



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:29 am GMT

PDB ID : 3W3N  
Title : Crystal structure of human TLR8 in complex with Resiquimod (R848) crystal form 3  
Authors : Tanji, H.; Ohto, U.; Shimizu, T.  
Deposited on : 2012-12-22  
Resolution : 2.10 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

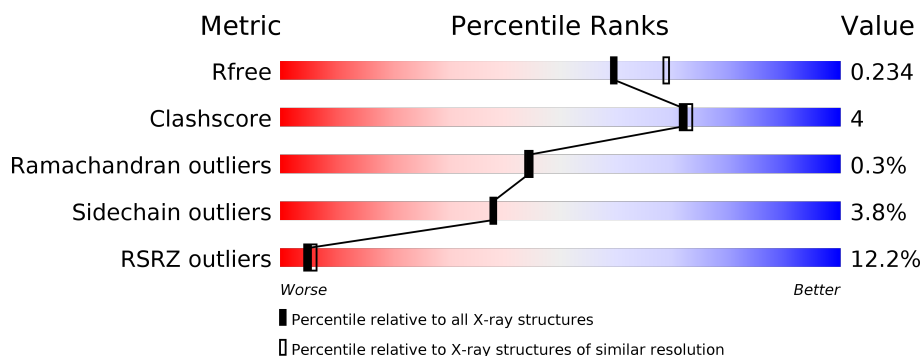
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	
1	B	811	

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
4	NAG	A	1015	-	-	-	X
4	NAG	B	917	-	-	-	X
4	NAG	B	921	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13256 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	751	Total	C	N	O	S	0	0	0
			6039	3861	1025	1134	19			
1	B	749	Total	C	N	O	S	0	0	0
			5994	3836	1019	1120	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	24	SER	-	EXPRESSION TAG	UNP Q9NR97
A	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	26	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	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	24	SER	-	EXPRESSION TAG	UNP Q9NR97
B	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	26	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

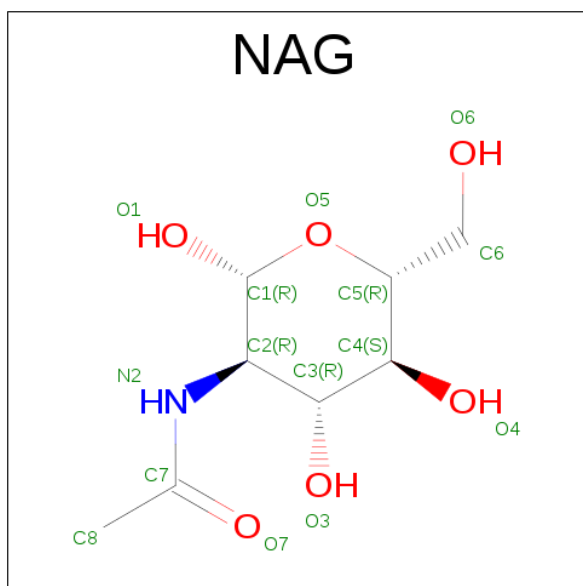
- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			61	34	2	25		
2	A	5	Total	C	N	O	0	0
			61	34	2	25		
2	B	5	Total	C	N	O	0	0
			61	34	2	25		
2	B	5	Total	C	N	O	0	0
			61	34	2	25		

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

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



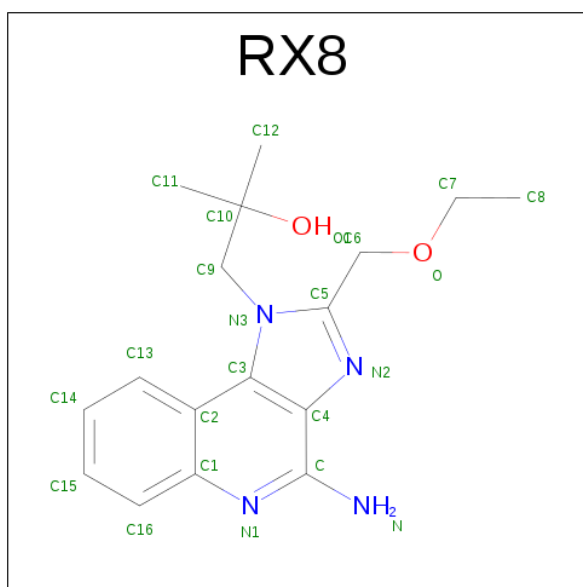
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is 1-[4-AMINO-2-(ETHOXYMETHYL)-1H-IMIDAZO[4,5-C]QUINOLIN-1-YL]-2-METHYLPROPAN-2-OL (three-letter code: RX8) (formula: C<sub>17</sub>H<sub>22</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			23	17	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			23	17	4	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

