



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2017 – 10:37 PM EDT

PDB ID : 2YLA
Title : INHIBITION OF THE PNEUMOCOCCAL VIRULENCE FACTOR STRH AND MOLECULAR INSIGHTS INTO N-GLYCAN RECOGNITION AND HYDROLYSIS
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Deposited on : unknown
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

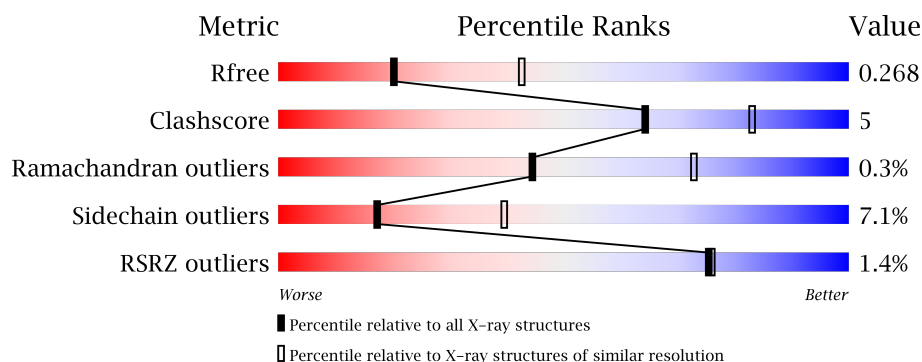
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	442	
1	B	442	
1	C	442	
1	D	442	

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	1101	-	-	-	X
2	NAG	A	1103	-	-	-	X
2	NAG	A	1105	-	-	-	X
2	NAG	B	1101	-	-	-	X
2	NAG	B	1103	-	-	-	X
2	NAG	B	1105	-	-	-	X
2	NAG	C	1104	-	-	-	X
2	NAG	D	1103	-	-	-	X
2	NAG	D	1105	-	-	-	X
4	MAN	A	1104	-	-	-	X
4	MAN	B	1104	-	-	-	X
4	MAN	C	1103	-	-	-	X
4	MAN	D	1104	-	-	-	X
5	EDO	A	1107	-	-	-	X
5	EDO	B	1107	-	-	-	X
5	EDO	B	1109	-	-	-	X
5	EDO	B	1113	-	-	-	X
5	EDO	B	1114	-	-	-	X
5	EDO	B	1115	-	-	-	X
5	EDO	C	1105	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14253 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 BETA-N-ACETYLHEXOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	21	2	0
			3321	2128	542	639	12			
1	B	417	Total	C	N	O	S	13	0	0
			3317	2126	539	640	12			
1	C	408	Total	C	N	O	S	16	2	0
			3267	2097	532	626	12			
1	D	408	Total	C	N	O	S	28	1	0
			3261	2092	531	626	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	623	GLY	-	expression tag	UNP P49610
A	624	SER	-	expression tag	UNP P49610
A	625	HIS	-	expression tag	UNP P49610
A	626	MET	-	expression tag	UNP P49610
A	805	GLN	GLU	engineered mutation	UNP P49610
B	623	GLY	-	expression tag	UNP P49610
B	624	SER	-	expression tag	UNP P49610
B	625	HIS	-	expression tag	UNP P49610
B	626	MET	-	expression tag	UNP P49610
B	805	GLN	GLU	engineered mutation	UNP P49610
C	623	GLY	-	expression tag	UNP P49610
C	624	SER	-	expression tag	UNP P49610
C	625	HIS	-	expression tag	UNP P49610
C	626	MET	-	expression tag	UNP P49610
C	805	GLN	GLU	engineered mutation	UNP P49610
D	623	GLY	-	expression tag	UNP P49610
D	624	SER	-	expression tag	UNP P49610
D	625	HIS	-	expression tag	UNP P49610
D	626	MET	-	expression tag	UNP P49610
D	805	GLN	GLU	engineered mutation	UNP P49610

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



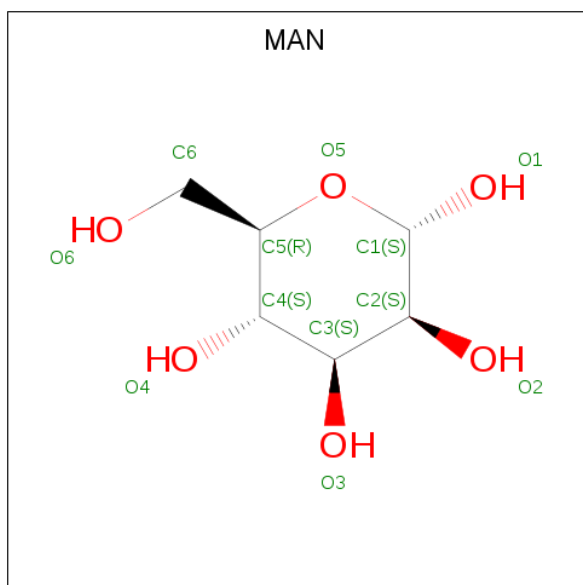
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



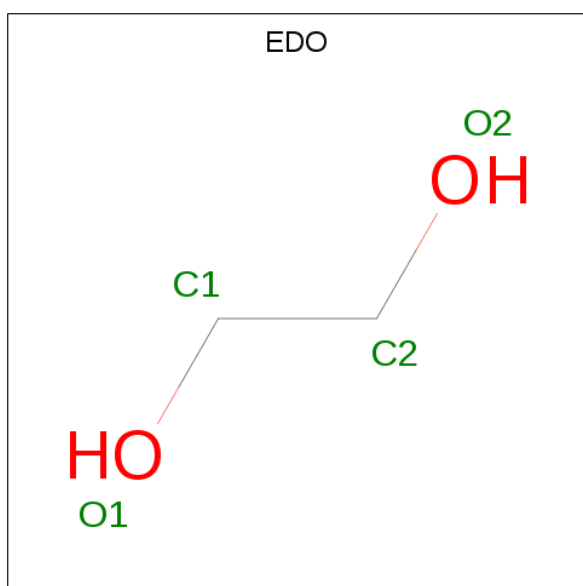
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

