Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:20 AM GMT

PDB ID	:	3LPO
Title	:	Crystal structure of the N-terminal domain of sucrase-isomaltase
Authors	:	Sim, L.; Rose, D.R.
Deposited on	:	2010-02-05
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

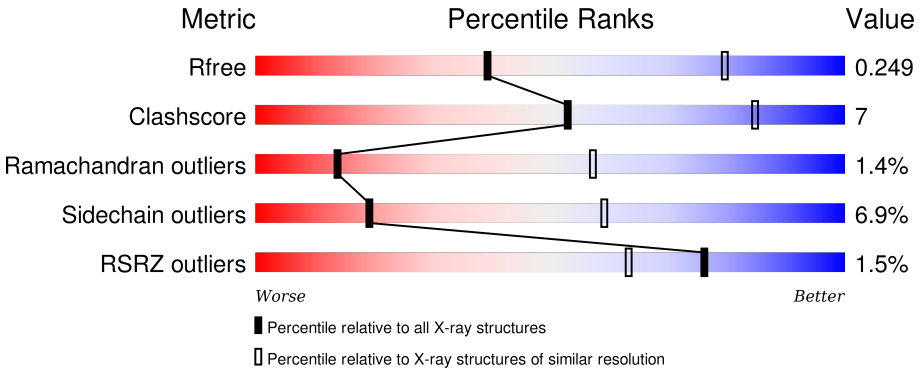
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 <=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	80% 14%
1	B	898	3% 79% 16%
1	C	898	80% 14%
1	D	898	80% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	2001	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27668 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	870	Total	C	N	O	S	0	0	0
			6853	4402	1146	1276	29			
1	B	870	Total	C	N	O	S	0	0	0
			6784	4353	1138	1264	29			
1	C	870	Total	C	N	O	S	0	0	0
			6904	4429	1157	1290	28			
1	D	870	Total	C	N	O	S	0	0	0
			6879	4414	1153	1283	29			

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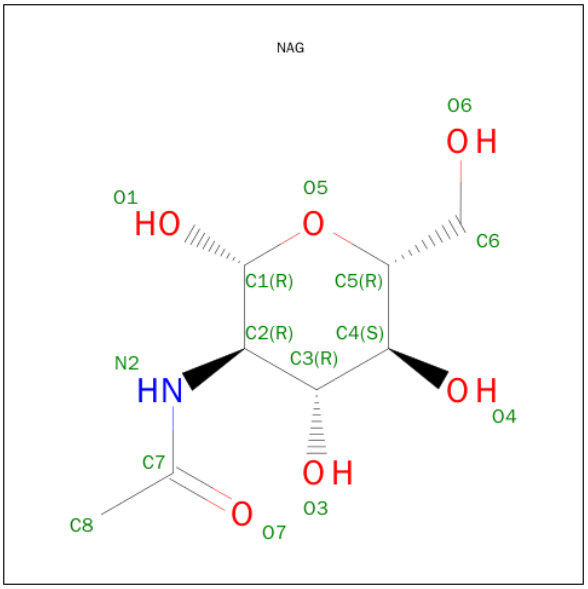
Chain	Residue	Modelled	Actual	Comment	Reference
D	22	PHE	-	EXPRESSION TAG	UNP P14410
D	23	GLN	-	EXPRESSION TAG	UNP P14410
D	24	SER	-	EXPRESSION TAG	UNP P14410
D	25	GLY	-	EXPRESSION TAG	UNP P14410
D	26	ILE	-	EXPRESSION TAG	UNP P14410
D	27	ARG	-	EXPRESSION TAG	UNP P14410
D	28	ARG	-	EXPRESSION TAG	UNP P14410

- Molecule 2 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

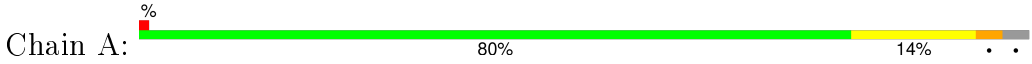
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		
4	C	5	Total	C	N	O	0	0
			61	34	2	25		

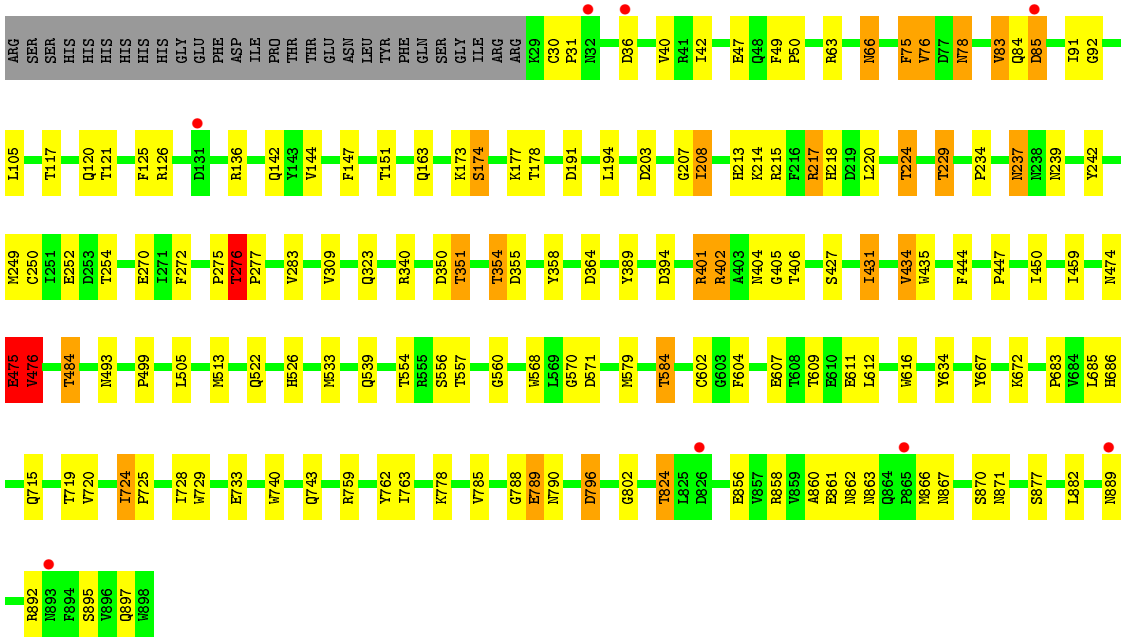
3 Residue-property plots (i)

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

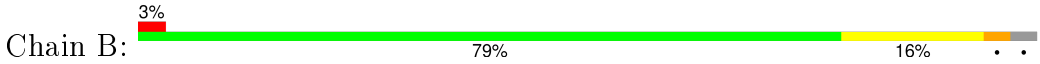
Chain A:

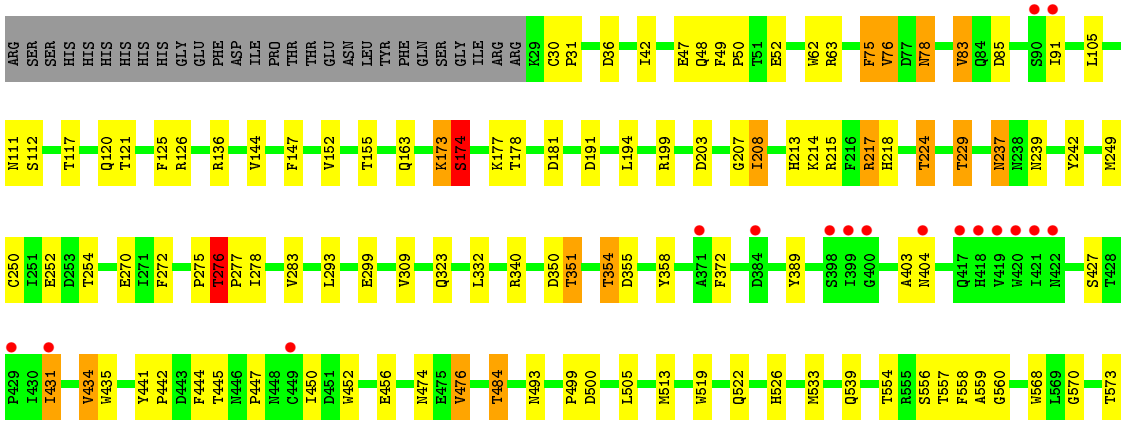


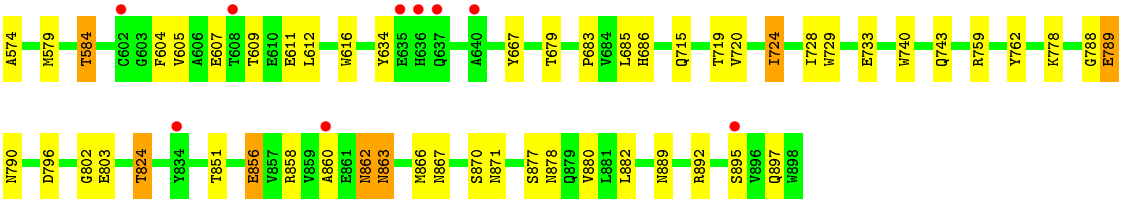


- Molecule 1: Sucrase-isomaltase

Chain B:

