W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 08:48 PM GMT

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PDB ID	:	4Z0C
Title	:	Crystal structure of TLR13-ssRNA13 complex
Authors	:	Song, W.; Han, Z.; Chai, J.
Deposited on	:	2015-03-26
Resolution	:	2.30 Å(reported)

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
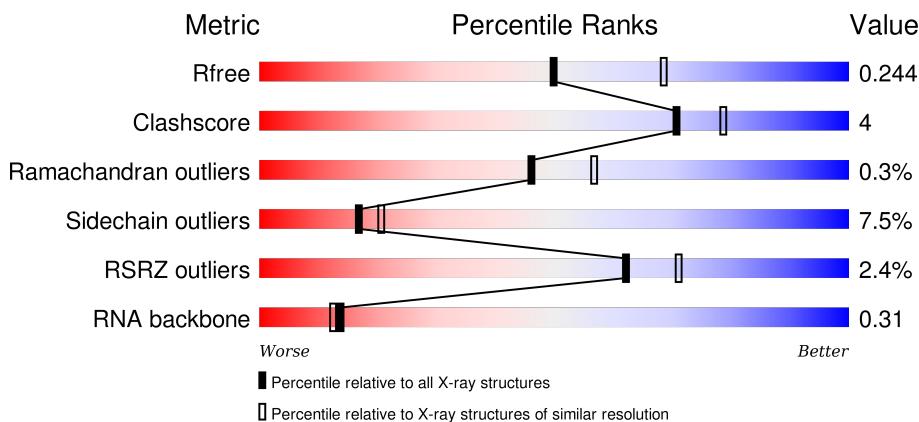
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)
RNA backbone	2183	1011 (2.84-1.76)

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 <=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	709	
1	D	709	
2	B	13	
2	C	13	
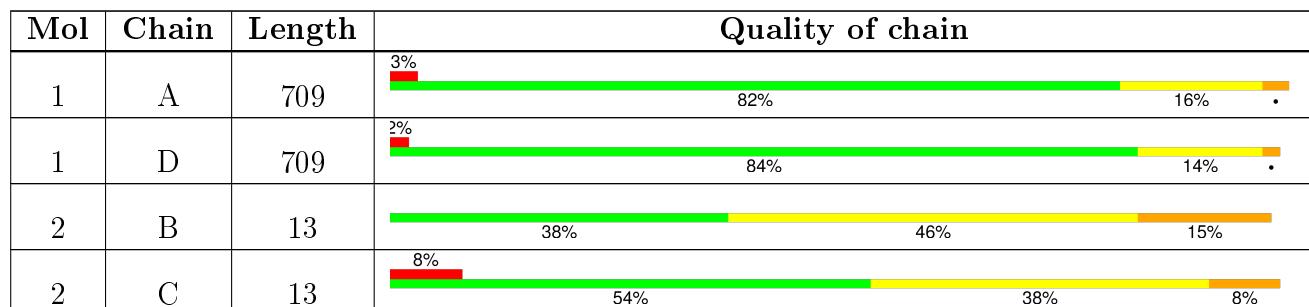
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	905	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12821 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 Toll-like receptor 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	709	Total	C	N	O	S	0	0	0
			5724	3672	984	1048	20			
1	D	709	Total	C	N	O	S	0	0	0
			5730	3675	987	1048	20			

- Molecule 2 is a RNA chain called DNA (5'-R(P*AP*CP*GP*GP*AP*AP*AP*GP*AP*CP *CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			279	125	55	86	13			
2	C	13	Total	C	N	O	P	0	0	0
			279	125	55	86	13			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
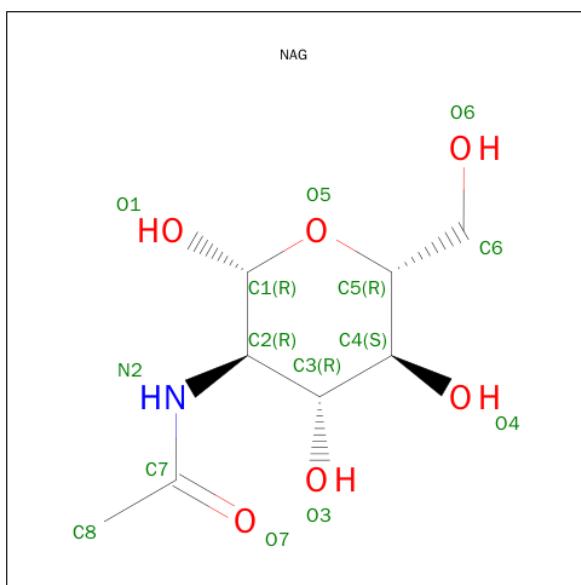
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0
3	D	1	Total 14	C 8	N 1	O 5	0	0

