



Full wwPDB X-ray Structure Validation 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 full wwPDB validation 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>

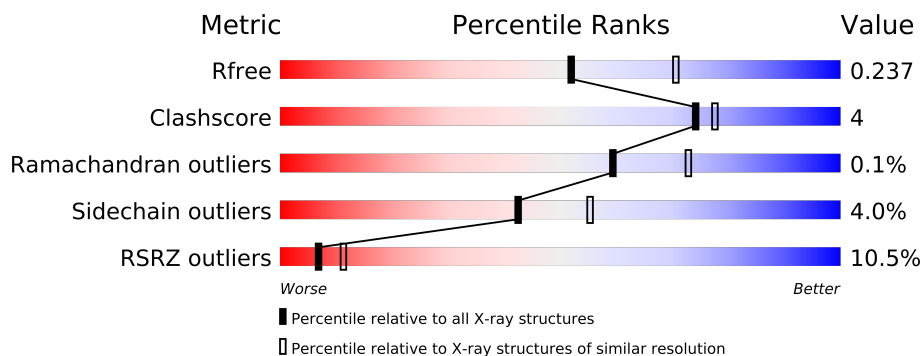
The following versions of software and data (see [references](#)) were used in the production of this report:

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:

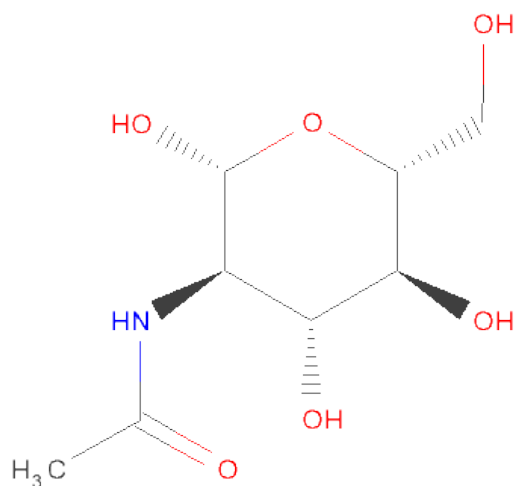
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	24	SER	-	EXPRESSION TAG	UNP Q9NR97
A	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
A	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
A	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
A	830	LEU	-	EXPRESSION TAG	UNP 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: $C_8H_{15}NO_6$).



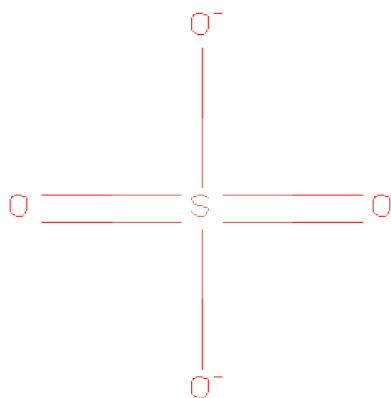
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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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).



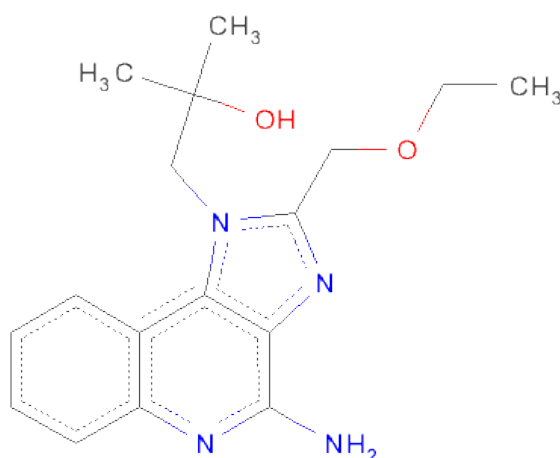
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5	4 1		

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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.

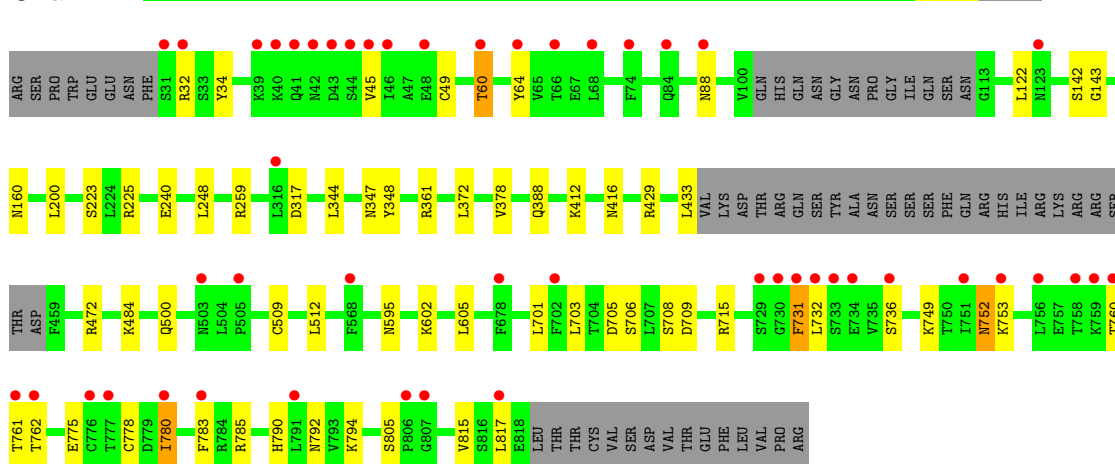
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	269	Total 269	O 269	0	0
7	B	240	Total 240	O 240	0	0
7	C	214	Total 214	O 214	0	0
7	D	172	Total 172	O 172	0	0

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 ($\text{RSRZ} > 2$). 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.