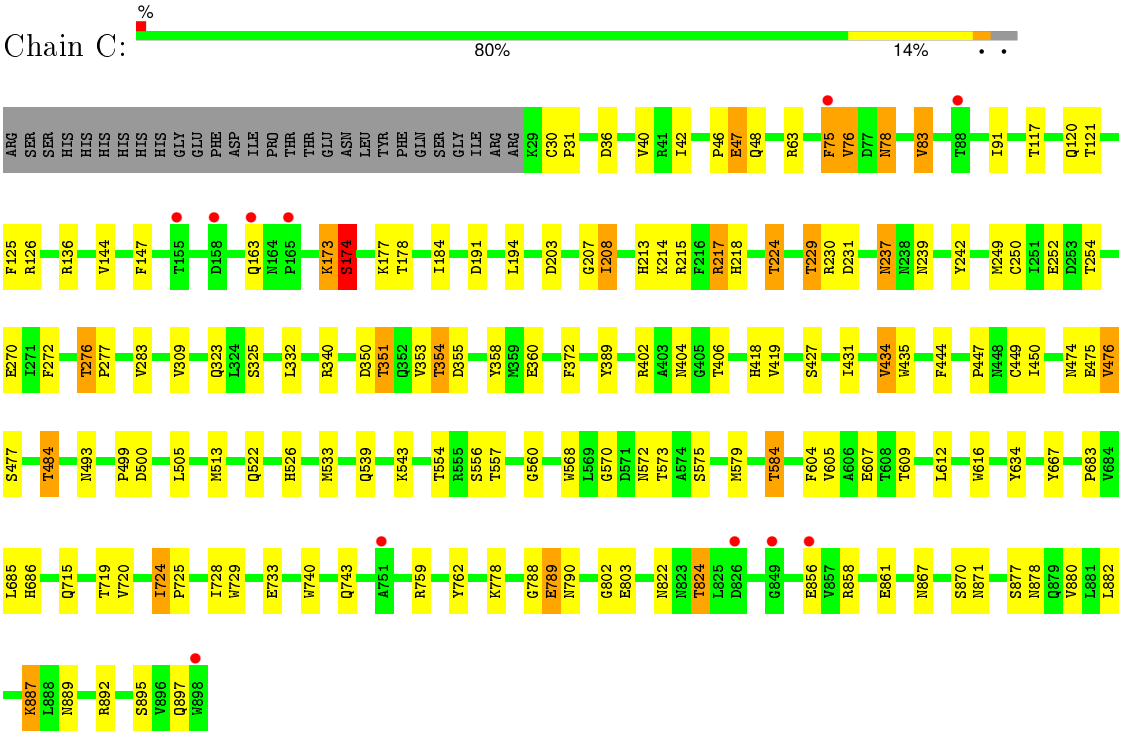






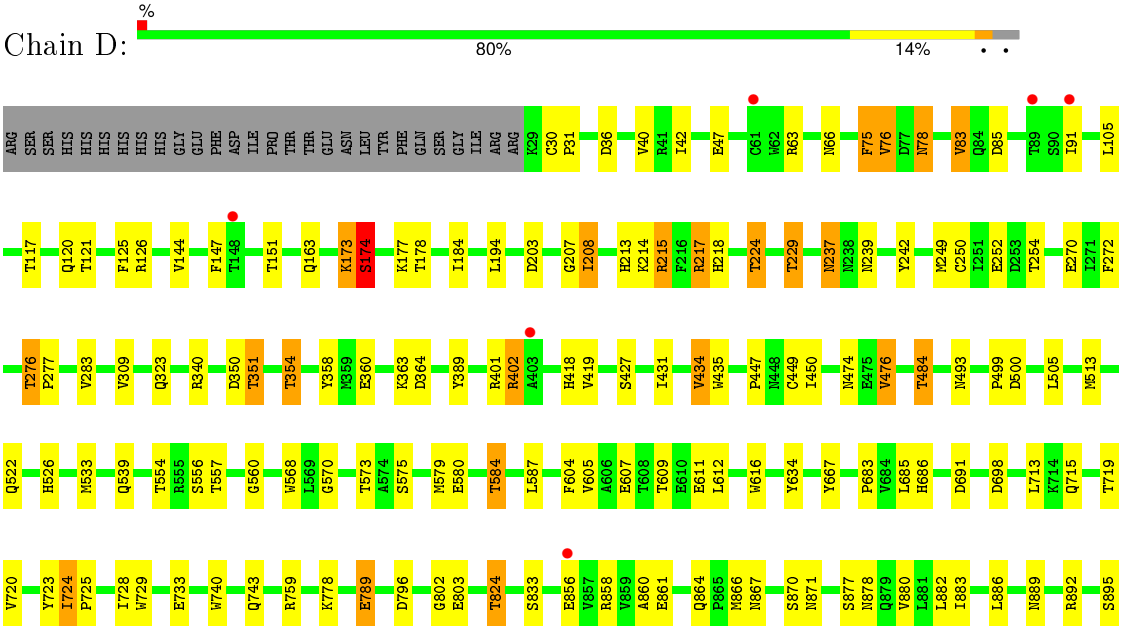
- Molecule 1: Sucrase-isomaltase

Chain C:



- Molecule 1: Sucrase-isomaltase

Chain D:




V896
Q897
W898

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.34Å 172.59Å 343.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.83 – 3.20 45.54 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.83-3.20) 99.7 (45.54-3.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.251 0.224 , 0.249	Depositor DCC
R_{free} test set	3802 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 16.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 75840 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	27668	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, 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	0.51	1/7054 (0.0%)	0.61	1/9644 (0.0%)
1	B	0.58	0/6980	0.61	0/9545
1	C	0.52	0/7105	0.61	0/9707
1	D	0.50	0/7080	0.61	0/9675
All	All	0.53	1/28219 (0.0%)	0.61	1/38571 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	602	CYS	CB-SG	-5.20	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	276	THR	N-CA-CB	5.59	120.92	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	475	GLU	Peptide

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	6853	0	6381	90	0
1	B	6784	0	6276	88	0
1	C	6904	0	6474	90	0
1	D	6879	0	6424	86	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	28	0	26	1	0
3	A	28	0	25	0	0
3	C	28	0	25	1	0
4	A	61	0	52	0	0
4	C	61	0	52	4	0
All	All	27668	0	25774	352	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 7.

