Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:10 PM GMT

PDB ID	:	4R07
Title	:	Crystal structure of human TLR8 in complex with ORN06
Authors	:	Tanji, H.; Ohto, U.; Shibata, T.; Taoka, M.; Yamauchi, Y.; Isobe, T.; Miyake, K.; Shimizu, T.
Deposited on	:	2014-07-30
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

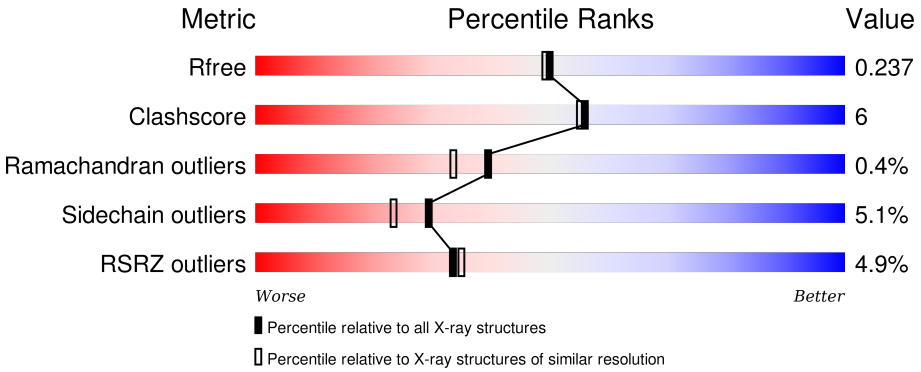
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	2% 79% 12% • 8%
1	B	811	3% 79% 10% • 9%
1	C	811	7% 75% 14% • 9%
1	D	811	6% 75% 13% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	C	910	-	-	-	X
6	NAG	C	915	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26233 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			6014	3847	1019	1129	19			
1	B	738	Total	C	N	O	S	0	0	0
			5949	3808	1009	1113	19			
1	C	738	Total	C	N	O	S	0	0	0
			5946	3806	1007	1114	19			
1	D	735	Total	C	N	O	S	0	0	0
			5925	3794	1004	1108	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	-	EXPRESSION TAG	UNP Q9NR97
A	23	SER	-	EXPRESSION TAG	UNP Q9NR97
A	24	PRO	-	EXPRESSION TAG	UNP Q9NR97
A	25	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	22	ARG	-	EXPRESSION TAG	UNP Q9NR97
B	23	SER	-	EXPRESSION TAG	UNP Q9NR97
B	24	PRO	-	EXPRESSION TAG	UNP Q9NR97
B	25	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	22	ARG	-	EXPRESSION TAG	UNP Q9NR97

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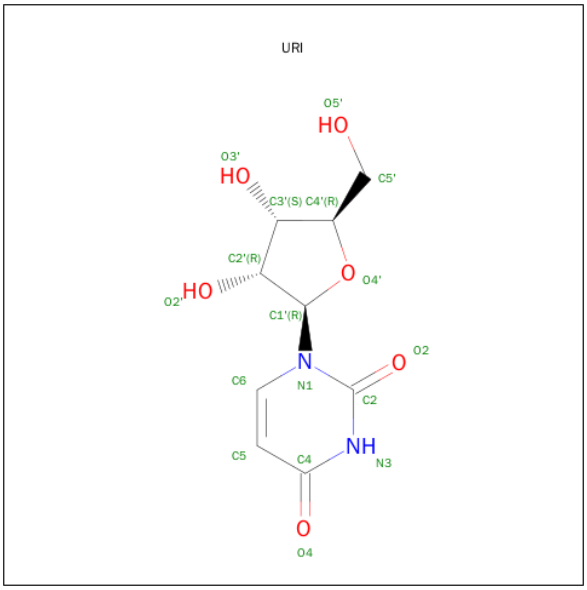
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	SER	-	EXPRESSION TAG	UNP Q9NR97
C	24	PRO	-	EXPRESSION TAG	UNP Q9NR97
C	25	TRP	-	EXPRESSION TAG	UNP Q9NR97
C	828	GLU	-	EXPRESSION TAG	UNP Q9NR97
C	829	PHE	-	EXPRESSION TAG	UNP Q9NR97
C	830	LEU	-	EXPRESSION TAG	UNP Q9NR97
C	831	VAL	-	EXPRESSION TAG	UNP Q9NR97
C	832	PRO	-	EXPRESSION TAG	UNP Q9NR97
C	833	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	22	ARG	-	EXPRESSION TAG	UNP Q9NR97
D	23	SER	-	EXPRESSION TAG	UNP Q9NR97
D	24	PRO	-	EXPRESSION TAG	UNP Q9NR97
D	25	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 URIDINE (three-letter code: URI) (formula: $C_9H_{12}N_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 17 9 2 6	0	0
2	B	1	Total C N O 17 9 2 6	0	0

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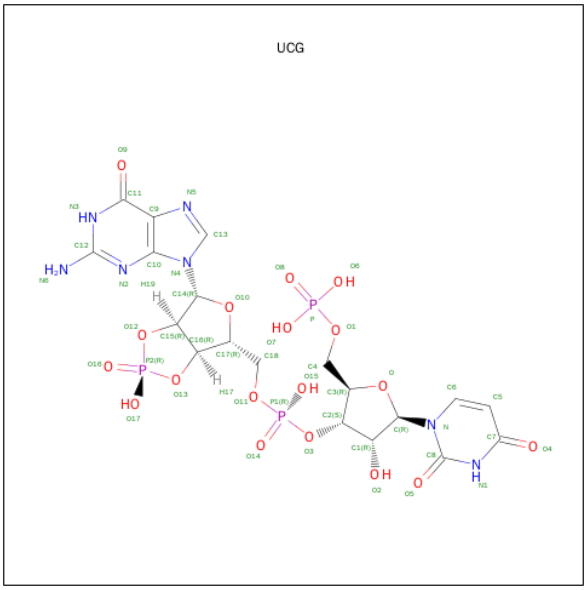
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 17 9 2 6	0	0
2	D	1	Total C N O 17 9 2 6	0	0

- Molecule 3 is 3'-O-[(R)-{[(2R,3AR,4R,6R,6AR)-6-(2-AMINO-6-OXO-1,6-DIHYDRO-9H-PURIN-9-YL)-2-HYDROXY-2-OXIDOTETRAHYDROFURO[3,4-D][1,3,2]DIOXAPHOSPHOL-4-YL]METHOXY}(HYDROXY)PHOSPHORYL]URIDINE 5'-(DIHYDROGEN PHOSPHATE) (three-letter code: UCG) (formula: $C_{19}H_{24}N_7O_{18}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 47 19 7 18 3	0	0
3	B	1	Total C N O P 47 19 7 18 3	0	0
3	C	1	Total C N O P 47 19 7 18 3	0	0
3	D	1	Total C N O P 47 19 7 18 3	0	0

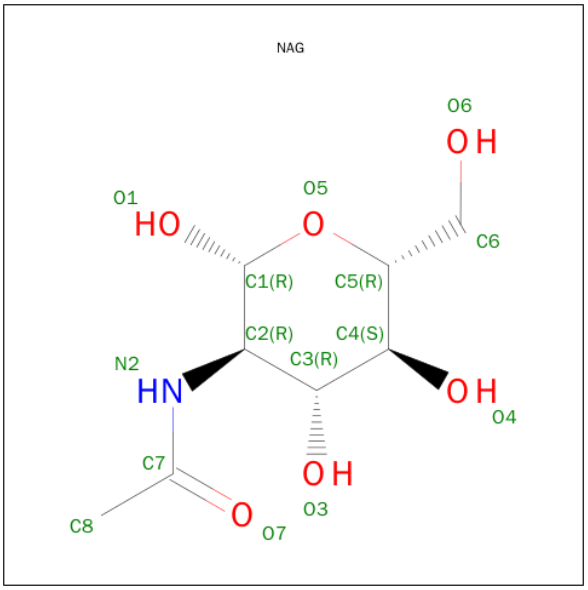
- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

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

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

- Molecule 9 is water.

