



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:45 pm GMT

PDB ID : 3OGV
Title : Complex structure of beta-galactosidase from *Trichoderma reesei* with PETG
Authors : Maksimainen, M.; Rouvinen, J.
Deposited on : 2010-08-17
Resolution : 1.40 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 : trunk28620
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) : recalc28949

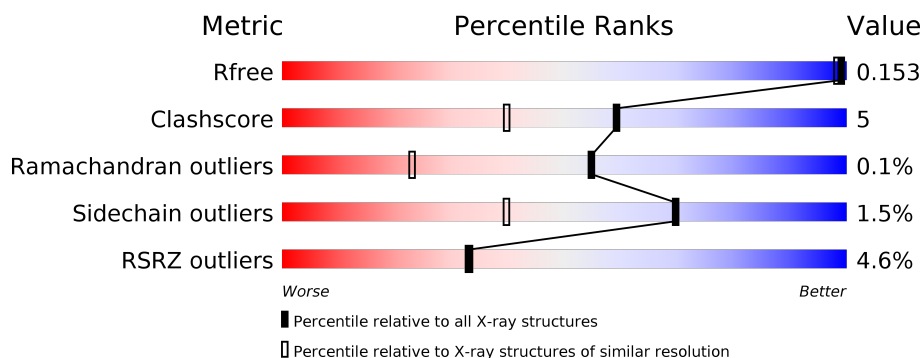
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1307 (1.40-1.40)
Clashscore	112137	1411 (1.40-1.40)
Ramachandran outliers	110173	1373 (1.40-1.40)
Sidechain outliers	110143	1372 (1.40-1.40)
RSRZ outliers	101464	1315 (1.40-1.40)

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	1003	<div> <div>4%</div> <div>82%</div> <div>14%</div> <div>••</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	A	1031	-	-	-	X
5	NAG	A	1040	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	1041	-	-	-	X
6	NAG	A	1043	-	-	-	X

2 Entry composition [i](#)

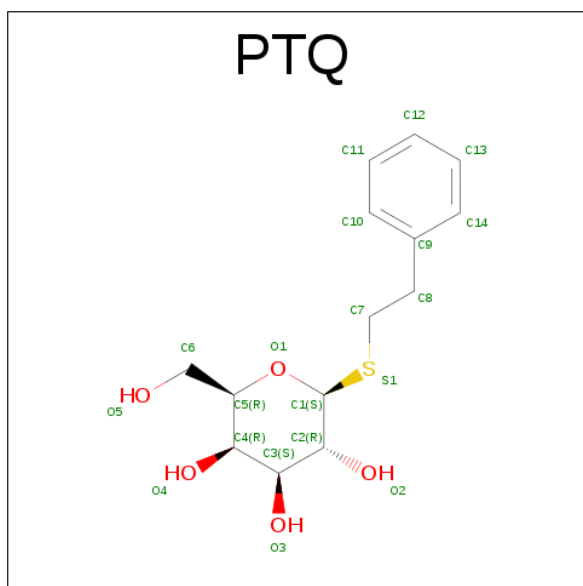
There are 7 unique types of molecules in this entry. The entry contains 9065 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	986	Total	C	N	O	S	0	10	0
			7674	4937	1292	1437	8			

- Molecule 2 is SUGAR (2-PHENYLETHYL 1-THIO-BETA-D-GALACTOPYRANOSIDE) (three-letter code: PTQ) (formula: C₁₄H₂₀O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			20	14	5	1		

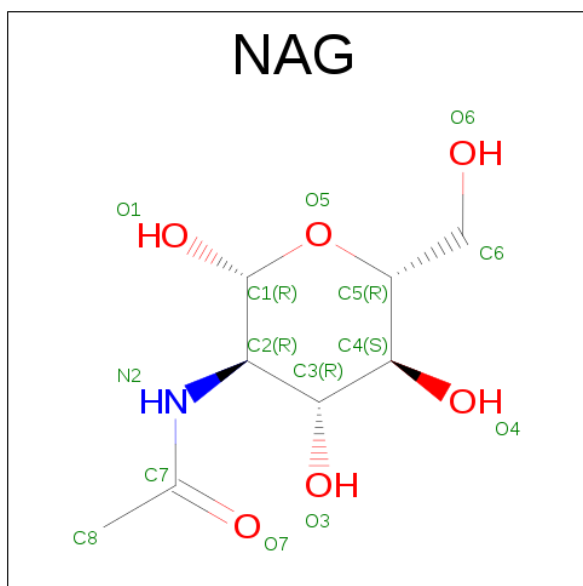
- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 4 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