All (352) 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:B:275:PRO:O	1:B:276:THR:HG22	1.29	1.32
1:B:860:ALA:HB2	1:B:866:MET:HG3	1.40	1.03
1:A:522:GLN:HE21	1:A:526:HIS:HD2	1.16	0.93
1:C:822:ASN:HD21	4:C:1001:NAG:H2	1.33	0.92
1:B:474:ASN:HB3	1:B:556:SER:HB3	1.50	0.92
1:A:402:ARG:CG	1:A:402:ARG:HH11	1.82	0.91
1:D:323:GLN:HG2	1:D:351:THR:HG23	1.53	0.91
1:C:522:GLN:HE21	1:C:526:HIS:HD2	1.18	0.90
1:A:402:ARG:HG2	1:A:402:ARG:HH11	1.34	0.89
1:D:522:GLN:HE21	1:D:526:HIS:HD2	1.16	0.88
1:C:474:ASN:HB3	1:C:556:SER:HB3	1.57	0.87
1:B:522:GLN:HE21	1:B:526:HIS:HD2	1.21	0.86
1:B:275:PRO:O	1:B:276:THR:CG2	2.21	0.85
1:A:474:ASN:HB3	1:A:556:SER:HB3	1.58	0.85
1:C:323:GLN:HG2	1:C:351:THR:HG23	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLN:HG2	1:A:351:THR:HG23	1.56	0.85
1:D:474:ASN:HB3	1:D:556:SER:HB3	1.58	0.85
1:B:48:GLN:HG3	1:C:48:GLN:HG3	1.58	0.83
1:B:323:GLN:HG2	1:B:351:THR:HG23	1.60	0.82
1:A:522:GLN:NE2	1:A:526:HIS:HD2	1.80	0.80
1:D:860:ALA:HB2	1:D:866:MET:CG	2.13	0.79
1:C:522:GLN:HE21	1:C:526:HIS:CD2	2.02	0.78
1:C:522:GLN:NE2	1:C:526:HIS:HD2	1.82	0.78
1:A:522:GLN:HE21	1:A:526:HIS:CD2	2.02	0.77
1:B:276:THR:HG21	1:B:278:ILE:HD12	1.67	0.77
1:B:522:GLN:HE21	1:B:526:HIS:CD2	2.03	0.76
1:B:237:ASN:HD22	1:B:239:ASN:H	1.31	0.76
1:D:224:THR:HG23	1:D:272:PHE:HD1	1.51	0.75
1:D:522:GLN:HE21	1:D:526:HIS:CD2	2.02	0.75
1:B:224:THR:HG23	1:B:272:PHE:HD1	1.50	0.75
1:C:237:ASN:HD22	1:C:239:ASN:H	1.35	0.75
1:B:117:THR:HG23	1:B:125:PHE:HE1	1.51	0.75
1:D:522:GLN:NE2	1:D:526:HIS:HD2	1.83	0.74
1:A:237:ASN:HD22	1:A:239:ASN:H	1.36	0.73
1:D:117:THR:HG23	1:D:125:PHE:HE1	1.53	0.73
1:D:237:ASN:HD22	1:D:239:ASN:H	1.36	0.73
1:C:117:THR:HG23	1:C:125:PHE:HE1	1.53	0.72
1:A:117:THR:HG23	1:A:125:PHE:HE1	1.52	0.72
1:A:224:THR:HG23	1:A:272:PHE:HD1	1.54	0.71
1:B:522:GLN:NE2	1:B:526:HIS:HD2	1.87	0.71
1:D:860:ALA:HB2	1:D:866:MET:HG3	1.72	0.71
1:C:224:THR:HG23	1:C:272:PHE:HD1	1.54	0.70
1:B:354:THR:HG21	1:B:389:TYR:OH	1.92	0.70
1:A:402:ARG:HG2	1:A:402:ARG:NH1	1.98	0.69
1:C:229:THR:HG22	1:C:526:HIS:CE1	2.28	0.68
1:B:824:THR:HB	1:B:897:GLN:HG2	1.75	0.68
1:C:887:LYS:HB2	1:C:887:LYS:NZ	2.09	0.67
1:C:824:THR:HB	1:C:897:GLN:HG2	1.77	0.66
1:A:474:ASN:ND2	1:A:554:THR:OG1	2.28	0.66
1:A:856:GLU:HG2	1:A:858:ARG:NH1	2.10	0.66
1:C:889:ASN:HB2	1:C:892:ARG:HH21	1.60	0.66
1:C:822:ASN:ND2	4:C:1001:NAG:H2	2.10	0.66
1:A:354:THR:HG21	1:A:389:TYR:OH	1.95	0.65
1:D:434:VAL:HG12	1:D:435:TRP:H	1.62	0.65
1:B:474:ASN:ND2	1:B:554:THR:OG1	2.29	0.65
1:A:824:THR:HB	1:A:897:GLN:HG2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HG12	1:B:111:ASN:ND2	2.12	0.65
1:D:76:VAL:H	1:D:78:ASN:ND2	1.95	0.65
1:C:207:GLY:O	1:C:218:HIS:HE1	1.80	0.64
1:B:889:ASN:HB2	1:B:892:ARG:HH21	1.63	0.64
1:B:229:THR:HG22	1:B:526:HIS:CE1	2.32	0.64
1:A:889:ASN:HB2	1:A:892:ARG:HH21	1.62	0.64
1:C:856:GLU:HG2	1:C:858:ARG:NH1	2.13	0.64
1:B:860:ALA:CB	1:B:866:MET:HG3	2.23	0.63
1:C:177:LYS:HE3	1:C:252:GLU:HB3	1.79	0.63
1:D:860:ALA:HB2	1:D:866:MET:HG2	1.79	0.63
1:D:824:THR:HB	1:D:897:GLN:HG2	1.81	0.63
1:A:207:GLY:O	1:A:218:HIS:HE1	1.82	0.63
1:B:177:LYS:HE3	1:B:252:GLU:HB3	1.80	0.63
1:D:856:GLU:HG2	1:D:858:ARG:NH1	2.14	0.63
1:A:474:ASN:C	1:A:476:VAL:H	2.00	0.62
1:C:354:THR:HG21	1:C:389:TYR:OH	2.00	0.62
1:D:740:TRP:HA	1:D:743:GLN:NE2	2.13	0.62
1:D:354:THR:HG21	1:D:389:TYR:OH	1.99	0.62
1:C:740:TRP:HA	1:C:743:GLN:NE2	2.14	0.61
1:C:475:GLU:CD	1:C:475:GLU:H	2.04	0.61
1:C:203:ASP:O	1:C:217:ARG:NH1	2.33	0.61
1:B:856:GLU:HG2	1:B:858:ARG:NH1	2.15	0.61
1:C:493:ASN:HD21	1:C:513:MET:H	1.47	0.60
1:D:889:ASN:HB2	1:D:892:ARG:HH21	1.65	0.60
1:A:860:ALA:HB2	1:A:866:MET:HG2	1.82	0.60
1:D:203:ASP:O	1:D:217:ARG:NH1	2.34	0.60
1:A:740:TRP:HA	1:A:743:GLN:NE2	2.17	0.60
1:B:434:VAL:HG12	1:B:435:TRP:H	1.67	0.60
1:B:275:PRO:C	1:B:276:THR:HG22	2.18	0.60
1:C:474:ASN:C	1:C:476:VAL:H	2.04	0.60
1:B:740:TRP:HA	1:B:743:GLN:NE2	2.17	0.59
1:D:207:GLY:O	1:D:218:HIS:HE1	1.84	0.59
1:C:360:GLU:OE1	1:C:402:ARG:NH2	2.31	0.59
1:A:142:GLN:NE2	1:A:142:GLN:HA	2.18	0.59
1:A:493:ASN:HD21	1:A:513:MET:H	1.51	0.58
1:C:214:LYS:O	1:C:584:THR:HG21	2.03	0.58
1:B:207:GLY:O	1:B:218:HIS:HE1	1.86	0.58
1:D:474:ASN:C	1:D:476:VAL:H	2.07	0.58
1:D:208:ILE:O	1:D:213:HIS:HE1	1.87	0.58
1:D:177:LYS:HE3	1:D:252:GLU:HB3	1.86	0.58
1:A:208:ILE:O	1:A:213:HIS:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASP:O	1:A:217:ARG:NH1	2.36	0.58
1:D:419:VAL:HG13	1:D:449:CYS:HA	1.84	0.58
1:A:177:LYS:HE3	1:A:252:GLU:HB3	1.85	0.58
1:B:208:ILE:O	1:B:213:HIS:HE1	1.86	0.57
1:D:214:LYS:O	1:D:584:THR:HG21	2.04	0.56
1:D:724:ILE:HG12	1:D:740:TRP:HB3	1.86	0.56
1:D:474:ASN:ND2	1:D:554:THR:OG1	2.39	0.56
1:C:117:THR:HG23	1:C:125:PHE:CE1	2.40	0.56
1:D:229:THR:HG22	1:D:526:HIS:CE1	2.41	0.56
1:A:434:VAL:HG12	1:A:435:TRP:H	1.71	0.56
1:B:724:ILE:HG12	1:B:740:TRP:HB3	1.88	0.56
1:A:672:LYS:HE3	1:A:796:ASP:OD1	2.05	0.56
1:C:822:ASN:HD21	4:C:1001:NAG:C2	2.10	0.56
1:B:474:ASN:C	1:B:476:VAL:H	2.10	0.56
1:C:729:TRP:CZ3	1:C:759:ARG:HB2	2.41	0.56
1:D:434:VAL:HG12	1:D:435:TRP:N	2.21	0.55
1:B:203:ASP:O	1:B:217:ARG:NH1	2.40	0.55
1:C:208:ILE:O	1:C:213:HIS:HE1	1.89	0.55
1:D:493:ASN:HD21	1:D:513:MET:H	1.53	0.55
1:D:419:VAL:HG12	1:D:449:CYS:SG	2.47	0.55
1:C:431:ILE:HB	1:C:484:THR:HB	1.89	0.55
