Full wwPDB X-ray Structure Validation Report (i)

Nov 25, 2024 – 06:49 PM EST

PDB ID	:	3LPP
Title	:	Crystal complex of N-terminal sucrase-isomaltase with kotalanol
Authors	:	Sim, L.; Rose, D.R.
Deposited on	:	2010-02-05
Resolution	:	2.15 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:

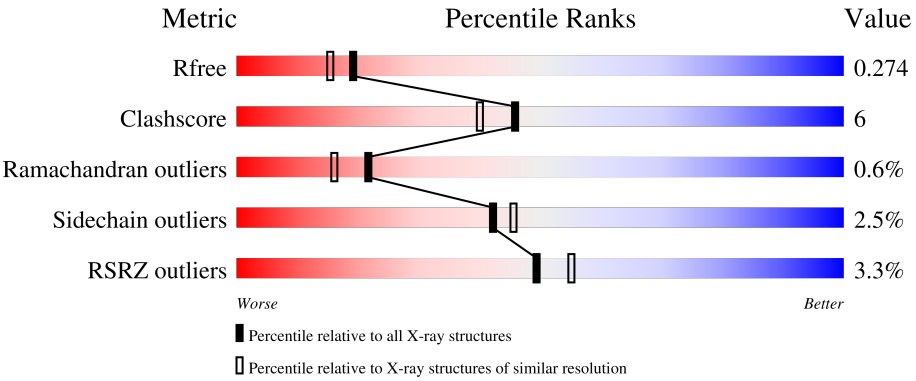
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.15 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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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%

Mol	Chain	Length	Quality of chain
1	A	898	3% 85% 11%
1	B	898	2% 83% 13%
1	C	898	3% 85% 12%
1	D	898	5% 80% 14% 5%
2	E	4	100%
2	H	4	25% 75%

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Mol	Chain	Length	Quality of chain
3	F	2	100%
3	G	2	50% 50%
3	I	2	100%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 30064 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 Sucrase-isomaltase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	871	Total	C	N	O	S	0	0	0
			7035	4503	1183	1320	29			
1	B	869	Total	C	N	O	S	0	0	0
			7015	4491	1177	1318	29			
1	C	871	Total	C	N	O	S	0	0	0
			7029	4500	1180	1320	29			
1	D	853	Total	C	N	O	S	0	0	0
			6882	4416	1150	1289	27			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	expression tag	UNP P14410
A	2	SER	-	expression tag	UNP P14410
A	3	SER	-	expression tag	UNP P14410
A	4	HIS	-	expression tag	UNP P14410
A	5	HIS	-	expression tag	UNP P14410
A	6	HIS	-	expression tag	UNP P14410
A	7	HIS	-	expression tag	UNP P14410
A	8	HIS	-	expression tag	UNP P14410
A	9	HIS	-	expression tag	UNP P14410
A	10	GLY	-	expression tag	UNP P14410
A	11	GLU	-	expression tag	UNP P14410
A	12	PHE	-	expression tag	UNP P14410
A	13	ASP	-	expression tag	UNP P14410
A	14	ILE	-	expression tag	UNP P14410
A	15	PRO	-	expression tag	UNP P14410
A	16	THR	-	expression tag	UNP P14410
A	17	THR	-	expression tag	UNP P14410
A	18	GLU	-	expression tag	UNP P14410
A	19	ASN	-	expression tag	UNP P14410
A	20	LEU	-	expression tag	UNP P14410
A	21	TYR	-	expression tag	UNP P14410

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	PHE	-	expression tag	UNP P14410
A	23	GLN	-	expression tag	UNP P14410
A	24	SER	-	expression tag	UNP P14410
A	25	GLY	-	expression tag	UNP P14410
A	26	ILE	-	expression tag	UNP P14410
A	27	ARG	-	expression tag	UNP P14410
A	28	ARG	-	expression tag	UNP P14410
B	1	ARG	-	expression tag	UNP P14410
B	2	SER	-	expression tag	UNP P14410
B	3	SER	-	expression tag	UNP P14410
B	4	HIS	-	expression tag	UNP P14410
B	5	HIS	-	expression tag	UNP P14410
B	6	HIS	-	expression tag	UNP P14410
B	7	HIS	-	expression tag	UNP P14410
B	8	HIS	-	expression tag	UNP P14410
B	9	HIS	-	expression tag	UNP P14410
B	10	GLY	-	expression tag	UNP P14410
B	11	GLU	-	expression tag	UNP P14410
B	12	PHE	-	expression tag	UNP P14410
B	13	ASP	-	expression tag	UNP P14410
B	14	ILE	-	expression tag	UNP P14410
B	15	PRO	-	expression tag	UNP P14410
B	16	THR	-	expression tag	UNP P14410
B	17	THR	-	expression tag	UNP P14410
B	18	GLU	-	expression tag	UNP P14410
B	19	ASN	-	expression tag	UNP P14410
B	20	LEU	-	expression tag	UNP P14410
B	21	TYR	-	expression tag	UNP P14410
B	22	PHE	-	expression tag	UNP P14410
B	23	GLN	-	expression tag	UNP P14410
B	24	SER	-	expression tag	UNP P14410
B	25	GLY	-	expression tag	UNP P14410
B	26	ILE	-	expression tag	UNP P14410
B	27	ARG	-	expression tag	UNP P14410
B	28	ARG	-	expression tag	UNP P14410
C	1	ARG	-	expression tag	UNP P14410
C	2	SER	-	expression tag	UNP P14410
C	3	SER	-	expression tag	UNP P14410
C	4	HIS	-	expression tag	UNP P14410
C	5	HIS	-	expression tag	UNP P14410
C	6	HIS	-	expression tag	UNP P14410
C	7	HIS	-	expression tag	UNP P14410

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	HIS	-	expression tag	UNP P14410
C	9	HIS	-	expression tag	UNP P14410
C	10	GLY	-	expression tag	UNP P14410
C	11	GLU	-	expression tag	UNP P14410
C	12	PHE	-	expression tag	UNP P14410
C	13	ASP	-	expression tag	UNP P14410
C	14	ILE	-	expression tag	UNP P14410
C	15	PRO	-	expression tag	UNP P14410
C	16	THR	-	expression tag	UNP P14410
C	17	THR	-	expression tag	UNP P14410
C	18	GLU	-	expression tag	UNP P14410
C	19	ASN	-	expression tag	UNP P14410
C	20	LEU	-	expression tag	UNP P14410
C	21	TYR	-	expression tag	UNP P14410
C	22	PHE	-	expression tag	UNP P14410
C	23	GLN	-	expression tag	UNP P14410
C	24	SER	-	expression tag	UNP P14410
C	25	GLY	-	expression tag	UNP P14410
C	26	ILE	-	expression tag	UNP P14410
C	27	ARG	-	expression tag	UNP P14410
C	28	ARG	-	expression tag	UNP P14410
D	1	ARG	-	expression tag	UNP P14410
D	2	SER	-	expression tag	UNP P14410
D	3	SER	-	expression tag	UNP P14410
D	4	HIS	-	expression tag	UNP P14410
D	5	HIS	-	expression tag	UNP P14410
D	6	HIS	-	expression tag	UNP P14410
D	7	HIS	-	expression tag	UNP P14410
D	8	HIS	-	expression tag	UNP P14410
D	9	HIS	-	expression tag	UNP P14410
D	10	GLY	-	expression tag	UNP P14410
D	11	GLU	-	expression tag	UNP P14410
D	12	PHE	-	expression tag	UNP P14410
D	13	ASP	-	expression tag	UNP P14410
D	14	ILE	-	expression tag	UNP P14410
D	15	PRO	-	expression tag	UNP P14410
D	16	THR	-	expression tag	UNP P14410
D	17	THR	-	expression tag	UNP P14410
D	18	GLU	-	expression tag	UNP P14410
D	19	ASN	-	expression tag	UNP P14410
D	20	LEU	-	expression tag	UNP P14410
D	21	TYR	-	expression tag	UNP P14410

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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	PHE	-	expression tag	UNP P14410
D	23	GLN	-	expression tag	UNP P14410
D	24	SER	-	expression tag	UNP P14410
D	25	GLY	-	expression tag	UNP P14410
D	26	ILE	-	expression tag	UNP P14410
D	27	ARG	-	expression tag	UNP P14410
D	28	ARG	-	expression tag	UNP P14410

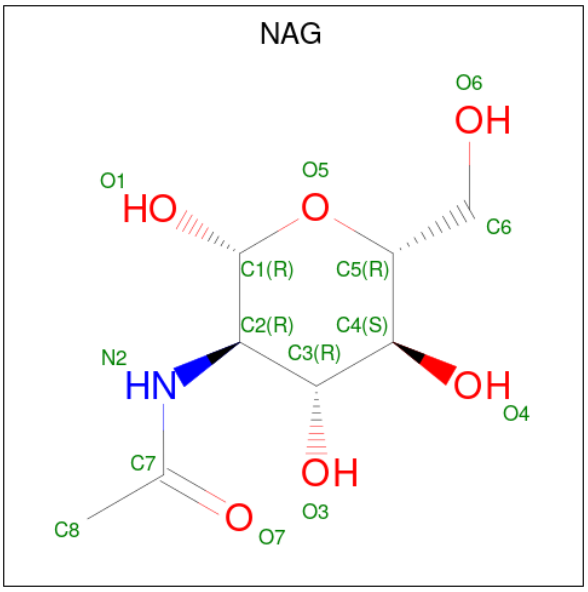
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

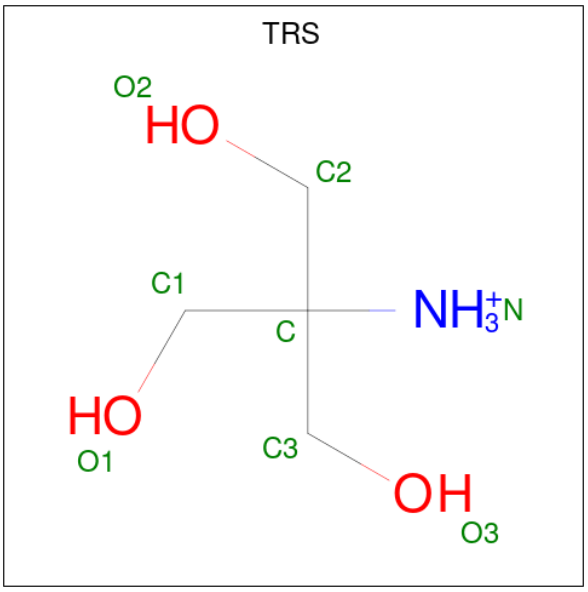
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



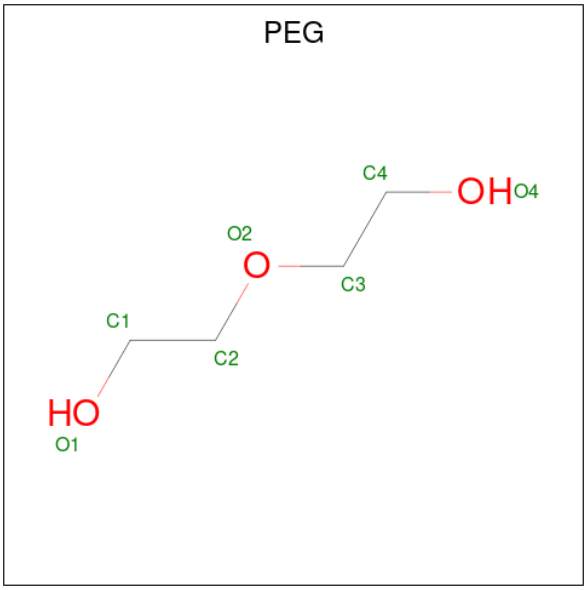
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 8 4 1 3	0	0
5	C	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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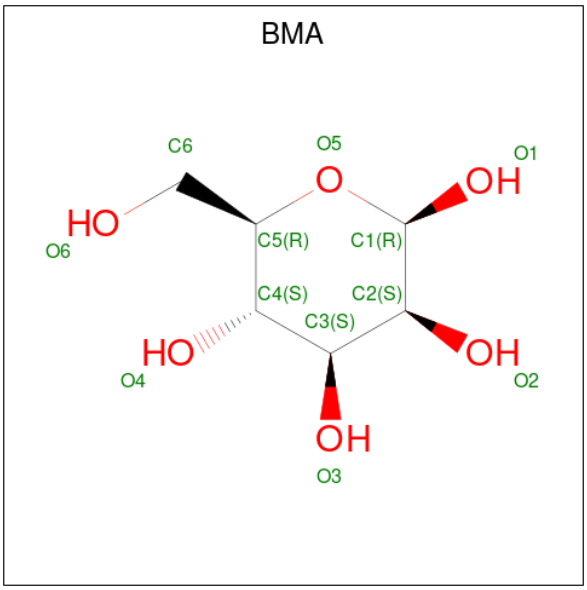
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

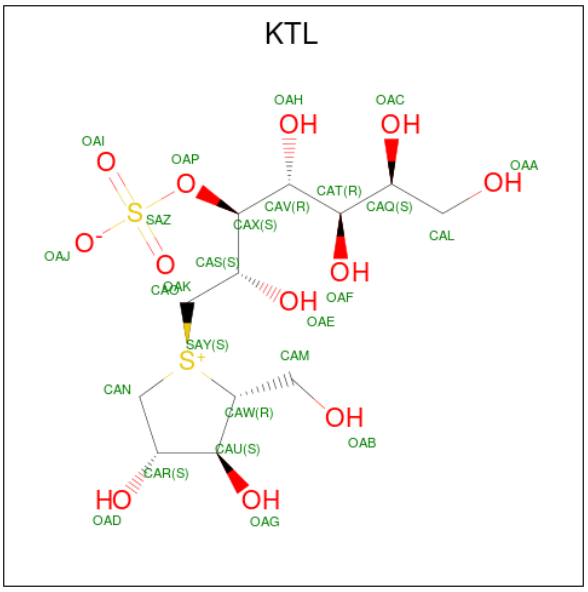
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 11 6 5	0	0

- Molecule 9 is (1S,2R,3R,4S)-1-{(1S)-2-[(2R,3S,4S)-3,4-dihydroxy-2-(hydroxymethyl)tetrahydrothiophenium-1-yl]-1-hydroxyethyl}-2,3,4,5-tetrahydroxypentyl sulfate (three-letter code: KTL) (formula: $C_{12}H_{24}O_{12}S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O	S	0	0
			26	12	12	2		
9	D	1	Total	C	O	S	0	0
			26	12	12	2		

- Molecule 10 is water.

