



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:06 PM GMT

PDB ID : 3W3J  
Title : Crystal structure of human TLR8 in complex with CL097  
Authors : Tanji, H.; Ohto, U.; Shimizu, T.  
Deposited on : 2012-12-22  
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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

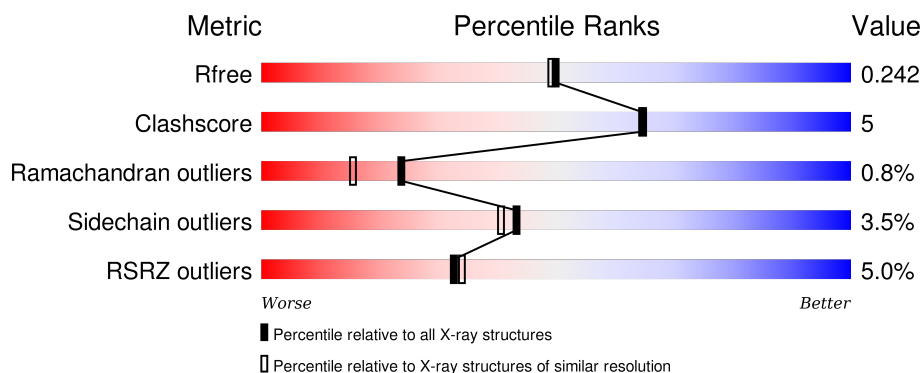
# 1 Overall quality at a glance

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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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>6%</div> <div>76%</div> <div>14%</div> <div>8%</div> </div>
1	B	811	<div> <div>3%</div> <div>79%</div> <div>12%</div> <div>8%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1011	-	-	-	X
4	NAG	B	908	-	-	-	X
4	NAG	B	913	-	-	-	X
7	SO4	A	1018	-	-	-	X
7	SO4	A	1021	-	-	-	X
7	SO4	B	919	-	-	-	X
7	SO4	B	922	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13299 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
			5988	3832	1018	1119	19			
1	B	746	Total	C	N	O	S	0	0	0
			5982	3830	1017	1116	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

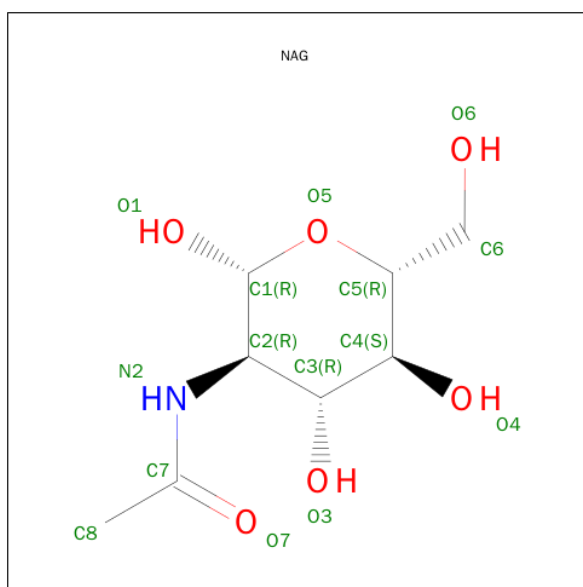
- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- 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		
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		

Continued on next page...

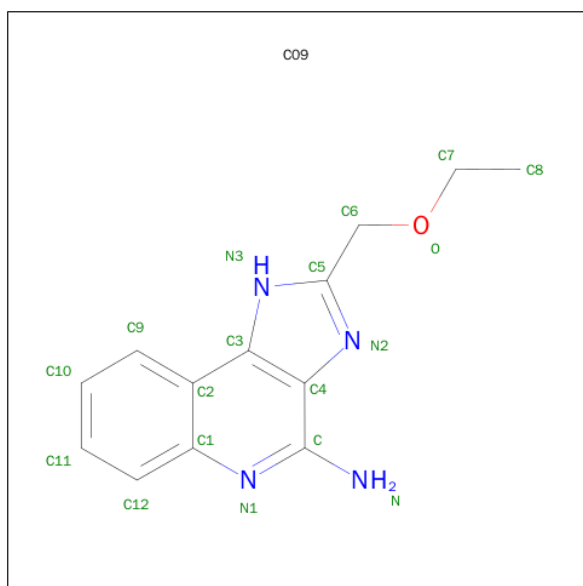
*Continued from previous page...*

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

- Molecule 6 is 2-(ETHOXYMETHYL)-1H-IMIDAZO[4,5-C]QUINOLIN-4-AMINE (three-letter code: C09) (formula: C<sub>13</sub>H<sub>14</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			18	13	4	1		
6	B	1	Total	C	N	O	0	0
			18	13	4	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



