	0	3,3,3	0.68	0
3	SO4	BBB	507	-	4,4,4	0.35	0	6,6,6	0.12	0
4	ACT	BBB	514	-	3,3,3	0.94	0	3,3,3	1.03	0
4	ACT	BBB	515	-	3,3,3	1.07	0	3,3,3	0.58	0
3	SO4	AAA	503	-	4,4,4	0.40	0	6,6,6	0.24	0
3	SO4	BBB	501	-	4,4,4	0.53	0	6,6,6	0.16	0
4	ACT	BBB	516	-	3,3,3	1.20	0	3,3,3	0.71	0
3	SO4	AAA	504	-	4,4,4	0.37	0	6,6,6	0.18	0
5	NAG	BBB	511	1	14,14,15	0.84	0	17,19,21	1.99	4 (23%)
3	SO4	AAA	513	-	4,4,4	0.35	0	6,6,6	0.05	0
3	SO4	BBB	503	-	4,4,4	0.37	0	6,6,6	0.07	0
4	ACT	BBB	513[A]	-	3,3,3	1.15	0	3,3,3	0.64	0
4	ACT	AAA	515	-	3,3,3	1.01	0	3,3,3	0.75	0
4	ACT	BBB	512	-	3,3,3	1.09	0	3,3,3	0.89	0
3	SO4	AAA	505	-	4,4,4	0.36	0	6,6,6	0.14	0
4	ACT	AAA	516	-	3,3,3	1.16	0	3,3,3	0.91	0
4	ACT	AAA	509	-	3,3,3	1.12	0	3,3,3	0.79	0
3	SO4	AAA	518	-	4,4,4	0.44	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	BBB	511	1	-	0/6/23/26	0/1/1/1
5	NAG	AAA	521	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	BBB	511	NAG	C1-O5-C5	4.43	118.19	112.19
5	BBB	511	NAG	O3-C3-C2	-3.93	101.34	109.47
5	AAA	521	NAG	O5-C5-C6	2.92	111.78	107.20
5	AAA	521	NAG	C2-N2-C7	2.91	127.04	122.90
5	BBB	511	NAG	O5-C1-C2	-2.67	107.07	111.29
5	BBB	511	NAG	C1-C2-N2	-2.41	106.37	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	517	ACT	2	0
4	AAA	512	ACT	1	0
3	BBB	505	SO4	1	0
4	BBB	506	ACT	2	0
4	AAA	510	ACT	2	0
4	BBB	517	ACT	2	0
3	BBB	507	SO4	1	0
3	AAA	503	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	497/497 (100%)	-0.15	1 (0%)	95	94	20, 31, 51, 74	6 (1%)
1	BBB	497/497 (100%)	-0.13	5 (1%)	82	82	22, 31, 53, 75	4 (0%)
All	All	994/994 (100%)	-0.14	6 (0%)	89	89	20, 31, 52, 75	10 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	317	LEU	3.6
1	AAA	347	PHE	3.6
1	BBB	312	TRP	3.1
1	BBB	1	ALA	2.7
1	BBB	30	THR	2.2
1	BBB	34[A]	LEU	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)

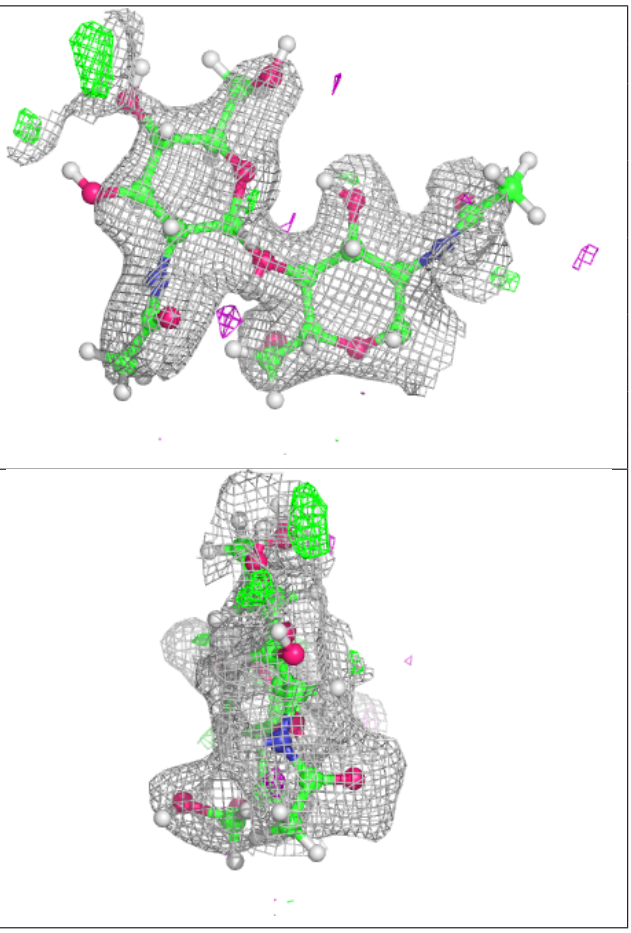
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	A	2	14/15	0.82	0.15	53,82,98,100	3
2	NAG	B	1	14/15	0.86	0.11	37,44,50,52	2
2	NAG	A	1	14/15	0.87	0.10	41,47,55,55	2
2	NAG	B	2	14/15	0.88	0.14	50,70,85,87	3