1:A:724:ILE:HG12	1:A:740:TRP:HB3	1.88	0.55
1:B:683:PRO:HG2	1:B:686:HIS:CD2	2.42	0.55
1:B:276:THR:HG21	1:B:278:ILE:CD1	2.37	0.54
1:A:91:ILE:HG23	1:A:147:PHE:HE2	1.72	0.54
1:D:83:VAL:HG13	1:D:163:GLN:HA	1.90	0.54
1:C:683:PRO:HG2	1:C:686:HIS:CD2	2.43	0.54
1:D:418:HIS:CD2	2:D:3001:NAG:H62	2.43	0.53
1:A:214:LYS:O	1:A:584:THR:HG21	2.08	0.53
1:A:229:THR:HG22	1:A:526:HIS:CE1	2.43	0.53
1:C:419:VAL:HG13	1:C:449:CYS:SG	2.49	0.53
1:C:474:ASN:ND2	1:C:554:THR:OG1	2.41	0.53
1:A:30:CYS:HB3	1:A:63:ARG:NH2	2.24	0.53
1:B:860:ALA:HB2	1:B:866:MET:CG	2.28	0.52
1:B:83:VAL:HG13	1:B:163:GLN:HA	1.92	0.52
1:B:493:ASN:HD21	1:B:513:MET:H	1.57	0.52
1:C:724:ILE:HG12	1:C:740:TRP:HB3	1.91	0.52
1:D:360:GLU:OE2	1:D:402:ARG:HG3	2.10	0.52
1:B:76:VAL:H	1:B:78:ASN:ND2	2.06	0.52
1:C:522:GLN:NE2	1:C:526:HIS:CD2	2.68	0.52
1:D:30:CYS:HB3	1:D:63:ARG:NH2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:MET:HE3	1:B:612:LEU:HD12	1.90	0.52
1:C:42:ILE:HG22	1:C:75:PHE:CE2	2.44	0.52
1:B:434:VAL:HG12	1:B:435:TRP:N	2.25	0.52
1:A:683:PRO:HG2	1:A:686:HIS:CD2	2.44	0.52
1:B:91:ILE:HG23	1:B:147:PHE:HE2	1.75	0.52
1:C:83:VAL:HG13	1:C:163:GLN:HA	1.92	0.51
1:C:309:VAL:HG12	1:C:560:GLY:HA3	1.91	0.51
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.73	0.51
1:B:431:ILE:HB	1:B:484:THR:HB	1.93	0.51
1:A:83:VAL:HG13	1:A:163:GLN:HA	1.92	0.51
1:B:354:THR:HG23	1:B:358:TYR:CD2	2.46	0.51
1:C:607:GLU:HG2	1:C:634:TYR:HB3	1.91	0.51
1:D:354:THR:HG23	1:D:358:TYR:CD2	2.46	0.51
1:D:323:GLN:HG2	1:D:351:THR:CG2	2.35	0.51
1:D:117:THR:HG23	1:D:125:PHE:CE1	2.41	0.51
1:D:402:ARG:CG	1:D:402:ARG:HH11	2.24	0.51
1:B:214:LYS:O	1:B:584:THR:HG21	2.11	0.51
1:C:76:VAL:H	1:C:78:ASN:ND2	2.08	0.51
1:A:354:THR:HG23	1:A:358:TYR:CD2	2.45	0.51
1:B:309:VAL:HG12	1:B:560:GLY:HA3	1.93	0.51
1:C:573:THR:HG23	1:C:605:VAL:HB	1.92	0.50
1:C:354:THR:HG23	1:C:358:TYR:CD2	2.47	0.50
1:A:431:ILE:HB	1:A:484:THR:HB	1.92	0.50
1:A:522:GLN:NE2	1:A:526:HIS:CD2	2.68	0.50
1:D:522:GLN:NE2	1:D:526:HIS:CD2	2.71	0.50
1:B:309:VAL:CG1	1:B:560:GLY:HA3	2.41	0.50
1:D:431:ILE:HB	1:D:484:THR:HB	1.92	0.50
1:A:434:VAL:HG12	1:A:435:TRP:N	2.27	0.50
1:C:120:GLN:NE2	1:C:126:ARG:HD2	2.27	0.50
1:D:42:ILE:HG22	1:D:75:PHE:CE2	2.47	0.50
1:B:30:CYS:HA	1:B:76:VAL:HG21	1.93	0.49
1:A:609:THR:HG22	1:A:611:GLU:H	1.77	0.49
1:C:609:THR:HB	1:C:612:LEU:H	1.77	0.49
1:C:270:GLU:HG3	1:C:499:PRO:CB	2.43	0.49
1:D:729:TRP:CZ3	1:D:759:ARG:HB2	2.47	0.49
1:A:309:VAL:CG1	1:A:560:GLY:HA3	2.42	0.49
1:A:76:VAL:H	1:A:78:ASN:ND2	2.11	0.49
1:B:729:TRP:CZ3	1:B:759:ARG:HB2	2.48	0.49
1:A:117:THR:HG23	1:A:125:PHE:CE1	2.41	0.49
1:C:579:MET:HE3	1:C:612:LEU:HD12	1.94	0.49
1:D:363:LYS:NZ	1:D:401:ARG:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:SER:HB2	1:C:353:VAL:HB	1.95	0.49
1:D:91:ILE:HG23	1:D:147:PHE:HE2	1.78	0.49
1:D:587:LEU:HD13	1:D:683:PRO:HB3	1.95	0.49
1:D:309:VAL:CG1	1:D:560:GLY:HA3	2.43	0.49
1:A:249:MET:HG2	1:A:250:CYS:N	2.27	0.49
1:C:249:MET:HG2	1:C:250:CYS:N	2.28	0.48
1:C:355:ASP:O	1:C:358:TYR:HD2	1.96	0.48
1:B:30:CYS:HB3	1:B:63:ARG:NH2	2.28	0.48
1:B:224:THR:HG23	1:B:272:PHE:CD1	2.39	0.48
1:C:242:TYR:CE2	1:C:570:GLY:HA3	2.48	0.48
1:A:728:ILE:HD12	1:A:789:GLU:H	1.78	0.48
1:D:309:VAL:HG12	1:D:560:GLY:HA3	1.96	0.48
1:C:91:ILE:HG23	1:C:147:PHE:HE2	1.79	0.48
1:D:683:PRO:HG2	1:D:686:HIS:CD2	2.48	0.48
1:D:276:THR:N	1:D:277:PRO:HA	2.28	0.48
1:B:117:THR:HG23	1:B:125:PHE:CE1	2.39	0.48
1:A:276:THR:N	1:A:277:PRO:HA	2.28	0.48
1:C:728:ILE:HD12	1:C:789:GLU:H	1.78	0.48
1:C:579:MET:HG3	1:C:616:TRP:CD2	2.49	0.48
1:A:401:ARG:NH1	1:A:405:GLY:O	2.33	0.48
1:D:579:MET:HE3	1:D:612:LEU:HD12	1.96	0.48
1:C:759:ARG:HD3	1:C:762:TYR:CE2	2.49	0.47
1:C:309:VAL:CG1	1:C:560:GLY:HA3	2.44	0.47
1:A:364:ASP:OD2	1:A:394:ASP:O	2.32	0.47
1:B:30:CYS:HB3	1:B:31:PRO:HD2	1.95	0.47
1:D:609:THR:HG22	1:D:611:GLU:H	1.79	0.47
1:B:452:TRP:O	1:B:456:GLU:HG2	2.15	0.47
1:B:52:GLU:HG3	1:B:62:TRP:CD1	2.49	0.47
1:A:42:ILE:HG22	1:A:75:PHE:CE2	2.50	0.47
1:A:579:MET:HE3	1:A:612:LEU:HD12	1.96	0.47
1:D:76:VAL:H	1:D:78:ASN:HD21	1.63	0.47
1:D:419:VAL:CG1	1:D:449:CYS:SG	3.03	0.47
1:D:30:CYS:HA	1:D:76:VAL:HG21	1.96	0.47
1:A:740:TRP:HA	1:A:743:GLN:HE22	1.79	0.47
1:A:667:TYR:OH	1:A:802:GLY:HA2	2.15	0.47
1:C:887:LYS:HB2	1:C:887:LYS:HZ1	1.80	0.47
1:A:275:PRO:O	1:A:276:THR:HG23	2.14	0.47
1:D:579:MET:HG3	1:D:616:TRP:CD2	2.49	0.47
1:D:609:THR:HB	1:D:612:LEU:H	1.80	0.47
1:B:293:LEU:N	1:B:293:LEU:HD12	2.30	0.47
1:C:224:THR:HG23	1:C:272:PHE:CD1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:THR:HG23	1:D:272:PHE:CD1	2.39	0.47
1:A:609:THR:HB	1:A:612:LEU:H	1.79	0.47
1:A:607:GLU:HG2	1:A:634:TYR:HB3	1.97	0.47
1:A:270:GLU:HG3	1:A:499:PRO:CB	2.45	0.47
1:A:579:MET:HG3	1:A:616:TRP:CD2	2.50	0.46
1:C:230:ARG:HG3	1:C:231:ASP:N	2.31	0.46
1:D:728:ILE:HD12	1:D:789:GLU:H	1.80	0.46
1:B:522:GLN:NE2	1:B:526:HIS:CD2	2.73	0.46
1:B:447:PRO:O	1:B:450:ILE:HG12	2.15	0.46
1:C:822:ASN:ND2	4:C:1001:NAG:C2	2.76	0.46
1:D:173:LYS:O	1:D:174:SER:C	2.54	0.46
1:C:276:THR:N	1:C:277:PRO:HA	2.30	0.46
1:B:120:GLN:NE2	1:B:126:ARG:HD2	2.31	0.46
1:D:580:GLU:HG3	1:D:713:LEU:HD13	1.96	0.46
1:A:444:PHE:CE2	1:A:533:MET:HG3	2.51	0.46
1:B:728:ILE:HD12	1:B:789:GLU:H	1.81	0.46
1:B:474:ASN:CB	1:B:556:SER:HB3	2.35	0.46
1:D:270:GLU:HG3	1:D:499:PRO:CB	2.46	0.46
