



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 6, 2018 – 11:16 AM EDT

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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

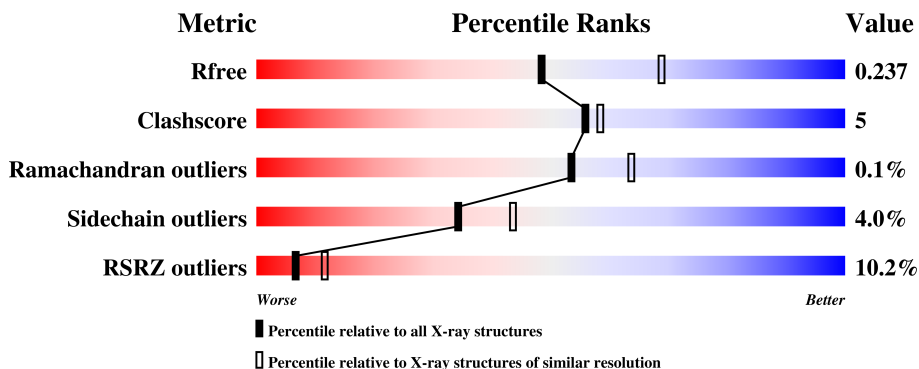
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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}	111664	1763 (2.36-2.32)
Clashscore	122126	1858 (2.36-2.32)
Ramachandran outliers	120053	1834 (2.36-2.32)
Sidechain outliers	120020	1835 (2.36-2.32)
RSRZ outliers	108989	1737 (2.36-2.32)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	811	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div> </div>
1	B	811	<div> <div>9%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div> </div>
1	C	811	<div> <div>12%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 7%</div> </div> </div>
1	D	811	<div> <div>11%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26024 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	0	0
			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:

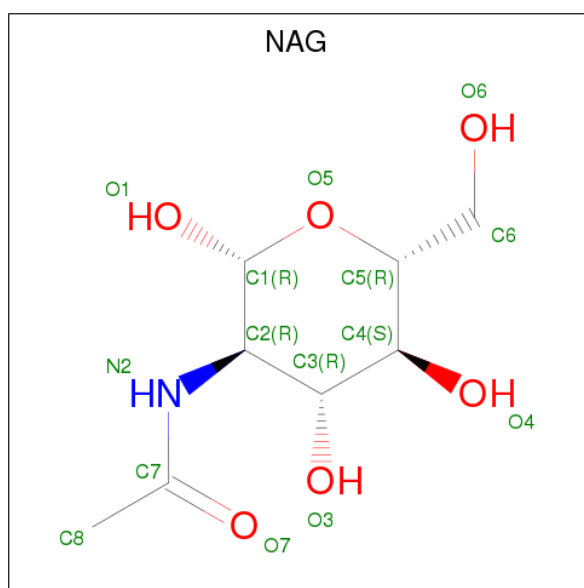
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	24	SER	-	EXPRESSION TAG	UNP Q9NR97
A	25	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	26	TRP	-	EXPRESSION TAG	UNP Q9NR97
A	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
A	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
A	830	LEU	-	EXPRESSION TAG	UNP 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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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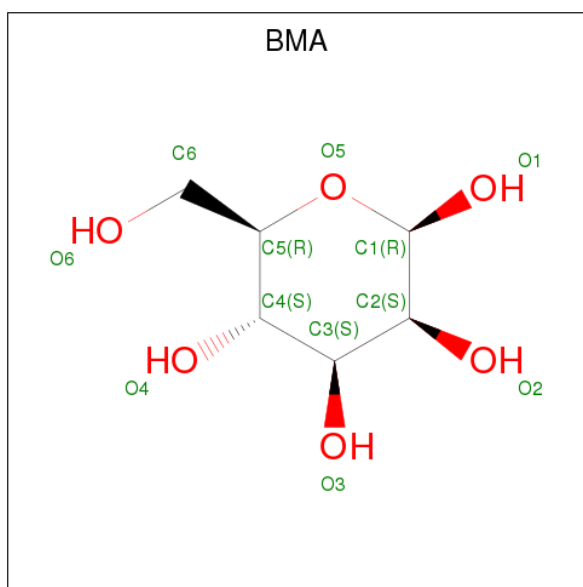
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

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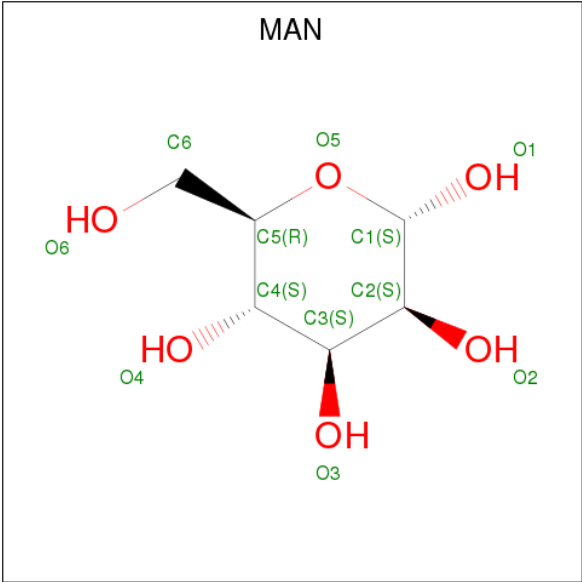
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



