



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:13 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 validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

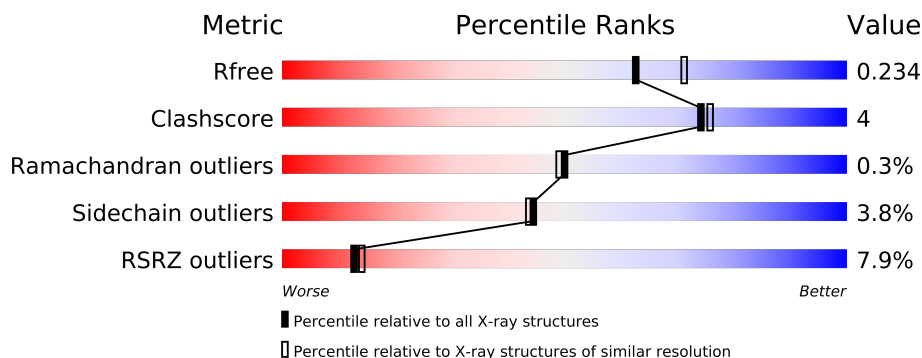
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	811	
1	B	811	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	A	1009	-	X
4	NAG	A	1015	-	X
4	NAG	A	1016	-	X
4	NAG	B	917	-	X
4	NAG	B	920	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13256 atoms, of which 0 are hydrogen and 0 are deuterium.

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 61	C 34	N 2	O 25	0	0
2	A	5	Total 61	C 34	N 2	O 25	0	0
2	B	5	Total 61	C 34	N 2	O 25	0	0
2	B	5	Total 61	C 34	N 2	O 25	0	0

There are 40 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
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
B	23	ARG	-	EXPRESSION TAG	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
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

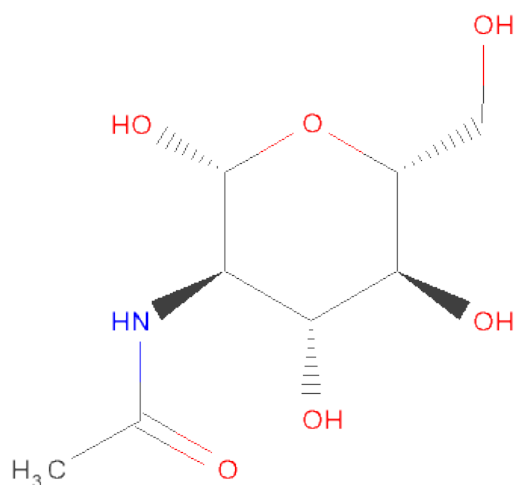
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

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		

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



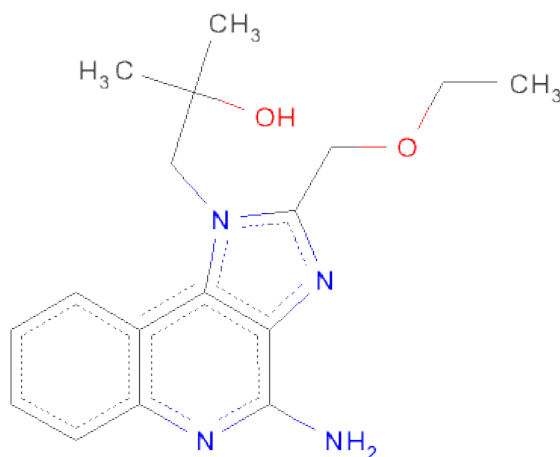
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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

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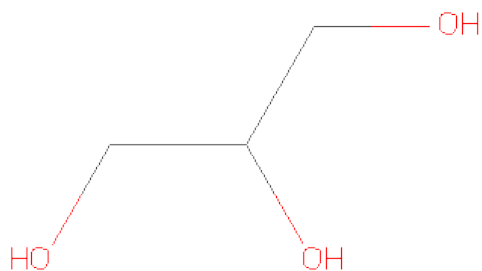
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- 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: C₁₇H₂₂N₄O₂).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is water.