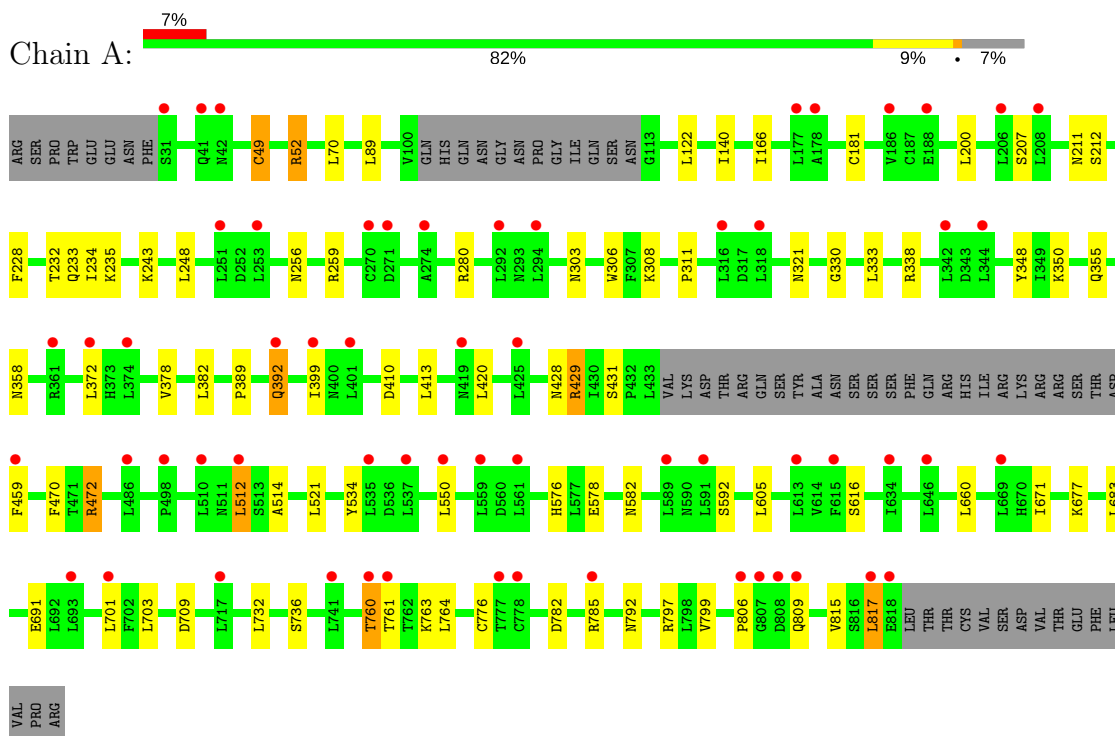
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	419	Total	O	0	0
			419	419		
7	B	248	Total	O	0	0
			248	248		