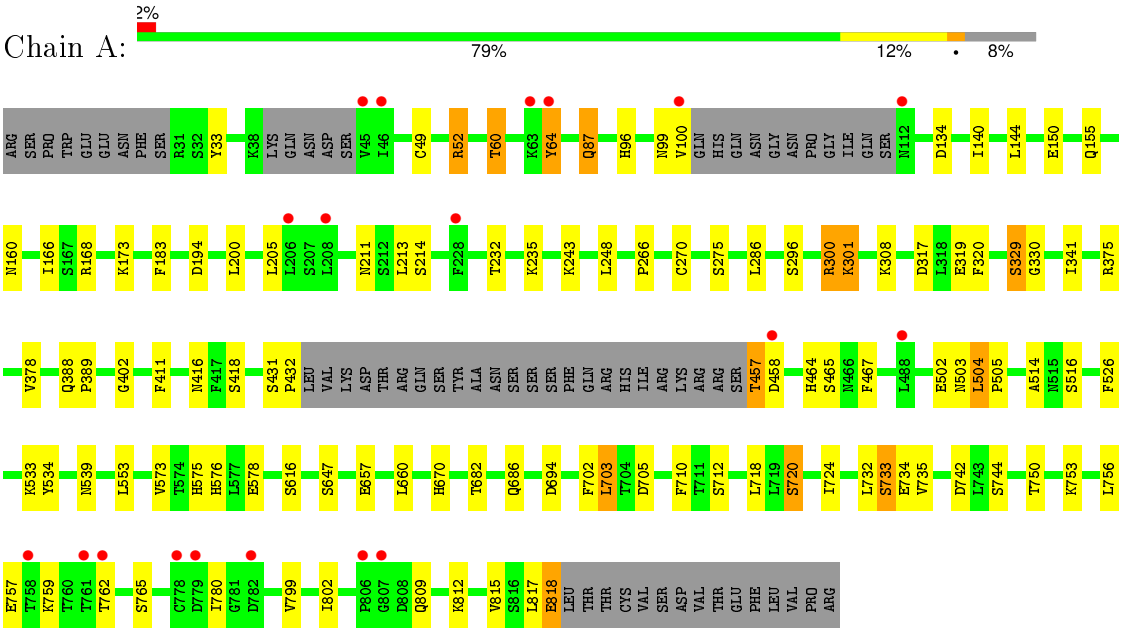
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	469	Total	O	0	0
			469	469		
9	B	374	Total	O	0	0
			374	374		
9	C	314	Total	O	0	0
			314	314		
9	D	277	Total	O	0	0
			277	277		

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

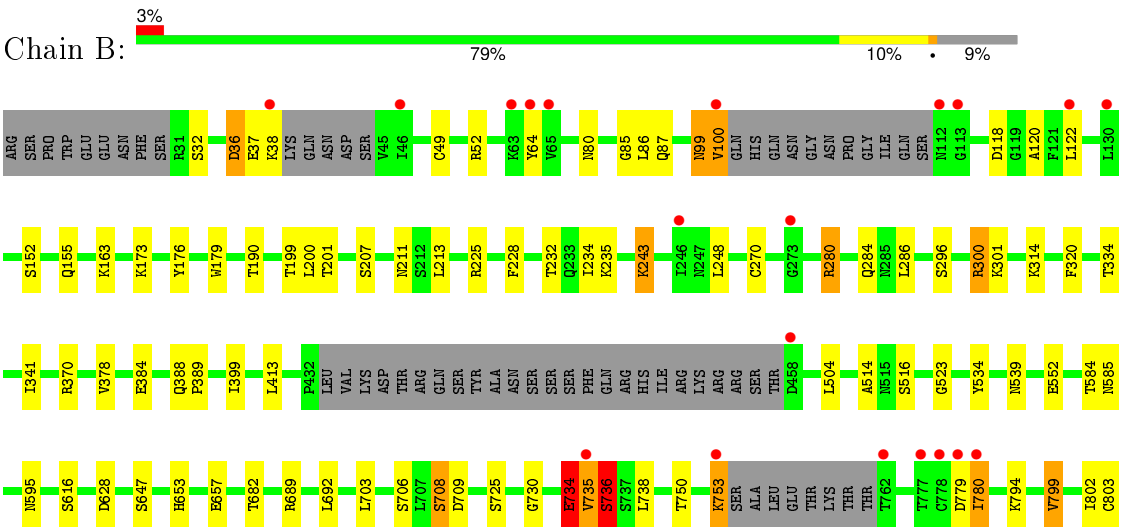
- Molecule 1: Toll-like receptor 8

Chain A:



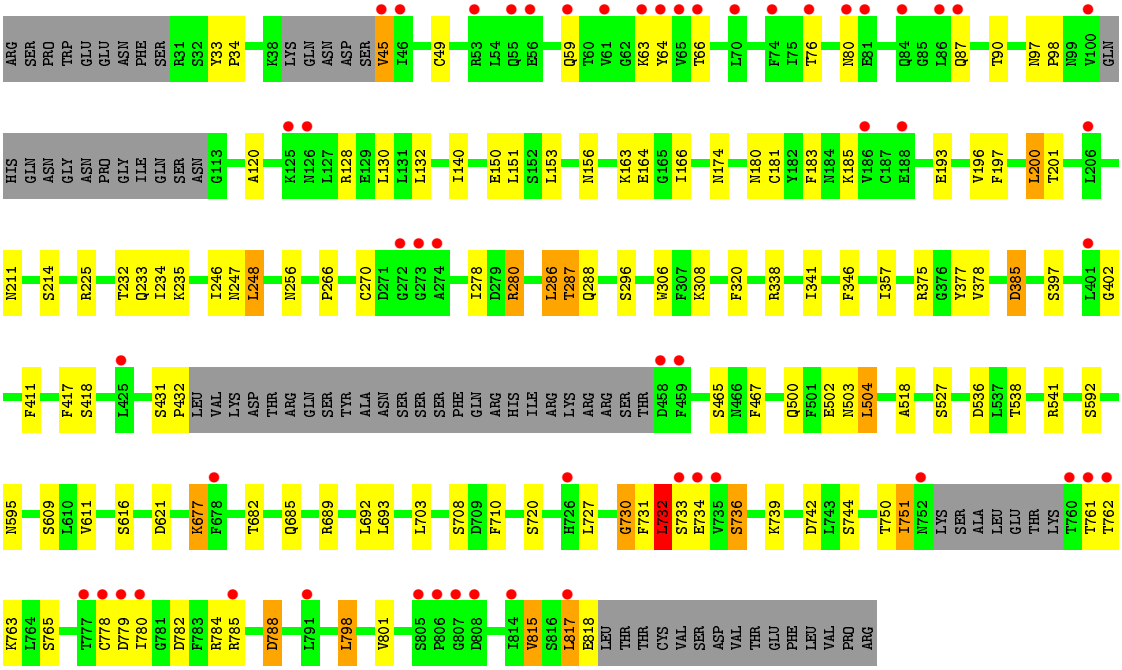
- Molecule 1: Toll-like receptor 8

Chain B:



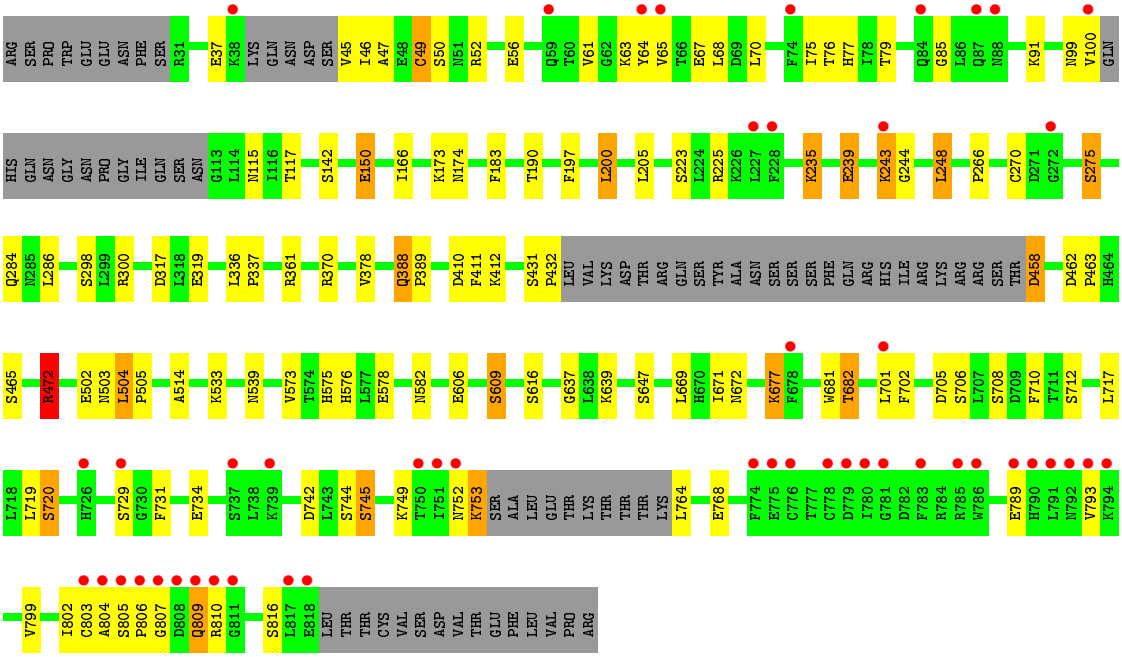
- Molecule 1: Toll-like receptor 8

Chain C:



- Molecule 1: Toll-like receptor 8

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.66Å 141.12Å 169.53Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	33.74 – 2.00 33.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (33.74-2.00) 97.5 (33.74-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.188 , 0.234 0.195 , 0.237	Depositor DCC
R_{free} test set	13522 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.8	EDS
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 267493 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26233	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.60	0/6138	0.69	0/8326
1	B	0.57	0/6072	0.71	3/8234 (0.0%)
1	C	0.54	0/6069	0.66	1/8232 (0.0%)
1	D	0.53	0/6048	0.64	1/8202 (0.0%)
All	All	0.56	0/24327	0.68	5/32994 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	4
1	D	0	1
All	All	0	9

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	628	ASP	CB-CG-OD1	6.22	123.89	118.30
1	C	621	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	472	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	805	SER	C-N-CD	-5.03	109.54	120.60
1	B	300	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	SER	Peptide
1	B	734	GLU	Peptide
1	B	85	GLY	Peptide
1	B	99	ASN	Peptide
1	C	417	PHE	Peptide
1	C	45	VAL	Peptide
1	C	730	GLY	Peptide
1	C	801	VAL	Peptide
1	D	99	ASN	Peptide