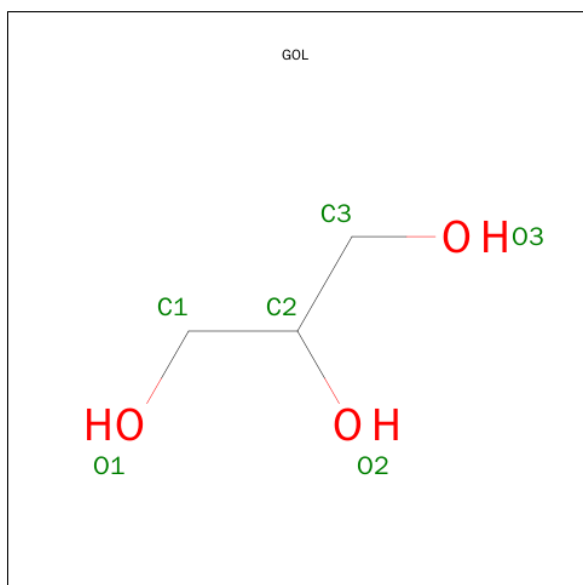
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 9 is water.

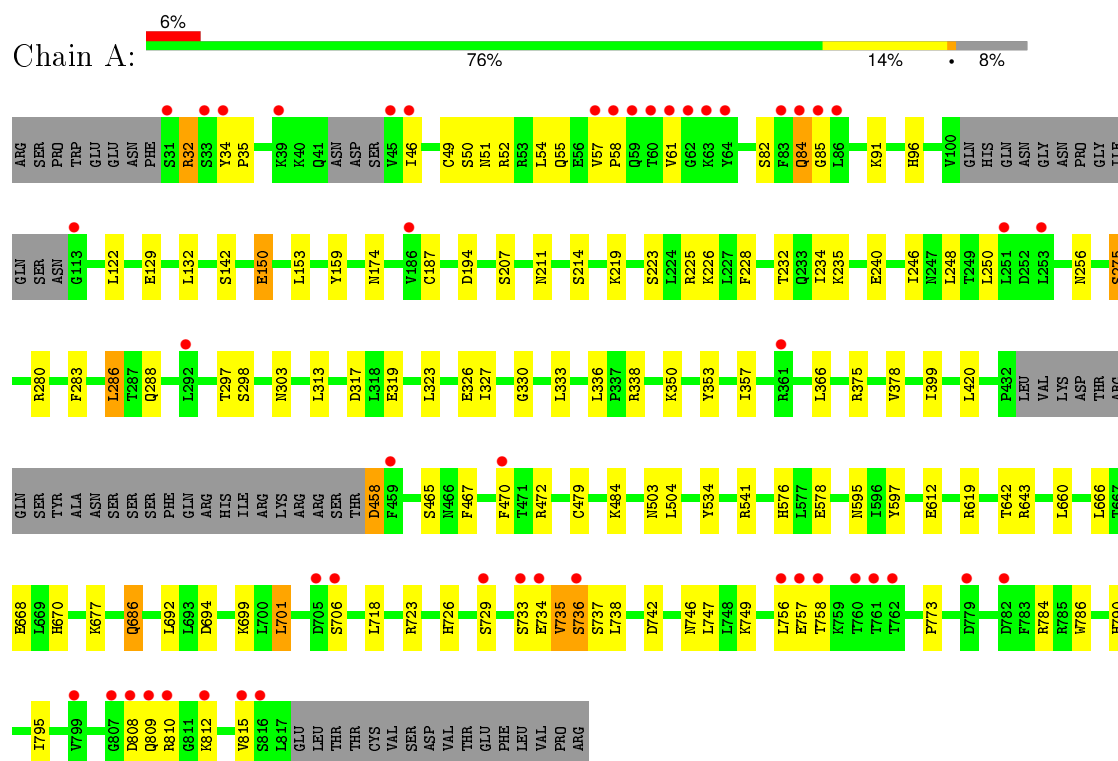
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	438	Total	O	0	0
			438	438		
9	B	423	Total	O	0	0
			423	423		



