



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:01 am GMT

PDB ID : 3W3M  
Title : Crystal structure of human TLR8 in complex with Resiquimod (R848) crystal form 2  
Authors : Tanji, H.; Ohto, U.; Shimizu, T.  
Deposited on : 2012-12-22  
Resolution : 2.70 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](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.

---

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

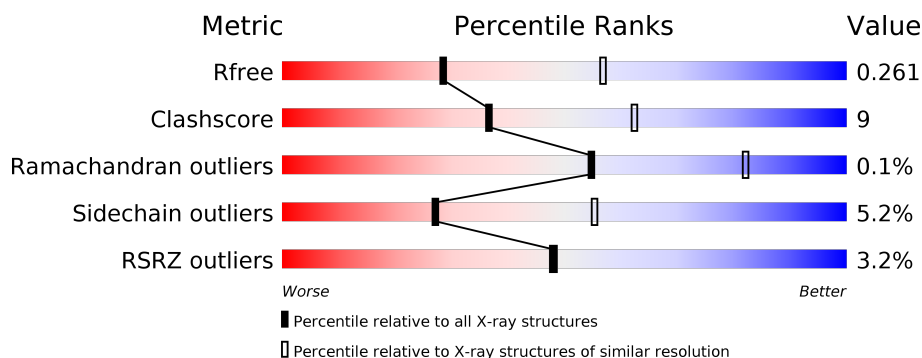
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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>3%</div> <div>69%</div> <div>22%</div> <div>7%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6348 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.

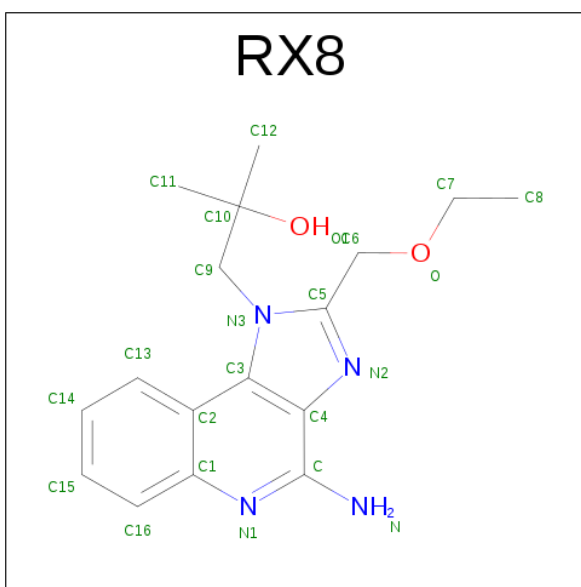
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			6035	3859	1025	1132	19			

There are 10 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

- Molecule 2 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
2	A	1	Total	C	N	O	0	0
			23	17	4	2		

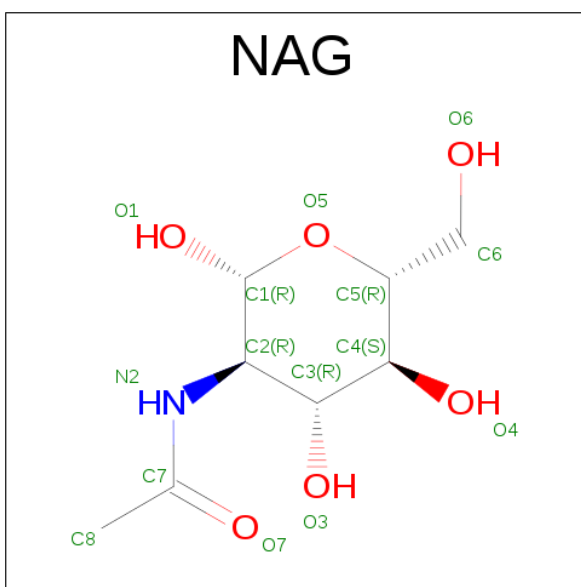
- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