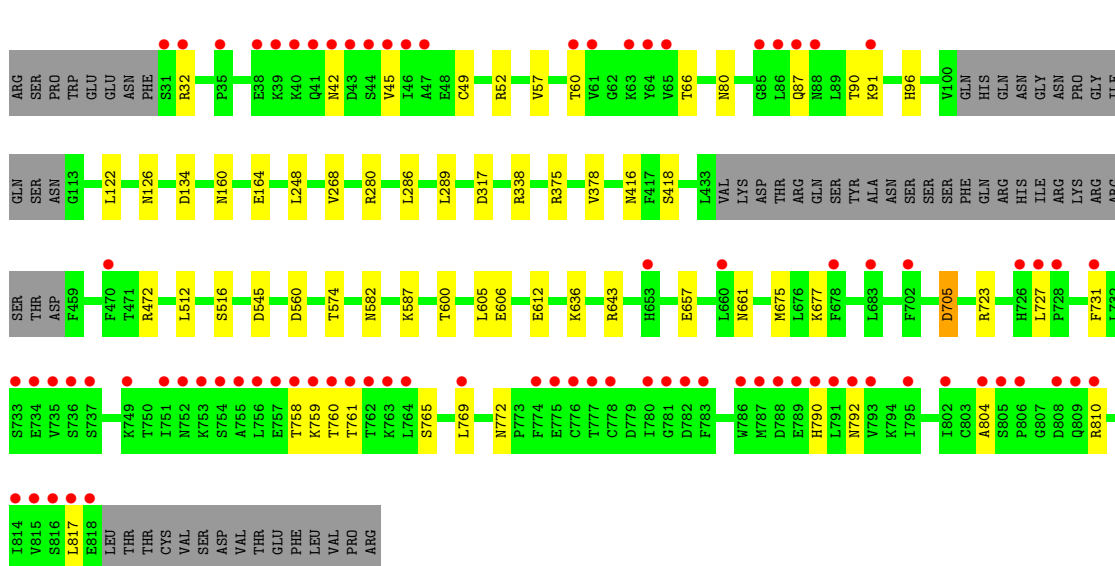
• Molecule 1: Toll-like receptor 8

Chain A:



• Molecule 1: Toll-like receptor 8

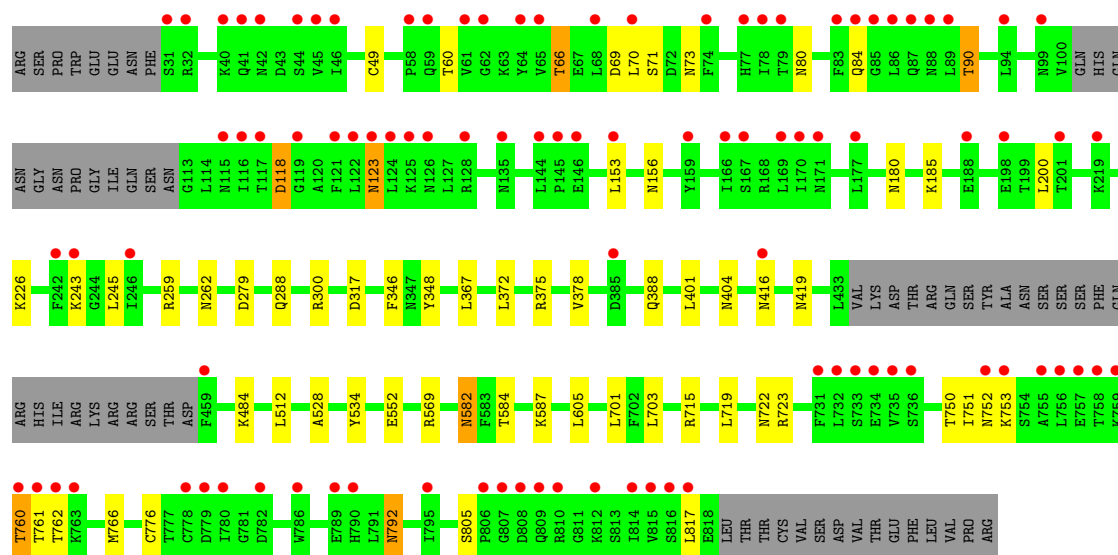
Chain B:



• Molecule 1: Toll-like receptor 8

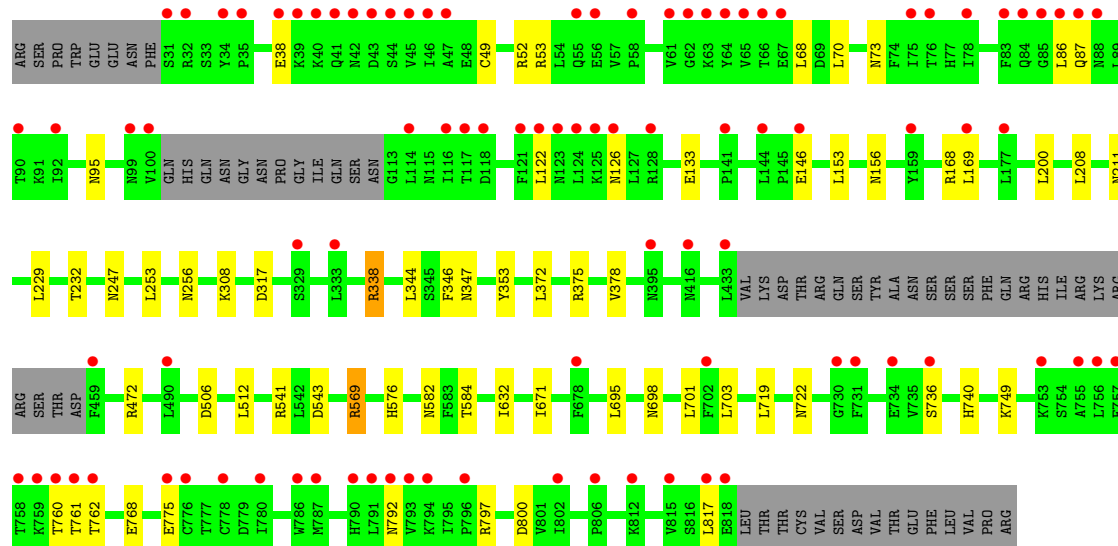
Chain C:





● 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.

