Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 10:58 PM EDT

PDB ID	:	6BYJ
Title	:	Structure of human 14-3-3 gamma bound to O-GlcNAc peptide
Authors	:	Schumacher, M.A.
Deposited on	:	2017-12-20
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

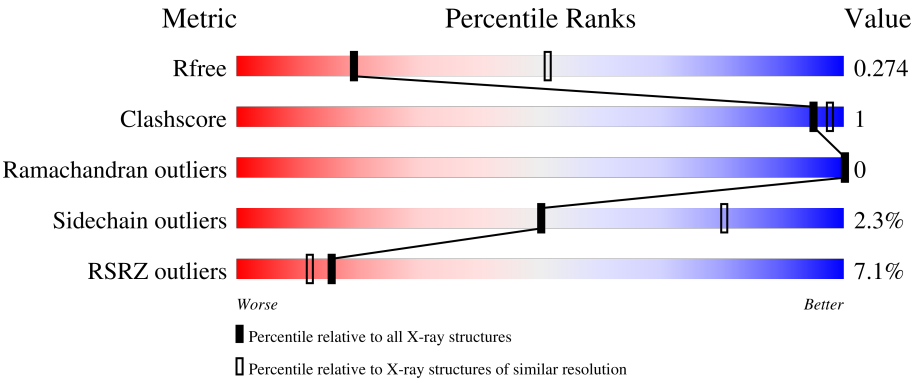
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	2% 98%
1	B	240	6% 97%
1	C	240	% 94% 5%
1	D	240	2% 96%
1	E	240	7% 96%

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Mol	Chain	Length	Quality of chain
1	F	240	19% 95%
2	G	20	10% 30% 35% 35%
2	P	20	25% 25% 10% 65%
2	T	20	35% 10% 15% 10% 65%

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	NAG	G	601	-	-	X	-
3	NAG	P	601	-	-	-	X
3	NAG	T	601	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22960 atoms, of which 11240 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.

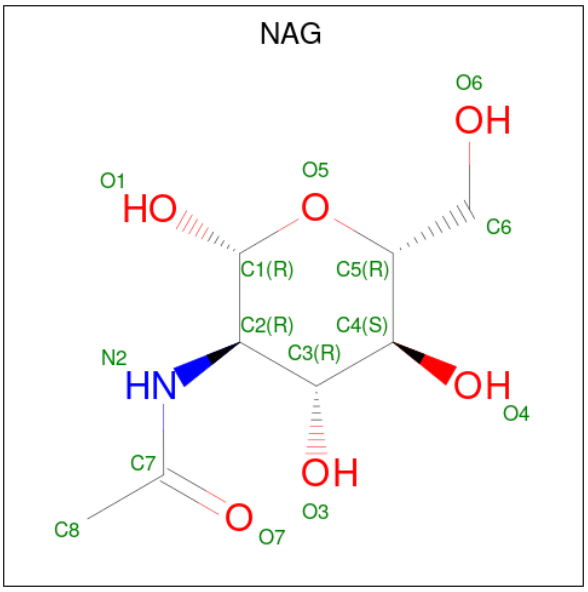
- Molecule 1 is a protein called 14-3-3 protein gamma.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	240	Total	C	H	N	O	S	0	0	0
			3826	1205	1887	330	395	9			
1	B	238	Total	C	H	N	O	S	0	0	0
			3802	1197	1879	328	389	9			
1	C	238	Total	C	H	N	O	S	0	0	0
			3802	1197	1879	328	389	9			
1	D	238	Total	C	H	N	O	S	0	0	0
			3802	1197	1879	328	389	9			
1	E	237	Total	C	H	N	O	S	0	0	0
			3790	1193	1875	327	386	9			
1	F	232	Total	C	H	N	O	S	0	0	0
			3717	1171	1841	320	376	9			

- Molecule 2 is a protein called TSTTATPPVSQASSTTTSTW O-GlcNac peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	13	Total	C	N	O	0	0	0
			86	51	14	21			
2	P	7	Total	C	N	O	0	0	0
			47	29	8	10			
2	T	7	Total	C	N	O	0	0	0
			46	26	8	12			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