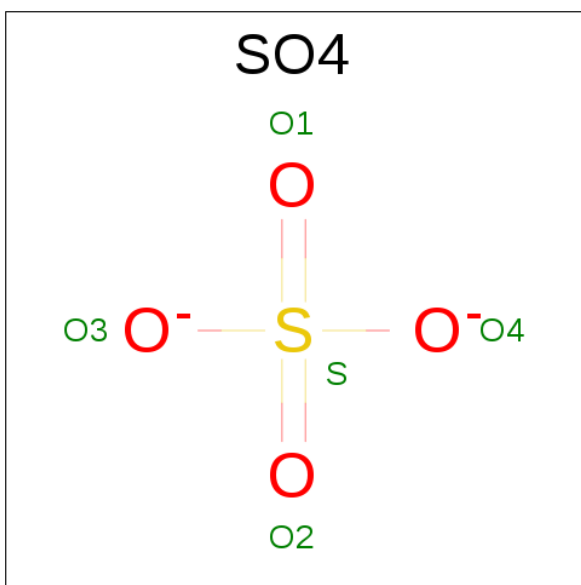
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

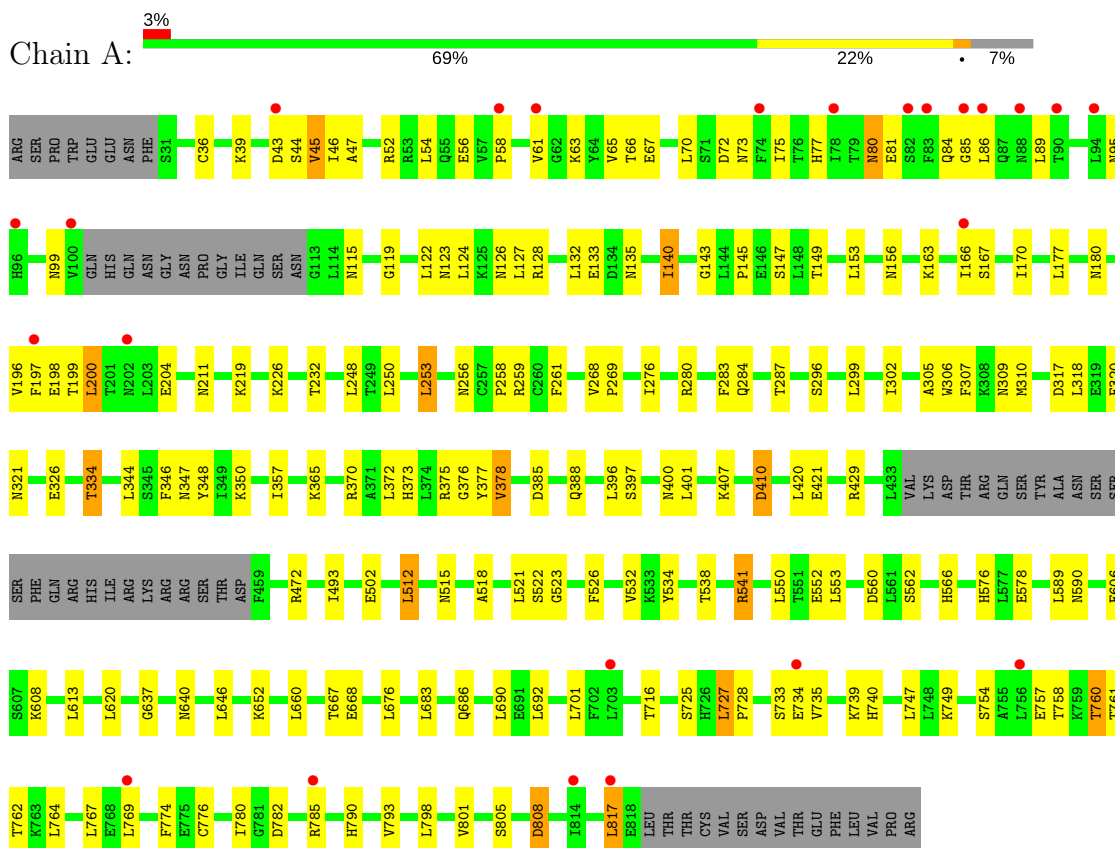
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	68	Total	O	0	0
			68	68		

