



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 04:38 AM GMT

PDB ID : 3W3L
Title : Crystal structure of human TLR8 in complex with Resiquimod (R848) crystal form 1
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2012-12-22
Resolution : 2.33 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>

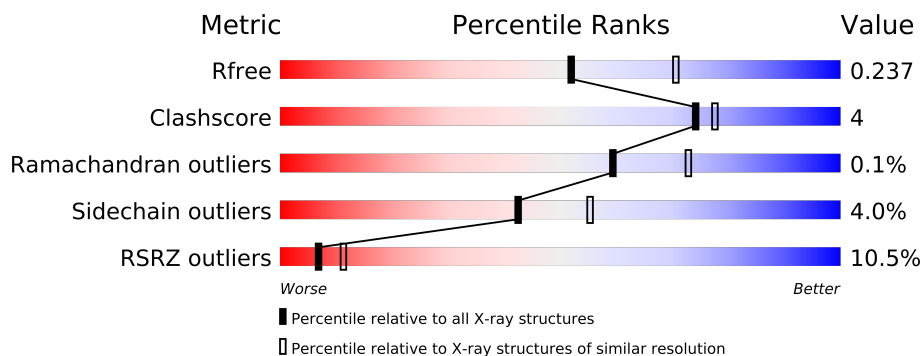
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.33 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	4049 (2.38-2.30)
Clashscore	79885	1094 (2.36-2.32)
Ramachandran outliers	78287	1080 (2.36-2.32)
Sidechain outliers	78261	1081 (2.36-2.32)
RSRZ outliers	66119	4050 (2.38-2.30)

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	
1	C	811	
1	D	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
5	SO4	A	1019	-	X
5	SO4	B	1020	-	X
5	SO4	B	1021	-	X
5	SO4	C	918	-	X
5	SO4	D	921	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26024 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
			6038	3862	1025	1132	19			
1	B	751	Total	C	N	O	S	0	0	0
			6035	3859	1025	1132	19			
1	C	751	Total	C	N	O	S	0	0	0
			6035	3859	1025	1132	19			
1	D	751	Total	C	N	O	S	0	0	0
			6035	3859	1025	1132	19			

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
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
C	23	ARG	-	EXPRESSION TAG	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	SER	-	EXPRESSION TAG	UNP Q9NR97
C	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
C	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
C	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
C	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
C	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
C	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
C	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
C	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	24	SER	-	EXPRESSION TAG	UNP Q9NR97
D	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
D	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
D	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
D	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
D	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
D	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	833	ARG	-	EXPRESSION TAG	UNP Q9NR97

- Molecule 2 is 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		
2	C	5	Total	C	N	O	0	0
			61	34	2	25		
2	C	5	Total	C	N	O	0	0
			61	34	2	25		
2	D	5	Total	C	N	O	0	0
			61	34	2	25		
2	D	5	Total	C	N	O	0	0
			61	34	2	25		

There are 80 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
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
C	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
C	24	SER	-	EXPRESSION TAG	UNP Q9NR97
C	25	PRO	-	EXPRESSION TAG	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
C	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
C	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
C	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
C	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
C	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
C	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
C	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
C	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
C	24	SER	-	EXPRESSION TAG	UNP Q9NR97
C	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
C	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
C	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
C	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
C	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
C	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
C	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
C	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	24	SER	-	EXPRESSION TAG	UNP Q9NR97
D	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
D	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
D	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
D	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
D	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
D	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	24	SER	-	EXPRESSION TAG	UNP Q9NR97
D	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
D	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
D	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
D	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
D	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
D	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	833	ARG	-	EXPRESSION TAG	UNP Q9NR97

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

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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		
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	D	3	Total	C	N	O	0	0
			39	22	2	15		

There are 40 discrepancies between the modelled and reference sequences:

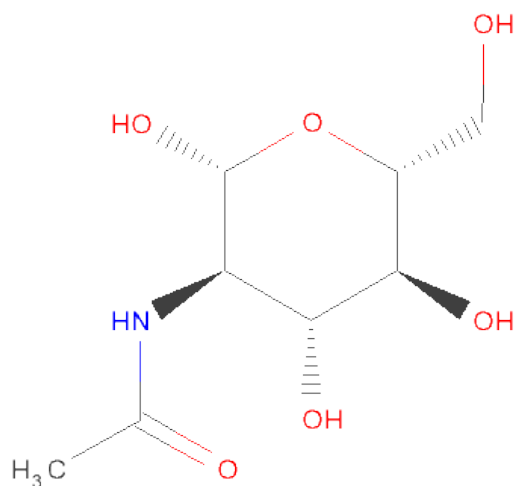
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	24	SER	-	EXPRESSION TAG	UNP Q9NR97
A	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
A	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
A	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
A	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
A	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
A	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
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
C	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
C	24	SER	-	EXPRESSION TAG	UNP Q9NR97
C	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
C	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
C	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
C	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
C	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
C	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
C	832	PRO	-	EXPRESSION TAG	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
C	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	24	SER	-	EXPRESSION TAG	UNP Q9NR97
D	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
D	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
D	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
D	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
D	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
D	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	833	ARG	-	EXPRESSION TAG	UNP Q9NR97

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



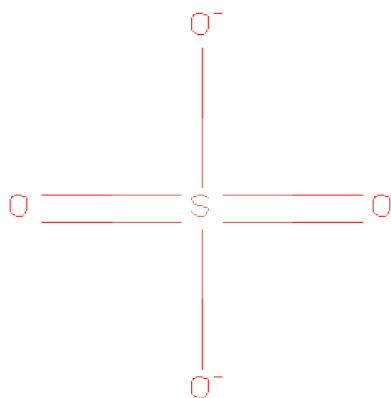
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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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		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



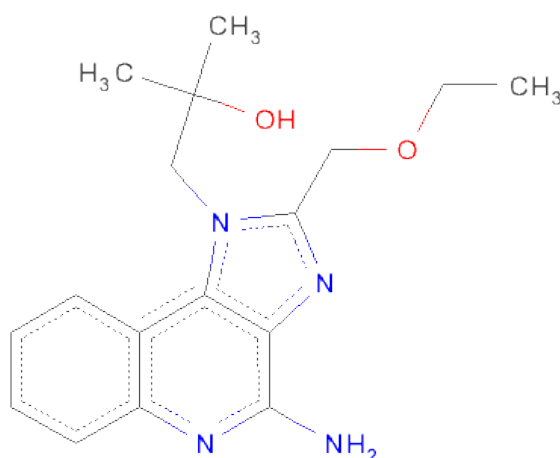
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5	4 1		

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

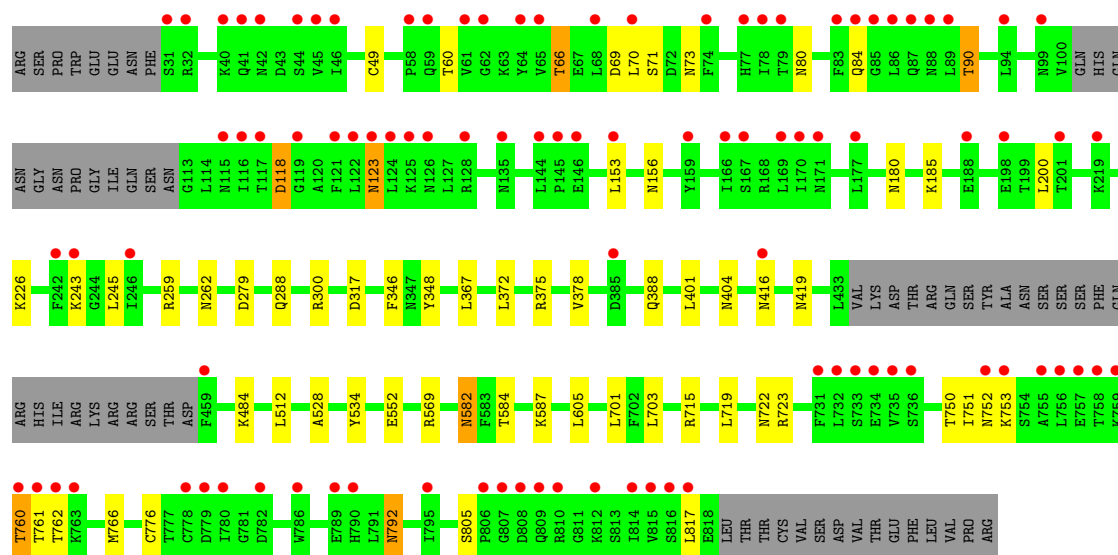
- Molecule 6 is 1-[4-AMINO-2-(ETHOXYMETHYL)-1H-IMIDAZO[4,5-C]QUINOLIN-1-YL]-2-METHYLPROPAN-2-OL (three-letter code: RX8) (formula: C₁₇H₂₂N₄O₂).