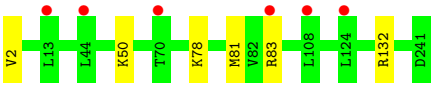
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C N O 14 8 1 5	0	0
3	P	1	Total C N O 14 8 1 5	0	0
3	T	1	Total C N O 14 8 1 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

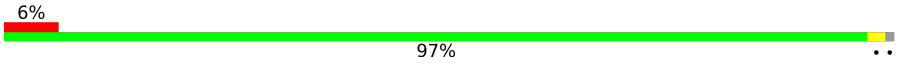
• Molecule 1: 14-3-3 protein gamma

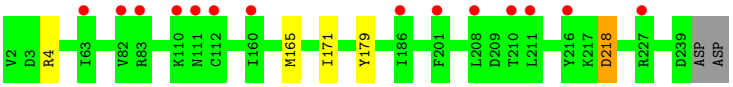
Chain A:



• Molecule 1: 14-3-3 protein gamma

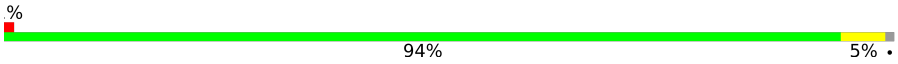
Chain B:





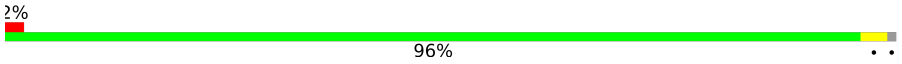
• Molecule 1: 14-3-3 protein gamma

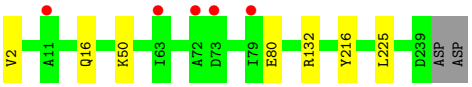
Chain C:



• Molecule 1: 14-3-3 protein gamma

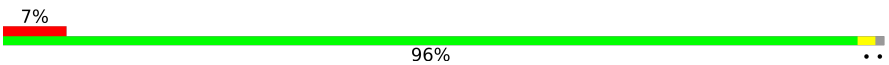
Chain D:

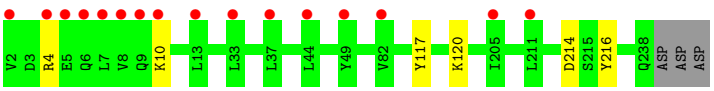




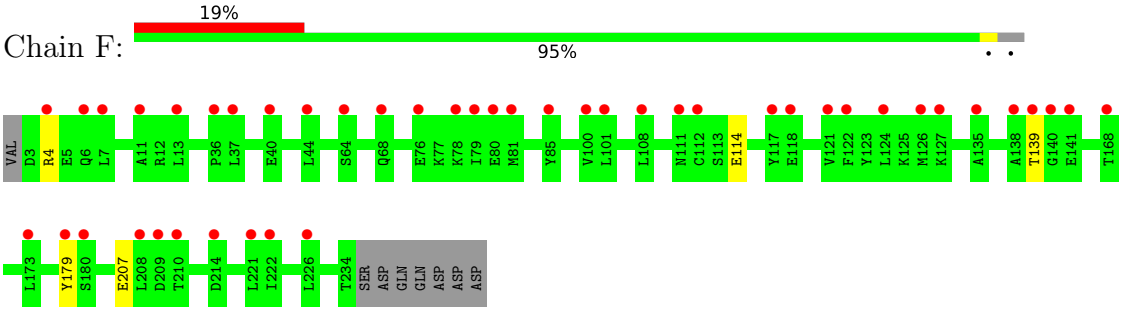
• Molecule 1: 14-3-3 protein gamma

Chain E:

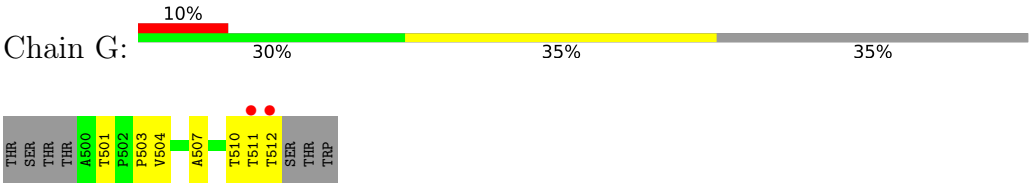




• Molecule 1: 14-3-3 protein gamma



• Molecule 2: TSTTATPPVSQASSTTTSTW O-GlcNac peptide



• Molecule 2: TSTTATPPVSQASSTTTSTW O-GlcNac peptide

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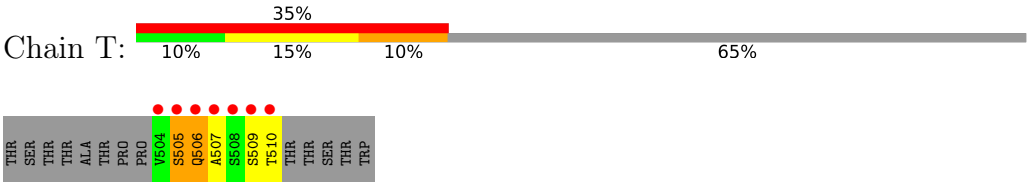

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	122.27Å 122.27Å 314.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.94 – 2.90 113.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (113.94-2.90) 100.0 (113.94-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.228 , 0.269 0.235 , 0.274	Depositor DCC
R_{free} test set	2000 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å^2)	91.2	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22960	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: NAG

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	0.22	0/1967	0.36	0/2655
1	B	0.23	0/1951	0.38	0/2633
1	C	0.23	0/1951	0.37	0/2633
1	D	0.22	0/1951	0.36	0/2633
1	E	0.22	0/1943	0.35	0/2622
1	F	0.22	0/1904	0.37	0/2569
2	G	0.34	0/87	0.53	0/121
2	P	0.25	0/48	0.42	0/65
2	T	0.53	0/45	0.62	0/60
All	All	0.22	0/11847	0.37	0/15991

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1939	1887	1891	4	0
1	B	1923	1879	1883	2	0
1	C	1923	1879	1883	5	1
1	D	1923	1879	1883	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1915	1875	1879	0	0
1	F	1876	1841	1845	0	1
2	G	86	0	82	5	0
2	P	47	0	45	3	0
2	T	46	0	42	7	0
3	G	14	0	13	8	0
3	P	14	0	13	4	0
3	T	14	0	13	6	0
All	All	11720	11240	11472	27	1

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 1.

All (27) 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)
2:G:507:ALA:HB2	3:G:601:NAG:H82	1.33	1.07
2:T:507:ALA:HB2	3:T:601:NAG:H83	1.56	0.88
2:P:507:ALA:HB2	3:P:601:NAG:H81	1.54	0.88
2:G:507:ALA:HB2	3:G:601:NAG:C8	2.05	0.87
2:G:507:ALA:CB	3:G:601:NAG:H82	2.12	0.77
2:T:507:ALA:HB2	3:T:601:NAG:C8	2.18	0.73
2:P:507:ALA:HB2	3:P:601:NAG:C8	2.22	0.70
1:C:57:ARG:NH2	1:C:136:GLU:OE1	2.34	0.60
1:C:43:ASN:HB2	2:T:509:SER:HB3	1.84	0.59
2:T:505:SER:HB2	3:T:601:NAG:N2	2.17	0.59
1:D:225:LEU:HD22	2:P:504:VAL:HG21	1.85	0.58
2:T:505:SER:HB2	3:T:601:NAG:HN2	1.68	0.58
1:C:4:ARG:NH2	1:C:41:GLU:OE1	2.37	0.57
1:C:132:ARG:HH22	3:T:601:NAG:H2	1.70	0.56
1:D:50:LYS:HD3	3:P:601:NAG:H83	1.88	0.55
1:D:132:ARG:HH12	3:P:601:NAG:H4	1.72	0.54
1:A:132:ARG:NH2	3:G:601:NAG:O3	2.44	0.50
2:G:511:THR:O	2:G:512:THR:OG1	2.27	0.50
2:G:503:PRO:HD2	3:G:601:NAG:O6	2.12	0.48
1:C:34:ASN:OD1	1:C:111:ASN:ND2	2.47	0.47
1:A:50:LYS:HD3	3:G:601:NAG:H83	1.98	0.45
2:T:506:GLN:HG2	2:T:507:ALA:N	2.30	0.45
1:B:218:ASP:N	1:B:218:ASP:OD1	2.50	0.44
1:A:132:ARG:NH1	3:G:601:NAG:O4	2.50	0.42
1:B:165:MET:HE1	1:B:171:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HH12	3:G:601:NAG:C4	2.32	0.41
2:T:505:SER:CB	3:T:601:NAG:N2	2.84	0.40