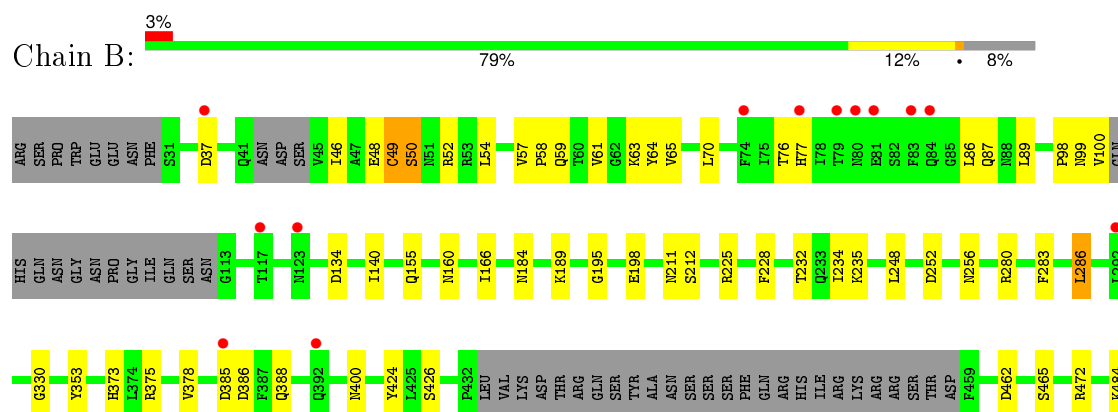
### 3 Residue-property plots

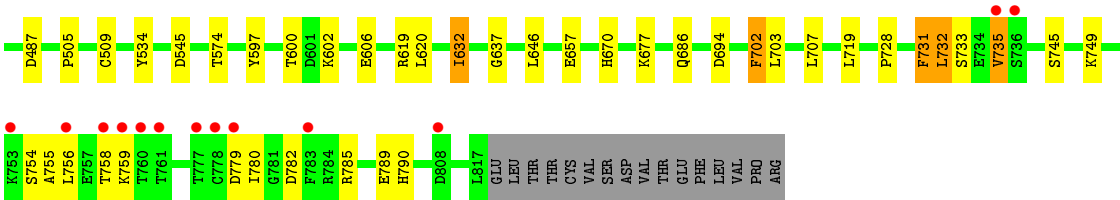
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 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, $\alpha$ , $\beta$ , $\gamma$	71.38Å 148.75Å 85.77Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	40.43 – 2.00 40.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.43-2.00) 97.9 (40.43-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.191 , 0.237 0.202 , 0.242	Depositor DCC
$R_{free}$ test set	5748 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 114604 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, BMA, NAG, C09, SO4, MAN

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	0.32	0/6112	0.50	0/8290
1	B	0.33	0/6106	0.51	0/8282
All	All	0.33	0/12218	0.50	0/16572

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	5988	0	5937	73	0
1	B	5982	0	5940	51	0
2	A	50	0	43	1	0
2	B	50	0	43	1	0
3	A	28	0	25	1	0
3	B	28	0	25	0	0
4	A	56	0	52	0	0
4	B	56	0	52	0	1
5	A	39	0	34	0	0
5	B	39	0	34	0	0
6	A	18	0	14	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	18	0	14	0	0
7	A	40	0	0	4	0
7	B	40	0	0	2	0
8	B	6	0	8	0	0
9	A	438	0	0	15	1
9	B	423	0	0	10	0
All	All	13299	0	12221	125	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 5.

The worst 5 of 125 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:386:ASP:OD2	9:B:1204:HOH:O	2.06	0.73
1:B:782:ASP:OD1	1:B:785:ARG:NH2	2.23	0.71
1:A:280:ARG:HD2	1:A:303:ASN:HD21	1.55	0.70
1:B:52:ARG:NH2	9:B:1320:HOH:O	2.24	0.70
1:A:150:GLU:HG2	1:A:174:ASN:HB2	1.77	0.67

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)
4:B:914:NAG:O3	9:A:1474:HOH:O[1_655]	2.06	0.14

## 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	739/811 (91%)	698 (94%)	34 (5%)	7 (1%)	21 13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	738/811 (91%)	688 (93%)	45 (6%)	5 (1%)	26	19
All	All	1477/1622 (91%)	1386 (94%)	79 (5%)	12 (1%)	24	15

