



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:21 AM GMT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

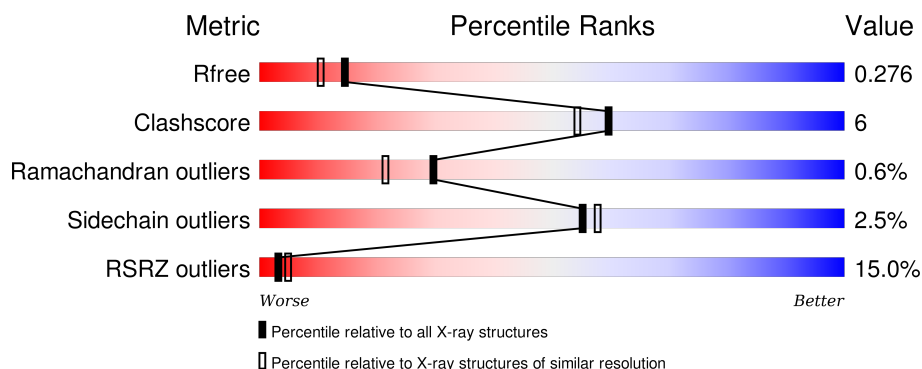
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	898	<div> <div>5%</div> <div>85%</div> <div>11%</div> <div>• •</div> </div>
1	B	898	<div> <div>5%</div> <div>83%</div> <div>13%</div> <div>• •</div> </div>
1	C	898	<div> <div>7%</div> <div>85%</div> <div>12%</div> <div>• •</div> </div>
1	D	898	<div> <div>40%</div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1002	-	-	-	X
3	NAG	C	3001	-	-	-	X
5	TRS	C	6001	-	-	-	X

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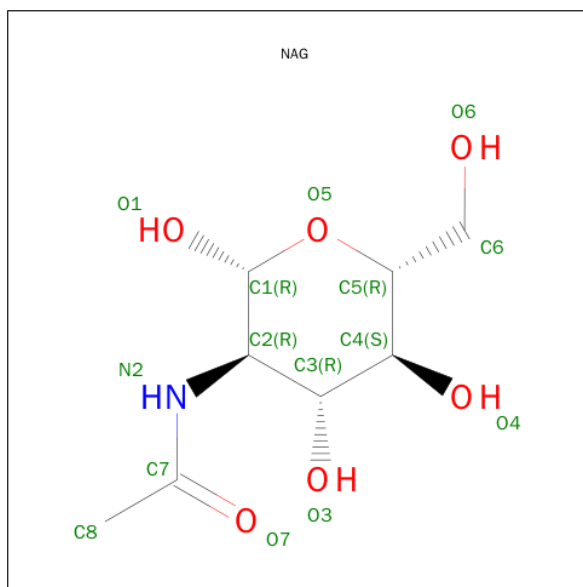
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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	PHE	-	EXPRESSION TAG	UNP P14410
D	23	GLN	-	EXPRESSION TAG	UNP P14410
D	24	SER	-	EXPRESSION TAG	UNP P14410
D	25	GLY	-	EXPRESSION TAG	UNP P14410
D	26	ILE	-	EXPRESSION TAG	UNP P14410
D	27	ARG	-	EXPRESSION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

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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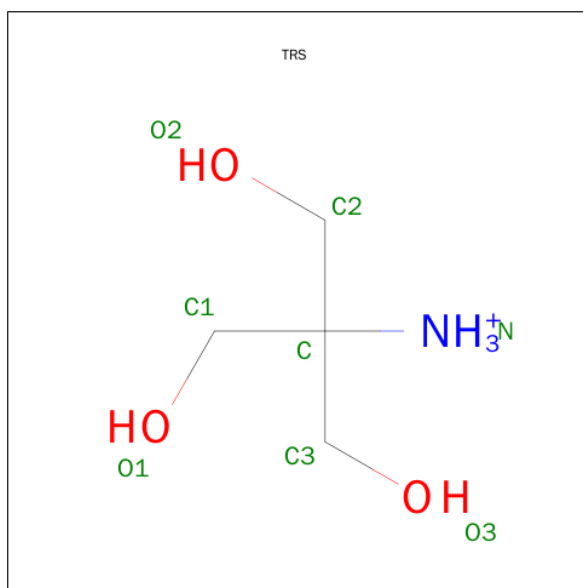
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