All (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
1:B:286:LEU:O	7:B:1199:HOH:O	2.08	0.70
1:A:595:ASN:ND2	7:A:1221:HOH:O	2.23	0.69
1:A:429:ARG:NH1	7:A:1276:HOH:O	2.26	0.69
1:A:160:ASN:ND2	7:A:1150:HOH:O	2.28	0.67
1:C:582:ASN:ND2	7:C:1190:HOH:O	2.28	0.66
1:C:723:ARG:NH1	5:C:918:SO4:O3	2.29	0.66
1:B:587:LYS:NZ	7:B:1217:HOH:O	2.28	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:569:ARG:NH2	7:D:1158:HOH:O	2.29	0.65
1:B:164:GLU:N	1:B:164:GLU:OE1	2.29	0.65
1:C:766:MET:SD	7:C:1205:HOH:O	2.55	0.65
1:D:346:PHE:N	1:D:375:ARG:O	2.30	0.65
1:A:775:GLU:OE1	1:A:805:SER:OG	2.15	0.64
1:A:223:SER:O	1:A:225:ARG:NH1	2.30	0.64
1:B:80:ASN:ND2	7:B:1233:HOH:O	2.30	0.63
1:B:606:GLU:OE2	7:B:1266:HOH:O	2.16	0.63
1:A:500:GLN:NE2	7:A:1168:HOH:O	2.31	0.62
1:B:87:GLN:O	1:B:126:ASN:ND2	2.33	0.62
1:B:32:ARG:NH2	1:B:790:HIS:O	2.33	0.62
1:C:587:LYS:NZ	7:C:1210:HOH:O	2.34	0.61
1:B:657:GLU:OE1	1:B:657:GLU:N	2.34	0.60
1:C:118:ASP:OD1	1:C:118:ASP:N	2.35	0.60
1:D:153:LEU:O	1:D:156:ASN:ND2	2.36	0.58
1:C:760:THR:OG1	1:C:761:THR:N	2.37	0.57
1:D:53:ARG:NH1	1:D:800:ASP:OD1	2.37	0.57
1:C:226:LYS:NZ	2:C:903:NAG:O7	2.38	0.57
1:D:253:LEU:O	1:D:256:ASN:ND2	2.37	0.57
1:D:70:LEU:O	1:D:73:ASN:ND2	2.38	0.57
1:A:361:ARG:NH1	7:A:1255:HOH:O	2.38	0.56
1:B:375:ARG:NH1	7:B:1200:HOH:O	2.38	0.56
1:B:723:ARG:NH1	5:B:1019:SO4:O1	2.38	0.56
1:A:484:LYS:NZ	7:A:1231:HOH:O	2.38	0.56
1:B:612:GLU:OE2	1:B:643:ARG:NH1	2.39	0.56
1:D:87:GLN:O	1:D:126:ASN:ND2	2.38	0.56
1:B:91:LYS:NZ	7:B:1110:HOH:O	2.39	0.55
1:C:346:PHE:N	1:C:375:ARG:O	2.39	0.55
1:B:792:ASN:OD1	1:B:792:ASN:N	2.39	0.55
1:C:719:LEU:O	1:C:722:ASN:ND2	2.40	0.54
1:C:792:ASN:N	1:C:792:ASN:OD1	2.41	0.54
1:A:749:LYS:O	1:A:775:GLU:N	2.41	0.53
1:A:705:ASP:OD1	1:A:705:ASP:N	2.42	0.52
1:D:146:GLU:OE1	1:D:146:GLU:N	2.43	0.52
1:B:769:LEU:O	1:B:772:ASN:ND2	2.42	0.51
1:D:576:HIS:NE2	7:D:1045:HOH:O	2.34	0.51
1:D:792:ASN:N	1:D:792:ASN:OD1	2.43	0.51
1:D:95:ASN:OD1	1:D:133:GLU:N	2.44	0.51
1:D:208:LEU:O	1:D:211:ASN:ND2	2.44	0.50
1:B:804:ALA:O	1:B:810:ARG:NH1	2.44	0.50
1:C:715:ARG:NH1	7:C:1189:HOH:O	2.44	0.50
1:A:792:ASN:N	1:A:792:ASN:OD1	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:84:GLN:N	1:C:84:GLN:OE1	2.45	0.49
1:A:731:PHE:CG	1:A:732:LEU:N	2.80	0.49
1:B:760:THR:OG1	1:B:761:THR:N	2.46	0.48
1:C:66:THR:OG1	1:C:90:THR:OG1	2.31	0.48
1:C:388:GLN:NE2	7:C:1118:HOH:O	2.46	0.48
1:D:695:LEU:O	1:D:698:ASN:ND2	2.45	0.48
1:A:706:SER:OG	1:A:709:ASP:OD2	2.30	0.48
1:B:96:HIS:ND1	1:B:134:ASP:OD2	2.46	0.48
1:C:776:CYS:N	1:C:805:SER:O	2.47	0.48
1:D:719:LEU:O	1:D:722:ASN:ND2	2.47	0.48
1:C:300:ARG:NE	7:C:1031:HOH:O	2.46	0.47
1:A:715:ARG:NE	7:A:1342:HOH:O	2.47	0.47
1:D:749:LYS:O	1:D:775:GLU:N	2.47	0.47
1:D:344:LEU:O	1:D:347:ASN:ND2	2.47	0.47
1:D:506:ASP:N	7:D:1122:HOH:O	2.48	0.47
1:D:740:HIS:NE2	1:D:768:GLU:OE2	2.49	0.46
1:C:552:GLU:N	1:C:552:GLU:OE1	2.49	0.45
1:C:153:LEU:O	1:C:156:ASN:ND2	2.49	0.45
1:A:752:ASN:OD1	1:A:752:ASN:N	2.50	0.45
1:A:780:ILE:O	1:A:783:PHE:N	2.49	0.45
1:B:582:ASN:ND2	7:B:1336:HOH:O	2.49	0.44
1:C:752:ASN:OD1	1:C:753:LYS:N	2.50	0.44
1:A:143:GLY:N	7:A:1277:HOH:O	2.49	0.44
1:C:180:ASN:O	1:C:185:LYS:NZ	2.51	0.44
1:B:545:ASP:OD1	1:B:574:THR:OG1	2.36	0.44
1:C:750:THR:OG1	1:C:751:ILE:N	2.51	0.43
1:D:760:THR:OG1	1:D:761:THR:N	2.52	0.43
1:B:600:THR:OG1	1:C:262:ASN:OD1	2.37	0.43
1:D:543:ASP:OD2	6:D:901:RX8:N1	2.51	0.43
1:D:229:LEU:O	1:D:232:THR:OG1	2.36	0.43
1:A:344:LEU:O	1:A:347:ASN:ND2	2.52	0.43
1:B:560:ASP:OD2	2:B:1010:NAG:N2	2.52	0.42
1:C:401:LEU:O	1:C:404:ASN:ND2	2.51	0.42
1:D:146:GLU:OE2	1:D:168:ARG:NH2	2.52	0.42
1:A:32:ARG:NH2	1:A:790:HIS:O	2.51	0.42
1:C:528:ALA:N	7:C:1080:HOH:O	2.52	0.42
1:C:484:LYS:NZ	7:C:1143:HOH:O	2.52	0.42
1:B:636:LYS:NZ	1:B:661:ASN:OD1	2.53	0.41
1:D:247:ASN:N	7:D:1052:HOH:O	2.53	0.41
1:B:66:THR:O	1:B:90:THR:N	2.54	0.41
1:C:69:ASP:OD1	1:C:71:SER:OG	2.38	0.41
1:D:584:THR:N	7:D:1025:HOH:O	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:70:LEU:O	1:C:73:ASN:ND2	2.54	0.41
1:A:259:ARG:NH2	1:A:348:TYR:O	2.54	0.41
1:C:288:GLN:N	7:C:1083:HOH:O	2.54	0.41
1:B:286:LEU:C	7:B:1199:HOH:O	2.56	0.40
1:B:675:MET:O	1:B:677:LYS:NZ	2.54	0.40
1:C:259:ARG:NH2	1:C:348:TYR:O	2.55	0.40
1:B:57:VAL:N	7:B:1293:HOH:O	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	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

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	49	CYS
1	A	60	THR
1	A	64	TYR
1	A	88	ASN
1	A	122	LEU
1	A	142	SER
1	A	200	LEU
1	A	240	GLU
1	A	248	LEU
1	A	317	ASP
1	A	372	LEU
1	A	388	GLN
1	A	412	LYS
1	A	416	ASN
1	A	433	LEU
1	A	472	ARG
1	A	509	CYS
1	A	512	LEU
1	A	602	LYS
1	A	605	LEU
1	A	701	LEU
1	A	703	LEU
1	A	731	PHE
1	A	736	SER
1	A	752	ASN

