



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:04 am GMT

PDB ID : 4R07  
Title : Crystal structure of human TLR8 in complex with ORN06  
Authors : Tanji, H.; Ohto, U.; Shibata, T.; Taoka, M.; Yamauchi, Y.; Isobe, T.; Miyake, K.; Shimizu, T.  
Deposited on : 2014-07-30  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

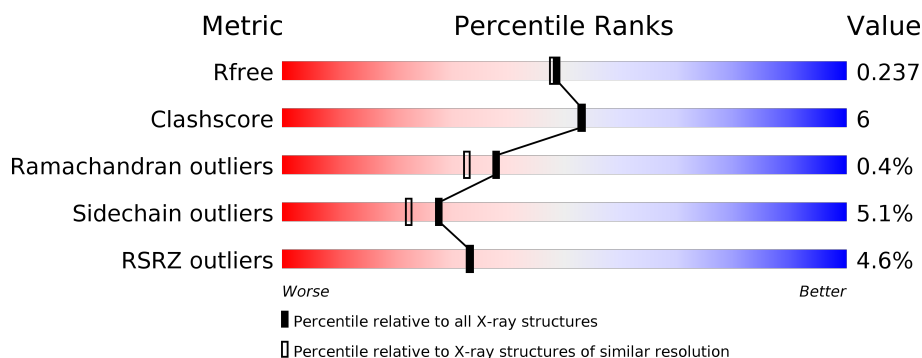
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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  $\geq 3$ , 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	811	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	811	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	811	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	811	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>•</div> <div>9%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	C	910	-	-	-	X
6	NAG	C	915	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26233 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 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			6014	3847	1019	1129	19			
1	B	738	Total	C	N	O	S	0	0	0
			5949	3808	1009	1113	19			
1	C	738	Total	C	N	O	S	0	0	0
			5946	3806	1007	1114	19			
1	D	735	Total	C	N	O	S	0	0	0
			5925	3794	1004	1108	19			

There are 40 discrepancies between the modelled and reference sequences:

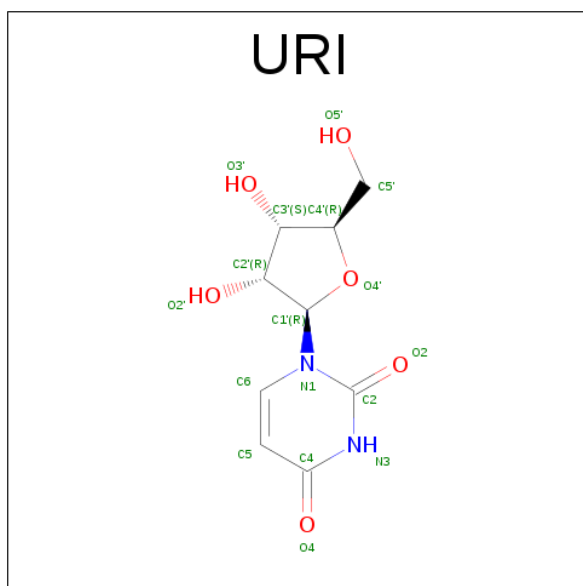
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	23	SER	-	EXPRESSION TAG	UNP Q9NR97
A	24	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	25	TRP	-	EXPRESSION TAG	UNP Q9NR97
A	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
A	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
A	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
A	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
A	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	22	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	23	SER	-	EXPRESSION TAG	UNP Q9NR97
B	24	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	25	TRP	-	EXPRESSION TAG	UNP Q9NR97
B	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
B	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
B	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
B	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
B	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
C	22	ARG	-	EXPRESSION TAG	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
C	23	SER	-	EXPRESSION TAG	UNP Q9NR97
C	24	PRO	-	EXPRESSION TAG	UNP Q9NR97
C	25	TRP	-	EXPRESSION TAG	UNP Q9NR97
C	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
C	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
C	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
C	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
C	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
C	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	22	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	23	SER	-	EXPRESSION TAG	UNP Q9NR97
D	24	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	25	TRP	-	EXPRESSION TAG	UNP Q9NR97
D	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
D	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
D	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
D	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
D	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	833	ARG	-	EXPRESSION TAG	UNP Q9NR97

- Molecule 2 is URIDINE (three-letter code: URI) (formula: C<sub>9</sub>H<sub>12</sub>N<sub>2</sub>O<sub>6</sub>).