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

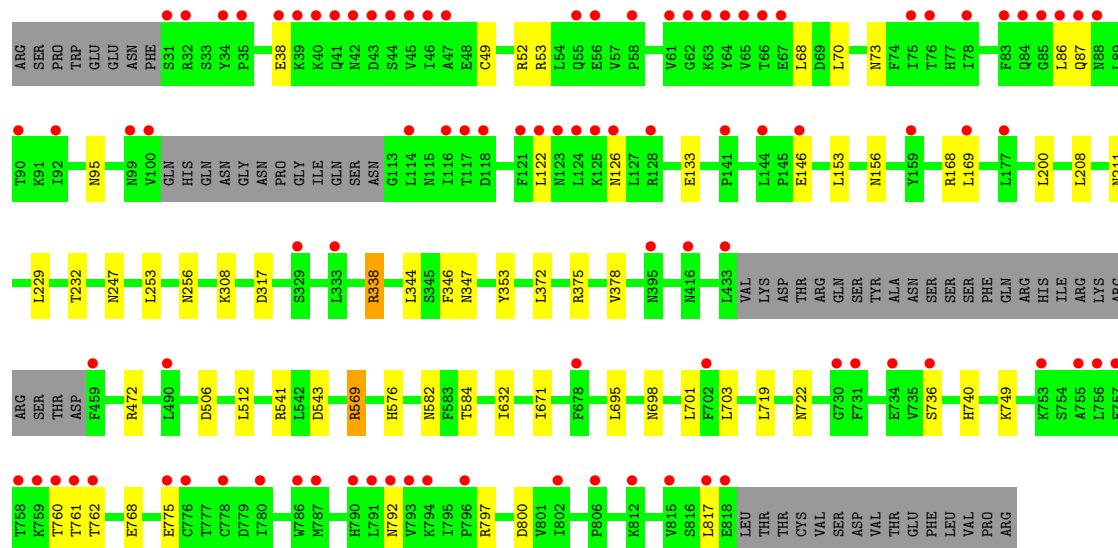
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	269	Total 269	O 269	0	0
7	B	240	Total 240	O 240	0	0
7	C	214	Total 214	O 214	0	0
7	D	172	Total 172	O 172	0	0



● Molecule 1: Toll-like receptor 8

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.47Å 138.87Å 169.66Å 90.00° 92.43° 90.00°	Depositor
Resolution (Å)	45.08 – 2.33 45.07 – 2.33	Depositor EDS
% Data completeness (in resolution range)	93.1 (45.08-2.33) 93.1 (45.07-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.196 , 0.239 0.198 , 0.237	Depositor DCC
R_{free} test set	7988 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.8	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 159447 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26024	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 3.10% 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, 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	0.35	0/6163	0.61	1/8360 (0.0%)
1	B	0.34	0/6160	0.60	0/8356
1	C	0.33	0/6160	0.58	0/8356
1	D	0.31	0/6160	0.57	0/8356
All	All	0.33	0/24643	0.59	1/33428 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	753	LYS	CD-CE-NZ	-5.75	98.49	111.70

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	6038	0	0	21	2
1	B	6035	0	0	28	0
1	C	6035	0	0	31	0
1	D	6035	0	0	24	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	122	0	0	0	0
2	B	122	0	0	1	0
2	C	122	0	0	1	0
2	D	122	0	0	0	0
3	A	39	0	0	0	0
3	B	39	0	0	0	0
3	C	39	0	0	0	0
3	D	39	0	0	0	0
4	A	56	0	0	0	0
4	B	56	0	0	0	0
4	C	42	0	0	0	0
4	D	56	0	0	0	0
5	A	10	0	0	0	0
5	B	15	0	0	1	0
5	C	5	0	0	1	0
5	D	10	0	0	0	0
6	B	23	0	0	0	0
6	C	23	0	0	0	0
6	D	46	0	0	1	0
7	A	269	0	0	8	0
7	B	240	0	0	10	0
7	C	214	0	0	9	0
7	D	172	0	0	5	0
All	All	26024	0	0	103	2