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total 117	O 117	0	0
4	D	207	Total 207	O 207	0	0
4	B	18	Total 18	O 18	0	0
4	C	19	Total 19	O 19	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Toll-like receptor 13
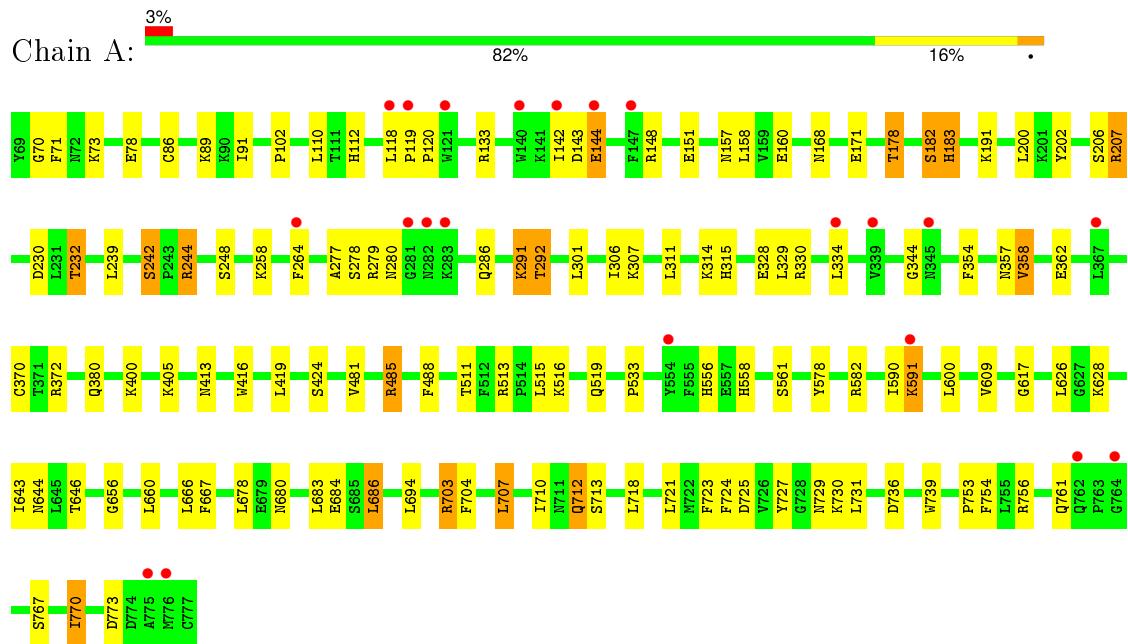

- Molecule 1: Toll-like receptor 13
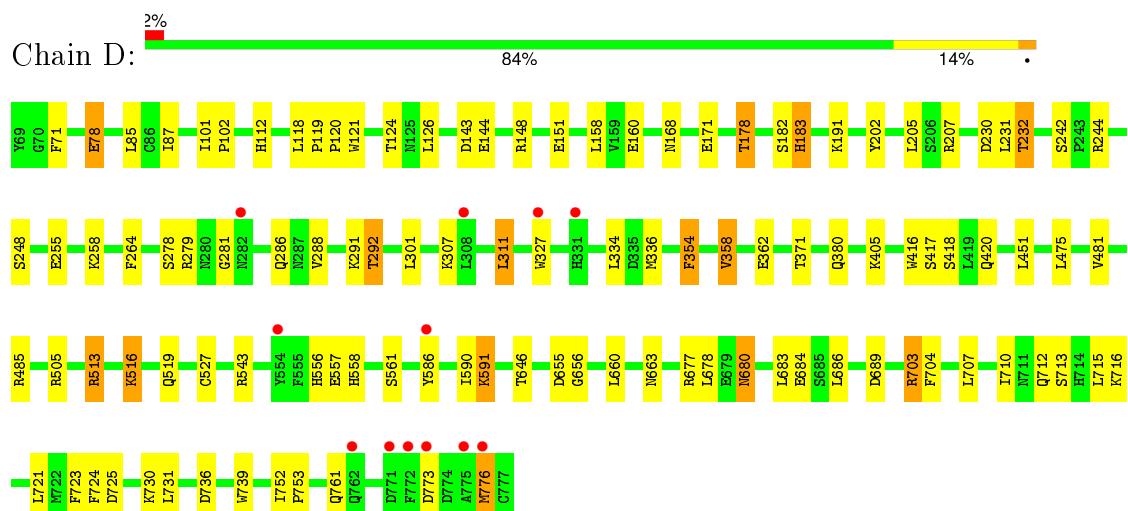
- Molecule 2: DNA (5'-R(P*AP*CP*GP*GP*AP*AP*AP*GP*AP*CP*CP*CP*C)-3')

