



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:07 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 full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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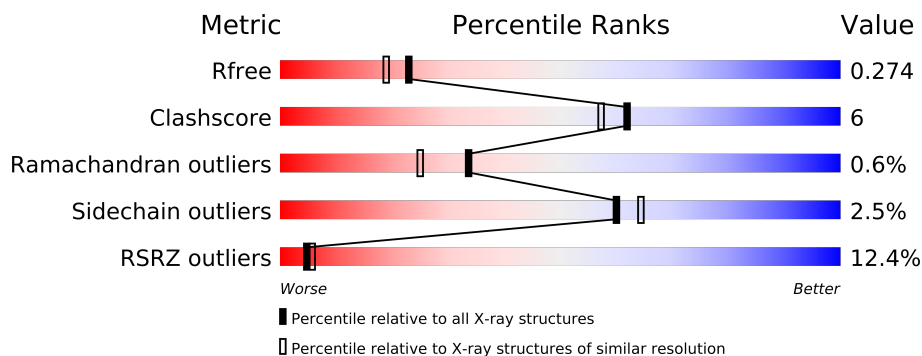
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	898	
1	B	898	
1	C	898	
1	D	898	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	4001	-	X
3	NAG	C	3001	-	X
5	TRS	C	6001	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 30064 atoms, of which 0 are hydrogen and 0 are deuterium.

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 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		

There are 56 discrepancies between the modelled and reference sequences:

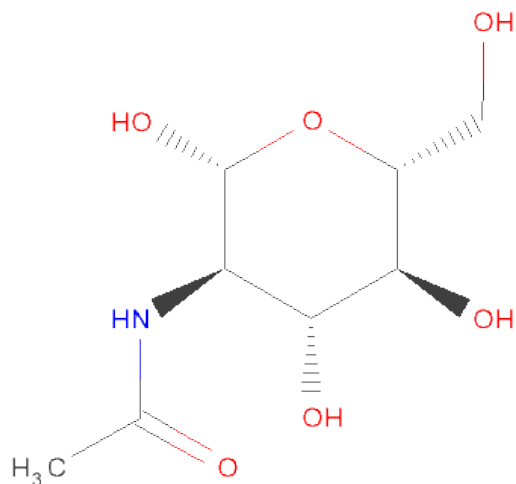
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	EXPRESSION TAG	UNP P14410
A	2	SER	-	EXPRESSION TAG	UNP P14410
A	3	SER	-	EXPRESSION TAG	UNP P14410
A	4	HIS	-	EXPRESSION TAG	UNP P14410
A	5	HIS	-	EXPRESSION TAG	UNP P14410
A	6	HIS	-	EXPRESSION TAG	UNP P14410
A	7	HIS	-	EXPRESSION TAG	UNP P14410
A	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
A	22	PHE	-	EXPRESSION TAG	UNP P14410
A	23	GLN	-	EXPRESSION TAG	UNP P14410

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

- 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		
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		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	EXPRESSION TAG	UNP P14410

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

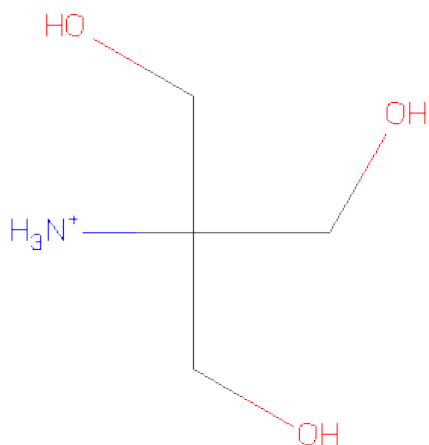
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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	THR	-	EXPRESSION TAG	UNP P14410
B	17	THR	-	EXPRESSION TAG	UNP P14410
B	18	GLU	-	EXPRESSION TAG	UNP P14410
B	19	ASN	-	EXPRESSION TAG	UNP P14410
B	20	LEU	-	EXPRESSION TAG	UNP P14410
B	21	TYR	-	EXPRESSION 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
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
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

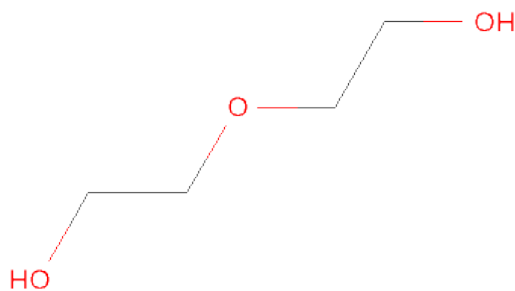
- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	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		

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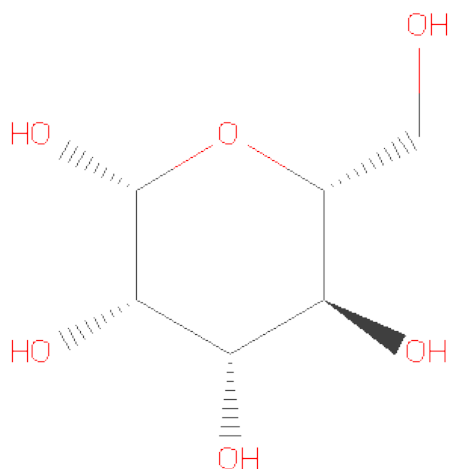
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

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

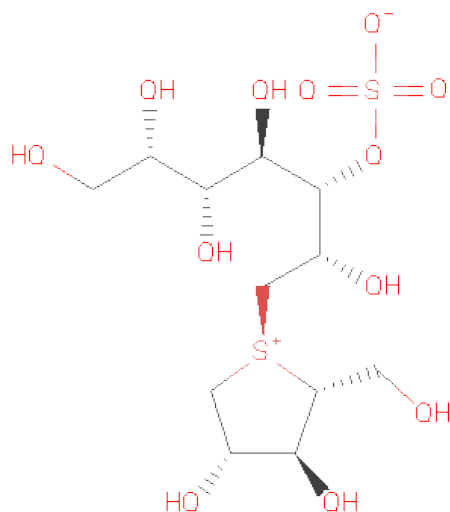
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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-TETRAHYDROXYPENTYLSULFATE (three-letter code: KTL) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>12</sub>S<sub>2</sub>).



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

- Molecule 10 is water.