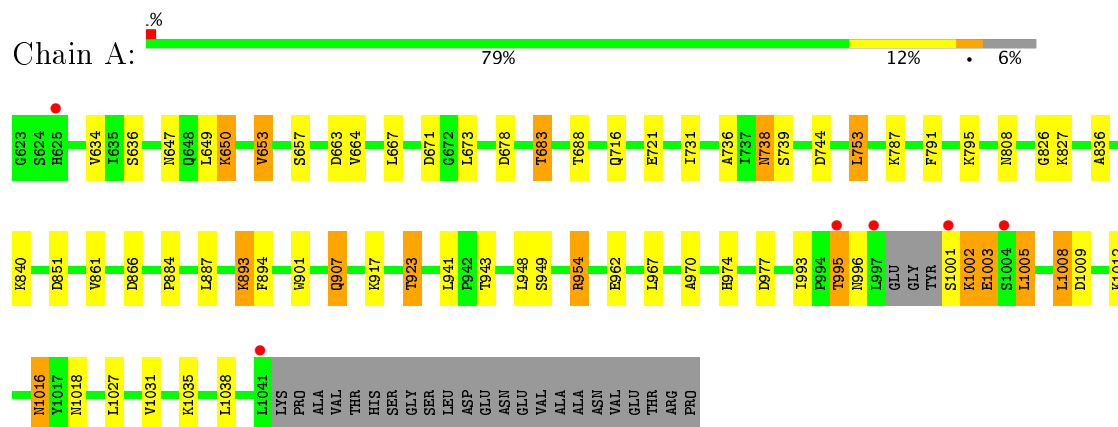
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	172	Total O 174 174	0	2
6	B	197	Total O 200 200	0	3
6	C	235	Total O 237 237	0	2
6	D	168	Total O 170 170	0	2

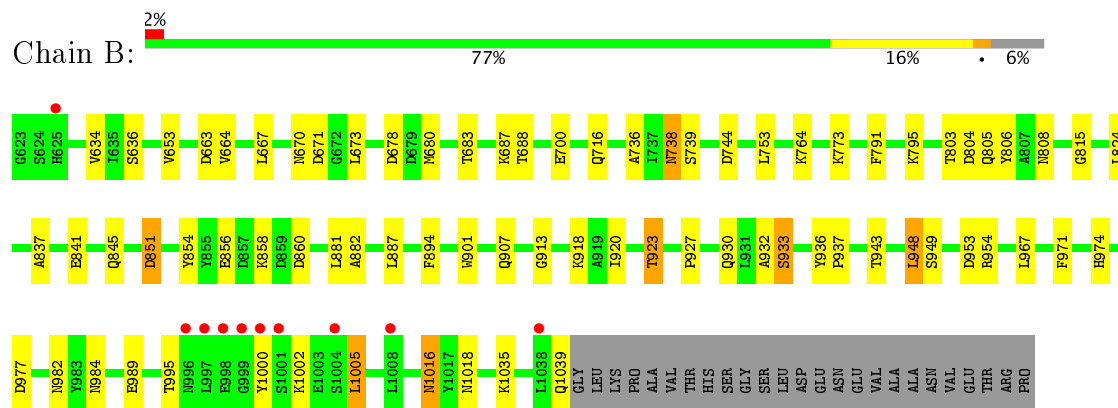
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

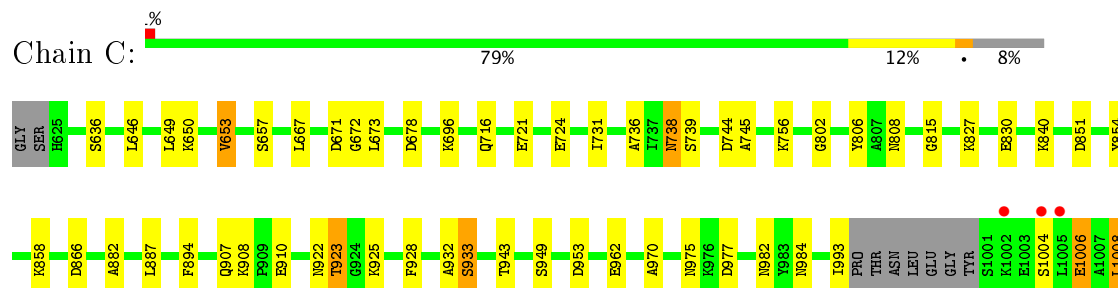
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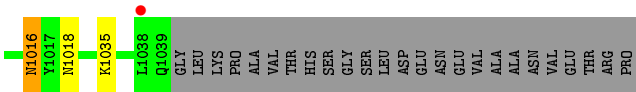


• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

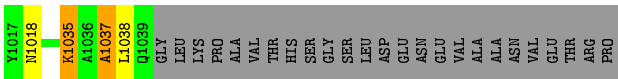
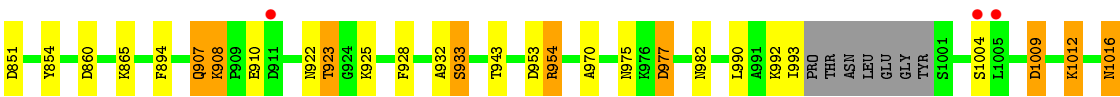
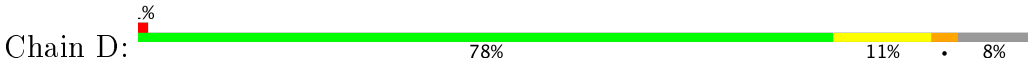


• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE





● Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.56Å 115.71Å 132.21Å 90.00° 99.67° 90.00°	Depositor
Resolution (Å)	29.97 – 2.70 29.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.97-2.70) 100.0 (29.98-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.223 , 0.273 0.221 , 0.268	Depositor DCC
R_{free} test set	2792 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14253	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.09 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.4880e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.64	9/3394 (0.3%)	0.60	7/4583 (0.2%)
1	B	0.56	4/3392 (0.1%)	0.53	2/4583 (0.0%)
1	C	1.13	5/3342 (0.1%)	0.63	7/4510 (0.2%)
1	D	1.32	12/3333 (0.4%)	0.66	7/4499 (0.2%)
All	All	0.97	30/13461 (0.2%)	0.61	23/18175 (0.1%)

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

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

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	724	GLU	CG-CD	50.47	2.27	1.51
1	D	756	LYS	CE-NZ	-47.28	0.30	1.49
1	D	1037	ALA	CA-CB	-31.76	0.85	1.52
1	C	908	LYS	CD-CE	-27.67	0.82	1.51
1	D	908	LYS	CD-CE	-22.56	0.94	1.51
1	D	696	LYS	CE-NZ	-20.50	0.97	1.49
1	D	1012	LYS	CD-CE	20.18	2.01	1.51
1	B	1005	LEU	CA-CB	-18.67	1.10	1.53
1	C	1006	GLU	CB-CG	-18.59	1.16	1.52
1	D	1009	ASP	CB-CG	-17.57	1.14	1.51
1	B	764	LYS	CE-NZ	-15.78	1.09	1.49
1	A	827	LYS	CD-CE	-14.98	1.13	1.51
1	C	1004	SER	CB-OG	-14.93	1.22	1.42
1	D	773	LYS	CE-NZ	-14.82	1.11	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1002	LYS	CA-CB	-13.06	1.25	1.53
1	D	990	LEU	CG-CD2	-12.64	1.05	1.51
1	A	1002	LYS	CE-NZ	-12.47	1.17	1.49
1	A	995	THR	CB-OG1	10.72	1.64	1.43
1	A	1003	GLU	CB-CG	-10.53	1.32	1.52
1	A	1009	ASP	CB-CG	9.78	1.72	1.51
1	A	995	THR	CB-CG2	8.67	1.80	1.52
1	B	995	THR	CA-CB	7.96	1.74	1.53
1	D	764	LYS	CE-NZ	7.85	1.68	1.49
1	D	992	LYS	CE-NZ	-6.97	1.31	1.49
1	A	1008	LEU	CG-CD2	-6.62	1.27	1.51
1	D	1035	LYS	CB-CG	-6.00	1.36	1.52
1	D	1038	LEU	CG-CD2	-5.47	1.31	1.51
1	C	1035	LYS	CD-CE	-5.28	1.38	1.51
1	B	858	LYS	CE-NZ	-5.18	1.36	1.49
1	A	1012	LYS	CE-NZ	-5.04	1.36	1.49