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 103 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:289:LEU:N	7:B:1199:HOH:O	2.09	0.84
1:A:34:TYR:O	1:A:60:THR:OG1	1.99	0.79
1:C:80:ASN:O	1:C:84:GLN:NE2	2.17	0.78
1:C:123:ASN:OD1	1:C:123:ASN:N	2.20	0.74
1:B:705:ASP:OD1	1:B:705:ASP:N	2.22	0.72

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	Distance(Å)	Clash(Å)
1:A:760:THR:OG1	1:D:308:LYS:O[2_645]	2.13	0.07
1:A:708:SER:O	1:D:338:ARG:NH2[2_645]	2.18	0.02

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%)	720 (97%)	24 (3%)	1 (0%)	59	73
1	B	745/811 (92%)	722 (97%)	22 (3%)	1 (0%)	59	73
1	C	745/811 (92%)	723 (97%)	21 (3%)	1 (0%)	59	73
1	D	745/811 (92%)	723 (97%)	21 (3%)	1 (0%)	59	73
All	All	2980/3244 (92%)	2888 (97%)	88 (3%)	4 (0%)	59	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	VAL
1	B	378	VAL
1	C	378	VAL
1	D	378	VAL

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%)	660 (95%)	34 (5%)	35	43
1	B	693/755 (92%)	668 (96%)	25 (4%)	47	60
1	C	693/755 (92%)	666 (96%)	27 (4%)	43	57
1	D	693/755 (92%)	668 (96%)	25 (4%)	47	60
All	All	2773/3020 (92%)	2662 (96%)	111 (4%)	42	55

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	516	SER
1	C	90	THR
1	D	582	ASN
1	B	605	LEU
1	B	759	LYS