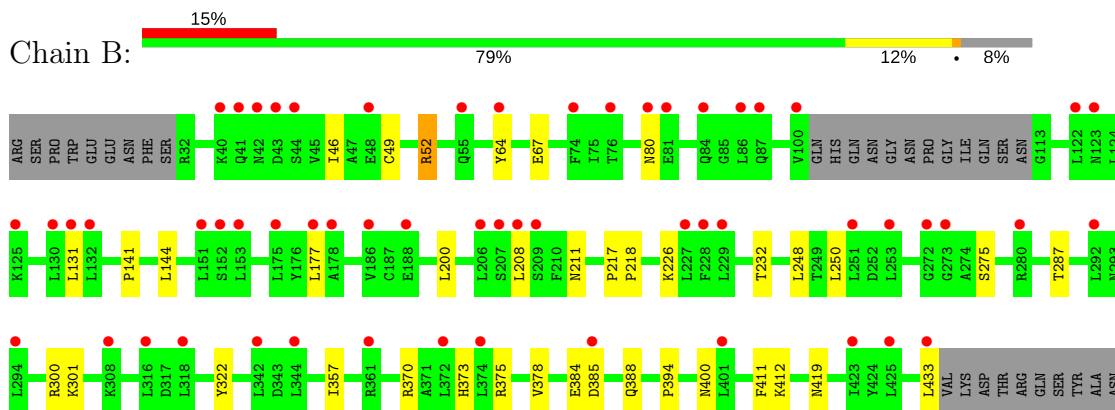
### 3 Residue-property plots [i](#)

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.

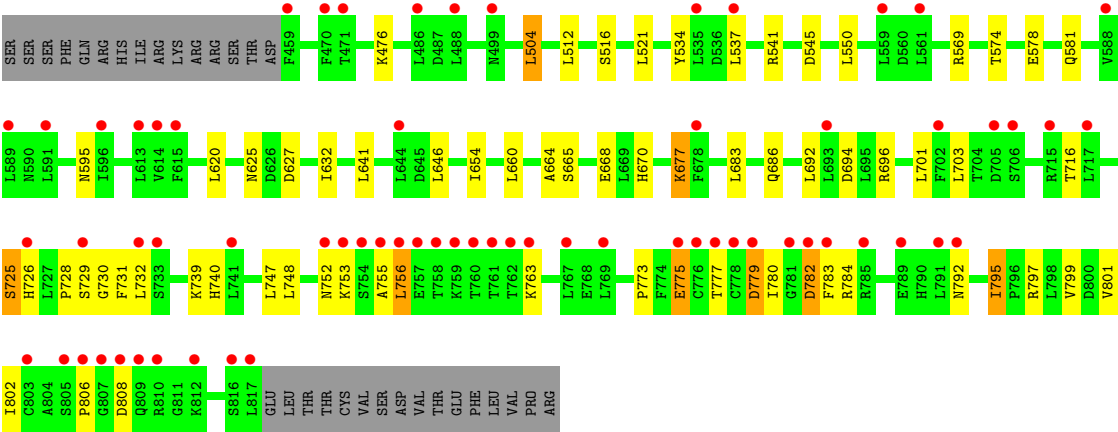
#### • Molecule 1: Toll-like receptor 8



#### • Molecule 1: Toll-like receptor 8







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.22Å 100.78Å 265.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.39 – 2.10 28.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (28.39-2.10) 95.7 (28.39-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.200 , 0.233 0.198 , 0.234	Depositor DCC
$R_{free}$ test set	6494 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: MAN, GOL, BMA, NAG, RX8

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	0.27	0/6164	0.47	0/8361
1	B	0.27	0/6119	0.46	0/8302
All	All	0.27	0/12283	0.46	0/16663

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	6039	0	6005	41	0
1	B	5994	0	5937	57	0
2	A	122	0	104	0	0
2	B	122	0	104	0	0
3	A	39	0	34	0	0
3	B	39	0	34	1	0
4	A	84	0	78	1	0
4	B	98	0	91	0	0
5	A	23	0	22	1	0
5	B	23	0	22	3	0
6	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	419	0	0	10	0
7	B	248	0	0	9	0
All	All	13256	0	12439	100	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 100 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ALA:O	7:B:1025:HOH:O	1.89	0.91
1:B:625:ASN:OD1	7:B:1187:HOH:O	1.95	0.83
1:A:333:LEU:O	7:A:1220:HOH:O	2.05	0.74
1:B:775:GLU:O	1:B:780:ILE:HD11	1.91	0.71
1:A:691:GLU:OE2	7:A:1158:HOH:O	2.09	0.70

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	745/811 (92%)	711 (95%)	32 (4%)	2 (0%)	44	44
1	B	743/811 (92%)	710 (96%)	31 (4%)	2 (0%)	44	44
All	All	1488/1622 (92%)	1421 (96%)	63 (4%)	4 (0%)	44	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	797	ARG
1	A	378	VAL