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	724	GLU	CB-CG-CD	-16.62	69.32	114.20
1	D	764	LYS	CD-CE-NZ	-15.43	76.21	111.70
1	A	995	THR	CA-CB-CG2	-13.57	93.40	112.40
1	D	908	LYS	CG-CD-CE	13.29	151.78	111.90
1	C	908	LYS	CG-CD-CE	10.85	144.45	111.90
1	A	995	THR	OG1-CB-CG2	-9.96	87.10	110.00
1	B	995	THR	N-CA-CB	-9.56	92.13	110.30
1	A	1035	LYS	CG-CD-CE	9.48	140.35	111.90
1	D	1012	LYS	CD-CE-NZ	9.45	133.43	111.70
1	C	1008	LEU	CA-CB-CG	9.23	136.53	115.30
1	D	1038	LEU	CB-CG-CD2	-9.20	95.37	111.00
1	D	990	LEU	CB-CG-CD1	-9.11	95.52	111.00
1	A	1008	LEU	CD1-CG-CD2	8.21	135.13	110.50
1	C	1006	GLU	CA-CB-CG	8.09	131.19	113.40
1	D	1012	LYS	CG-CD-CE	-7.30	89.99	111.90
1	C	724	GLU	CG-CD-OE2	-7.20	103.90	118.30
1	C	724	GLU	CG-CD-OE1	7.02	132.34	118.30
1	A	1009	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	1008	LEU	CB-CG-CD1	5.52	120.38	111.00
1	A	1002	LYS	N-CA-CB	5.12	119.83	110.60
1	B	1005	LEU	N-CA-CB	5.11	120.62	110.40
1	D	990	LEU	CD1-CG-CD2	5.05	125.64	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	827	LYS	CG-CD-CE	5.02	126.96	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	803	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3321	0	3252	40	0
1	B	3317	0	3240	36	0
1	C	3267	0	3207	24	0
1	D	3261	0	3194	25	0
2	A	43	0	40	1	0
2	B	43	0	40	2	0
2	C	29	0	27	0	0
2	D	43	0	40	0	0
3	A	11	0	8	0	0
3	B	11	0	8	0	0
3	C	11	0	9	0	0
3	D	11	0	8	0	0
4	A	11	0	9	0	0
4	B	11	0	9	0	0
4	C	11	0	9	0	0
4	D	11	0	9	0	0
5	A	8	0	12	0	0
5	B	40	0	60	2	0
5	C	8	0	12	1	0
5	D	4	0	6	0	0
6	A	174	0	0	0	0
6	B	200	0	0	0	0
6	C	237	0	0	0	0
6	D	170	0	0	0	0
All	All	14253	0	13199	128	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 5.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:982:ASN:HD21	1:B:984:ASN:HD22	1.21	0.87
1:A:907:GLN:NE2	1:A:954:ARG:HH12	1.79	0.80
1:D:907:GLN:NE2	1:D:954:ARG:HH12	1.85	0.75
1:B:678:ASP:H	1:B:716:GLN:HE21	1.34	0.73
1:B:845:GLN:HB2	5:B:1114:EDO:H11	1.70	0.73
1:A:1016:ASN:HD22	1:A:1018:ASN:H	1.35	0.73
1:A:907:GLN:HE22	1:A:954:ARG:HH12	1.39	0.71
1:B:678:ASP:H	1:B:716:GLN:NE2	1.88	0.69
1:A:678:ASP:H	1:A:716:GLN:NE2	1.90	0.69
1:A:683:THR:HG23	1:A:688:THR:HG22	1.74	0.69
1:D:1016:ASN:HD22	1:D:1018:ASN:H	1.40	0.69
1:D:678:ASP:H	1:D:716:GLN:NE2	1.92	0.68
1:A:901:TRP:HB3	1:A:948:LEU:HD12	1.76	0.67
1:B:1016:ASN:HD22	1:B:1018:ASN:H	1.42	0.66
1:C:982:ASN:HD21	1:C:984:ASN:HD22	1.42	0.66
1:A:893:LYS:HE2	1:A:893:LYS:H	1.61	0.66
1:D:750:MET:HB2	1:D:755:ILE:HD12	1.76	0.66
1:A:948:LEU:HD21	1:A:967:LEU:HG	1.79	0.64
1:C:738:ASN:HD22	1:C:739:SER:H	1.45	0.64
1:A:1016:ASN:ND2	1:A:1018:ASN:H	1.98	0.62
1:B:738:ASN:HD22	1:B:739:SER:H	1.45	0.62
1:A:996:ASN:HD21	1:A:1005:LEU:HD11	1.65	0.61
1:A:993:ILE:HG22	1:A:1038:LEU:HD13	1.83	0.60
1:B:948:LEU:HD21	1:B:967:LEU:HG	1.85	0.59
1:B:791:PHE:O	1:B:795:LYS:HD2	2.04	0.58
1:B:653:VAL:HG12	1:B:664:VAL:HG21	1.85	0.58
1:B:982:ASN:ND2	1:B:984:ASN:HD22	1.99	0.57
1:D:738:ASN:HD22	1:D:739:SER:H	1.52	0.57
1:B:837:ALA:HB1	5:B:1110:EDO:H11	1.85	0.57
1:D:1016:ASN:ND2	1:D:1018:ASN:H	2.03	0.57
1:D:907:GLN:HE21	1:D:954:ARG:HH12	1.53	0.57
1:A:923:THR:HG22	1:A:974:HIS:CD2	2.41	0.55
1:C:678:ASP:H	1:C:716:GLN:NE2	2.05	0.55
1:B:927:PRO:HG2	1:B:930:GLN:HB2	1.89	0.55
1:B:907:GLN:NE2	1:B:954:ARG:HH12	2.05	0.54
1:C:667:LEU:HA	1:C:736:ALA:HB3	1.88	0.54
1:C:1016:ASN:HD22	1:C:1018:ASN:H	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1016:ASN:ND2	1:B:1018:ASN:H	2.05	0.53
1:B:738:ASN:HD22	1:B:739:SER:N	2.07	0.52
1:A:826:GLY:HA2	1:A:861:VAL:HG11	1.92	0.52
1:D:678:ASP:H	1:D:716:GLN:HE21	1.57	0.51
1:D:699:ILE:HG23	1:D:712:THR:HG21	1.92	0.51
1:D:854:TYR:OH	1:D:865:LYS:HE2	2.11	0.51
1:D:894:PHE:HB2	1:D:943:THR:HG22	1.92	0.51
1:B:894:PHE:HB2	1:B:943:THR:HG22	1.91	0.51
1:D:738:ASN:HD22	1:D:739:SER:N	2.09	0.51
1:B:773:LYS:HE3	1:B:824:LEU:HD21	1.92	0.50
1:A:653:VAL:HG12	1:A:664:VAL:HG21	1.92	0.50