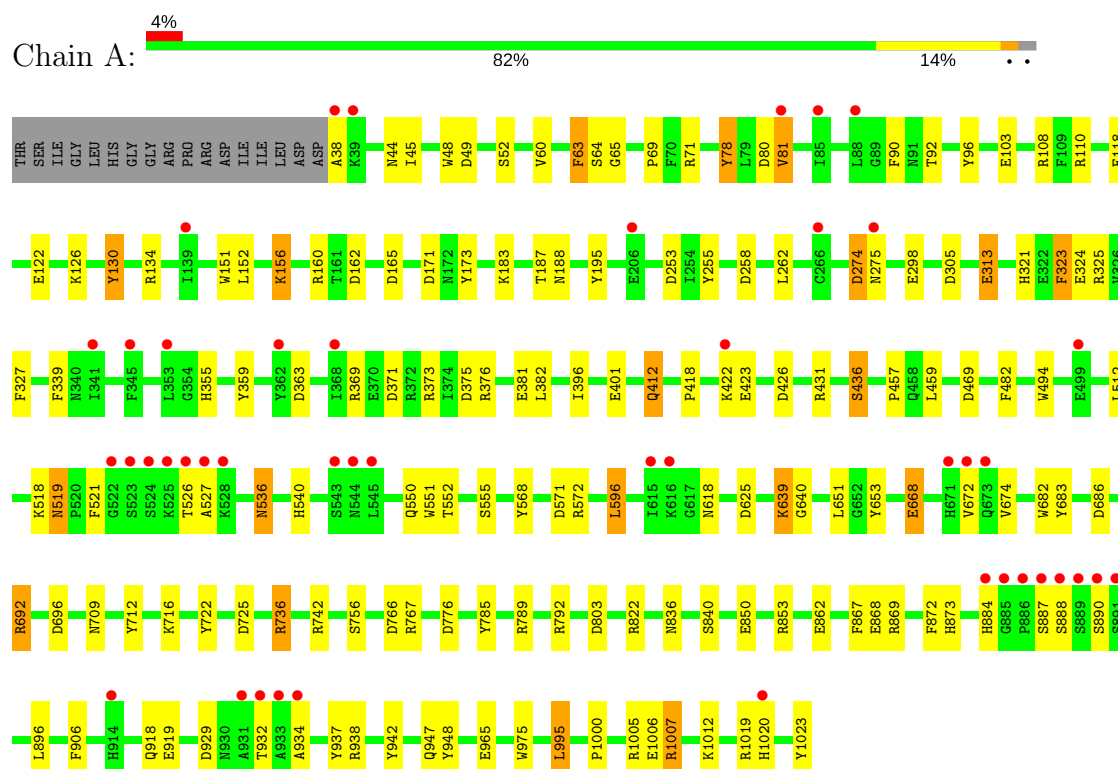
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1138	Total	O	0	0
			1138	1138		

3 Residue-property plots [i](#)

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

• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.60Å 68.70Å 81.70Å 108.50° 97.70° 114.50°	Depositor
Resolution (Å)	42.76 – 1.40 42.76 – 1.35	Depositor EDS
% Data completeness (in resolution range)	95.0 (42.76-1.40) 77.7 (42.76-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.132 , 0.166 0.145 , 0.153	Depositor DCC
R_{free} test set	11034 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	10.9	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9065	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GLC, BMA, NAG, PTQ, 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	1.49	46/7915 (0.6%)	1.38	87/10787 (0.8%)