1:B:42:ILE:HG22	1:B:75:PHE:CE2	2.51	0.46
1:B:609:THR:HB	1:B:612:LEU:H	1.80	0.46
1:B:573:THR:HG23	1:B:605:VAL:HB	1.97	0.46
1:B:740:TRP:HA	1:B:743:GLN:HE22	1.80	0.45
1:C:447:PRO:O	1:C:450:ILE:HG12	2.16	0.45
1:A:861:GLU:OE2	1:A:892:ARG:HD2	2.16	0.45
1:D:573:THR:HG23	1:D:605:VAL:HB	1.98	0.45
1:B:579:MET:HG3	1:B:616:TRP:CD2	2.51	0.45
1:B:173:LYS:O	1:B:174:SER:C	2.54	0.45
1:A:30:CYS:HB3	1:A:31:PRO:HD2	1.98	0.45
1:D:883:ILE:HG22	1:D:886:LEU:HD11	1.99	0.45
1:D:242:TYR:CE2	1:D:570:GLY:HA3	2.52	0.45
1:A:120:GLN:NE2	1:A:126:ARG:HD2	2.31	0.45
1:A:66:ASN:OD1	1:A:66:ASN:N	2.50	0.45
1:B:276:THR:N	1:B:277:PRO:HA	2.32	0.45
1:C:30:CYS:HB3	1:C:63:ARG:NH2	2.32	0.45
1:D:120:GLN:NE2	1:D:126:ARG:HD2	2.32	0.45
1:A:724:ILE:O	1:A:724:ILE:HG13	2.17	0.44
1:C:418:HIS:HB2	3:C:3002:NAG:H61	1.98	0.44
1:A:475:GLU:O	1:A:476:VAL:HG23	2.17	0.44
1:D:724:ILE:HA	1:D:725:PRO:HD3	1.75	0.44
1:A:862:ASN:HB3	1:A:863:ASN:H	1.58	0.44
1:A:759:ARG:HD3	1:A:762:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLU:OE2	1:B:679:THR:OG1	2.27	0.44
1:C:30:CYS:HB3	1:C:31:PRO:HD2	1.98	0.44
1:C:878:ASN:HB3	1:C:880:VAL:HG23	2.00	0.44
1:A:49:PHE:HA	1:A:50:PRO:HD3	1.85	0.44
1:C:207:GLY:O	1:C:218:HIS:CE1	2.67	0.44
1:A:309:VAL:HG12	1:A:560:GLY:HA3	2.00	0.44
1:B:270:GLU:HG3	1:B:499:PRO:CB	2.48	0.44
1:B:607:GLU:HG2	1:B:634:TYR:HB3	2.00	0.44
1:A:474:ASN:C	1:A:476:VAL:N	2.68	0.43
1:D:740:TRP:HA	1:D:743:GLN:HE22	1.82	0.43
1:B:152:VAL:HG12	1:B:155:THR:HG22	2.00	0.43
1:B:242:TYR:CE2	1:B:570:GLY:HA3	2.52	0.43
1:C:474:ASN:C	1:C:476:VAL:N	2.71	0.43
1:A:355:ASP:O	1:A:358:TYR:HD2	2.01	0.43
1:B:609:THR:HG22	1:B:611:GLU:H	1.83	0.43
1:B:355:ASP:O	1:B:358:TYR:HD2	2.01	0.43
1:D:878:ASN:HB3	1:D:880:VAL:HG23	2.00	0.43
1:D:607:GLU:HG2	1:D:634:TYR:HB3	2.00	0.43
1:C:740:TRP:HA	1:C:743:GLN:HE22	1.84	0.43
1:A:729:TRP:CZ3	1:A:759:ARG:HB2	2.53	0.43
1:B:444:PHE:CE2	1:B:533:MET:HG3	2.53	0.43
1:D:402:ARG:CG	1:D:402:ARG:NH1	2.82	0.43
1:D:866:MET:HB2	1:D:866:MET:HE3	1.64	0.43
1:A:724:ILE:HA	1:A:725:PRO:HD3	1.72	0.43
1:C:213:HIS:O	1:C:214:LYS:HB2	2.18	0.43
1:B:249:MET:HG2	1:B:250:CYS:N	2.34	0.43
1:C:889:ASN:HB2	1:C:892:ARG:NH2	2.32	0.43
1:C:42:ILE:HG22	1:C:75:PHE:CD2	2.54	0.43
1:C:40:VAL:O	1:C:40:VAL:CG1	2.67	0.43
1:B:136:ARG:HH12	1:B:191:ASP:HA	1.83	0.43
1:B:270:GLU:HG3	1:B:499:PRO:HB2	2.00	0.43
1:C:173:LYS:O	1:C:174:SER:C	2.57	0.43
1:D:184:ILE:HA	1:D:184:ILE:HD12	1.83	0.43
1:A:40:VAL:HG12	1:A:40:VAL:O	2.19	0.43
1:D:447:PRO:O	1:D:450:ILE:HG12	2.17	0.43
1:A:224:THR:HG23	1:A:272:PHE:CD1	2.43	0.43
1:D:215:ARG:NH1	1:D:698:ASP:OD2	2.51	0.43
1:D:249:MET:HG2	1:D:250:CYS:N	2.34	0.43
1:D:474:ASN:OD1	1:D:533:MET:SD	2.78	0.42
1:C:360:GLU:CD	1:C:402:ARG:HH21	2.16	0.42
1:C:444:PHE:CE2	1:C:533:MET:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:GLY:O	1:B:790:ASN:N	2.53	0.42
1:C:434:VAL:HG12	1:C:435:TRP:H	1.82	0.42
1:D:667:TYR:OH	1:D:802:GLY:HA2	2.19	0.42
1:D:474:ASN:C	1:D:476:VAL:N	2.71	0.42
1:A:242:TYR:CE2	1:A:570:GLY:HA3	2.54	0.42
1:A:788:GLY:O	1:A:790:ASN:N	2.53	0.42
1:C:667:TYR:OH	1:C:802:GLY:HA2	2.19	0.42
1:A:203:ASP:HB3	1:A:220:LEU:HD11	2.02	0.42
1:D:30:CYS:HB3	1:D:31:PRO:HD2	2.01	0.42
1:C:724:ILE:HA	1:C:725:PRO:HD3	1.74	0.42
1:C:788:GLY:O	1:C:790:ASN:N	2.53	0.42
1:C:474:ASN:OD1	1:C:533:MET:SD	2.78	0.42
1:B:759:ARG:HD3	1:B:762:TYR:CE2	2.55	0.42
1:A:763:ILE:HG12	1:A:785:VAL:HG22	2.02	0.42
1:C:332:LEU:HB2	1:C:372:PHE:HA	2.02	0.41
1:A:234:PRO:HD2	1:A:571:ASP:O	2.20	0.41
1:C:136:ARG:HH12	1:C:191:ASP:HA	1.85	0.41
1:A:323:GLN:HG2	1:A:351:THR:CG2	2.40	0.41
1:A:40:VAL:O	1:A:40:VAL:CG1	2.67	0.41
1:B:332:LEU:HB2	1:B:372:PHE:HA	2.02	0.41
1:B:667:TYR:OH	1:B:802:GLY:HA2	2.20	0.41
1:D:40:VAL:CG1	1:D:40:VAL:O	2.68	0.41
1:D:861:GLU:OE2	1:D:892:ARG:HD2	2.21	0.41
1:A:136:ARG:HH12	1:A:191:ASP:HA	1.86	0.41
1:A:92:GLY:HA3	1:A:117:THR:HG22	2.02	0.41
1:C:572:ASN:O	1:C:604:PHE:HB3	2.21	0.41
1:D:691:ASP:OD2	1:D:723:TYR:OH	2.33	0.41
1:B:445:THR:HB	1:B:519:TRP:CE2	2.56	0.41
1:A:84:GLN:O	1:A:85:ASP:HB3	2.21	0.41
1:D:42:ILE:HG22	1:D:75:PHE:CD2	2.56	0.41
1:D:40:VAL:HG12	1:D:40:VAL:O	2.21	0.41
1:B:441:TYR:HA	1:B:442:PRO:HD3	1.90	0.41
1:B:181:ASP:HB3	1:B:199:ARG:HB3	2.03	0.41
1:C:323:GLN:HG2	1:C:351:THR:CG2	2.41	0.41
1:C:861:GLU:OE2	1:C:892:ARG:HD2	2.21	0.41
1:B:76:VAL:H	1:B:78:ASN:HD21	1.69	0.41
1:D:91:ILE:CG2	1:D:147:PHE:HE2	2.34	0.41
1:C:40:VAL:O	1:C:40:VAL:HG12	2.21	0.41
1:B:49:PHE:HA	1:B:50:PRO:HD3	1.87	0.41
1:B:878:ASN:HB3	1:B:880:VAL:HG23	2.03	0.41
1:B:558:PHE:CG	1:B:559:ALA:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ILE:CG2	1:A:147:PHE:HE2	2.33	0.40
1:C:46:PRO:HD2	1:C:47:GLU:HG3	2.02	0.40
1:A:474:ASN:O	1:A:476:VAL:N	2.54	0.40
1:A:889:ASN:HB2	1:A:892:ARG:NH2	2.34	0.40
1:A:447:PRO:O	1:A:450:ILE:HG12	2.21	0.40
1:C:42:ILE:HG22	1:C:75:PHE:HE2	1.87	0.40
1:A:83:VAL:CG1	1:A:163:GLN:HA	2.52	0.40
1:C:184:ILE:HD12	1:C:184:ILE:HA	1.87	0.40
1:B:862:ASN:HB3	1:B:863:ASN:H	1.65	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	868/898 (97%)	802 (92%)	55 (6%)	11 (1%)	15	59
1	B	868/898 (97%)	802 (92%)	51 (6%)	15 (2%)	11	52
1	C	868/898 (97%)	804 (93%)	53 (6%)	11 (1%)	15	59
1	D	868/898 (97%)	805 (93%)	50 (6%)	13 (2%)	13	55
All	All	3472/3592 (97%)	3213 (92%)	209 (6%)	50 (1%)	14	57