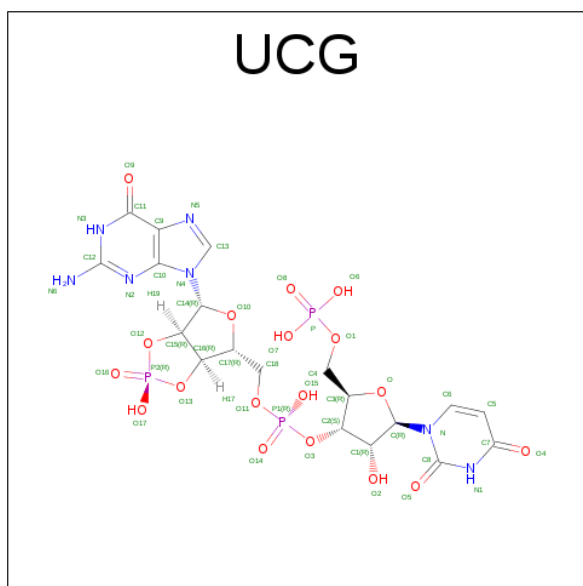
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	9	2	6		
2	B	1	Total	C	N	O	0	0
			17	9	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			17	9	2	6		
2	D	1	Total	C	N	O	0	0
			17	9	2	6		

- Molecule 3 is 3'-O-[(R)-{[(2R,3AR,4R,6R,6AR)-6-(2-AMINO-6-OXO-1,6-DIHYDRO-9H-PURIN-9-YL)-2-HYDROXY-2-OXIDOTETRAHYDROFURO[3,4-D][1,3,2]DIOXAPHOSPHOL-4-YL]METHOXY}(HYDROXY)PHOSPHORYL]URIDINE 5'-(DIHYDROGEN PHOSPHATE) (three-letter code: UCG) (formula: C<sub>19</sub>H<sub>24</sub>N<sub>7</sub>O<sub>18</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			47	19	7	18	3		
3	B	1	Total	C	N	O	P	0	0
			47	19	7	18	3		
3	C	1	Total	C	N	O	P	0	0
			47	19	7	18	3		
3	D	1	Total	C	N	O	P	0	0
			47	19	7	18	3		

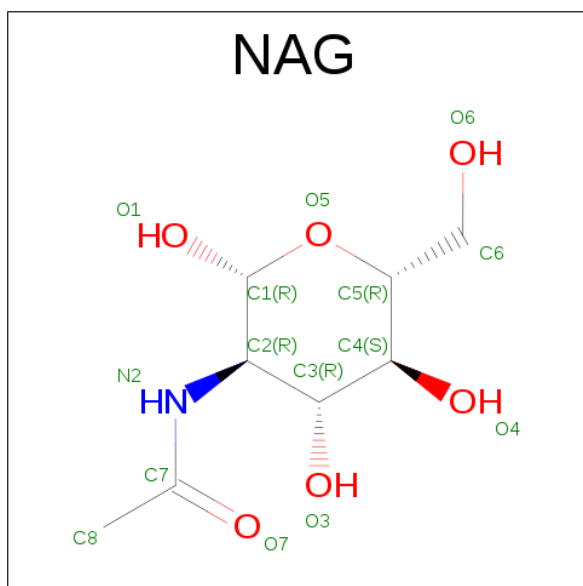
- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	3	Total	C	N	O	0	0
			39	22	2	15		
8	B	3	Total	C	N	O	0	0
			39	22	2	15		
8	C	3	Total	C	N	O	0	0
			39	22	2	15		
8	C	3	Total	C	N	O	0	0
			39	22	2	15		
8	D	3	Total	C	N	O	0	0
			39	22	2	15		

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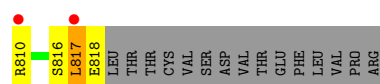
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	3	Total	C	N	O	0	0
			39	22	2	15		

