



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:21 AM GMT

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

This is a 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 ⓘ symbol.

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

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

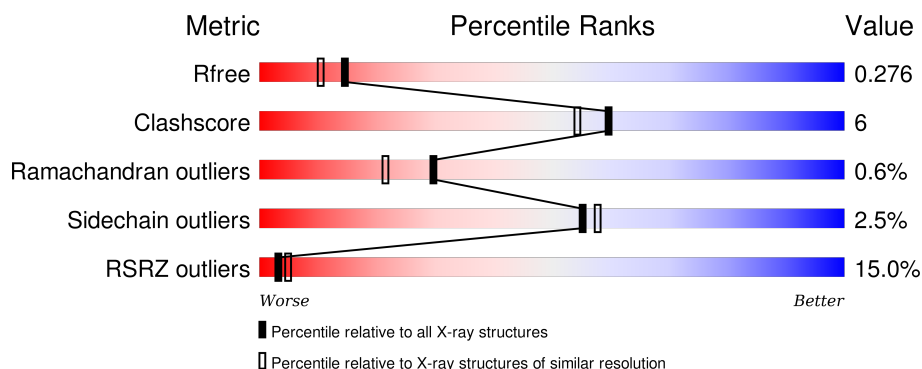
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

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

2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sucrase-isomaltase.

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

There are 112 discrepancies between the modelled and reference sequences:

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

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

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

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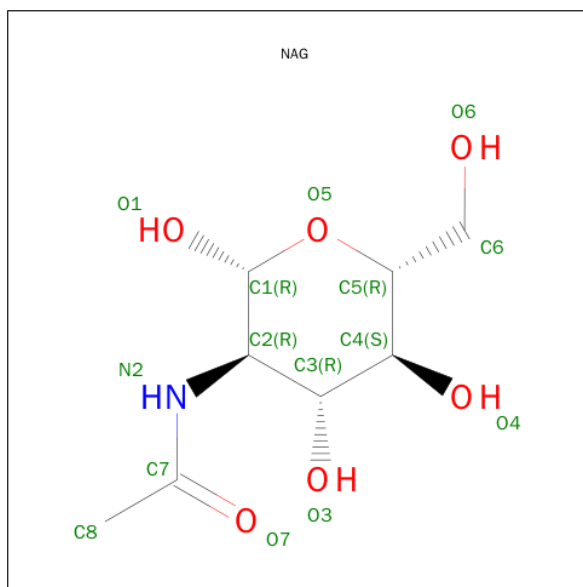
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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	PHE	-	EXPRESSION TAG	UNP P14410
D	23	GLN	-	EXPRESSION TAG	UNP P14410
D	24	SER	-	EXPRESSION TAG	UNP P14410
D	25	GLY	-	EXPRESSION TAG	UNP P14410
D	26	ILE	-	EXPRESSION TAG	UNP P14410
D	27	ARG	-	EXPRESSION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

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

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

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



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

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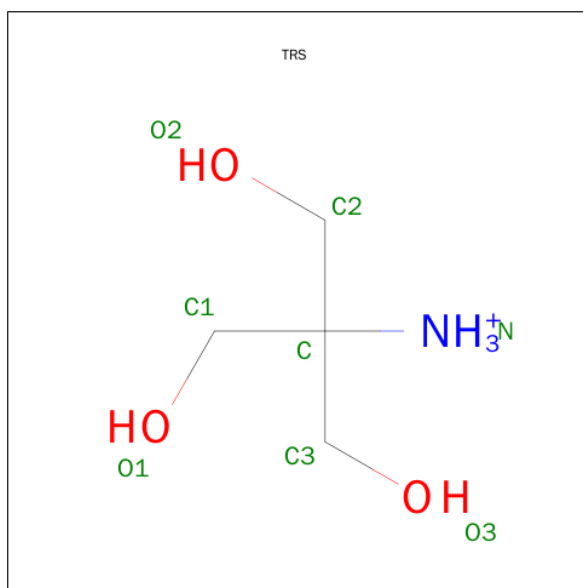
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

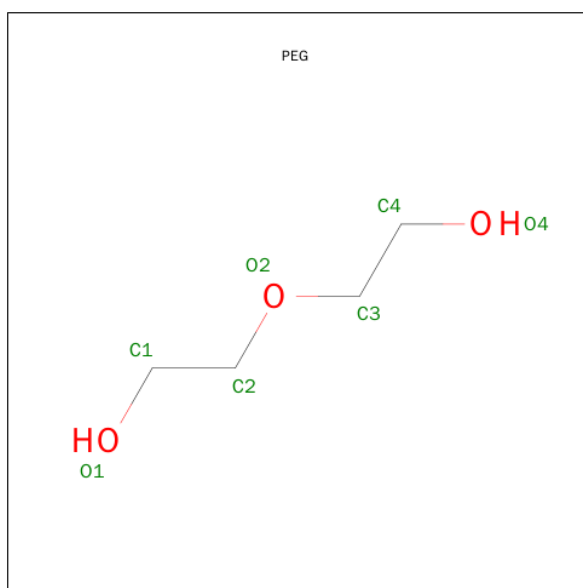
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

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



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: $C_4H_{10}O_3$).