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	THR
1	A	789	GLU
1	B	276	THR
1	B	789	GLU
1	C	276	THR
1	C	789	GLU

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Mol	Chain	Res	Type
1	D	276	THR
1	D	789	GLU
1	A	76	VAL
1	A	208	ILE
1	B	76	VAL
1	B	208	ILE
1	C	76	VAL
1	C	208	ILE
1	D	208	ILE
1	A	174	SER
1	A	404	ASN
1	B	174	SER
1	B	404	ASN
1	C	174	SER
1	A	604	PHE
1	B	803	GLU
1	D	66	ASN
1	D	76	VAL
1	D	174	SER
1	D	604	PHE
1	A	475	GLU
1	B	85	ASP
1	B	403	ALA
1	B	500	ASP
1	B	574	ALA
1	C	500	ASP
1	C	803	GLU
1	D	803	GLU
1	A	476	VAL
1	B	604	PHE
1	C	404	ASN
1	D	85	ASP
1	D	500	ASP
1	A	434	VAL
1	B	434	VAL
1	C	434	VAL
1	C	476	VAL
1	D	144	VAL
1	D	434	VAL
1	D	476	VAL
1	A	144	VAL
1	B	144	VAL

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Mol	Chain	Res	Type
1	B	476	VAL
1	C	144	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	720/797 (90%)	668 (93%)	52 (7%)	18	57
1	B	703/797 (88%)	652 (93%)	51 (7%)	17	57
1	C	734/797 (92%)	687 (94%)	47 (6%)	22	62
1	D	728/797 (91%)	678 (93%)	50 (7%)	19	59
All	All	2885/3188 (90%)	2685 (93%)	200 (7%)	19	59

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	47	GLU
1	A	66	ASN
1	A	75	PHE
1	A	78	ASN
1	A	83	VAL
1	A	85	ASP
1	A	105	LEU
1	A	121	THR
1	A	151	THR
1	A	173	LYS
1	A	174	SER
1	A	178	THR
1	A	194	LEU
1	A	215	ARG
1	A	217	ARG
1	A	224	THR
1	A	229	THR
1	A	237	ASN

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Mol	Chain	Res	Type
1	A	254	THR
1	A	283	VAL
1	A	340	ARG
1	A	350	ASP
1	A	351	THR
1	A	354	THR
1	A	401	ARG
1	A	402	ARG
1	A	406	THR
1	A	427	SER
1	A	431	ILE
1	A	476	VAL
1	A	484	THR
1	A	505	LEU
1	A	539	GLN
1	A	557	THR
1	A	568	TRP
1	A	584	THR
1	A	685	LEU
1	A	715	GLN
1	A	719	THR
1	A	720	VAL
1	A	724	ILE
1	A	733	GLU
1	A	778	LYS
1	A	796	ASP
1	A	824	THR
1	A	867	ASN
1	A	870	SER
1	A	871	ASN
1	A	877	SER
1	A	882	LEU
1	A	895	SER
1	B	36	ASP
1	B	47	GLU
1	B	75	PHE
1	B	78	ASN
1	B	83	VAL
1	B	105	LEU
1	B	112	SER
1	B	121	THR
1	B	173	LYS