### 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.77Å 106.00Å 72.32Å 90.00° 106.94° 90.00°	Depositor
Resolution (Å)	41.84 – 2.70 41.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (41.84-2.70) 97.8 (41.84-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.220 , 0.255 0.223 , 0.261	Depositor DCC
$R_{free}$ test set	1339 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, RX8, BMA, NAG, SO4

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	0.28	0/6160	0.53	0/8356

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 [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	6035	0	6002	111	2
2	A	23	0	22	3	0
3	A	122	0	104	1	0
4	A	39	0	34	0	0
5	A	56	0	52	0	0
6	A	5	0	0	0	0
7	A	68	0	0	4	1
All	All	6348	0	6214	113	2

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 9.

All (113) 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:334:THR:HG22	1:A:365:LYS:HG2	1.66	0.77
1:A:344:LEU:O	1:A:347:ASN:ND2	2.23	0.72
1:A:276:ILE:HG22	1:A:299:LEU:HD11	1.75	0.69
1:A:606:GLU:HG2	1:A:637:GLY:HA3	1.75	0.67
1:A:318:LEU:O	1:A:321:ASN:ND2	2.28	0.66
1:A:61:VAL:HG21	1:A:86:LEU:HD11	1.78	0.65
1:A:177:LEU:O	1:A:180:ASN:ND2	2.30	0.65
1:A:72:ASP:OD1	1:A:99:ASN:ND2	2.29	0.64
1:A:199:THR:HG23	1:A:200:LEU:HD13	1.79	0.64
1:A:284:GLN:O	1:A:309:ASN:ND2	2.31	0.64
1:A:760:THR:OG1	1:A:761:THR:N	2.31	0.63
1:A:576:HIS:NE2	7:A:1040:HOH:O	2.31	0.62
1:A:733:SER:OG	1:A:757:GLU:O	2.18	0.60
1:A:197:PHE:HA	1:A:200:LEU:HD22	1.82	0.60
1:A:140:ILE:HD12	1:A:166:ILE:HD11	1.84	0.59
1:A:734:GLU:H	1:A:758:THR:HG23	1.68	0.59
2:A:901:RX8:H9	2:A:901:RX8:H19	1.86	0.58
1:A:782:ASP:OD1	1:A:785:ARG:NH2	2.37	0.58
1:A:45:VAL:HG22	1:A:65:VAL:HA	1.86	0.58
1:A:410:ASP:OD1	1:A:410:ASP:N	2.37	0.57
1:A:44:SER:OG	1:A:45:VAL:N	2.36	0.57
1:A:660:LEU:HD21	1:A:683:LEU:HD22	1.87	0.56
1:A:526:PHE:HB2	1:A:553:LEU:HD21	1.88	0.56
1:A:80:ASN:N	1:A:80:ASN:OD1	2.27	0.56
1:A:66:THR:HG22	1:A:67:GLU:HG3	1.87	0.56
1:A:56:GLU:HA	1:A:75:ILE:HG23	1.88	0.55
1:A:493:ILE:O	1:A:515:ASN:HB3	2.07	0.54
3:A:913:BMA:H62	3:A:914:MAN:H3	1.89	0.54
1:A:538:THR:HG22	1:A:562:SER:HB2	1.88	0.54
1:A:518:ALA:HA	1:A:541:ARG:O	2.08	0.54
1:A:769:LEU:HD23	1:A:774:PHE:HZ	1.71	0.54
1:A:378:VAL:HG11	2:A:901:RX8:H2	1.88	0.53
1:A:780:ILE:HD11	1:A:817:LEU:HD13	1.89	0.53
1:A:253:LEU:O	1:A:256:ASN:ND2	2.30	0.53
1:A:226:LYS:HG2	1:A:250:LEU:HB3	1.91	0.53
1:A:259:ARG:NH1	1:A:321:ASN:O	2.42	0.53
1:A:84:GLN:OE1	1:A:123:ASN:ND2	2.42	0.53
1:A:798:LEU:HA	1:A:801:VAL:HG22	1.91	0.52
1:A:385:ASP:HA	1:A:388:GLN:HG2	1.93	0.51
1:A:739:LYS:NZ	7:A:1025:HOH:O	2.44	0.51
1:A:124:LEU:HD23	1:A:126:ASN:H	1.76	0.51
1:A:77:HIS:HE1	1:A:115:ASN:HD22	1.58	0.50