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

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

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	GLU	CD-OE1	11.05	1.37	1.25
1	A	551	TRP	CB-CG	8.83	1.66	1.50
1	A	324	GLU	CD-OE1	8.36	1.34	1.25
1	A	436	SER	CA-CB	8.24	1.65	1.52
1	A	325	ARG	CG-CD	7.67	1.71	1.51
1	A	151	TRP	CE3-CZ3	7.30	1.50	1.38
1	A	862	GLU	CG-CD	7.27	1.62	1.51
1	A	942	TYR	CD2-CE2	7.22	1.50	1.39
1	A	381	GLU	CD-OE2	6.75	1.33	1.25
1	A	789	ARG	CZ-NH2	6.72	1.41	1.33
1	A	118	GLU	CD-OE1	6.66	1.32	1.25
1	A	948	TYR	CD2-CE2	6.62	1.49	1.39
1	A	44	ASN	CB-CG	-6.45	1.36	1.51
1	A	162	ASP	CB-CG	-6.44	1.38	1.51
1	A	785	TYR	CD2-CE2	6.44	1.49	1.39
1	A	103	GLU	CD-OE1	-6.44	1.18	1.25
1	A	313	GLU	CD-OE2	-6.33	1.18	1.25
1	A	325	ARG	CB-CG	-6.27	1.35	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	868	GLU	CD-OE2	6.17	1.32	1.25
1	A	840	SER	CB-OG	-6.06	1.34	1.42
1	A	862	GLU	CB-CG	-5.85	1.41	1.52
1	A	975	TRP	CE3-CZ3	5.78	1.48	1.38
1	A	255	TYR	CE2-CZ	5.78	1.46	1.38
1	A	324	GLU	CG-CD	-5.77	1.43	1.51
1	A	110	ARG	CZ-NH1	5.71	1.40	1.33
1	A	65	GLY	N-CA	5.66	1.54	1.46
1	A	674	VAL	CB-CG1	5.63	1.64	1.52
1	A	937	TYR	CD1-CE1	5.60	1.47	1.39
1	A	48	TRP	CD2-CE2	5.60	1.48	1.41
1	A	555	SER	CA-CB	5.59	1.61	1.52
1	A	942	TYR	CE1-CZ	-5.53	1.31	1.38
1	A	712	TYR	CD2-CE2	5.52	1.47	1.39
1	A	494	TRP	CD2-CE2	5.46	1.48	1.41
1	A	482	PHE	CE1-CZ	5.46	1.47	1.37
1	A	872	PHE	CD2-CE2	5.43	1.50	1.39
1	A	653	TYR	CE2-CZ	5.37	1.45	1.38
1	A	850	GLU	CD-OE2	-5.32	1.19	1.25
1	A	756[A]	SER	CB-OG	-5.29	1.35	1.42
1	A	756[B]	SER	CB-OG	-5.29	1.35	1.42
1	A	457	PRO	N-CA	5.23	1.56	1.47
1	A	436	SER	CB-OG	5.20	1.49	1.42
1	A	568	TYR	CE1-CZ	5.16	1.45	1.38
1	A	668	GLU	CD-OE1	5.16	1.31	1.25
1	A	323	PHE	CD2-CE2	5.16	1.49	1.39
1	A	572	ARG	CZ-NH1	5.10	1.39	1.33
1	A	78	TYR	CE2-CZ	-5.05	1.31	1.38

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	ARG	NE-CZ-NH2	-13.98	113.31	120.30
1	A	938	ARG	NE-CZ-NH2	-13.69	113.45	120.30
1	A	938	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	A	431	ARG	NE-CZ-NH1	11.73	126.16	120.30
1	A	162	ASP	CB-CG-OD2	-11.16	108.26	118.30
1	A	686	ASP	CB-CG-OD1	11.10	128.29	118.30
1	A	822	ARG	NE-CZ-NH1	10.83	125.71	120.30
1	A	572	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	766	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	A	869	ARG	NE-CZ-NH1	8.80	124.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	A	162	ASP	CB-CG-OD1	8.64	126.08	118.30
1	A	431	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	110	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	A	1019	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	766	ASP	CB-CG-OD1	7.92	125.43	118.30
1	A	134	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	152	LEU	CB-CG-CD2	7.85	124.35	111.00
1	A	722	TYR	CB-CG-CD1	7.83	125.70	121.00
1	A	469	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	80	ASP	CB-CG-OD2	7.65	125.19	118.30
1	A	274	ASP	CB-CG-OD1	7.36	124.93	118.30
1	A	324	GLU	OE1-CD-OE2	-7.32	114.52	123.30
1	A	313	GLU	CG-CD-OE1	7.14	132.59	118.30
1	A	130	TYR	CG-CD2-CE2	-7.14	115.58	121.30
1	A	995	LEU	CA-CB-CG	7.05	131.52	115.30
1	A	369	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	160	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	339	PHE	CB-CG-CD2	-6.87	115.99	120.80
1	A	195	TYR	CD1-CE1-CZ	-6.76	113.72	119.80
1	A	258	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	A	363	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	A	872	PHE	CB-CG-CD2	-6.69	116.12	120.80
1	A	426	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	156	LYS	CD-CE-NZ	-6.63	96.45	111.70
1	A	692	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	965	GLU	OE1-CD-OE2	6.54	131.14	123.30
1	A	942	TYR	CB-CG-CD1	-6.48	117.11	121.00
1	A	571	ASP	CB-CG-OD1	6.48	124.14	118.30
1	A	596[A]	LEU	CB-CG-CD2	-6.43	100.07	111.00
1	A	596[B]	LEU	CB-CG-CD2	-6.43	100.07	111.00
1	A	165	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	96	TYR	CG-CD2-CE2	6.38	126.40	121.30
1	A	696	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	359	TYR	CD1-CE1-CZ	-6.25	114.17	119.80
1	A	995	LEU	CB-CG-CD1	6.21	121.55	111.00
1	A	325	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	323	PHE	CB-CG-CD1	-6.15	116.49	120.80
1	A	305	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	776	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	375	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	722	TYR	CB-CG-CD2	-5.88	117.47	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	PHE	CB-CG-CD1	5.87	124.91	120.80
1	A	725	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	822	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	929	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	371	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	313	GLU	CG-CD-OE2	-5.83	106.64	118.30
1	A	1005	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	382	LEU	CB-CG-CD2	-5.76	101.21	111.00
1	A	867	PHE	CB-CG-CD1	-5.76	116.77	120.80
1	A	906	PHE	CB-CG-CD1	-5.73	116.79	120.80
1	A	942	TYR	CZ-CE2-CD2	-5.72	114.66	119.80
1	A	49	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	373	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	110	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	71	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	736	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	869	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	803	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	173	TYR	CZ-CE2-CD2	-5.40	114.94	119.80
1	A	572	ARG	CD-NE-CZ	5.38	131.14	123.60
1	A	376	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	171	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	686	ASP	OD1-CG-OD2	-5.32	113.19	123.30
1	A	683	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	90	PHE	CB-CG-CD1	5.23	124.46	120.80
1	A	625	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	81[A]	VAL	CA-CB-CG2	-5.16	103.16	110.90
1	A	81[B]	VAL	CA-CB-CG2	-5.16	103.16	110.90
1	A	426	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	253	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	195	TYR	CG-CD2-CE2	-5.13	117.20	121.30
1	A	853	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	896	LEU	CB-CG-CD2	5.08	119.64	111.00
1	A	258	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	255	TYR	CB-CG-CD1	-5.01	117.99	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	736	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	7674	0	7490	83	2
2	A	20	0	20	1	0
3	A	83	0	70	2	0
4	A	94	0	79	0	0
5	A	28	0	26	0	0
6	A	28	0	25	1	0
7	A	1138	0	0	44	3
All	All	9065	0	7710	84	5