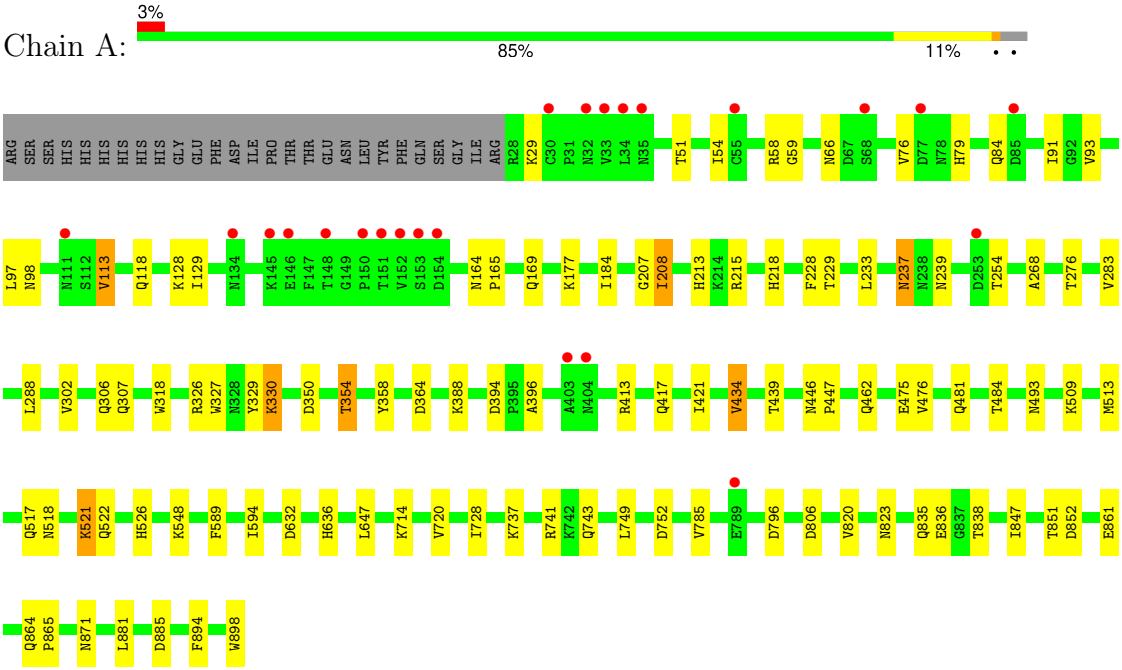
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	529	Total	O	0	0
			529	529		
10	B	514	Total	O	0	0
			514	514		
10	C	458	Total	O	0	0
			458	458		
10	D	226	Total	O	0	0
			226	226		

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. 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. 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.

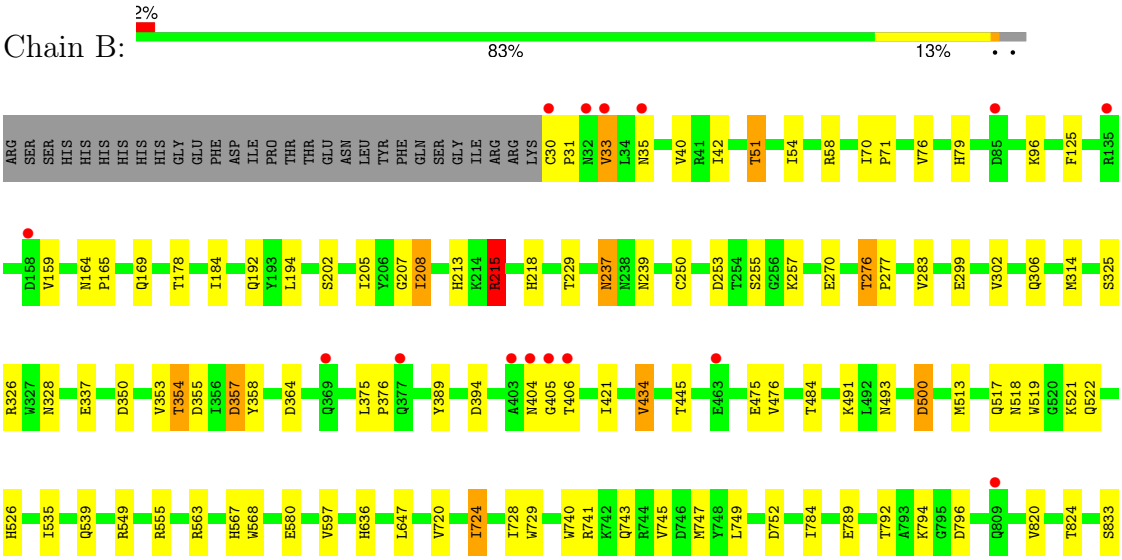
- Molecule 1: Sucrase-isomaltase

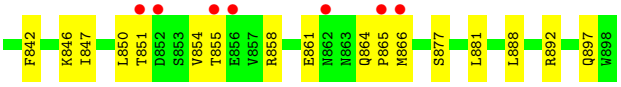
Chain A:



- Molecule 1: Sucrase-isomaltase

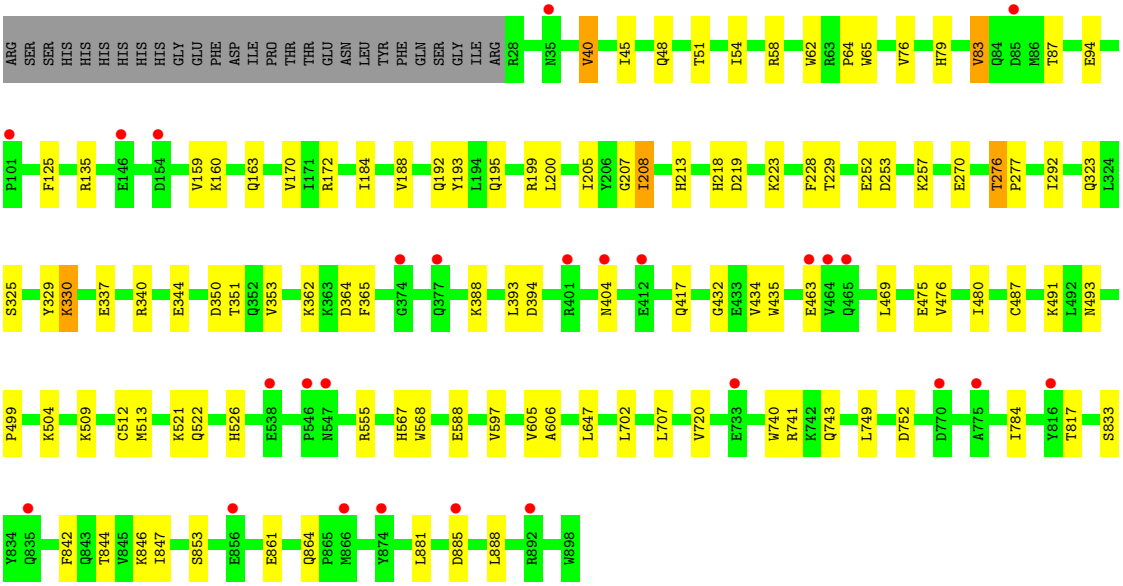
Chain B:





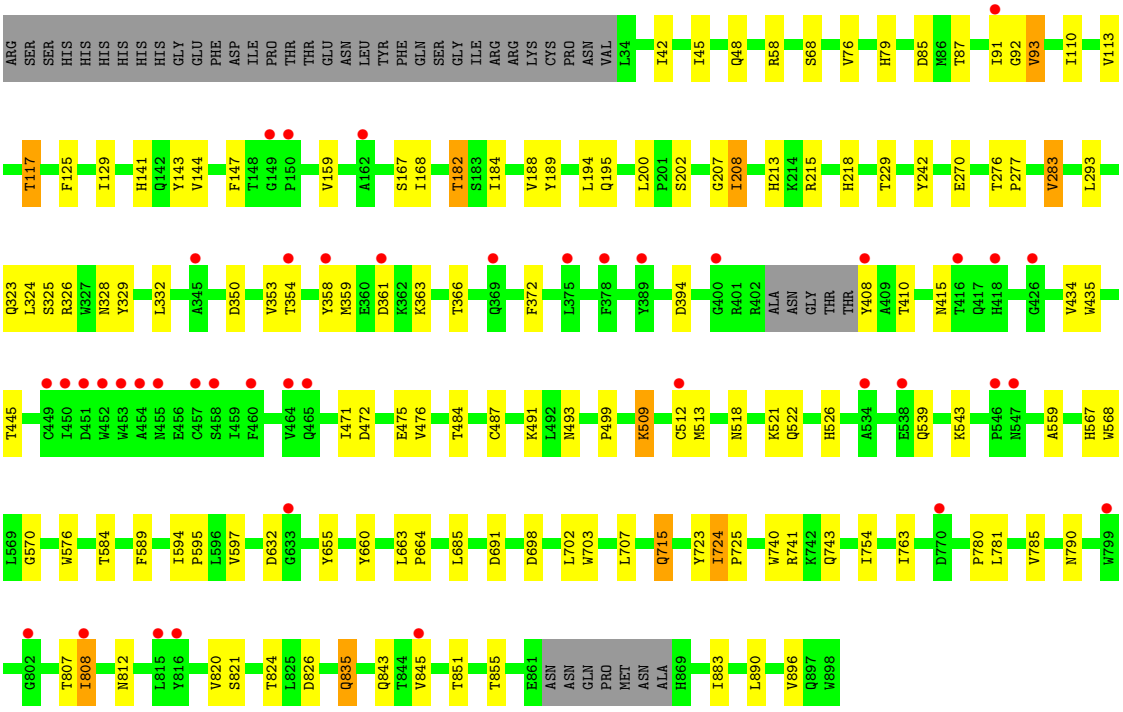
• Molecule 1: Sucrase-isomaltase

Chain C:



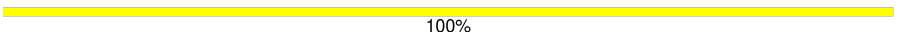
• Molecule 1: Sucrase-isomaltase

Chain D:



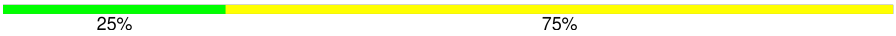
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



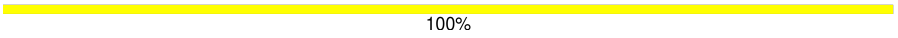
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

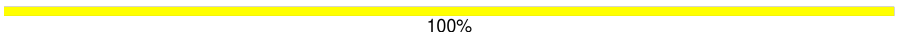


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.40Å 165.76Å 341.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.15 19.95 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.8 (19.95-2.15) 94.7 (19.95-2.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.223 0.240 , 0.274	Depositor DCC
R_{free} test set	10150 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 31.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	30064	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: TRS, MAN, NAG, BMA, PEG, KTL, CL

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	0.59	0/7236	0.65	1/9868 (0.0%)
1	B	0.55	0/7216	0.64	1/9843 (0.0%)
1	C	0.55	0/7230	0.63	0/9861
1	D	0.44	0/7079	0.57	0/9653
All	All	0.54	0/28761	0.62	2/39225 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	233	LEU	CA-CB-CG	5.03	126.87	115.30

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	A	7035	0	6734	67	0
1	B	7015	0	6711	86	0
1	C	7029	0	6724	69	0
1	D	6882	0	6573	95	0
2	E	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	50	0	43	0	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
3	I	28	0	25	0	0
4	A	28	0	26	0	0
4	B	14	0	13	0	0
4	C	42	0	39	0	0
5	A	8	0	12	0	0
5	C	8	0	12	0	0
6	A	7	0	10	0	0
6	B	7	0	10	3	0
6	C	7	0	10	3	0
6	D	7	0	10	0	0
7	A	1	0	0	0	0
8	B	11	0	10	1	0
9	B	26	0	24	0	0
9	D	26	0	24	2	0
10	A	529	0	0	9	0
10	B	514	0	0	11	0
10	C	458	0	0	12	0
10	D	226	0	0	9	0
All	All	30064	0	27103	316	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 6.