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	6014	0	5989	68	0
1	B	5949	0	5920	70	1
1	C	5946	0	5916	84	0
1	D	5925	0	5895	75	0
2	A	17	0	12	1	0
2	B	17	0	12	1	0
2	C	17	0	12	1	0
2	D	17	0	12	1	0
3	A	47	0	20	4	0
3	B	47	0	20	6	0
3	C	47	0	20	5	0
3	D	47	0	20	1	0
4	A	50	0	43	1	0
4	C	50	0	43	1	0
5	A	39	0	34	0	0
6	A	70	0	65	0	0
6	B	70	0	65	1	0
6	C	56	0	52	0	0
6	D	56	0	52	2	0
7	A	28	0	25	0	0
7	B	28	0	25	0	0
7	D	28	0	25	0	0
8	B	78	0	68	0	0
8	C	78	0	68	0	0
8	D	78	0	68	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	469	0	0	11	0
9	B	374	0	0	11	0
9	C	314	0	0	14	0
9	D	277	0	0	12	0
All	All	26233	0	24481	304	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (304) 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:D:75:ILE:HG22	9:D:1225:HOH:O	1.52	1.09
1:A:33:TYR:O	1:A:60:THR:HG21	1.59	1.02
1:A:33:TYR:O	1:A:60:THR:CG2	2.11	0.96
1:D:77:HIS:N	9:D:1225:HOH:O	2.00	0.92
1:B:708:SER:HB3	1:B:735:VAL:HG22	1.52	0.90
1:B:341:ILE:CD1	3:B:902:UCG:H5	2.05	0.87
1:B:734:GLU:HA	1:B:734:GLU:OE1	1.75	0.86
1:B:370:ARG:NE	9:B:1246:HOH:O	2.10	0.85
1:D:472:ARG:HH11	1:D:472:ARG:HG3	1.40	0.85
1:B:708:SER:HB3	1:B:735:VAL:CG2	2.07	0.84
1:C:595:ASN:ND2	9:C:1121:HOH:O	2.09	0.84
1:B:804:ALA:O	1:B:810:ARG:NH1	2.12	0.82
1:C:341:ILE:CD1	3:C:902:UCG:H5	2.11	0.81
1:C:341:ILE:HD13	3:C:902:UCG:H5	1.63	0.81
1:A:799:VAL:O	1:A:802:ILE:HD11	1.81	0.81
1:B:735:VAL:HB	1:B:736:SER:HB3	1.62	0.80
1:C:734:GLU:O	9:C:1148:HOH:O	1.99	0.78
1:D:50:SER:O	9:D:1247:HOH:O	2.02	0.78
1:B:99:ASN:O	1:B:100:VAL:HB	1.84	0.78
1:A:720:SER:OG	1:A:744:SER:OG	2.01	0.77
1:C:730:GLY:O	1:C:734:GLU:HB2	1.85	0.76
1:A:60:THR:CG2	1:A:60:THR:O	2.33	0.76
1:B:735:VAL:HG12	1:B:736:SER:HB2	1.68	0.74
1:A:341:ILE:HD11	3:A:902:UCG:C6	2.17	0.74
1:A:60:THR:HG22	1:A:60:THR:O	1.86	0.74
1:A:516:SER:OG	9:A:1252:HOH:O	2.06	0.74
1:D:502:GLU:OE1	9:D:1254:HOH:O	2.06	0.73
1:D:244:GLY:N	9:D:1196:HOH:O	1.82	0.73
1:A:660:LEU:HD22	1:A:686:GLN:HG3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:ASN:HB3	9:C:1047:HOH:O	1.88	0.71
1:B:516:SER:OG	9:B:1181:HOH:O	2.06	0.71
1:A:341:ILE:CD1	3:A:902:UCG:H5	2.19	0.71
1:A:235:LYS:HD2	1:A:270:CYS:SG	2.30	0.71
1:B:730:GLY:O	1:B:734:GLU:HB2	1.93	0.69
1:B:341:ILE:HD13	3:B:902:UCG:H5	1.74	0.69
1:D:745:SER:OG	9:D:1223:HOH:O	2.11	0.69
1:C:720:SER:HB2	1:C:742:ASP:OD2	1.94	0.68
1:D:225:ARG:O	1:D:248:LEU:HD22	1.94	0.68
1:A:33:TYR:O	1:A:60:THR:HG22	1.94	0.68
1:C:185:LYS:O	9:C:1287:HOH:O	2.12	0.68
1:B:734:GLU:OE2	1:B:735:VAL:HG13	1.94	0.68
6:D:913:NAG:O3	6:D:913:NAG:H82	1.94	0.68
1:D:150:GLU:HG2	1:D:174:ASN:HB2	1.76	0.67
1:D:190:THR:O	9:D:1248:HOH:O	2.14	0.65
1:B:341:ILE:HD12	3:B:902:UCG:H5	1.76	0.65
1:D:76:THR:N	9:D:1225:HOH:O	2.30	0.64
1:A:144:LEU:O	1:A:168:ARG:NH2	2.29	0.64
1:A:657:GLU:OE2	9:A:1224:HOH:O	2.15	0.63
1:A:817:LEU:HG	1:A:818:GLU:N	2.12	0.62
1:C:411:PHE:HB3	1:C:504:LEU:HD13	1.82	0.62
1:B:314:LYS:HD2	3:B:902:UCG:O5	1.98	0.62
1:D:799:VAL:O	1:D:802:ILE:HD11	1.98	0.62
1:A:341:ILE:HD13	3:A:902:UCG:H5	1.82	0.62
1:C:140:ILE:HD13	1:C:166:ILE:HD11	1.82	0.62
1:A:52:ARG:HG2	1:A:799:VAL:HG11	1.82	0.61
1:B:235:LYS:HD2	1:B:270:CYS:SG	2.40	0.61
1:D:472:ARG:HG3	1:D:472:ARG:NH1	2.05	0.61
1:D:63:LYS:HD2	1:D:85:GLY:O	2.01	0.61
1:A:194:ASP:OD1	9:A:1151:HOH:O	2.16	0.61
1:C:788:ASP:OD2	9:C:1254:HOH:O	2.16	0.60
1:A:329:SER:OG	1:A:330:GLY:N	2.28	0.60
1:A:341:ILE:HD11	3:A:902:UCG:C5	2.32	0.59
1:B:243:LYS:HA	1:B:243:LYS:HE3	1.83	0.59
1:C:385:ASP:HA	9:C:1279:HOH:O	2.01	0.59
1:B:595:ASN:OD1	9:B:1231:HOH:O	2.16	0.59
1:B:653:HIS:HA	9:B:1255:HOH:O	2.03	0.59
1:B:735:VAL:CB	1:B:736:SER:CB	2.82	0.58
1:D:806:PRO:HD2	1:D:809:GLN:HB2	1.86	0.57
1:C:225:ARG:NH1	1:C:247:ASN:HB3	2.19	0.57
1:D:370:ARG:HH21	6:D:909:NAG:H81	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:ALA:O	1:D:810:ARG:HD2	2.04	0.57
1:C:66:THR:O	1:C:90:THR:HG22	2.05	0.57
1:D:731:PHE:HA	1:D:734:GLU:HG2	1.86	0.56
1:A:388:GLN:HB2	1:A:389:PRO:HD3	1.86	0.56
1:D:458:ASP:N	9:D:1155:HOH:O	2.39	0.56
1:B:243:LYS:HA	1:B:243:LYS:CE	2.37	0.55
1:D:606:GLU:HG2	1:D:637:GLY:HA3	1.87	0.55
1:C:59:GLN:NE2	9:C:1293:HOH:O	2.24	0.55
1:C:782:ASP:OD2	1:C:785:ARG:NH1	2.40	0.55
1:D:411:PHE:HB3	1:D:504:LEU:HD13	1.88	0.55
1:B:735:VAL:HB	1:B:736:SER:CB	2.32	0.54
1:C:211:ASN:O	1:C:232:THR:HA	2.08	0.54
1:D:682:THR:HA	1:D:710:PHE:CD1	2.43	0.53
1:B:706:SER:HB3	1:B:709:ASP:OD2	2.08	0.53
1:B:735:VAL:CG1	1:B:736:SER:HB2	2.37	0.53
1:B:388:GLN:HB2	1:B:389:PRO:HD3	1.90	0.53
1:B:52:ARG:HG2	1:B:799:VAL:HG21	1.89	0.53
1:C:692:LEU:HD23	1:C:692:LEU:C	2.28	0.53
1:B:708:SER:CB	1:B:735:VAL:CG2	2.84	0.53
1:C:225:ARG:O	1:C:248:LEU:HD22	2.09	0.53
1:A:300:ARG:O	1:A:301:LYS:HD2	2.08	0.53
1:C:762:THR:O	1:C:762:THR:HG23	2.08	0.53
1:D:720:SER:HB3	1:D:744:SER:OG	2.09	0.53
1:A:703:LEU:HD13	1:A:724:ILE:HD12	1.90	0.53
1:D:79:THR:HG22	1:D:117:THR:HG21	1.90	0.52
1:C:225:ARG:HD3	1:C:247:ASN:O	2.09	0.52
1:B:199:THR:O	1:B:201:THR:HG23	2.10	0.52
1:B:753:LYS:H	1:B:753:LYS:CD	2.22	0.52
1:D:67:GLU:HG2	1:D:91:LYS:HB3	1.91	0.52
1:D:243:LYS:HB3	9:D:1196:HOH:O	2.10	0.52
1:D:183:PHE:HB3	1:D:266:PRO:HG2	1.90	0.52
1:C:130:LEU:HD21	1:C:132:LEU:HD11	1.92	0.52
3:D:902:UCG:H15	3:D:902:UCG:H8	1.91	0.52
1:C:720:SER:HA	1:C:744:SER:O	2.10	0.52
1:D:752:ASN:CG	1:D:753:LYS:H	2.13	0.52
1:B:735:VAL:CA	1:B:736:SER:CB	2.88	0.52
1:A:464:HIS:ND1	9:A:1394:HOH:O	2.34	0.52
1:B:296:SER:HA	1:B:320:PHE:O	2.10	0.52
1:D:647:SER:HA	1:D:672:ASN:O	2.10	0.51
1:C:357:ILE:HG13	1:C:377:TYR:CZ	2.45	0.51
1:C:385:ASP:OD2	1:C:385:ASP:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:729:SER:O	1:D:731:PHE:N	2.43	0.51
1:A:733:SER:CB	1:A:762:THR:HG22	2.40	0.51
1:C:750:THR:CG2	1:C:751:ILE:N	2.73	0.51
1:D:317:ASP:OD1	1:D:319:GLU:OE1	2.29	0.51
1:D:197:PHE:HA	1:D:200:LEU:HD22	1.93	0.50
1:A:733:SER:HB3	1:A:762:THR:HG22	1.94	0.50
1:C:80:ASN:HA	1:C:120:ALA:O	2.12	0.50
1:A:733:SER:OG	1:A:762:THR:HG22	2.12	0.50
1:C:235:LYS:HD3	1:C:270:CYS:SG	2.52	0.50
1:D:764:LEU:O	1:D:793:VAL:HG22	2.11	0.50
1:B:300:ARG:NE	9:B:1129:HOH:O	2.24	0.50
1:A:616:SER:HA	1:A:647:SER:O	2.11	0.50
1:A:411:PHE:HB3	1:A:504:LEU:HD13	1.93	0.50
1:B:370:ARG:CZ	9:B:1246:HOH:O	2.56	0.50
1:C:181:CYS:HB3	9:C:1077:HOH:O	2.12	0.50
1:A:96:HIS:HB3	9:A:1260:HOH:O	2.11	0.50
1:B:808:ASP:OD1	1:B:809:GLN:N	2.44	0.49
1:A:734:GLU:HG2	9:A:1257:HOH:O	2.11	0.49
1:D:816:SER:O	1:D:816:SER:OG	2.22	0.49
1:C:692:LEU:HD23	1:C:693:LEU:N	2.27	0.49
2:D:901:URI:O2	2:D:901:URI:H2'	2.12	0.49
1:B:234:ILE:HG22	1:B:234:ILE:O	2.11	0.49
1:D:45:VAL:HG23	1:D:65:VAL:HA	1.93	0.49
1:C:784:ARG:HH12	1:C:817:LEU:HA	1.78	0.49
1:C:739:LYS:HD2	1:C:763:LYS:HB3	1.93	0.49
1:D:166:ILE:CG2	1:D:200:LEU:HD21	2.43	0.48
1:D:720:SER:HA	1:D:744:SER:O	2.14	0.48
1:C:798:LEU:HD12	1:C:798:LEU:H	1.79	0.48
1:B:799:VAL:O	1:B:802:ILE:HD11	2.12	0.48
1:C:150:GLU:HG2	1:C:174:ASN:HB2	1.94	0.48
1:C:682:THR:HG22	1:C:710:PHE:CZ	2.47	0.48
1:D:49:CYS:HB3	1:D:70:LEU:HD23	1.94	0.48
1:B:735:VAL:CB	1:B:736:SER:HB2	2.44	0.48