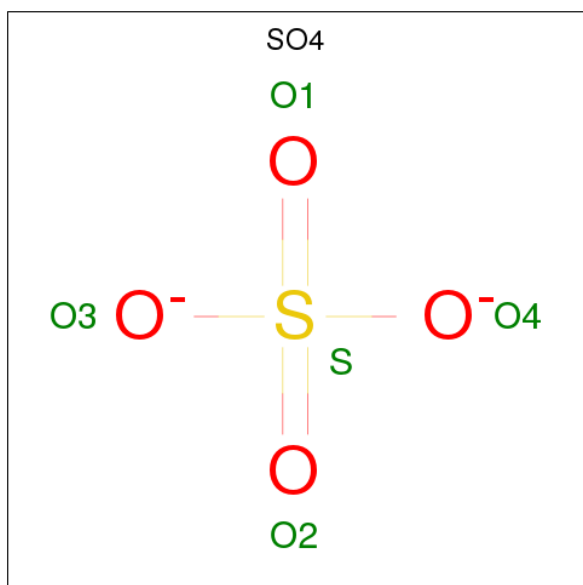
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

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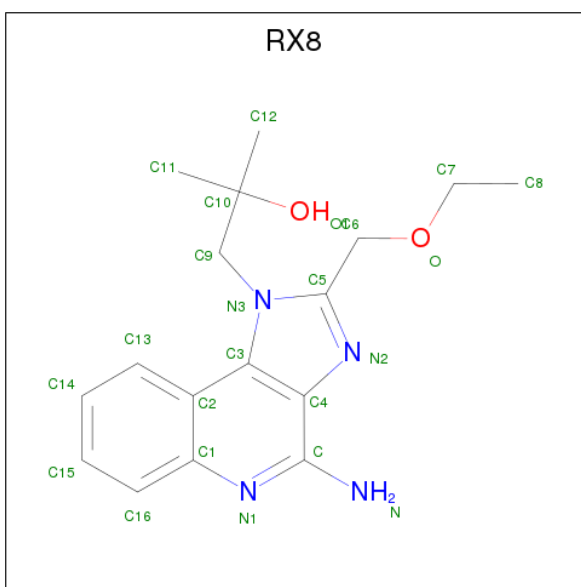
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

- 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		
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	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		

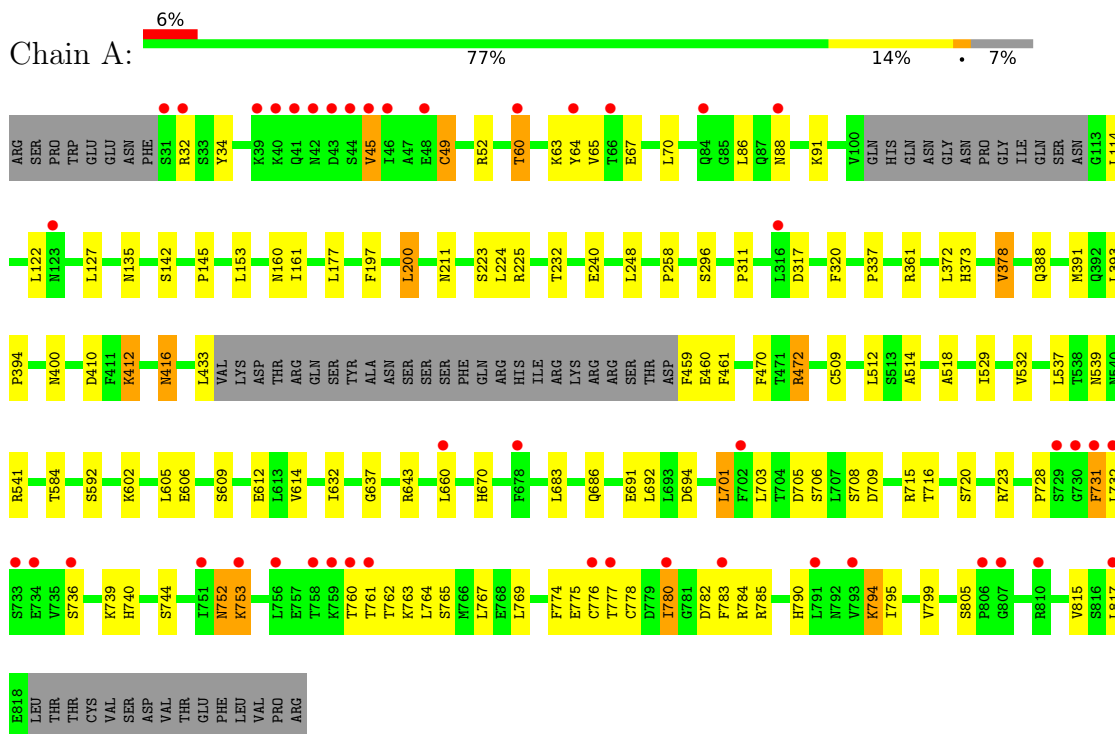
- Molecule 7 is water.