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Mol	Chain	Res	Type
1	B	378	VAL
1	A	330	GLY

### 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	694/755 (92%)	670 (96%)	24 (4%)	41	42
1	B	683/755 (90%)	654 (96%)	29 (4%)	34	33
All	All	1377/1510 (91%)	1324 (96%)	53 (4%)	38	38

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	817	LEU
1	B	248	LEU
1	B	775	GLU
1	B	49	CYS
1	B	80	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	790	HIS
1	B	809	GLN
1	B	309	ASN
1	A	233	GLN
1	B	499	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

26 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$
2	NAG	A	1001	1,2	14,14,15	0.56	0	15,19,21	0.87	1 (6%)
2	NAG	A	1002	2	14,14,15	0.65	0	15,19,21	0.86	1 (6%)
2	BMA	A	1003	2	11,11,12	0.80	1 (9%)	13,15,17	0.95	1 (7%)
2	MAN	A	1004	2	11,11,12	0.61	0	13,15,17	0.54	0
2	MAN	A	1005	2	11,11,12	0.63	0	13,15,17	0.75	1 (7%)
3	NAG	A	1006	1,3	14,14,15	0.55	0	15,19,21	0.80	0
3	NAG	A	1007	3	14,14,15	0.59	0	15,19,21	0.86	0
3	BMA	A	1008	3	11,11,12	0.58	0	13,15,17	0.79	0
2	NAG	A	1010	1,2	14,14,15	0.58	0	15,19,21	1.04	1 (6%)
2	NAG	A	1011	2	14,14,15	0.59	0	15,19,21	0.77	0
2	BMA	A	1012	2	11,11,12	1.32	2 (18%)	13,15,17	1.88	2 (15%)
2	MAN	A	1013	2	11,11,12	0.77	0	13,15,17	1.31	2 (15%)
2	MAN	A	1014	2	11,11,12	0.55	0	13,15,17	1.22	2 (15%)
2	NAG	B	902	1,2	14,14,15	0.50	0	15,19,21	0.81	1 (6%)
2	NAG	B	903	2	14,14,15	0.66	0	15,19,21	0.90	1 (6%)
2	BMA	B	904	2	11,11,12	0.82	1 (9%)	13,15,17	1.08	2 (15%)
2	MAN	B	905	2	11,11,12	0.67	0	13,15,17	0.67	0
2	MAN	B	906	2	11,11,12	0.65	0	13,15,17	0.72	0
3	NAG	B	907	1,3	14,14,15	0.51	0	15,19,21	0.91	1 (6%)
3	NAG	B	908	3	14,14,15	0.61	0	15,19,21	0.87	0
3	BMA	B	909	3	11,11,12	0.68	0	13,15,17	0.67	0
2	NAG	B	911	1,2	14,14,15	0.50	0	15,19,21	0.89	1 (6%)
2	NAG	B	912	2	14,14,15	0.60	0	15,19,21	1.00	1 (6%)
2	BMA	B	913	2	11,11,12	0.84	1 (9%)	13,15,17	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	B	914	2	11,11,12	0.67	0	13,15,17	0.79	0
2	MAN	B	915	2	11,11,12	0.60	0	13,15,17	1.02	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1004	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1005	2	-	0/2/19/22	0/1/1/1
3	NAG	A	1006	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1007	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1008	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1010	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1011	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1012	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1013	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1014	2	-	0/2/19/22	0/1/1/1
2	NAG	B	902	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	903	2	-	0/6/23/26	0/1/1/1
2	BMA	B	904	2	-	0/2/19/22	0/1/1/1
2	MAN	B	905	2	-	0/2/19/22	0/1/1/1
2	MAN	B	906	2	-	0/2/19/22	0/1/1/1
3	NAG	B	907	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	908	3	-	0/6/23/26	0/1/1/1
3	BMA	B	909	3	-	0/2/19/22	0/1/1/1
2	NAG	B	911	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	912	2	-	0/6/23/26	0/1/1/1
2	BMA	B	913	2	-	0/2/19/22	0/1/1/1
2	MAN	B	914	2	-	0/2/19/22	0/1/1/1
2	MAN	B	915	2	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1012	BMA	O5-C1	-3.06	1.38	1.43
2	A	1003	BMA	O5-C1	-2.21	1.40	1.43
2	B	904	BMA	O5-C1	-2.21	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	913	BMA	O5-C1	-2.14	1.40	1.43
2	A	1012	BMA	C4-C5	2.44	1.58	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1010	NAG	O5-C1-C2	-3.27	106.92	111.47
2	A	1013	MAN	O5-C1-C2	-2.96	106.15	110.79
2	A	1014	MAN	O5-C1-C2	-2.88	106.28	110.79
2	A	1013	MAN	C1-O5-C5	-2.64	108.53	112.17
2	B	903	NAG	O5-C1-C2	-2.59	107.87	111.47