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASN:O	1:A:232:THR:HA	2.11	0.50
1:A:348:TYR:HB3	1:A:376:GLY:O	2.12	0.50
1:A:776:CYS:N	1:A:805:SER:O	2.21	0.49
1:A:668:GLU:HG3	1:A:692:LEU:HD23	1.94	0.49
1:A:808:ASP:N	1:A:808:ASP:OD1	2.41	0.49
1:A:66:THR:O	1:A:89:LEU:HA	2.13	0.49
1:A:258:PRO:HD2	1:A:269:PRO:HA	1.95	0.49
1:A:54:LEU:HD13	1:A:58:PRO:HD3	1.95	0.48
1:A:357:ILE:HG13	1:A:377:TYR:CE1	2.48	0.48
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.95	0.48
1:A:541:ARG:HB3	1:A:566:HIS:CB	2.44	0.48
1:A:70:LEU:O	1:A:73:ASN:ND2	2.46	0.48
1:A:280:ARG:CZ	1:A:305:ALA:HB1	2.44	0.48
1:A:63:LYS:HD2	1:A:85:GLY:O	2.13	0.47
1:A:397:SER:HA	1:A:420:LEU:HA	1.97	0.47
1:A:283:PHE:HD2	1:A:306:TRP:HB3	1.78	0.47
1:A:346:PHE:N	1:A:375:ARG:O	2.27	0.47
1:A:764:LEU:HD21	1:A:767:LEU:HD13	1.96	0.47
1:A:526:PHE:CB	1:A:553:LEU:HD21	2.45	0.47
1:A:769:LEU:HD23	1:A:774:PHE:CZ	2.50	0.46
1:A:89:LEU:CD1	1:A:124:LEU:HD11	2.46	0.46
1:A:378:VAL:HG21	2:A:901:RX8:H9	1.97	0.46
1:A:119:GLY:HA2	1:A:143:GLY:O	2.16	0.46
1:A:521:LEU:HD13	1:A:550:LEU:HD21	1.97	0.46
1:A:357:ILE:HG22	7:A:1016:HOH:O	2.15	0.46
1:A:716:THR:HG23	1:A:740:HIS:HB3	1.98	0.46
1:A:198:GLU:HG3	1:A:219:LYS:HB3	1.97	0.46
1:A:180:ASN:HB2	1:A:211:ASN:OD1	2.16	0.46
1:A:512:LEU:HD12	1:A:512:LEU:HA	1.74	0.46
1:A:61:VAL:HG23	1:A:86:LEU:HD21	1.97	0.46
1:A:86:LEU:HB3	1:A:89:LEU:HD11	1.98	0.45
1:A:122:LEU:HA	1:A:145:PRO:HG3	1.99	0.45
1:A:132:LEU:O	1:A:135:ASN:ND2	2.50	0.45
1:A:39:LYS:HG3	1:A:46:ILE:HG23	2.00	0.44
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.98	0.44