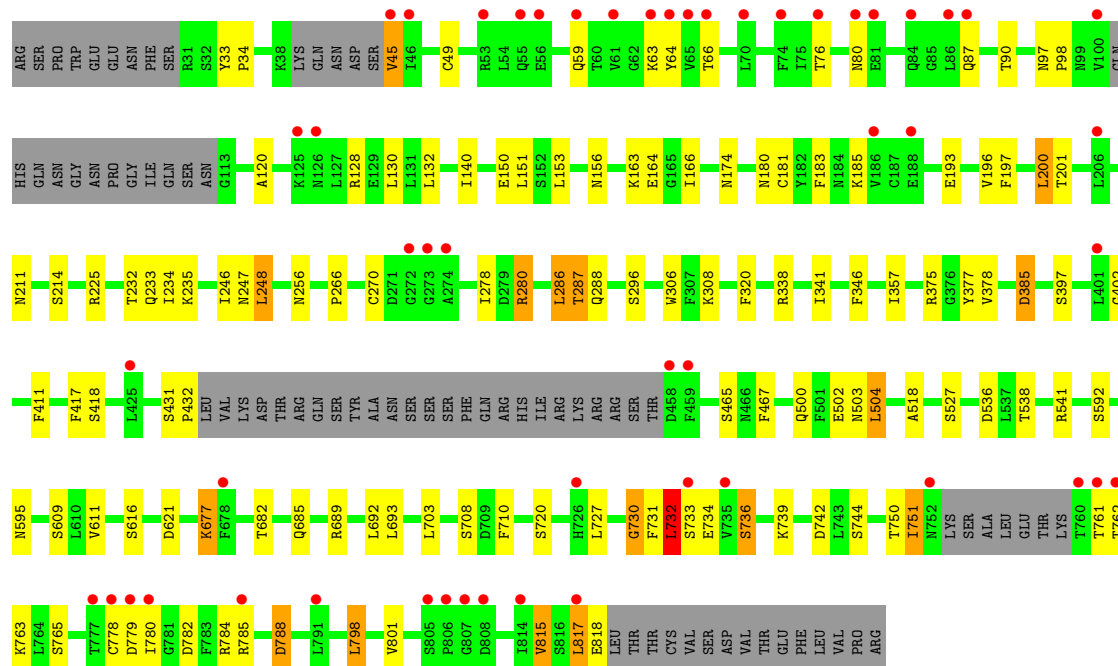
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	469	Total	O	0	0
			469	469		
9	B	374	Total	O	0	0
			374	374		
9	C	314	Total	O	0	0
			314	314		
9	D	277	Total	O	0	0
			277	277		

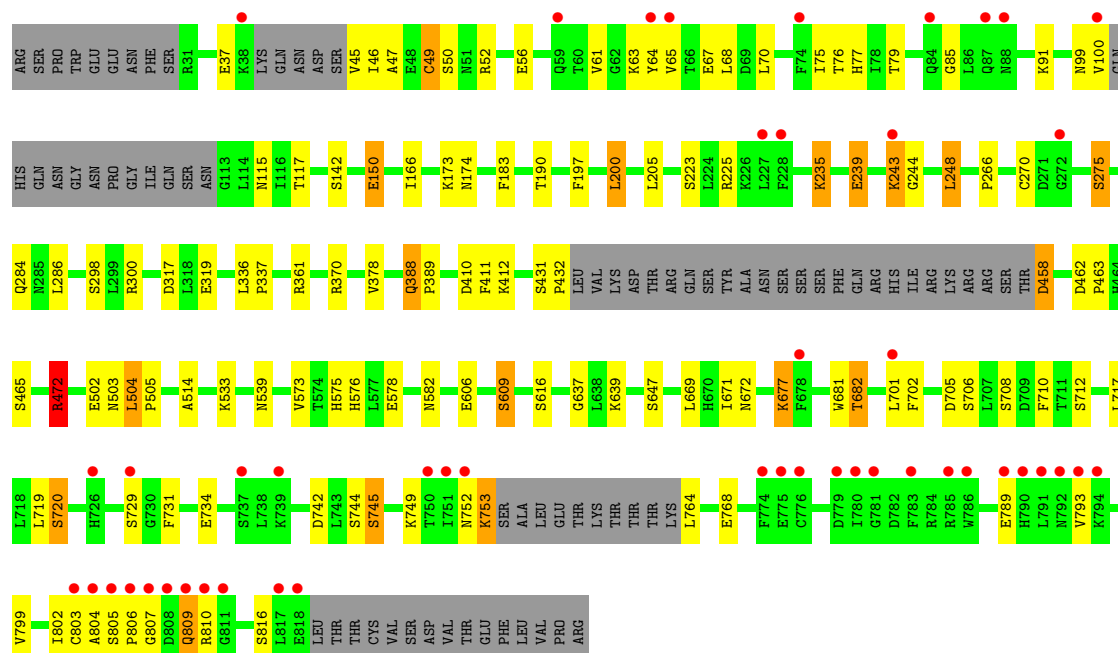
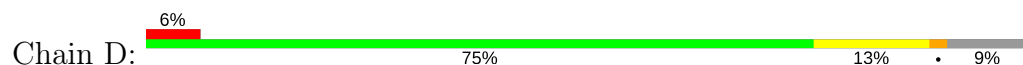