All (316) 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:C:487:CYS:HG	1:C:512:CYS:HG	1.05	1.01
1:B:741:ARG:H	1:B:743:GLN:HE21	1.13	0.93
1:C:741:ARG:H	1:C:743:GLN:HE21	1.13	0.88
1:C:51:THR:HG22	10:C:920:HOH:O	1.75	0.87
1:B:51:THR:HG21	10:C:1095:HOH:O	1.75	0.85
1:C:323:GLN:HG2	1:C:351:THR:OG1	1.81	0.81
1:A:741:ARG:H	1:A:743:GLN:HE21	1.30	0.79
1:B:205:ILE:HG12	10:B:1299:HOH:O	1.83	0.79
1:C:270:GLU:HG3	1:C:499:PRO:HB3	1.65	0.77
1:A:354:THR:CG2	1:A:358:TYR:CD2	2.68	0.76
1:B:237:ASN:HD22	1:B:239:ASN:H	1.35	0.74
1:A:237:ASN:HD22	1:A:239:ASN:H	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:GLN:HE21	1:D:526:HIS:HD2	1.35	0.74
1:C:493:ASN:HD21	1:C:513:MET:H	1.36	0.73
1:D:91:ILE:HG23	1:D:147:PHE:HE2	1.53	0.73
1:B:563:ARG:NH1	10:B:1727:HOH:O	2.22	0.73
1:D:896:VAL:HG23	10:D:923:HOH:O	1.89	0.73
1:B:404:ASN:C	1:B:406:THR:H	1.90	0.72
1:D:475:GLU:N	1:D:476:VAL:HA	2.05	0.71
1:B:493:ASN:HD21	1:B:513:MET:H	1.39	0.71
1:D:434:VAL:HG12	1:D:435:TRP:H	1.56	0.70
1:B:475:GLU:N	1:B:476:VAL:HA	2.07	0.69
1:D:113:VAL:CG1	1:D:129:ILE:CG2	2.71	0.69
1:A:51:THR:HG22	10:A:993:HOH:O	1.93	0.69
1:C:229:THR:O	1:C:526:HIS:HE1	1.76	0.69
1:D:141:HIS:HD2	1:D:143:TYR:H	1.41	0.68
1:A:481:GLN:HE22	1:A:509:LYS:H	1.40	0.68
1:B:724:ILE:CD1	1:B:729:TRP:CD1	2.76	0.68
1:B:861:GLU:O	1:B:864:GLN:HG2	1.93	0.67
1:A:475:GLU:N	1:A:476:VAL:HA	2.09	0.67
1:C:351:THR:HG22	1:C:388:LYS:HB2	1.77	0.67
1:D:724:ILE:HD11	1:D:741:ARG:HA	1.75	0.67
1:A:229:THR:O	1:A:526:HIS:HE1	1.77	0.67
1:D:270:GLU:HG3	1:D:499:PRO:HB3	1.78	0.66
1:D:493:ASN:HD21	1:D:513:MET:H	1.43	0.66
1:B:51:THR:HG22	1:B:54:ILE:H	1.59	0.66
1:B:229:THR:O	1:B:526:HIS:HE1	1.79	0.66
1:B:493:ASN:ND2	1:B:513:MET:H	1.92	0.66
1:A:647:LEU:HD11	1:A:752:ASP:HB3	1.78	0.66
1:B:741:ARG:HH12	1:B:789:GLU:HG2	1.61	0.66
1:D:780:PRO:HB3	1:D:843:GLN:HG3	1.78	0.64
1:D:229:THR:O	1:D:526:HIS:HE1	1.81	0.64
1:A:354:THR:HG22	1:A:358:TYR:CD2	2.33	0.64
1:A:481:GLN:NE2	1:A:509:LYS:H	1.95	0.64
1:D:821:SER:O	1:D:824:THR:HG22	1.98	0.63
1:D:113:VAL:HG11	1:D:129:ILE:CG2	2.28	0.62
1:B:741:ARG:H	1:B:743:GLN:NE2	1.91	0.62
1:B:864:GLN:HB2	1:B:865:PRO:HD2	1.82	0.62
1:D:141:HIS:HE1	1:D:559:ALA:O	1.83	0.62
1:D:58:ARG:O	1:D:79:HIS:HE1	1.83	0.61
1:B:299:GLU:HG2	10:B:1251:HOH:O	1.99	0.61
1:B:724:ILE:HD13	1:B:729:TRP:CD1	2.35	0.61
1:A:835:GLN:O	1:A:838:THR:HB	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:846:LYS:HD2	6:C:7001:PEG:H11	1.83	0.61
1:C:218:HIS:HD2	10:C:940:HOH:O	1.83	0.61
1:B:250:CYS:HB2	10:B:1299:HOH:O	2.00	0.60
1:B:302:VAL:HG12	1:B:306:GLN:NE2	2.16	0.60
1:C:135:ARG:HH22	1:D:491:LYS:HZ2	1.46	0.60
1:C:135:ARG:HH22	1:D:491:LYS:NZ	1.99	0.60
1:C:493:ASN:ND2	1:C:513:MET:H	1.99	0.60
1:D:141:HIS:CD2	1:D:143:TYR:H	2.18	0.60
1:A:493:ASN:HD21	1:A:513:MET:H	1.50	0.60
1:A:237:ASN:ND2	1:A:239:ASN:H	1.98	0.59
1:B:354:THR:HG23	1:B:358:TYR:CD2	2.35	0.59
1:D:394:ASP:HB3	10:D:1353:HOH:O	2.01	0.59
1:D:323:GLN:HE21	1:D:353:VAL:HG21	1.68	0.59
1:B:207:GLY:O	1:B:218:HIS:HE1	1.85	0.59
1:A:493:ASN:ND2	1:A:513:MET:H	2.00	0.59
1:A:522:GLN:HE21	1:A:526:HIS:HD2	1.50	0.59
1:C:170:VAL:HG21	1:C:292:ILE:HD13	1.83	0.59
1:D:741:ARG:H	1:D:743:GLN:HE21	1.49	0.59
1:D:207:GLY:O	1:D:218:HIS:HE1	1.85	0.58
1:D:471:ILE:HG23	10:D:941:HOH:O	2.02	0.58
1:D:113:VAL:CG1	1:D:129:ILE:HG23	2.32	0.58
1:B:302:VAL:HG12	1:B:306:GLN:HE21	1.69	0.58
1:C:784:ILE:CD1	6:C:7001:PEG:H12	2.33	0.58
1:A:207:GLY:O	1:A:218:HIS:HE1	1.87	0.57
1:B:854:VAL:HG21	1:B:881:LEU:HD22	1.86	0.57
1:A:84:GLN:HG3	1:A:98:ASN:OD1	2.04	0.57
1:D:354:THR:CG2	1:D:358:TYR:HB3	2.34	0.57
1:D:167:SER:HB2	1:D:182:THR:HG22	1.87	0.57
1:D:91:ILE:HG23	1:D:147:PHE:CE2	2.37	0.57
1:A:522:GLN:NE2	1:A:526:HIS:HD2	2.03	0.56
1:C:79:HIS:HD2	10:C:1112:HOH:O	1.86	0.56
1:D:354:THR:HG21	1:D:358:TYR:HB3	1.87	0.56
1:A:91:ILE:HD12	1:A:118:GLN:HG2	1.87	0.56
1:C:475:GLU:N	1:C:476:VAL:HA	2.19	0.56
1:C:125:PHE:CE1	1:C:159:VAL:HG21	2.41	0.56
1:C:847:ILE:HD12	1:C:881:LEU:HD23	1.87	0.56
1:A:228:PHE:CD1	1:A:268:ALA:HB2	2.42	0.55
1:B:215:ARG:NH2	1:B:580:GLU:OE2	2.38	0.55
1:D:724:ILE:HD11	1:D:741:ARG:CA	2.36	0.55
1:A:864:GLN:HB3	1:A:865:PRO:HD2	1.89	0.55
1:B:404:ASN:C	1:B:406:THR:N	2.59	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG12	1:A:306:GLN:NE2	2.22	0.54
1:B:325:SER:HB2	1:B:353:VAL:HB	1.88	0.54
1:C:51:THR:HG21	10:C:938:HOH:O	2.07	0.54
1:B:237:ASN:ND2	1:B:239:ASN:H	2.04	0.54
1:D:493:ASN:ND2	1:D:513:MET:H	2.05	0.54
1:C:87:THR:HG23	1:C:94:GLU:HB2	1.89	0.54
1:B:354:THR:HG21	1:B:389:TYR:OH	2.08	0.54
1:D:522:GLN:NE2	1:D:526:HIS:HD2	2.03	0.54
1:A:208:ILE:O	1:A:213:HIS:HE1	1.91	0.54
1:A:329:TYR:O	1:A:330:LYS:HB2	2.08	0.53
1:C:337:GLU:HA	1:C:340:ARG:HG2	1.90	0.53
1:A:184:ILE:HG22	10:A:955:HOH:O	2.08	0.53
1:C:207:GLY:O	1:C:218:HIS:HE1	1.92	0.53
1:D:125:PHE:CE1	1:D:159:VAL:HG21	2.43	0.53
1:D:168:ILE:H	1:D:182:THR:CG2	2.22	0.53
1:D:58:ARG:O	1:D:79:HIS:CE1	2.62	0.53
1:D:323:GLN:NE2	10:D:1307:HOH:O	2.41	0.53
1:B:79:HIS:HD2	10:B:945:HOH:O	1.92	0.53
1:D:522:GLN:HE21	1:D:526:HIS:CD2	2.22	0.53
1:D:664:PRO:HA	10:D:1088:HOH:O	2.07	0.53
1:A:354:THR:HG23	1:A:358:TYR:HB3	1.90	0.53
1:B:784:ILE:HD11	6:B:7001:PEG:H41	1.90	0.53
1:A:806:ASP:HA	10:A:1169:HOH:O	2.08	0.52
1:B:125:PHE:CE1	1:B:159:VAL:HG21	2.44	0.52
1:A:302:VAL:HG12	1:A:306:GLN:HE21	1.73	0.52
1:D:724:ILE:HG12	1:D:740:TRP:HB3	1.92	0.52
1:C:58:ARG:O	1:C:79:HIS:HE1	1.91	0.52
1:B:276:THR:N	1:B:277:PRO:HA	2.25	0.51
1:D:703:TRP:HB2	1:D:707:LEU:HB3	1.91	0.51
1:B:364:ASP:OD2	1:B:394:ASP:O	2.29	0.51
1:B:555:ARG:O	1:B:567:HIS:CE1	2.63	0.51
1:B:51:THR:HB	10:B:988:HOH:O	2.10	0.51
1:D:741:ARG:H	1:D:743:GLN:NE2	2.09	0.51
1:B:824:THR:OG1	1:B:897:GLN:HG2	2.10	0.51
1:C:219:ASP:OD2	1:C:223:LYS:HE2	2.11	0.51
1:A:354:THR:CG2	1:A:358:TYR:HB3	2.41	0.51
1:D:168:ILE:H	1:D:182:THR:HG22	1.76	0.51
1:A:714:LYS:HE2	10:A:1124:HOH:O	2.11	0.50
1:D:487:CYS:SG	1:D:512:CYS:SG	3.10	0.50
1:D:208:ILE:O	1:D:213:HIS:HE1	1.95	0.50
1:D:781:LEU:HD12	1:D:890:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:ILE:HD11	1:B:741:ARG:HA	1.94	0.50
1:D:76:VAL:HG12	1:D:76:VAL:O	2.12	0.50
8:B:3003:BMA:C1	3:G:2:NAG:O4	2.60	0.50
1:C:323:GLN:CG	1:C:351:THR:OG1	2.55	0.50
1:C:522:GLN:HE21	1:C:526:HIS:HD2	1.58	0.50
1:A:113:VAL:HG13	1:A:129:ILE:HG23	1.94	0.49
1:B:647:LEU:HD11	1:B:752:ASP:HB3	1.92	0.49
1:B:858:ARG:HB3	1:B:866:MET:HG3	1.94	0.49
1:D:790:ASN:ND2	10:D:1421:HOH:O	2.44	0.49
1:A:354:THR:HG23	1:A:358:TYR:CD2	2.48	0.49
1:C:40:VAL:HG13	10:C:1204:HOH:O	2.12	0.49
1:C:784:ILE:HD11	6:C:7001:PEG:H12	1.93	0.49
1:D:332:LEU:HB2	1:D:372:PHE:HA	1.94	0.49
1:B:784:ILE:CD1	6:B:7001:PEG:H41	2.42	0.49
1:C:193:TYR:OH	1:C:195:GLN:NE2	2.38	0.49
1:C:555:ARG:O	1:C:567:HIS:CE1	2.65	0.49
1:A:823:ASN:HD22	1:A:898:TRP:HE1	1.58	0.49
1:C:404:ASN:ND2	10:C:1128:HOH:O	2.44	0.49
1:D:215:ARG:NH1	1:D:698:ASP:OD2	2.45	0.49
1:B:326:ARG:HH11	1:B:636:HIS:CD2	2.31	0.49
1:B:375:LEU:HB3	1:B:376:PRO:HD3	1.94	0.49
1:C:362:LYS:HD2	1:C:435:TRP:HB3	1.94	0.49
1:D:325:SER:HB2	1:D:353:VAL:HB	1.95	0.49
1:D:408:TYR:CZ	1:D:410:THR:HB	2.48	0.49
1:B:192:GLN:HE22	1:B:491:LYS:HB2	1.78	0.49
1:C:192:GLN:HE22	1:C:491:LYS:HB2	1.78	0.48
1:A:861:GLU:HG3	1:A:894:PHE:CE1	2.49	0.48
1:D:445:THR:OG1	1:D:518:ASN:HB3	2.12	0.48
1:A:237:ASN:HD22	1:A:237:ASN:C	2.17	0.48
1:B:337:GLU:HG3	10:B:999:HOH:O	2.14	0.48
1:B:846:LYS:HD2	6:B:7001:PEG:H42	1.95	0.48
1:A:847:ILE:HD12	1:A:881:LEU:HD23	1.96	0.47
1:A:522:GLN:NE2	1:A:526:HIS:CD2	2.82	0.47
1:B:792:THR:HG23	1:B:820:VAL:O	2.15	0.47
1:D:567:HIS:O	1:D:597:VAL:HA	2.15	0.47
1:B:720:VAL:CG1	1:B:749:LEU:HD12	2.44	0.47
1:D:92:GLY:HA3	1:D:117:THR:HG22	1.96	0.47
1:D:200:LEU:HB2	1:D:277:PRO:HG2	1.97	0.47
1:D:270:GLU:HG3	1:D:499:PRO:CB	2.44	0.47
1:A:518:ASN:ND2	10:A:1543:HOH:O	2.45	0.47
1:B:255:SER:OG	1:B:257:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:781:LEU:CD1	1:D:890:LEU:HD11	2.45	0.47
1:C:329:TYR:O	1:C:330:LYS:HB2	2.15	0.47
1:D:785:VAL:HG11	1:D:820:VAL:HG21	1.96	0.47
1:C:83:VAL:HG13	1:C:163:GLN:HA	1.97	0.46
1:A:51:THR:HG23	1:A:54:ILE:H	1.79	0.46
1:D:141:HIS:CD2	1:D:144:VAL:H	2.33	0.46
1:C:720:VAL:HG12	1:C:749:LEU:HD12	1.96	0.46
1:A:364:ASP:OD2	1:A:394:ASP:O	2.33	0.46
1:B:522:GLN:HE21	1:B:526:HIS:HD2	1.63	0.46
1:D:472:ASP:OD2	9:D:5001:KTL:H22	2.16	0.46
1:D:724:ILE:HD11	1:D:741:ARG:N	2.31	0.46
1:B:850:LEU:HD11	1:B:881:LEU:HB2	1.97	0.46
1:C:51:THR:HG23	1:C:54:ILE:H	1.81	0.46
1:D:576:TRP:NE1	1:D:715:GLN:HG3	2.31	0.46
1:B:270:GLU:OE1	1:B:500:ASP:N	2.45	0.46
1:D:724:ILE:HD11	1:D:740:TRP:C	2.36	0.46
1:A:58:ARG:O	1:A:79:HIS:HE1	1.99	0.46
1:B:169:GLN:HG3	1:B:178:THR:HG23	1.97	0.46
1:C:861:GLU:O	1:C:864:GLN:HB2	2.16	0.46
1:C:842:PHE:HB2	1:C:888:LEU:HB2	1.98	0.45
1:B:40:VAL:O	1:B:42:ILE:HD12	2.16	0.45
1:B:567:HIS:O	1:B:597:VAL:HA	2.16	0.45
1:A:720:VAL:CG1	1:A:749:LEU:HD12	2.47	0.45
1:A:396:ALA:HB1	1:A:439:THR:HB	1.97	0.45
1:D:702:LEU:HA	1:D:707:LEU:O	2.17	0.45
1:D:845:VAL:HG23	1:D:883:ILE:HB	1.99	0.45
1:A:354:THR:CG2	1:A:358:TYR:HD2	2.26	0.45
1:A:446:ASN:HA	1:A:447:PRO:HD2	1.86	0.45
1:B:421:ILE:HG12	1:B:517:GLN:HG2	1.99	0.45
1:C:62:TRP:CZ2	1:C:64:PRO:HG3	2.51	0.45
1:C:567:HIS:O	1:C:597:VAL:HA	2.16	0.45
1:D:45:ILE:CG2	1:D:48:GLN:HG2	2.47	0.45
1:A:318:TRP:CE3	1:A:388:LYS:HG3	2.52	0.45
1:B:394:ASP:HB3	10:B:1069:HOH:O	2.16	0.45
1:C:172:ARG:HD3	1:C:257:LYS:HD3	1.98	0.45
1:C:188:VAL:HB	1:C:195:GLN:HB3	1.98	0.45
1:D:194:LEU:HB2	1:D:283:VAL:HG13	1.98	0.45
1:B:354:THR:CG2	1:B:358:TYR:CD2	2.99	0.44
1:C:208:ILE:O	1:C:213:HIS:HE1	1.99	0.44
1:D:141:HIS:HD2	1:D:144:VAL:H	1.65	0.44
1:D:188:VAL:HB	1:D:195:GLN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HE3	10:A:1083:HOH:O	2.17	0.44
1:D:595:PRO:HD2	10:D:969:HOH:O	2.16	0.44
1:B:33:VAL:HG13	1:B:35:ASN:H	1.81	0.44
1:C:741:ARG:N	1:C:743:GLN:HE21	1.95	0.44
1:A:521:LYS:HB2	1:A:521:LYS:HE2	1.68	0.44
1:B:720:VAL:HG13	1:B:747:MET:HB3	1.99	0.44
1:D:835:GLN:N	1:D:835:GLN:OE1	2.51	0.44
1:B:720:VAL:HG11	1:B:749:LEU:HD12	1.99	0.44
1:C:720:VAL:CG1	1:C:749:LEU:HD12	2.47	0.44
1:D:167:SER:CB	1:D:182:THR:HG22	2.47	0.44
1:D:724:ILE:HA	1:D:725:PRO:HD3	1.72	0.44
1:C:200:LEU:HD12	1:C:205:ILE:HD11	1.98	0.44
1:D:323:GLN:OE1	10:D:974:HOH:O	2.21	0.44
1:D:660:TYR:HA	1:D:663:LEU:HG	2.00	0.44
1:B:355:ASP:O	1:B:358:TYR:HD2	2.01	0.43
1:C:364:ASP:HB3	1:C:365:PHE:CD2	2.52	0.43
1:D:42:ILE:HD13	1:D:184:ILE:O	2.18	0.43
1:B:164:ASN:HA	1:B:165:PRO:HA	1.80	0.43
1:C:160:LYS:HB2	10:C:1369:HOH:O	2.17	0.43
1:B:864:GLN:CB	1:B:865:PRO:HD2	2.47	0.43
1:C:394:ASP:HB3	10:C:1006:HOH:O	2.17	0.43
1:A:851:THR:HG22	10:A:1300:HOH:O	2.19	0.43
1:B:30:CYS:HA	1:B:31:PRO:HD3	1.91	0.43
1:B:535:ILE:O	1:B:539:GLN:HG2	2.18	0.43
1:C:702:LEU:HA	1:C:707:LEU:O	2.18	0.43
1:A:413:ARG:O	1:A:417:GLN:HG2	2.18	0.43
1:B:724:ILE:CD1	1:B:729:TRP:HD1	2.31	0.43
1:A:326:ARG:HH11	1:A:636:HIS:CD2	2.36	0.43
1:A:785:VAL:HG11	1:A:820:VAL:HG21	2.00	0.43
1:C:325:SER:HB2	1:C:353:VAL:HB	2.00	0.43
1:D:110:ILE:HD12	1:D:189:TYR:CD2	2.54	0.43
1:D:522:GLN:NE2	1:D:526:HIS:CD2	2.82	0.43
1:A:394:ASP:HB3	10:A:933:HOH:O	2.19	0.43
1:A:720:VAL:HG11	1:A:749:LEU:HD12	2.01	0.43
1:A:728:ILE:HG23	1:A:737:LYS:HE2	2.00	0.43
1:B:404:ASN:HB2	10:B:1242:HOH:O	2.19	0.43
1:C:647:LEU:HD11	1:C:752:ASP:HB3	2.01	0.43
1:D:113:VAL:CG1	1:D:129:ILE:HG22	2.49	0.43
1:B:58:ARG:O	1:B:79:HIS:HE1	2.02	0.42
1:B:96:LYS:HG3	10:B:1144:HOH:O	2.18	0.42
1:C:504:LYS:HE2	1:C:504:LYS:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:VAL:HG12	1:D:117:THR:HB	2.00	0.42
1:C:555:ARG:O	1:C:567:HIS:HE1	2.03	0.42
1:C:844:THR:HG22	10:C:1159:HOH:O	2.19	0.42
1:A:871:ASN:ND2	1:A:885:ASP:OD1	2.51	0.42
1:B:847:ILE:HD13	1:B:881:LEU:HD23	2.00	0.42
1:C:213:HIS:ND1	1:C:588:GLU:OE2	2.52	0.42
1:D:359:MET:HA	1:D:366:THR:O	2.19	0.42
1:A:327:TRP:CD2	1:A:632:ASP:HB2	2.54	0.42
1:B:70:ILE:HA	1:B:71:PRO:HD3	1.91	0.42
1:D:361:ASP:HB2	1:D:363:LYS:HD2	2.01	0.42
1:B:229:THR:O	1:B:526:HIS:CE1	2.67	0.42
1:C:45:ILE:CG2	1:C:48:GLN:HG2	2.49	0.42
1:C:252:GLU:O	1:C:253:ASP:HB3	2.19	0.42
1:C:521:LYS:HB2	1:C:521:LYS:HE2	1.47	0.42
1:D:807:THR:O	1:D:812:ASN:N	2.49	0.42
1:A:207:GLY:O	1:A:218:HIS:CE1	2.71	0.42
1:B:861:GLU:OE2	1:B:892:ARG:HD2	2.20	0.42
1:A:29:LYS:HE3	1:A:59:GLY:HA2	2.02	0.42
1:D:326:ARG:HG2	1:D:329:TYR:CE1	2.55	0.42
1:A:97:LEU:HB2	1:A:113:VAL:HG12	2.01	0.41
1:B:208:ILE:O	1:B:213:HIS:HE1	2.02	0.41
1:B:354:THR:HB	1:B:389:TYR:HE1	1.85	0.41
1:C:393:LEU:HD12	1:C:469:LEU:HD22	2.01	0.41
1:A:548:LYS:HA	1:A:548:LYS:HD3	1.89	0.41
1:D:326:ARG:HG2	1:D:329:TYR:CZ	2.55	0.41
1:A:462:GLN:NE2	10:A:1084:HOH:O	2.53	0.41
1:C:417:GLN:NE2	10:C:1286:HOH:O	2.53	0.41
1:C:605:VAL:O	1:C:606:ALA:HB3	2.20	0.41
1:A:164:ASN:HA	1:A:165:PRO:HA	1.86	0.41
1:C:184:ILE:HD13	1:C:199:ARG:CZ	2.50	0.41
1:D:328:ASN:ND2	1:D:632:ASP:OD1	2.52	0.41
1:D:691:ASP:OD1	1:D:723:TYR:OH	2.20	0.41
1:C:276:THR:N	1:C:277:PRO:HA	2.35	0.41
1:C:740:TRP:HA	1:C:743:GLN:NE2	2.36	0.41
1:B:728:ILE:CD1	1:B:789:GLU:HG3	2.51	0.41
1:D:808:ILE:H	1:D:808:ILE:HG12	1.74	0.41
1:B:328:ASN:HA	1:B:357:ASP:CG	2.41	0.41
1:B:740:TRP:CG	1:B:745:VAL:HG11	2.55	0.41
1:A:58:ARG:O	1:A:79:HIS:CE1	2.74	0.41
1:B:445:THR:HB	1:B:519:TRP:CG	2.55	0.41
1:D:655:TYR:CZ	1:D:754:ILE:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:763:ILE:HD11	1:D:820:VAL:HG23	2.02	0.41
1:A:128:LYS:HA	1:A:288:LEU:O	2.20	0.41
1:B:794:LYS:HD3	10:B:951:HOH:O	2.20	0.41
1:B:842:PHE:HB2	1:B:888:LEU:HB2	2.03	0.41
1:D:509:LYS:HZ3	9:D:5001:KTL:CAL	2.34	0.41
1:B:724:ILE:O	1:B:724:ILE:HG13	2.21	0.40
1:C:432:GLY:HA2	1:C:480:ILE:HD11	2.03	0.40
1:D:218:HIS:HD2	10:D:963:HOH:O	2.03	0.40
1:A:421:ILE:HG12	1:A:517:GLN:HG2	2.02	0.40
1:A:589:PHE:CD2	1:A:594:ILE:HD12	2.57	0.40
1:B:253:ASP:OD1	1:B:255:SER:OG	2.32	0.40
1:D:242:TYR:CE2	1:D:570:GLY:HA3	2.56	0.40
1:D:589:PHE:HD2	1:D:594:ILE:HD12	1.86	0.40
1:B:445:THR:OG1	1:B:518:ASN:HB3	2.21	0.40
1:C:257:LYS:HE3	10:C:1344:HOH:O	2.19	0.40
1:B:314:MET:O	1:B:549:ARG:HD3	2.21	0.40
1:D:354:THR:HG22	1:D:358:TYR:HB3	2.03	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	A	869/898 (97%)	831 (96%)	32 (4%)	6 (1%)	19	13
1	B	867/898 (96%)	825 (95%)	36 (4%)	6 (1%)	19	13
1	C	869/898 (97%)	825 (95%)	38 (4%)	6 (1%)	19	13
1	D	847/898 (94%)	800 (94%)	45 (5%)	2 (0%)	44	44
All	All	3452/3592 (96%)	3281 (95%)	151 (4%)	20 (1%)	22	16