Chain B:

• Molecule 2: DNA (5'-R(P*AP*CP*GP*GP*AP*AP*AP*GP*AP*CP*CP*CP*C)-3')

Chain C:
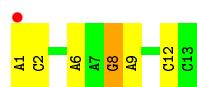
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.55Å 115.21Å 167.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 2.30 45.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (45.90-2.30) 92.4 (45.90-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.244 0.192 , 0.244	Depositor DCC
R_{free} test set	4484 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.989	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.6	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 89721 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12821	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/5845	0.61	1/7918 (0.0%)
1	D	0.45	0/5851	0.62	0/7925
2	B	0.68	0/312	1.21	1/484 (0.2%)
2	C	0.61	0/312	1.35	1/484 (0.2%)
All	All	0.45	0/12320	0.67	3/16811 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	8	G	O4'-C1'-N9	6.81	113.65	108.20
2	B	2	C	P-O3'-C3'	5.72	126.56	119.70
1	A	70	GLY	N-CA-C	-5.37	99.68	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5724	0	5782	61	0
1	D	5730	0	5789	46	0
2	B	279	0	144	3	0
2	C	279	0	144	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	210	0	192	5	0
3	D	238	0	218	3	0
4	A	117	0	0	3	0
4	B	18	0	0	0	0
4	C	19	0	0	0	0
4	D	207	0	0	6	0
All	All	12821	0	12269	108	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 4.

The worst 5 of 108 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:279:ARG:NH1	4:A:1001:HOH:O	2.11	0.82
1:D:689:ASP:OD1	1:D:716:LYS:NZ	2.13	0.81
1:D:148:ARG:NH1	1:D:171:GLU:HG2	1.97	0.80
1:A:556:HIS:CD2	1:A:558:HIS:H	2.01	0.78
3:D:917:NAG:O4	4:D:1001:HOH:O	2.04	0.75

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	707/709 (100%)	657 (93%)	48 (7%)	2 (0%)	46	57
1	D	707/709 (100%)	650 (92%)	55 (8%)	2 (0%)	46	57
All	All	1414/1418 (100%)	1307 (92%)	103 (7%)	4 (0%)	46	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	773	ASP
1	A	656	GLY
1	D	656	GLY
1	A	773	ASP

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	662/663 (100%)	610 (92%)	52 (8%)	15	19
1	D	663/663 (100%)	615 (93%)	48 (7%)	18	22
All	All	1325/1326 (100%)	1225 (92%)	100 (8%)	17	21

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	718	LEU
1	D	151	GLU
1	D	710	ILE
1	A	730	LYS
1	A	767	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	556	HIS
1	A	597	GLN
1	D	556	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	13/13 (100%)	5 (38%)	2 (15%)
2	C	13/13 (100%)	3 (23%)	2 (15%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	26/26 (100%)	8 (30%)	4 (15%)

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	C
2	B	3	G
2	B	9	A
2	B	12	C
2	B	13	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1	A
2	B	2	C
2	C	1	A
2	C	8	G