1:B:989:GLU:CD	1:B:1035:LYS:HG2	2.32	0.50
1:C:982:ASN:ND2	1:C:984:ASN:HD22	2.09	0.50
1:C:636:SER:HB3	1:C:949:SER:HA	1.94	0.49
1:D:683:THR:HG23	1:D:688:THR:HG22	1.94	0.49
1:B:923:THR:HG22	1:B:974:HIS:CD2	2.47	0.49
1:A:893:LYS:CE	1:A:893:LYS:H	2.25	0.49
2:B:1103:NAG:C8	2:B:1103:NAG:H3	2.43	0.49
1:B:901:TRP:HB3	1:B:948:LEU:HD12	1.94	0.49
1:C:932:ALA:O	1:C:933:SER:HB3	2.12	0.49
1:D:634:VAL:HG22	1:D:663:ASP:HB2	1.95	0.49
1:C:922:ASN:HA	1:C:925:LYS:HB2	1.95	0.49
1:C:1016:ASN:ND2	1:C:1018:ASN:H	2.10	0.48
1:B:936:TYR:CD1	1:B:937:PRO:HA	2.48	0.48
1:A:923:THR:CG2	1:A:974:HIS:HD2	2.27	0.47
1:A:1016:ASN:HD22	1:A:1016:ASN:C	2.17	0.47
1:A:657:SER:HA	1:A:731:ILE:HD11	1.96	0.47
1:A:678:ASP:H	1:A:716:GLN:HE21	1.61	0.47
1:C:657:SER:HA	1:C:731:ILE:HD11	1.95	0.47
1:C:923:THR:HG21	1:C:970:ALA:HB1	1.97	0.47
1:D:791:PHE:O	1:D:795:LYS:HD2	2.14	0.47
1:D:1016:ASN:C	1:D:1016:ASN:HD22	2.18	0.47
1:D:977:ASP:N	1:D:977:ASP:OD1	2.45	0.47
1:A:667:LEU:HA	1:A:736:ALA:HB3	1.96	0.46
1:A:791:PHE:O	1:A:795:LYS:HD2	2.16	0.46
1:C:928:PHE:HB2	1:C:975:ASN:ND2	2.30	0.46
1:B:634:VAL:HG22	1:B:663:ASP:HB2	1.98	0.46
1:A:894:PHE:HB2	1:A:943:THR:HG22	1.97	0.46
1:C:806:TYR:O	1:C:815:GLY:HA3	2.15	0.46
1:C:894:PHE:HB2	1:C:943:THR:HG22	1.97	0.45
1:A:647[A]:ASN:HA	1:A:650:LYS:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:TYR:O	1:B:815:GLY:HA3	2.16	0.45
1:D:932:ALA:O	1:D:933:SER:HB3	2.17	0.45
1:B:977:ASP:N	1:B:977:ASP:OD1	2.40	0.45
1:A:923:THR:HG21	1:A:970:ALA:HB1	1.98	0.44
1:A:923:THR:CG2	1:A:974:HIS:CD2	3.00	0.44
1:B:913:GLY:O	1:B:918:LYS:HD2	2.17	0.44
2:B:1103:NAG:H3	2:B:1103:NAG:H83	1.99	0.44
1:C:756:LYS:HG2	5:C:1106:EDO:H11	1.98	0.44
1:B:851:ASP:HA	1:B:881:LEU:HD22	1.98	0.44
1:B:636:SER:HB3	1:B:949:SER:HA	1.99	0.44
1:B:683:THR:HG23	1:B:688:THR:HG22	2.00	0.44
1:A:738:ASN:HD22	1:A:739:SER:N	2.15	0.44
1:C:738:ASN:ND2	1:C:802:GLY:HA3	2.33	0.44
2:A:1103:NAG:C8	2:A:1103:NAG:H3	2.48	0.43
1:D:667:LEU:HA	1:D:736:ALA:HB3	2.00	0.43
1:B:923:THR:HG23	1:B:971:PHE:HA	2.00	0.43
1:A:1001:SER:O	1:A:1005:LEU:HB2	2.19	0.43
1:A:977:ASP:N	1:A:977:ASP:OD1	2.44	0.43
1:D:907:GLN:NE2	1:D:954:ARG:NH1	2.61	0.43
1:B:667:LEU:HA	1:B:736:ALA:HB3	2.00	0.43
1:C:977:ASP:OD1	1:C:977:ASP:N	2.48	0.43
1:D:923:THR:HG21	1:D:970:ALA:CB	2.48	0.43
1:A:649:LEU:O	1:A:653:VAL:HG13	2.18	0.43
1:B:932:ALA:O	1:B:933:SER:HB3	2.19	0.43
1:D:762:PHE:C	1:D:764:LYS:H	2.23	0.42
1:B:670:ASN:O	1:B:671:ASP:HB2	2.20	0.42
1:A:884:PRO:HB2	1:A:941:LEU:CD1	2.50	0.42
1:C:923:THR:HG21	1:C:970:ALA:CB	2.49	0.42
1:A:738:ASN:HD22	1:A:739:SER:H	1.66	0.42
1:C:646:LEU:O	1:C:650:LYS:HB2	2.19	0.42
1:C:854:TYR:O	1:C:882:ALA:HB2	2.19	0.42
1:A:647[B]:ASN:ND2	1:A:647[B]:ASN:C	2.73	0.42
1:C:672:GLY:HA2	1:C:745:ALA:HB2	2.00	0.42
1:A:907:GLN:HE22	1:A:954:ARG:NH1	2.12	0.42
1:D:922:ASN:HA	1:D:925:LYS:HB2	2.02	0.42
1:A:1027:LEU:O	1:A:1031:VAL:HG23	2.20	0.41
1:B:854:TYR:O	1:B:882:ALA:HB2	2.20	0.41
1:A:636:SER:HB3	1:A:949:SER:HA	2.02	0.41
1:B:982:ASN:HD21	1:B:984:ASN:ND2	2.02	0.41
1:A:836:ALA:O	1:A:840:LYS:HG3	2.20	0.41
1:A:923:THR:HG21	1:A:970:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:TYR:CG	1:B:937:PRO:HA	2.56	0.41
1:D:928:PHE:HB2	1:D:975:ASN:ND2	2.35	0.41
1:A:634:VAL:HG22	1:A:663:ASP:HB2	2.02	0.41
1:C:649:LEU:O	1:C:653:VAL:HG12	2.20	0.41
1:C:840:LYS:HE2	1:C:866:ASP:HB2	2.02	0.41
1:D:923:THR:HG21	1:D:970:ALA:HB1	2.03	0.40
1:A:753:LEU:HA	1:A:753:LEU:HD12	1.92	0.40
1:B:920:ILE:O	1:B:923:THR:HB	2.21	0.40
1:A:840:LYS:HE2	1:A:866:ASP:HB2	2.02	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	414/442 (94%)	397 (96%)	16 (4%)	1 (0%)	51	79
1	B	415/442 (94%)	396 (95%)	17 (4%)	2 (0%)	32	60
1	C	406/442 (92%)	389 (96%)	16 (4%)	1 (0%)	51	79
1	D	405/442 (92%)	387 (96%)	17 (4%)	1 (0%)	51	79
All	All	1640/1768 (93%)	1569 (96%)	66 (4%)	5 (0%)	44	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	804	ASP
1	D	1037	ALA
1	A	671	ASP
1	B	805	GLN
1	C	671	ASP