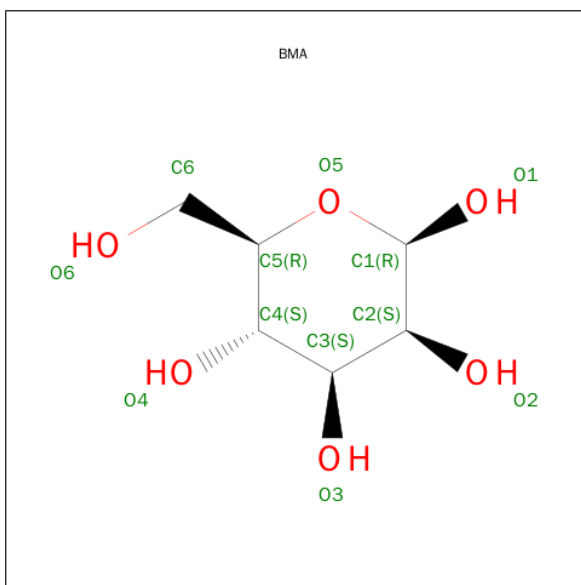


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

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

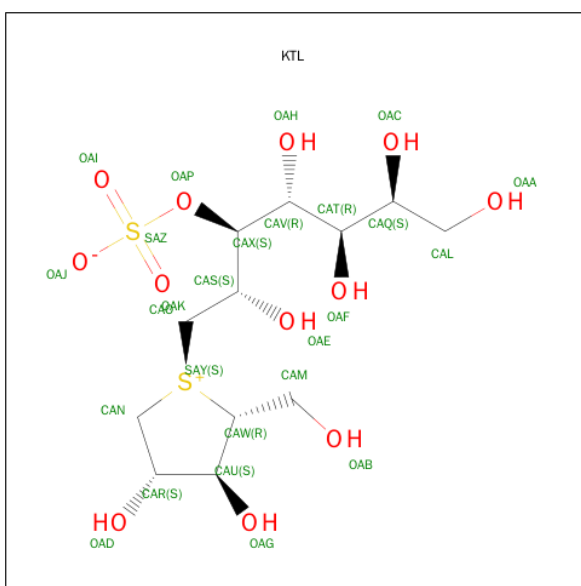
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

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



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

- Molecule 9 is (1S,2R,3R,4S)-1-[(1S)-2-[(2R,3S,4S)-3,4-DIHYDROXY-2-(HYDROXYMETHYL)TETRAHYDROTHIOPHENIUM-1-YL]-1-HYDROXYETHYL]-2,3,4,5-TETRAHYDROXYPENTYL SULFATE (three-letter code: KTL) (formula: C₁₂H₂₄O₁₂S₂).



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

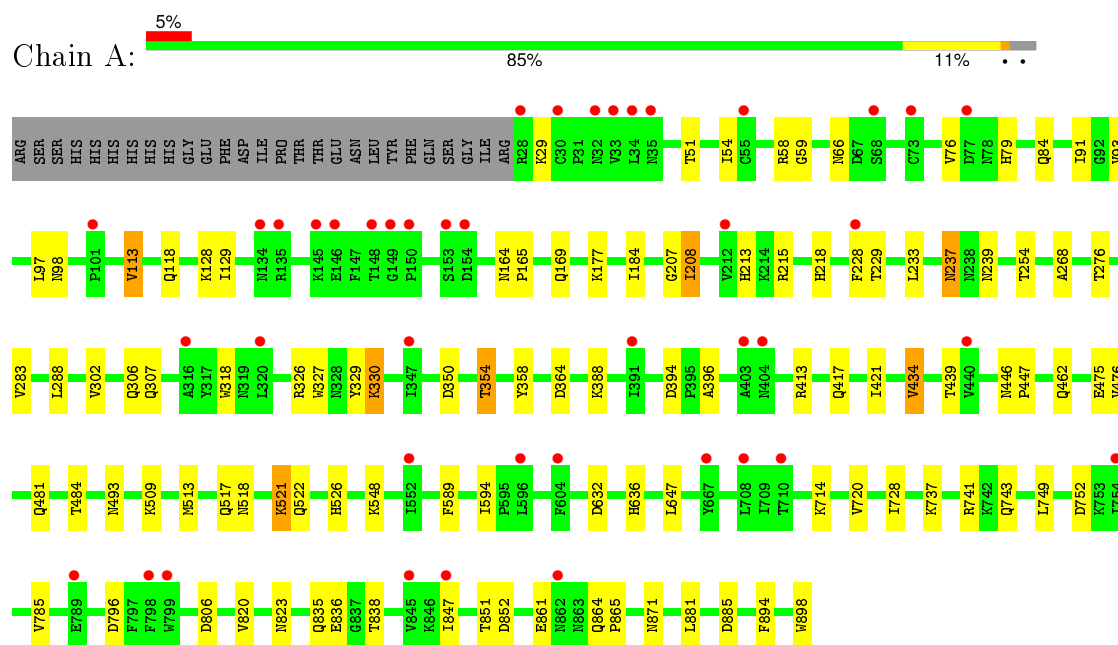
- Molecule 10 is water.

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

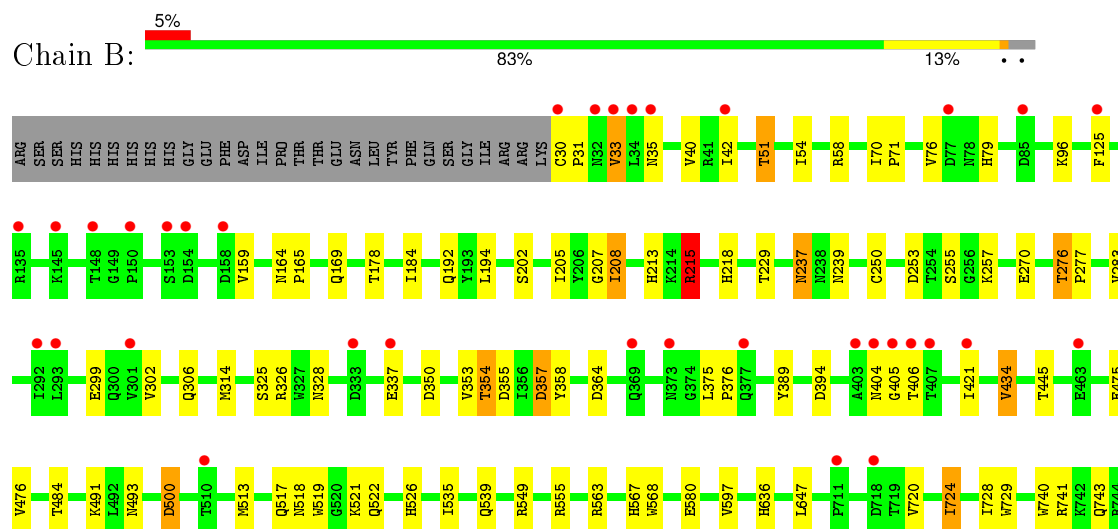
3 Residue-property plots

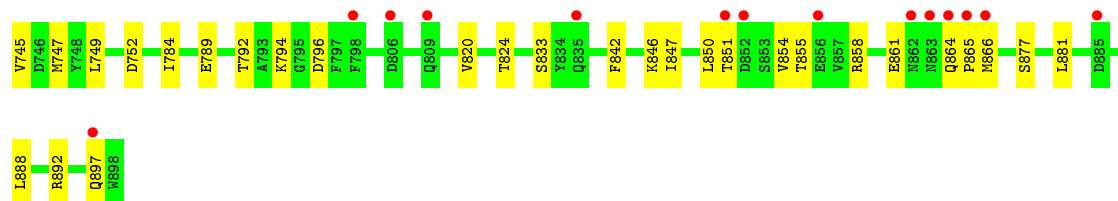
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Sucrase-isomaltase