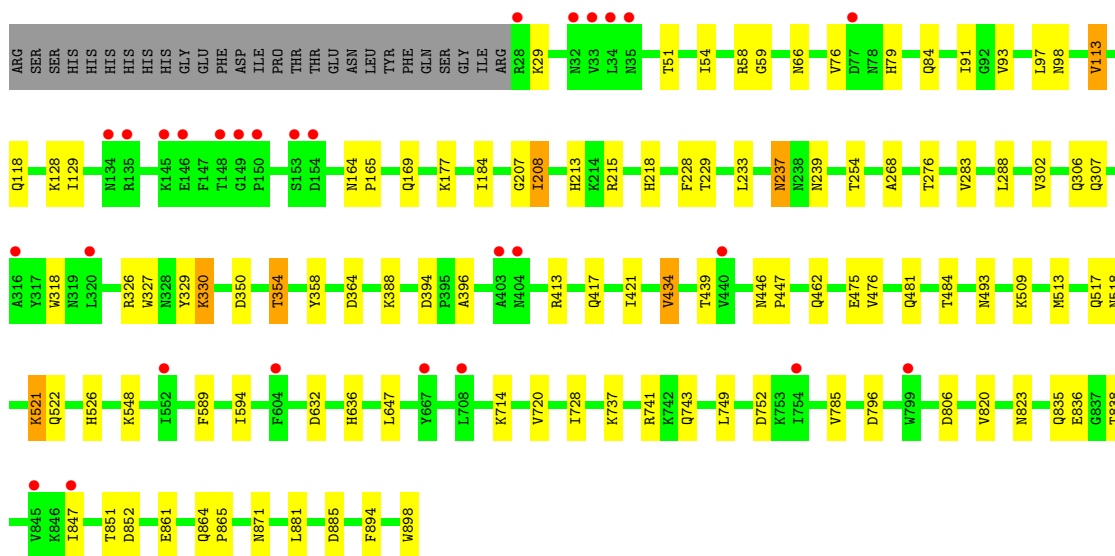
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	529	Total	O	0	0
			529	529		
10	B	514	Total	O	0	0
			514	514		
10	C	458	Total	O	0	0
			458	458		
10	D	226	Total	O	0	0
			226	226		

### 3 Residue-property plots

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.

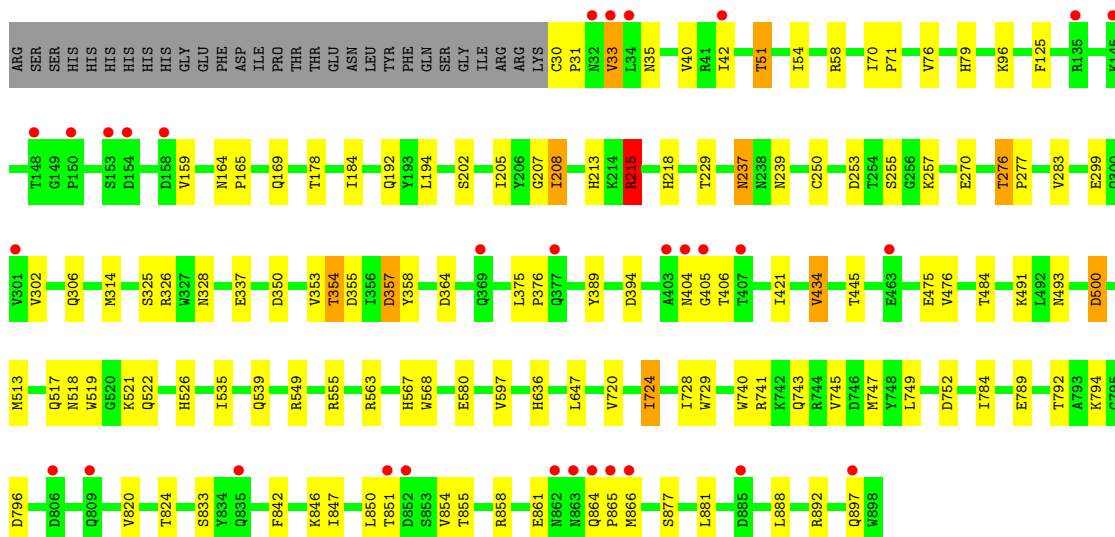
#### • Molecule 1: Sucrase-isomaltase

Chain A: 



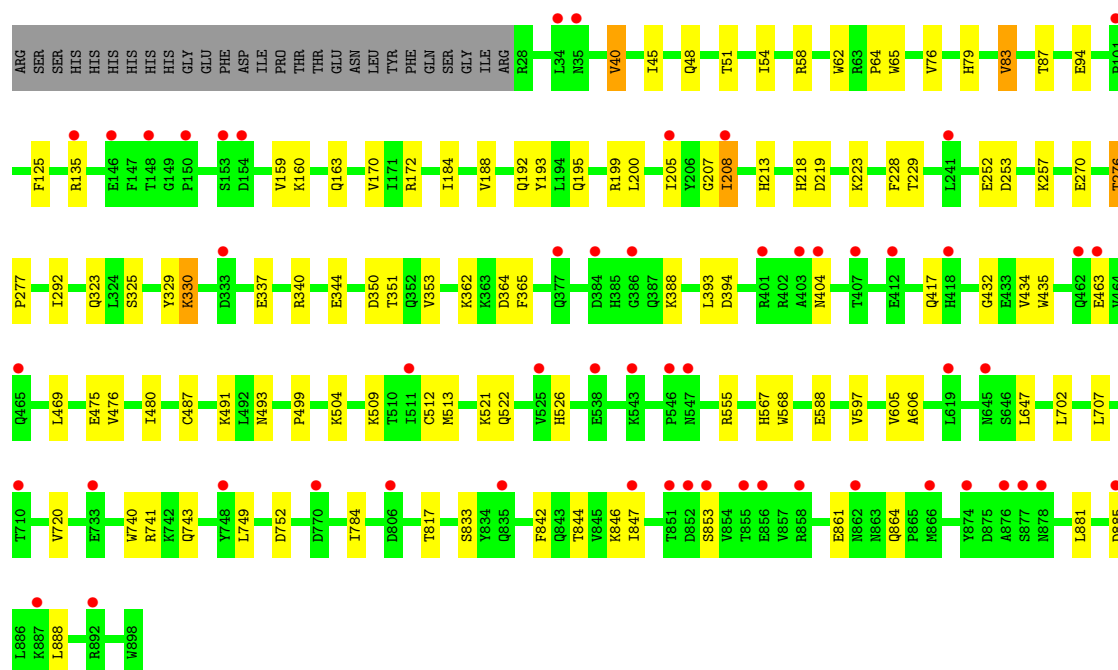
#### • Molecule 1: Sucrase-isomaltase

Chain B: 