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 ⓘ

52 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	0.79	1 (8%)	15,19,21	1.04	0
2	NAG	A	1002	2	12,14,15	0.68	1 (8%)	15,19,21	0.89	0
2	BMA	A	1003	2	10,11,12	0.71	0	11,15,17	0.94	1 (9%)
2	MAN	A	1004	2	10,11,12	0.71	0	11,15,17	0.95	1 (9%)
2	MAN	A	1005	2	10,11,12	0.81	0	11,15,17	0.76	0
3	NAG	A	1006	1,3	12,14,15	0.62	0	15,19,21	1.29	3 (20%)
3	NAG	A	1007	3	12,14,15	0.73	1 (8%)	15,19,21	1.24	2 (13%)
3	BMA	A	1008	3	10,11,12	0.69	0	11,15,17	1.18	1 (9%)
2	NAG	A	1010	1,2	12,14,15	0.75	1 (8%)	15,19,21	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1011	2	12,14,15	0.72	0	15,19,21	1.32	3 (20%)
2	BMA	A	1012	2	10,11,12	1.01	0	11,15,17	1.04	0
2	MAN	A	1013	2	10,11,12	0.84	1 (10%)	11,15,17	1.20	1 (9%)
2	MAN	A	1014	2	10,11,12	0.70	0	11,15,17	0.89	0
2	NAG	B	1001	1,2	12,14,15	0.76	1 (8%)	15,19,21	1.06	1 (6%)
2	NAG	B	1002	2	12,14,15	0.76	1 (8%)	15,19,21	0.88	0
2	BMA	B	1003	2	10,11,12	0.57	0	11,15,17	0.95	0
2	MAN	B	1004	2	10,11,12	0.73	0	11,15,17	0.78	0
2	MAN	B	1005	2	10,11,12	0.76	0	11,15,17	1.05	1 (9%)
3	NAG	B	1006	1,3	12,14,15	0.70	0	15,19,21	1.40	3 (20%)
3	NAG	B	1007	3	12,14,15	0.70	1 (8%)	15,19,21	1.15	1 (6%)
3	BMA	B	1008	3	10,11,12	0.85	0	11,15,17	1.22	1 (9%)
2	NAG	B	1010	1,2	12,14,15	0.67	1 (8%)	15,19,21	1.17	2 (13%)
2	NAG	B	1011	2	12,14,15	0.89	1 (8%)	15,19,21	0.90	1 (6%)
2	BMA	B	1012	2	10,11,12	0.89	0	11,15,17	1.07	1 (9%)
2	MAN	B	1013	2	10,11,12	0.85	1 (10%)	11,15,17	0.93	1 (9%)
2	MAN	B	1014	2	10,11,12	0.72	0	11,15,17	0.84	0
2	NAG	C	902	1,2	12,14,15	0.66	0	15,19,21	1.31	2 (13%)
2	NAG	C	903	2	12,14,15	0.73	1 (8%)	15,19,21	1.07	0
2	BMA	C	904	2	10,11,12	0.70	0	11,15,17	1.06	0
2	MAN	C	905	2	10,11,12	0.81	1 (10%)	11,15,17	0.80	0
2	MAN	C	906	2	10,11,12	0.78	0	11,15,17	0.82	1 (9%)
3	NAG	C	907	1,3	12,14,15	0.63	0	15,19,21	0.94	1 (6%)
3	NAG	C	908	3	12,14,15	0.76	1 (8%)	15,19,21	1.00	0
3	BMA	C	909	3	10,11,12	0.78	0	11,15,17	1.26	3 (27%)
2	NAG	C	911	1,2	12,14,15	0.79	1 (8%)	15,19,21	0.92	1 (6%)
2	NAG	C	912	2	12,14,15	0.75	1 (8%)	15,19,21	0.85	0
2	BMA	C	913	2	10,11,12	0.90	0	11,15,17	1.07	1 (9%)
2	MAN	C	914	2	10,11,12	0.80	0	11,15,17	1.16	1 (9%)
2	MAN	C	915	2	10,11,12	0.68	0	11,15,17	0.96	1 (9%)
2	NAG	D	903	1,2	12,14,15	0.66	0	15,19,21	1.08	1 (6%)
2	NAG	D	904	2	12,14,15	0.64	0	15,19,21	1.07	2 (13%)
2	BMA	D	905	2	10,11,12	0.86	1 (10%)	11,15,17	0.96	0
2	MAN	D	906	2	10,11,12	0.73	0	11,15,17	0.72	0
2	MAN	D	907	2	10,11,12	0.83	1 (10%)	11,15,17	0.87	0
3	NAG	D	908	1,3	12,14,15	0.66	0	15,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	909	3	12,14,15	0.72	1 (8%)	15,19,21	1.33	4 (26%)
3	BMA	D	910	3	10,11,12	0.78	0	11,15,17	1.19	1 (9%)
2	NAG	D	912	1,2	12,14,15	0.82	1 (8%)	15,19,21	0.94	0
2	NAG	D	913	2	12,14,15	0.69	0	15,19,21	0.95	1 (6%)
2	BMA	D	914	2	10,11,12	0.78	0	11,15,17	0.83	0
2	MAN	D	915	2	10,11,12	0.77	0	11,15,17	0.94	1 (9%)
2	MAN	D	916	2	10,11,12	0.71	0	11,15,17	0.84	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
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	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	B	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1004	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1005	2	-	0/2/19/22	0/1/1/1
3	NAG	B	1006	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1007	3	-	0/6/23/26	0/1/1/1
3	BMA	B	1008	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1010	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1011	2	-	0/6/23/26	0/1/1/1
2	BMA	B	1012	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1013	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1014	2	-	0/2/19/22	0/1/1/1
2	NAG	C	902	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	903	2	-	0/6/23/26	0/1/1/1
2	BMA	C	904	2	-	0/2/19/22	0/1/1/1
2	MAN	C	905	2	-	0/2/19/22	0/1/1/1
2	MAN	C	906	2	-	0/2/19/22	0/1/1/1
3	NAG	C	907	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	908	3	-	0/6/23/26	0/1/1/1
3	BMA	C	909	3	-	0/2/19/22	0/1/1/1
2	NAG	C	911	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	912	2	-	0/6/23/26	0/1/1/1
2	BMA	C	913	2	-	0/2/19/22	0/1/1/1
2	MAN	C	914	2	-	0/2/19/22	0/1/1/1
2	MAN	C	915	2	-	0/2/19/22	0/1/1/1
2	NAG	D	903	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	904	2	-	0/6/23/26	0/1/1/1
2	BMA	D	905	2	-	0/2/19/22	0/1/1/1
2	MAN	D	906	2	-	0/2/19/22	0/1/1/1
2	MAN	D	907	2	-	0/2/19/22	0/1/1/1
3	NAG	D	908	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	909	3	-	0/6/23/26	0/1/1/1
3	BMA	D	910	3	-	0/2/19/22	0/1/1/1
2	NAG	D	912	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	913	2	-	0/6/23/26	0/1/1/1
2	BMA	D	914	2	-	0/2/19/22	0/1/1/1
2	MAN	D	915	2	-	0/2/19/22	0/1/1/1
2	MAN	D	916	2	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	911	NAG	O5-C5	-2.42	1.40	1.45
3	C	908	NAG	O5-C5	-2.37	1.41	1.45
2	A	1001	NAG	O5-C5	-2.35	1.41	1.45
2	D	912	NAG	O5-C5	-2.31	1.41	1.45
2	C	903	NAG	O5-C5	-2.31	1.41	1.45