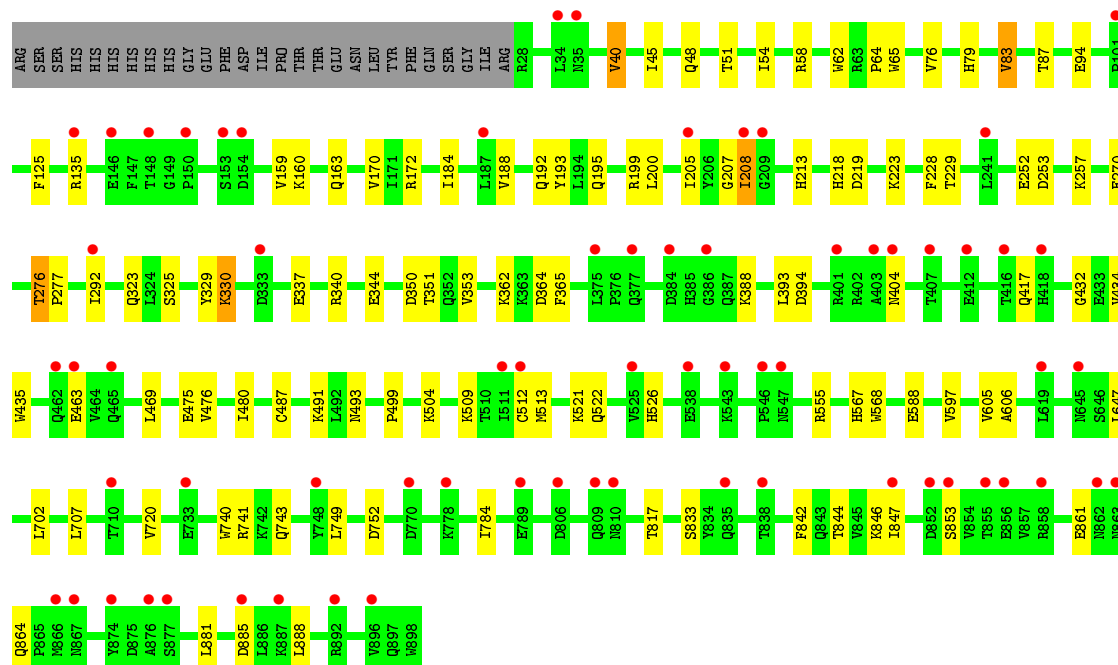
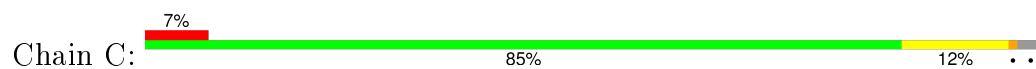


• Molecule 1: Sucrase-isomaltase

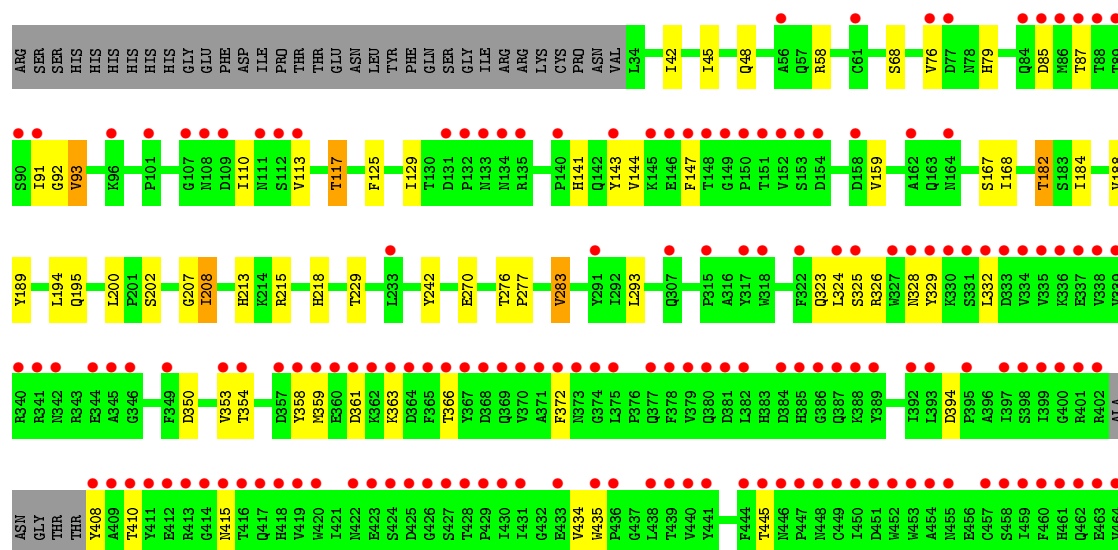
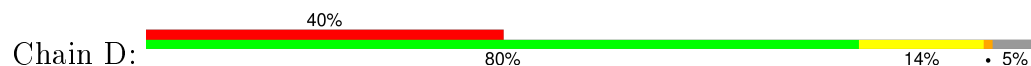