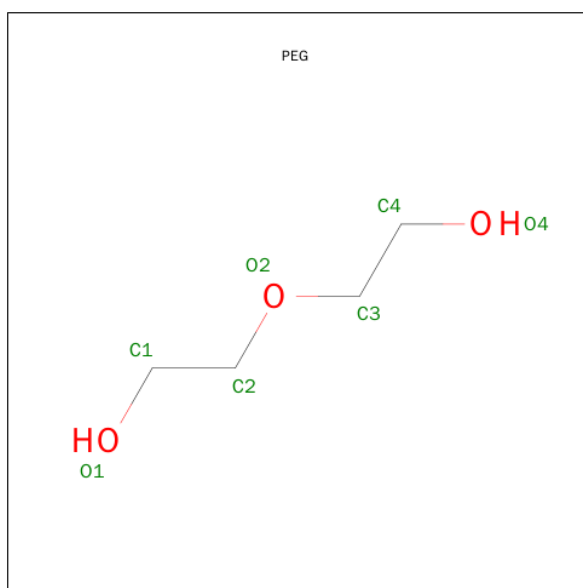
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



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

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

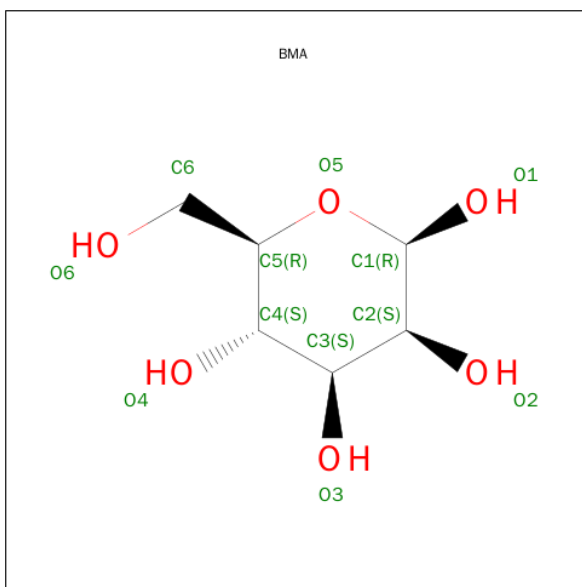


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

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

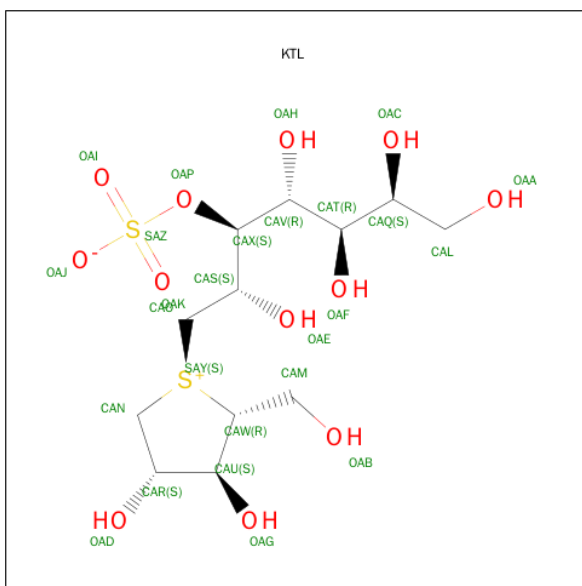
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

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



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

- 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: C₁₂H₂₄O₁₂S₂).