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

32 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	A	901	1,3	14,14,15	0.83	1 (7%)	15,19,21	1.12	1 (6%)
3	NAG	A	902	3	14,14,15	0.54	0	15,19,21	1.34	1 (6%)
3	NAG	A	903	1	14,14,15	0.44	0	15,19,21	1.55	2 (13%)
3	NAG	A	904	1	14,14,15	0.60	0	15,19,21	0.70	0
3	NAG	A	905	1	14,14,15	0.45	0	15,19,21	1.31	1 (6%)
3	NAG	A	906	1	14,14,15	0.48	0	15,19,21	1.26	2 (13%)
3	NAG	A	907	1,3	14,14,15	0.56	0	15,19,21	1.60	3 (20%)
3	NAG	A	908	3	14,14,15	0.50	0	15,19,21	1.02	1 (6%)
3	NAG	A	909	-	14,14,15	0.75	1 (7%)	15,19,21	1.21	3 (20%)
3	NAG	A	910	1	14,14,15	0.44	0	15,19,21	1.47	1 (6%)
3	NAG	A	911	1	14,14,15	0.57	0	15,19,21	0.97	0
3	NAG	A	912	1,3	14,14,15	0.63	0	15,19,21	1.17	1 (6%)
3	NAG	A	913	3	14,14,15	0.52	0	15,19,21	1.17	3 (20%)
3	NAG	A	914	-	14,14,15	0.47	0	15,19,21	0.96	0
3	NAG	A	915	1	14,14,15	0.46	0	15,19,21	0.81	0
3	NAG	D	901	1,3	14,14,15	0.63	0	15,19,21	0.77	0
3	NAG	D	902	3	14,14,15	0.69	0	15,19,21	1.53	3 (20%)
3	NAG	D	903	1	14,14,15	0.56	0	15,19,21	0.93	1 (6%)
3	NAG	D	904	1	14,14,15	0.48	0	15,19,21	1.19	1 (6%)
3	NAG	D	905	1	14,14,15	0.62	0	15,19,21	1.13	1 (6%)
3	NAG	D	906	1,3	14,14,15	0.50	0	15,19,21	0.90	0
3	NAG	D	907	3	14,14,15	0.59	0	15,19,21	0.98	1 (6%)
3	NAG	D	908	1	14,14,15	0.59	0	15,19,21	1.30	2 (13%)
3	NAG	D	909	1	14,14,15	0.59	0	15,19,21	1.68	2 (13%)
3	NAG	D	910	1,3	14,14,15	0.68	0	15,19,21	1.68	3 (20%)
3	NAG	D	911	3	14,14,15	0.59	0	15,19,21	1.05	1 (6%)
3	NAG	D	912	1	14,14,15	0.55	0	15,19,21	1.03	1 (6%)
3	NAG	D	913	1	14,14,15	0.50	0	15,19,21	1.03	1 (6%)
3	NAG	D	914	1	14,14,15	0.47	0	15,19,21	0.84	0
3	NAG	D	915	1	14,14,15	0.62	0	15,19,21	1.54	2 (13%)
3	NAG	D	916	1	14,14,15	0.58	0	15,19,21	1.16	1 (6%)
3	NAG	D	917	1	14,14,15	0.47	0	15,19,21	1.28	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	902	3	-	0/6/23/26	0/1/1/1
3	NAG	A	903	1	-	0/6/23/26	0/1/1/1
3	NAG	A	904	1	-	0/6/23/26	0/1/1/1
3	NAG	A	905	1	-	0/6/23/26	0/1/1/1
3	NAG	A	906	1	-	0/6/23/26	0/1/1/1
3	NAG	A	907	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	908	3	-	0/6/23/26	0/1/1/1
3	NAG	A	909	-	-	0/6/23/26	0/1/1/1
3	NAG	A	910	1	-	0/6/23/26	0/1/1/1
3	NAG	A	911	1	-	0/6/23/26	0/1/1/1
3	NAG	A	912	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	913	3	-	0/6/23/26	0/1/1/1
3	NAG	A	914	-	-	0/6/23/26	0/1/1/1
3	NAG	A	915	1	-	0/6/23/26	0/1/1/1
3	NAG	D	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	902	3	-	0/6/23/26	0/1/1/1
3	NAG	D	903	1	-	0/6/23/26	0/1/1/1
3	NAG	D	904	1	-	0/6/23/26	0/1/1/1
3	NAG	D	905	1	-	0/6/23/26	0/1/1/1
3	NAG	D	906	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	907	3	-	0/6/23/26	0/1/1/1
3	NAG	D	908	1	-	0/6/23/26	0/1/1/1
3	NAG	D	909	1	-	0/6/23/26	0/1/1/1
3	NAG	D	910	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	911	3	-	0/6/23/26	0/1/1/1
3	NAG	D	912	1	-	0/6/23/26	0/1/1/1
3	NAG	D	913	1	-	0/6/23/26	0/1/1/1
3	NAG	D	914	1	-	0/6/23/26	0/1/1/1
3	NAG	D	915	1	-	0/6/23/26	0/1/1/1
3	NAG	D	916	1	-	0/6/23/26	0/1/1/1
3	NAG	D	917	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	909	NAG	O5-C1	-2.04	1.40	1.43
3	A	901	NAG	C1-C2	2.14	1.55	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	909	NAG	C2-N2-C7	-4.67	117.03	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	910	NAG	C3-C4-C5	-4.34	102.50	110.23
3	D	915	NAG	C2-N2-C7	-4.11	117.76	123.11
3	A	907	NAG	C2-N2-C7	-3.87	118.07	123.11
3	D	908	NAG	C2-N2-C7	-3.16	119.00	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	904	NAG	1	0
3	A	909	NAG	2	0
3	A	912	NAG	1	0
3	A	914	NAG	1	0
3	D	901	NAG	1	0
3	D	906	NAG	1	0
3	D	917	NAG	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	709/709 (100%)	0.14	21 (2%)	54	63	15, 38, 64, 121	0
1	D	709/709 (100%)	0.04	12 (1%)	73	79	15, 31, 57, 105	0
2	B	13/13 (100%)	-0.05	0	100	100	27, 34, 55, 71	0
2	C	13/13 (100%)	-0.45	1 (7%)	16	23	29, 32, 54, 72	0
All	All	1444/1444 (100%)	0.08	34 (2%)	62	71	15, 34, 62, 121	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	GLY	4.8
1	D	554	TYR	4.3
1	A	339	VAL	3.9
1	D	776	MET	3.8
1	A	282	ASN	3.8