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

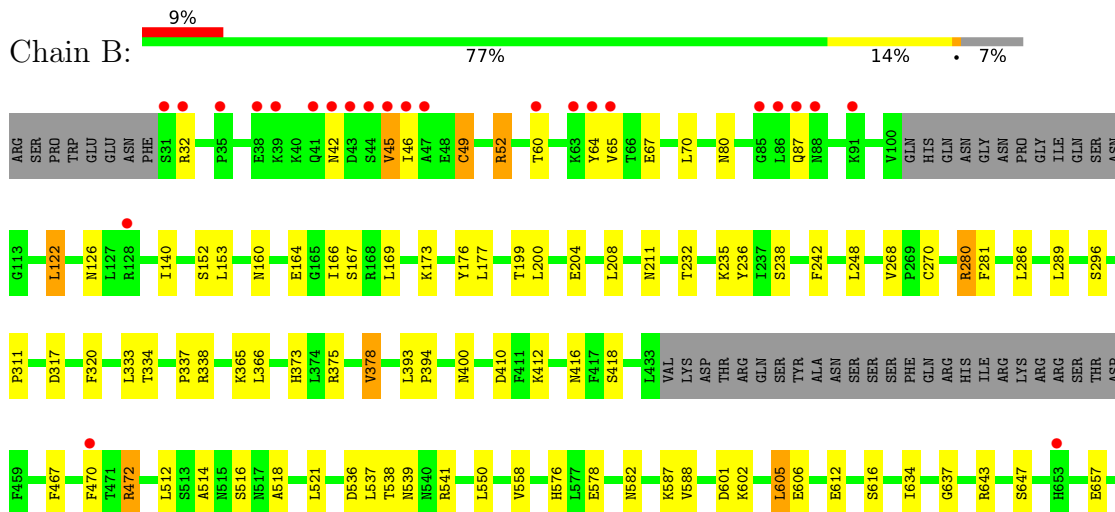
3 Residue-property plots [i](#)

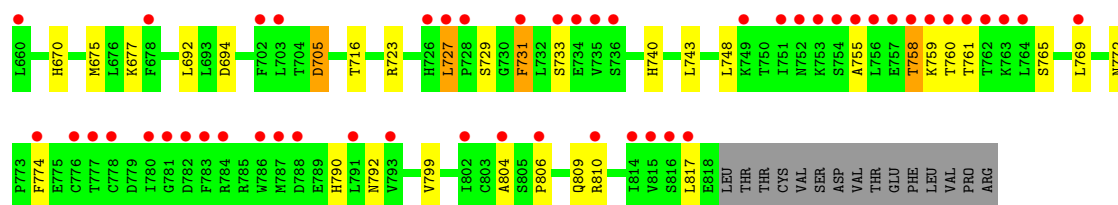
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Toll-like receptor 8

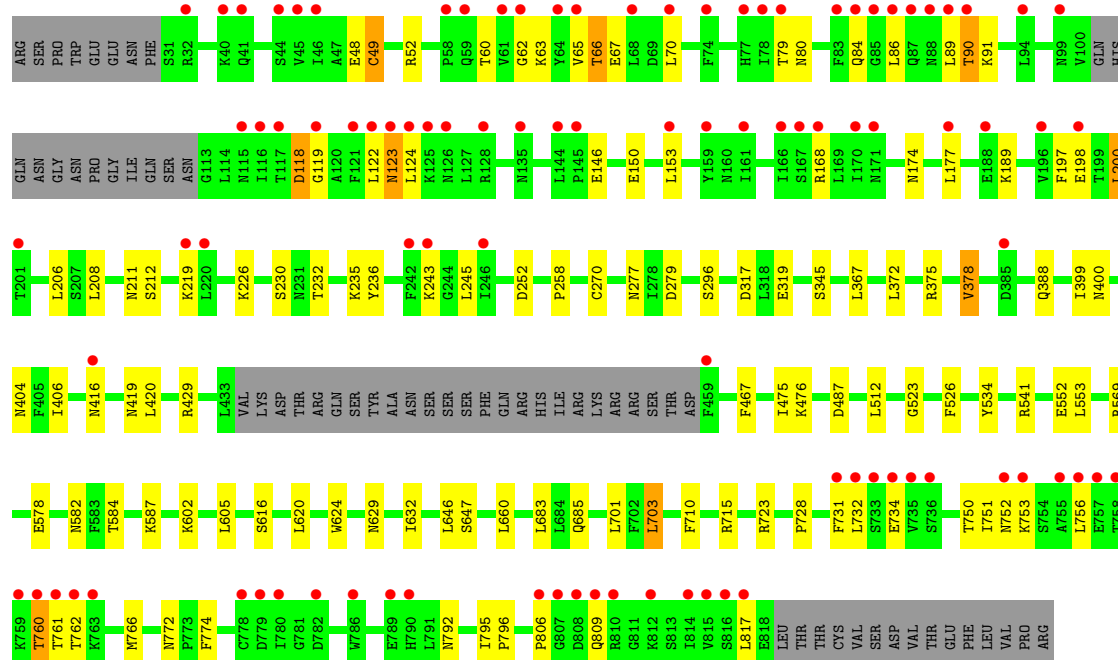
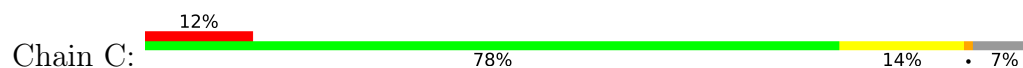