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 (84) 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:A:108:ARG:HD2	7:A:2107:HOH:O	1.34	1.22
1:A:1012:LYS:HE3	7:A:1986:HOH:O	1.42	1.19
1:A:1020:HIS:CD2	7:A:2077:HOH:O	2.04	1.11
1:A:69:PRO:HG2	7:A:1597:HOH:O	1.50	1.10
1:A:1006:GLU:HG3	7:A:1815:HOH:O	1.51	1.07
1:A:412:GLN:HG3	7:A:2209:HOH:O	1.60	0.98
1:A:188:ASN:HB2	7:A:1524:HOH:O	1.64	0.96
1:A:1020:HIS:HD2	7:A:2077:HOH:O	1.47	0.92
1:A:38:ALA:HB3	7:A:1875:HOH:O	1.70	0.92
1:A:262:LEU:HD11	1:A:327:PHE:CZ	2.06	0.90
1:A:934:ALA:HB1	7:A:1813:HOH:O	1.72	0.89
1:A:188:ASN:CB	7:A:1524:HOH:O	2.22	0.85
1:A:518:LYS:NZ	7:A:2093:HOH:O	1.97	0.82
1:A:38:ALA:N	7:A:1928:HOH:O	2.15	0.79
1:A:1006:GLU:CG	7:A:1815:HOH:O	2.15	0.77
1:A:412:GLN:CG	7:A:2209:HOH:O	2.24	0.77
1:A:1006:GLU:HG3	7:A:1857:HOH:O	1.86	0.76
1:A:1020:HIS:HD2	7:A:1518:HOH:O	1.68	0.76
1:A:122:GLU:HG2	7:A:2207:HOH:O	1.86	0.75
1:A:459:LEU:CD1	7:A:1670:HOH:O	2.34	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60[A]:VAL:HG21	1:A:596[A]:LEU:HD13	1.67	0.74
1:A:422:LYS:HG2	1:A:423:GLU:HG3	1.70	0.73
1:A:183:LYS:HE2	7:A:1588:HOH:O	1.89	0.71
1:A:108:ARG:NH1	7:A:2107:HOH:O	1.87	0.71
1:A:767:ARG:HD3	7:A:1982:HOH:O	1.92	0.70
1:A:1006:GLU:CD	7:A:1815:HOH:O	2.30	0.69
1:A:716:LYS:NZ	7:A:1840:HOH:O	2.26	0.68
1:A:651:LEU:HD23	1:A:651:LEU:N	2.13	0.64
1:A:262:LEU:CD1	1:A:327:PHE:CZ	2.81	0.63
1:A:1020:HIS:CD2	7:A:1518:HOH:O	2.48	0.63
1:A:742:ARG:CG	7:A:1564:HOH:O	2.46	0.63
1:A:887:SER:O	1:A:888:SER:OG	2.16	0.62
1:A:1023:TYR:HB2	7:A:2206:HOH:O	1.99	0.62
1:A:918:GLN:HG3	1:A:1007:ARG:HE	1.64	0.61
1:A:60[A]:VAL:HG21	1:A:596[A]:LEU:CD1	2.32	0.60
1:A:1012:LYS:CE	7:A:1986:HOH:O	2.22	0.60
1:A:38:ALA:CB	7:A:1875:HOH:O	2.38	0.59
1:A:668:GLU:CG	7:A:1891:HOH:O	2.50	0.58
1:A:651:LEU:HD23	1:A:651:LEU:H	1.69	0.58
1:A:873:HIS:CD2	1:A:873:HIS:H	2.23	0.57
1:A:668:GLU:HG2	7:A:1891:HOH:O	2.04	0.56
1:A:742:ARG:HG2	7:A:1564:HOH:O	2.06	0.55
1:A:512:LEU:HD11	1:A:550:GLN:HG2	1.89	0.54
1:A:262:LEU:HD13	1:A:323:PHE:HE1	1.72	0.54
1:A:692:ARG:HD2	7:A:1422:HOH:O	2.08	0.54
1:A:262:LEU:HD11	1:A:327:PHE:HZ	1.65	0.52
1:A:412:GLN:CD	7:A:2209:HOH:O	2.47	0.52