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	THR
1	B	276	THR
1	C	276	THR
1	D	276	THR
1	A	66	ASN
1	A	208	ILE
1	B	208	ILE
1	C	208	ILE
1	C	330	LYS
1	D	208	ILE
1	C	228	PHE
1	A	330	LYS
1	B	76	VAL
1	A	76	VAL
1	C	76	VAL
1	B	500	ASP
1	A	434	VAL
1	B	405	GLY
1	C	434	VAL
1	B	434	VAL

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	772/797 (97%)	756 (98%)	16 (2%)	48	53
1	B	770/797 (97%)	749 (97%)	21 (3%)	40	42
1	C	771/797 (97%)	759 (98%)	12 (2%)	58	64
1	D	751/797 (94%)	724 (96%)	27 (4%)	30	29
All	All	3064/3188 (96%)	2988 (98%)	76 (2%)	42	45

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	VAL
1	A	113	VAL

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Mol	Chain	Res	Type
1	A	169	GLN
1	A	215	ARG
1	A	237	ASN
1	A	254	THR
1	A	283	VAL
1	A	307	GLN
1	A	350	ASP
1	A	354	THR
1	A	434	VAL
1	A	484	THR
1	A	521	LYS
1	A	796	ASP
1	A	836	GLU
1	A	852	ASP
1	B	33	VAL
1	B	51	THR
1	B	184	ILE
1	B	194	LEU
1	B	202	SER
1	B	215	ARG
1	B	237	ASN
1	B	283	VAL
1	B	350	ASP
1	B	354	THR
1	B	357	ASP
1	B	434	VAL
1	B	484	THR
1	B	521	LYS
1	B	568	TRP
1	B	724	ILE
1	B	796	ASP
1	B	833	SER
1	B	851	THR
1	B	855	THR
1	B	877	SER
1	C	40	VAL
1	C	65	TRP
1	C	83	VAL
1	C	344	GLU
1	C	350	ASP
1	C	463	GLU
1	C	509	LYS

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Mol	Chain	Res	Type
1	C	568	TRP
1	C	817	THR
1	C	833	SER
1	C	853	SER
1	C	885	ASP
1	D	68	SER
1	D	85	ASP
1	D	87	THR
1	D	93	VAL
1	D	117	THR
1	D	182	THR
1	D	202	SER
1	D	283	VAL
1	D	293	LEU
1	D	324	LEU
1	D	350	ASP
1	D	415	ASN
1	D	484	THR
1	D	509	LYS
1	D	521	LYS
1	D	539	GLN
1	D	543	LYS
1	D	568	TRP
1	D	584	THR
1	D	685	LEU
1	D	715	GLN
1	D	724	ILE
1	D	808	ILE
1	D	826	ASP
1	D	835	GLN
1	D	851	THR
1	D	855	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	48	GLN
1	A	79	HIS
1	A	98	ASN
1	A	192	GLN
1	A	195	GLN

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Mol	Chain	Res	Type
1	A	218	HIS
1	A	237	ASN
1	A	267	ASN
1	A	319	ASN
1	A	418	HIS
1	A	448	ASN
1	A	462	GLN
1	A	465	GLN
1	A	481	GLN
1	A	493	ASN
1	A	518	ASN
1	A	522	GLN
1	A	526	HIS
1	A	636	HIS
1	A	654	GLN
1	A	743	GLN
1	A	791	ASN
1	A	823	ASN
1	B	39	ASN
1	B	48	GLN
1	B	79	HIS
1	B	108	ASN
1	B	192	GLN
1	B	195	GLN
1	B	218	HIS
1	B	237	ASN
1	B	267	ASN
1	B	448	ASN
1	B	455	ASN
1	B	462	GLN
1	B	493	ASN
1	B	518	ASN
1	B	526	HIS
1	B	636	HIS
1	B	715	GLN
1	B	743	GLN
1	B	790	ASN
1	B	823	ASN
1	C	32	ASN
1	C	39	ASN
1	C	48	GLN
1	C	79	HIS

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Mol	Chain	Res	Type
1	C	123	ASN
1	C	142	GLN
1	C	163	GLN
1	C	169	GLN
1	C	192	GLN
1	C	195	GLN
1	C	218	HIS
1	C	267	ASN
1	C	404	ASN
1	C	417	GLN
1	C	448	ASN
1	C	493	ASN
1	C	518	ASN
1	C	526	HIS
1	C	636	HIS
1	C	644	GLN
1	C	715	GLN
1	C	743	GLN
1	C	791	ASN
1	D	39	ASN
1	D	48	GLN
1	D	79	HIS
1	D	123	ASN
1	D	141	HIS
1	D	192	GLN
1	D	195	GLN
1	D	218	HIS
1	D	267	ASN
1	D	319	ASN
1	D	323	GLN
1	D	448	ASN
1	D	455	ASN
1	D	493	ASN
1	D	518	ASN
1	D	526	HIS
1	D	539	GLN
1	D	564	HIS
1	D	636	HIS
1	D	743	GLN
1	D	790	ASN
1	D	791	ASN
1	D	823	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