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	NAG	O5-C5-C6	3.41	110.56	106.98
3	B	1006	NAG	O5-C5-C6	3.37	110.52	106.98
2	D	903	NAG	O5-C5-C6	3.34	110.49	106.98
3	D	909	NAG	O5-C5-C6	3.22	110.36	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	914	MAN	O5-C5-C6	3.18	110.32	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

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	1009	1	12,14,15	0.72	1 (8%)	15,19,21	0.82	0
4	NAG	A	1015	1	12,14,15	0.61	0	15,19,21	0.92	1 (6%)
4	NAG	A	1016	1	12,14,15	0.64	0	15,19,21	1.19	3 (20%)
4	NAG	A	1017	1	12,14,15	0.62	0	15,19,21	0.87	0
5	SO4	A	1018	-	4,4,4	0.25	0	6,6,6	0.08	0
5	SO4	A	1019	-	4,4,4	0.13	0	6,6,6	0.16	0
4	NAG	B	1009	1	12,14,15	0.68	1 (8%)	15,19,21	0.99	0
4	NAG	B	1015	1	12,14,15	0.60	0	15,19,21	1.02	1 (6%)
4	NAG	B	1016	1	12,14,15	0.70	0	15,19,21	1.17	1 (6%)
4	NAG	B	1017	1	12,14,15	0.62	0	15,19,21	0.96	1 (6%)
6	RX8	B	1018	-	25,25,25	1.61	5 (20%)	37,37,37	1.70	6 (16%)
5	SO4	B	1019	-	4,4,4	0.21	0	6,6,6	0.08	0
5	SO4	B	1020	-	4,4,4	0.09	0	6,6,6	0.25	0
5	SO4	B	1021	-	4,4,4	0.03	0	6,6,6	0.33	0
6	RX8	C	901	-	25,25,25	1.55	4 (16%)	37,37,37	1.53	4 (10%)
4	NAG	C	910	1	12,14,15	0.66	0	15,19,21	0.75	0
4	NAG	C	916	1	12,14,15	0.73	0	15,19,21	1.30	2 (13%)
4	NAG	C	917	1	12,14,15	0.70	1 (8%)	15,19,21	0.96	1 (6%)
5	SO4	C	918	-	4,4,4	0.22	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	RX8	D	901	-	25,25,25	1.52	4 (16%)	37,37,37	1.51	4 (10%)
6	RX8	D	902	-	25,25,25	1.59	5 (20%)	37,37,37	1.44	6 (16%)
4	NAG	D	911	1	12,14,15	0.66	1 (8%)	15,19,21	0.75	0
4	NAG	D	917	1	12,14,15	0.73	1 (8%)	15,19,21	1.01	1 (6%)
4	NAG	D	918	1	12,14,15	0.63	0	15,19,21	0.97	0
4	NAG	D	919	1	12,14,15	0.58	0	15,19,21	0.91	1 (6%)
5	SO4	D	920	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	D	921	-	4,4,4	0.08	0	6,6,6	0.20	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	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
5	SO4	A	1018	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1019	-	-	0/0/0/0	0/0/0/0
4	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1015	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1016	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1017	1	-	0/6/23/26	0/1/1/1
6	RX8	B	1018	-	-	0/9/9/9	0/0/3/3
5	SO4	B	1019	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1020	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1021	-	-	0/0/0/0	0/0/0/0
6	RX8	C	901	-	-	2/9/9/9	0/0/3/3
4	NAG	C	910	1	-	0/6/23/26	0/1/1/1
4	NAG	C	916	1	-	0/6/23/26	0/1/1/1
4	NAG	C	917	1	-	0/6/23/26	0/1/1/1
5	SO4	C	918	-	-	0/0/0/0	0/0/0/0
6	RX8	D	901	-	-	0/9/9/9	0/0/3/3
6	RX8	D	902	-	-	2/9/9/9	0/0/3/3
4	NAG	D	911	1	-	0/6/23/26	0/1/1/1
4	NAG	D	917	1	-	0/6/23/26	0/1/1/1
4	NAG	D	918	1	-	0/6/23/26	0/1/1/1
4	NAG	D	919	1	-	0/6/23/26	0/1/1/1
5	SO4	D	920	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	D	921	-	-	0/0/0/0	0/0/0/0