• Molecule 1: Sucrase-isomaltase



• Molecule 1: Sucrase-isomaltase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.40 Å 165.76 Å 341.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.15 19.94 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.8 (19.95-2.15) 94.8 (19.94-2.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.15 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.223 0.243 , 0.276	Depositor DCC
R_{free} test set	10150 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 202412 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30064	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CL, KTL, TRS, PEG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/7236	0.65	1/9868 (0.0%)
1	B	0.55	0/7216	0.64	1/9843 (0.0%)
1	C	0.55	0/7230	0.63	0/9861
1	D	0.44	0/7079	0.57	0/9653
All	All	0.54	0/28761	0.62	2/39225 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7035	0	6734	67	0
1	B	7015	0	6711	86	0
1	C	7029	0	6724	69	0
1	D	6882	0	6573	95	0
2	A	50	0	43	0	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:CYS:HG	1:C:512:CYS:HG	1.05	1.01
1:B:741:ARG:H	1:B:743:GLN:HE21	1.13	0.93
1:C:741:ARG:H	1:C:743:GLN:HE21	1.13	0.88
1:C:51:THR:HG22	10:C:920:HOH:O	1.75	0.87
1:B:51:THR:HG21	10:C:1095:HOH:O	1.75	0.85
1:C:323:GLN:HG2	1:C:351:THR:OG1	1.81	0.81
1:A:741:ARG:H	1:A:743:GLN:HE21	1.30	0.79
1:B:205:ILE:HG12	10:B:1299:HOH:O	1.83	0.79
1:C:270:GLU:HG3	1:C:499:PRO:HB3	1.65	0.77
1:A:354:THR:CG2	1:A:358:TYR:CD2	2.68	0.76
1:B:237:ASN:HD22	1:B:239:ASN:H	1.35	0.74
1:A:237:ASN:HD22	1:A:239:ASN:H	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:GLN:HE21	1:D:526:HIS:HD2	1.35	0.74
1:C:493:ASN:HD21	1:C:513:MET:H	1.36	0.73
1:D:91:ILE:HG23	1:D:147:PHE:HE2	1.53	0.73
1: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:846:LYS:HD2	6:C:7001:PEG:H11	1.83	0.61
1:C:218:HIS:HD2	10:C:940:HOH:O	1.83	0.61
1:B:250:CYS:HB2	10:B:1299:HOH:O	2.00	0.60
1:B:302:VAL:HG12	1:B:306:GLN:NE2	2.16	0.60
1:C:135:ARG:HH22	1:D:491:LYS:HZ2	1.46	0.60
1:C:135:ARG:HH22	1:D:491:LYS:NZ	1.99	0.60
1:C:493:ASN:ND2	1:C:513:MET:H	1.99	0.60
1:D:141:HIS:CD2	1:D:143:TYR:H	2.18	0.60
1:A:493:ASN:HD21	1:A:513:MET:H	1.50	0.60
1:A:237:ASN:ND2	1:A:239:ASN:H	1.98	0.59
1:B:354:THR:HG23	1:B:358:TYR:CD2	2.35	0.59
1:D:394:ASP:HB3	10:D:1353:HOH:O	2.01	0.59
1:D:323:GLN:HE21	1:D:353:VAL:HG21	1.68	0.59
1:B:207:GLY:O	1:B:218:HIS:HE1	1.85	0.59
1:A: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG12	1:A:306:GLN:NE2	2.22	0.54
1:C:51:THR:HG21	10:C:938:HOH:O	2.07	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:ILE:HD11	1:B:741:ARG:HA	1.94	0.50
1:D:76:VAL:HG12	1:D:76:VAL:O	2.12	0.50
1:C:323:GLN:CG	1:C:351:THR:OG1	2.55	0.50
1:C:522:GLN:HE21	1:C:526:HIS:HD2	1.58	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HE3	10:A:1083:HOH:O	2.17	0.44
1:D:595:PRO:HD2	10:D:969:HOH:O	2.16	0.44
1:B:33:VAL:HG13	1:B:35:ASN:H	1.81	0.44
1:C:741:ARG:N	1:C:743:GLN:HE21	1.95	0.44
1:B:720:VAL:HG13	1:B:747:MET:HB3	1.99	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