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		

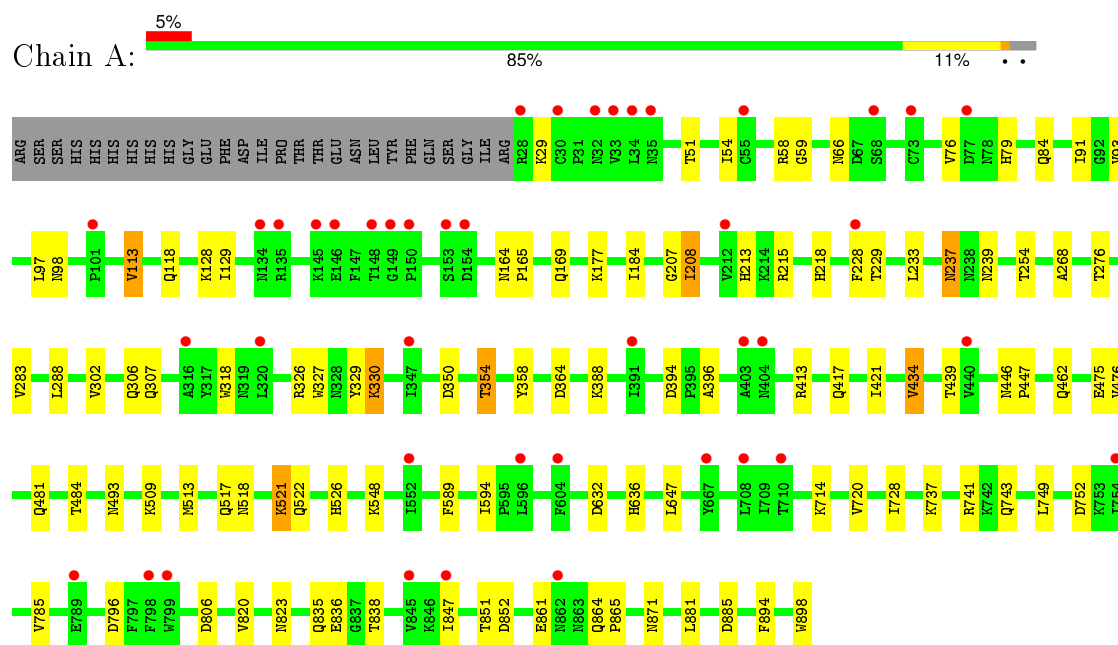
- Molecule 10 is water.