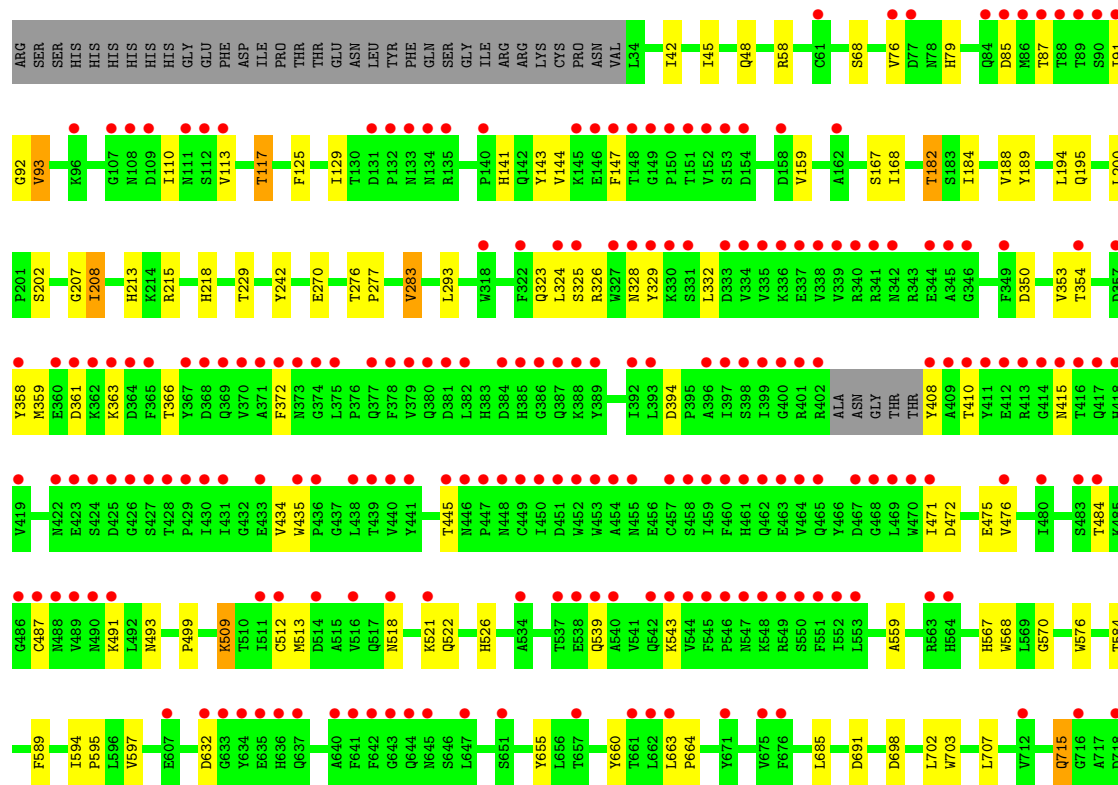
- Molecule 1: Sucrase-isomaltase

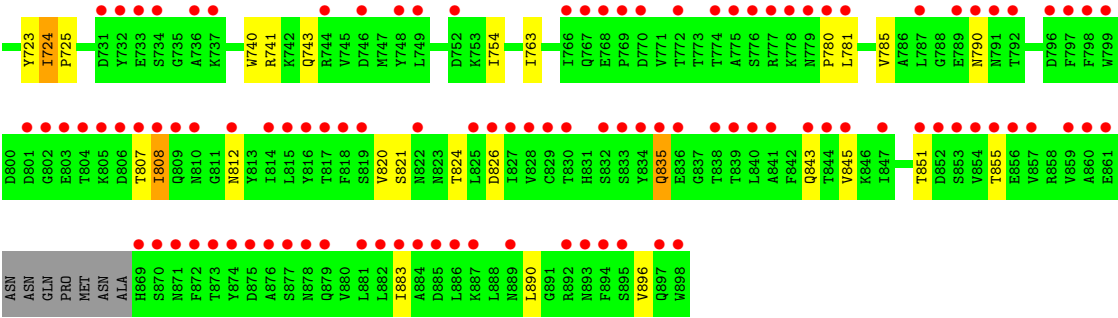
Chain C:



- Molecule 1: Sucrase-isomaltase

Chain D:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.40Å 165.76Å 341.40Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	10140 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 13.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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, 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6882	0	6573	95	0
2	A	50	0	43	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (316) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:D:896:VAL:HG23	10:D:923:HOH:O	1.89	0.73
1:B:563:ARG:NH1	10:B:1727:HOH:O	2.22	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:B:741:ARG:HH12	1:B:789:GLU:HG2	1.61	0.66
1:A:647:LEU:HD11	1:A:752:ASP:HB3	1.78	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:D:141:HIS:HE1	1:D:559:ALA:O	1.83	0.62
1:B:864:GLN:HB2	1:B:865:PRO:HD2	1.82	0.62
1:D:58:ARG:O	1:D:79:HIS:HE1	1.83	0.61
1:B:724:ILE:HD13	1:B:729:TRP:CD1	2.35	0.61
1:B:299:GLU:HG2	10:B:1251:HOH:O	1.99	0.61
1:A:835:GLN:O	1:A:838:THR:HB	2.01	0.61
1:C:846:LYS:HD2	6:C:7001:PEG:H11	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:522:GLN:HE21	1:A:526:HIS:HD2	1.50	0.59
1:A:493:ASN:ND2	1:A:513:MET:H	2.00	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:471:ILE:HG23	10:D:941:HOH:O	2.02	0.58
1:D:207:GLY:O	1:D:218:HIS:HE1	1.85	0.58
1:D:113:VAL:CG1	1:D:129:ILE:HG23	2.32	0.58
1:C:784:ILE:CD1	6:C:7001:PEG:H12	2.33	0.58
1:B:302:VAL:HG12	1:B:306:GLN:HE21	1.69	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:D:354:THR:HG21	1:D:358:TYR:HB3	1.87	0.56
1:C:79:HIS:HD2	10:C:1112:HOH:O	1.86	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:D:724:ILE:HD11	1:D:741:ARG:CA	2.36	0.55
1:B:215:ARG:NH2	1:B:580:GLU:OE2	2.38	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
1:A:302:VAL:HG12	1:A:306:GLN:NE2	2.22	0.54
1:C:51:THR:HG21	10:C:938:HOH:O	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:325:SER:HB2	1:B:353:VAL:HB	1.88	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:C:337:GLU:HA	1:C:340:ARG:HG2	1.90	0.53
1:A:329:TYR:O	1:A:330:LYS:HB2	2.08	0.53
1:C:207:GLY:O	1:C:218:HIS:HE1	1.92	0.53
1:D:168:ILE:H	1:D:182:THR:CG2	2.22	0.53
1:D:125:PHE:CE1	1:D:159:VAL:HG21	2.43	0.53
1:A:184:ILE:HG22	10:A:955:HOH:O	2.08	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:D:522:GLN:HE21	1:D:526:HIS:CD2	2.22	0.53
1:B:79:HIS:HD2	10:B:945:HOH:O	1.92	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
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
1:C:323:GLN:CG	1:C:351:THR:OG1	2.55	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:522:GLN:HE21	1:C:526:HIS:HD2	1.58	0.50
4:B:3002:NAG:O4	8:B:3003:BMA:C1	2.60	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: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:C:40:VAL:HG13	10:C:1204:HOH:O	2.12	0.49
1:B:784:ILE:CD1	6:B:7001:PEG:H41	2.42	0.49
1:C:555:ARG:O	1:C:567:HIS:CE1	2.65	0.49
1:C:193:TYR:OH	1:C:195:GLN:NE2	2.38	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:C:362:LYS:HD2	1:C:435:TRP:HB3	1.94	0.49
1:B:375:LEU:HB3	1:B:376:PRO:HD3	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:D:567:HIS:O	1:D:597:VAL:HA	2.15	0.47
1:B:792:THR:HG23	1:B:820:VAL:O	2.15	0.47
1:D:270:GLU:HG3	1:D:499:PRO:CB	2.44	0.47
1:D:92:GLY:HA3	1:D:117:THR:HG22	1.96	0.47
1:B:720:VAL:CG1	1:B:749:LEU:HD12	2.44	0.47
1:D:200:LEU:HB2	1:D:277:PRO:HG2	1.97	0.47
1:D:781:LEU:CD1	1:D:890:LEU:HD11	2.45	0.47
1:B:255:SER:OG	1:B:257:LYS:HE2	2.15	0.47
1:A:518:ASN:ND2	10:A:1543:HOH:O	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:724:ILE:HD11	1:D:741:ARG:N	2.31	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:C:51:THR:HG23	1:C:54:ILE:H	1.81	0.46
1:B:850:LEU:HD11	1:B:881:LEU:HB2	1.97	0.46
1:D:576:TRP:NE1	1:D:715:GLN:HG3	2.31	0.46
1:D:724:ILE:HD11	1:D:740:TRP:C	2.36	0.46
1:B:270:GLU:OE1	1:B:500:ASP:N	2.45	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:567:HIS:O	1:B:597:VAL:HA	2.16	0.45
1:B:40:VAL:O	1:B:42:ILE:HD12	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: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:C:62:TRP:CZ2	1:C:64:PRO:HG3	2.51	0.45
1:B:394:ASP:HB3	10:B:1069:HOH:O	2.16	0.45
1:C:188:VAL:HB	1:C:195:GLN:HB3	1.98	0.45
1:C:172:ARG:HD3	1:C:257:LYS:HD3	1.98	0.45
1:A:318:TRP:CE3	1:A:388:LYS:HG3	2.52	0.45
1:D:194:LEU:HB2	1:D:283:VAL:HG13	1.98	0.45
1:D:141:HIS:HD2	1:D:144:VAL:H	1.65	0.44
1:B:354:THR:CG2	1:B:358:TYR:CD2	2.99	0.44
1:D:188:VAL:HB	1:D:195:GLN:HB3	1.99	0.44
1:C:208:ILE:O	1:C:213:HIS:HE1	1.99	0.44
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:B:720:VAL:HG13	1:B:747:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:835:GLN:OE1	1:D:835:GLN:N	2.51	0.44
1:A:521:LYS:HE2	1:A:521:LYS:HB2	1.68	0.44
1:D:724:ILE:HA	1:D:725:PRO:HD3	1.72	0.44
1:D:167:SER:CB	1:D:182:THR:HG22	2.47	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:323:GLN:OE1	10:D:974:HOH:O	2.21	0.44
1:C:200:LEU:HD12	1:C:205:ILE:HD11	1.98	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: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:B:30:CYS:HA	1:B:31:PRO:HD3	1.91	0.43
1:A:851:THR:HG22	10:A:1300:HOH:O	2.19	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:C:325:SER:HB2	1:C:353:VAL:HB	2.00	0.43
1:A:785:VAL:HG11	1:A:820:VAL:HG21	2.00	0.43
1:A:326:ARG:HH11	1:A:636:HIS:CD2	2.36	0.43
1:D:522:GLN:NE2	1:D:526:HIS:CD2	2.82	0.43
1:D:110:ILE:HD12	1:D:189:TYR:CD2	2.54	0.43
1:B:404:ASN:HB2	10:B:1242:HOH:O	2.19	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:D:113:VAL:CG1	1:D:129:ILE:HG22	2.49	0.43
1:C:647:LEU:HD11	1:C:752:ASP:HB3	2.01	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:D:93:VAL:HG12	1:D:117:THR:HB	2.00	0.42
1:C:504:LYS:HE2	1:C:504:LYS:HB3	1.83	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:871:ASN:ND2	1:A:885:ASP:OD1	2.51	0.42
1:D:361:ASP:HB2	1:D:363:LYS:HD2	2.01	0.42
1:B:70:ILE:HA	1:B:71:PRO:HD3	1.91	0.42
1:A:327:TRP:CD2	1:A:632:ASP:HB2	2.54	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:D:807:THR:O	1:D:812:ASN:N	2.49	0.42
1:C:521:LYS:HB2	1:C:521:LYS:HE2	1.47	0.42
1:B:861:GLU:OE2	1:B:892:ARG:HD2	2.20	0.42
1:A:207:GLY:O	1:A:218:HIS:CE1	2.71	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:B:354:THR:HB	1:B:389:TYR:HE1	1.85	0.41
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:C:393:LEU:HD12	1:C:469:LEU:HD22	2.01	0.41
1:D:326:ARG:HG2	1:D:329:TYR:CZ	2.55	0.41
1:A:548:LYS:HD3	1:A:548:LYS:HA	1.89	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:462:GLN:NE2	10:A:1084:HOH:O	2.53	0.41
1:D:691:ASP:OD1	1:D:723:TYR:OH	2.20	0.41
1:D:328:ASN:ND2	1:D:632:ASP:OD1	2.52	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:C:740:TRP:HA	1:C:743:GLN:NE2	2.36	0.41
1:C:276:THR:N	1:C:277:PRO:HA	2.35	0.41
1:B:728:ILE:CD1	1:B:789:GLU:HG3	2.51	0.41
1:D:808:ILE:HG12	1:D:808:ILE:H	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:D:763:ILE:HD11	1:D:820:VAL:HG23	2.02	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
1:D:509:LYS:HZ3	9:D:5001:KTL:CAL	2.34	0.41
1:A:128:LYS:HA	1:A:288:LEU:O	2.20	0.41
1:B:842:PHE:HB2	1:B:888:LEU:HB2	2.03	0.41
1:B:794:LYS:HD3	10:B:951:HOH:O	2.20	0.41
1:B:724:ILE:HG13	1:B:724:ILE:O	2.21	0.40
1:D:218:HIS:HD2	10:D:963:HOH:O	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:432:GLY:HA2	1:C:480:ILE:HD11	2.03	0.40
1:A:421:ILE:HG12	1:A:517:GLN:HG2	2.02	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:A:589:PHE:CD2	1:A:594:ILE:HD12	2.57	0.40
1:D:589:PHE:HD2	1:D:594:ILE:HD12	1.86	0.40
1:C:257:LYS:HE3	10:C:1344:HOH:O	2.19	0.40
1:B:445:THR:OG1	1:B:518:ASN:HB3	2.21	0.40
1:D:354:THR:HG22	1:D:358:TYR:HB3	2.03	0.40
1:B:314:MET:O	1:B:549:ARG:HD3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	869/898 (97%)	831 (96%)	32 (4%)	6 (1%)	30	20
1	B	867/898 (96%)	825 (95%)	36 (4%)	6 (1%)	30	20
1	C	869/898 (97%)	825 (95%)	38 (4%)	6 (1%)	30	20
1	D	847/898 (94%)	800 (94%)	45 (5%)	2 (0%)	56	55
All	All	3452/3592 (96%)	3281 (95%)	151 (4%)	20 (1%)	33	25