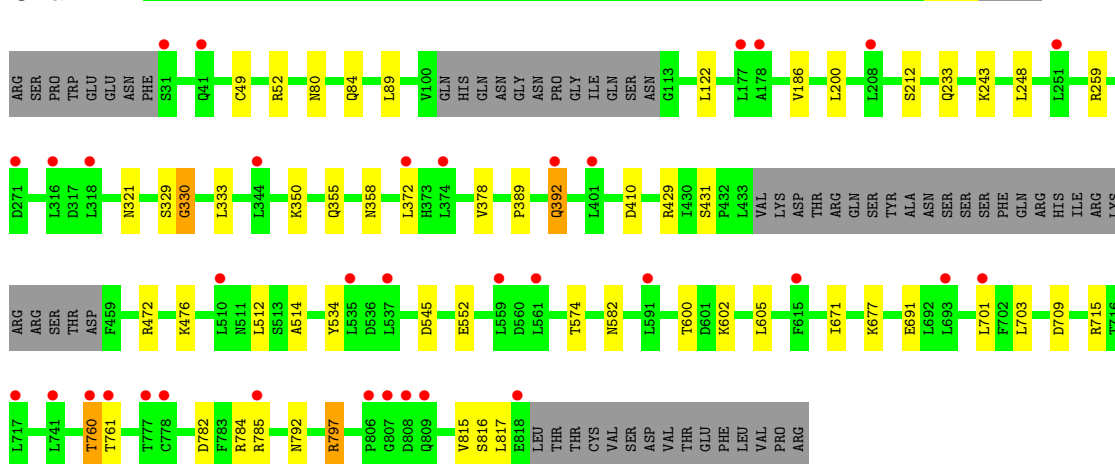
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	419	Total	O	0	0
			419	419		
7	B	248	Total	O	0	0
			248	248		

3 Residue-property plots

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.

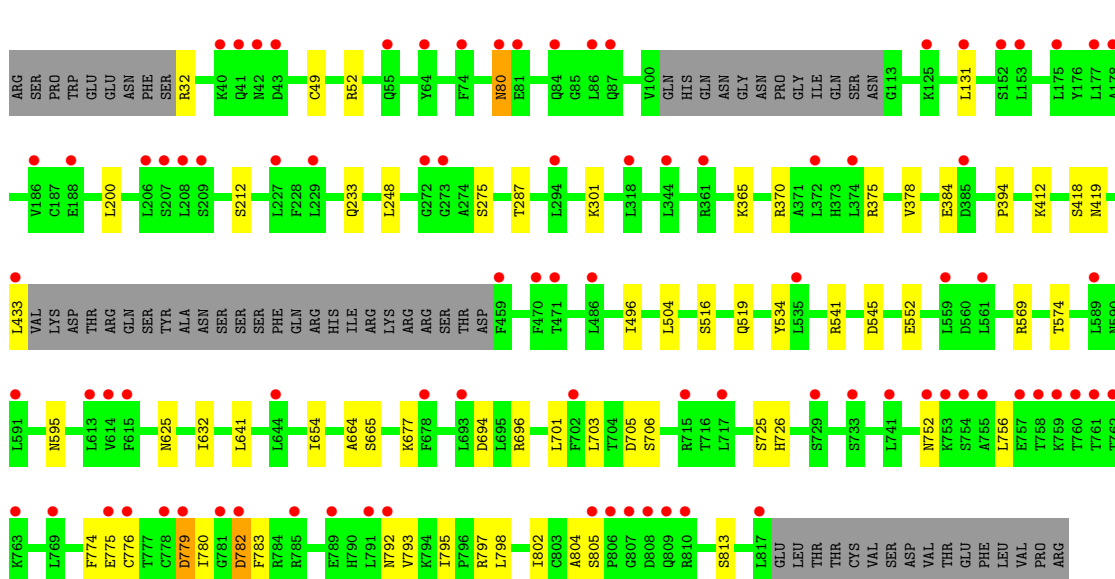
• Molecule 1: Toll-like receptor 8

Chain A:



• Molecule 1: Toll-like receptor 8

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.200 , 0.233 0.201 , 0.234	Depositor DCC
R_{free} test set	6495 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 129652 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13256	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6039	0	0	25	0
1	B	5994	0	0	26	0
2	A	122	0	0	0	0
2	B	122	0	0	0	0
3	A	39	0	0	0	0
3	B	39	0	0	0	0
4	A	84	0	0	1	0
4	B	98	0	0	0	0
5	A	23	0	0	0	0
5	B	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	6	0	0	0	0
7	A	419	0	0	13	0
7	B	248	0	0	8	0
All	All	13256	0	0	51	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 51 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:355:GLN:NE2	7:A:1476:HOH:O	2.16	0.77
1:B:370:ARG:NH1	7:B:1094:HOH:O	2.17	0.77
1:A:784:ARG:NE	7:A:1444:HOH:O	2.18	0.75

There are no symmetry-related clashes.

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	745/811 (92%)	711 (95%)	32 (4%)	2 (0%)	50	49
1	B	743/811 (92%)	710 (96%)	31 (4%)	2 (0%)	50	49
All	All	1488/1622 (92%)	1421 (96%)	63 (4%)	4 (0%)	50	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	797	ARG
1	A	378	VAL
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%)	48	48
1	B	683/755 (90%)	654 (96%)	29 (4%)	40	38
All	All	1377/1510 (91%)	1324 (96%)	53 (4%)	44	44

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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	12,14,15	0.70	1 (8%)	15,19,21	0.80	0
2	NAG	A	1002	2	12,14,15	0.74	0	15,19,21	0.91	1 (6%)
2	BMA	A	1003	2	10,11,12	0.51	0	11,15,17	1.01	0
2	MAN	A	1004	2	10,11,12	0.79	0	11,15,17	0.71	1 (9%)
2	MAN	A	1005	2	10,11,12	0.78	0	11,15,17	0.97	1 (9%)
3	NAG	A	1006	1,3	12,14,15	0.66	0	15,19,21	1.10	2 (13%)
3	NAG	A	1007	3	12,14,15	0.71	1 (8%)	15,19,21	0.73	0
3	BMA	A	1008	3	10,11,12	0.43	0	11,15,17	0.98	0
2	NAG	A	1010	1,2	12,14,15	0.73	1 (8%)	15,19,21	0.84	0
2	NAG	A	1011	2	12,14,15	0.71	0	15,19,21	0.91	0
2	BMA	A	1012	2	10,11,12	0.92	1 (10%)	11,15,17	1.71	3 (27%)
2	MAN	A	1013	2	10,11,12	0.83	1 (10%)	11,15,17	0.89	0
2	MAN	A	1014	2	10,11,12	0.73	0	11,15,17	0.91	0
2	NAG	B	902	1,2	12,14,15	0.67	0	15,19,21	0.96	1 (6%)
2	NAG	B	903	2	12,14,15	0.76	1 (8%)	15,19,21	1.08	1 (6%)
2	BMA	B	904	2	10,11,12	0.57	0	11,15,17	0.97	1 (9%)
2	MAN	B	905	2	10,11,12	0.82	1 (10%)	11,15,17	0.96	1 (9%)
2	MAN	B	906	2	10,11,12	0.80	0	11,15,17	1.03	1 (9%)
3	NAG	B	907	1,3	12,14,15	0.66	0	15,19,21	0.88	1 (6%)
3	NAG	B	908	3	12,14,15	0.72	1 (8%)	15,19,21	0.70	0
3	BMA	B	909	3	10,11,12	0.55	0	11,15,17	1.02	0
2	NAG	B	911	1,2	12,14,15	0.64	0	15,19,21	0.83	1 (6%)
2	NAG	B	912	2	12,14,15	0.72	0	15,19,21	0.96	0
2	BMA	B	913	2	10,11,12	0.62	0	11,15,17	0.88	0
2	MAN	B	914	2	10,11,12	0.81	1 (10%)	11,15,17	0.66	0
2	MAN	B	915	2	10,11,12	0.78	0	11,15,17	0.96	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	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1012	BMA	C4-C5	2.36	1.58	1.53
3	B	908	NAG	O5-C5	-2.22	1.41	1.45
3	A	1007	NAG	O5-C5	-2.20	1.41	1.45
2	A	1001	NAG	O5-C5	-2.18	1.41	1.45
2	B	903	NAG	O5-C5	-2.18	1.41	1.45