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	344/363 (95%)	320 (93%)	24 (7%)	18	40
1	B	343/363 (94%)	321 (94%)	22 (6%)	20	45
1	C	338/363 (93%)	316 (94%)	22 (6%)	20	44
1	D	337/363 (93%)	309 (92%)	28 (8%)	13	30
All	All	1362/1452 (94%)	1266 (93%)	96 (7%)	17	40

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	650	LYS
1	A	653	VAL
1	A	673	LEU
1	A	683	THR
1	A	721	GLU
1	A	738	ASN
1	A	744	ASP
1	A	753	LEU
1	A	787	LYS
1	A	808	ASN
1	A	851	ASP
1	A	887	LEU
1	A	893	LYS
1	A	907	GLN
1	A	917	LYS
1	A	923	THR
1	A	954	ARG
1	A	962	GLU
1	A	995	THR
1	A	1002	LYS
1	A	1003	GLU
1	A	1005	LEU
1	A	1008	LEU
1	A	1016	ASN

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Mol	Chain	Res	Type
1	B	673	LEU
1	B	680	MET
1	B	687	LYS
1	B	700	GLU
1	B	738	ASN
1	B	744	ASP
1	B	753	LEU
1	B	808	ASN
1	B	841	GLU
1	B	851	ASP
1	B	856	GLU
1	B	860	ASP
1	B	887	LEU
1	B	923	THR
1	B	933	SER
1	B	948	LEU
1	B	953	ASP
1	B	1000	TYR
1	B	1002	LYS
1	B	1005	LEU
1	B	1016	ASN
1	B	1039	GLN
1	C	653	VAL
1	C	673	LEU
1	C	696	LYS
1	C	721	GLU
1	C	738	ASN
1	C	744	ASP
1	C	808	ASN
1	C	827	LYS
1	C	830	GLU
1	C	851	ASP
1	C	858	LYS
1	C	887	LEU
1	C	907	GLN
1	C	910	GLU
1	C	923	THR
1	C	933	SER
1	C	953	ASP
1	C	962	GLU
1	C	993	ILE
1	C	1006	GLU

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Mol	Chain	Res	Type
1	C	1008	LEU
1	C	1016	ASN
1	D	625	HIS
1	D	650	LYS
1	D	653	VAL
1	D	654	ASP
1	D	673	LEU
1	D	687	LYS
1	D	738	ASN
1	D	744	ASP
1	D	753	LEU
1	D	808	ASN
1	D	827	LYS
1	D	851	ASP
1	D	860	ASP
1	D	907	GLN
1	D	908	LYS
1	D	910	GLU
1	D	923	THR
1	D	933	SER
1	D	953	ASP
1	D	954	ARG
1	D	977	ASP
1	D	982	ASN
1	D	993	ILE
1	D	1004	SER
1	D	1009	ASP
1	D	1012	LYS
1	D	1016	ASN
1	D	1035	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	632	ASN
1	A	670	ASN
1	A	716	GLN
1	A	738	ASN
1	A	862	GLN
1	A	907	GLN
1	A	922	ASN
1	A	929	ASN