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	66	72
1	B	770/797 (97%)	749 (97%)	21 (3%)	57	60
1	C	771/797 (97%)	759 (98%)	12 (2%)	75	81
1	D	751/797 (94%)	724 (96%)	27 (4%)	47	47
All	All	3064/3188 (96%)	2988 (98%)	76 (2%)	60	64

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

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Some 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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	12,14,15	0.75	1 (8%)	15,19,21	1.30	3 (20%)
2	NAG	A	1002	2	12,14,15	0.48	0	15,19,21	1.00	1 (6%)
2	BMA	A	1003	2	10,11,12	0.72	0	11,15,17	1.33	2 (18%)
2	MAN	A	1004	2	10,11,12	0.73	0	11,15,17	0.78	0
4	NAG	A	3001	1,4	12,14,15	0.66	0	15,19,21	1.15	2 (13%)
4	NAG	A	3002	4	12,14,15	0.55	0	15,19,21	0.82	0
4	NAG	B	3001	1,4	12,14,15	0.67	0	15,19,21	0.94	1 (6%)
4	NAG	B	3002	4	12,14,15	0.70	1 (8%)	15,19,21	1.26	2 (13%)
2	NAG	C	1001	1,2	12,14,15	0.85	1 (8%)	15,19,21	0.85	0
2	NAG	C	1002	2	12,14,15	0.66	0	15,19,21	0.62	0
2	BMA	C	1003	2	10,11,12	0.59	0	11,15,17	0.99	1 (9%)
2	MAN	C	1004	2	10,11,12	0.78	0	11,15,17	0.98	0
4	NAG	D	2001	1,4	12,14,15	0.54	0	15,19,21	1.85	5 (33%)
4	NAG	D	2002	4	12,14,15	0.51	0	15,19,21	1.76	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	NAG	O5-C5	-2.31	1.41	1.45
2	A	1001	NAG	O5-C5	-2.04	1.41	1.45
4	B	3002	NAG	O5-C5	-2.04	1.41	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2002	NAG	O5-C5-C4	5.55	117.70	110.65
4	D	2001	NAG	O5-C5-C4	3.64	115.28	110.65
2	A	1003	BMA	C4-C3-C2	3.50	115.21	110.50
4	D	2001	NAG	C6-C5-C4	-2.87	106.06	113.00
4	D	2001	NAG	C3-C2-N2	-2.69	107.66	111.76
2	A	1001	NAG	O5-C5-C4	-2.65	107.30	110.65
4	D	2001	NAG	O5-C5-C6	-2.64	104.21	106.98
4	D	2001	NAG	C3-C4-C5	2.61	114.86	110.20
4	A	3001	NAG	O5-C5-C4	2.56	113.91	110.65
2	A	1001	NAG	O5-C5-C6	2.50	109.61	106.98
2	A	1001	NAG	C3-C2-N2	-2.49	107.96	111.76
4	B	3002	NAG	O5-C5-C4	2.49	113.82	110.65
4	D	2002	NAG	C3-C4-C5	2.42	114.52	110.20
2	A	1003	BMA	C3-C4-C5	2.35	114.39	110.20
4	B	3001	NAG	O5-C5-C6	2.33	109.43	106.98
2	A	1002	NAG	O5-C5-C6	2.20	109.29	106.98
4	B	3002	NAG	C3-C2-N2	-2.19	108.43	111.76
4	A	3001	NAG	C3-C2-N2	-2.15	108.49	111.76
4	D	2002	NAG	C2-N2-C7	-2.07	119.62	123.09
2	C	1003	BMA	C4-C3-C2	2.06	113.27	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	12,14,15	0.73	1 (8%)	15,19,21	0.82	0
3	NAG	A	4001	1	12,14,15	0.62	0	15,19,21	1.51	3 (20%)
5	TRS	A	6001	-	7,7,7	1.14	1 (14%)	9,9,9	1.13	1 (11%)
6	PEG	A	7001	-	6,6,6	0.52	0	5,5,5	0.38	0
3	NAG	B	2001	1	12,14,15	0.52	0	15,19,21	1.81	5 (33%)
8	BMA	B	3003	-	10,11,12	0.55	0	11,15,17	0.81	0
9	KTL	B	5001	-	26,26,26	2.44	5 (19%)	38,38,38	2.16	8 (21%)
6	PEG	B	7001	-	6,6,6	0.38	0	5,5,5	0.47	0
3	NAG	C	2001	1	12,14,15	0.55	0	15,19,21	1.45	1 (6%)
3	NAG	C	3001	1	12,14,15	0.51	0	15,19,21	0.76	0
3	NAG	C	4001	1	12,14,15	0.58	0	15,19,21	1.25	1 (6%)
5	TRS	C	6001	-	7,7,7	0.98	1 (14%)	9,9,9	0.61	0
6	PEG	C	7001	-	6,6,6	0.45	0	5,5,5	0.23	0
9	KTL	D	5001	-	26,26,26	2.59	4 (15%)	38,38,38	1.96	5 (13%)
6	PEG	D	7001	-	6,6,6	0.43	0	5,5,5	0.29	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	-	-	0/29/45/45	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0/29/45/45	0/1/1/1
6	PEG	D	7001	-	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	5001	KTL	CAW-SAY	-8.08	1.66	1.84
9	D	5001	KTL	CAN-SAY	-7.99	1.66	1.82
9	B	5001	KTL	CAW-SAY	-7.40	1.68	1.84
9	B	5001	KTL	CAN-SAY	-7.25	1.67	1.82
9	D	5001	KTL	CAO-SAY	-5.45	1.66	1.82
9	B	5001	KTL	CAO-SAY	-5.24	1.67	1.82
9	D	5001	KTL	OAP-SAZ	2.79	1.64	1.59
5	A	6001	TRS	C-N	-2.73	1.46	1.50
9	B	5001	KTL	OAP-CAX	-2.55	1.42	1.46
5	C	6001	TRS	C-N	-2.51	1.47	1.50
3	A	2001	NAG	O5-C5	-2.23	1.41	1.45
9	B	5001	KTL	OAP-SAZ	2.02	1.63	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	5001	KTL	CAO-SAY-CAN	8.87	110.01	101.64
9	D	5001	KTL	CAO-SAY-CAN	7.15	108.39	101.64
9	D	5001	KTL	CAN-SAY-CAW	6.98	103.69	93.48
9	B	5001	KTL	CAN-SAY-CAW	5.76	101.90	93.48
3	C	2001	NAG	O5-C5-C6	4.45	111.65	106.98
3	B	2001	NAG	C6-C5-C4	-3.94	103.48	113.00
9	B	5001	KTL	CAM-CAW-SAY	3.72	113.79	110.08
3	C	4001	NAG	O5-C5-C6	3.61	110.77	106.98
3	B	2001	NAG	O5-C5-C4	3.22	114.74	110.65
3	A	4001	NAG	C4-C3-C2	-3.11	103.71	111.32
9	B	5001	KTL	OAD-CAR-CAN	3.02	114.69	109.14
3	A	4001	NAG	C2-N2-C7	2.86	127.88	123.09
3	A	4001	NAG	C3-C2-N2	2.76	115.97	111.76
5	A	6001	TRS	C1-C-N	-2.36	101.89	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	NAG	C3-C2-N2	-2.32	108.23	111.76
9	B	5001	KTL	CAN-CAR-CAU	-2.32	104.25	106.42
3	B	2001	NAG	C3-C4-C5	2.26	114.25	110.20
3	B	2001	NAG	O5-C5-C6	2.23	109.32	106.98
9	D	5001	KTL	OAP-SAZ-OAI	2.15	110.58	104.58
9	D	5001	KTL	CAQ-CAT-CAV	2.14	115.92	112.43
9	B	5001	KTL	OAP-SAZ-OAI	2.14	110.56	104.58
9	D	5001	KTL	OAP-CAX-CAV	2.13	111.14	106.37
9	B	5001	KTL	CAR-CAN-SAY	-2.08	103.13	107.25
9	B	5001	KTL	OAG-CAU-CAW	2.01	113.55	109.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	871/898 (96%)	0.51	28 (3%)	45 49	4, 10, 19, 36	0
1	B	869/898 (96%)	0.48	31 (3%)	41 44	3, 11, 20, 37	0
1	C	871/898 (96%)	0.57	55 (6%)	19 22	5, 11, 21, 30	0
1	D	853/898 (94%)	1.71	318 (37%)	1 1	3, 11, 20, 27	0
All	All	3464/3592 (96%)	0.81	432 (12%)	5 5	3, 11, 20, 37	0