All (1) 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)
1:C:114:GLU:OE2	1:F:139:THR:OG1[3_555]	2.19	0.01

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	238/240 (99%)	233 (98%)	5 (2%)	0	100	100
1	B	236/240 (98%)	230 (98%)	6 (2%)	0	100	100
1	C	236/240 (98%)	230 (98%)	6 (2%)	0	100	100
1	D	236/240 (98%)	225 (95%)	11 (5%)	0	100	100
1	E	235/240 (98%)	227 (97%)	8 (3%)	0	100	100
1	F	230/240 (96%)	222 (96%)	8 (4%)	0	100	100
2	G	11/20 (55%)	8 (73%)	3 (27%)	0	100	100
2	P	5/20 (25%)	5 (100%)	0	0	100	100
2	T	5/20 (25%)	3 (60%)	2 (40%)	0	100	100
All	All	1432/1500 (96%)	1383 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	212/212 (100%)	208 (98%)	4 (2%)	57 84
1	B	210/212 (99%)	207 (99%)	3 (1%)	67 89
1	C	210/212 (99%)	207 (99%)	3 (1%)	67 89
1	D	210/212 (99%)	206 (98%)	4 (2%)	57 84
1	E	209/212 (99%)	203 (97%)	6 (3%)	42 76
1	F	204/212 (96%)	200 (98%)	4 (2%)	55 82
2	G	11/18 (61%)	8 (73%)	3 (27%)	0 1
2	P	6/18 (33%)	6 (100%)	0	100 100
2	T	6/18 (33%)	3 (50%)	3 (50%)	0 0
All	All	1278/1326 (96%)	1248 (98%)	30 (2%)	50 80

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	78	LYS
1	A	81	MET
1	A	83	ARG
1	B	4	ARG
1	B	179	TYR
1	B	218	ASP
1	C	68	GLN
1	C	179	TYR
1	C	237	GLN
1	D	2	VAL
1	D	16	GLN
1	D	80	GLU
1	D	216	TYR
1	E	4	ARG
1	E	10	LYS
1	E	117	TYR
1	E	120	LYS

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Mol	Chain	Res	Type
1	E	214	ASP
1	E	216	TYR
1	F	4	ARG
1	F	114	GLU
1	F	179	TYR
1	F	207	GLU
2	G	501	THR
2	G	504	VAL
2	G	510	THR
2	T	505	SER
2	T	506	GLN
2	T	510	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	158	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	NAG	P	601	2	14,14,15	0.33	0	17,19,21	0.35	0
3	NAG	G	601	2	14,14,15	0.33	0	17,19,21	0.43	0
3	NAG	T	601	2	14,14,15	0.60	0	17,19,21	0.63	1 (5%)