1:A:302:ILE:N	1:A:326:GLU:OE2	2.36	0.44
1:A:81:GLU:N	1:A:81:GLU:OE1	2.50	0.44
1:A:296:SER:HA	1:A:320:PHE:O	2.18	0.44
1:A:167:SER:HB3	1:A:199:THR:HG21	2.00	0.43
1:A:163:LYS:HA	1:A:196:VAL:HG23	2.00	0.43
1:A:36:CYS:HB3	1:A:47:ALA:HB1	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:HIS:CE1	1:A:115:ASN:HD22	2.35	0.43
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.19	0.43
1:A:725:SER:N	7:A:1023:HOH:O	2.17	0.43
1:A:620:LEU:HD11	1:A:646:LEU:HD22	2.01	0.43
1:A:258:PRO:HA	1:A:296:SER:O	2.18	0.43
1:A:259:ARG:NH2	1:A:348:TYR:O	2.37	0.43
1:A:370:ARG:O	1:A:396:LEU:HD12	2.19	0.43
1:A:608:LYS:O	1:A:640:ASN:HB2	2.19	0.43
1:A:589:LEU:HD23	1:A:613:LEU:HD13	2.01	0.43
1:A:89:LEU:HD13	1:A:124:LEU:HD11	2.02	0.42
1:A:727:LEU:HA	1:A:728:PRO:HD3	1.86	0.42
1:A:95:ASN:OD1	1:A:133:GLU:N	2.52	0.42
1:A:283:PHE:HB3	1:A:310:MET:HE3	2.02	0.41
1:A:128:ARG:HD2	1:A:149:THR:HG23	2.02	0.41
1:A:407:LYS:HE2	1:A:429:ARG:HH11	1.84	0.41
1:A:692:LEU:HD13	1:A:716:THR:HB	2.02	0.41
1:A:302:ILE:HD11	1:A:307:PHE:CZ	2.55	0.41
1:A:153:LEU:O	1:A:156:ASN:ND2	2.34	0.41
1:A:401:LEU:HA	1:A:401:LEU:HD23	1.95	0.41
1:A:560:ASP:OD1	1:A:590:ASN:HB3	2.19	0.41
1:A:798:LEU:H	1:A:798:LEU:HD12	1.84	0.41
1:A:318:LEU:HB2	1:A:344:LEU:HD23	2.03	0.41
1:A:652:LYS:O	1:A:676:LEU:HA	2.21	0.41
1:A:754:SER:HA	1:A:757:GLU:HG2	2.03	0.41
1:A:523:GLY:O	1:A:552:GLU:HB3	2.21	0.41
1:A:309:ASN:OD1	1:A:309:ASN:N	2.54	0.41
1:A:667:THR:HA	1:A:690:LEU:HA	2.03	0.41
1:A:749:LYS:O	1:A:774:PHE:HA	2.21	0.41
1:A:86:LEU:CB	1:A:89:LEU:HD11	2.51	0.40
1:A:261:PHE:CD2	1:A:350:LYS:HE2	2.56	0.40