1:A:122:GLU:HG3	7:A:1791:HOH:O	2.10	0.51
1:A:108:ARG:CD	7:A:2107:HOH:O	2.15	0.51
3:A:1028:MAN:H62	7:A:1934:HOH:O	2.10	0.51
1:A:672:VAL:HG23	1:A:1000:PRO:HG3	1.93	0.51
1:A:126:LYS:HE2	7:A:1815:HOH:O	2.11	0.50
1:A:742:ARG:NH2	1:A:836:ASN:O	2.45	0.50
1:A:401:GLU:HB2	1:A:418:PRO:HG2	1.95	0.49
1:A:536:ASN:ND2	1:A:552:THR:H	2.11	0.49
1:A:651:LEU:CD2	1:A:651:LEU:N	2.76	0.49
1:A:668:GLU:HG3	7:A:1891:HOH:O	2.11	0.48
1:A:156:LYS:HE3	1:A:709:ASN:OD1	2.14	0.47
1:A:792:ARG:NH1	7:A:2212:HOH:O	2.43	0.47
1:A:313:GLU:OE2	7:A:2052:HOH:O	2.20	0.47
1:A:45[B]:ILE:HD12	1:A:187:THR:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:HIS:HD2	7:A:1209:HOH:O	1.98	0.46
1:A:672:VAL:CG2	1:A:1000:PRO:HG3	2.47	0.45
1:A:639:LYS:HE2	1:A:640:GLY:N	2.32	0.44
1:A:521:PHE:CD1	1:A:527:ALA:HB1	2.52	0.44
1:A:52:SER:HB3	1:A:396:ILE:HG23	2.00	0.44
1:A:64:SER:HA	1:A:92:THR:O	2.17	0.43
1:A:682:TRP:O	1:A:884:HIS:HD2	2.01	0.43
1:A:518:LYS:O	1:A:519:ASN:C	2.58	0.42
1:A:92:THR:HA	1:A:130:TYR:O	2.20	0.42
1:A:639:LYS:HE2	1:A:640:GLY:H	1.85	0.42
1:A:321:HIS:HE1	3:A:1029:MAN:O4	2.03	0.42
1:A:183:LYS:HG3	7:A:1531:HOH:O	2.20	0.41
1:A:78:TYR:O	1:A:81[A]:VAL:CG2	2.68	0.41
1:A:918:GLN:NE2	1:A:919:GLU:OE2	2.44	0.41
1:A:298:GLU:OE1	2:A:1024:PTQ:H1	2.20	0.41
1:A:742:ARG:HH11	1:A:742:ARG:HD2	1.64	0.41
1:A:436:SER:OG	6:A:1042:NAG:H5	2.21	0.41
1:A:274:ASP:O	1:A:275:ASN:HB2	2.20	0.41
1:A:262:LEU:HD13	1:A:323:PHE:CE1	2.55	0.40
1:A:78:TYR:O	1:A:81[A]:VAL:HG22	2.21	0.40
1:A:536:ASN:HD21	1:A:552:THR:H	1.69	0.40
1:A:887:SER:C	1:A:888:SER:HG	2.21	0.40
1:A:459:LEU:HD13	7:A:1670:HOH:O	2.13	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1305:HOH:O	7:A:2204:HOH:O[1_556]	1.72	0.48
1:A:540:HIS:CE1	1:A:1020:HIS:CE1[1_544]	1.88	0.32
7:A:1300:HOH:O	7:A:2160:HOH:O[1_455]	2.10	0.10
1:A:540:HIS:CE1	1:A:1020:HIS:NE2[1_544]	2.12	0.08
7:A:1873:HOH:O	7:A:1988:HOH:O[1_655]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	994/1003 (99%)	965 (97%)	28 (3%)	1 (0%)	55 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	519	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	815/819 (100%)	803 (98%)	12 (2%)	70 40