14 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	E	1	1,2	14,14,15	0.65	0	17,19,21	0.99	1 (5%)
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	1.18	2 (11%)
2	BMA	E	3	2	11,11,12	0.75	0	15,15,17	1.17	3 (20%)
2	MAN	E	4	2	11,11,12	0.56	0	15,15,17	0.95	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.57	0	17,19,21	1.20	1 (5%)
3	NAG	F	2	3	14,14,15	0.45	0	17,19,21	1.19	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.61	0	17,19,21	1.00	0
3	NAG	G	2	3	14,14,15	0.56	0	17,19,21	1.39	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.68	0	17,19,21	1.06	2 (11%)
2	NAG	H	2	2	14,14,15	0.49	0	17,19,21	1.49	1 (5%)
2	BMA	H	3	2	11,11,12	0.62	0	15,15,17	1.30	1 (6%)
2	MAN	H	4	2	11,11,12	0.65	0	15,15,17	0.77	0
3	NAG	I	1	1,3	14,14,15	0.69	1 (7%)	17,19,21	2.32	3 (17%)
3	NAG	I	2	3	14,14,15	0.45	0	17,19,21	2.50	5 (29%)

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	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	C1-C2	2.05	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	2	NAG	C1-O5-C5	8.32	123.34	112.19
3	I	1	NAG	C1-O5-C5	7.76	122.58	112.19
2	H	2	NAG	C1-O5-C5	5.59	119.68	112.19
2	H	3	BMA	C1-O5-C5	3.98	117.52	112.19
3	F	2	NAG	C1-O5-C5	3.98	117.52	112.19
3	G	2	NAG	C1-O5-C5	3.97	117.51	112.19
3	I	2	NAG	O5-C1-C2	3.43	116.59	111.29
2	E	2	NAG	C1-O5-C5	3.27	116.57	112.19
3	F	1	NAG	C1-O5-C5	3.09	116.33	112.19
3	I	1	NAG	C6-C5-C4	-2.83	106.06	113.02
3	I	2	NAG	O5-C5-C4	2.83	117.70	110.83
2	E	4	MAN	C1-O5-C5	2.77	115.90	112.19
3	I	1	NAG	C3-C4-C5	2.55	114.86	110.23
2	H	1	NAG	C1-O5-C5	2.53	115.57	112.19
2	E	3	BMA	C1-O5-C5	2.48	115.51	112.19
2	E	3	BMA	C2-C3-C4	2.47	115.21	110.86
3	I	2	NAG	C2-N2-C7	-2.45	119.62	122.90
3	I	2	NAG	C3-C4-C5	2.36	114.52	110.23
2	E	3	BMA	C3-C4-C5	2.29	114.39	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C4-C3-C2	-2.12	107.91	111.02
2	H	1	NAG	C4-C3-C2	2.04	114.01	111.02
2	E	1	NAG	C4-C3-C2	2.01	113.96	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

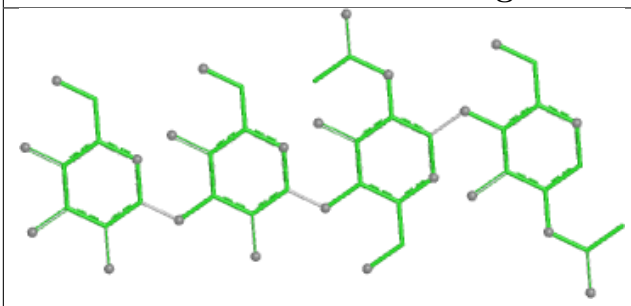
There are no ring outliers.

1 monomer is involved in 1 short contact:

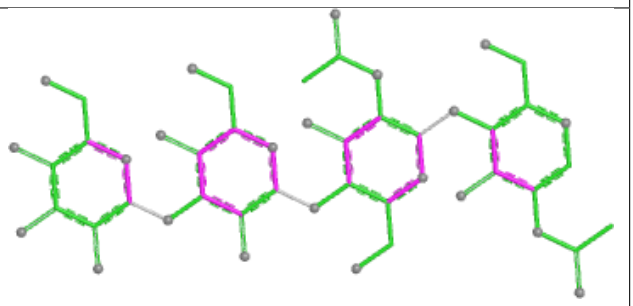
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0