2:B:901:URI:H1'	9:B:1238:HOH:O	2.14	0.48
1:B:735:VAL:HA	1:B:736:SER:HB2	1.96	0.48
1:B:817:LEU:HD22	9:B:1095:HOH:O	2.14	0.48
1:D:410:ASP:OD1	1:D:412:LYS:HE3	2.14	0.47
1:B:384:GLU:HA	1:B:413:LEU:HB3	1.96	0.47
1:C:341:ILE:HD12	3:C:902:UCG:C8	2.44	0.47
1:D:502:GLU:O	1:D:503:ASN:HB2	2.14	0.47
1:D:431:SER:HB2	1:D:432:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:LYS:HD2	1:D:270:CYS:SG	2.53	0.47
1:C:287:THR:CG2	1:C:288:GLN:HE21	2.27	0.47
1:A:375:ARG:HA	1:A:402:GLY:O	2.15	0.47
1:B:780:ILE:HG23	1:B:780:ILE:O	2.15	0.47
1:D:205:LEU:HD23	1:D:205:LEU:C	2.34	0.47
1:D:742:ASP:HA	1:D:768:GLU:HB2	1.97	0.47
2:C:901:URI:O5'	1:D:573:VAL:HA	2.15	0.47
1:D:705:ASP:OD1	1:D:706:SER:N	2.48	0.47
1:A:211:ASN:O	1:A:232:THR:HA	2.15	0.47
1:C:287:THR:HG22	9:C:1261:HOH:O	2.15	0.46
1:C:234:ILE:O	1:C:256:ASN:HB3	2.16	0.46
1:B:523:GLY:O	1:B:552:GLU:HB3	2.16	0.46
1:C:280:ARG:HH11	1:C:280:ARG:HG3	1.80	0.46
1:B:523:GLY:HA2	1:B:552:GLU:OE1	2.16	0.46
1:A:718:LEU:HA	1:A:742:ASP:HB3	1.97	0.46
1:C:45:VAL:HG11	1:C:64:TYR:CD2	2.49	0.46
1:B:692:LEU:HD23	1:B:692:LEU:C	2.36	0.46
1:B:616:SER:HA	1:B:647:SER:O	2.15	0.46
1:A:52:ARG:HG2	1:A:799:VAL:HG21	1.98	0.46
1:A:99:ASN:O	1:A:100:VAL:HB	2.15	0.46
1:A:87:GLN:CG	9:A:1135:HOH:O	2.64	0.46
1:A:140:ILE:HD13	1:A:166:ILE:HD11	1.97	0.46
1:D:606:GLU:CG	1:D:637:GLY:HA3	2.46	0.46
1:B:514:ALA:HA	1:B:539:ASN:O	2.16	0.46
1:B:341:ILE:HD12	3:B:902:UCG:C8	2.46	0.45
1:A:52:ARG:CG	1:A:799:VAL:HG21	2.47	0.45
6:B:914:NAG:H61	9:B:1164:HOH:O	2.16	0.45
1:C:500:GLN:OE1	9:C:1136:HOH:O	2.21	0.45
1:C:341:ILE:CD1	3:C:902:UCG:C8	2.95	0.45
1:B:152:SER:HA	1:B:176:TYR:HB2	1.99	0.45
1:B:753:LYS:H	1:B:753:LYS:CE	2.29	0.45
1:D:77:HIS:CD2	1:D:115:ASN:HB3	2.51	0.45
1:D:805:SER:HB2	1:D:806:PRO:HA	1.98	0.45
1:C:467:PHE:HB3	4:C:903:NAG:H81	1.99	0.45
1:A:183:PHE:HB3	1:A:266:PRO:HG2	1.97	0.45
1:C:502:GLU:O	1:C:503:ASN:HB2	2.17	0.45
1:D:514:ALA:HA	1:D:539:ASN:O	2.17	0.45
1:B:809:GLN:O	1:B:810:ARG:C	2.55	0.44
1:A:205:LEU:C	1:A:205:LEU:HD23	2.38	0.44
1:D:56:GLU:HA	1:D:75:ILE:HG23	1.99	0.44
1:A:296:SER:HA	1:A:320:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:SER:HA	1:D:298:SER:HB2	1.98	0.44
1:A:87:GLN:HG3	9:A:1135:HOH:O	2.17	0.44
1:A:732:LEU:HD12	1:A:756:LEU:HD23	2.00	0.44
8:D:903:NAG:H61	9:D:1125:HOH:O	2.17	0.44
1:B:657:GLU:OE2	9:B:1045:HOH:O	2.21	0.44
1:C:731:PHE:O	1:C:732:LEU:C	2.55	0.44
1:B:817:LEU:HG	1:B:818:GLU:H	1.82	0.44
1:B:155:GLN:HA	1:B:179:TRP:O	2.18	0.44
1:C:163:LYS:HG3	1:C:193:GLU:OE2	2.18	0.44
1:D:336:LEU:N	1:D:337:PRO:CD	2.79	0.44
1:D:37:GLU:HA	1:D:46:ILE:O	2.18	0.44
1:D:677:LYS:HE3	1:D:701:LEU:HD11	1.99	0.44
1:C:762:THR:CG2	1:C:762:THR:O	2.66	0.44
1:C:183:PHE:HB3	1:C:266:PRO:HG2	1.99	0.44
1:A:502:GLU:O	1:A:503:ASN:HB2	2.17	0.44
1:D:576:HIS:HB3	1:D:578:GLU:OE1	2.17	0.44
1:C:730:GLY:O	1:C:734:GLU:CB	2.60	0.44
1:C:225:ARG:CZ	1:C:247:ASN:HB3	2.48	0.44
1:D:45:VAL:CG2	1:D:65:VAL:HA	2.48	0.44
1:A:317:ASP:OD1	1:A:319:GLU:OE1	2.36	0.44
1:D:802:ILE:HG22	1:D:803:CYS:O	2.18	0.44
1:B:753:LYS:H	1:B:753:LYS:HD2	1.83	0.44
1:C:689:ARG:NE	9:C:1285:HOH:O	2.50	0.44
1:D:609:SER:N	9:D:1250:HOH:O	2.51	0.44
1:B:341:ILE:HD11	3:B:902:UCG:C6	2.47	0.43
1:B:808:ASP:OD1	1:B:809:GLN:HG2	2.18	0.43
1:A:213:LEU:O	1:A:214:SER:HB2	2.17	0.43
1:A:809:GLN:O	1:A:812:LYS:HG3	2.18	0.43
1:D:197:PHE:O	1:D:200:LEU:HB2	2.18	0.43
1:A:576:HIS:HB3	1:A:578:GLU:OE1	2.19	0.43
1:B:99:ASN:O	1:B:100:VAL:CB	2.63	0.43
1:C:280:ARG:NH1	1:C:280:ARG:HG3	2.34	0.43
1:A:533:LYS:NZ	9:A:1053:HOH:O	2.51	0.43
1:A:300:ARG:NH2	9:A:1218:HOH:O	2.52	0.43
1:C:677:LYS:H	1:C:677:LYS:HG2	1.71	0.43
1:A:300:ARG:NE	9:A:1218:HOH:O	1.98	0.43
1:C:201:THR:HB	9:C:1080:HOH:O	2.17	0.43
1:A:514:ALA:HA	1:A:539:ASN:O	2.19	0.43
1:B:190:THR:HB	1:B:213:LEU:HD23	2.00	0.43
1:C:518:ALA:HA	1:C:541:ARG:O	2.18	0.43
1:B:736:SER:H	1:B:738:LEU:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ASP:OD1	1:A:319:GLU:HG3	2.19	0.43
1:C:708:SER:HB3	1:C:734:GLU:HG2	2.00	0.42
1:B:584:THR:HG22	1:B:585:ASN:OD1	2.19	0.42
1:D:388:GLN:N	1:D:389:PRO:CD	2.82	0.42
1:C:736:SER:O	1:C:763:LYS:HG3	2.18	0.42
1:A:431:SER:HB2	1:A:432:PRO:CD	2.50	0.42
1:D:717:LEU:HD21	1:D:719:LEU:HD11	2.01	0.42
1:C:727:LEU:HD12	1:C:751:ILE:HG23	2.02	0.42
1:D:431:SER:HB2	1:D:432:PRO:HD2	2.01	0.42
1:C:151:LEU:HD21	1:C:153:LEU:HD11	2.02	0.42
1:A:467:PHE:HB3	4:A:903:NAG:H81	2.00	0.42
1:C:214:SER:HA	1:C:233:GLN:O	2.19	0.42
1:D:616:SER:HA	1:D:647:SER:O	2.18	0.42
1:C:536:ASP:OD1	1:C:538:THR:HG23	2.20	0.42
1:A:705:ASP:OD1	1:A:705:ASP:C	2.57	0.42
1:C:278:ILE:HB	1:C:306:TRP:CZ2	2.53	0.42
1:A:660:LEU:CD2	1:A:686:GLN:HG3	2.45	0.42
1:A:134:ASP:HA	1:A:155:GLN:O	2.19	0.42
1:C:296:SER:HA	1:C:320:PHE:O	2.20	0.42
1:B:399:ILE:O	1:B:399:ILE:HG23	2.20	0.42
1:D:462:ASP:HA	1:D:463:PRO:HD3	1.93	0.42
1:B:36:ASP:OD2	1:B:52:ARG:NH2	2.52	0.42
1:A:703:LEU:HD13	1:A:703:LEU:N	2.34	0.42
1:D:458:ASP:OD1	1:D:458:ASP:N	2.53	0.41
1:C:750:THR:HG23	1:C:751:ILE:N	2.34	0.41
1:A:457:THR:HB	1:A:458:ASP:H	1.62	0.41
1:C:727:LEU:HD23	1:C:727:LEU:HA	1.96	0.41
1:C:734:GLU:CG	9:C:1148:HOH:O	2.68	0.41
1:A:734:GLU:HB3	1:A:735:VAL:HG23	2.03	0.41
1:C:197:PHE:HA	1:C:200:LEU:HD22	2.02	0.41
1:D:669:LEU:HD21	1:D:671:ILE:HD11	2.02	0.41
1:D:729:SER:C	1:D:731:PHE:N	2.74	0.41
1:A:64:TYR:N	1:A:64:TYR:CD1	2.86	0.41
1:A:526:PHE:HB3	1:A:553:LEU:HD21	2.03	0.41
1:B:735:VAL:CA	1:B:736:SER:HB2	2.51	0.41
1:D:472:ARG:HH11	1:D:472:ARG:CG	2.23	0.41
1:C:736:SER:HB3	1:C:761:THR:HG23	2.01	0.41
1:C:320:PHE:HA	1:C:346:PHE:O	2.21	0.41
1:C:527:SER:O	9:C:1154:HOH:O	2.21	0.41
1:C:815:VAL:O	1:C:815:VAL:CG1	2.68	0.41
1:D:573:VAL:O	1:D:575:HIS:CE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:SER:HA	1:C:616:SER:O	2.21	0.41
1:C:286:LEU:HD12	1:C:286:LEU:HA	1.90	0.41
1:B:802:ILE:HG22	1:B:803:CYS:O	2.20	0.41
1:A:682:THR:HG22	1:A:710:PHE:CZ	2.56	0.41
1:C:97:ASN:HA	1:C:98:PRO:HA	1.83	0.41
1:C:341:ILE:HD11	3:C:902:UCG:C6	2.51	0.41
1:D:79:THR:HG22	1:D:117:THR:CG2	2.51	0.41
1:C:739:LYS:HB3	1:C:739:LYS:HE3	1.85	0.41
1:C:518:ALA:HB2	1:C:541:ARG:HD2	2.03	0.41
1:C:33:TYR:CG	1:C:34:PRO:HA	2.56	0.41
1:B:163:LYS:HE2	9:B:1081:HOH:O	2.21	0.41
1:D:239:GLU:HG3	1:D:284:GLN:HE21	1.86	0.41
1:B:32:SER:CB	1:B:37:GLU:HG3	2.51	0.41
1:A:670:HIS:HA	1:A:694:ASP:HB3	2.03	0.41
1:B:80:ASN:HA	1:B:120:ALA:O	2.21	0.41
1:B:211:ASN:O	1:B:232:THR:HA	2.22	0.40
1:C:375:ARG:HA	1:C:402:GLY:O	2.21	0.40
1:A:388:GLN:CB	1:A:389:PRO:HD3	2.50	0.40
1:C:431:SER:HB2	1:C:432:PRO:CD	2.52	0.40
1:C:196:VAL:O	1:C:196:VAL:HG22	2.20	0.40
1:B:735:VAL:HA	1:B:736:SER:CB	2.50	0.40
1:C:685:GLN:HE21	1:C:710:PHE:HD1	1.69	0.40
1:A:573:VAL:O	1:A:575:HIS:CE1	2.74	0.40
1:D:223:SER:O	1:D:225:ARG:NH1	2.53	0.40
1:D:637:GLY:HA2	1:D:639:LYS:HE3	2.04	0.40
1:B:207:SER:HA	1:B:228:PHE:HB2	2.03	0.40
1:C:156:ASN:C	1:C:180:ASN:OD1	2.60	0.40
2:A:901:URI:O2	2:A:901:URI:H2'	2.21	0.40
1:D:47:ALA:HB3	1:D:68:LEU:HD12	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ARG:NH1	1:B:709:ASP:OD2[1_455]	2.03	0.17