- Molecule 1: Toll-like receptor 8

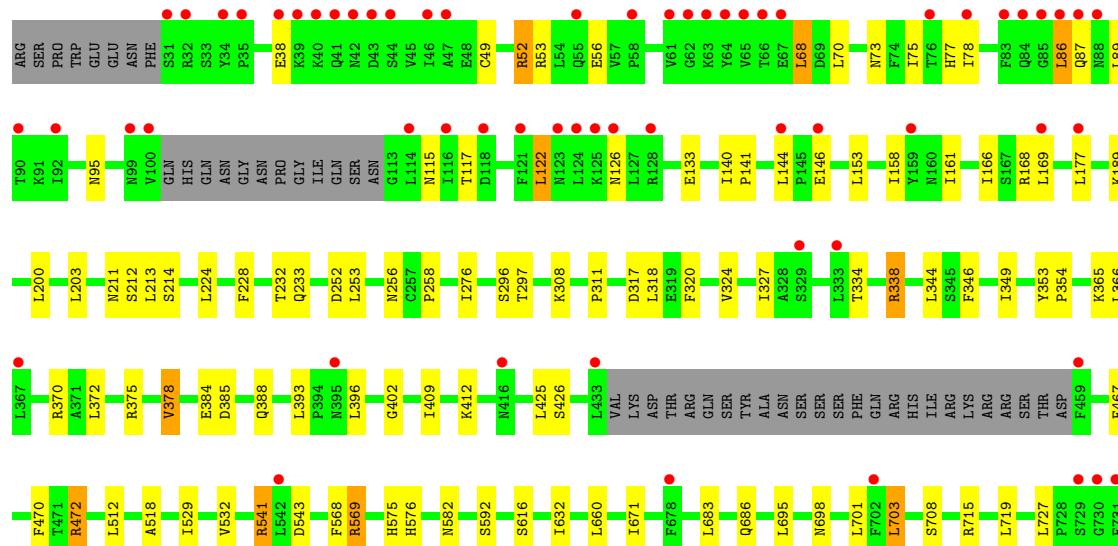
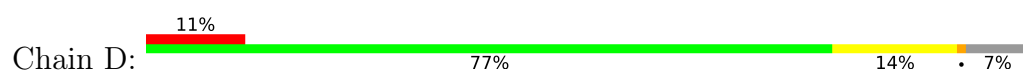


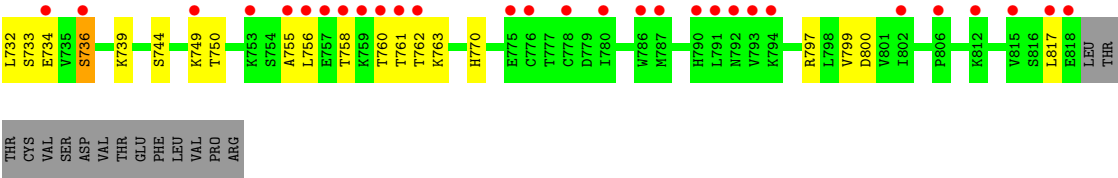


• Molecule 1: Toll-like receptor 8



• Molecule 1: Toll-like receptor 8





THR
CYS
VAL
SER
ASP
VAL
THR
GLU
PHE
LEU
VAL
PRO
ARG

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 1.8.1_1168	Depositor
R, R_{free}	0.196 , 0.239 0.198 , 0.237	Depositor DCC
R_{free} test set	7995 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.35	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 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6038	0	6012	65	2
1	B	6035	0	6003	73	0
1	C	6035	0	6004	66	0
1	D	6035	0	6003	68	2
2	A	140	0	124	0	0
2	B	140	0	124	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	126	0	111	3	0
2	D	140	0	124	1	0
3	A	33	0	26	0	0
3	B	33	0	26	0	0
3	C	33	0	26	0	0
3	D	33	0	26	0	0
4	A	44	0	40	0	0
4	B	44	0	40	0	0
4	C	44	0	40	0	0
4	D	44	0	40	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	22	3	0
6	C	23	0	22	2	0
6	D	46	0	44	5	0
7	A	269	0	0	3	0
7	B	240	0	0	9	0
7	C	214	0	0	4	0
7	D	172	0	0	2	0
All	All	26024	0	24857	274	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 274 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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:N	1:C:123:ASN:OD1	2.20	0.74
1:D:749:LYS:HG3	1:D:750:THR:HG22	1.71	0.73
1:D:52:ARG:HG2	1:D:799:VAL:HG21	1.70	0.73