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Mol	Chain	Res	Type
1	A	974	HIS
1	A	996	ASN
1	A	1016	ASN
1	A	1033	ASN
1	B	670	ASN
1	B	716	GLN
1	B	738	ASN
1	B	808	ASN
1	B	845	GLN
1	B	907	GLN
1	B	922	ASN
1	B	929	ASN
1	B	974	HIS
1	B	975	ASN
1	B	982	ASN
1	B	1016	ASN
1	B	1033	ASN
1	C	670	ASN
1	C	716	GLN
1	C	738	ASN
1	C	907	GLN
1	C	922	ASN
1	C	929	ASN
1	C	974	HIS
1	C	975	ASN
1	C	982	ASN
1	C	1016	ASN
1	C	1033	ASN
1	D	670	ASN
1	D	716	GLN
1	D	738	ASN
1	D	808	ASN
1	D	907	GLN
1	D	922	ASN
1	D	974	HIS
1	D	975	ASN
1	D	982	ASN
1	D	1016	ASN
1	D	1033	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	1101	3	15,15,15	0.53	0	21,21,21	1.64	5 (23%)
3	BMA	A	1102	2,4	11,11,12	0.90	0	13,15,17	0.91	0
2	NAG	A	1103	3	14,14,15	0.60	0	15,19,21	2.24	4 (26%)
4	MAN	A	1104	3,2	11,11,12	0.54	0	13,15,17	0.97	1 (7%)
2	NAG	A	1105	4	14,14,15	0.70	1 (7%)	15,19,21	2.34	3 (20%)
5	EDO	A	1106	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	1107	-	3,3,3	0.47	0	2,2,2	0.33	0
2	NAG	B	1101	3	15,15,15	0.45	0	21,21,21	0.85	1 (4%)
3	BMA	B	1102	2,4	11,11,12	0.92	0	13,15,17	0.89	0
2	NAG	B	1103	3	14,14,15	0.55	0	15,19,21	2.10	3 (20%)
4	MAN	B	1104	3,2	11,11,12	0.55	0	13,15,17	1.24	1 (7%)
2	NAG	B	1105	4	14,14,15	0.65	1 (7%)	15,19,21	2.24	4 (26%)
5	EDO	B	1106	-	3,3,3	0.45	0	2,2,2	0.33	0
5	EDO	B	1107	-	3,3,3	0.50	0	2,2,2	0.29	0
5	EDO	B	1108	-	3,3,3	0.49	0	2,2,2	0.31	0
5	EDO	B	1109	-	3,3,3	0.46	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	1110	-	3,3,3	0.48	0	2,2,2	0.34	0
5	EDO	B	1111	-	3,3,3	0.49	0	2,2,2	0.26	0
5	EDO	B	1112	-	3,3,3	0.45	0	2,2,2	0.32	0
5	EDO	B	1113	-	3,3,3	0.48	0	2,2,2	0.34	0
5	EDO	B	1114	-	3,3,3	0.48	0	2,2,2	0.17	0
5	EDO	B	1115	-	3,3,3	0.47	0	2,2,2	0.33	0
2	NAG	C	1101	3	15,15,15	0.57	0	21,21,21	1.43	4 (19%)
3	BMA	C	1102	2,4	11,11,12	0.83	0	13,15,17	0.91	1 (7%)
4	MAN	C	1103	3,2	11,11,12	0.51	0	13,15,17	1.03	1 (7%)
2	NAG	C	1104	4	14,14,15	0.65	1 (7%)	15,19,21	2.26	3 (20%)
5	EDO	C	1105	-	3,3,3	0.47	0	2,2,2	0.35	0
5	EDO	C	1106	-	3,3,3	0.45	0	2,2,2	0.34	0
2	NAG	D	1101	3	15,15,15	0.57	0	21,21,21	1.43	4 (19%)
3	BMA	D	1102	2,4	11,11,12	0.86	0	13,15,17	0.92	0
2	NAG	D	1103	3	14,14,15	0.58	0	15,19,21	1.27	2 (13%)
4	MAN	D	1104	3,2	11,11,12	0.57	0	13,15,17	0.94	1 (7%)
2	NAG	D	1105	4	14,14,15	0.72	1 (7%)	15,19,21	2.22	4 (26%)
5	EDO	D	1106	-	3,3,3	0.48	0	2,2,2	0.30	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
2	NAG	A	1101	3	-	0/6/26/26	0/1/1/1
3	BMA	A	1102	2,4	-	0/2/19/22	0/1/1/1
2	NAG	A	1103	3	-	0/6/23/26	0/1/1/1
4	MAN	A	1104	3,2	-	0/2/19/22	0/1/1/1
2	NAG	A	1105	4	-	0/6/23/26	0/1/1/1
5	EDO	A	1106	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1107	-	-	0/1/1/1	0/0/0/0
2	NAG	B	1101	3	-	0/6/26/26	0/1/1/1
3	BMA	B	1102	2,4	-	0/2/19/22	0/1/1/1
2	NAG	B	1103	3	-	0/6/23/26	0/1/1/1
4	MAN	B	1104	3,2	-	0/2/19/22	0/1/1/1
2	NAG	B	1105	4	-	0/6/23/26	0/1/1/1
5	EDO	B	1106	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1107	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1108	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1109	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1110	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1111	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1112	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1113	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1114	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1115	-	-	0/1/1/1	0/0/0/0
2	NAG	C	1101	3	-	0/6/26/26	0/1/1/1
3	BMA	C	1102	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1103	3,2	-	0/2/19/22	0/1/1/1
2	NAG	C	1104	4	-	0/6/23/26	0/1/1/1
5	EDO	C	1105	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1106	-	-	0/1/1/1	0/0/0/0
2	NAG	D	1101	3	-	0/6/26/26	0/1/1/1
3	BMA	D	1102	2,4	-	0/2/19/22	0/1/1/1
2	NAG	D	1103	3	-	0/6/23/26	0/1/1/1
4	MAN	D	1104	3,2	-	0/2/19/22	0/1/1/1
2	NAG	D	1105	4	-	0/6/23/26	0/1/1/1
5	EDO	D	1106	-	-	0/1/1/1	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1105	NAG	C1-C2	2.06	1.55	1.52
2	C	1104	NAG	C1-C2	2.08	1.55	1.52
2	A	1105	NAG	C1-C2	2.25	1.55	1.52
2	D	1105	NAG	C1-C2	2.33	1.55	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1103	NAG	O7-C7-C8	-2.39	117.70	122.06
2	D	1101	NAG	O7-C7-C8	-2.39	117.71	122.06
2	B	1103	NAG	O7-C7-C8	-2.37	117.75	122.06
2	D	1103	NAG	C1-O5-C5	-2.37	108.91	112.17
2	C	1101	NAG	O7-C7-C8	-2.27	117.92	122.06