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	P	601	2	-	2/6/23/26	0/1/1/1
3	NAG	G	601	2	-	4/6/23/26	0/1/1/1
3	NAG	T	601	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	601	NAG	C1-O5-C5	2.03	114.95	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	601	NAG	C4-C5-C6-O6
3	P	601	NAG	O5-C5-C6-O6
3	T	601	NAG	C4-C5-C6-O6
3	T	601	NAG	O5-C5-C6-O6
3	G	601	NAG	C4-C5-C6-O6
3	G	601	NAG	O5-C5-C6-O6
3	G	601	NAG	C1-C2-N2-C7
3	G	601	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	601	NAG	4	0
3	G	601	NAG	8	0
3	T	601	NAG	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	240/240 (100%)	0.60	6 (2%) 57 55	52, 79, 143, 193	0
1	B	238/240 (99%)	0.66	14 (5%) 22 18	57, 91, 164, 208	0
1	C	238/240 (99%)	0.57	3 (1%) 77 77	55, 87, 142, 173	0
1	D	238/240 (99%)	0.51	5 (2%) 63 61	63, 99, 159, 205	0
1	E	237/240 (98%)	0.57	16 (6%) 17 13	79, 106, 157, 231	0
1	F	232/240 (96%)	1.11	45 (19%) 1 0	95, 161, 215, 282	0
2	G	13/20 (65%)	1.72	2 (15%) 2 1	84, 108, 139, 144	0
2	P	7/20 (35%)	2.65	5 (71%) 0 0	121, 126, 139, 142	0
2	T	7/20 (35%)	4.54	7 (100%) 0 0	135, 137, 145, 149	0
All	All	1450/1500 (96%)	0.71	103 (7%) 16 12	52, 100, 184, 282	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	THR	9.1
1	F	208	LEU	8.7
1	F	226	LEU	8.0
1	F	209	ASP	6.9
2	T	508	SER	6.8
2	G	512	THR	6.0
1	B	112	CYS	5.9
1	F	111	ASN	5.5
1	F	121	VAL	5.4
2	T	509	SER	5.3
1	F	112	CYS	5.3
1	F	117	TYR	5.1
1	F	135	ALA	5.0
1	F	140	GLY	4.7
1	B	111	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
2	T	507	ALA	4.6
1	E	9	GLN	4.6
1	C	72	ALA	4.6
1	F	80	GLU	4.6
2	P	504	VAL	4.5
1	F	44	LEU	4.5
1	F	4	ARG	4.4
1	E	4	ARG	4.4
2	T	504	VAL	4.3
1	F	76	GLU	4.3
2	P	505	SER	4.3
1	F	122	PHE	4.2
1	F	173	LEU	4.1
1	E	8	VAL	4.1
1	B	110	LYS	4.0
2	T	510	THR	3.9
1	F	124	LEU	3.9
1	F	141	GLU	3.8
1	A	70	THR	3.7
2	G	511	THR	3.7
1	E	13	LEU	3.6
2	T	506	GLN	3.6
1	F	222	ILE	3.5
1	B	216	TYR	3.5
2	P	503	PRO	3.4
2	T	505	SER	3.2
1	F	179	TYR	3.1
1	E	6	GLN	3.1
1	B	211	LEU	3.1
2	P	502	PRO	3.1
1	E	10	LYS	3.0
1	F	126	MET	3.0
1	F	85	TYR	3.0
1	F	68	GLN	2.9
1	F	221	LEU	2.9
1	F	180	SER	2.8
1	E	33	LEU	2.7
1	F	13	LEU	2.7
1	F	210	THR	2.6
1	F	108	LEU	2.6
1	F	118	GLU	2.6
1	E	7	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	36	PRO	2.6
1	F	138	ALA	2.6
1	B	82	VAL	2.6
1	F	127	LYS	2.6
1	A	44	LEU	2.5
1	F	79	ILE	2.5
1	F	139	THR	2.5
1	F	11	ALA	2.5
1	F	81	MET	2.5
1	F	168	THR	2.5
1	B	201	PHE	2.4
1	D	72	ALA	2.4
1	F	6	GLN	2.4
1	F	40	GLU	2.4
1	E	2	VAL	2.4
2	P	508	SER	2.4
1	E	44	LEU	2.4
1	D	73	ASP	2.3
1	E	5	GLU	2.3
1	B	208	LEU	2.3
1	A	13	LEU	2.3
1	F	101	LEU	2.3
1	D	63	ILE	2.3
1	E	211	LEU	2.3
1	C	160	ILE	2.2
1	F	100	VAL	2.2
1	F	64	SER	2.2
1	B	63	ILE	2.2
1	A	124	LEU	2.2
1	F	214	ASP	2.1
1	B	83	ARG	2.1
1	C	13	LEU	2.1
1	E	37	LEU	2.1
1	F	78	LYS	2.1
1	E	49	TYR	2.1
1	D	11	ALA	2.1
1	D	79	ILE	2.1
1	E	205	ILE	2.1
1	A	108	LEU	2.1
1	A	83	ARG	2.1
1	B	160	ILE	2.1
1	B	227	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	186	ILE	2.0
1	E	82	VAL	2.0
1	F	7	LEU	2.0
1	F	37	LEU	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	T	601	14/15	0.71	0.46	105,130,144,162	0
3	NAG	P	601	14/15	0.72	0.77	111,130,148,151	0
3	NAG	G	601	14/15	0.77	0.40	73,103,134,149	0

6.5 Other polymers (i)

There are no such residues in this entry.