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	735	VAL
1	A	736	SER
1	A	757	GLU
1	A	734	GLU
1	B	99	ASN

### 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	683/755 (90%)	657 (96%)	26 (4%)	40	36
1	B	683/755 (90%)	661 (97%)	22 (3%)	46	44
All	All	1366/1510 (90%)	1318 (96%)	48 (4%)	43	40

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	686	GLN
1	B	46	ILE
1	B	735	VAL
1	A	701	LEU
1	A	729	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	B	87	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 ⓘ

18 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	0.62	0	15,19,21	0.80	0
2	NAG	A	1002	2	14,14,15	0.57	0	15,19,21	0.77	0
2	BMA	A	1003	2	11,11,12	0.93	1 (9%)	14,15,17	1.08	0
2	MAN	A	1004	2	11,11,12	0.49	0	14,15,17	2.24	2 (14%)
3	NAG	A	1005	1,3	14,14,15	0.59	0	15,19,21	0.90	1 (6%)
3	NAG	A	1006	3	14,14,15	0.60	0	15,19,21	0.59	0
5	NAG	A	1008	1,5	14,14,15	0.60	0	15,19,21	1.03	1 (6%)
5	NAG	A	1009	5	14,14,15	0.57	0	15,19,21	1.11	2 (13%)
5	BMA	A	1010	5	11,11,12	0.73	0	14,15,17	0.67	0
2	NAG	B	902	1,2	14,14,15	0.60	0	15,19,21	1.48	1 (6%)
2	NAG	B	903	2	14,14,15	0.48	0	15,19,21	0.94	1 (6%)
2	BMA	B	904	2	11,11,12	1.31	1 (9%)	14,15,17	1.55	3 (21%)
2	MAN	B	905	2	11,11,12	0.52	0	14,15,17	1.95	1 (7%)
3	NAG	B	906	1,3	14,14,15	0.93	1 (7%)	15,19,21	1.39	1 (6%)
3	NAG	B	907	3	14,14,15	0.56	0	15,19,21	1.24	2 (13%)
5	NAG	B	909	1,5	14,14,15	0.61	0	15,19,21	0.91	1 (6%)
5	NAG	B	910	5	14,14,15	0.52	0	15,19,21	0.93	0
5	BMA	B	911	5	11,11,12	0.99	1 (9%)	14,15,17	1.04	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
3	NAG	A	1005	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1006	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1008	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1009	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1010	5	-	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	1/1/1/1
3	NAG	B	906	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	907	3	-	0/6/23/26	0/1/1/1
5	NAG	B	909	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	910	5	-	0/6/23/26	0/1/1/1
5	BMA	B	911	5	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	904	BMA	O5-C1	-3.44	1.38	1.43
3	B	906	NAG	O5-C1	-2.98	1.38	1.43
2	A	1003	BMA	O5-C1	-2.16	1.40	1.43
5	B	911	BMA	O5-C5	2.17	1.48	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	907	NAG	C2-N2-C7	-2.52	119.80	123.04
5	A	1009	NAG	C2-N2-C7	-2.15	120.28	123.04
2	B	904	BMA	C2-C3-C4	2.02	114.47	111.04
5	A	1009	NAG	C1-O5-C5	2.07	114.88	112.25
3	A	1005	NAG	C2-N2-C7	2.18	125.84	123.04

There are no chirality outliers.

There are no torsion outliers.



All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	905	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	1	0
3	A	1005	NAG	1	0
2	B	905	MAN	1	0