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	PHE
1	A	355	HIS
1	A	412	GLN
1	A	526	THR
1	A	536	ASN
1	A	618	ASN
1	A	639	LYS
1	A	890	SER
1	A	932	THR
1	A	947	GLN
1	A	995	LEU
1	A	1007	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	HIS
1	A	412	GLN
1	A	413	ASN
1	A	536	ASN
1	A	618	ASN
1	A	673	GLN
1	A	836	ASN
1	A	873	HIS
1	A	884	HIS
1	A	1015	HIS
1	A	1020	HIS

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 ⓘ

17 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	$\# Z > 2$
3	NAG	A	1025	1,3	14,14,15	0.50	0	15,19,21	1.81	4 (26%)
3	NAG	A	1026	3	14,14,15	0.74	0	15,19,21	1.44	4 (26%)
3	BMA	A	1027	3	11,11,12	1.21	1 (9%)	13,15,17	1.03	1 (7%)
3	MAN	A	1028	3	11,11,12	0.86	0	13,15,17	1.09	1 (7%)
3	MAN	A	1029	3	11,11,12	0.97	0	13,15,17	1.64	1 (7%)
3	MAN	A	1030	3	11,11,12	1.28	2 (18%)	13,15,17	1.48	2 (15%)
3	MAN	A	1031	3	11,11,12	1.11	0	13,15,17	2.45	6 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1032	1,4	14,14,15	1.89	4 (28%)	15,19,21	1.63	2 (13%)
4	NAG	A	1033	4	14,14,15	0.77	0	15,19,21	1.39	2 (13%)
4	BMA	A	1034	4	11,11,12	1.03	1 (9%)	13,15,17	1.36	3 (23%)
4	MAN	A	1035	4	11,11,12	1.15	1 (9%)	13,15,17	2.23	4 (30%)
4	MAN	A	1036	4	11,11,12	0.96	1 (9%)	13,15,17	1.78	5 (38%)
4	MAN	A	1037	4	11,11,12	1.05	1 (9%)	13,15,17	1.67	3 (23%)
4	MAN	A	1038	4	11,11,12	0.81	0	13,15,17	1.30	3 (23%)
4	GLC	A	1039	4	11,11,12	0.81	1 (9%)	13,15,17	2.16	4 (30%)
6	NAG	A	1042	1,6	14,14,15	1.05	1 (7%)	15,19,21	2.04	5 (33%)
6	NAG	A	1043	6	14,14,15	0.56	0	15,19,21	1.63	4 (26%)