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:THR:OG1	1:D:308:LYS:O[2_645]	2.13	0.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:SER:O	1:D:338:ARG:NH2[2_645]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	745/811 (92%)	720 (97%)	24 (3%)	1 (0%)	53	64
1	B	745/811 (92%)	722 (97%)	22 (3%)	1 (0%)	53	64
1	C	745/811 (92%)	723 (97%)	21 (3%)	1 (0%)	53	64
1	D	745/811 (92%)	723 (97%)	21 (3%)	1 (0%)	53	64
All	All	2980/3244 (92%)	2888 (97%)	88 (3%)	4 (0%)	53	64

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	694/755 (92%)	660 (95%)	34 (5%)	27	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	693/755 (92%)	668 (96%)	25 (4%)	38	48
1	C	693/755 (92%)	666 (96%)	27 (4%)	35	45
1	D	693/755 (92%)	668 (96%)	25 (4%)	38	48
All	All	2773/3020 (92%)	2662 (96%)	111 (4%)	34	43

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. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	581	GLN
1	D	160	ASN
1	C	595	ASN
1	B	191	ASN
1	C	77	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

79 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1001	1,2	14,14,15	0.71	0	17,19,21	1.18	1 (5%)
2	NAG	A	1002	3,2	14,14,15	0.62	0	17,19,21	0.85	0
3	BMA	A	1003	2,4	11,11,12	0.98	1 (9%)	15,15,17	1.05	1 (6%)
4	MAN	A	1004	3	11,11,12	0.57	0	15,15,17	0.97	1 (6%)
4	MAN	A	1005	3	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
2	NAG	A	1006	1,2	14,14,15	0.53	0	17,19,21	1.08	1 (5%)
2	NAG	A	1007	3,2	14,14,15	0.72	0	17,19,21	1.10	1 (5%)
3	BMA	A	1008	2	11,11,12	0.93	1 (9%)	15,15,17	1.07	1 (6%)
2	NAG	A	1009	1	14,14,15	0.57	0	17,19,21	0.74	0
2	NAG	A	1010	1,2	14,14,15	0.64	0	17,19,21	0.96	0
2	NAG	A	1011	3,2	14,14,15	0.52	0	17,19,21	1.69	3 (17%)
3	BMA	A	1012	2,4	11,11,12	1.42	1 (9%)	15,15,17	0.83	0
4	MAN	A	1013	3	11,11,12	0.70	0	15,15,17	1.05	1 (6%)
4	MAN	A	1014	3	11,11,12	0.51	0	15,15,17	1.16	2 (13%)
2	NAG	A	1015	1	14,14,15	0.46	0	17,19,21	0.96	1 (5%)
2	NAG	A	1016	1	14,14,15	0.55	0	17,19,21	1.21	2 (11%)
2	NAG	A	1017	1	14,14,15	0.50	0	17,19,21	0.94	1 (5%)
5	SO4	A	1018	-	4,4,4	0.15	0	6,6,6	0.09	0
5	SO4	A	1019	-	4,4,4	0.24	0	6,6,6	0.10	0
2	NAG	B	1001	1,2	14,14,15	0.60	0	17,19,21	1.17	1 (5%)
2	NAG	B	1002	3,2	14,14,15	0.74	0	17,19,21	1.01	1 (5%)
3	BMA	B	1003	2,4	11,11,12	0.88	1 (9%)	15,15,17	1.08	1 (6%)
4	MAN	B	1004	3	11,11,12	0.59	0	15,15,17	0.71	0
4	MAN	B	1005	3	11,11,12	0.62	0	15,15,17	0.92	1 (6%)
2	NAG	B	1006	1,2	14,14,15	0.55	0	17,19,21	1.28	3 (17%)
2	NAG	B	1007	3,2	14,14,15	0.63	0	17,19,21	1.24	1 (5%)
3	BMA	B	1008	2	11,11,12	1.09	1 (9%)	15,15,17	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1009	1	14,14,15	0.53	0	17,19,21	1.22	1 (5%)
2	NAG	B	1010	1,2	14,14,15	0.54	0	17,19,21	1.08	1 (5%)
2	NAG	B	1011	3,2	14,14,15	0.69	0	17,19,21	0.79	0
3	BMA	B	1012	2,4	11,11,12	1.41	1 (9%)	15,15,17	0.93	1 (6%)
4	MAN	B	1013	3	11,11,12	0.69	0	15,15,17	0.84	0
4	MAN	B	1014	3	11,11,12	0.51	0	15,15,17	1.02	1 (6%)
2	NAG	B	1015	1	14,14,15	0.46	0	17,19,21	1.03	1 (5%)
2	NAG	B	1016	1	14,14,15	0.51	0	17,19,21	1.19	2 (11%)
2	NAG	B	1017	1	14,14,15	0.54	0	17,19,21	0.75	0
6	RX8	B	1018	-	22,25,25	1.63	3 (13%)	25,37,37	1.33	5 (20%)
5	SO4	B	1019	-	4,4,4	0.17	0	6,6,6	0.10	0
5	SO4	B	1020	-	4,4,4	0.20	0	6,6,6	0.25	0
5	SO4	B	1021	-	4,4,4	0.21	0	6,6,6	0.29	0
6	RX8	C	901	-	22,25,25	1.56	3 (13%)	25,37,37	1.07	3 (12%)
2	NAG	C	902	1,2	14,14,15	0.54	0	17,19,21	1.15	2 (11%)
2	NAG	C	903	3,2	14,14,15	0.58	0	17,19,21	1.07	0
3	BMA	C	904	2,4	11,11,12	0.94	1 (9%)	15,15,17	0.93	0
4	MAN	C	905	3	11,11,12	0.62	0	15,15,17	0.71	0
4	MAN	C	906	3	11,11,12	0.68	0	15,15,17	0.79	0
2	NAG	C	907	1,2	14,14,15	0.55	0	17,19,21	0.90	0
2	NAG	C	908	3,2	14,14,15	0.69	0	17,19,21	1.14	1 (5%)
3	BMA	C	909	2	11,11,12	1.01	1 (9%)	15,15,17	0.92	0
2	NAG	C	910	1	14,14,15	0.56	0	17,19,21	0.83	1 (5%)
2	NAG	C	911	1,2	14,14,15	0.62	0	17,19,21	1.02	1 (5%)
2	NAG	C	912	3,2	14,14,15	0.64	0	17,19,21	0.74	0
3	BMA	C	913	2,4	11,11,12	1.15	1 (9%)	15,15,17	0.97	0
4	MAN	C	914	3	11,11,12	0.70	0	15,15,17	1.05	2 (13%)
4	MAN	C	915	3	11,11,12	0.46	0	15,15,17	1.06	1 (6%)
2	NAG	C	916	1	14,14,15	0.63	0	17,19,21	1.17	2 (11%)
2	NAG	C	917	1	14,14,15	0.58	0	17,19,21	0.85	0
5	SO4	C	918	-	4,4,4	0.17	0	6,6,6	0.11	0
6	RX8	D	901	-	22,25,25	1.54	3 (13%)	25,37,37	1.20	3 (12%)
6	RX8	D	902	-	22,25,25	1.57	3 (13%)	25,37,37	1.19	4 (16%)
2	NAG	D	903	1,2	14,14,15	0.50	0	17,19,21	1.09	2 (11%)
2	NAG	D	904	3,2	14,14,15	0.55	0	17,19,21	1.06	1 (5%)
3	BMA	D	905	2,4	11,11,12	1.27	1 (9%)	15,15,17	0.70	0
4	MAN	D	906	3	11,11,12	0.54	0	15,15,17	0.87	0
4	MAN	D	907	3	11,11,12	0.70	0	15,15,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	908	1,2	14,14,15	0.49	0	17,19,21	0.73	0