All (432) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	PRO	7.5
1	D	547	ASN	7.3
1	D	808	ILE	7.2
1	D	455	ASN	6.8
1	D	546	PRO	6.6
1	D	370	VAL	6.4
1	D	416	THR	6.4
1	D	450	ILE	6.4
1	D	361	ASP	6.3
1	D	855	THR	6.2
1	D	400	GLY	6.1
1	D	458	SER	6.1
1	A	148	THR	6.0
1	D	408	TYR	6.0
1	D	874	TYR	5.9
1	D	154	ASP	5.9
1	D	802	GLY	5.9
1	D	822	ASN	5.8
1	D	345	ALA	5.7
1	D	418	HIS	5.7
1	D	91	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	462	GLN	5.6
1	D	149	GLY	5.5
1	B	865	PRO	5.5
1	D	452	TRP	5.5
1	D	464	VAL	5.4
1	D	789	GLU	5.4
1	D	876	ALA	5.4
1	B	403	ALA	5.4
1	D	834	TYR	5.4
1	D	454	ALA	5.3
1	D	816	TYR	5.3
1	D	851	THR	5.3
1	B	32	ASN	5.2
1	D	633	GLY	5.2
1	D	465	GLN	5.2
1	D	427	SER	5.1
1	D	873	THR	5.1
1	D	378	PHE	5.1
1	D	451	ASP	5.0
1	D	853	SER	5.0
1	B	33	VAL	5.0
1	D	892	ARG	4.9
1	D	447	PRO	4.8
1	D	409	ALA	4.8
1	D	872	PHE	4.7
1	D	435	TRP	4.7
1	D	770	ASP	4.7
1	D	877	SER	4.6
1	D	372	PHE	4.6
1	D	135	ARG	4.6
1	D	799	TRP	4.6
1	D	852	ASP	4.6
1	D	538	GLU	4.5
1	D	542	GLN	4.5
1	D	373	ASN	4.4
1	D	516	VAL	4.4
1	D	768	GLU	4.4
1	D	380	GLN	4.4
1	D	375	LEU	4.4
1	D	854	VAL	4.4
1	D	448	ASN	4.4
1	D	413	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	417	GLN	4.3
1	D	367	TYR	4.3
1	B	866	MET	4.3
1	D	148	THR	4.3
1	D	835	GLN	4.3
1	D	333	ASP	4.3
1	D	457	CYS	4.3
1	D	484	THR	4.3
1	D	426	GLY	4.2
1	D	369	GLN	4.2
1	D	382	LEU	4.2
1	D	401	ARG	4.2
1	D	486	GLY	4.2
1	D	548	LYS	4.2
1	D	534	ALA	4.2
1	D	438	LEU	4.2
1	D	733	GLU	4.2
1	D	885	ASP	4.2
1	D	362	LYS	4.2
1	D	344	GLU	4.2
1	D	371	ALA	4.2
1	D	870	SER	4.2
1	D	386	GLY	4.1
1	D	792	THR	4.1
1	D	453	TRP	4.1
1	D	810	ASN	4.1
1	D	84	GLN	4.1
1	D	884	ALA	4.0
1	D	640	ALA	4.0
1	C	154	ASP	4.0
1	D	446	ASN	4.0
1	D	897	GLN	4.0
1	B	404	ASN	4.0
1	D	718	ASP	4.0
1	D	859	VAL	3.9
1	C	401	ARG	3.9
1	D	839	THR	3.9
1	D	843	GLN	3.9
1	D	545	PHE	3.9
1	D	449	CYS	3.9
1	D	881	LEU	3.9
1	D	769	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	836	GLU	3.8
1	D	87	THR	3.8
1	D	861	GLU	3.8
1	A	32	ASN	3.8
1	C	546	PRO	3.8
1	C	547	ASN	3.7
1	D	132	PRO	3.7
1	D	431	ILE	3.7
1	D	90	SER	3.7
1	D	385	HIS	3.7
1	C	34	LEU	3.7
1	D	328	ASN	3.7
1	D	331	SER	3.7
1	D	518	ASN	3.7
1	D	419	VAL	3.7
1	C	35	ASN	3.6
1	D	152	VAL	3.6
1	D	381	ASP	3.6
1	D	671	TYR	3.6
1	D	543	LYS	3.6
1	B	862	ASN	3.6
1	D	856	GLU	3.6
1	A	404	ASN	3.6
1	D	460	PHE	3.6
1	D	398	SER	3.5
1	D	384	ASP	3.5
1	D	809	GLN	3.5
1	D	641	PHE	3.5
1	D	746	ASP	3.5
1	D	645	ASN	3.5
1	D	153	SER	3.5
1	D	358	TYR	3.5
1	C	856	GLU	3.4
1	D	550	SER	3.4
1	D	318	TRP	3.4
1	D	734	SER	3.4
1	D	780	PRO	3.4
1	D	812	ASN	3.4
1	D	878	ASN	3.4
1	D	76	VAL	3.4
1	D	470	TRP	3.4
1	C	153	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	790	ASN	3.4
1	A	403	ALA	3.4
1	D	338	VAL	3.4
1	D	807	THR	3.3
1	D	748	TYR	3.3
1	C	876	ALA	3.3
1	D	77	ASP	3.3
1	D	354	THR	3.3
1	B	407	THR	3.3
1	D	337	GLU	3.3
1	A	33	VAL	3.3
1	D	377	GLN	3.3
1	D	387	GLN	3.3
1	D	838	THR	3.3
1	D	336	LYS	3.3
1	D	145	LYS	3.3
1	D	89	THR	3.2
1	D	365	PHE	3.2
1	D	845	VAL	3.2
1	D	894	PHE	3.2
1	C	465	GLN	3.2
1	D	887	LYS	3.2
1	D	425	ASP	3.2
1	D	399	ILE	3.2
1	D	815	LEU	3.2
1	B	863	ASN	3.2
1	D	818	PHE	3.2
1	C	377	GLN	3.1
1	C	101	PRO	3.1
1	D	414	GLY	3.1
1	D	829	CYS	3.1
1	D	412	GLU	3.1
1	D	429	PRO	3.1
1	A	146	GLU	3.1
1	D	85	ASP	3.1
1	D	393	LEU	3.1
1	D	787	LEU	3.1
1	D	374	GLY	3.1
1	D	643	GLY	3.1
1	D	397	ILE	3.1
1	D	540	ALA	3.1
1	D	657	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	864	GLN	3.1
1	D	814	ILE	3.1
1	A	150	PRO	3.0
1	D	112	SER	3.0
1	D	88	THR	3.0
1	D	647	LEU	3.0
1	D	886	LEU	3.0
1	D	389	TYR	3.0
1	D	162	ALA	3.0
1	D	716	GLY	3.0
1	D	436	PRO	3.0
1	D	551	PHE	3.0
1	D	830	THR	3.0
1	D	329	TYR	3.0
1	D	334	VAL	3.0
1	D	731	ASP	3.0
1	D	844	THR	3.0
1	D	801	ASP	2.9
1	C	866	MET	2.9
1	C	892	ARG	2.9
1	D	803	GLU	2.9
1	D	468	GLY	2.9
1	D	146	GLU	2.9
1	A	153	SER	2.9
1	D	847	ILE	2.9