## 5.6 Ligand geometry [i](#)

27 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	1007	1	14,14,15	0.57	0	15,19,21	0.89	0
4	NAG	A	1011	1	14,14,15	0.44	0	15,19,21	1.03	1 (6%)
4	NAG	A	1012	1	14,14,15	0.54	0	15,19,21	0.84	1 (6%)
4	NAG	A	1013	1	14,14,15	0.54	0	15,19,21	0.74	0
6	C09	A	1014	-	16,20,20	1.58	3 (18%)	14,28,28	1.49	2 (14%)
7	SO4	A	1015	-	4,4,4	0.27	0	6,6,6	0.12	0
7	SO4	A	1016	-	4,4,4	0.23	0	6,6,6	0.18	0
7	SO4	A	1017	-	4,4,4	0.25	0	6,6,6	0.10	0
7	SO4	A	1018	-	4,4,4	0.25	0	6,6,6	0.10	0
7	SO4	A	1019	-	4,4,4	0.24	0	6,6,6	0.09	0
7	SO4	A	1020	-	4,4,4	0.23	0	6,6,6	0.12	0
7	SO4	A	1021	-	4,4,4	0.24	0	6,6,6	0.19	0
7	SO4	A	1022	-	4,4,4	0.15	0	6,6,6	0.14	0
6	C09	B	901	-	16,20,20	1.59	3 (18%)	14,28,28	1.60	2 (14%)
4	NAG	B	908	1	14,14,15	0.60	0	15,19,21	0.92	1 (6%)
4	NAG	B	912	1	14,14,15	0.60	0	15,19,21	0.64	0
4	NAG	B	913	1	14,14,15	0.51	0	15,19,21	0.82	0
4	NAG	B	914	1	14,14,15	0.51	0	15,19,21	1.02	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	B	915	-	4,4,4	0.21	0	6,6,6	0.11	0
7	SO4	B	916	-	4,4,4	0.27	0	6,6,6	0.09	0
7	SO4	B	917	-	4,4,4	0.25	0	6,6,6	0.07	0
7	SO4	B	918	-	4,4,4	0.23	0	6,6,6	0.07	0
7	SO4	B	919	-	4,4,4	0.23	0	6,6,6	0.11	0
7	SO4	B	920	-	4,4,4	0.22	0	6,6,6	0.06	0
7	SO4	B	921	-	4,4,4	0.25	0	6,6,6	0.08	0
7	SO4	B	922	-	4,4,4	0.23	0	6,6,6	0.10	0
8	GOL	B	923	-	5,5,5	0.35	0	5,5,5	0.28	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
4	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1011	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1012	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1013	1	-	0/6/23/26	0/1/1/1
6	C09	A	1014	-	-	0/2/4/4	0/3/3/3
7	SO4	A	1015	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1016	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1017	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1018	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1019	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1020	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1021	-	-	0/0/0/0	0/0/0/0
7	SO4	A	1022	-	-	0/0/0/0	0/0/0/0
6	C09	B	901	-	-	0/2/4/4	0/3/3/3
4	NAG	B	908	1	-	0/6/23/26	0/1/1/1
4	NAG	B	912	1	-	0/6/23/26	0/1/1/1
4	NAG	B	913	1	-	0/6/23/26	0/1/1/1
4	NAG	B	914	1	-	0/6/23/26	0/1/1/1
7	SO4	B	915	-	-	0/0/0/0	0/0/0/0
7	SO4	B	916	-	-	0/0/0/0	0/0/0/0
7	SO4	B	917	-	-	0/0/0/0	0/0/0/0
7	SO4	B	918	-	-	0/0/0/0	0/0/0/0
7	SO4	B	919	-	-	0/0/0/0	0/0/0/0
7	SO4	B	920	-	-	0/0/0/0	0/0/0/0
7	SO4	B	921	-	-	0/0/0/0	0/0/0/0
7	SO4	B	922	-	-	0/0/0/0	0/0/0/0
8	GOL	B	923	-	-	0/4/4/4	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	901	C09	C2-C3	-3.47	1.37	1.45
6	A	1014	C09	C2-C3	-3.18	1.38	1.45
6	A	1014	C09	C4-N2	-2.86	1.34	1.38
6	B	901	C09	C4-N2	-2.43	1.35	1.38
6	B	901	C09	C2-C1	3.37	1.48	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	901	C09	O-C6-C5	-2.44	103.68	110.86
6	A	1014	C09	O-C6-C5	-2.39	103.81	110.86
4	B	908	NAG	C2-N2-C7	-2.05	120.40	123.04
4	A	1012	NAG	C1-O5-C5	2.43	115.33	112.25
4	B	914	NAG	C1-O5-C5	2.55	115.49	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1016	SO4	1	0
7	A	1020	SO4	1	0
7	A	1021	SO4	1	0
7	A	1022	SO4	1	0
4	B	914	NAG	0	1
7	B	917	SO4	1	0
7	B	920	SO4	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, 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%)	0.22	48 (6%) 23 24	16, 36, 71, 92	0
1	B	746/811 (91%)	0.09	26 (3%) 48 49	16, 34, 64, 91	0
All	All	1493/1622 (92%)	0.16	74 (4%) 32 34	16, 35, 69, 92	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	758	THR	10.1
1	B	759	LYS	6.9
1	A	62	GLY	6.0
1	A	64	TYR	5.5
1	A	758	THR	5.3