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1018	RX8	C2-C3	4.94	1.49	1.40
6	D	902	RX8	C2-C3	4.73	1.49	1.40
6	D	901	RX8	C2-C3	4.65	1.49	1.40
6	C	901	RX8	C2-C3	4.38	1.48	1.40
6	C	901	RX8	C2-C1	-2.90	1.37	1.41

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	901	RX8	C9-N3-C5	-4.92	124.42	127.34
6	B	1018	RX8	C9-N3-C5	-4.86	124.46	127.34
6	B	1018	RX8	C6-O-C7	4.76	122.77	112.57
6	B	1018	RX8	C-N1-C1	4.61	122.39	118.42
6	D	901	RX8	C-N1-C1	4.52	122.31	118.42

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	902	RX8	O-C6-C5-N3
6	D	902	RX8	O-C6-C5-N2
6	C	901	RX8	O-C6-C5-N2
6	C	901	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%)	0.53	48 (6%)	19 28	11, 33, 87, 120	0
1	B	751/811 (92%)	0.56	84 (11%)	6 10	9, 33, 93, 127	0
1	C	751/811 (92%)	0.75	97 (12%)	4 7	11, 43, 92, 115	0
1	D	751/811 (92%)	0.76	94 (12%)	5 8	14, 49, 91, 115	0
All	All	3004/3244 (92%)	0.65	323 (10%)	7 10	9, 39, 92, 127	0

The worst 5 of 323 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	761	THR	14.8
1	C	88	ASN	14.2
1	C	756	LEU	13.9
1	B	733	SER	12.1
1	C	86	LEU	12.0