All (2) 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:A:280:ARG:NH2	1:A:734:GLU:OE2[3_455]	2.08	0.12
1:A:429:ARG:NH2	7:A:1060:HOH:O[2_555]	2.11	0.09

## 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%)	714 (96%)	30 (4%)	1 (0%)	55	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	VAL

### 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	693/755 (92%)	657 (95%)	36 (5%)	27	55

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	45	VAL
1	A	52	ARG
1	A	80	ASN
1	A	127	LEU
1	A	140	ILE
1	A	147	SER
1	A	170	ILE
1	A	200	LEU
1	A	204	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	248	LEU
1	A	253	LEU
1	A	268	VAL
1	A	287	THR
1	A	317	ASP
1	A	334	THR
1	A	372	LEU
1	A	410	ASP
1	A	421	GLU
1	A	472	ARG
1	A	502	GLU
1	A	512	LEU
1	A	522	SER
1	A	532	VAL
1	A	534	TYR
1	A	541	ARG
1	A	701	LEU
1	A	727	LEU
1	A	735	VAL
1	A	747	LEU
1	A	760	THR
1	A	762	THR
1	A	790	HIS
1	A	793	VAL
1	A	808	ASP
1	A	817	LEU

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

Mol	Chain	Res	Type
1	A	77	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

13 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	NAG	A	902	1,3	14,14,15	0.52	0	15,19,21	0.77	1 (6%)
3	NAG	A	903	3	14,14,15	0.52	0	15,19,21	0.85	0
3	BMA	A	904	3	11,11,12	0.62	0	13,15,17	0.75	1 (7%)
3	MAN	A	905	3	11,11,12	0.62	0	13,15,17	0.86	0
3	MAN	A	906	3	11,11,12	0.65	0	13,15,17	0.77	1 (7%)
4	NAG	A	907	1,4	14,14,15	0.48	0	15,19,21	0.83	0
4	NAG	A	908	4	14,14,15	0.58	0	15,19,21	1.02	1 (6%)
4	BMA	A	909	4	11,11,12	0.71	0	13,15,17	0.70	0
3	NAG	A	911	1,3	14,14,15	1.28	1 (7%)	15,19,21	2.02	3 (20%)
3	NAG	A	912	3	14,14,15	1.60	3 (21%)	15,19,21	2.44	7 (46%)
3	BMA	A	913	3	11,11,12	1.48	2 (18%)	13,15,17	2.52	7 (53%)
3	MAN	A	914	3	11,11,12	0.70	0	13,15,17	0.76	0
3	MAN	A	915	3	11,11,12	0.54	0	13,15,17	0.86	0

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	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	903	3	-	0/6/23/26	0/1/1/1
3	BMA	A	904	3	-	0/2/19/22	0/1/1/1
3	MAN	A	905	3	-	0/2/19/22	0/1/1/1
3	MAN	A	906	3	-	0/2/19/22	0/1/1/1
4	NAG	A	907	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	908	4	-	0/6/23/26	0/1/1/1
4	BMA	A	909	4	-	0/2/19/22	0/1/1/1
3	NAG	A	911	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	912	3	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	A	913	3	-	0/2/19/22	0/1/1/1
3	MAN	A	914	3	-	0/2/19/22	0/1/1/1
3	MAN	A	915	3	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	913	BMA	O5-C1	-3.12	1.38	1.43
3	A	912	NAG	O5-C1	-2.39	1.39	1.43
3	A	912	NAG	O7-C7	-2.24	1.18	1.23
3	A	912	NAG	C8-C7	-2.20	1.45	1.50
3	A	911	NAG	O7-C7	-2.16	1.18	1.23
3	A	913	BMA	O2-C2	-2.00	1.39	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	912	NAG	O5-C1-C2	-4.70	104.93	111.47
3	A	913	BMA	O5-C1-C2	-4.45	103.82	110.79
3	A	911	NAG	O5-C1-C2	-4.13	105.72	111.47
3	A	913	BMA	O2-C2-C1	-4.02	100.99	109.18
3	A	912	NAG	O3-C3-C4	-3.95	101.77	110.36
3	A	912	NAG	C6-C5-C4	-3.57	104.66	113.00
3	A	911	NAG	C3-C4-C5	-2.94	105.04	110.22
3	A	913	BMA	O2-C2-C3	-2.87	104.53	110.17
3	A	912	NAG	O4-C4-C3	-2.74	104.40	110.36
3	A	912	NAG	O7-C7-C8	-2.45	117.60	122.06
3	A	906	MAN	O5-C1-C2	-2.28	107.22	110.79
3	A	913	BMA	C6-C5-C4	-2.19	107.88	113.00
3	A	913	BMA	O4-C4-C5	-2.12	103.94	109.28
3	A	902	NAG	O5-C1-C2	-2.03	108.64	111.47
3	A	904	BMA	O2-C2-C3	-2.01	106.23	110.17
3	A	913	BMA	C3-C4-C5	2.07	113.86	110.22
3	A	912	NAG	C8-C7-N2	2.21	120.11	116.11
4	A	908	NAG	C4-C3-C2	2.52	114.72	111.02
3	A	912	NAG	C1-O5-C5	3.67	117.23	112.17
3	A	913	BMA	C1-O5-C5	4.65	118.58	112.17
3	A	911	NAG	C1-O5-C5	4.69	118.63	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	913	BMA	1	0
3	A	914	MAN	1	0