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	739/811 (91%)	700 (95%)	37 (5%)	2 (0%)	46	41
1	B	728/811 (90%)	678 (93%)	47 (6%)	3 (0%)	39	33
1	C	728/811 (90%)	665 (91%)	59 (8%)	4 (0%)	34	26
1	D	725/811 (89%)	668 (92%)	53 (7%)	4 (1%)	30	22
All	All	2920/3244 (90%)	2711 (93%)	196 (7%)	13 (0%)	39	33

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	736	SER
1	C	378	VAL
1	D	243	LYS
1	B	284	GLN
1	C	732	LEU
1	A	378	VAL
1	B	378	VAL
1	C	779	ASP
1	D	378	VAL
1	C	815	VAL
1	D	505	PRO
1	D	807	GLY
1	A	505	PRO

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	693/755 (92%)	658 (95%)	35 (5%)	29	23
1	B	685/755 (91%)	649 (95%)	36 (5%)	28	22
1	C	685/755 (91%)	651 (95%)	34 (5%)	30	24
1	D	682/755 (90%)	646 (95%)	36 (5%)	28	22
All	All	2745/3020 (91%)	2604 (95%)	141 (5%)	29	23

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	CYS
1	A	52	ARG
1	A	60	THR
1	A	64	TYR
1	A	87	GLN
1	A	150	GLU
1	A	160	ASN
1	A	173	LYS
1	A	200	LEU
1	A	243	LYS
1	A	248	LEU
1	A	275	SER
1	A	286	LEU
1	A	300	ARG
1	A	301	LYS
1	A	308	LYS
1	A	329	SER
1	A	416	ASN
1	A	457	THR
1	A	465	SER
1	A	504	LEU
1	A	534	TYR
1	A	702	PHE
1	A	703	LEU
1	A	712	SER
1	A	720	SER
1	A	733	SER
1	A	750	THR
1	A	753	LYS
1	A	757	GLU
1	A	759	LYS
1	A	765	SER
1	A	780	ILE