• Molecule 1: Toll-like receptor 8



• Molecule 1: Toll-like receptor 8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.66Å 141.12Å 169.53Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	33.74 – 2.00 33.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (33.74-2.00) 97.5 (33.74-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.188 , 0.234 0.195 , 0.237	Depositor DCC
$R_{free}$ test set	13522 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: UCG, MAN, BMA, NAG, URI

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	0.60	0/6138	0.69	0/8326
1	B	0.57	0/6072	0.71	3/8234 (0.0%)
1	C	0.54	0/6069	0.66	1/8232 (0.0%)
1	D	0.53	0/6048	0.64	1/8202 (0.0%)
All	All	0.56	0/24327	0.68	5/32994 (0.0%)

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
1	B	0	3
1	C	0	4
1	D	0	1
All	All	0	9

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	ASP	CB-CG-OD1	6.22	123.89	118.30
1	C	621	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	472	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	805	SER	C-N-CD	-5.03	109.54	120.60
1	B	300	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	SER	Peptide
1	B	734	GLU	Peptide
1	B	85	GLY	Peptide
1	B	99	ASN	Peptide
1	C	45	VAL	Peptide

## 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	6014	0	5989	68	0
1	B	5949	0	5920	70	1
1	C	5946	0	5916	84	0
1	D	5925	0	5895	75	0
2	A	17	0	12	1	0
2	B	17	0	12	1	0
2	C	17	0	12	1	0
2	D	17	0	12	1	0
3	A	47	0	20	4	0
3	B	47	0	20	6	0
3	C	47	0	20	5	0
3	D	47	0	20	1	0
4	A	50	0	43	1	0
4	C	50	0	43	1	0
5	A	39	0	34	0	0
6	A	70	0	65	0	0
6	B	70	0	65	1	0
6	C	56	0	52	0	0
6	D	56	0	52	2	0
7	A	28	0	25	0	0
7	B	28	0	25	0	0
7	D	28	0	25	0	0
8	B	78	0	68	0	0
8	C	78	0	68	0	0
8	D	78	0	68	1	0
9	A	469	0	0	11	0
9	B	374	0	0	11	0
9	C	314	0	0	14	0
9	D	277	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	26233	0	24481	304	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 6.

The worst 5 of 304 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:D:75:ILE:HG22	9:D:1225:HOH:O	1.52	1.09
1:A:33:TYR:O	1:A:60:THR:HG21	1.59	1.02
1:A:33:TYR:O	1:A:60:THR:CG2	2.11	0.96
1:D:77:HIS:N	9:D:1225:HOH:O	2.00	0.92
1:B:708:SER:HB3	1:B:735:VAL:HG22	1.52	0.90

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:B:280:ARG:NH1	1:B:709:ASP:OD2[1_455]	2.03	0.17

## 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	739/811 (91%)	700 (95%)	37 (5%)	2 (0%)	44	40
1	B	728/811 (90%)	678 (93%)	47 (6%)	3 (0%)	38	33
1	C	728/811 (90%)	665 (91%)	59 (8%)	4 (0%)	32	26
1	D	725/811 (89%)	668 (92%)	53 (7%)	4 (1%)	28	21
All	All	2920/3244 (90%)	2711 (93%)	196 (7%)	13 (0%)	38	33

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	736	SER
1	C	378	VAL
1	D	243	LYS
1	B	284	GLN
1	C	732	LEU

### 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	693/755 (92%)	658 (95%)	35 (5%)	28	22
1	B	685/755 (91%)	649 (95%)	36 (5%)	26	21
1	C	685/755 (91%)	651 (95%)	34 (5%)	28	23
1	D	682/755 (90%)	646 (95%)	36 (5%)	26	21
All	All	2745/3020 (91%)	2604 (95%)	141 (5%)	28	22

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	750	THR
1	C	246	ILE
1	D	681	TRP
1	B	779	ASP
1	C	49	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	288	GLN
1	D	809	GLN
1	D	123	ASN
1	B	135	ASN
1	D	686	GLN