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Mol	Chain	Res	Type
1	A	761	THR
1	A	762	THR
1	A	778	CYS
1	A	780	ILE
1	A	785	ARG
1	A	794	LYS
1	A	815	VAL
1	A	817	LEU
1	B	42	ASN
1	B	45	VAL
1	B	49	CYS
1	B	52	ARG
1	B	60	THR
1	B	122	LEU
1	B	160	ASN
1	B	248	LEU
1	B	268	VAL
1	B	280	ARG
1	B	317	ASP
1	B	338	ARG
1	B	416	ASN
1	B	418	SER
1	B	472	ARG
1	B	512	LEU
1	B	516	SER
1	B	605	LEU
1	B	705	ASP
1	B	727	LEU
1	B	731	PHE
1	B	758	THR
1	B	759	LYS
1	B	765	SER
1	B	817	LEU
1	C	49	CYS
1	C	60	THR
1	C	66	THR
1	C	90	THR
1	C	118	ASP
1	C	123	ASN
1	C	200	LEU
1	C	243	LYS
1	C	245	LEU

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Mol	Chain	Res	Type
1	C	279	ASP
1	C	317	ASP
1	C	367	LEU
1	C	372	LEU
1	C	416	ASN
1	C	419	ASN
1	C	512	LEU
1	C	534	TYR
1	C	569	ARG
1	C	582	ASN
1	C	584	THR
1	C	605	LEU
1	C	701	LEU
1	C	703	LEU
1	C	760	THR
1	C	762	THR
1	C	792	ASN
1	C	817	LEU
1	D	38	GLU
1	D	49	CYS
1	D	52	ARG
1	D	68	LEU
1	D	86	LEU
1	D	122	LEU
1	D	169	LEU
1	D	200	LEU
1	D	317	ASP
1	D	338	ARG
1	D	353	TYR
1	D	372	LEU
1	D	472	ARG
1	D	512	LEU
1	D	541	ARG
1	D	569	ARG
1	D	582	ASN
1	D	632	ILE
1	D	671	ILE
1	D	701	LEU
1	D	703	LEU
1	D	736	SER
1	D	762	THR
1	D	797	ARG

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Mol	Chain	Res	Type
1	D	817	LEU

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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
2	A	1010	NAG	O5-C5	-2.30	1.41	1.45
2	B	1002	NAG	O5-C5	-2.24	1.41	1.45
3	B	1007	NAG	O5-C5	-2.20	1.41	1.45
2	C	912	NAG	O5-C5	-2.18	1.41	1.45
2	B	1013	MAN	O5-C5	-2.15	1.41	1.45
2	B	1011	NAG	O5-C5	-2.15	1.41	1.45
3	A	1007	NAG	O5-C5	-2.13	1.41	1.45
2	A	1013	MAN	O5-C5	-2.12	1.41	1.45
2	D	907	MAN	O5-C5	-2.11	1.41	1.45
2	D	905	BMA	O5-C5	-2.10	1.41	1.45
3	D	909	NAG	O5-C5	-2.09	1.41	1.45
2	A	1002	NAG	O5-C5	-2.08	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	NAG	O5-C5	-2.08	1.41	1.45
2	C	905	MAN	O5-C5	-2.06	1.41	1.45
2	B	1010	NAG	O5-C5	-2.04	1.41	1.45

All (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
2	C	914	MAN	O5-C5-C6	3.18	110.32	106.98
2	B	1005	MAN	O5-C5-C6	3.07	110.21	106.98
3	B	1007	NAG	C2-N2-C7	-3.07	117.94	123.09
3	D	910	BMA	O5-C5-C6	3.05	110.18	106.98
3	A	1006	NAG	C2-N2-C7	-2.96	118.12	123.09
3	A	1006	NAG	O5-C5-C6	2.96	110.08	106.98
2	A	1011	NAG	O5-C5-C4	2.80	114.21	110.65
3	A	1007	NAG	O5-C5-C6	2.77	109.89	106.98
2	B	1001	NAG	O5-C5-C6	2.68	109.79	106.98
2	D	904	NAG	O5-C5-C6	2.57	109.68	106.98
3	B	1008	BMA	C4-C3-C2	2.57	113.96	110.50
3	B	1006	NAG	C2-N2-C7	-2.57	118.78	123.09
2	D	913	NAG	O5-C5-C6	2.44	109.54	106.98
2	B	1010	NAG	C3-C2-N2	-2.42	108.08	111.76
3	A	1008	BMA	O5-C5-C6	2.40	109.50	106.98
2	A	1011	NAG	C3-C2-N2	-2.39	108.12	111.76
2	A	1003	BMA	O2-C2-C3	-2.39	105.02	110.18
3	A	1007	NAG	O5-C5-C4	-2.37	107.64	110.65
2	D	915	MAN	O5-C5-C6	2.36	109.46	106.98
2	C	915	MAN	O5-C5-C6	2.35	109.45	106.98
2	C	902	NAG	C3-C2-N2	-2.35	108.18	111.76
3	C	907	NAG	C3-C2-N2	-2.35	108.19	111.76
2	B	1012	BMA	O5-C5-C6	-2.31	104.56	106.98
2	A	1013	MAN	C3-C4-C5	2.30	114.31	110.20
2	B	1011	NAG	O5-C5-C6	2.29	109.38	106.98
2	B	1013	MAN	O5-C5-C6	2.27	109.37	106.98
2	B	1010	NAG	O5-C5-C6	2.27	109.37	106.98
3	D	909	NAG	O5-C5-C4	-2.26	107.78	110.65
3	C	909	BMA	C4-C3-C2	2.25	113.53	110.50
2	C	913	BMA	C4-C3-C2	2.25	113.53	110.50
2	A	1011	NAG	C3-C4-C5	2.24	114.20	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	909	BMA	O5-C5-C6	2.22	109.31	106.98
3	A	1006	NAG	C3-C2-N2	-2.18	108.44	111.76
3	D	909	NAG	C3-C2-N2	-2.17	108.46	111.76
3	C	909	BMA	O5-C5-C4	-2.14	107.94	110.65
2	D	904	NAG	C3-C2-N2	-2.12	108.54	111.76
2	A	1004	MAN	O5-C5-C6	2.10	109.18	106.98
2	C	911	NAG	O5-C5-C6	2.06	109.15	106.98
3	B	1006	NAG	C6-C5-C4	-2.06	108.02	113.00
2	C	906	MAN	O5-C5-C6	2.03	109.11	106.98
3	D	909	NAG	C2-N2-C7	-2.03	119.69	123.09