2	A	1101	NAG	O7-C7-C8	-2.17	118.10	122.06
2	A	1103	NAG	O5-C1-C2	-2.05	108.62	111.47
3	C	1102	BMA	C1-C2-C3	2.00	112.19	109.65
2	D	1101	NAG	C1-C2-N2	2.01	113.06	110.73
2	D	1105	NAG	C1-C2-N2	2.06	114.01	110.49
2	B	1101	NAG	O5-C5-C6	2.08	111.39	106.41
2	A	1101	NAG	C3-C2-N2	2.12	114.67	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1105	NAG	C1-C2-N2	2.23	114.30	110.49
4	D	1104	MAN	C1-O5-C5	2.25	115.27	112.17
2	C	1101	NAG	C1-C2-N2	2.38	113.48	110.73
2	D	1103	NAG	C2-N2-C7	2.52	126.62	122.94
2	B	1105	NAG	O5-C1-C2	2.64	115.14	111.47
4	C	1103	MAN	C1-O5-C5	2.64	115.81	112.17
2	C	1104	NAG	C2-N2-C7	2.90	127.17	122.94
4	A	1104	MAN	C1-O5-C5	2.91	116.17	112.17
4	B	1104	MAN	C1-O5-C5	3.05	116.37	112.17
2	A	1101	NAG	C8-C7-N2	3.06	121.64	116.11
2	C	1101	NAG	C8-C7-N2	3.12	121.74	116.11
2	D	1101	NAG	C8-C7-N2	3.16	121.81	116.11
2	B	1103	NAG	C8-C7-N2	3.20	121.88	116.11
2	C	1104	NAG	O5-C1-C2	3.23	115.97	111.47
2	D	1105	NAG	C2-N2-C7	3.24	127.67	122.94
2	D	1101	NAG	C2-N2-C7	3.25	131.43	123.19
2	A	1103	NAG	C8-C7-N2	3.27	122.02	116.11
2	B	1105	NAG	C2-N2-C7	3.30	127.76	122.94
2	C	1101	NAG	C2-N2-C7	3.38	131.75	123.19
2	A	1105	NAG	C2-N2-C7	3.44	127.97	122.94
2	A	1101	NAG	C2-N2-C7	3.54	132.15	123.19
2	D	1105	NAG	O5-C1-C2	3.59	116.46	111.47
2	A	1101	NAG	C1-C2-N2	3.90	115.25	110.73
2	A	1105	NAG	O5-C1-C2	4.09	117.17	111.47
2	D	1105	NAG	C1-O5-C5	6.17	120.66	112.17
2	A	1105	NAG	C1-O5-C5	6.47	121.08	112.17
2	B	1103	NAG	C2-N2-C7	6.53	132.47	122.94
2	B	1105	NAG	C1-O5-C5	6.74	121.45	112.17
2	A	1103	NAG	C2-N2-C7	6.91	133.03	122.94
2	C	1104	NAG	C1-O5-C5	6.96	121.76	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1103	NAG	1	0
2	B	1103	NAG	2	0
5	B	1110	EDO	1	0
5	B	1114	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1106	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	416/442 (94%)	-0.26	6 (1%) 75 76	4, 12, 35, 46	14 (3%)
1	B	417/442 (94%)	-0.19	10 (2%) 59 60	3, 11, 41, 54	17 (4%)
1	C	408/442 (92%)	-0.30	4 (0%) 82 82	4, 11, 34, 52	13 (3%)
1	D	408/442 (92%)	-0.28	3 (0%) 87 88	5, 13, 39, 53	21 (5%)
All	All	1649/1768 (93%)	-0.26	23 (1%) 75 76	3, 12, 37, 54	65 (3%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1000	TYR	5.7
1	B	1008	LEU	5.3
1	B	996	ASN	5.1
1	B	997	LEU	4.4
1	B	1001	SER	3.9
1	D	1004	SER	3.9
1	A	997	LEU	3.7
1	B	1004	SER	3.7
1	B	625	HIS	3.2
1	B	998	GLU	2.9
1	C	1038	LEU	2.9
1	A	1041	LEU	2.8
1	A	625	HIS	2.7
1	A	995	THR	2.5
1	D	1005	LEU	2.4
1	C	1004	SER	2.2
1	B	1038	LEU	2.2
1	A	1001	SER	2.1
1	B	999	GLY	2.1
1	D	911	ASP	2.1
1	C	1005	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1004	SER	2.1
1	C	1002	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	1101	15/15	0.64	0.44	23.10	70,71,72,72	0
5	EDO	B	1114	4/4	0.69	0.43	19.77	29,30,30,31	0
2	NAG	A	1103	14/15	0.58	0.51	14.86	72,72,72,72	0
2	NAG	B	1103	14/15	0.70	0.44	14.37	62,63,63,63	0
2	NAG	D	1103	14/15	0.69	0.42	13.66	64,64,64,64	0
4	MAN	B	1104	11/12	0.82	0.30	12.85	54,56,57,57	0
5	EDO	A	1107	4/4	0.74	0.47	11.87	63,63,63,63	0
5	EDO	C	1105	4/4	0.88	0.26	9.82	20,20,21,21	0
5	EDO	B	1115	4/4	0.86	0.24	9.79	41,42,42,42	0
5	EDO	B	1113	4/4	0.67	0.40	9.12	85,85,85,85	0
4	MAN	C	1103	11/12	0.81	0.27	7.34	53,55,56,56	0
2	NAG	B	1101	15/15	0.65	0.45	6.31	61,62,62,62	0
2	NAG	D	1105	14/15	0.82	0.33	5.51	56,57,57,58	0
2	NAG	B	1105	14/15	0.87	0.31	4.79	50,52,53,53	0
4	MAN	D	1104	11/12	0.78	0.27	4.02	59,60,61,61	0
5	EDO	B	1109	4/4	0.91	0.26	3.83	31,31,31,31	0
5	EDO	B	1107	4/4	0.81	0.23	3.77	27,28,28,28	0
2	NAG	A	1105	14/15	0.90	0.27	3.22	62,62,63,63	0
2	NAG	C	1104	14/15	0.90	0.27	3.09	49,50,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MAN	A	1104	11/12	0.78	0.28	2.76	65,66,67,67	0
5	EDO	B	1112	4/4	0.86	0.28	1.89	49,49,49,49	0
5	EDO	D	1106	4/4	0.76	0.30	-	38,38,38,38	0
3	BMA	D	1102	11/12	0.69	0.41	-	62,63,64,64	0
2	NAG	D	1101	15/15	0.62	0.43	-	64,65,66,66	0
3	BMA	C	1102	11/12	0.65	0.39	-	57,58,59,59	0
5	EDO	B	1110	4/4	0.79	0.42	-	36,37,37,37	0
5	EDO	C	1106	4/4	0.88	0.29	-	42,42,42,43	0
5	EDO	A	1106	4/4	0.75	0.26	-	37,37,37,37	0
2	NAG	C	1101	15/15	0.76	0.39	-	60,61,62,62	0
5	EDO	B	1108	4/4	0.79	0.25	-	39,39,39,39	0
3	BMA	B	1102	11/12	0.72	0.36	-	58,61,61,61	0
3	BMA	A	1102	11/12	0.59	0.41	-	68,70,70,71	0
5	EDO	B	1111	4/4	0.71	0.39	-	36,36,36,37	0
5	EDO	B	1106	4/4	0.88	0.40	-	43,43,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.