## 5.6 Ligand geometry [i](#)

6 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	RX8	A	901	-	22,25,25	1.61	3 (13%)	24,37,37	1.04	4 (16%)
5	NAG	A	910	1	14,14,15	0.54	0	15,19,21	0.89	0
5	NAG	A	916	1	14,14,15	0.47	0	15,19,21	0.74	0
5	NAG	A	917	1	14,14,15	0.46	0	15,19,21	0.79	0
5	NAG	A	918	1	14,14,15	0.53	0	15,19,21	0.57	0
6	SO4	A	919	-	4,4,4	0.14	0	6,6,6	0.06	0

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	RX8	A	901	-	-	0/5/9/9	0/3/3/3
5	NAG	A	910	1	-	0/6/23/26	0/1/1/1
5	NAG	A	916	1	-	0/6/23/26	0/1/1/1
5	NAG	A	917	1	-	0/6/23/26	0/1/1/1
5	NAG	A	918	1	-	0/6/23/26	0/1/1/1
6	SO4	A	919	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	RX8	O1-C10	-2.49	1.38	1.44
2	A	901	RX8	C-N	2.36	1.43	1.34
2	A	901	RX8	C2-C3	5.04	1.49	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	RX8	C2-C1-N1	-2.08	120.75	123.08
2	A	901	RX8	C2-C3-N3	2.05	134.76	130.42
2	A	901	RX8	O-C6-C5	2.14	117.16	110.96
2	A	901	RX8	C6-O-C7	2.44	119.69	112.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	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 ⓘ

### 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<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%)	0.18	24 (3%)	48 48	21, 54, 99, 122	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	GLY	5.2
1	A	83	PHE	4.6
1	A	166	ILE	4.3
1	A	86	LEU	4.0
1	A	202	ASN	3.5
1	A	43	ASP	3.4
1	A	61	VAL	3.4
1	A	100	VAL	3.4
1	A	756	LEU	3.2
1	A	82	SER	3.2
1	A	769	LEU	3.0
1	A	734	GLU	3.0
1	A	197	PHE	2.9
1	A	58	PRO	2.7
1	A	74	PHE	2.6
1	A	817	LEU	2.5
1	A	94	LEU	2.4
1	A	88	ASN	2.4
1	A	96	HIS	2.3
1	A	90	THR	2.3
1	A	78	ILE	2.2
1	A	814	ILE	2.1
1	A	785	ARG	2.0
1	A	703	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](#)

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
3	NAG	A	903	14/15	0.96	0.20	0.41	34,41,48,50	0
3	NAG	A	902	14/15	0.94	0.19	0.27	37,47,50,50	0
4	NAG	A	907	14/15	0.97	0.14	-0.61	28,32,40,43	0
3	NAG	A	912	14/15	0.98	0.13	-1.12	21,33,44,47	0
3	NAG	A	911	14/15	0.97	0.10	-2.17	17,30,37,41	0
4	NAG	A	908	14/15	0.93	0.19	-	54,64,70,71	0
4	BMA	A	909	11/12	0.92	0.17	-	68,70,75,77	0
3	BMA	A	904	11/12	0.96	0.12	-	45,48,55,63	0
3	MAN	A	906	11/12	0.85	0.17	-	69,72,78,82	0
3	MAN	A	914	11/12	0.76	0.16	-	87,89,92,93	0
3	BMA	A	913	11/12	0.95	0.09	-	57,67,82,87	0
3	MAN	A	905	11/12	0.86	0.14	-	50,54,56,57	0
3	MAN	A	915	11/12	0.83	0.23	-	81,86,90,91	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(Å <sup>2</sup> )	Q<0.9
5	NAG	A	917	14/15	0.87	0.22	1.92	45,60,71,72	0
5	NAG	A	918	14/15	0.96	0.18	1.07	32,47,56,57	0
2	RX8	A	901	23/23	0.98	0.19	0.33	28,36,51,52	0
5	NAG	A	910	14/15	0.93	0.13	-1.13	54,59,75,79	0
6	SO4	A	919	5/5	0.85	0.27	-	113,114,115,117	0
5	NAG	A	916	14/15	0.87	0.16	-	60,71,73,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.