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

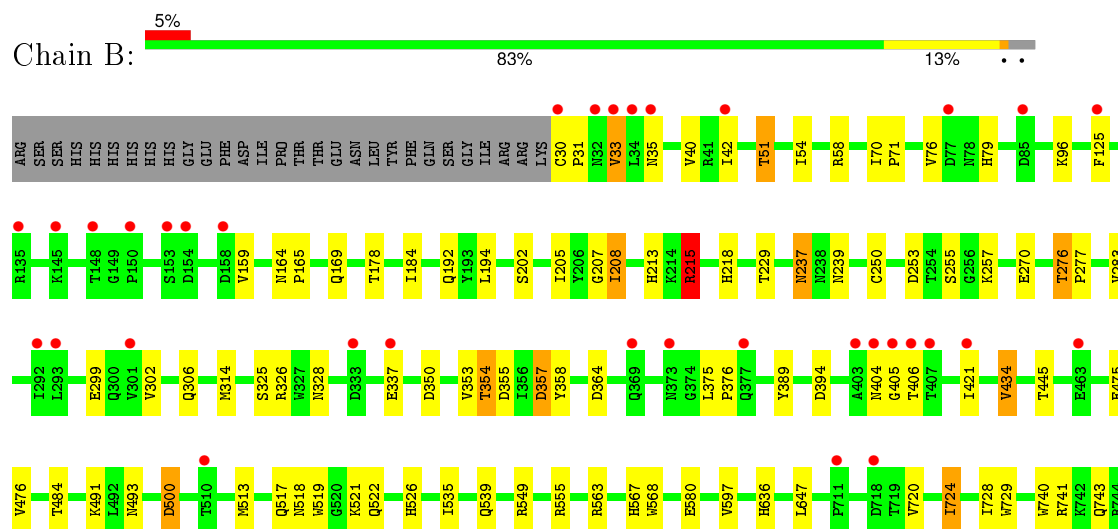
3 Residue-property plots

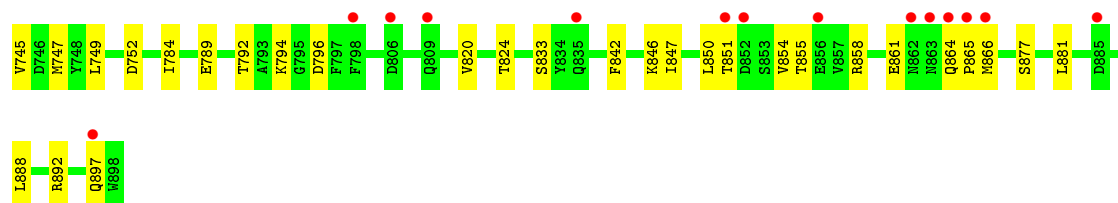
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Sucrase-isomaltase

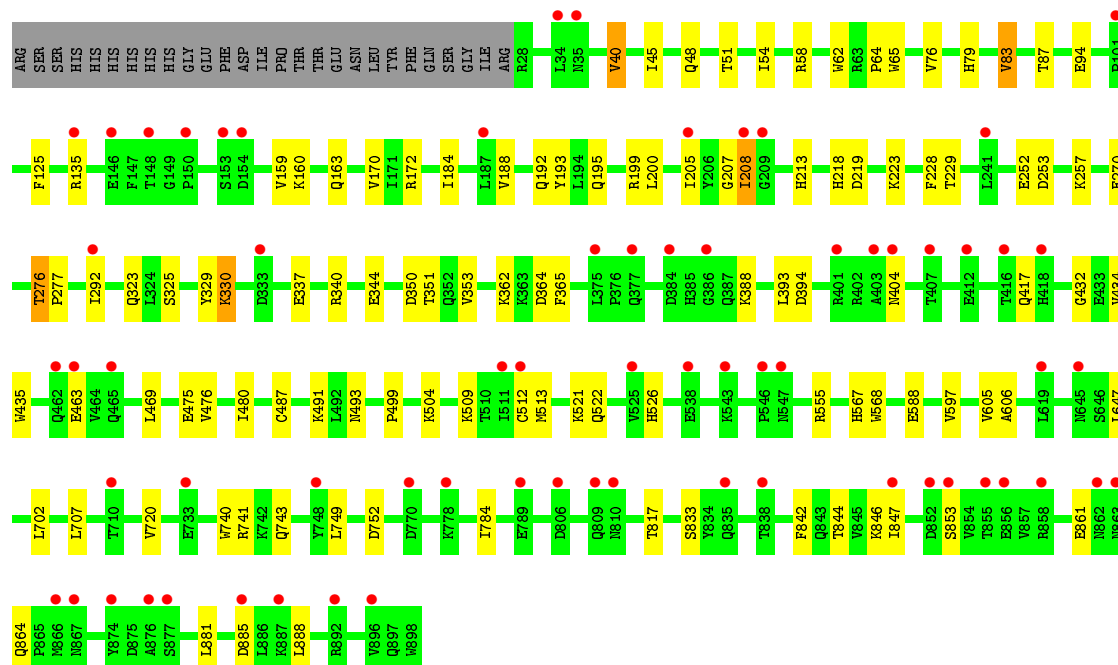
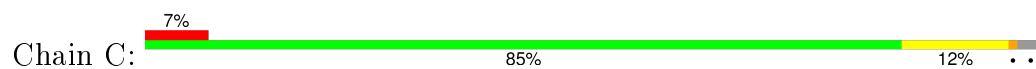