### 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 ⓘ

35 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	$\# Z  > 2$
4	NAG	A	903	1,4	14,14,15	0.82	1 (7%)	15,19,21	1.29	2 (13%)
4	NAG	A	904	4	14,14,15	0.75	1 (7%)	15,19,21	1.56	3 (20%)
4	BMA	A	905	4	11,11,12	0.57	0	13,15,17	3.26	6 (46%)
4	MAN	A	906	4	11,11,12	0.78	0	13,15,17	1.39	3 (23%)
5	BMA	A	907	5	11,11,12	0.54	0	13,15,17	0.81	0
5	NAG	A	908	1,5	14,14,15	0.98	1 (7%)	15,19,21	1.06	1 (6%)
5	NAG	A	909	5	14,14,15	0.82	0	15,19,21	1.67	3 (20%)
7	NAG	A	911	1,7	14,14,15	0.96	1 (7%)	15,19,21	1.26	2 (13%)
7	NAG	A	912	7	14,14,15	0.79	1 (7%)	15,19,21	1.97	4 (26%)
8	NAG	B	903	1,8	14,14,15	0.66	0	15,19,21	1.61	3 (20%)
8	NAG	B	904	8	14,14,15	0.78	0	15,19,21	1.62	3 (20%)
8	BMA	B	905	8	11,11,12	0.70	0	13,15,17	1.61	3 (23%)
8	NAG	B	906	1,8	14,14,15	0.74	0	15,19,21	1.30	4 (26%)
8	NAG	B	907	8	14,14,15	1.01	1 (7%)	15,19,21	1.55	3 (20%)
8	BMA	B	908	8	11,11,12	0.28	0	13,15,17	0.95	1 (7%)
7	NAG	B	910	1,7	14,14,15	0.83	0	15,19,21	1.33	2 (13%)
7	NAG	B	911	7	14,14,15	0.79	1 (7%)	15,19,21	1.45	4 (26%)
4	NAG	C	903	1,4	14,14,15	1.08	1 (7%)	15,19,21	2.01	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	904	4	14,14,15	0.77	0	15,19,21	1.30	2 (13%)
4	BMA	C	905	4	11,11,12	0.33	0	13,15,17	1.30	2 (15%)
4	MAN	C	906	4	11,11,12	0.84	0	13,15,17	1.56	3 (23%)
8	NAG	C	907	1,8	14,14,15	0.49	0	15,19,21	1.11	1 (6%)
8	NAG	C	908	8	14,14,15	1.01	1 (7%)	15,19,21	1.26	0
8	BMA	C	909	8	11,11,12	0.44	0	13,15,17	1.08	1 (7%)
8	NAG	C	911	1,8	14,14,15	0.75	0	15,19,21	0.93	0
8	NAG	C	912	8	14,14,15	0.51	0	15,19,21	1.32	2 (13%)
8	BMA	C	913	8	11,11,12	0.56	0	13,15,17	1.13	0
8	NAG	D	903	1,8	14,14,15	0.77	0	15,19,21	2.27	5 (33%)
8	NAG	D	904	8	14,14,15	0.75	0	15,19,21	1.28	1 (6%)
8	BMA	D	905	8	11,11,12	0.60	0	13,15,17	2.35	6 (46%)
8	NAG	D	906	1,8	14,14,15	0.64	0	15,19,21	1.55	2 (13%)
8	NAG	D	907	8	14,14,15	1.09	1 (7%)	15,19,21	1.30	2 (13%)
8	BMA	D	908	8	11,11,12	0.50	0	13,15,17	0.74	0
7	NAG	D	910	1,7	14,14,15	1.24	2 (14%)	15,19,21	2.03	4 (26%)
7	NAG	D	911	7	14,14,15	0.68	1 (7%)	15,19,21	1.11	1 (6%)

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
4	NAG	A	903	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	904	4	-	0/6/23/26	0/1/1/1
4	BMA	A	905	4	-	0/2/19/22	0/1/1/1
4	MAN	A	906	4	-	0/2/19/22	0/1/1/1
5	BMA	A	907	5	-	0/2/19/22	0/1/1/1
5	NAG	A	908	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	909	5	-	0/6/23/26	0/1/1/1
7	NAG	A	911	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	912	7	-	0/6/23/26	0/1/1/1
8	NAG	B	903	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	904	8	-	0/6/23/26	0/1/1/1
8	BMA	B	905	8	-	0/2/19/22	0/1/1/1
8	NAG	B	906	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	907	8	-	0/6/23/26	0/1/1/1
8	BMA	B	908	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	910	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	911	7	-	0/6/23/26	0/1/1/1
4	NAG	C	903	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	904	4	-	0/6/23/26	0/1/1/1
4	BMA	C	905	4	-	0/2/19/22	0/1/1/1
4	MAN	C	906	4	-	0/2/19/22	0/1/1/1
8	NAG	C	907	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	908	8	-	0/6/23/26	0/1/1/1
8	BMA	C	909	8	-	0/2/19/22	0/1/1/1
8	NAG	C	911	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	912	8	-	0/6/23/26	0/1/1/1
8	BMA	C	913	8	-	0/2/19/22	0/1/1/1
8	NAG	D	903	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	904	8	-	0/6/23/26	0/1/1/1
8	BMA	D	905	8	-	0/2/19/22	0/1/1/1
8	NAG	D	906	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	907	8	-	0/6/23/26	0/1/1/1
8	BMA	D	908	8	-	0/2/19/22	0/1/1/1
7	NAG	D	910	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	911	7	-	0/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	908	NAG	O5-C1	-2.94	1.38	1.43
7	D	910	NAG	O5-C1	-2.89	1.39	1.43
4	A	903	NAG	O5-C1	-2.67	1.39	1.43
5	A	908	NAG	O5-C1	-2.52	1.39	1.43
4	C	903	NAG	O5-C1	-2.49	1.39	1.43