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
3	B	907	NAG	1	0

## 5.6 Ligand geometry [i](#)

16 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	$\# Z  > 2$
4	NAG	A	1009	1	14,14,15	0.52	0	15,19,21	0.76	0
4	NAG	A	1015	1	14,14,15	0.49	0	15,19,21	1.26	2 (13%)
4	NAG	A	1016	1	14,14,15	0.51	0	15,19,21	0.76	0
4	NAG	A	1017	1	14,14,15	0.47	0	15,19,21	2.00	2 (13%)
4	NAG	A	1018	1	14,14,15	0.58	0	15,19,21	0.93	1 (6%)
4	NAG	A	1019	1	14,14,15	0.54	0	15,19,21	0.88	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	RX8	A	1020	-	22,25,25	1.58	3 (13%)	24,37,37	1.10	4 (16%)
6	GOL	A	1021	-	5,5,5	0.36	0	5,5,5	0.23	0
5	RX8	B	901	-	22,25,25	1.53	3 (13%)	24,37,37	1.05	2 (8%)
4	NAG	B	910	1	14,14,15	0.50	0	15,19,21	1.09	1 (6%)
4	NAG	B	916	1	14,14,15	0.46	0	15,19,21	1.00	1 (6%)
4	NAG	B	917	1	14,14,15	0.52	0	15,19,21	0.86	0
4	NAG	B	918	1	14,14,15	0.57	0	15,19,21	0.57	0
4	NAG	B	919	1	14,14,15	0.43	0	15,19,21	1.73	5 (33%)
4	NAG	B	920	1	14,14,15	0.48	0	15,19,21	0.71	0
4	NAG	B	921	1	14,14,15	0.44	0	15,19,21	1.30	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	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1015	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1016	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1017	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1018	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1019	1	-	0/6/23/26	0/1/1/1
5	RX8	A	1020	-	-	0/5/9/9	0/3/3/3
6	GOL	A	1021	-	-	0/4/4/4	0/0/0/0
5	RX8	B	901	-	-	0/5/9/9	0/3/3/3
4	NAG	B	910	1	-	0/6/23/26	0/1/1/1
4	NAG	B	916	1	-	0/6/23/26	0/1/1/1
4	NAG	B	917	1	-	0/6/23/26	0/1/1/1
4	NAG	B	918	1	-	0/6/23/26	0/1/1/1
4	NAG	B	919	1	-	0/6/23/26	0/1/1/1
4	NAG	B	920	1	-	0/6/23/26	0/1/1/1
4	NAG	B	921	1	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1020	RX8	O1-C10	-2.61	1.37	1.44
5	B	901	RX8	O1-C10	-2.57	1.38	1.44
5	B	901	RX8	C-N	2.26	1.43	1.34
5	A	1020	RX8	C-N	2.30	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	901	RX8	C2-C3	4.79	1.48	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	919	NAG	C6-C5-C4	-2.72	106.63	113.00
4	A	1015	NAG	C2-N2-C7	-2.57	119.19	122.94
4	B	919	NAG	O5-C1-C2	-2.29	108.29	111.47
5	B	901	RX8	C3-C2-C1	-2.27	117.92	119.65
4	B	916	NAG	C2-N2-C7	-2.20	119.74	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1018	NAG	1	0
5	A	1020	RX8	1	0
5	B	901	RX8	3	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, 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	751/811 (92%)	0.29	60 (7%) 13 17	19, 35, 62, 92	0
1	B	749/811 (92%)	0.71	123 (16%) 2 3	21, 46, 87, 107	0
All	All	1500/1622 (92%)	0.50	183 (12%) 5 6	19, 40, 78, 107	0