1	D	796	ASP	2.9
1	D	644	GLN	2.9
1	D	488	ASN	2.9
1	D	368	ASP	2.9
1	D	752	ASP	2.9
1	D	410	THR	2.9
1	C	887	LYS	2.9
1	D	879	GLN	2.9
1	D	675	VAL	2.9
1	D	882	LEU	2.9
1	B	851	THR	2.9
1	D	324	LEU	2.8
1	D	549	ARG	2.8
1	B	885	ASP	2.8
1	D	346	GLY	2.8
1	D	476	VAL	2.8
1	D	676	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	853	SER	2.8
1	D	766	ILE	2.8
1	D	360	GLU	2.8
1	D	840	LEU	2.8
1	D	564	HIS	2.8
1	C	146	GLU	2.8
1	D	607	GLU	2.8
1	A	77	ASP	2.8
1	A	34	LEU	2.8
1	C	403	ALA	2.8
1	B	405	GLY	2.8
1	B	852	ASP	2.8
1	D	430	ILE	2.8
1	C	874	TYR	2.8
1	A	149	GLY	2.8
1	C	407	THR	2.7
1	D	151	THR	2.7
1	D	772	THR	2.7
1	D	826	ASP	2.7
1	D	133	ASN	2.7
1	C	855	THR	2.7
1	D	778	LYS	2.7
1	C	835	GLN	2.7
1	D	487	CYS	2.7
1	D	544	VAL	2.7
1	D	469	LEU	2.7
1	D	552	ILE	2.7
1	B	369	GLN	2.7
1	D	632	ASP	2.7
1	C	241	LEU	2.7
1	D	781	LEU	2.7
1	D	736	ALA	2.7
1	C	384	ASP	2.7
1	D	806	ASP	2.7
1	D	113	VAL	2.7
1	D	340	ARG	2.7
1	D	871	ASN	2.6
1	D	388	LYS	2.6
1	C	885	ASP	2.6
1	D	483	SER	2.6
1	D	898	TRP	2.6
1	D	411	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	423	GLU	2.6
1	C	852	ASP	2.6
1	D	379	VAL	2.6
1	D	489	VAL	2.6
1	D	563	ARG	2.6
1	A	35	ASN	2.6
1	D	341	ARG	2.6
1	C	877	SER	2.6
1	C	418	HIS	2.6
1	D	817	THR	2.6
1	A	754	ILE	2.6
1	D	779	ASN	2.6
1	D	433	GLU	2.6
1	D	463	GLU	2.6
1	D	440	VAL	2.6
1	D	662	LEU	2.6
1	B	809	GLN	2.6
1	C	412	GLU	2.6
1	A	28	ARG	2.6
1	A	134	ASN	2.6
1	D	512	CYS	2.6
1	A	154	ASP	2.5
1	B	135	ARG	2.5
1	A	667	TYR	2.5
1	C	150	PRO	2.5
1	C	847	ILE	2.5
1	D	134	ASN	2.5
1	D	893	ASN	2.5
1	C	710	THR	2.5
1	C	135	ARG	2.5
1	D	424	SER	2.5
1	D	651	SER	2.5
1	C	404	ASN	2.5
1	D	767	GLN	2.5
1	D	364	ASP	2.5
1	D	825	LEU	2.5
1	C	858	ARG	2.5
1	B	154	ASP	2.5
1	D	467	ASP	2.5
1	D	107	GLY	2.4
1	D	461	HIS	2.4
1	D	339	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	415	ASN	2.4
1	B	835	GLN	2.4
1	B	463	GLU	2.4
1	D	791	ASN	2.4
1	D	402	ARG	2.4
1	D	459	ILE	2.4
1	D	663	LEU	2.4
1	D	732	TYR	2.4
1	D	327	TRP	2.4
1	D	445	THR	2.4
1	C	543	LYS	2.4
1	A	847	ILE	2.4
1	D	357	ASP	2.4
1	D	439	THR	2.4
1	A	799	TRP	2.4
1	D	635	GLU	2.4
1	D	428	THR	2.4
1	C	205	ILE	2.4
1	C	619	LEU	2.3
1	D	108	ASN	2.3
1	D	797	PHE	2.3
1	B	42	ILE	2.3
1	D	109	ASP	2.3
1	D	335	VAL	2.3
1	D	441	TYR	2.3
1	D	744	ARG	2.3
1	D	392	ILE	2.3
1	D	819	SER	2.3
1	D	833	SER	2.3
1	D	634	TYR	2.3
1	D	860	ALA	2.3
1	C	463	GLU	2.3
1	D	883	ILE	2.3
1	B	377	GLN	2.3
1	D	804	THR	2.3
1	D	61	CYS	2.3
1	D	539	GLN	2.3
1	D	805	LYS	2.3
1	B	148	THR	2.3
1	D	828	VAL	2.3
1	D	396	ALA	2.3
1	D	776	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	832	SER	2.3
1	D	661	THR	2.3
1	D	857	VAL	2.2
1	D	775	ALA	2.2
1	D	330	LYS	2.2
1	D	749	LEU	2.2
1	C	538	GLU	2.2
1	B	153	SER	2.2
1	C	645	ASN	2.2
1	C	770	ASP	2.2
1	D	480	ILE	2.2
1	D	111	ASN	2.2
1	D	363	LYS	2.2
1	D	777	ARG	2.2
1	D	349	PHE	2.2
1	D	889	ASN	2.2
1	D	471	ILE	2.2
1	A	145	LYS	2.2
1	B	145	LYS	2.2
1	D	131	ASP	2.2
1	D	841	ALA	2.2
1	D	712	VAL	2.2
1	C	148	THR	2.2
1	B	806	ASP	2.2
1	D	827	ILE	2.2
1	C	878	ASN	2.2
1	D	537	THR	2.2
1	D	869	HIS	2.2
1	D	322	PHE	2.1
1	D	737	LYS	2.1
1	B	34	LEU	2.1
1	C	733	GLU	2.1
1	D	553	LEU	2.1
1	C	208	ILE	2.1
1	D	86	MET	2.1
1	B	158	ASP	2.1
1	C	862	ASN	2.1
1	D	875	ASP	2.1
1	A	845	VAL	2.1
1	D	521	LYS	2.1
1	D	422	ASN	2.1
1	C	462	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	96	LYS	2.1
1	D	774	THR	2.1
1	C	525	VAL	2.1
1	C	511	ILE	2.1
1	B	301	VAL	2.1
1	B	897	GLN	2.1
1	D	147	PHE	2.1
1	D	642	PHE	2.1
1	B	150	PRO	2.1
1	A	708	LEU	2.1
1	A	135	ARG	2.1
1	D	342	ASN	2.1
1	D	490	ASN	2.1
1	C	748	TYR	2.1
1	C	386	GLY	2.1
1	A	320	LEU	2.1
1	D	637	GLN	2.1
1	D	636	HIS	2.1
1	A	604	PHE	2.1
1	A	552	ILE	2.0
1	D	511	ILE	2.0
1	D	491	LYS	2.0
1	D	895	SER	2.0
1	C	806	ASP	2.0
1	D	514	ASP	2.0
1	A	440	VAL	2.0
1	D	798	PHE	2.0
1	A	316	ALA	2.0
1	C	851	THR	2.0
1	C	333	ASP	2.0
1	D	140	PRO	2.0
1	D	158	ASP	2.0
1	D	325	SER	2.0