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	903	NAG	O5-C1-C2	-6.00	103.12	111.47
8	D	903	NAG	O6-C6-C5	-4.77	95.30	111.34
7	D	910	NAG	C1-C2-N2	-4.67	102.51	110.49
7	A	912	NAG	C3-C4-C5	-4.40	102.46	110.22
8	D	903	NAG	O5-C1-C2	-4.27	105.53	111.47

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
4	A	903	NAG	1	0
4	C	903	NAG	1	0
8	D	903	NAG	1	0

## 5.6 Ligand geometry

26 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	URI	A	901	-	14,18,18	0.99	1 (7%)	15,26,26	2.71	3 (20%)
3	UCG	A	902	-	41,52,52	1.51	9 (21%)	50,82,82	2.05	14 (28%)
6	NAG	A	910	1	14,14,15	0.60	0	15,19,21	1.74	4 (26%)
6	NAG	A	913	1	14,14,15	0.84	0	15,19,21	1.22	1 (6%)
6	NAG	A	914	1	14,14,15	0.54	0	15,19,21	1.41	2 (13%)
6	NAG	A	915	1	14,14,15	0.50	0	15,19,21	1.11	2 (13%)
6	NAG	A	916	1	14,14,15	0.75	0	15,19,21	2.18	4 (26%)
2	URI	B	901	-	14,18,18	1.23	2 (14%)	15,26,26	2.66	2 (13%)
3	UCG	B	902	-	41,52,52	1.47	7 (17%)	50,82,82	2.17	13 (26%)
6	NAG	B	909	1	14,14,15	0.83	1 (7%)	15,19,21	0.93	0
6	NAG	B	912	1	14,14,15	0.81	1 (7%)	15,19,21	1.77	4 (26%)
6	NAG	B	913	1	14,14,15	0.67	0	15,19,21	1.34	2 (13%)
6	NAG	B	914	1	14,14,15	0.52	0	15,19,21	1.83	4 (26%)
6	NAG	B	915	1	14,14,15	0.92	1 (7%)	15,19,21	2.49	3 (20%)
2	URI	C	901	-	14,18,18	0.74	0	15,26,26	2.42	4 (26%)
3	UCG	C	902	-	41,52,52	1.56	9 (21%)	50,82,82	1.89	9 (18%)
6	NAG	C	910	1	14,14,15	0.48	0	15,19,21	1.58	3 (20%)
6	NAG	C	914	1	14,14,15	0.84	0	15,19,21	1.23	1 (6%)
6	NAG	C	915	1	14,14,15	0.62	0	15,19,21	1.05	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	C	916	1	14,14,15	0.73	0	15,19,21	1.96	4 (26%)
2	URI	D	901	-	14,18,18	0.97	1 (7%)	15,26,26	2.55	3 (20%)
3	UCG	D	902	-	41,52,52	1.41	9 (21%)	50,82,82	1.97	13 (26%)
6	NAG	D	909	1	14,14,15	0.63	0	15,19,21	1.66	2 (13%)
6	NAG	D	912	1	14,14,15	0.94	1 (7%)	15,19,21	1.52	3 (20%)
6	NAG	D	913	1	14,14,15	0.59	0	15,19,21	1.91	5 (33%)
6	NAG	D	914	1	14,14,15	0.74	0	15,19,21	1.73	2 (13%)