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

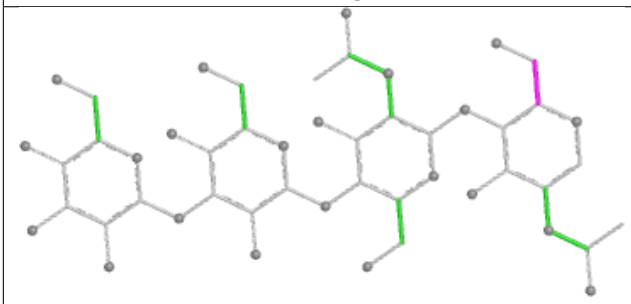
Oligosaccharide Chain E



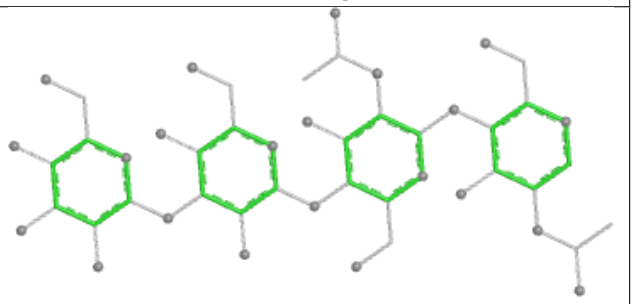
Bond lengths



Bond angles

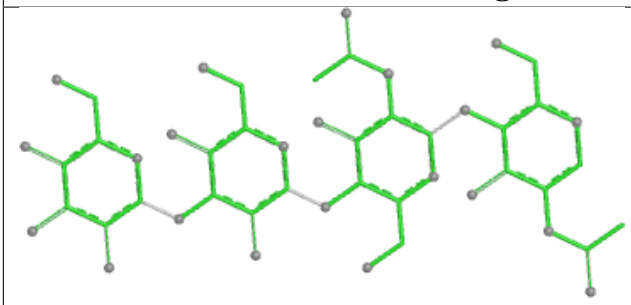


Torsions

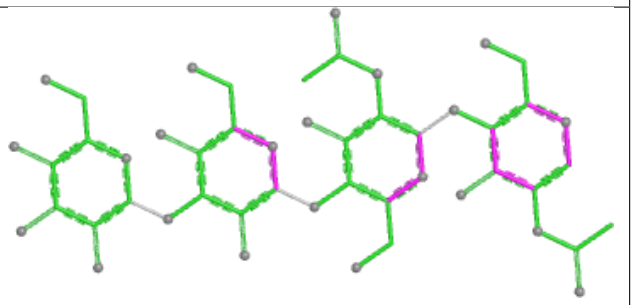


Rings

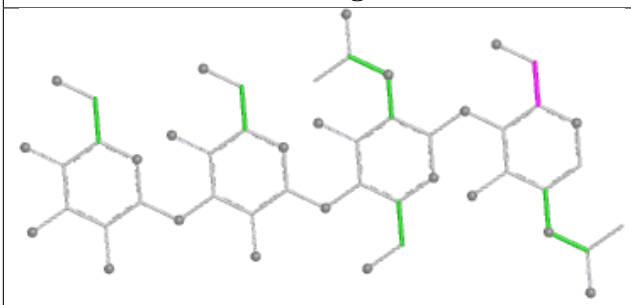
Oligosaccharide Chain H



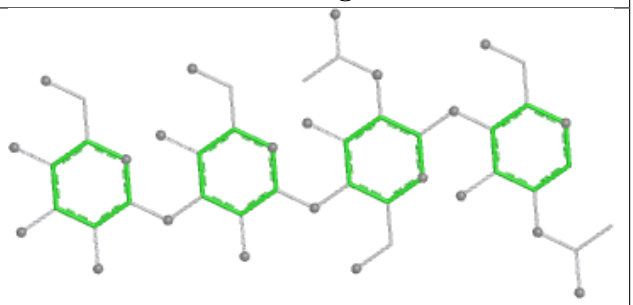
Bond lengths



Bond angles

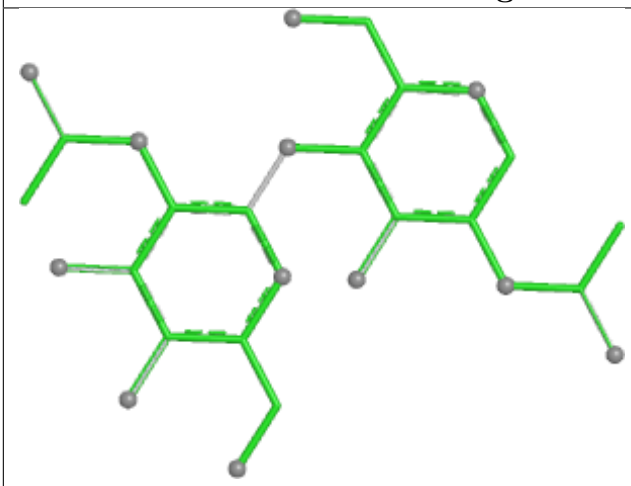


Torsions

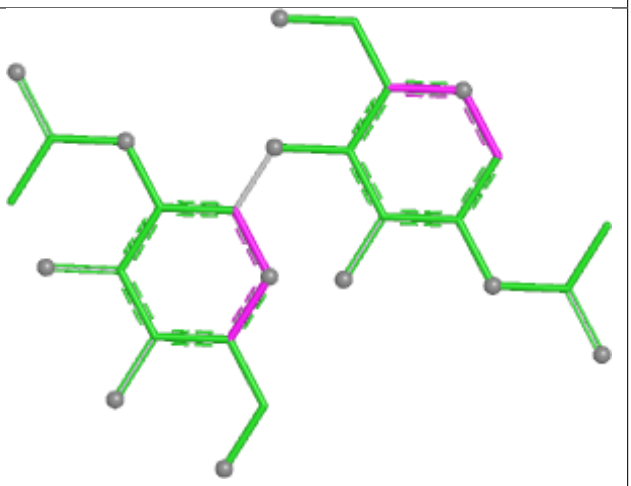


Rings

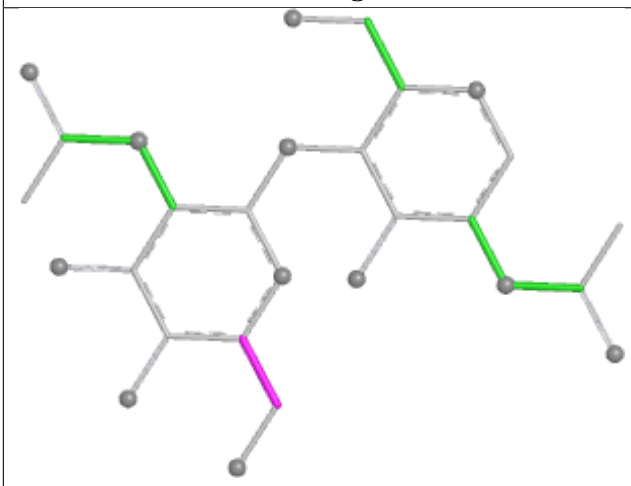
Oligosaccharide Chain F



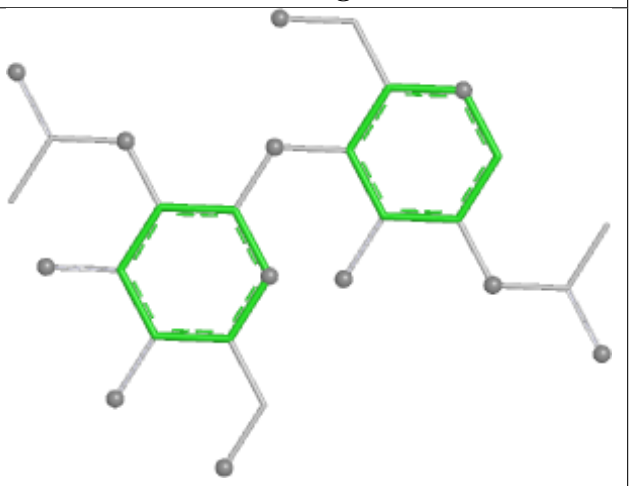
Bond lengths



Bond angles

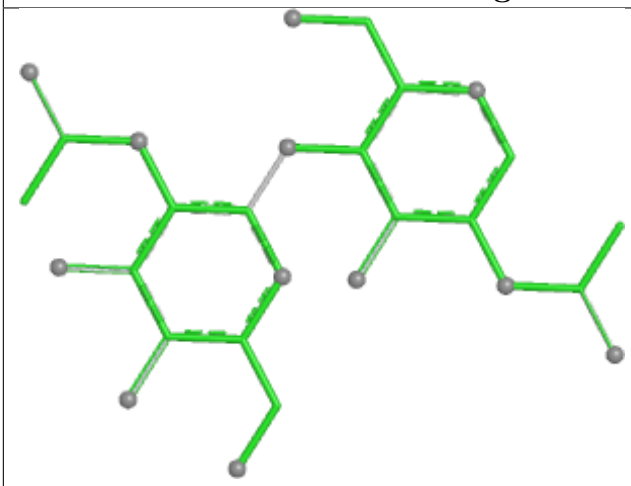


Torsions

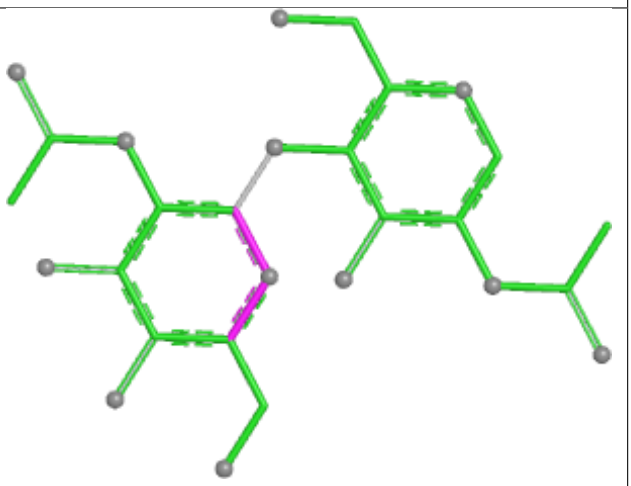


Rings

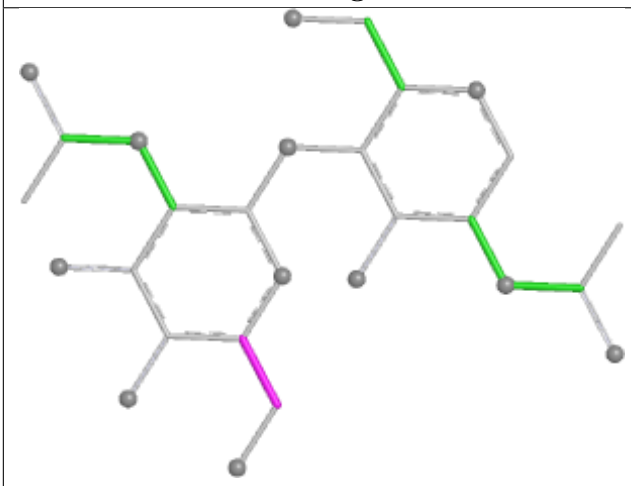
Oligosaccharide Chain G



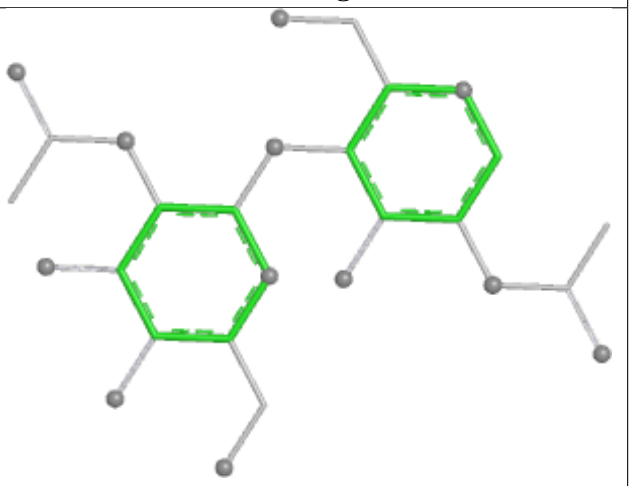
Bond lengths



Bond angles

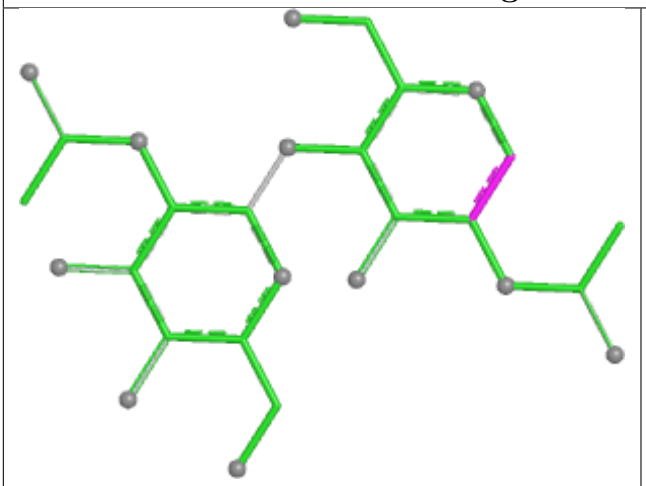


Torsions

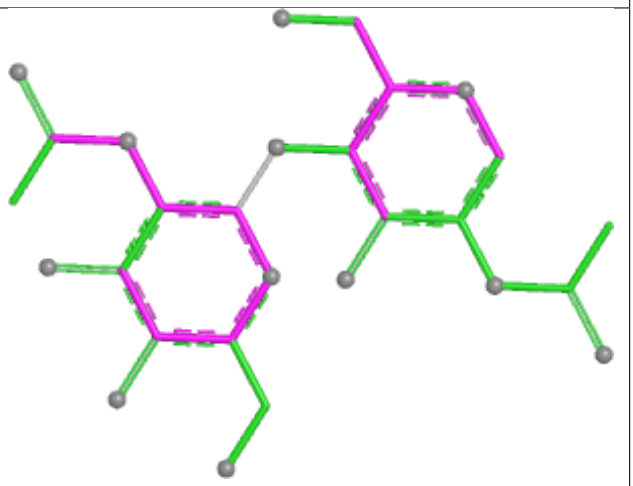


Rings

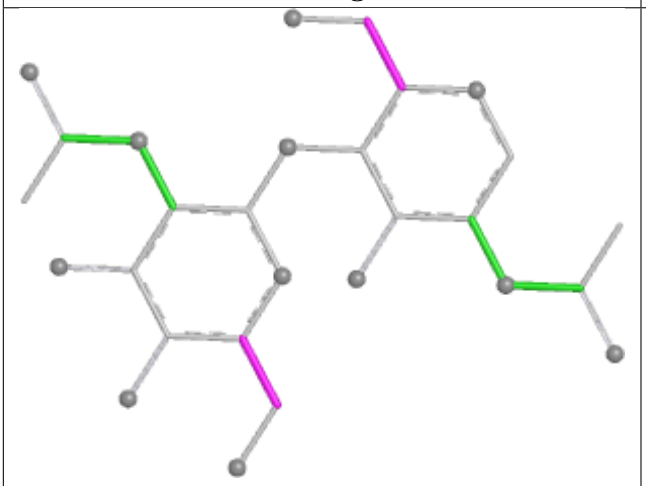
Oligosaccharide Chain I



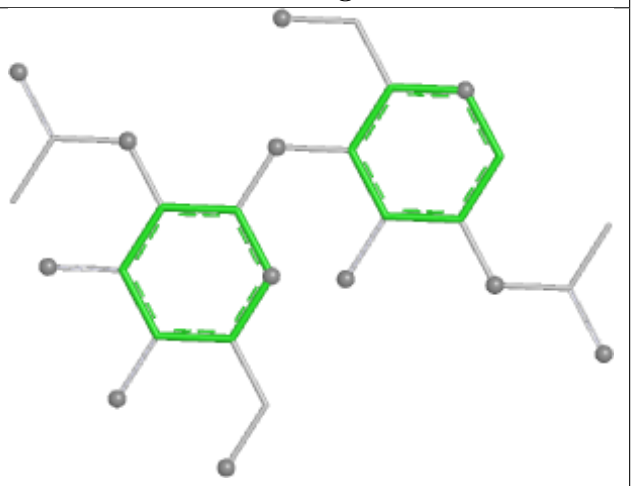
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\#\|Z\| > 2$
9	KTL	D	5001	-	21,26,26	1.86	2 (9%)	25,38,38	0.97	2 (8%)
4	NAG	C	2001	1	14,14,15	0.56	0	17,19,21	0.84	1 (5%)
6	PEG	A	7001	-	6,6,6	0.53	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	KTL	B	5001	-	21,26,26	1.77	1 (4%)	25,38,38	1.13	3 (12%)
6	PEG	D	7001	-	6,6,6	0.44	0	5,5,5	0.28	0
5	TRS	A	6001	-	7,7,7	0.48	0	9,9,9	1.05	1 (11%)
4	NAG	A	2001	1	14,14,15	0.56	0	17,19,21	2.00	1 (5%)
5	TRS	C	6001	-	7,7,7	0.33	0	9,9,9	0.45	0
4	NAG	A	4001	1	14,14,15	0.70	0	17,19,21	2.40	5 (29%)
4	NAG	B	2001	1	14,14,15	0.49	0	17,19,21	2.14	4 (23%)
4	NAG	C	4001	1	14,14,15	0.66	0	17,19,21	1.20	1 (5%)
8	BMA	B	3003	-	11,11,12	0.47	0	15,15,17	0.60	0
4	NAG	C	3001	1	14,14,15	0.48	0	17,19,21	1.28	1 (5%)
6	PEG	C	7001	-	6,6,6	0.46	0	5,5,5	0.25	0
6	PEG	B	7001	-	6,6,6	0.38	0	5,5,5	0.49	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
9	KTL	D	5001	-	-	12/28/45/45	0/1/1/1
4	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
6	PEG	A	7001	-	-	2/4/4/4	-
9	KTL	B	5001	-	-	6/28/45/45	0/1/1/1
6	PEG	D	7001	-	-	1/4/4/4	-
5	TRS	A	6001	-	-	0/9/9/9	-
4	NAG	A	2001	1	-	4/6/23/26	0/1/1/1
5	TRS	C	6001	-	-	0/9/9/9	-
4	NAG	A	4001	1	-	3/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	C	4001	1	-	2/6/23/26	0/1/1/1
8	BMA	B	3003	-	-	0/2/19/22	0/1/1/1
4	NAG	C	3001	1	-	0/6/23/26	0/1/1/1
6	PEG	C	7001	-	-	1/4/4/4	-
6	PEG	B	7001	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	5001	KTL	CAN-SAY	-7.84	1.66	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	5001	KTL	CAN-SAY	-7.09	1.67	1.82
9	D	5001	KTL	OAP-SAZ	2.40	1.64	1.57

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	NAG	C1-O5-C5	7.46	122.19	112.19
4	B	2001	NAG	C1-O5-C5	5.76	119.91	112.19
4	A	4001	NAG	C1-C2-N2	5.23	118.67	110.43
4	A	4001	NAG	C4-C3-C2	-4.99	103.71	111.02
4	A	4001	NAG	O5-C1-C2	-4.03	105.06	111.29
4	C	3001	NAG	C1-O5-C5	3.93	117.45	112.19
4	B	2001	NAG	C6-C5-C4	-3.89	103.48	113.02
4	A	4001	NAG	C2-N2-C7	3.72	127.88	122.90
4	C	4001	NAG	C1-O5-C5	3.61	117.02	112.19
4	B	2001	NAG	O5-C1-C2	-2.95	106.73	111.29
4	A	4001	NAG	C1-O5-C5	2.84	115.99	112.19
9	B	5001	KTL	OAD-CAR-CAN	2.57	114.69	109.66
9	B	5001	KTL	CAN-CAR-CAU	-2.51	104.25	106.43
5	A	6001	TRS	C1-C-N	-2.46	101.89	108.17
9	D	5001	KTL	OAP-CAX-CAS	2.34	110.47	106.35
9	D	5001	KTL	CAQ-CAT-CAV	2.24	115.92	112.48
4	B	2001	NAG	C3-C4-C5	2.21	114.25	110.23
9	B	5001	KTL	OAG-CAU-CAW	2.05	113.55	109.22
4	C	2001	NAG	O5-C5-C6	2.05	111.65	107.66

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4001	NAG	C1-C2-N2-C7
9	B	5001	KTL	OAB-CAM-CAW-CAU
9	B	5001	KTL	OAB-CAM-CAW-SAY
9	B	5001	KTL	OAF-CAT-CAV-CAX
9	D	5001	KTL	OAB-CAM-CAW-CAU
9	D	5001	KTL	OAB-CAM-CAW-SAY
9	D	5001	KTL	OAF-CAT-CAV-CAX
9	D	5001	KTL	CAQ-CAT-CAV-CAX
9	D	5001	KTL	OAA-CAL-CAQ-CAT
4	C	4001	NAG	C4-C5-C6-O6
9	D	5001	KTL	OAC-CAQ-CAT-CAV
9	D	5001	KTL	CAL-CAQ-CAT-OAF

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Mol	Chain	Res	Type	Atoms
9	D	5001	KTL	CAL-CAQ-CAT-CAV
9	D	5001	KTL	OAF-CAT-CAV-OAH
9	B	5001	KTL	CAQ-CAT-CAV-CAX
4	A	2001	NAG	O5-C5-C6-O6
4	C	4001	NAG	O5-C5-C6-O6
9	D	5001	KTL	OAA-CAL-CAQ-OAC
6	B	7001	PEG	O1-C1-C2-O2
4	A	2001	NAG	C4-C5-C6-O6
9	D	5001	KTL	OAC-CAQ-CAT-OAF
6	A	7001	PEG	O2-C3-C4-O4
9	B	5001	KTL	OAF-CAT-CAV-OAH
6	B	7001	PEG	O2-C3-C4-O4
9	D	5001	KTL	CAQ-CAT-CAV-OAH
4	A	4001	NAG	C4-C5-C6-O6
4	A	4001	NAG	O5-C5-C6-O6
6	A	7001	PEG	O1-C1-C2-O2
6	B	7001	PEG	C4-C3-O2-C2
6	C	7001	PEG	C1-C2-O2-C3
6	D	7001	PEG	C4-C3-O2-C2
4	A	2001	NAG	C8-C7-N2-C2
4	A	2001	NAG	O7-C7-N2-C2
9	B	5001	KTL	OAA-CAL-CAQ-OAC

There are no ring outliers.

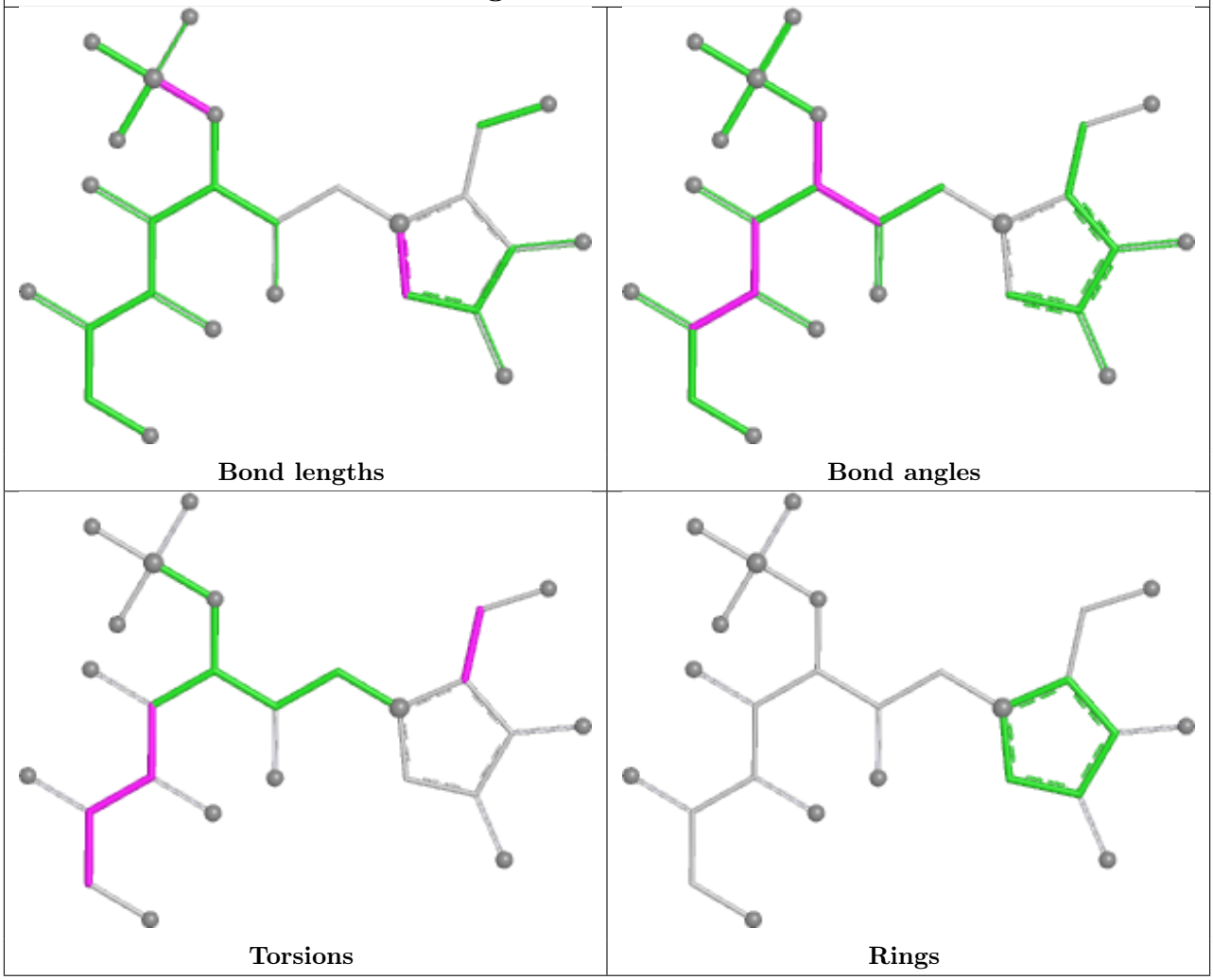
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	5001	KTL	2	0
8	B	3003	BMA	1	0
6	C	7001	PEG	3	0
6	B	7001	PEG	3	0