All (20) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

14 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1001	1,2	14,14,15	0.64	0	15,19,21	0.95	0
2	NAG	A	1002	2	14,14,15	0.45	0	15,19,21	1.28	2 (13%)
2	BMA	A	1003	2	11,11,12	0.77	0	14,15,17	1.25	3 (21%)
2	MAN	A	1004	2	11,11,12	0.55	0	14,15,17	1.02	1 (7%)
4	NAG	A	3001	1,4	14,14,15	0.56	0	15,19,21	1.18	1 (6%)
4	NAG	A	3002	4	14,14,15	0.43	0	15,19,21	1.29	1 (6%)
4	NAG	B	3001	1,4	14,14,15	0.59	0	15,19,21	0.93	0
4	NAG	B	3002	4	14,14,15	0.54	0	15,19,21	1.44	1 (6%)
2	NAG	C	1001	1,2	14,14,15	0.65	0	15,19,21	1.05	1 (6%)
2	NAG	C	1002	2	14,14,15	0.47	0	15,19,21	1.66	1 (6%)
2	BMA	C	1003	2	11,11,12	0.60	0	14,15,17	1.43	1 (7%)
2	MAN	C	1004	2	11,11,12	0.64	0	14,15,17	0.82	0
4	NAG	D	2001	1,4	14,14,15	0.66	0	15,19,21	2.51	3 (20%)
4	NAG	D	2002	4	14,14,15	0.43	0	15,19,21	2.52	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1004	2	-	0/2/19/22	0/1/1/1
4	NAG	A	3001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3002	4	-	0/6/23/26	0/1/1/1
4	NAG	B	3001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	3002	4	-	0/6/23/26	0/1/1/1
2	NAG	C	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	C	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	C	1004	2	-	0/2/19/22	0/1/1/1
4	NAG	D	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2002	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2001	NAG	C6-C5-C4	-2.82	106.06	113.02
4	D	2002	NAG	C2-N2-C7	-2.66	119.62	123.04
2	A	1002	NAG	C4-C3-C2	-2.13	107.91	111.23
2	A	1003	BMA	C3-C4-C5	2.41	114.39	110.20
2	A	1003	BMA	C2-C3-C4	2.45	115.21	111.04
4	D	2002	NAG	C3-C4-C5	2.48	114.52	110.20
2	A	1003	BMA	C1-O5-C5	2.57	115.51	112.25
2	C	1001	NAG	C1-O5-C5	2.62	115.57	112.25
4	D	2001	NAG	C3-C4-C5	2.68	114.86	110.20
2	A	1004	MAN	C1-O5-C5	2.88	115.90	112.25
4	A	3001	NAG	C1-O5-C5	3.22	116.33	112.25
2	A	1002	NAG	C1-O5-C5	3.40	116.57	112.25
4	B	3002	NAG	C1-O5-C5	4.15	117.51	112.25
2	C	1003	BMA	C1-O5-C5	4.15	117.52	112.25
4	A	3002	NAG	C1-O5-C5	4.15	117.52	112.25
2	C	1002	NAG	C1-O5-C5	5.86	119.68	112.25
4	D	2001	NAG	C1-O5-C5	8.14	122.58	112.25
4	D	2002	NAG	C1-O5-C5	8.74	123.34	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	2001	1	14,14,15	0.52	0	15,19,21	2.18	1 (6%)
3	NAG	A	4001	1	14,14,15	0.67	0	15,19,21	1.98	4 (26%)
5	TRS	A	6001	-	7,7,7	1.14	1 (14%)	9,9,9	1.47	1 (11%)
6	PEG	A	7001	-	6,6,6	0.52	0	5,5,5	0.38	0
3	NAG	B	2001	1	14,14,15	0.47	0	15,19,21	2.11	3 (20%)
8	BMA	B	3003	-	11,11,12	0.48	0	14,15,17	0.64	0
9	KTL	B	5001	-	22,26,26	1.80	1 (4%)	24,38,38	0.94	1 (4%)
6	PEG	B	7001	-	6,6,6	0.38	0	5,5,5	0.50	0
3	NAG	C	2001	1	14,14,15	0.54	0	15,19,21	0.82	0
3	NAG	C	3001	1	14,14,15	0.46	0	15,19,21	1.33	1 (6%)
3	NAG	C	4001	1	14,14,15	0.63	0	15,19,21	1.27	1 (6%)
5	TRS	C	6001	-	7,7,7	0.96	1 (14%)	9,9,9	0.69	0
6	PEG	C	7001	-	6,6,6	0.46	0	5,5,5	0.25	0
9	KTL	D	5001	-	22,26,26	1.90	2 (9%)	24,38,38	0.82	1 (4%)
6	PEG	D	7001	-	6,6,6	0.43	0	5,5,5	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
3	NAG	A	4001	1	-	0/6/23/26	0/1/1/1
5	TRS	A	6001	-	-	0/9/9/9	0/0/0/0

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

All (5) bond length outliers are listed below:

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

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4001	NAG	C4-C3-C2	-4.84	103.71	111.23
3	B	2001	NAG	C6-C5-C4	-3.87	103.48	113.02
5	A	6001	TRS	C1-C-N	-3.40	101.89	108.09
9	D	5001	KTL	CAQ-CAT-CAV	2.12	115.92	112.47
3	A	4001	NAG	C3-C2-N2	2.26	115.97	110.56
3	B	2001	NAG	C3-C4-C5	2.32	114.25	110.20
3	A	4001	NAG	C1-O5-C5	2.95	115.99	112.25
9	B	5001	KTL	OAD-CAR-CAN	3.15	114.69	109.15
3	C	4001	NAG	C1-O5-C5	3.76	117.02	112.25
3	A	4001	NAG	C2-N2-C7	3.77	127.88	123.04
3	C	3001	NAG	C1-O5-C5	4.10	117.45	112.25
3	B	2001	NAG	C1-O5-C5	6.03	119.91	112.25
3	A	2001	NAG	C1-O5-C5	7.83	122.19	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	871/898 (96%)	0.60	42 (4%) 34 45	4, 10, 19, 36	0
1	B	869/898 (96%)	0.58	48 (5%) 29 39	3, 11, 20, 37	0
1	C	871/898 (96%)	0.67	67 (7%) 16 22	5, 11, 21, 30	0
1	D	853/898 (94%)	1.93	363 (42%) 0 1	3, 11, 20, 27	0
All	All	3464/3592 (96%)	0.94	520 (15%) 3 5	3, 11, 20, 37	0