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Mol	Chain	Res	Type
1	A	815	VAL
1	A	818	GLU
1	B	36	ASP
1	B	38	LYS
1	B	49	CYS
1	B	64	TYR
1	B	86	LEU
1	B	87	GLN
1	B	100	VAL
1	B	118	ASP
1	B	122	LEU
1	B	173	LYS
1	B	200	LEU
1	B	225	ARG
1	B	243	LYS
1	B	248	LEU
1	B	280	ARG
1	B	286	LEU
1	B	301	LYS
1	B	334	THR
1	B	504	LEU
1	B	534	TYR
1	B	682	THR
1	B	689	ARG
1	B	703	LEU
1	B	708	SER
1	B	725	SER
1	B	734	GLU
1	B	735	VAL
1	B	736	SER
1	B	750	THR
1	B	753	LYS
1	B	779	ASP
1	B	780	ILE
1	B	794	LYS
1	B	799	VAL
1	B	816	SER
1	B	817	LEU
1	C	49	CYS
1	C	63	LYS
1	C	76	THR
1	C	87	GLN

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Mol	Chain	Res	Type
1	C	128	ARG
1	C	164	GLU
1	C	200	LEU
1	C	246	ILE
1	C	248	LEU
1	C	280	ARG
1	C	286	LEU
1	C	287	THR
1	C	308	LYS
1	C	338	ARG
1	C	385	ASP
1	C	397	SER
1	C	418	SER
1	C	465	SER
1	C	504	LEU
1	C	609	SER
1	C	611	VAL
1	C	677	LYS
1	C	703	LEU
1	C	732	LEU
1	C	733	SER
1	C	736	SER
1	C	751	ILE
1	C	765	SER
1	C	778	CYS
1	C	780	ILE
1	C	788	ASP
1	C	798	LEU
1	C	817	LEU
1	C	818	GLU
1	D	49	CYS
1	D	52	ARG
1	D	61	VAL
1	D	64	TYR
1	D	100	VAL
1	D	142	SER
1	D	150	GLU
1	D	173	LYS
1	D	200	LEU
1	D	235	LYS
1	D	239	GLU
1	D	248	LEU

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Mol	Chain	Res	Type
1	D	275	SER
1	D	286	LEU
1	D	300	ARG
1	D	361	ARG
1	D	388	GLN
1	D	458	ASP
1	D	465	SER
1	D	472	ARG
1	D	504	LEU
1	D	533	LYS
1	D	582	ASN
1	D	609	SER
1	D	677	LYS
1	D	681	TRP
1	D	682	THR
1	D	702	PHE
1	D	708	SER
1	D	712	SER
1	D	720	SER
1	D	745	SER
1	D	749	LYS
1	D	753	LYS
1	D	789	GLU
1	D	809	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	84	GLN
1	B	135	ASN
1	C	288	GLN
1	D	123	ASN
1	D	686	GLN
1	D	809	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

35 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	$\#\|Z\|>2$
4	NAG	A	903	1,4	14,14,15	0.80	1 (7%)	15,19,21	1.25	1 (6%)
4	NAG	A	904	4	14,14,15	0.74	1 (7%)	15,19,21	1.38	2 (13%)
4	BMA	A	905	4	11,11,12	0.55	0	14,15,17	3.28	6 (42%)
4	MAN	A	906	4	11,11,12	0.76	0	14,15,17	1.39	3 (21%)
5	BMA	A	907	5	11,11,12	0.53	0	14,15,17	0.84	0
5	NAG	A	908	1,5	14,14,15	0.95	1 (7%)	15,19,21	1.00	1 (6%)
5	NAG	A	909	5	14,14,15	0.80	0	15,19,21	1.72	3 (20%)
7	NAG	A	911	1,7	14,14,15	0.94	1 (7%)	15,19,21	0.63	0
7	NAG	A	912	7	14,14,15	0.77	1 (7%)	15,19,21	1.86	2 (13%)
8	NAG	B	903	1,8	14,14,15	0.65	0	15,19,21	1.53	2 (13%)
8	NAG	B	904	8	14,14,15	0.77	0	15,19,21	1.35	4 (26%)
8	BMA	B	905	8	11,11,12	0.68	0	14,15,17	1.61	3 (21%)
8	NAG	B	906	1,8	14,14,15	0.73	0	15,19,21	1.12	2 (13%)
8	NAG	B	907	8	14,14,15	0.99	1 (7%)	15,19,21	1.54	3 (20%)
8	BMA	B	908	8	11,11,12	0.27	0	14,15,17	0.94	1 (7%)
7	NAG	B	910	1,7	14,14,15	0.81	0	15,19,21	0.99	0
7	NAG	B	911	7	14,14,15	0.77	1 (7%)	15,19,21	1.38	3 (20%)
4	NAG	C	903	1,4	14,14,15	1.06	1 (7%)	15,19,21	1.38	3 (20%)
4	NAG	C	904	4	14,14,15	0.75	0	15,19,21	1.15	1 (6%)
4	BMA	C	905	4	11,11,12	0.32	0	14,15,17	1.30	1 (7%)
4	MAN	C	906	4	11,11,12	0.82	0	14,15,17	1.50	3 (21%)
8	NAG	C	907	1,8	14,14,15	0.49	0	15,19,21	0.80	0
8	NAG	C	908	8	14,14,15	0.98	1 (7%)	15,19,21	1.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BMA	C	909	8	11,11,12	0.43	0	14,15,17	1.10	1 (7%)
8	NAG	C	911	1,8	14,14,15	0.73	0	15,19,21	0.95	0
8	NAG	C	912	8	14,14,15	0.50	0	15,19,21	1.14	1 (6%)
8	BMA	C	913	8	11,11,12	0.55	0	14,15,17	1.13	0
8	NAG	D	903	1,8	14,14,15	0.77	0	15,19,21	2.11	4 (26%)
8	NAG	D	904	8	14,14,15	0.73	0	15,19,21	0.99	0
8	BMA	D	905	8	11,11,12	0.58	0	14,15,17	2.36	5 (35%)
8	NAG	D	906	1,8	14,14,15	0.62	0	15,19,21	1.33	2 (13%)
8	NAG	D	907	8	14,14,15	1.06	1 (7%)	15,19,21	1.39	3 (20%)
8	BMA	D	908	8	11,11,12	0.49	0	14,15,17	0.80	1 (7%)
7	NAG	D	910	1,7	14,14,15	1.21	2 (14%)	15,19,21	1.96	4 (26%)
7	NAG	D	911	7	14,14,15	0.67	1 (7%)	15,19,21	1.04	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	903	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	904	4	-	0/6/23/26	0/1/1/1
4	BMA	A	905	4	-	0/2/19/22	0/1/1/1
4	MAN	A	906	4	-	0/2/19/22	0/1/1/1
5	BMA	A	907	5	-	0/2/19/22	0/1/1/1
5	NAG	A	908	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	909	5	-	0/6/23/26	0/1/1/1
7	NAG	A	911	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	912	7	-	0/6/23/26	0/1/1/1
8	NAG	B	903	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	904	8	-	0/6/23/26	0/1/1/1
8	BMA	B	905	8	-	0/2/19/22	0/1/1/1
8	NAG	B	906	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	907	8	-	0/6/23/26	0/1/1/1
8	BMA	B	908	8	-	0/2/19/22	0/1/1/1
7	NAG	B	910	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	911	7	-	0/6/23/26	0/1/1/1
4	NAG	C	903	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	904	4	-	0/6/23/26	0/1/1/1
4	BMA	C	905	4	-	0/2/19/22	0/1/1/1
4	MAN	C	906	4	-	0/2/19/22	0/1/1/1
8	NAG	C	907	1,8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	908	8	-	0/6/23/26	0/1/1/1
8	BMA	C	909	8	-	0/2/19/22	0/1/1/1
8	NAG	C	911	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	912	8	-	0/6/23/26	0/1/1/1
8	BMA	C	913	8	-	0/2/19/22	0/1/1/1
8	NAG	D	903	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	904	8	-	0/6/23/26	0/1/1/1
8	BMA	D	905	8	-	0/2/19/22	0/1/1/1
8	NAG	D	906	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	907	8	-	0/6/23/26	0/1/1/1
8	BMA	D	908	8	-	0/2/19/22	0/1/1/1
7	NAG	D	910	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	911	7	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	908	NAG	O5-C1	-2.87	1.38	1.43
7	D	910	NAG	O5-C1	-2.83	1.39	1.43
4	A	903	NAG	O5-C1	-2.61	1.39	1.43
5	A	908	NAG	O5-C1	-2.46	1.39	1.43
4	C	903	NAG	O5-C1	-2.44	1.39	1.43
7	A	911	NAG	O5-C1	-2.35	1.39	1.43
7	B	911	NAG	O5-C1	-2.29	1.39	1.43
7	D	910	NAG	C2-N2	-2.25	1.42	1.46
8	D	907	NAG	O5-C1	-2.25	1.40	1.43
7	A	912	NAG	O5-C1	-2.16	1.40	1.43
4	A	904	NAG	O5-C1	-2.02	1.40	1.43
8	B	907	NAG	O5-C1	-2.02	1.40	1.43
7	D	911	NAG	O5-C1	-2.02	1.40	1.43