The worst 5 of 183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	761	THR	9.6
1	B	759	LYS	8.0
1	B	64	TYR	6.9
1	B	754	SER	6.3
1	B	778	CYS	6.3

### 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(Å <sup>2</sup> )	Q<0.9
2	NAG	A	1002	14/15	0.96	0.10	-0.41	19,23,32,35	0
2	NAG	B	902	14/15	0.95	0.14	-0.76	27,29,35,37	0
2	NAG	B	903	14/15	0.95	0.10	-1.03	30,33,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	911	14/15	0.91	0.12	-1.29	23,31,34,41	0
2	NAG	A	1001	14/15	0.97	0.09	-1.53	17,21,29,31	0
3	NAG	B	907	14/15	0.96	0.08	-1.94	22,28,36,37	0
3	NAG	A	1006	14/15	0.96	0.08	-2.69	20,23,28,34	0
2	NAG	A	1010	14/15	0.97	0.08	-3.15	18,21,27,28	0
3	BMA	B	909	11/12	0.85	0.33	-	69,72,73,74	0
3	BMA	A	1008	11/12	0.89	0.32	-	63,67,69,69	0
2	NAG	B	912	14/15	0.88	0.12	-	30,34,43,43	0
2	MAN	B	914	11/12	0.68	0.37	-	73,79,84,86	0
2	BMA	A	1003	11/12	0.92	0.13	-	32,43,54,56	0
3	NAG	A	1007	14/15	0.92	0.16	-	36,49,53,56	0
2	MAN	B	906	11/12	0.89	0.31	-	70,73,76,77	0
2	MAN	A	1004	11/12	0.79	0.22	-	33,39,47,55	0
2	BMA	B	904	11/12	0.93	0.20	-	39,56,63,64	0
2	MAN	B	905	11/12	0.81	0.24	-	45,60,66,67	0
3	NAG	B	908	14/15	0.86	0.19	-	44,57,67,72	0
2	BMA	B	913	11/12	0.87	0.24	-	49,63,71,74	0
2	MAN	A	1014	11/12	0.85	0.35	-	69,73,76,76	0
2	BMA	A	1012	11/12	0.93	0.23	-	40,55,67,75	0
2	MAN	A	1013	11/12	0.65	0.38	-	67,73,81,82	0
2	MAN	A	1005	11/12	0.83	0.29	-	56,66,71,76	0
2	NAG	A	1011	14/15	0.94	0.10	-	21,26,36,47	0
2	MAN	B	915	11/12	0.86	0.41	-	72,78,86,87	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, 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
4	NAG	B	917	14/15	0.93	0.31	6.34	50,60,73,76	0
4	NAG	A	1015	14/15	0.89	0.29	4.13	52,64,74,75	0
4	NAG	B	921	14/15	0.77	0.30	2.52	68,72,74,77	0
4	NAG	B	916	14/15	0.90	0.27	1.69	64,75,83,83	0
6	GOL	A	1021	6/6	0.76	0.15	1.01	66,71,73,74	0
5	RX8	B	901	23/23	0.94	0.12	0.35	22,29,41,45	0
4	NAG	B	918	14/15	0.92	0.13	0.26	44,52,56,57	0
4	NAG	A	1018	14/15	0.97	0.12	0.03	36,42,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	919	14/15	0.91	0.22	-0.07	52,57,63,69	0
5	RX8	A	1020	23/23	0.96	0.10	-0.53	22,32,41,42	0
4	NAG	A	1019	14/15	0.94	0.10	-0.74	29,31,34,34	0
4	NAG	A	1016	14/15	0.87	0.34	-	62,65,67,69	0
4	NAG	B	910	14/15	0.91	0.12	-	44,60,67,75	0
4	NAG	A	1017	14/15	0.86	0.37	-	62,68,75,78	0
4	NAG	A	1009	14/15	0.91	0.20	-	48,56,68,73	0
4	NAG	B	920	14/15	0.89	0.33	-	77,82,86,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.