All (520) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	PRO	8.8
1	D	546	PRO	8.2
1	D	808	ILE	7.9
1	D	345	ALA	7.8
1	D	547	ASN	7.8
1	A	148	THR	7.7
1	D	802	GLY	7.6
1	D	361	ASP	7.5
1	D	408	TYR	7.0
1	D	400	GLY	7.0
1	D	455	ASN	6.9
1	D	450	ILE	6.8
1	D	418	HIS	6.8
1	D	416	THR	6.8
1	B	33	VAL	6.7
1	D	855	THR	6.7
1	D	452	TRP	6.6
1	D	851	THR	6.4
1	D	91	ILE	6.4
1	B	32	ASN	6.4
1	D	149	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
1	D	876	ALA	6.4
1	D	154	ASP	6.4
1	D	822	ASN	6.4
1	D	834	TYR	6.3
1	D	873	THR	6.2
1	D	378	PHE	6.2
1	D	874	TYR	6.2
1	D	370	VAL	6.2
1	D	458	SER	6.1
1	D	462	GLN	6.1
1	B	403	ALA	6.1
1	B	865	PRO	6.0
1	D	633	GLY	5.8
1	D	454	ALA	5.7
1	D	464	VAL	5.7
1	D	799	TRP	5.7
1	D	789	GLU	5.7
1	D	816	TYR	5.6
1	D	892	ARG	5.5
1	D	885	ASP	5.5
1	C	546	PRO	5.4
1	D	884	ALA	5.4
1	D	409	ALA	5.4
1	D	427	SER	5.3
1	D	872	PHE	5.3
1	D	877	SER	5.2
1	D	333	ASP	5.2
1	D	447	PRO	5.2
1	D	451	ASP	5.2
1	D	135	ARG	5.2
1	D	435	TRP	5.1
1	D	548	LYS	5.1
1	D	542	GLN	5.1
1	D	375	LEU	5.0
1	D	465	GLN	5.0
1	D	344	GLU	5.0
1	D	770	ASP	5.0
1	D	853	SER	4.9
1	D	839	THR	4.9
1	D	426	GLY	4.9
1	D	372	PHE	4.8
1	D	417	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	457	CYS	4.8
1	D	852	ASP	4.8
1	D	413	ARG	4.7
1	D	76	VAL	4.7
1	D	371	ALA	4.7
1	D	640	ALA	4.7
1	D	516	VAL	4.7
1	D	641	PHE	4.7
1	D	484	THR	4.7
1	D	380	GLN	4.6
1	D	835	GLN	4.6
1	D	545	PHE	4.6
1	D	373	ASN	4.6
1	D	792	THR	4.6
1	D	768	GLU	4.6
1	D	843	GLN	4.6
1	D	769	PRO	4.6
1	D	384	ASP	4.6
1	D	446	ASN	4.6
1	D	538	GLU	4.5
1	D	449	CYS	4.5
1	D	438	LEU	4.5
1	C	547	ASN	4.5
1	D	367	TYR	4.5
1	D	401	ARG	4.5
1	D	897	GLN	4.5
1	C	154	ASP	4.5
1	B	866	MET	4.4
1	D	362	LYS	4.4
1	C	401	ARG	4.4
1	D	486	GLY	4.4
1	D	148	THR	4.4
1	D	382	LEU	4.3
1	C	153	SER	4.3
1	D	338	VAL	4.3
1	D	718	ASP	4.3
1	C	876	ALA	4.3
1	D	87	THR	4.3
1	D	733	GLU	4.3
1	D	331	SER	4.2
1	D	448	ASN	4.2
1	D	84	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	132	PRO	4.2
1	D	810	ASN	4.2
1	D	534	ALA	4.2
1	D	152	VAL	4.2
1	D	854	VAL	4.2
1	D	859	VAL	4.2
1	D	365	PHE	4.2
1	D	453	TRP	4.2
1	D	881	LEU	4.1
1	D	385	HIS	4.1
1	D	358	TYR	4.1
1	D	381	ASP	4.1
1	D	518	ASN	4.1
1	D	377	GLN	4.1
1	D	354	THR	4.1
1	A	404	ASN	4.1
1	D	836	GLU	4.1
1	D	657	THR	4.1
1	B	404	ASN	4.0
1	D	470	TRP	4.0
1	D	856	GLU	4.0
1	D	861	GLU	4.0
1	D	460	PHE	4.0
1	A	33	VAL	4.0
1	D	807	THR	4.0
1	D	369	GLN	3.9
1	D	398	SER	3.9
1	D	870	SER	3.9
1	D	809	GLN	3.9
1	D	334	VAL	3.9
1	A	32	ASN	3.9
1	D	386	GLY	3.9
1	D	431	ILE	3.9
1	D	812	ASN	3.9
1	D	425	ASP	3.9
1	D	878	ASN	3.8
1	D	829	CYS	3.8
1	C	35	ASN	3.8
1	D	162	ALA	3.8
1	D	318	TRP	3.8
1	D	734	SER	3.8
1	D	645	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	543	LYS	3.8
1	D	780	PRO	3.8
1	B	862	ASN	3.8
1	D	746	ASP	3.8
1	C	856	GLU	3.8
1	D	153	SER	3.8
1	D	894	PHE	3.8
1	D	85	ASP	3.7
1	D	90	SER	3.7
1	D	838	THR	3.7
1	D	337	GLU	3.7
1	D	886	LEU	3.7
1	A	146	GLU	3.7
1	C	101	PRO	3.7
1	D	88	THR	3.7
1	D	790	ASN	3.7
1	C	34	LEU	3.7
1	D	787	LEU	3.7
1	D	845	VAL	3.6
1	D	844	THR	3.6
1	D	731	ASP	3.6
1	D	419	VAL	3.6
1	D	647	LEU	3.6
1	D	671	TYR	3.6
1	D	374	GLY	3.6
1	D	882	LEU	3.6
1	D	412	GLU	3.6
1	A	149	GLY	3.6
1	D	468	GLY	3.6
1	D	544	VAL	3.6
1	A	150	PRO	3.6
1	D	748	TYR	3.6
1	B	864	GLN	3.6
1	D	399	ILE	3.5
1	B	852	ASP	3.5
1	D	414	GLY	3.5
1	D	360	GLU	3.5
1	A	403	ALA	3.5
1	D	368	ASP	3.5
1	D	551	PHE	3.5
1	D	476	VAL	3.5
1	D	145	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	328	ASN	3.5
1	D	469	LEU	3.5
1	D	549	ARG	3.5
1	D	814	ILE	3.5
1	D	830	THR	3.4
1	C	377	GLN	3.4
1	D	112	SER	3.4
1	B	851	THR	3.4
1	A	134	ASN	3.4
1	D	716	GLY	3.4
1	D	736	ALA	3.4
1	D	77	ASP	3.4