• Molecule 1: Sucrase-isomaltase

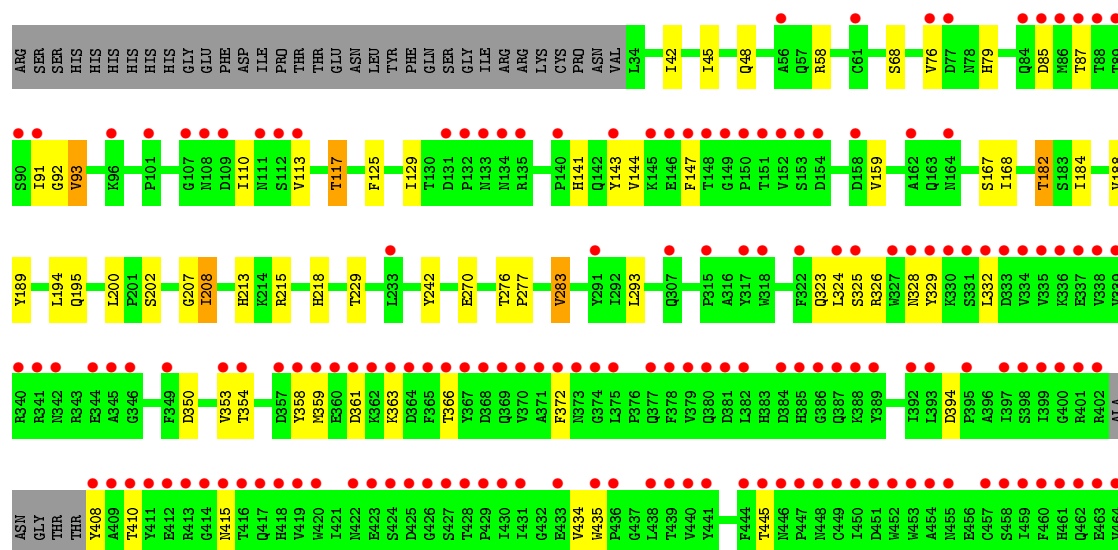
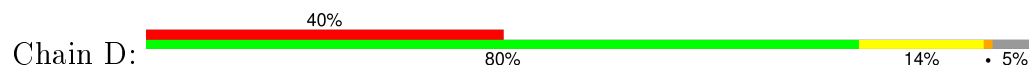




• Molecule 1: Sucrase-isomaltase



• Molecule 1: Sucrase-isomaltase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.40 Å 165.76 Å 341.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.15 19.94 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.8 (19.95-2.15) 94.8 (19.94-2.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.15 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.223 0.243 , 0.276	Depositor DCC
R_{free} test set	10150 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 202412 reflections (0.000%)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, CL, KTL, TRS, PEG, MAN

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(°)	Ideal(°)
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	A	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	50	0	43	0	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
3	C	42	0	39	0	0
4	A	28	0	25	0	0
4	B	28	0	25	1	0
4	D	28	0	25	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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	869/898 (97%)	831 (96%)	32 (4%)	6 (1%)	26	18
1	B	867/898 (96%)	825 (95%)	36 (4%)	6 (1%)	26	18
1	C	869/898 (97%)	825 (95%)	38 (4%)	6 (1%)	26	18
1	D	847/898 (94%)	800 (94%)	45 (5%)	2 (0%)	52	51
All	All	3452/3592 (96%)	3281 (95%)	151 (4%)	20 (1%)	30	21

5 of 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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	772/797 (97%)	756 (98%)	16 (2%)	61	65
1	B	770/797 (97%)	749 (97%)	21 (3%)	52	53
1	C	771/797 (97%)	759 (98%)	12 (2%)	70	76
1	D	751/797 (94%)	724 (96%)	27 (4%)	42	40
All	All	3064/3188 (96%)	2988 (98%)	76 (2%)	55	58

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	851	THR
1	C	463	GLU
1	D	724	ILE
1	B	855	THR
1	C	65	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	715	GLN
1	C	163	GLN
1	D	539	GLN
1	B	743	GLN
1	C	39	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 carbohydrates 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	1001	1,2	14,14,15	0.64	0	15,19,21	0.95	0
2	NAG	A	1002	2	14,14,15	0.45	0	15,19,21	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	A	1003	2	11,11,12	0.77	0	14,15,17	1.25	3 (21%)
2	MAN	A	1004	2	11,11,12	0.55	0	14,15,17	1.02	1 (7%)
4	NAG	A	3001	1,4	14,14,15	0.56	0	15,19,21	1.18	1 (6%)
4	NAG	A	3002	4	14,14,15	0.43	0	15,19,21	1.29	1 (6%)
4	NAG	B	3001	1,4	14,14,15	0.59	0	15,19,21	0.93	0
4	NAG	B	3002	4	14,14,15	0.54	0	15,19,21	1.44	1 (6%)
2	NAG	C	1001	1,2	14,14,15	0.65	0	15,19,21	1.05	1 (6%)
2	NAG	C	1002	2	14,14,15	0.47	0	15,19,21	1.66	1 (6%)
2	BMA	C	1003	2	11,11,12	0.60	0	14,15,17	1.43	1 (7%)
2	MAN	C	1004	2	11,11,12	0.64	0	14,15,17	0.82	0
4	NAG	D	2001	1,4	14,14,15	0.66	0	15,19,21	2.51	3 (20%)
4	NAG	D	2002	4	14,14,15	0.43	0	15,19,21	2.52	3 (20%)