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(Å²)	Q<0.9
3	NAG	D	905	14/15	0.88	0.19	4.61	24,40,50,57	0
3	NAG	D	908	14/15	0.86	0.17	1.42	52,62,76,77	0
3	NAG	D	914	14/15	0.95	0.16	0.71	23,31,35,40	0
3	NAG	A	905	14/15	0.85	0.17	0.54	28,44,55,61	0
3	NAG	A	904	14/15	0.94	0.24	0.50	46,56,64,64	0
3	NAG	A	913	14/15	0.86	0.15	0.42	33,40,45,51	0
3	NAG	A	909	14/15	0.84	0.17	0.31	34,54,61,61	0
3	NAG	D	909	14/15	0.93	0.14	0.28	26,32,38,40	0
3	NAG	A	901	14/15	0.97	0.13	0.01	27,33,38,39	0
3	NAG	D	902	14/15	0.91	0.12	-0.06	23,30,35,35	0
3	NAG	A	907	14/15	0.95	0.13	-0.31	19,31,45,56	0
3	NAG	D	912	14/15	0.94	0.13	-0.42	26,36,45,47	0
3	NAG	D	910	14/15	0.95	0.11	-0.54	18,27,39,43	0
3	NAG	D	901	14/15	0.98	0.11	-0.77	15,25,32,34	0
3	NAG	A	902	14/15	0.90	0.12	-1.68	29,35,38,39	0
3	NAG	D	906	14/15	0.97	0.10	-2.61	24,33,45,48	0
3	NAG	A	906	14/15	0.92	0.10	-3.08	38,46,51,53	0
3	NAG	A	910	14/15	0.83	0.21	-	40,57,65,69	0
3	NAG	A	914	14/15	0.78	0.15	-	63,73,82,83	0
3	NAG	D	916	14/15	0.87	0.20	-	63,71,87,89	0
3	NAG	A	912	14/15	0.94	0.10	-	28,34,41,42	0
3	NAG	A	915	14/15	0.76	0.42	-	68,73,80,82	0
3	NAG	D	907	14/15	0.87	0.15	-	33,47,53,59	0
3	NAG	A	908	14/15	0.91	0.13	-	44,51,60,66	0
3	NAG	D	917	14/15	0.92	0.13	-	39,49,57,62	0
3	NAG	D	915	14/15	0.94	0.10	-	16,39,45,52	0
3	NAG	A	903	14/15	0.82	0.11	-	62,70,82,82	0
3	NAG	D	913	14/15	0.88	0.12	-	35,55,65,73	0
3	NAG	D	904	14/15	0.87	0.13	-	41,61,67,75	0
3	NAG	D	911	14/15	0.91	0.14	-	42,49,61,65	0
3	NAG	D	903	14/15	0.85	0.15	-	51,63,71,74	0
3	NAG	A	911	14/15	0.94	0.14	-	46,54,57,63	0

6.5 Other polymers (i)

There are no such residues in this entry.