2	NAG	D	909	3,2	14,14,15	0.61	0	17,19,21	1.00	2 (11%)
3	BMA	D	910	2	11,11,12	0.81	0	15,15,17	0.80	0
2	NAG	D	911	1	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
2	NAG	D	912	1,2	14,14,15	0.65	0	17,19,21	1.14	1 (5%)
2	NAG	D	913	3,2	14,14,15	0.64	0	17,19,21	0.75	0
3	BMA	D	914	2,4	11,11,12	1.02	1 (9%)	15,15,17	0.77	0
4	MAN	D	915	3	11,11,12	0.69	0	15,15,17	1.04	1 (6%)
4	MAN	D	916	3	11,11,12	0.50	0	15,15,17	0.95	1 (6%)
2	NAG	D	917	1	14,14,15	0.57	0	17,19,21	0.87	0
2	NAG	D	918	1	14,14,15	0.45	0	17,19,21	0.98	1 (5%)
2	NAG	D	919	1	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
5	SO4	D	920	-	4,4,4	0.16	0	6,6,6	0.08	0
5	SO4	D	921	-	4,4,4	0.21	0	6,6,6	0.22	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	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1003	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1004	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1005	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1006	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1007	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1008	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1010	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1011	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1012	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1013	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1014	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1015	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1016	1	-	0/6/23/26	0/1/1/1
2	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
2	NAG	B	1001	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1002	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1003	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1004	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1005	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1006	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1007	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1008	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1010	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1011	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1012	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1013	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1014	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1015	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1016	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1017	1	-	0/6/23/26	0/1/1/1
6	RX8	B	1018	-	-	0/5/9/9	0/3/3/3
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	-	-	0/5/9/9	0/3/3/3
2	NAG	C	902	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	903	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	904	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	905	3	-	0/2/19/22	0/1/1/1
4	MAN	C	906	3	-	0/2/19/22	0/1/1/1
2	NAG	C	907	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	908	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	909	2	-	0/2/19/22	0/1/1/1
2	NAG	C	910	1	-	0/6/23/26	0/1/1/1
2	NAG	C	911	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	912	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	913	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	914	3	-	0/2/19/22	0/1/1/1
4	MAN	C	915	3	-	0/2/19/22	0/1/1/1
2	NAG	C	916	1	-	0/6/23/26	0/1/1/1
2	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	-	-	0/5/9/9	0/3/3/3
6	RX8	D	902	-	-	0/5/9/9	0/3/3/3
2	NAG	D	903	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	904	3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	D	905	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	906	3	-	0/2/19/22	0/1/1/1
4	MAN	D	907	3	-	0/2/19/22	0/1/1/1
2	NAG	D	908	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	909	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	910	2	-	0/2/19/22	0/1/1/1
2	NAG	D	911	1	-	0/6/23/26	0/1/1/1
2	NAG	D	912	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	913	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	914	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	915	3	-	0/2/19/22	0/1/1/1
4	MAN	D	916	3	-	0/2/19/22	0/1/1/1
2	NAG	D	917	1	-	0/6/23/26	0/1/1/1
2	NAG	D	918	1	-	0/6/23/26	0/1/1/1
2	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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1012	BMA	O5-C1	-4.01	1.37	1.43
3	A	1012	BMA	O5-C1	-3.76	1.37	1.43
3	D	905	BMA	O5-C1	-3.64	1.37	1.43
6	B	1018	RX8	O1-C10	-2.77	1.37	1.44
3	C	913	BMA	O5-C1	-2.72	1.39	1.43