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	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1004	2	-	0/2/19/22	0/1/1/1
4	NAG	A	3001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3002	4	-	0/6/23/26	0/1/1/1
4	NAG	B	3001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	3002	4	-	0/6/23/26	0/1/1/1
2	NAG	C	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	C	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	C	1004	2	-	0/2/19/22	0/1/1/1
4	NAG	D	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2002	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2001	NAG	C6-C5-C4	-2.82	106.06	113.02
4	D	2002	NAG	C2-N2-C7	-2.66	119.62	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	NAG	C4-C3-C2	-2.13	107.91	111.23
2	A	1003	BMA	C3-C4-C5	2.41	114.39	110.20
2	A	1003	BMA	C2-C3-C4	2.45	115.21	111.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3002	NAG	1	0

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	$\# Z > 2$
3	NAG	A	2001	1	14,14,15	0.52	0	15,19,21	2.18	1 (6%)
3	NAG	A	4001	1	14,14,15	0.67	0	15,19,21	1.98	4 (26%)
5	TRS	A	6001	-	7,7,7	1.14	1 (14%)	9,9,9	1.47	1 (11%)
6	PEG	A	7001	-	6,6,6	0.52	0	5,5,5	0.38	0
3	NAG	B	2001	1	14,14,15	0.47	0	15,19,21	2.11	3 (20%)
8	BMA	B	3003	-	11,11,12	0.48	0	14,15,17	0.64	0
9	KTL	B	5001	-	22,26,26	1.80	1 (4%)	24,38,38	0.94	1 (4%)
6	PEG	B	7001	-	6,6,6	0.38	0	5,5,5	0.50	0
3	NAG	C	2001	1	14,14,15	0.54	0	15,19,21	0.82	0
3	NAG	C	3001	1	14,14,15	0.46	0	15,19,21	1.33	1 (6%)
3	NAG	C	4001	1	14,14,15	0.63	0	15,19,21	1.27	1 (6%)
5	TRS	C	6001	-	7,7,7	0.96	1 (14%)	9,9,9	0.69	0
6	PEG	C	7001	-	6,6,6	0.46	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	KTL	D	5001	-	22,26,26	1.90	2 (9%)	24,38,38	0.82	1 (4%)
6	PEG	D	7001	-	6,6,6	0.43	0	5,5,5	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
3	NAG	A	4001	1	-	0/6/23/26	0/1/1/1
5	TRS	A	6001	-	-	0/9/9/9	0/0/0/0
6	PEG	A	7001	-	-	0/4/4/4	0/0/0/0
3	NAG	B	2001	1	-	0/6/23/26	0/1/1/1
8	BMA	B	3003	-	-	0/2/19/22	0/1/1/1
9	KTL	B	5001	-	-	0/28/45/45	0/1/1/1
6	PEG	B	7001	-	-	0/4/4/4	0/0/0/0
3	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
3	NAG	C	3001	1	-	0/6/23/26	0/1/1/1
3	NAG	C	4001	1	-	0/6/23/26	0/1/1/1
5	TRS	C	6001	-	-	0/9/9/9	0/0/0/0
6	PEG	C	7001	-	-	0/4/4/4	0/0/0/0
9	KTL	D	5001	-	-	0/28/45/45	0/1/1/1
6	PEG	D	7001	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	5001	KTL	CAN-SAY	-8.24	1.66	1.82
9	B	5001	KTL	CAN-SAY	-7.47	1.67	1.82
5	A	6001	TRS	C-N	-2.67	1.46	1.50
5	C	6001	TRS	C-N	-2.46	1.47	1.50
9	D	5001	KTL	OAP-SAZ	2.31	1.64	1.57