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

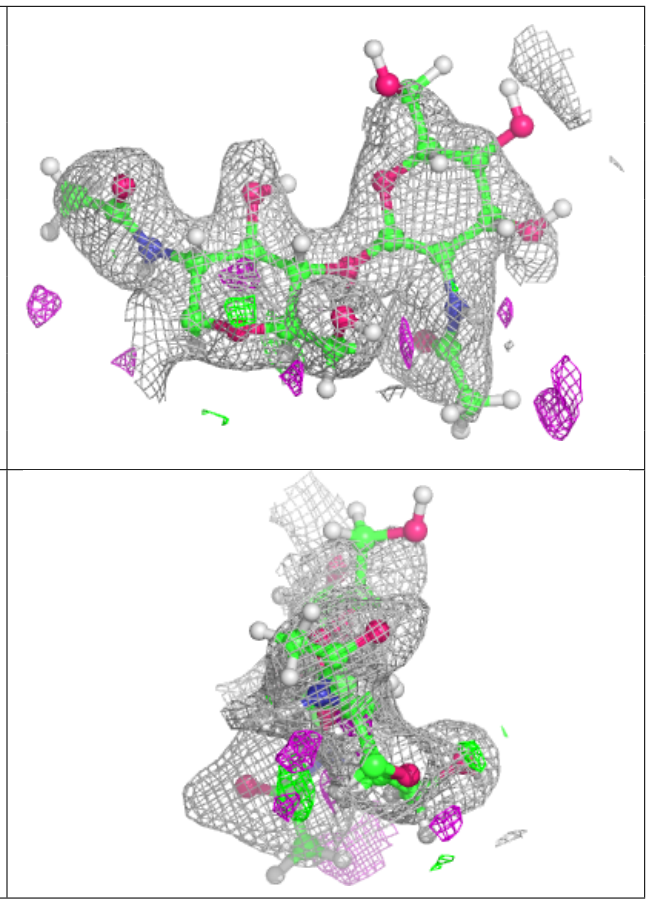
Electron density around Chain A:

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



Electron density around Chain B:

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



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
4	ACT	AAA	512	4/4	0.49	0.15	56,60,61,65	0
5	NAG	AAA	521	14/15	0.51	0.41	99,118,122,124	3
4	ACT	BBB	515	4/4	0.67	0.19	74,77,80,85	0
4	ACT	BBB	516	4/4	0.73	0.28	43,62,66,82	0
4	ACT	AAA	514	4/4	0.75	0.18	61,68,72,73	0
4	ACT	BBB	512	4/4	0.77	0.11	56,59,64,69	0
4	ACT	AAA	509	4/4	0.77	0.14	56,67,70,72	0
5	NAG	BBB	511	14/15	0.78	0.15	50,66,83,86	3
4	ACT	AAA	516	4/4	0.83	0.09	48,50,53,58	0
4	ACT	AAA	515	4/4	0.83	0.11	64,66,73,75	0
3	SO4	BBB	518	5/5	0.84	0.22	117,121,127,129	0
4	ACT	AAA	510	4/4	0.85	0.12	41,50,53,62	0
3	SO4	BBB	507	5/5	0.86	0.20	95,97,108,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	BBB	514	4/4	0.89	0.08	50,56,58,66	0
4	ACT	BBB	506	4/4	0.89	0.16	42,43,55,61	0
3	SO4	AAA	513	5/5	0.89	0.11	89,99,102,102	0
4	ACT	BBB	513[A]	4/4	0.89	0.17	42,43,44,47	7
4	ACT	BBB	513[B]	4/4	0.89	0.17	37,38,39,40	7
3	SO4	AAA	518	5/5	0.90	0.13	39,46,49,51	5
4	ACT	BBB	519	4/4	0.90	0.10	54,64,65,70	0
3	SO4	AAA	504	5/5	0.91	0.09	69,73,75,84	0
3	SO4	AAA	511	5/5	0.91	0.11	92,93,101,101	0
4	ACT	AAA	517	4/4	0.93	0.12	52,53,57,63	0
3	SO4	BBB	505	5/5	0.93	0.09	63,71,83,83	0
4	ACT	BBB	508	4/4	0.93	0.15	53,59,60,65	0
4	ACT	BBB	517	4/4	0.94	0.10	47,47,52,59	0
3	SO4	AAA	506	5/5	0.94	0.09	65,65,66,82	0
3	SO4	AAA	505	5/5	0.94	0.09	61,63,75,76	0
3	SO4	BBB	502	5/5	0.94	0.10	50,59,69,70	0
3	SO4	AAA	508	5/5	0.96	0.09	54,56,62,62	5
3	SO4	BBB	504	5/5	0.96	0.11	54,60,68,71	0
3	SO4	AAA	503	5/5	0.96	0.08	45,55,61,62	0
3	SO4	BBB	503	5/5	0.97	0.08	51,53,56,62	0
7	NA	BBB	521	1/1	0.97	0.07	40,40,40,40	0
3	SO4	AAA	502	5/5	0.98	0.07	52,56,61,64	0
3	SO4	AAA	507	5/5	0.98	0.06	56,56,59,59	0
3	SO4	AAA	501	5/5	0.99	0.08	35,37,41,46	0
6	K	BBB	520	1/1	0.99	0.04	44,44,44,44	0
3	SO4	BBB	501	5/5	0.99	0.10	37,42,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.