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

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

All (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
6	D	902	RX8	C2-C1	-2.90	1.37	1.41
6	B	1018	RX8	C2-C1	-2.76	1.37	1.41
6	D	901	RX8	C-N	2.69	1.43	1.35
6	C	901	RX8	C-N	2.65	1.43	1.35
6	D	901	RX8	C2-C1	-2.63	1.37	1.41
6	B	1018	RX8	C-N	2.62	1.43	1.35
6	D	902	RX8	C-N	2.54	1.43	1.35
6	B	1018	RX8	O1-C10	-2.50	1.37	1.44
6	C	901	RX8	O1-C10	-2.40	1.37	1.44
6	D	901	RX8	O1-C10	-2.31	1.38	1.44
4	C	917	NAG	O5-C5	-2.20	1.41	1.45
6	D	902	RX8	O1-C10	-2.18	1.38	1.44
4	B	1009	NAG	O5-C5	-2.14	1.41	1.45
4	A	1009	NAG	O5-C5	-2.07	1.41	1.45
4	D	917	NAG	O5-C5	-2.05	1.41	1.45
4	D	911	NAG	O5-C5	-2.04	1.41	1.45
6	D	902	RX8	C6-C5	2.04	1.52	1.50
6	B	1018	RX8	C3-N3	2.02	1.41	1.39

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
6	C	901	RX8	C-N1-C1	4.32	122.14	118.42
6	D	901	RX8	C6-O-C7	4.14	121.43	112.57
6	D	902	RX8	C-N1-C1	4.07	121.93	118.42
6	D	902	RX8	C6-O-C7	3.83	120.76	112.57
6	D	901	RX8	C9-N3-C5	-3.75	125.12	127.34
6	C	901	RX8	C6-O-C7	3.74	120.57	112.57
6	D	902	RX8	C9-N3-C5	-3.60	125.20	127.34
4	C	916	NAG	O5-C5-C6	3.42	110.57	106.98
4	B	1015	NAG	O5-C5-C6	3.10	110.23	106.98
4	B	1017	NAG	O5-C5-C6	2.78	109.90	106.98
6	B	1018	RX8	C2-C1-N1	-2.64	120.62	123.02
4	D	917	NAG	O5-C5-C6	2.61	109.72	106.98
4	D	919	NAG	O5-C5-C6	2.52	109.62	106.98
4	C	916	NAG	C2-N2-C7	-2.50	118.89	123.09
6	B	1018	RX8	C2-C3-N3	2.49	135.68	130.42
4	A	1016	NAG	O5-C5-C6	2.47	109.57	106.98
4	A	1015	NAG	O5-C5-C6	2.47	109.57	106.98
6	D	901	RX8	C2-C1-N1	-2.43	120.81	123.02
6	D	902	RX8	C2-C1-N1	-2.39	120.85	123.02
6	C	901	RX8	C2-C1-N1	-2.38	120.85	123.02
6	D	902	RX8	O-C6-C5	2.32	118.08	111.00
6	D	902	RX8	C2-C3-N3	2.20	135.08	130.42
4	B	1016	NAG	C2-N2-C7	-2.17	119.45	123.09
6	B	1018	RX8	O-C6-C5	2.14	117.53	111.00
4	C	917	NAG	O5-C5-C6	2.10	109.18	106.98
4	A	1016	NAG	C6-C5-C4	-2.05	108.05	113.00
4	A	1016	NAG	C3-C2-N2	-2.02	108.68	111.76