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4001	NAG	C4-C3-C2	-4.84	103.71	111.23
3	B	2001	NAG	C6-C5-C4	-3.87	103.48	113.02
5	A	6001	TRS	C1-C-N	-3.40	101.89	108.09
9	D	5001	KTL	CAQ-CAT-CAV	2.12	115.92	112.47
3	A	4001	NAG	C3-C2-N2	2.26	115.97	110.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	3003	BMA	1	0
6	B	7001	PEG	3	0
6	C	7001	PEG	3	0
9	D	5001	KTL	2	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	A	871/898 (96%)	0.60	42 (4%) 34 45	4, 10, 19, 36	0
1	B	869/898 (96%)	0.58	48 (5%) 29 39	3, 11, 20, 37	0
1	C	871/898 (96%)	0.67	67 (7%) 16 22	5, 11, 21, 30	0
1	D	853/898 (94%)	1.93	363 (42%) 0 1	3, 11, 20, 27	0
All	All	3464/3592 (96%)	0.94	520 (15%) 3 5	3, 11, 20, 37	0

The worst 5 of 520 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	PRO	8.8
1	D	546	PRO	8.2
1	D	808	ILE	7.9
1	D	345	ALA	7.8
1	D	547	ASN	7.8

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	1002	14/15	0.92	0.18	2.81	12,13,18,20	0
4	NAG	B	3001	14/15	0.90	0.17	1.18	19,20,22,24	0
4	NAG	D	2001	14/15	0.88	0.14	0.04	4,14,19,23	0
2	MAN	C	1004	11/12	0.88	0.14	-0.13	11,13,16,16	0
2	BMA	C	1003	11/12	0.88	0.12	-0.48	14,16,20,23	0
4	NAG	A	3001	14/15	0.94	0.12	-0.99	9,13,15,18	0
2	MAN	A	1004	11/12	0.92	0.10	-2.28	15,17,18,19	0
2	NAG	C	1001	14/15	0.83	0.23	-	14,16,17,19	0
2	NAG	A	1001	14/15	0.81	0.24	-	16,20,24,25	0
4	NAG	B	3002	14/15	0.88	0.15	-	25,27,28,29	0
2	NAG	C	1002	14/15	0.89	0.20	-	12,15,18,21	0
4	NAG	A	3002	14/15	0.86	0.32	-	24,27,29,30	0
4	NAG	D	2002	14/15	0.73	0.32	-	24,27,31,32	0
2	BMA	A	1003	11/12	0.90	0.12	-	15,17,18,20	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	3001	14/15	0.80	0.29	2.63	22,25,26,27	0
5	TRS	C	6001	8/8	0.88	0.18	2.12	20,20,20,21	0
5	TRS	A	6001	8/8	0.86	0.19	0.99	10,12,13,15	0
6	PEG	A	7001	7/7	0.90	0.15	0.15	21,22,25,25	0
6	PEG	B	7001	7/7	0.90	0.12	0.11	20,20,21,22	0
9	KTL	D	5001	26/26	0.89	0.18	-0.47	20,24,26,27	0
6	PEG	C	7001	7/7	0.85	0.12	-0.78	18,22,25,27	0
3	NAG	B	2001	14/15	0.88	0.12	-0.83	9,16,18,21	0
9	KTL	B	5001	26/26	0.93	0.13	-0.86	10,18,23,25	0
6	PEG	D	7001	7/7	0.81	0.15	-1.23	37,37,38,38	0
7	CL	A	8001	1/1	0.98	0.09	-5.14	3,3,3,3	0
3	NAG	A	2001	14/15	0.66	0.19	-	31,33,34,34	0
3	NAG	C	2001	14/15	0.88	0.16	-	16,22,26,27	0
3	NAG	A	4001	14/15	0.80	0.34	-	24,27,28,30	0
3	NAG	C	4001	14/15	0.84	0.30	-	35,40,41,42	0
8	BMA	B	3003	11/12	0.55	0.23	-	61,62,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.