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1012	BMA	O5-C5-C6	-4.08	102.70	106.98
2	B	903	NAG	O5-C5-C6	3.31	110.45	106.98
2	B	906	MAN	O5-C5-C6	2.94	110.07	106.98
2	A	1005	MAN	O5-C5-C6	2.88	110.00	106.98
3	A	1006	NAG	O5-C5-C6	2.87	109.99	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

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	12,14,15	0.69	1 (8%)	15,19,21	0.79	0
4	NAG	A	1015	1	12,14,15	0.65	0	15,19,21	1.06	2 (13%)
4	NAG	A	1016	1	12,14,15	0.67	0	15,19,21	0.85	1 (6%)
4	NAG	A	1017	1	12,14,15	0.61	0	15,19,21	1.08	1 (6%)
4	NAG	A	1018	1	12,14,15	0.74	1 (8%)	15,19,21	0.81	0
4	NAG	A	1019	1	12,14,15	0.57	0	15,19,21	1.05	2 (13%)
5	RX8	A	1020	-	25,25,25	1.57	4 (16%)	37,37,37	1.50	5 (13%)
6	GOL	A	1021	-	5,5,5	0.35	0	5,5,5	0.25	0
5	RX8	B	901	-	25,25,25	1.52	4 (16%)	37,37,37	1.38	5 (13%)
4	NAG	B	910	1	12,14,15	0.65	0	15,19,21	0.95	1 (6%)
4	NAG	B	916	1	12,14,15	0.64	0	15,19,21	0.93	1 (6%)
4	NAG	B	917	1	12,14,15	0.68	1 (8%)	15,19,21	0.94	0
4	NAG	B	918	1	12,14,15	0.73	1 (8%)	15,19,21	0.90	1 (6%)
4	NAG	B	919	1	12,14,15	0.57	0	15,19,21	1.46	3 (20%)
4	NAG	B	920	1	12,14,15	0.64	0	15,19,21	1.03	1 (6%)
4	NAG	B	921	1	12,14,15	0.58	0	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	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1015	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	2/9/9/9	0/0/3/3
6	GOL	A	1021	-	-	0/4/4/4	0/0/0/0
5	RX8	B	901	-	-	2/9/9/9	0/0/3/3
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 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1020	RX8	C2-C3	4.72	1.49	1.40
5	B	901	RX8	C2-C3	4.49	1.48	1.40
5	B	901	RX8	C2-C1	-2.91	1.37	1.41
5	A	1020	RX8	C2-C1	-2.74	1.37	1.41
5	A	1020	RX8	C-N	2.63	1.43	1.35

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1020	RX8	C-N1-C1	4.56	122.34	118.42
5	B	901	RX8	C-N1-C1	4.48	122.28	118.42
5	A	1020	RX8	C9-N3-C5	-4.32	124.78	127.34
5	B	901	RX8	C9-N3-C5	-3.67	125.16	127.34
5	A	1020	RX8	C6-O-C7	3.50	120.07	112.57

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	RX8	O-C6-C5-N2
5	B	901	RX8	O-C6-C5-N3
5	A	1020	RX8	O-C6-C5-N2
5	A	1020	RX8	O-C6-C5-N3

There are no ring outliers.