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	912	NAG	O5-C1-C2	-3.69	106.42	111.52
2	B	1007	NAG	C2-N2-C7	-3.43	117.94	122.94
2	B	1001	NAG	O5-C1-C2	-3.33	106.92	111.52
2	A	1006	NAG	C2-N2-C7	-3.31	118.12	122.94
2	B	1002	NAG	O5-C1-C2	-3.16	107.17	111.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	NAG	1	0
6	B	1018	RX8	3	0
5	B	1019	SO4	1	0
6	C	901	RX8	2	0
2	C	902	NAG	1	0
2	C	903	NAG	1	0
2	C	907	NAG	1	0
5	C	918	SO4	1	0
6	D	901	RX8	3	0
6	D	902	RX8	2	0
2	D	903	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.44	45 (5%) 22 31	11, 33, 87, 120	0
1	B	751/811 (92%)	0.47	74 (9%) 7 12	9, 33, 93, 127	0
1	C	751/811 (92%)	0.67	97 (12%) 3 6	11, 43, 92, 115	0
1	D	751/811 (92%)	0.67	90 (11%) 4 8	14, 49, 91, 115	0
All	All	3004/3244 (92%)	0.56	306 (10%) 7 11	9, 39, 92, 127	0

The worst 5 of 306 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	761	THR	15.8
1	C	756	LEU	12.9
1	C	88	ASN	12.6
1	B	758	THR	12.1
1	C	86	LEU	11.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	B	1021	5/5	0.71	0.26	107,108,110,110	0
4	MAN	B	1005	11/12	0.78	0.21	61,65,73,76	0
4	MAN	B	1013	11/12	0.79	0.27	72,75,80,81	0
3	BMA	A	1008	11/12	0.80	0.18	64,72,77,79	0
4	MAN	D	915	11/12	0.80	0.20	64,74,78,78	0
3	BMA	B	1008	11/12	0.80	0.17	59,64,78,78	0
4	MAN	C	914	11/12	0.80	0.16	69,76,80,82	0
4	MAN	C	906	11/12	0.80	0.15	69,72,74,74	0
3	BMA	D	910	11/12	0.82	0.19	59,64,102,102	0
4	MAN	D	906	11/12	0.82	0.12	41,51,59,59	0
2	NAG	D	909	14/15	0.83	0.19	44,56,61,61	0
3	BMA	C	909	11/12	0.83	0.17	69,72,75,75	0
2	NAG	A	1015	14/15	0.84	0.26	63,67,69,74	0
5	SO4	B	1020	5/5	0.84	0.17	97,98,99,102	0
2	NAG	A	1017	14/15	0.84	0.20	47,64,67,70	0
4	MAN	A	1014	11/12	0.85	0.23	66,72,75,76	0
5	SO4	D	921	5/5	0.85	0.20	106,106,107,111	0
4	MAN	A	1013	11/12	0.85	0.18	59,66,67,68	0
2	NAG	B	1015	14/15	0.86	0.20	71,78,82,83	0
4	MAN	C	915	11/12	0.86	0.15	67,68,70,70	0
5	SO4	D	920	5/5	0.86	0.22	104,105,106,106	0
4	MAN	D	916	11/12	0.86	0.23	70,74,76,76	0
2	NAG	D	918	14/15	0.86	0.29	66,68,71,74	0
4	MAN	B	1014	11/12	0.87	0.18	66,69,77,77	0
3	BMA	C	904	11/12	0.88	0.10	54,59,62,65	0
2	NAG	C	916	14/15	0.88	0.14	40,46,50,53	0
4	MAN	D	907	11/12	0.88	0.21	80,82,85,88	0
4	MAN	B	1004	11/12	0.88	0.13	29,41,45,48	0
5	SO4	A	1019	5/5	0.89	0.21	100,102,104,105	0