### 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
5	NAG	A	1009	14/15	0.96	0.13	1.53	22,25,39,46	0
5	NAG	B	909	14/15	0.96	0.10	0.18	18,22,28,30	0
3	NAG	B	906	14/15	0.94	0.12	0.16	15,24,30,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	1008	14/15	0.95	0.10	0.16	16,21,26,27	0
3	NAG	A	1005	14/15	0.94	0.11	0.02	17,22,29,36	0
2	NAG	A	1001	14/15	0.97	0.15	-0.12	21,27,31,32	0
2	NAG	A	1002	14/15	0.97	0.12	-0.12	23,31,35,40	0
2	NAG	B	902	14/15	0.94	0.11	-0.74	18,20,29,34	0
2	NAG	B	903	14/15	0.95	0.09	-0.75	21,25,30,33	0
2	BMA	A	1003	11/12	0.88	0.10	-	44,48,53,53	0
5	BMA	A	1010	11/12	0.91	0.20	-	45,52,55,56	0
5	NAG	B	910	14/15	0.94	0.11	-	23,26,36,42	0
5	BMA	B	911	11/12	0.86	0.19	-	48,54,59,59	0
2	MAN	B	905	11/12	0.83	0.27	-	54,58,60,63	0
2	BMA	B	904	11/12	0.86	0.14	-	34,46,54,54	0
3	NAG	B	907	14/15	0.86	0.19	-	42,52,61,66	0
2	MAN	A	1004	11/12	0.82	0.12	-	54,56,58,58	0
3	NAG	A	1006	14/15	0.74	0.29	-	44,52,62,65	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
4	NAG	B	908	14/15	0.84	0.21	12.46	49,58,67,71	0
7	SO4	A	1018	5/5	0.95	0.26	10.58	91,92,93,94	0
4	NAG	A	1011	14/15	0.86	0.31	7.47	52,57,65,67	0
7	SO4	B	922	5/5	0.90	0.21	4.55	85,85,86,87	0
7	SO4	A	1021	5/5	0.91	0.17	2.79	82,83,85,85	0
7	SO4	B	919	5/5	0.89	0.17	2.64	85,85,86,87	0
4	NAG	B	913	14/15	0.91	0.16	2.32	38,41,46,47	0
4	NAG	B	912	14/15	0.87	0.16	1.88	50,57,61,62	0
7	SO4	A	1022	5/5	0.96	0.22	1.72	78,79,82,82	0
4	NAG	A	1012	14/15	0.90	0.14	1.13	38,45,49,49	0
4	NAG	A	1007	14/15	0.92	0.15	0.60	40,49,61,67	0
4	NAG	A	1013	14/15	0.94	0.11	0.19	43,50,56,61	0
6	C09	B	901	18/18	0.97	0.13	0.12	17,22,27,29	0
4	NAG	B	914	14/15	0.93	0.12	-0.12	32,46,60,63	0
7	SO4	B	915	5/5	0.97	0.11	-0.13	38,41,52,53	0
6	C09	A	1014	18/18	0.97	0.13	-0.26	15,21,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	A	1017	5/5	0.96	0.10	-0.51	67,68,70,71	0
7	SO4	B	920	5/5	0.97	0.12	-0.63	65,65,68,70	0
7	SO4	B	916	5/5	0.97	0.08	-0.94	54,56,59,61	0
7	SO4	A	1016	5/5	0.98	0.07	-2.84	42,46,50,57	0
7	SO4	B	918	5/5	0.94	0.08	-	84,87,88,89	0
8	GOL	B	923	6/6	0.81	0.19	-	38,43,46,50	0
7	SO4	A	1020	5/5	0.90	0.32	-	95,97,97,99	0
7	SO4	A	1015	5/5	0.98	0.13	-	34,40,46,50	0
7	SO4	B	917	5/5	0.94	0.13	-	63,64,66,67	0
7	SO4	A	1019	5/5	0.92	0.23	-	84,84,85,86	0
7	SO4	B	921	5/5	0.92	0.18	-	89,89,90,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.