1	D	429	PRO	3.4
1	C	465	GLN	3.4
1	D	676	PHE	3.4
1	D	89	THR	3.4
1	D	336	LYS	3.4
1	D	393	LEU	3.4
1	D	564	HIS	3.4
1	D	436	PRO	3.4
1	C	384	ASP	3.3
1	D	847	ILE	3.3
1	D	550	SER	3.3
1	D	803	GLU	3.3
1	A	34	LEU	3.3
1	A	28	ARG	3.3
1	A	153	SER	3.3
1	D	815	LEU	3.3
1	D	146	GLU	3.3
1	D	887	LYS	3.3
1	D	818	PHE	3.3
1	D	898	TRP	3.3
1	B	407	THR	3.3
1	C	866	MET	3.2
1	A	799	TRP	3.2
1	D	879	GLN	3.2
1	D	411	TYR	3.2
1	D	324	LEU	3.2
1	D	133	ASN	3.2
1	C	403	ALA	3.2
1	C	852	ASP	3.2
1	C	892	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	540	ALA	3.2
1	D	439	THR	3.2
1	D	379	VAL	3.2
1	D	840	LEU	3.2
1	D	424	SER	3.2
1	B	863	ASN	3.2
1	D	552	ILE	3.2
1	D	632	ASP	3.1
1	D	134	ASN	3.1
1	D	389	TYR	3.1
1	D	871	ASN	3.1
1	B	405	GLY	3.1
1	D	387	GLN	3.1
1	D	512	CYS	3.1
1	C	241	LEU	3.1
1	D	675	VAL	3.0
1	B	809	GLN	3.0
1	C	877	SER	3.0
1	D	817	THR	3.0
1	D	397	ILE	3.0
1	C	855	THR	3.0
1	D	410	THR	3.0
1	D	423	GLU	3.0
1	D	339	VAL	3.0
1	D	346	GLY	3.0
1	D	643	GLY	3.0
1	D	388	LYS	3.0
1	D	327	TRP	3.0
1	D	796	ASP	3.0
1	D	806	ASP	3.0
1	D	428	THR	3.0
1	C	835	GLN	3.0
1	C	853	SER	3.0
1	A	754	ILE	3.0
1	D	445	THR	3.0
1	C	150	PRO	3.0
1	B	885	ASP	3.0
1	D	893	ASN	3.0
1	D	826	ASP	2.9
1	D	663	LEU	2.9
1	A	667	TYR	2.9
1	A	35	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	418	HIS	2.9
1	D	801	ASP	2.9
1	D	651	SER	2.9
1	D	322	PHE	2.9
1	D	553	LEU	2.9
1	A	77	ASP	2.9
1	D	440	VAL	2.9
1	D	732	TYR	2.9
1	C	412	GLU	2.9
1	D	467	ASP	2.9
1	D	480	ILE	2.9
1	D	662	LEU	2.9
1	D	644	GLN	2.9
1	C	148	THR	2.9
1	C	885	ASP	2.9
1	D	433	GLU	2.9
1	D	61	CYS	2.9
1	D	151	THR	2.9
1	C	407	THR	2.8
1	D	459	ILE	2.8
1	D	781	LEU	2.8
1	D	825	LEU	2.8
1	C	887	LYS	2.8
1	D	661	THR	2.8
1	B	463	GLU	2.8
1	D	635	GLU	2.8
1	D	767	GLN	2.8
1	D	804	THR	2.8
1	D	752	ASP	2.8
1	B	42	ILE	2.8
1	D	772	THR	2.8
1	C	146	GLU	2.8
1	D	402	ARG	2.8
1	B	154	ASP	2.8
1	D	340	ARG	2.8
1	D	489	VAL	2.8
1	C	874	TYR	2.7
1	D	776	SER	2.7
1	C	404	ASN	2.7
1	D	774	THR	2.7
1	D	766	ILE	2.7
1	A	154	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	369	GLN	2.7
1	D	483	SER	2.7
1	C	645	ASN	2.7
1	C	867	ASN	2.7
1	C	135	ARG	2.7
1	D	329	TYR	2.7
1	D	335	VAL	2.7
1	D	353	VAL	2.7
1	D	111	ASN	2.7
1	D	415	ASN	2.7
1	D	821	SER	2.7
1	A	847	ILE	2.7
1	D	107	GLY	2.7
1	D	778	LYS	2.7
1	D	364	ASP	2.7
1	C	710	THR	2.7
1	D	349	PHE	2.7
1	C	619	LEU	2.6
1	D	392	ILE	2.6
1	D	113	VAL	2.6
1	D	461	HIS	2.6
1	D	779	ASN	2.6
1	A	145	LYS	2.6
1	D	744	ARG	2.6
1	D	833	SER	2.6
1	D	363	LYS	2.6
1	D	634	TYR	2.6
1	B	377	GLN	2.6
1	D	471	ILE	2.6
1	D	883	ILE	2.6
1	D	463	GLU	2.6
1	D	782	GLY	2.6
1	D	791	ASN	2.6
1	D	819	SER	2.6
1	D	488	ASN	2.6
1	D	487	CYS	2.6
1	C	511	ILE	2.6
1	C	858	ARG	2.6
1	D	341	ARG	2.6
1	A	320	LEU	2.5
1	C	205	ILE	2.5
1	D	828	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	832	SER	2.5
1	D	563	ARG	2.5
1	B	806	ASP	2.5
1	D	514	ASP	2.5
1	D	712	VAL	2.5
1	B	150	PRO	2.5
1	B	148	THR	2.5
1	D	775	ALA	2.5
1	D	798	PHE	2.5
1	C	862	ASN	2.5
1	C	847	ILE	2.5
1	D	330	LYS	2.5
1	D	737	LYS	2.5
1	C	463	GLU	2.5
1	D	607	GLU	2.5
1	B	158	ASP	2.5
1	A	798	PHE	2.5
1	D	660	TYR	2.5
1	D	491	LYS	2.5
1	D	777	ARG	2.5
1	D	479	PHE	2.5
1	D	332	LEU	2.5
1	D	430	ILE	2.5
1	D	719	THR	2.5
1	C	333	ASP	2.4
1	D	642	PHE	2.4
1	C	543	LYS	2.4
1	C	733	GLU	2.4
1	D	108	ASN	2.4
1	D	740	TRP	2.4
1	D	654	GLN	2.4
1	B	85	ASP	2.4
1	D	357	ASP	2.4
1	C	208	ILE	2.4
1	A	101	PRO	2.4
1	A	604	PHE	2.4
1	A	845	VAL	2.4
1	D	717	ALA	2.4
1	D	422	ASN	2.4
1	D	490	ASN	2.4
1	D	797	PHE	2.4
1	B	153	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	708	LEU	2.4
1	D	143	TYR	2.4
1	D	366	THR	2.4
1	D	636	HIS	2.4
1	D	841	ALA	2.3
1	D	131	ASP	2.3
1	B	145	LYS	2.3