2	NAG	B	1017	14/15	0.90	0.20	56,61,62,63	0
2	NAG	B	1009	14/15	0.90	0.14	48,60,68,68	0
3	BMA	D	914	11/12	0.90	0.11	49,57,66,72	0
2	NAG	B	1007	14/15	0.90	0.17	32,43,56,63	0
3	BMA	C	913	11/12	0.90	0.13	43,55,66,67	0
2	NAG	D	917	14/15	0.91	0.17	58,61,68,72	0
2	NAG	C	917	14/15	0.91	0.17	50,59,62,63	0
3	BMA	B	1012	11/12	0.92	0.12	48,55,62,69	0
4	MAN	C	905	11/12	0.92	0.09	51,57,59,60	0
2	NAG	D	911	14/15	0.92	0.13	49,54,59,61	0
3	BMA	A	1012	11/12	0.92	0.16	48,52,64,64	0
4	MAN	A	1005	11/12	0.92	0.10	68,70,73,74	0
2	NAG	C	910	14/15	0.93	0.10	31,46,52,54	0
2	NAG	D	919	14/15	0.93	0.14	41,51,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	C	918	5/5	0.93	0.17	89,91,92,93	0
2	NAG	A	1009	14/15	0.94	0.10	46,56,68,71	0
5	SO4	A	1018	5/5	0.94	0.11	91,93,94,94	0
2	NAG	A	1007	14/15	0.94	0.12	33,46,51,58	0
2	NAG	D	904	14/15	0.94	0.14	34,44,49,57	0
3	BMA	B	1003	11/12	0.94	0.10	32,36,45,52	0
3	BMA	D	905	11/12	0.95	0.11	59,61,73,77	0
2	NAG	C	908	14/15	0.95	0.10	31,46,59,66	0
2	NAG	B	1016	14/15	0.96	0.14	27,32,39,46	0
2	NAG	C	911	14/15	0.96	0.15	12,14,22,23	0
2	NAG	B	1010	14/15	0.96	0.12	14,17,28,32	0
4	MAN	A	1004	11/12	0.96	0.11	36,40,43,44	0
5	SO4	B	1019	5/5	0.96	0.07	86,87,88,89	0
2	NAG	C	903	14/15	0.96	0.13	29,41,51,55	0
2	NAG	A	1001	14/15	0.97	0.17	9,14,20,20	0
3	BMA	A	1003	11/12	0.97	0.10	38,41,58,64	0
6	RX8	B	1018	23/23	0.97	0.17	22,25,30,88	0
2	NAG	A	1010	14/15	0.97	0.09	15,20,24,24	0
2	NAG	B	1006	14/15	0.97	0.15	9,18,22,28	0
2	NAG	A	1006	14/15	0.97	0.12	11,16,18,26	0
2	NAG	D	912	14/15	0.97	0.12	17,19,27,32	0
2	NAG	D	903	14/15	0.97	0.16	34,37,52,54	0
6	RX8	C	901	23/23	0.97	0.17	8,14,18,21	0
2	NAG	C	902	14/15	0.97	0.14	30,36,38,41	0
2	NAG	B	1001	14/15	0.97	0.15	8,14,22,25	0
2	NAG	B	1011	14/15	0.97	0.11	16,31,38,41	0
6	RX8	D	901	23/23	0.97	0.18	11,17,22,23	0
2	NAG	D	913	14/15	0.97	0.11	19,27,40,40	0
2	NAG	A	1002	14/15	0.98	0.17	8,20,34,34	0
2	NAG	A	1011	14/15	0.98	0.09	17,24,32,42	0
2	NAG	B	1002	14/15	0.98	0.11	12,20,27,28	0
2	NAG	D	908	14/15	0.98	0.15	18,21,31,38	0
2	NAG	A	1016	14/15	0.98	0.11	26,34,41,48	0
2	NAG	C	912	14/15	0.98	0.10	14,22,31,37	0
2	NAG	C	907	14/15	0.98	0.11	13,18,30,35	0
6	RX8	D	902	23/23	0.98	0.20	25,28,38,44	0

6.5 Other polymers

There are no such residues in this entry.