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

All (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
1	D	761	THR	12.0
1	B	758	THR	11.8
1	B	760	THR	10.7
1	A	761	THR	10.3
1	D	64	TYR	10.2
1	C	758	THR	9.6
1	C	760	THR	9.5
1	A	756	LEU	9.2
1	D	756	LEU	9.1
1	B	759	LYS	8.7
1	D	760	THR	8.2
1	C	733	SER	8.0
1	B	817	LEU	8.0
1	D	42	ASN	8.0
1	C	83	PHE	7.9
1	B	64	TYR	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	41	GLN	7.5
1	C	45	VAL	7.4
1	D	41	GLN	7.3
1	B	731	PHE	7.2
1	B	756	LEU	7.0
1	C	759	LYS	6.9
1	D	85	GLY	6.6
1	C	65	VAL	6.6
1	D	46	ILE	6.6
1	C	757	GLU	6.5
1	D	817	LEU	6.5
1	C	734	GLU	6.3
1	C	78	ILE	6.3
1	A	817	LEU	6.2
1	B	762	THR	6.2
1	C	166	ILE	6.1
1	C	761	THR	6.1
1	D	759	LYS	6.1
1	A	43	ASP	6.0
1	A	40	LYS	6.0
1	B	783	PHE	5.9
1	A	39	LYS	5.9
1	B	39	LYS	5.8
1	B	734	GLU	5.7
1	C	116	ILE	5.7
1	B	763	LYS	5.7
1	D	88	ASN	5.5
1	C	85	GLY	5.5
1	A	64	TYR	5.5
1	B	42	ASN	5.5
1	C	123	ASN	5.2
1	B	735	VAL	5.2
1	A	678	PHE	5.2
1	A	733	SER	5.2
1	D	144	LEU	5.1
1	D	83	PHE	5.0
1	C	807	GLY	5.0
1	B	751	ILE	5.0
1	D	43	ASP	5.0
1	D	818	GLU	5.0
1	C	64	TYR	4.9
1	A	730	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	121	PHE	4.9
1	C	46	ILE	4.9
1	D	815	VAL	4.8
1	C	170	ILE	4.8
1	D	730	GLY	4.8
1	D	758	THR	4.8
1	B	804	ALA	4.8
1	D	121	PHE	4.7
1	A	732	LEU	4.7
1	B	727	LEU	4.6
1	D	38	GLU	4.5
1	B	736	SER	4.5
1	D	762	THR	4.5
1	B	41	GLN	4.5
1	B	810	ARG	4.4
1	C	41	GLN	4.3
1	D	736	SER	4.3
1	C	122	LEU	4.3
1	C	126	ASN	4.3
1	D	791	LEU	4.3
1	B	32	ARG	4.2
1	D	793	VAL	4.2
1	C	40	LYS	4.2
1	B	45	VAL	4.2
1	B	802	ILE	4.1
1	C	62	GLY	4.1
1	A	759	LYS	4.1
1	D	87	GLN	4.1
1	C	762	THR	4.1
1	B	702	PHE	4.1
1	D	44	SER	4.1
1	D	66	THR	4.1
1	C	736	SER	4.0
1	B	793	VAL	4.0
1	A	44	SER	4.0
1	C	786	TRP	4.0
1	C	124	LEU	4.0
1	B	815	VAL	4.0
1	B	757	GLU	4.0
1	B	728	PRO	3.9
1	B	43	ASP	3.9
1	C	763	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	39	LYS	3.9
1	A	42	ASN	3.9
1	B	780	ILE	3.8
1	D	778	CYS	3.8
1	C	144	LEU	3.8
1	D	100	VAL	3.8
1	B	782	ASP	3.8
1	C	779	ASP	3.8
1	B	46	ILE	3.8
1	D	78	ILE	3.8
1	D	86	LEU	3.7
1	D	678	PHE	3.7
1	A	45	VAL	3.7
1	A	31	SER	3.7
1	B	47	ALA	3.7
1	B	787	MET	3.7
1	B	788	ASP	3.7
1	D	702	PHE	3.7
1	D	62	GLY	3.7
1	B	87	GLN	3.7
1	C	731	PHE	3.6
1	D	128	ARG	3.6
1	B	786	TRP	3.5
1	D	61	VAL	3.5
1	B	806	PRO	3.5
1	D	65	VAL	3.5
1	D	31	SER	3.5
1	D	40	LYS	3.4
1	C	99	ASN	3.4
1	A	32	ARG	3.4
1	A	729	SER	3.4
1	B	753	LYS	3.4
1	C	814	ILE	3.4
1	B	678	PHE	3.4
1	D	58	PRO	3.4
1	A	66	THR	3.4
1	B	726	HIS	3.4
1	B	781	GLY	3.4
1	C	385	ASP	3.4
1	A	123	ASN	3.4
1	A	751	ILE	3.4
1	C	58	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	731	PHE	3.3
1	C	125	LYS	3.3
1	C	806	PRO	3.3
1	C	789	GLU	3.3
1	B	774	PHE	3.3
1	C	89	LEU	3.2
1	C	778	CYS	3.2
1	A	46	ILE	3.2
1	A	734	GLU	3.2
1	A	807	GLY	3.2
1	B	791	LEU	3.2
1	D	124	LEU	3.2
1	D	757	GLU	3.2
1	D	34	TYR	3.2
1	B	38	GLU	3.2
1	D	67	GLU	3.2
1	A	753	LYS	3.1
1	C	44	SER	3.1
1	C	243	LYS	3.1
1	A	88	ASN	3.1
1	A	760	THR	3.1
1	A	84	GLN	3.1