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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	751/811 (92%)	0.13	35 (4%) 30 33	19, 35, 62, 92	0
1	B	749/811 (92%)	0.55	87 (11%) 5 6	21, 46, 87, 107	0
All	All	1500/1622 (92%)	0.34	122 (8%) 13 13	19, 40, 78, 107	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	759	LYS	8.7
1	B	761	THR	7.2
1	B	64	TYR	6.6
1	B	758	THR	5.7
1	B	754	SER	5.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MAN	A	1004	11/12	0.20	5.83	33,39,47,55	0
2	MAN	B	905	11/12	0.22	3.16	45,60,66,67	0
3	NAG	B	908	14/15	0.20	0.85	44,57,67,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	1002	14/15	0.09	-0.48	19,23,32,35	0
2	NAG	B	902	14/15	0.14	-0.53	27,29,35,37	0
2	NAG	B	912	14/15	0.11	-0.61	30,34,43,43	0
2	NAG	B	903	14/15	0.10	-0.94	30,33,37,38	0
2	NAG	B	911	14/15	0.12	-1.09	23,31,34,41	0
2	NAG	A	1011	14/15	0.09	-1.11	21,26,36,47	0
3	NAG	A	1007	14/15	0.13	-1.14	36,49,53,56	0
2	NAG	A	1001	14/15	0.08	-1.52	17,21,29,31	0
3	NAG	A	1006	14/15	0.07	-2.35	20,23,28,34	0
3	NAG	B	907	14/15	0.07	-2.58	22,28,36,37	0
2	NAG	A	1010	14/15	0.07	-2.89	18,21,27,28	0
2	MAN	B	906	11/12	0.30	-	70,73,76,77	0
2	MAN	A	1005	11/12	0.28	-	56,66,71,76	0
2	BMA	B	904	11/12	0.17	-	39,56,63,64	0
2	MAN	B	915	11/12	0.35	-	72,78,86,87	0
3	BMA	B	909	11/12	0.34	-	69,72,73,74	0
3	BMA	A	1008	11/12	0.30	-	63,67,69,69	0
2	MAN	A	1014	11/12	0.35	-	69,73,76,76	0
2	BMA	A	1012	11/12	0.21	-	40,55,67,75	0
2	BMA	B	913	11/12	0.21	-	49,63,71,74	0
2	MAN	B	914	11/12	0.35	-	73,79,84,86	0
2	BMA	A	1003	11/12	0.12	-	32,43,54,56	0
2	MAN	A	1013	11/12	0.37	-	67,73,81,82	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	1009	14/15	0.17	9.77	48,56,68,73	0
4	NAG	B	920	14/15	0.32	5.72	77,82,86,87	0
4	NAG	A	1015	14/15	0.27	5.47	52,64,74,75	0
4	NAG	A	1016	14/15	0.31	5.06	62,65,67,69	0
4	NAG	B	917	14/15	0.26	4.46	50,60,73,76	0
4	NAG	B	921	14/15	0.25	1.52	68,72,74,77	0
6	GOL	A	1021	6/6	0.16	1.42	66,71,73,74	0
4	NAG	B	910	14/15	0.12	1.41	44,60,67,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	B	916	14/15	0.24	1.35	64,75,83,83	0
4	NAG	A	1017	14/15	0.37	1.04	62,68,75,78	0
5	RX8	B	901	23/23	0.12	0.50	22,29,41,45	0
4	NAG	B	919	14/15	0.23	0.14	52,57,63,69	0
4	NAG	B	918	14/15	0.12	-0.06	44,52,56,57	0
4	NAG	A	1018	14/15	0.10	-0.15	36,42,50,51	0
5	RX8	A	1020	23/23	0.10	-0.33	22,32,41,42	0
4	NAG	A	1019	14/15	0.09	-0.87	29,31,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.