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

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



### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	3002	14/15	0.31	6.02	24,27,29,30	0
4	NAG	D	2002	14/15	0.33	5.22	24,27,31,32	0
2	NAG	A	1001	14/15	0.23	4.38	16,20,24,25	0
2	NAG	C	1002	14/15	0.19	4.16	12,15,18,21	0
2	NAG	C	1001	14/15	0.23	3.29	14,16,17,19	0
2	NAG	A	1002	14/15	0.18	2.28	12,13,18,20	0
4	NAG	B	3001	14/15	0.19	1.52	19,20,22,24	0
2	MAN	C	1004	11/12	0.14	0.17	11,13,16,16	0
2	BMA	C	1003	11/12	0.13	0.05	14,16,20,23	0
4	NAG	D	2001	14/15	0.13	-0.14	4,14,19,23	0
4	NAG	A	3001	14/15	0.12	-1.02	9,13,15,18	0
2	BMA	A	1003	11/12	0.12	-1.25	15,17,18,20	0
4	NAG	B	3002	14/15	0.16	-1.75	25,27,28,29	0
2	MAN	A	1004	11/12	0.09	-2.24	15,17,18,19	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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	4001	14/15	0.33	10.28	24,27,28,30	0
3	NAG	C	3001	14/15	0.27	2.28	22,25,26,27	0
5	TRS	C	6001	8/8	0.17	2.08	20,20,20,21	0
3	NAG	C	4001	14/15	0.30	1.50	35,40,41,42	0
5	TRS	A	6001	8/8	0.19	0.87	10,12,13,15	0
3	NAG	C	2001	14/15	0.17	0.62	16,22,26,27	0
6	PEG	A	7001	7/7	0.15	0.02	21,22,25,25	0
6	PEG	B	7001	7/7	0.12	-0.02	20,20,21,22	0
3	NAG	A	2001	14/15	0.19	-0.18	31,33,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	KTL	D	5001	26/26	0.17	-0.66	20,24,26,27	0
6	PEG	C	7001	7/7	0.12	-0.83	18,22,25,27	0
9	KTL	B	5001	26/26	0.13	-0.93	10,18,23,25	0
3	NAG	B	2001	14/15	0.11	-1.17	9,16,18,21	0
6	PEG	D	7001	7/7	0.14	-1.36	37,37,38,38	0
7	CL	A	8001	1/1	0.12	-3.71	3,3,3,3	0
8	BMA	B	3003	11/12	0.22	-	61,62,63,63	0

## 6.5 Other polymers

There are no such residues in this entry.