1	B	135	ARG	2.3
1	D	515	ALA	2.3
1	D	860	ALA	2.3
1	C	386	GLY	2.3
1	D	537	THR	2.3
1	D	749	LEU	2.3
1	D	441	TYR	2.3
1	A	391	ILE	2.3
1	D	474	ASN	2.3
1	D	511	ILE	2.3
1	D	795	GLY	2.3
1	B	897	GLN	2.3
1	D	359	MET	2.3
1	B	77	ASP	2.3
1	D	857	VAL	2.3
1	A	862	ASN	2.3
1	D	539	GLN	2.3
1	C	209	GLY	2.3
1	D	869	HIS	2.3
1	A	55	CYS	2.3
1	B	30	CYS	2.3
1	B	856	GLU	2.3
1	D	889	ASN	2.3
1	D	880	VAL	2.2
1	A	552	ILE	2.2
1	B	718	ASP	2.2
1	D	805	LYS	2.2
1	B	835	GLN	2.2
1	B	711	PRO	2.2
1	C	770	ASP	2.2
1	D	639	PRO	2.2
1	A	710	THR	2.2
1	B	35	ASN	2.2
1	C	863	ASN	2.2
1	A	68	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	56	ALA	2.2
1	C	375	LEU	2.2
1	C	809	GLN	2.2
1	B	333	ASP	2.2
1	C	896	VAL	2.2
1	D	96	LYS	2.2
1	A	316	ALA	2.2
1	D	158	ASP	2.2
1	D	395	PRO	2.2
1	A	135	ARG	2.2
1	D	646	SER	2.2
1	D	109	ASP	2.2
1	A	789	GLU	2.2
1	C	538	GLU	2.2
1	D	420	TRP	2.2
1	D	164	ASN	2.2
1	D	753	LYS	2.2
1	D	140	PRO	2.2
1	D	739	PRO	2.2
1	D	533	MET	2.1
1	B	34	LEU	2.1
1	D	875	ASP	2.1
1	C	748	TYR	2.1
1	D	727	ALA	2.1
1	B	421	ILE	2.1
1	D	895	SER	2.1
1	D	602	CYS	2.1
1	C	462	GLN	2.1
1	D	625	PHE	2.1
1	D	101	PRO	2.1
1	D	521	LYS	2.1
1	D	649	VAL	2.1
1	B	292	ILE	2.1
1	D	325	SER	2.1
1	D	837	GLY	2.1
1	B	373	ASN	2.1
1	C	838	THR	2.1
1	D	888	LEU	2.1
1	D	610	GLU	2.1
1	D	147	PHE	2.1
1	D	655	TYR	2.1
1	D	667	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	233	LEU	2.1
1	D	890	LEU	2.1
1	D	315	PRO	2.1
1	A	228	PHE	2.1
1	D	86	MET	2.1
1	A	440	VAL	2.1
1	C	525	VAL	2.1
1	C	778	LYS	2.1
1	C	292	ILE	2.1
1	B	293	LEU	2.1
1	D	858	ARG	2.1
1	B	125	PHE	2.1
1	A	73	CYS	2.1
1	D	317	TYR	2.1
1	B	301	VAL	2.1
1	C	512	CYS	2.1
1	D	754	ILE	2.0
1	C	187	LEU	2.0
1	D	482	GLY	2.0
1	B	337	GLU	2.0
1	C	789	GLU	2.0
1	B	798	PHE	2.0
1	A	212	VAL	2.0
1	B	406	THR	2.0
1	C	416	THR	2.0
1	D	291	TYR	2.0
1	D	342	ASN	2.0
1	A	347	ILE	2.0
1	A	596	LEU	2.0
1	C	806	ASP	2.0
1	B	510	THR	2.0
1	D	307	GLN	2.0
1	D	637	GLN	2.0
1	D	444	PHE	2.0
1	C	810	ASN	2.0
1	A	30	CYS	2.0
1	D	849	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	1002	14/15	0.92	0.18	2.81	12,13,18,20	0
4	NAG	B	3001	14/15	0.90	0.17	1.18	19,20,22,24	0
4	NAG	D	2001	14/15	0.88	0.14	0.04	4,14,19,23	0
2	MAN	C	1004	11/12	0.88	0.14	-0.13	11,13,16,16	0
2	BMA	C	1003	11/12	0.88	0.12	-0.48	14,16,20,23	0
4	NAG	A	3001	14/15	0.94	0.12	-0.99	9,13,15,18	0
2	MAN	A	1004	11/12	0.92	0.10	-2.28	15,17,18,19	0
2	NAG	C	1001	14/15	0.83	0.23	-	14,16,17,19	0
2	NAG	A	1001	14/15	0.81	0.24	-	16,20,24,25	0
4	NAG	B	3002	14/15	0.88	0.15	-	25,27,28,29	0
2	NAG	C	1002	14/15	0.89	0.20	-	12,15,18,21	0
4	NAG	A	3002	14/15	0.86	0.32	-	24,27,29,30	0
4	NAG	D	2002	14/15	0.73	0.32	-	24,27,31,32	0
2	BMA	A	1003	11/12	0.90	0.12	-	15,17,18,20	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	C	3001	14/15	0.80	0.29	2.63	22,25,26,27	0
5	TRS	C	6001	8/8	0.88	0.18	2.12	20,20,20,21	0
5	TRS	A	6001	8/8	0.86	0.19	0.99	10,12,13,15	0
6	PEG	A	7001	7/7	0.90	0.15	0.15	21,22,25,25	0
6	PEG	B	7001	7/7	0.90	0.12	0.11	20,20,21,22	0
9	KTL	D	5001	26/26	0.89	0.18	-0.47	20,24,26,27	0
6	PEG	C	7001	7/7	0.85	0.12	-0.78	18,22,25,27	0
3	NAG	B	2001	14/15	0.88	0.12	-0.83	9,16,18,21	0
9	KTL	B	5001	26/26	0.93	0.13	-0.86	10,18,23,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	PEG	D	7001	7/7	0.81	0.15	-1.23	37,37,38,38	0
7	CL	A	8001	1/1	0.98	0.09	-5.14	3,3,3,3	0
3	NAG	A	2001	14/15	0.66	0.19	-	31,33,34,34	0
3	NAG	C	2001	14/15	0.88	0.16	-	16,22,26,27	0
3	NAG	A	4001	14/15	0.80	0.34	-	24,27,28,30	0
3	NAG	C	4001	14/15	0.84	0.30	-	35,40,41,42	0
8	BMA	B	3003	11/12	0.55	0.23	-	61,62,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.