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Mol	Chain	Res	Type
1	B	174	SER
1	B	178	THR
1	B	194	LEU
1	B	215	ARG
1	B	217	ARG
1	B	224	THR
1	B	229	THR
1	B	237	ASN
1	B	254	THR
1	B	276	THR
1	B	283	VAL
1	B	340	ARG
1	B	350	ASP
1	B	351	THR
1	B	354	THR
1	B	427	SER
1	B	431	ILE
1	B	484	THR
1	B	505	LEU
1	B	539	GLN
1	B	557	THR
1	B	568	TRP
1	B	584	THR
1	B	685	LEU
1	B	715	GLN
1	B	719	THR
1	B	720	VAL
1	B	724	ILE
1	B	733	GLU
1	B	778	LYS
1	B	796	ASP
1	B	824	THR
1	B	851	THR
1	B	856	GLU
1	B	862	ASN
1	B	863	ASN
1	B	867	ASN
1	B	870	SER
1	B	871	ASN
1	B	877	SER
1	B	882	LEU
1	B	895	SER

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Mol	Chain	Res	Type
1	C	36	ASP
1	C	47	GLU
1	C	75	PHE
1	C	78	ASN
1	C	83	VAL
1	C	121	THR
1	C	173	LYS
1	C	174	SER
1	C	178	THR
1	C	194	LEU
1	C	215	ARG
1	C	217	ARG
1	C	224	THR
1	C	229	THR
1	C	237	ASN
1	C	254	THR
1	C	283	VAL
1	C	340	ARG
1	C	350	ASP
1	C	351	THR
1	C	354	THR
1	C	406	THR
1	C	427	SER
1	C	477	SER
1	C	484	THR
1	C	505	LEU
1	C	539	GLN
1	C	543	LYS
1	C	557	THR
1	C	568	TRP
1	C	575	SER
1	C	584	THR
1	C	685	LEU
1	C	715	GLN
1	C	719	THR
1	C	720	VAL
1	C	724	ILE
1	C	733	GLU
1	C	778	LYS
1	C	824	THR
1	C	867	ASN
1	C	870	SER

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Mol	Chain	Res	Type
1	C	871	ASN
1	C	877	SER
1	C	882	LEU
1	C	887	LYS
1	C	895	SER
1	D	36	ASP
1	D	47	GLU
1	D	75	PHE
1	D	78	ASN
1	D	83	VAL
1	D	105	LEU
1	D	121	THR
1	D	151	THR
1	D	173	LYS
1	D	174	SER
1	D	178	THR
1	D	194	LEU
1	D	215	ARG
1	D	217	ARG
1	D	224	THR
1	D	229	THR
1	D	237	ASN
1	D	254	THR
1	D	283	VAL
1	D	340	ARG
1	D	350	ASP
1	D	351	THR
1	D	354	THR
1	D	364	ASP
1	D	402	ARG
1	D	427	SER
1	D	484	THR
1	D	505	LEU
1	D	539	GLN
1	D	557	THR
1	D	568	TRP
1	D	575	SER
1	D	584	THR
1	D	685	LEU
1	D	715	GLN
1	D	719	THR
1	D	720	VAL

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Mol	Chain	Res	Type
1	D	724	ILE
1	D	733	GLU
1	D	778	LYS
1	D	796	ASP
1	D	824	THR
1	D	833	SER
1	D	864	GLN
1	D	867	ASN
1	D	870	SER
1	D	871	ASN
1	D	877	SER
1	D	882	LEU
1	D	895	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	48	GLN
1	A	78	ASN
1	A	79	HIS
1	A	142	GLN
1	A	213	HIS
1	A	218	HIS
1	A	232	GLN
1	A	237	ASN
1	A	239	ASN
1	A	448	ASN
1	A	474	ASN
1	A	493	ASN
1	A	517	GLN
1	A	522	GLN
1	A	526	HIS
1	A	686	HIS
1	A	743	GLN
1	B	39	ASN
1	B	48	GLN
1	B	78	ASN
1	B	79	HIS
1	B	98	ASN
1	B	111	ASN
1	B	142	GLN

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Mol	Chain	Res	Type
1	B	164	ASN
1	B	213	HIS
1	B	218	HIS
1	B	232	GLN
1	B	237	ASN
1	B	239	ASN
1	B	474	ASN
1	B	493	ASN
1	B	517	GLN
1	B	526	HIS
1	B	743	GLN
1	B	823	ASN
1	B	871	ASN
1	C	39	ASN
1	C	48	GLN
1	C	78	ASN
1	C	79	HIS
1	C	142	GLN
1	C	169	GLN
1	C	192	GLN
1	C	213	HIS
1	C	218	HIS
1	C	232	GLN
1	C	237	ASN
1	C	239	ASN
1	C	474	ASN
1	C	493	ASN
1	C	517	GLN
1	C	522	GLN
1	C	526	HIS
1	C	743	GLN
1	C	822	ASN
1	C	823	ASN
1	C	897	GLN
1	D	39	ASN
1	D	48	GLN
1	D	78	ASN
1	D	79	HIS
1	D	142	GLN
1	D	169	GLN
1	D	213	HIS
1	D	218	HIS

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Mol	Chain	Res	Type
1	D	232	GLN
1	D	237	ASN
1	D	239	ASN
1	D	380	GLN
1	D	418	HIS
1	D	474	ASN
1	D	493	ASN
1	D	517	GLN
1	D	522	GLN
1	D	526	HIS
1	D	743	GLN
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 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	$\#\|Z\| > 2$
4	NAG	A	1001	1,4	14,14,15	0.65	0	15,19,21	2.39	4 (26%)
4	NAG	A	1002	4	14,14,15	0.61	0	15,19,21	0.90	0
4	BMA	A	1003	4	11,11,12	0.57	0	14,15,17	1.76	2 (14%)
4	MAN	A	1004	4	11,11,12	0.73	0	14,15,17	1.91	4 (28%)
4	MAN	A	1005	4	11,11,12	0.57	0	14,15,17	0.79	0
3	NAG	A	3001	1,3	14,14,15	0.62	0	15,19,21	1.02	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	3002	3	14,14,15	0.55	0	15,19,21	2.14	3 (20%)
4	NAG	C	1001	4	14,14,15	0.62	0	15,19,21	1.85	2 (13%)
4	NAG	C	1002	4	14,14,15	0.58	0	15,19,21	1.26	1 (6%)
4	BMA	C	1003	4	11,11,12	0.54	0	14,15,17	2.31	7 (50%)
4	MAN	C	1004	4	11,11,12	0.66	0	14,15,17	1.21	2 (14%)
4	MAN	C	1005	4	11,11,12	0.75	0	14,15,17	2.64	6 (42%)
3	NAG	C	3001	1,3	14,14,15	0.66	0	15,19,21	1.11	0
3	NAG	C	3002	3	14,14,15	0.42	0	15,19,21	2.22	2 (13%)