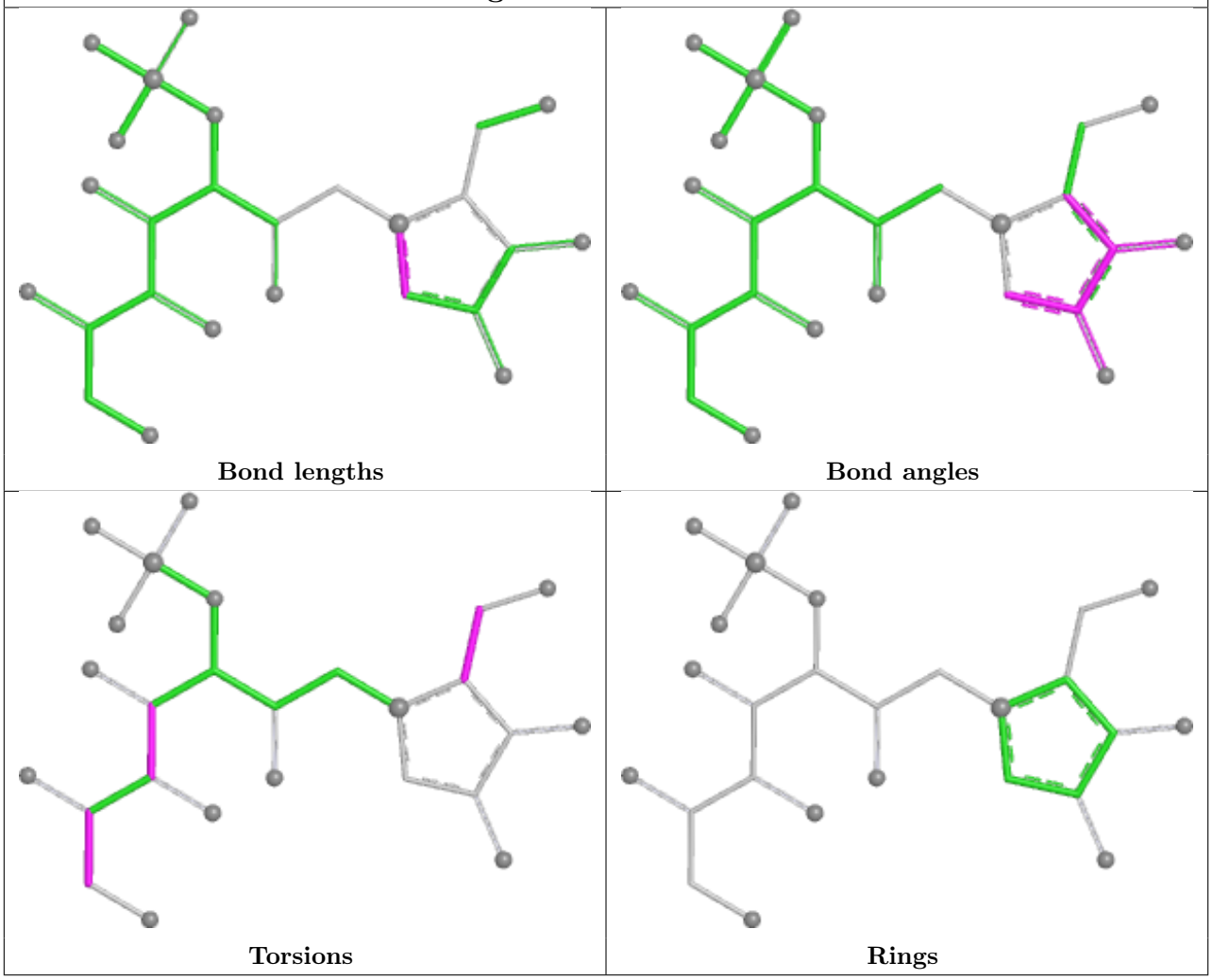
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 KTL D 5001



Ligand KTL B 5001



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

Warning: The R factor obtained from EDS is 0.2428, which does not match the depositor's R factor of 0.17693. Please interpret the results in this section carefully.

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	871/898 (96%)	0.05	23 (2%)	57	62	4, 10, 19, 36	0
1	B	869/898 (96%)	0.08	22 (2%)	58	63	3, 11, 20, 37	0
1	C	871/898 (96%)	0.16	26 (2%)	52	58	5, 11, 21, 30	0
1	D	853/898 (94%)	0.67	42 (4%)	36	41	3, 11, 20, 27	0
All	All	3464/3592 (96%)	0.24	113 (3%)	49	55	3, 11, 20, 37	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	865	PRO	4.6
1	B	403	ALA	4.6
1	D	150	PRO	4.3
1	A	148	THR	4.2
1	B	32	ASN	4.2
1	B	33	VAL	4.1
1	C	547	ASN	4.0
1	A	403	ALA	3.8
1	D	455	ASN	3.5
1	D	452	TRP	3.5
1	B	404	ASN	3.5
1	B	866	MET	3.4
1	D	802	GLY	3.4
1	A	404	ASN	3.4
1	A	146	GLU	3.3
1	A	32	ASN	3.2
1	B	862	ASN	3.2
1	B	463	GLU	3.2
1	A	33	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	416	THR	3.1
1	A	77	ASP	3.1
1	B	852	ASP	3.1
1	C	146	GLU	3.0
1	A	30	CYS	3.0
1	D	458	SER	3.0
1	C	856	GLU	3.0
1	A	85	ASP	2.9
1	D	149	GLY	2.9
1	D	345	ALA	2.7
1	C	412	GLU	2.7
1	C	465	GLN	2.7
1	D	816	TYR	2.7
1	A	154	ASP	2.7
1	B	30	CYS	2.7
1	C	775	ALA	2.7
1	C	401	ARG	2.7
1	C	546	PRO	2.6
1	D	457	CYS	2.6
1	B	369	GLN	2.6
1	D	418	HIS	2.6
1	A	35	ASN	2.6
1	C	835	GLN	2.6
1	D	375	LEU	2.6
1	C	463	GLU	2.6
1	C	538	GLU	2.6
1	A	134	ASN	2.6
1	C	377	GLN	2.6
1	D	534	ALA	2.5
1	D	451	ASP	2.5
1	D	91	ILE	2.5
1	A	153	SER	2.5
1	B	85	ASP	2.5
1	D	464	VAL	2.5
1	D	799	TRP	2.5
1	A	55	CYS	2.5
1	D	450	ILE	2.5
1	D	400	GLY	2.5
1	B	851	THR	2.5
1	D	808	ILE	2.4
1	C	464	VAL	2.4
1	D	449	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	866	MET	2.4
1	C	816	TYR	2.4
1	D	408	TYR	2.4
1	D	354	THR	2.3
1	D	426	GLY	2.3
1	A	68	SER	2.3
1	D	546	PRO	2.3
1	A	152	VAL	2.3
1	C	874	TYR	2.3
1	D	815	LEU	2.3
1	D	454	ALA	2.3
1	A	150	PRO	2.3
1	C	770	ASP	2.3
1	C	885	ASP	2.3
1	D	361	ASP	2.3
1	B	405	GLY	2.3
1	C	404	ASN	2.2
1	A	253	ASP	2.2
1	B	158	ASP	2.2
1	C	892	ARG	2.2
1	D	378	PHE	2.2
1	A	151	THR	2.2
1	D	770	ASP	2.2
1	D	633	GLY	2.2
1	C	35	ASN	2.2
1	B	377	GLN	2.2
1	D	538	GLU	2.2
1	D	453	TRP	2.2
1	D	547	ASN	2.2
1	B	856	GLU	2.1
1	D	460	PHE	2.1
1	A	34	LEU	2.1
1	B	855	THR	2.1
1	B	135	ARG	2.1
1	D	358	TYR	2.1
1	C	374	GLY	2.1
1	A	789	GLU	2.1
1	C	733	GLU	2.1
1	C	85	ASP	2.1
1	C	154	ASP	2.1
1	B	35	ASN	2.1
1	D	465	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	845	VAL	2.1
1	B	406	THR	2.1
1	D	162	ALA	2.1
1	C	101	PRO	2.1
1	B	809	GLN	2.1
1	D	369	GLN	2.1
1	D	389	TYR	2.0
1	A	111	ASN	2.0
1	A	145	LYS	2.0
1	D	512	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

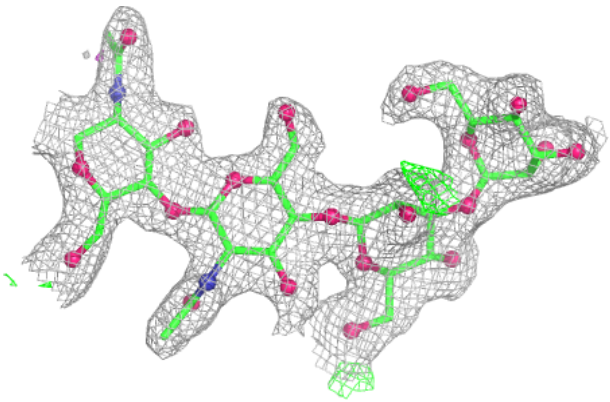
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

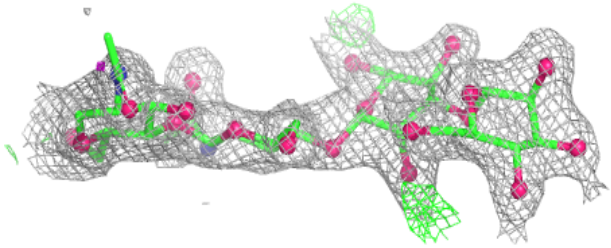
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	I	2	14/15	0.75	0.11	24,27,31,32	0
2	NAG	H	1	14/15	0.80	0.10	14,16,17,19	0
2	NAG	E	1	14/15	0.83	0.10	16,20,24,25	0
3	NAG	F	2	14/15	0.85	0.10	24,27,29,30	0
3	NAG	G	2	14/15	0.86	0.10	25,27,28,29	0
3	NAG	I	1	14/15	0.88	0.08	4,14,19,23	0
2	BMA	H	3	11/12	0.88	0.08	14,16,20,23	0
2	NAG	E	2	14/15	0.89	0.08	12,13,18,20	0
2	MAN	H	4	11/12	0.89	0.08	11,13,16,16	0
2	NAG	H	2	14/15	0.91	0.07	12,15,18,21	0
2	BMA	E	3	11/12	0.91	0.07	15,17,18,20	0
3	NAG	G	1	14/15	0.91	0.07	19,20,22,24	0
3	NAG	F	1	14/15	0.92	0.08	9,13,15,18	0
2	MAN	E	4	11/12	0.93	0.06	15,17,18,19	0

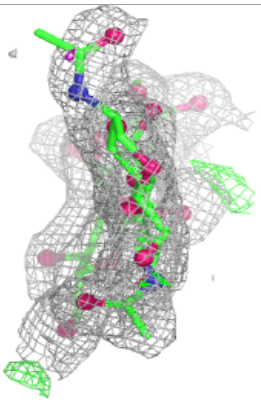
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

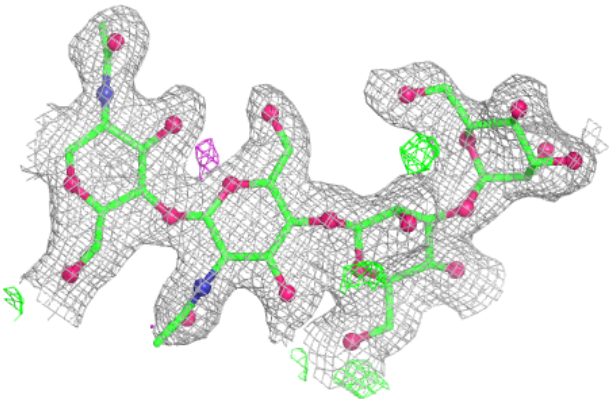


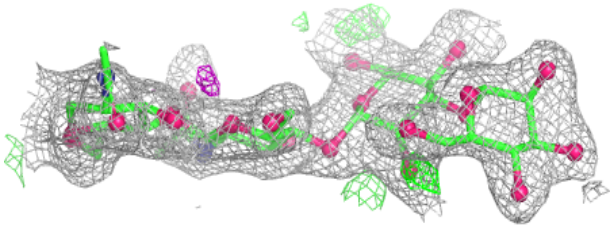


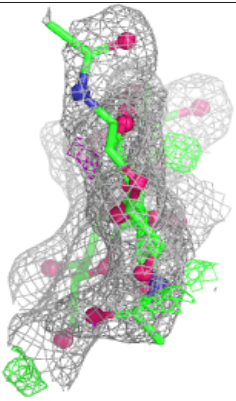


Electron density around Chain H:

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

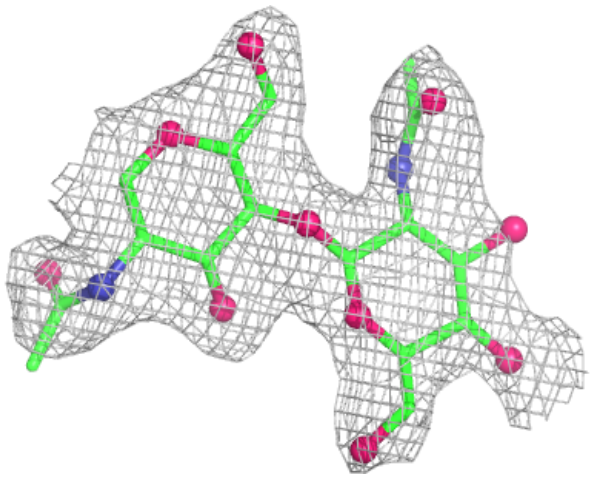


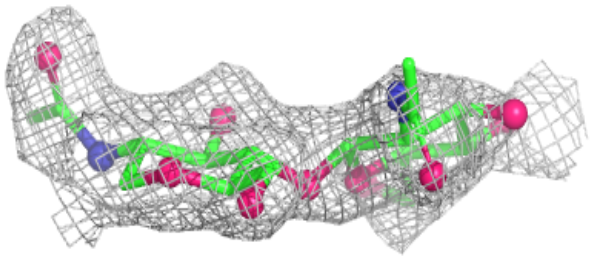


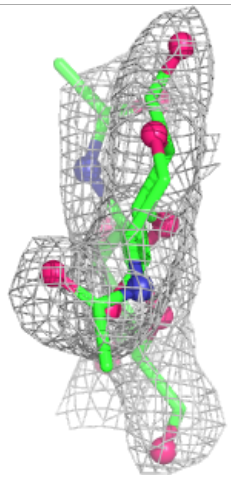


Electron density around Chain F:

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

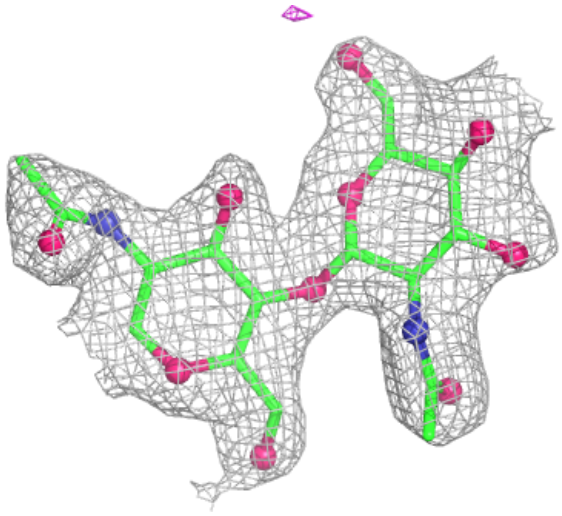


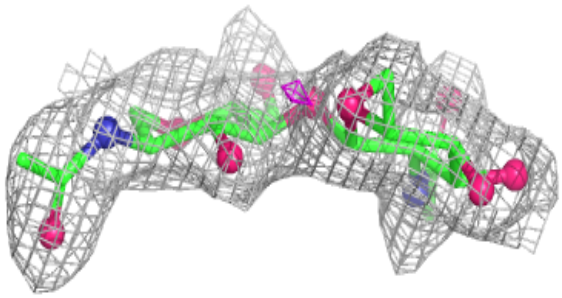


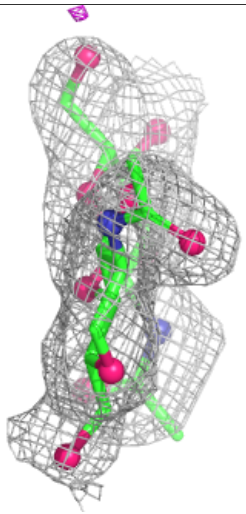


Electron density around Chain G:

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

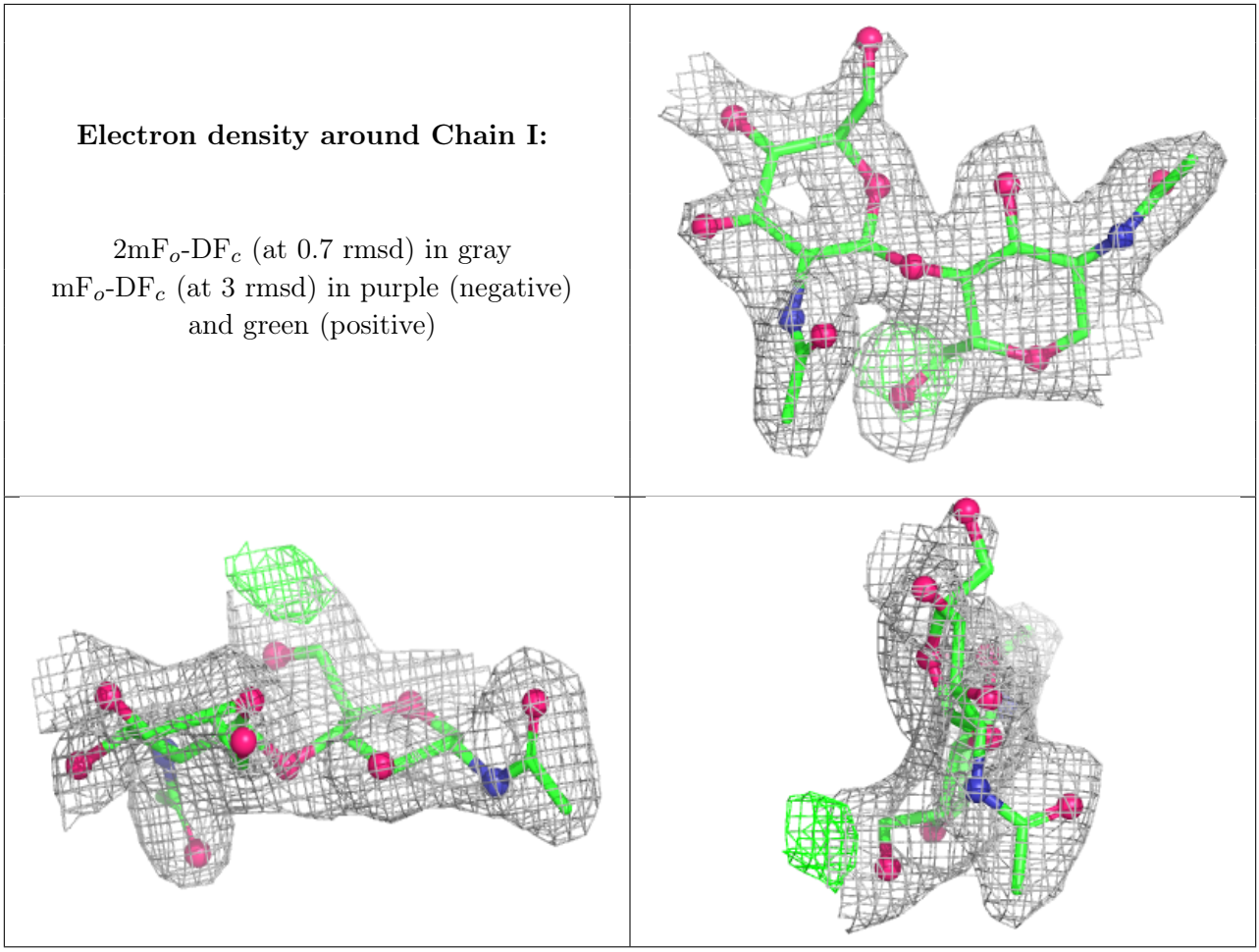






Electron density around Chain I:

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



6.4 Ligands

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
8	BMA	B	3003	11/12	0.62	0.19	61,62,63,63	0
4	NAG	A	2001	14/15	0.68	0.12	31,33,34,34	0
4	NAG	C	4001	14/15	0.73	0.12	35,40,41,42	0
4	NAG	A	4001	14/15	0.80	0.10	24,27,28,30	0
4	NAG	C	3001	14/15	0.80	0.10	22,25,26,27	0
6	PEG	D	7001	7/7	0.82	0.12	37,37,38,38	0
6	PEG	A	7001	7/7	0.85	0.13	21,22,25,25	0
6	PEG	C	7001	7/7	0.85	0.12	18,22,25,27	0
6	PEG	B	7001	7/7	0.87	0.13	20,20,21,22	0
5	TRS	A	6001	8/8	0.87	0.11	10,12,13,15	0
5	TRS	C	6001	8/8	0.87	0.09	20,20,20,21	0

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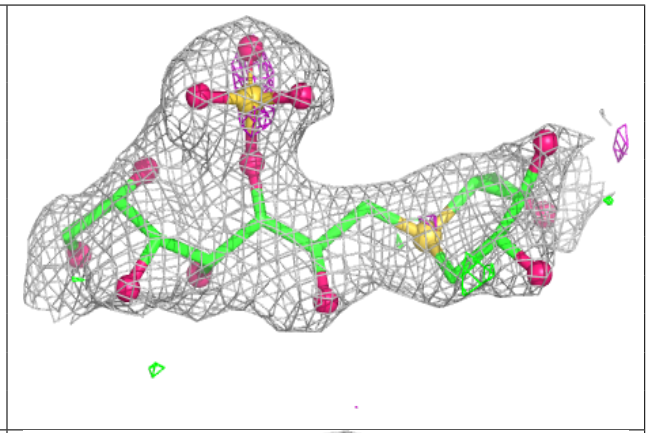
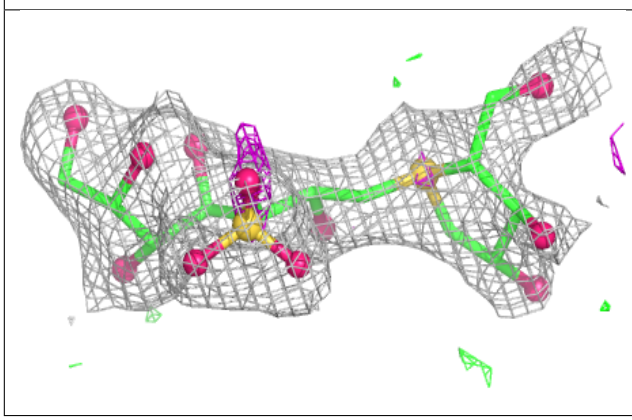
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	C	2001	14/15	0.87	0.08	16,22,26,27	0
9	KTL	D	5001	26/26	0.88	0.10	20,24,26,27	0
4	NAG	B	2001	14/15	0.89	0.08	9,16,18,21	0
9	KTL	B	5001	26/26	0.93	0.08	10,18,23,25	0
7	CL	A	8001	1/1	0.96	0.09	3,3,3,3	0

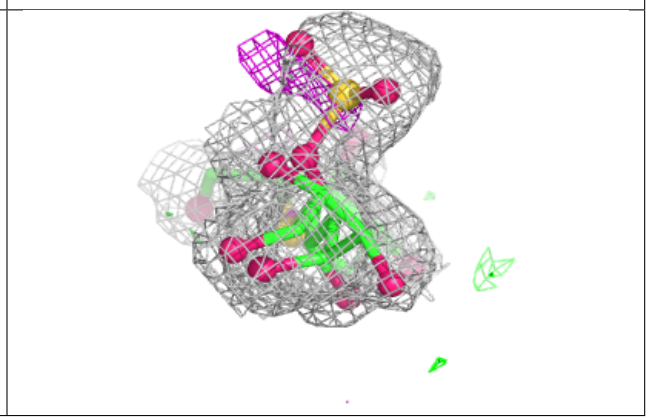
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KTL D 5001:

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

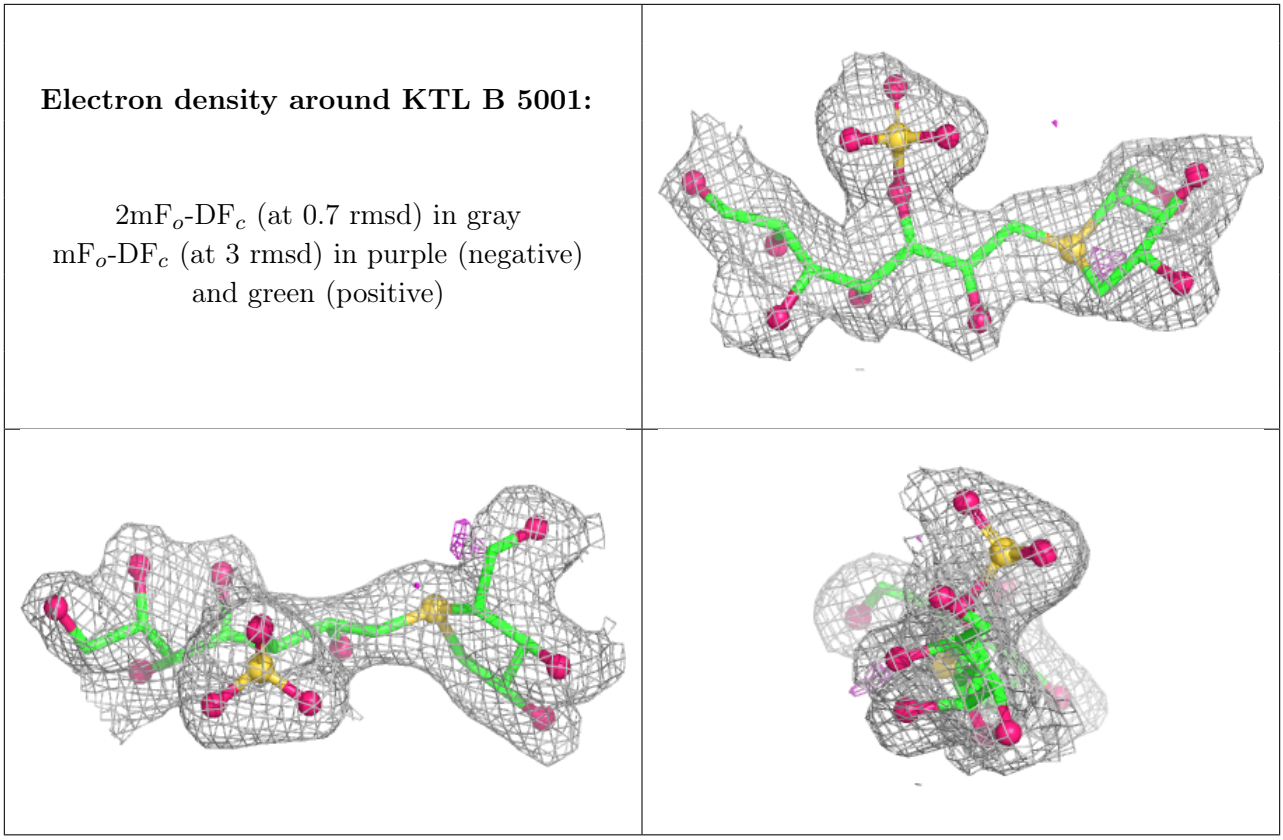






Electron density around KTL B 5001:

$2mF_o$-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.