1	D	32	ARG	3.1
1	C	42	ASN	3.0
1	D	416	ASN	3.0
1	C	246	ILE	3.0
1	B	653	HIS	3.0
1	D	459	PHE	3.0
1	A	777	THR	3.0
1	D	35	PRO	3.0
1	D	802	ILE	3.0
1	C	145	PRO	3.0
1	A	758	THR	3.0
1	C	79	THR	2.9
1	A	783	PHE	2.9
1	C	812	LYS	2.9
1	C	61	VAL	2.9
1	C	752	ASN	2.9
1	B	60	THR	2.9
1	B	776	CYS	2.9
1	C	167	SER	2.9
1	D	792	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	755	ALA	2.9
1	C	159	TYR	2.9
1	B	778	CYS	2.9
1	D	794	LYS	2.8
1	C	790	HIS	2.8
1	C	171	ASN	2.8
1	D	126	ASN	2.8
1	B	754	SER	2.8
1	B	814	ILE	2.8
1	C	459	PHE	2.8
1	A	74	PHE	2.8
1	B	470	PHE	2.8
1	D	47	ALA	2.8
1	A	505	PRO	2.8
1	C	94	LEU	2.8
1	C	201	THR	2.8
1	B	35	PRO	2.7
1	D	90	THR	2.7
1	C	119	GLY	2.7
1	D	159	TYR	2.7
1	D	329	SER	2.7
1	C	115	ASN	2.7
1	C	177	LEU	2.7
1	C	732	LEU	2.7
1	D	177	LEU	2.7
1	D	755	ALA	2.7
1	C	815	VAL	2.7
1	B	749	LYS	2.7
1	D	433	LEU	2.7
1	B	31	SER	2.7
1	D	123	ASN	2.7
1	D	63	LYS	2.7
1	D	790	HIS	2.7
1	B	65	VAL	2.7
1	B	764	LEU	2.7
1	D	169	LEU	2.7
1	D	116	ILE	2.7
1	D	787	MET	2.7
1	B	809	GLN	2.6
1	D	55	GLN	2.6
1	C	817	LEU	2.6
1	C	188	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	75	ILE	2.6
1	C	810	ARG	2.6
1	A	780	ILE	2.6
1	C	816	SER	2.6
1	C	146	GLU	2.6
1	C	242	PHE	2.6
1	B	88	ASN	2.6
1	B	752	ASN	2.6
1	A	736	SER	2.6
1	C	70	LEU	2.6
1	D	114	LEU	2.6
1	B	61	VAL	2.6
1	B	85	GLY	2.5
1	B	86	LEU	2.5
1	A	791	LEU	2.5
1	C	809	GLN	2.5
1	C	755	ALA	2.5
1	C	59	GLN	2.5
1	C	77	HIS	2.5
1	D	56	GLU	2.5
1	B	808	ASP	2.5
1	B	660	LEU	2.5
1	C	808	ASP	2.5
1	C	68	LEU	2.5
1	B	777	THR	2.4
1	C	198	GLU	2.4
1	B	769	LEU	2.4
1	A	776	CYS	2.4
1	C	782	ASP	2.4
1	C	219	LYS	2.4
1	D	780	ILE	2.4
1	D	141	PRO	2.4
1	D	806	PRO	2.4
1	C	117	THR	2.4
1	B	44	SER	2.4
1	D	146	GLU	2.4
1	D	753	LYS	2.3
1	A	68	LEU	2.3
1	D	333	LEU	2.3
1	B	816	SER	2.3
1	A	702	PHE	2.3
1	D	118	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	792	ASN	2.3
1	D	812	LYS	2.3
1	C	74	PHE	2.3
1	D	99	ASN	2.3
1	D	45	VAL	2.3
1	B	91	LYS	2.3
1	D	125	LYS	2.2
1	C	735	VAL	2.2
1	D	92	ILE	2.2
1	C	87	GLN	2.2
1	A	806	PRO	2.2
1	D	775	GLU	2.2
1	D	776	CYS	2.2
1	D	796	PRO	2.2
1	A	60	THR	2.2
1	B	775	GLU	2.2
1	C	416	ASN	2.2
1	D	395	ASN	2.2
1	C	153	LEU	2.2
1	B	683	LEU	2.2
1	B	63	LYS	2.2
1	D	734	GLU	2.2
1	A	48	GLU	2.2
1	C	31	SER	2.2
1	A	503	ASN	2.2
1	C	32	ARG	2.1
1	C	84	GLN	2.1
1	A	316	LEU	2.1
1	D	84	GLN	2.1
1	A	568	PHE	2.1
1	D	76	THR	2.1
1	C	135	ASN	2.1
1	D	786	TRP	2.1
1	C	169	LEU	2.1
1	D	122	LEU	2.1
1	C	795	ILE	2.1
1	B	789	GLU	2.1
1	D	490	LEU	2.1
1	C	753	LYS	2.1
1	A	762	THR	2.1
1	B	737	SER	2.1
1	B	790	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	805	SER	2.0
1	B	795	ILE	2.0
1	B	818	GLU	2.0
1	C	780	ILE	2.0
1	D	731	PHE	2.0
1	C	128	ARG	2.0
1	B	40	LYS	2.0
1	D	117	THR	2.0

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(Å 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

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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
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.