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(\AA^2)	Q<0.9
3	NAG	B	1007	14/15	0.16	5.25	32,43,56,63	0
3	NAG	B	1006	14/15	0.15	0.91	9,18,22,28	0
2	MAN	B	1004	11/12	0.12	0.77	29,41,45,48	0
2	NAG	D	903	14/15	0.16	0.61	34,37,52,54	0
2	NAG	B	1001	14/15	0.14	0.59	8,14,22,25	0
2	NAG	A	1002	14/15	0.17	0.40	8,20,34,34	0
2	NAG	C	903	14/15	0.13	0.01	29,41,51,55	0
2	NAG	C	902	14/15	0.14	-0.09	30,36,38,41	0
2	MAN	A	1004	11/12	0.11	-0.29	36,40,43,44	0
3	NAG	A	1006	14/15	0.13	-0.30	11,16,18,26	0
2	NAG	C	911	14/15	0.14	-0.35	12,14,22,23	0
3	NAG	D	909	14/15	0.18	-0.35	44,56,61,61	0
2	NAG	A	1001	14/15	0.16	-0.41	9,14,20,20	0
3	NAG	D	908	14/15	0.15	-0.52	18,21,31,38	0
2	NAG	B	1011	14/15	0.11	-0.61	16,31,38,41	0
2	NAG	D	913	14/15	0.11	-0.72	19,27,40,40	0
2	NAG	D	912	14/15	0.13	-0.77	17,19,27,32	0
2	NAG	D	904	14/15	0.14	-1.01	34,44,49,57	0
2	NAG	B	1010	14/15	0.12	-1.08	14,17,28,32	0
3	NAG	A	1007	14/15	0.13	-1.22	33,46,51,58	0
2	NAG	B	1002	14/15	0.11	-1.39	12,20,27,28	0
2	MAN	C	905	11/12	0.10	-1.45	51,57,59,60	0
3	NAG	C	907	14/15	0.11	-1.87	13,18,30,35	0
2	MAN	D	906	11/12	0.12	-1.99	41,51,59,59	0
2	NAG	A	1011	14/15	0.09	-2.07	17,24,32,42	0
2	NAG	A	1010	14/15	0.10	-2.23	15,20,24,24	0
3	NAG	C	908	14/15	0.11	-2.95	31,46,59,66	0
2	NAG	C	912	14/15	0.10	-8.39	14,22,31,37	0
2	MAN	A	1013	11/12	0.19	-	59,66,67,68	0
2	BMA	A	1003	11/12	0.10	-	38,41,58,64	0
3	BMA	A	1008	11/12	0.18	-	64,72,77,79	0
2	MAN	B	1005	11/12	0.21	-	61,65,73,76	0
2	MAN	B	1014	11/12	0.20	-	66,69,77,77	0
2	MAN	B	1013	11/12	0.31	-	72,75,80,81	0
2	BMA	D	905	11/12	0.11	-	59,61,73,77	0
2	MAN	C	906	11/12	0.15	-	69,72,74,74	0
2	MAN	C	915	11/12	0.18	-	67,68,70,70	0
2	BMA	B	1012	11/12	0.13	-	48,55,62,69	0
2	MAN	A	1005	11/12	0.10	-	68,70,73,74	0
2	BMA	A	1012	11/12	0.15	-	48,52,64,64	0
2	MAN	D	916	11/12	0.23	-	70,74,76,76	0
3	BMA	C	909	11/12	0.19	-	69,72,75,75	0
2	MAN	A	1014	11/12	0.24	-	66,72,75,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BMA	D	914	11/12	0.14	-	49,57,66,72	0
2	MAN	C	914	11/12	0.16	-	69,76,80,82	0
3	BMA	B	1008	11/12	0.17	-	59,64,78,78	0
2	BMA	C	904	11/12	0.10	-	54,59,62,65	0
2	MAN	D	915	11/12	0.21	-	64,74,78,78	0
3	BMA	D	910	11/12	0.19	-	59,64,102,102	0
2	MAN	D	907	11/12	0.21	-	80,82,85,88	0
2	BMA	C	913	11/12	0.14	-	43,55,66,67	0
2	BMA	B	1003	11/12	0.10	-	32,36,45,52	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
5	SO4	B	1021	5/5	0.28	6.25	107,108,110,110	0
5	SO4	A	1019	5/5	0.21	2.53	100,102,104,105	0
5	SO4	C	918	5/5	0.17	2.53	89,91,92,93	0
5	SO4	B	1020	5/5	0.17	2.46	97,98,99,102	0
5	SO4	D	921	5/5	0.20	2.17	106,106,107,111	0
4	NAG	D	918	14/15	0.28	1.42	66,68,71,74	0
6	RX8	D	901	23/23	0.18	0.93	11,17,22,23	0
4	NAG	A	1017	14/15	0.20	0.92	47,64,67,70	0
6	RX8	C	901	23/23	0.16	0.86	8,14,18,21	0
4	NAG	C	917	14/15	0.17	0.85	50,59,62,63	0
6	RX8	B	1018	23/23	0.16	0.82	22,25,30,88	0
4	NAG	B	1009	14/15	0.14	0.72	48,60,68,68	0
4	NAG	B	1016	14/15	0.14	0.65	27,32,39,46	0
4	NAG	B	1017	14/15	0.19	0.55	56,61,62,63	0
6	RX8	D	902	23/23	0.19	0.51	25,28,38,44	0
4	NAG	A	1015	14/15	0.25	0.33	63,67,69,74	0
5	SO4	D	920	5/5	0.21	0.22	104,105,106,106	0
4	NAG	D	917	14/15	0.17	0.13	58,61,68,72	0
4	NAG	C	916	14/15	0.13	0.03	40,46,50,53	0
4	NAG	D	919	14/15	0.15	-0.09	41,51,57,58	0
4	NAG	B	1015	14/15	0.20	-0.22	71,78,82,83	0
4	NAG	A	1016	14/15	0.11	-1.00	26,34,41,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	C	910	14/15	0.10	-1.01	31,46,52,54	0
4	NAG	A	1009	14/15	0.10	-1.08	46,56,68,71	0
4	NAG	D	911	14/15	0.14	-1.34	49,54,59,61	0
5	SO4	A	1018	5/5	0.10	-2.97	91,93,94,94	0
5	SO4	B	1019	5/5	0.07	-5.04	86,87,88,89	0

6.5 Other polymers ⓘ

There are no such residues in this entry.