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	1025	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1026	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1027	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1028	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1029	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1030	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1031	3	-	0/2/19/22	0/1/1/1
4	NAG	A	1032	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1033	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1034	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1035	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1036	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1037	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1038	4	-	0/2/19/22	0/1/1/1
4	GLC	A	1039	4	-	0/2/19/22	0/1/1/1
6	NAG	A	1042	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1043	6	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1032	NAG	O5-C1	-3.90	1.37	1.43
4	A	1035	MAN	O5-C1	-2.81	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1042	NAG	C1-C2	-2.78	1.48	1.52
4	A	1032	NAG	C2-N2	-2.33	1.42	1.46
3	A	1030	MAN	O2-C2	-2.28	1.38	1.43
3	A	1030	MAN	O5-C1	-2.20	1.40	1.43
4	A	1039	GLC	O5-C5	-2.02	1.39	1.43
4	A	1037	MAN	O5-C5	2.00	1.47	1.43
4	A	1036	MAN	C6-C5	2.34	1.59	1.51
4	A	1034	BMA	C4-C5	2.40	1.58	1.53
3	A	1027	BMA	O5-C1	2.47	1.47	1.43
4	A	1032	NAG	C4-C5	2.95	1.59	1.53
4	A	1032	NAG	C1-C2	3.50	1.57	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1031	MAN	C6-C5-C4	-5.72	99.62	113.00
6	A	1043	NAG	C3-C4-C5	-4.03	103.12	110.22
4	A	1033	NAG	O4-C4-C3	-3.83	102.03	110.36
3	A	1031	MAN	O6-C6-C5	-3.53	99.46	111.34
4	A	1037	MAN	C1-C2-C3	-3.46	105.27	109.65
4	A	1039	GLC	O5-C1-C2	-3.44	105.40	110.79
3	A	1025	NAG	O7-C7-C8	-3.38	115.90	122.06
3	A	1030	MAN	O3-C3-C2	-3.30	104.02	110.02
3	A	1025	NAG	C2-N2-C7	-3.24	118.21	122.94
3	A	1030	MAN	O2-C2-C3	-3.21	103.87	110.17
3	A	1026	NAG	O5-C1-C2	-2.68	107.74	111.47
3	A	1031	MAN	O4-C4-C5	-2.55	102.85	109.28
3	A	1025	NAG	O5-C1-C2	-2.54	107.94	111.47
4	A	1033	NAG	O5-C1-C2	-2.44	108.07	111.47
3	A	1028	MAN	O3-C3-C2	-2.43	105.59	110.02
3	A	1025	NAG	C1-O5-C5	-2.43	108.81	112.17
4	A	1038	MAN	O3-C3-C4	-2.43	105.07	110.36
3	A	1031	MAN	C1-C2-C3	-2.39	106.62	109.65
3	A	1026	NAG	O4-C4-C3	-2.37	105.19	110.36
6	A	1043	NAG	O5-C1-C2	-2.30	108.27	111.47
4	A	1034	BMA	C1-C2-C3	-2.25	106.80	109.65
4	A	1036	MAN	O2-C2-C3	-2.23	105.79	110.17
3	A	1026	NAG	C1-C2-N2	-2.20	106.72	110.49
6	A	1042	NAG	O7-C7-C8	-2.19	118.08	122.06
4	A	1039	GLC	C2-C3-C4	-2.17	107.09	110.88
3	A	1027	BMA	C1-O5-C5	-2.15	109.20	112.17
3	A	1026	NAG	C4-C3-C2	-2.10	107.94	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1037	MAN	O2-C2-C3	-2.08	106.10	110.17
4	A	1032	NAG	O5-C1-C2	-2.03	108.64	111.47
4	A	1035	MAN	O3-C3-C4	2.02	114.75	110.36
4	A	1034	BMA	C2-C3-C4	2.03	114.42	110.88
6	A	1043	NAG	C1-O5-C5	2.12	115.08	112.17
4	A	1038	MAN	C1-O5-C5	2.18	115.17	112.17
4	A	1039	GLC	C1-C2-C3	2.27	112.53	109.65
6	A	1042	NAG	C1-O5-C5	2.27	115.29	112.17
4	A	1036	MAN	O3-C3-C4	2.35	115.47	110.36
4	A	1038	MAN	C1-C2-C3	2.37	112.66	109.65
4	A	1037	MAN	O5-C1-C2	2.51	114.72	110.79
4	A	1036	MAN	O5-C1-C2	2.51	114.73	110.79
6	A	1043	NAG	C2-N2-C7	2.51	126.61	122.94
4	A	1036	MAN	C1-O5-C5	2.56	115.69	112.17
6	A	1042	NAG	C2-N2-C7	2.56	126.67	122.94
3	A	1031	MAN	O5-C1-C2	2.65	114.94	110.79
4	A	1034	BMA	O3-C3-C2	2.79	115.11	110.02
3	A	1031	MAN	C1-O5-C5	2.86	116.10	112.17
4	A	1032	NAG	C1-O5-C5	3.32	116.75	112.17
6	A	1042	NAG	C8-C7-N2	3.49	122.41	116.11
4	A	1035	MAN	C1-C2-C3	3.64	114.26	109.65
6	A	1042	NAG	C4-C3-C2	3.67	116.40	111.02
4	A	1036	MAN	C3-C4-C5	3.69	116.72	110.22
3	A	1029	MAN	C1-O5-C5	3.78	117.37	112.17
4	A	1035	MAN	O4-C4-C3	3.81	118.65	110.36
4	A	1035	MAN	C1-O5-C5	4.48	118.34	112.17
4	A	1039	GLC	C1-O5-C5	5.69	120.01	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1028	MAN	1	0
3	A	1029	MAN	1	0
6	A	1042	NAG	1	0

5.6 Ligand geometry

3 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	PTQ	A	1024	-	21,21,21	1.49	4 (19%)	26,28,28	1.52	5 (19%)
5	NAG	A	1040	1	14,14,15	1.25	1 (7%)	15,19,21	1.65	2 (13%)
5	NAG	A	1041	1	14,14,15	0.83	0	15,19,21	2.10	6 (40%)