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	URI	A	901	-	-	0/2/22/22	0/2/2/2
3	UCG	A	902	-	-	0/17/67/67	0/6/6/6
6	NAG	A	910	1	-	0/6/23/26	0/1/1/1
6	NAG	A	913	1	-	0/6/23/26	0/1/1/1
6	NAG	A	914	1	-	0/6/23/26	0/1/1/1
6	NAG	A	915	1	-	0/6/23/26	0/1/1/1
6	NAG	A	916	1	-	0/6/23/26	0/1/1/1
2	URI	B	901	-	-	0/2/22/22	0/2/2/2
3	UCG	B	902	-	-	0/17/67/67	0/6/6/6
6	NAG	B	909	1	-	0/6/23/26	0/1/1/1
6	NAG	B	912	1	-	0/6/23/26	0/1/1/1
6	NAG	B	913	1	-	0/6/23/26	0/1/1/1
6	NAG	B	914	1	-	0/6/23/26	0/1/1/1
6	NAG	B	915	1	-	0/6/23/26	0/1/1/1
2	URI	C	901	-	-	0/2/22/22	0/2/2/2
3	UCG	C	902	-	-	0/17/67/67	0/6/6/6
6	NAG	C	910	1	-	0/6/23/26	0/1/1/1
6	NAG	C	914	1	-	0/6/23/26	0/1/1/1
6	NAG	C	915	1	-	0/6/23/26	0/1/1/1
6	NAG	C	916	1	-	0/6/23/26	0/1/1/1
2	URI	D	901	-	-	0/2/22/22	0/2/2/2
3	UCG	D	902	-	-	0/17/67/67	0/6/6/6
6	NAG	D	909	1	-	0/6/23/26	0/1/1/1
6	NAG	D	912	1	-	0/6/23/26	0/1/1/1
6	NAG	D	913	1	-	0/6/23/26	0/1/1/1
6	NAG	D	914	1	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	UCG	C8-N1	-3.73	1.30	1.38
3	A	902	UCG	C8-N1	-3.14	1.31	1.38
3	C	902	UCG	O12-C15	-3.03	1.38	1.45
3	B	902	UCG	C6-N	-2.96	1.31	1.35
3	A	902	UCG	O12-C15	-2.88	1.38	1.45

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	915	NAG	O5-C1-C2	-7.57	100.94	111.47
3	C	902	UCG	C9-C11-N3	-4.53	117.03	123.48
6	B	912	NAG	C1-C2-N2	-4.33	103.09	110.49
3	B	902	UCG	C9-C11-N3	-4.18	117.53	123.48
3	B	902	UCG	N2-C12-N3	-4.00	121.62	127.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	URI	1	0
3	A	902	UCG	4	0
2	B	901	URI	1	0
3	B	902	UCG	6	0
6	B	914	NAG	1	0
2	C	901	URI	1	0
3	C	902	UCG	5	0
2	D	901	URI	1	0
3	D	902	UCG	1	0
6	D	909	NAG	1	0
6	D	913	NAG	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	747/811 (92%)	-0.13	17 (2%) 61 60	18, 32, 62, 90	0
1	B	738/811 (90%)	0.02	20 (2%) 55 54	19, 37, 70, 94	0
1	C	738/811 (90%)	0.25	52 (7%) 17 17	19, 43, 78, 112	0
1	D	735/811 (90%)	0.18	48 (6%) 20 20	21, 41, 86, 104	0
All	All	2958/3244 (91%)	0.08	137 (4%) 33 33	18, 38, 76, 112	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	TYR	8.1
1	C	761	THR	7.8
1	B	817	LEU	7.0
1	C	733	SER	6.4
1	D	64	TYR	6.2