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
4	NAG	A	1001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1002	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1004	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1005	4	-	0/2/19/22	0/1/1/1
3	NAG	A	3001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3002	3	-	0/6/23/26	0/1/1/1
4	NAG	C	1001	4	-	0/6/23/26	0/1/1/1
4	NAG	C	1002	4	-	0/6/23/26	0/1/1/1
4	BMA	C	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	C	1004	4	-	0/2/19/22	0/1/1/1
4	MAN	C	1005	4	-	0/2/19/22	0/1/1/1
3	NAG	C	3001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	3002	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1004	MAN	O3-C3-C2	-2.84	104.87	110.00
4	C	1003	BMA	O5-C1-C2	-2.81	106.30	110.86
3	A	3001	NAG	C3-C4-C5	-2.80	105.32	110.20
3	A	3002	NAG	O3-C3-C4	-2.78	104.07	110.34
4	A	1003	BMA	O6-C6-C5	-2.51	103.03	111.33
4	A	1004	MAN	O2-C2-C3	-2.48	105.14	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	NAG	O4-C4-C3	-2.18	105.42	110.34
4	C	1003	BMA	O5-C5-C6	-2.18	102.63	107.35
4	C	1003	BMA	O3-C3-C4	-2.16	105.47	110.34
4	C	1004	MAN	O5-C1-C2	-2.03	107.57	110.86
4	C	1005	MAN	O5-C5-C6	2.12	111.93	107.35
4	C	1004	MAN	C1-O5-C5	2.20	115.04	112.25
3	C	3002	NAG	O5-C5-C6	2.27	112.26	107.35
4	A	1001	NAG	C4-C3-C2	2.28	114.78	111.23
4	C	1005	MAN	O5-C1-C2	2.33	114.64	110.86
4	C	1003	BMA	C2-C3-C4	2.67	115.58	111.04
4	A	1001	NAG	C3-C4-C5	2.76	115.00	110.20
4	C	1003	BMA	C3-C4-C5	2.83	115.12	110.20
4	A	1004	MAN	C3-C4-C5	3.22	115.81	110.20
4	C	1003	BMA	C1-C2-C3	3.47	113.65	109.54
3	A	3002	NAG	C4-C3-C2	3.49	116.65	111.23
4	C	1002	NAG	C4-C3-C2	3.91	117.31	111.23
4	A	1004	MAN	C1-C2-C3	4.00	114.27	109.54
4	C	1005	MAN	C3-C4-C5	4.01	117.19	110.20
4	C	1005	MAN	C2-C3-C4	4.18	118.14	111.04
4	A	1003	BMA	C1-C2-C3	4.51	114.87	109.54
4	C	1001	NAG	C1-O5-C5	4.54	118.02	112.25
4	C	1005	MAN	C1-O5-C5	4.57	118.05	112.25
4	C	1003	BMA	C1-O5-C5	4.84	118.39	112.25
4	C	1001	NAG	C3-C4-C5	4.84	118.63	110.20
4	C	1005	MAN	C1-C2-C3	5.59	116.16	109.54
3	A	3002	NAG	C1-O5-C5	5.96	119.81	112.25
4	A	1001	NAG	C1-O5-C5	7.43	121.68	112.25
3	C	3002	NAG	C1-O5-C5	7.67	121.98	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1001	NAG	4	0
3	C	3002	NAG	1	0

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	2001	1	14,14,15	0.52	0	15,19,21	1.53	3 (20%)
2	NAG	B	2001	1	14,14,15	0.66	0	15,19,21	3.03	6 (40%)
2	NAG	C	2001	1	14,14,15	0.69	0	15,19,21	1.64	2 (13%)
2	NAG	D	2001	1	14,14,15	1.33	2 (14%)	15,19,21	3.96	6 (40%)
2	NAG	D	3001	1	14,14,15	0.61	0	15,19,21	1.32	2 (13%)

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	2001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	2001	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
2	NAG	D	2001	1	-	0/6/23/26	0/1/1/1
2	NAG	D	3001	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	NAG	C2-N2	2.23	1.50	1.46
2	D	2001	NAG	C1-C2	3.39	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2001	NAG	O7-C7-C8	-3.60	115.46	122.06
2	B	2001	NAG	O7-C7-C8	-2.47	117.52	122.06
2	D	3001	NAG	C3-C4-C5	-2.44	105.95	110.20
2	A	2001	NAG	O3-C3-C2	-2.21	104.73	109.11
2	A	2001	NAG	O7-C7-C8	-2.08	118.24	122.06
2	D	3001	NAG	C4-C3-C2	2.10	114.49	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	NAG	O7-C7-N2	2.37	126.70	121.86
2	D	2001	NAG	C3-C2-N2	2.49	116.52	110.56
2	B	2001	NAG	C4-C3-C2	2.73	115.48	111.23
2	C	2001	NAG	C2-N2-C7	2.78	126.62	123.04
2	D	2001	NAG	O3-C3-C2	3.35	115.76	109.11
2	B	2001	NAG	C3-C4-C5	3.41	116.14	110.20
2	A	2001	NAG	C1-O5-C5	4.04	117.38	112.25
2	D	2001	NAG	C8-C7-N2	4.07	123.89	116.11
2	C	2001	NAG	C1-O5-C5	4.84	118.39	112.25
2	D	2001	NAG	C1-O5-C5	5.31	118.98	112.25
2	B	2001	NAG	C2-N2-C7	6.17	130.97	123.04
2	B	2001	NAG	C1-O5-C5	7.47	121.73	112.25
2	D	2001	NAG	C2-N2-C7	12.33	138.89	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2001	NAG	C1

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
2	D	3001	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	870/898 (96%)	-0.06	8 (0%) 85 78	29, 49, 61, 69	0
1	B	870/898 (96%)	0.08	26 (2%) 54 39	29, 49, 61, 69	0
1	C	870/898 (96%)	0.00	11 (1%) 79 67	29, 49, 61, 69	0
1	D	870/898 (96%)	-0.07	6 (0%) 89 83	29, 49, 61, 69	0
All	All	3480/3592 (96%)	-0.01	51 (1%) 76 63	29, 49, 61, 69	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	148	THR	3.8
1	B	602	CYS	3.6
1	B	429	PRO	3.5
1	B	420	TRP	3.3
1	B	636	HIS	3.2
1	B	635	GLU	3.2
1	B	418	HIS	2.9
1	B	431	ILE	2.8
1	B	834	TYR	2.8
1	B	449	CYS	2.8
1	B	640	ALA	2.8
1	B	399	ILE	2.8
1	C	751	ALA	2.7
1	D	91	ILE	2.7
1	B	419	VAL	2.6
1	B	895	SER	2.6
1	A	131	ASP	2.6
1	B	860	ALA	2.6
1	C	88	THR	2.5
1	B	417	GLN	2.5
1	C	856	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	637	GLN	2.5
1	B	384	ASP	2.5
1	C	898	TRP	2.5
1	B	398	SER	2.4
1	A	889	ASN	2.4
1	B	404	ASN	2.4
1	A	36	ASP	2.4
1	B	91	ILE	2.4
1	B	90	SER	2.3
1	C	75	PHE	2.3
1	B	400	GLY	2.3
1	A	865	PRO	2.3
1	A	85	ASP	2.3
1	D	403	ALA	2.3
1	B	422	ASN	2.3
1	C	155	THR	2.2
1	A	893	ASN	2.2
1	C	826	ASP	2.2
1	A	826	ASP	2.2
1	C	165	PRO	2.2
1	D	89	THR	2.2
1	B	608	THR	2.1
1	C	849	GLY	2.1
1	C	163	GLN	2.1
1	D	856	GLU	2.1
1	B	371	ALA	2.1
1	D	61	CYS	2.0
1	C	158	ASP	2.0
1	A	32	ASN	2.0
1	B	421	ILE	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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	3001	14/15	0.96	0.29	0.90	57,59,60,62	0
4	MAN	A	1004	11/12	0.87	0.21	-0.02	52,54,55,55	0
4	MAN	C	1004	11/12	0.94	0.21	-0.15	60,61,63,63	0
3	NAG	C	3001	14/15	0.93	0.23	-0.19	55,60,62,64	0
4	NAG	A	1001	14/15	0.91	0.18	-	61,62,65,66	0
4	BMA	C	1003	11/12	0.88	0.20	-	64,67,71,75	0
4	NAG	C	1002	14/15	0.88	0.24	-	70,75,78,79	0
3	NAG	A	3002	14/15	0.90	0.34	-	62,63,65,65	0
3	NAG	C	3002	14/15	0.88	0.37	-	65,66,69,70	0
4	NAG	A	1002	14/15	0.91	0.26	-	60,63,66,66	0
4	MAN	A	1005	11/12	0.89	0.40	-	68,69,70,71	0
4	MAN	C	1005	11/12	0.82	0.25	-	74,76,76,77	0
4	NAG	C	1001	14/15	0.88	0.18	-	77,80,81,81	0
4	BMA	A	1003	11/12	0.93	0.28	-	56,59,64,67	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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	D	2001	14/15	0.79	0.19	-0.46	40,45,46,46	0
2	NAG	D	3001	14/15	0.91	0.17	-0.77	60,61,62,63	0
2	NAG	B	2001	14/15	0.86	0.17	-	48,51,53,53	0
2	NAG	C	2001	14/15	0.87	0.15	-	57,61,62,62	0
2	NAG	A	2001	14/15	0.88	0.18	-	48,50,53,55	0

6.5 Other polymers

There are no such residues in this entry.