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	PTQ	A	1024	-	-	0/8/28/28	0/2/2/2
5	NAG	A	1040	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1041	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1024	PTQ	C13-C14	-2.50	1.34	1.38
2	A	1024	PTQ	C1-C2	-2.08	1.49	1.53
2	A	1024	PTQ	C1-S1	2.34	1.84	1.80
2	A	1024	PTQ	O1-C5	2.97	1.51	1.44
5	A	1040	NAG	O7-C7	3.91	1.32	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1041	NAG	O7-C7-C8	-4.46	113.93	122.06
5	A	1040	NAG	C8-C7-N2	-3.36	110.05	116.11
5	A	1040	NAG	O6-C6-C5	-3.24	100.43	111.34
5	A	1041	NAG	O4-C4-C5	-3.15	101.36	109.28
2	A	1024	PTQ	O1-C5-C6	-2.79	99.72	106.41
5	A	1041	NAG	C2-N2-C7	-2.35	119.52	122.94
2	A	1024	PTQ	O4-C4-C3	-2.24	105.47	110.36
5	A	1041	NAG	O3-C3-C4	2.01	114.73	110.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1024	PTQ	C3-C4-C5	2.46	114.56	110.22
5	A	1041	NAG	C8-C7-N2	2.74	121.06	116.11
2	A	1024	PTQ	O1-C1-C2	2.79	114.11	110.28
5	A	1041	NAG	C4-C3-C2	3.04	115.48	111.02
2	A	1024	PTQ	C6-C5-C4	3.68	121.62	113.00

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
2	A	1024	PTQ	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	986/1003 (98%)	0.16	45 (4%) 33 33	6, 12, 26, 61	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	526	THR	11.9
1	A	933	ALA	10.1
1	A	932	THR	7.7
1	A	523	SER	7.0
1	A	525	LYS	6.9
1	A	931	ALA	5.7
1	A	543	SER	5.5
1	A	527	ALA	5.4
1	A	522	GLY	5.4
1	A	524	SER	4.5
1	A	888	SER	4.5
1	A	886	PRO	4.0
1	A	890	SER	3.8
1	A	545	LEU	3.6
1	A	528	LYS	3.1
1	A	885	GLY	2.9
1	A	891	SER	2.9
1	A	266	CYS	2.8
1	A	671	HIS	2.8
1	A	544	ASN	2.8
1	A	368	ILE	2.8
1	A	887	SER	2.8
1	A	673	GLN	2.8
1	A	345	PHE	2.8
1	A	275	ASN	2.7
1	A	422	LYS	2.7
1	A	39	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1020	HIS	2.6
1	A	362	TYR	2.6
1	A	889	SER	2.6
1	A	341	ILE	2.6
1	A	914	HIS	2.4
1	A	353	LEU	2.4
1	A	81[A]	VAL	2.4
1	A	616	LYS	2.3
1	A	206	GLU	2.3
1	A	672	VAL	2.3
1	A	499	GLU	2.2
1	A	88	LEU	2.2
1	A	38	ALA	2.2
1	A	139	ILE	2.1
1	A	85	ILE	2.1
1	A	615	ILE	2.0
1	A	934	ALA	2.0
1	A	884	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
6	NAG	A	1043	14/15	0.70	0.34	14.94	35,40,51,51	0
3	MAN	A	1031	11/12	0.93	0.14	2.41	15,16,22,25	0
6	NAG	A	1042	14/15	0.88	0.15	1.09	22,30,38,41	0
4	MAN	A	1037	11/12	0.96	0.10	0.77	12,13,16,16	0
4	NAG	A	1032	14/15	0.96	0.08	-0.23	11,13,22,28	0
4	GLC	A	1039	11/12	0.95	0.09	-0.23	13,15,19,21	0
3	MAN	A	1029	11/12	0.97	0.07	-0.37	10,12,19,29	0
3	NAG	A	1025	14/15	0.97	0.07	-1.02	8,11,18,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	1026	14/15	0.98	0.06	-1.57	8,10,15,16	0
4	NAG	A	1033	14/15	0.96	0.10	-	10,14,32,34	0
3	MAN	A	1028	11/12	0.96	0.07	-	9,11,16,22	0
4	MAN	A	1036	11/12	0.94	0.11	-	14,18,23,31	0
3	MAN	A	1030	11/12	0.89	0.27	-	21,25,36,37	0
4	MAN	A	1038	11/12	0.97	0.07	-	13,13,15,16	0
3	BMA	A	1027	11/12	0.98	0.06	-	9,11,14,15	0
4	BMA	A	1034	11/12	0.97	0.09	-	12,13,17,18	0
4	MAN	A	1035	11/12	0.82	0.24	-	27,31,37,40	0

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(\AA^2)	Q<0.9
5	NAG	A	1041	14/15	0.90	0.20	5.73	24,28,35,41	0
5	NAG	A	1040	14/15	0.79	0.23	3.52	28,36,45,48	0
2	PTQ	A	1024	20/20	0.97	0.09	-0.34	6,8,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.