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
8	NAG	B	903	14/15	0.97	0.15	1.12	26,30,36,52	0
4	NAG	A	903	14/15	0.97	0.17	1.02	19,21,25,29	0
4	NAG	C	903	14/15	0.97	0.14	0.37	28,31,36,46	0
8	NAG	D	903	14/15	0.97	0.15	0.09	24,26,31,35	0
7	NAG	B	910	14/15	0.96	0.13	-0.22	21,22,29,31	0
4	NAG	A	904	14/15	0.97	0.12	-0.38	24,28,34,38	0
8	NAG	D	906	14/15	0.97	0.09	-0.63	27,31,33,35	0
7	NAG	D	910	14/15	0.94	0.10	-0.69	27,30,35,49	0
7	NAG	A	911	14/15	0.96	0.09	-1.12	21,23,26,26	0
8	NAG	C	907	14/15	0.97	0.08	-1.13	22,24,26,26	0
8	NAG	D	904	14/15	0.97	0.07	-1.25	28,32,41,41	0
8	NAG	C	911	14/15	0.97	0.08	-1.34	24,26,29,32	0
4	NAG	C	904	14/15	0.94	0.09	-1.62	34,39,48,48	0
8	NAG	B	904	14/15	0.96	0.07	-1.65	31,35,41,42	0
8	NAG	B	906	14/15	0.98	0.07	-2.02	19,22,23,23	0
5	NAG	A	908	14/15	0.97	0.07	-2.23	20,23,25,26	0
7	NAG	B	911	14/15	0.96	0.09	-	32,36,40,48	0
8	BMA	D	905	11/12	0.90	0.10	-	40,48,56,56	0
8	BMA	B	908	11/12	0.93	0.17	-	39,45,54,61	0
8	NAG	B	907	14/15	0.97	0.09	-	23,26,33,42	0
4	MAN	C	906	11/12	0.89	0.22	-	60,70,80,95	0
7	NAG	A	912	14/15	0.92	0.15	-	29,36,42,52	0
5	NAG	A	909	14/15	0.94	0.12	-	26,30,34,36	0
8	BMA	C	913	11/12	0.83	0.30	-	57,64,72,75	0
8	BMA	D	908	11/12	0.88	0.32	-	47,57,62,64	0
8	NAG	D	907	14/15	0.96	0.14	-	31,36,44,52	0
8	BMA	C	909	11/12	0.93	0.30	-	41,47,51,57	0
4	MAN	A	906	11/12	0.88	0.15	-	34,44,49,53	0
4	BMA	C	905	11/12	0.89	0.15	-	44,50,64,65	0
8	NAG	C	908	14/15	0.94	0.13	-	25,30,35,39	0
5	BMA	A	907	11/12	0.91	0.28	-	40,46,54,56	0
8	BMA	B	905	11/12	0.83	0.12	-	41,50,53,59	0
7	NAG	D	911	14/15	0.93	0.11	-	33,39,45,49	0
4	BMA	A	905	11/12	0.90	0.10	-	36,42,49,51	0
8	NAG	C	912	14/15	0.93	0.17	-	34,40,46,47	0

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
6	NAG	C	915	14/15	0.95	0.17	5.68	33,46,55,57	0
6	NAG	C	910	14/15	0.94	0.17	2.85	43,51,60,64	0
3	UCG	A	902	47/47	0.90	0.15	1.81	26,41,85,94	0
6	NAG	A	916	14/15	0.94	0.18	1.64	35,46,57,58	0
3	UCG	B	902	47/47	0.85	0.20	1.50	31,51,91,100	0
6	NAG	D	913	14/15	0.86	0.15	1.26	50,58,70,72	0
6	NAG	D	912	14/15	0.89	0.12	0.53	43,54,65,68	0
6	NAG	B	914	14/15	0.95	0.11	0.29	34,41,44,57	0
6	NAG	A	910	14/15	0.97	0.11	0.19	35,39,42,48	0
3	UCG	D	902	47/47	0.89	0.14	0.03	33,48,79,96	0
2	URI	D	901	17/17	0.98	0.10	-0.21	21,24,31,31	0
2	URI	C	901	17/17	0.97	0.10	-0.51	26,33,42,44	0
2	URI	A	901	17/17	0.98	0.10	-0.55	19,22,29,31	0
6	NAG	D	909	14/15	0.98	0.08	-0.81	31,39,51,56	0
3	UCG	C	902	47/47	0.94	0.10	-0.91	34,42,61,70	0
6	NAG	B	913	14/15	0.94	0.08	-1.11	42,49,60,62	0
2	URI	B	901	17/17	0.98	0.07	-1.24	18,22,36,37	0
6	NAG	B	912	14/15	0.91	0.21	-	43,56,64,69	0
6	NAG	C	916	14/15	0.91	0.12	-	49,55,65,65	0
6	NAG	A	915	14/15	0.90	0.11	-	45,52,61,66	0
6	NAG	B	915	14/15	0.90	0.18	-	43,49,61,64	0
6	NAG	B	909	14/15	0.84	0.26	-	51,71,83,93	0
6	NAG	A	913	14/15	0.92	0.13	-	40,49,56,61	0
6	NAG	D	914	14/15	0.94	0.15	-	48,57,62,64	0
6	NAG	C	914	14/15	0.96	0.20	-	41,50,66,73	0
6	NAG	A	914	14/15	0.92	0.18	-	48,58,67,68	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.