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	903	NAG	O6-C6-C5	-4.85	95.30	111.33
7	A	912	NAG	C3-C4-C5	-4.44	102.46	110.20
7	D	910	NAG	O5-C5-C6	-4.12	98.43	107.35
5	A	909	NAG	O6-C6-C5	-3.60	99.45	111.33
8	D	907	NAG	O4-C4-C3	-3.06	103.45	110.34
8	B	907	NAG	O4-C4-C3	-3.03	103.52	110.34
4	A	904	NAG	O3-C3-C4	-2.99	103.62	110.34
7	B	911	NAG	C3-C4-C5	-2.97	105.02	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	912	NAG	C3-C4-C5	-2.88	105.17	110.20
8	B	905	BMA	O4-C4-C3	-2.81	104.02	110.34
7	D	911	NAG	C3-C2-N2	-2.69	104.12	110.56
8	B	904	NAG	C1-O5-C5	-2.62	108.93	112.25
8	B	907	NAG	C4-C3-C2	-2.56	107.25	111.23
8	D	906	NAG	O7-C7-C8	-2.54	117.41	122.06
8	D	907	NAG	C3-C2-N2	-2.51	104.54	110.56
8	D	903	NAG	C2-N2-C7	-2.51	119.81	123.04
8	B	903	NAG	C6-C5-C4	-2.51	106.83	113.02
8	B	907	NAG	O6-C6-C5	-2.50	103.09	111.33
4	A	903	NAG	O7-C7-C8	-2.49	117.49	122.06
7	D	910	NAG	C4-C3-C2	-2.49	107.36	111.23
8	D	905	BMA	C6-C5-C4	-2.48	106.91	113.02
4	A	905	BMA	C6-C5-C4	-2.43	107.01	113.02
4	A	904	NAG	O4-C4-C3	-2.41	104.91	110.34
5	A	909	NAG	O4-C4-C3	-2.40	104.93	110.34
7	B	911	NAG	C4-C3-C2	-2.38	107.52	111.23
4	C	903	NAG	C6-C5-C4	-2.36	107.18	113.02
5	A	908	NAG	O7-C7-C8	-2.33	117.79	122.06
8	B	908	BMA	O2-C2-C1	-2.32	104.56	109.21
4	C	903	NAG	O6-C6-C5	-2.26	103.88	111.33
8	D	907	NAG	O6-C6-C5	-2.19	104.09	111.33
8	B	904	NAG	C2-N2-C7	-2.17	120.25	123.04
4	A	905	BMA	O3-C3-C4	-2.17	105.45	110.34
4	A	906	MAN	C2-C3-C4	-2.15	107.39	111.04
8	B	904	NAG	C3-C4-C5	-2.14	106.47	110.20
8	D	908	BMA	C2-C3-C4	-2.13	107.43	111.04
8	C	909	BMA	O2-C2-C1	-2.12	104.95	109.21
4	C	906	MAN	O5-C1-C2	-2.07	107.50	110.86
8	D	903	NAG	O3-C3-C4	-2.06	105.69	110.34
7	B	911	NAG	O6-C6-C5	-2.05	104.55	111.33
8	B	906	NAG	O4-C4-C3	-2.04	105.74	110.34
4	C	906	MAN	O4-C4-C3	-2.02	105.78	110.34
4	C	904	NAG	O4-C4-C3	-2.00	105.83	110.34
8	B	904	NAG	O5-C5-C6	2.04	111.77	107.35
8	D	905	BMA	O3-C3-C2	2.05	113.70	110.00
8	D	906	NAG	O5-C5-C6	2.10	111.90	107.35
8	B	906	NAG	C8-C7-N2	2.17	120.26	116.11
4	A	906	MAN	O2-C2-C3	2.18	114.51	110.12
8	B	905	BMA	O3-C3-C2	2.25	114.06	110.00
4	A	906	MAN	O3-C3-C2	2.29	114.14	110.00
8	D	905	BMA	C1-C2-C3	2.31	112.28	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	905	BMA	C2-C3-C4	2.41	115.14	111.04
4	C	903	NAG	C1-O5-C5	2.44	115.35	112.25
7	D	910	NAG	C3-C4-C5	2.45	114.46	110.20
4	A	905	BMA	O5-C1-C2	2.52	114.95	110.86
4	C	905	BMA	C1-C2-C3	2.68	112.71	109.54
8	B	905	BMA	C1-C2-C3	3.13	113.24	109.54
5	A	909	NAG	C1-O5-C5	3.14	116.24	112.25
4	C	906	MAN	C3-C4-C5	3.28	115.91	110.20
8	B	903	NAG	C1-O5-C5	3.39	116.55	112.25
8	D	905	BMA	C3-C4-C5	3.96	117.10	110.20
7	D	910	NAG	C1-O5-C5	4.26	117.65	112.25
8	D	903	NAG	C1-O5-C5	4.28	117.68	112.25
7	A	912	NAG	C1-O5-C5	4.50	117.96	112.25
4	A	905	BMA	C3-C4-C5	4.53	118.09	110.20
8	D	905	BMA	C1-O5-C5	6.18	120.09	112.25
4	A	905	BMA	C1-O5-C5	9.88	124.79	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	NAG	1	0
4	C	903	NAG	1	0
8	D	903	NAG	1	0

5.6 Ligand geometry (i)

26 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	URI	A	901	-	12,18,18	1.01	1 (8%)	15,26,26	2.42	2 (13%)
3	UCG	A	902	-	39,52,52	1.50	7 (17%)	48,82,82	1.88	13 (27%)
6	NAG	A	910	1	14,14,15	0.59	0	15,19,21	1.62	2 (13%)
6	NAG	A	913	1	14,14,15	0.82	0	15,19,21	1.08	1 (6%)
6	NAG	A	914	1	14,14,15	0.53	0	15,19,21	1.30	1 (6%)
6	NAG	A	915	1	14,14,15	0.49	0	15,19,21	1.33	3 (20%)
6	NAG	A	916	1	14,14,15	0.73	0	15,19,21	2.28	4 (26%)
2	URI	B	901	-	12,18,18	1.23	2 (16%)	15,26,26	2.38	1 (6%)
3	UCG	B	902	-	39,52,52	1.40	7 (17%)	48,82,82	2.07	12 (25%)
6	NAG	B	909	1	14,14,15	0.81	1 (7%)	15,19,21	0.78	0
6	NAG	B	912	1	14,14,15	0.80	1 (7%)	15,19,21	1.23	1 (6%)
6	NAG	B	913	1	14,14,15	0.66	0	15,19,21	1.46	3 (20%)
6	NAG	B	914	1	14,14,15	0.51	0	15,19,21	1.88	4 (26%)
6	NAG	B	915	1	14,14,15	0.91	1 (7%)	15,19,21	1.69	2 (13%)
2	URI	C	901	-	12,18,18	0.66	0	15,26,26	2.26	3 (20%)
3	UCG	C	902	-	39,52,52	1.55	9 (23%)	48,82,82	1.77	7 (14%)
6	NAG	C	910	1	14,14,15	0.48	0	15,19,21	1.62	3 (20%)
6	NAG	C	914	1	14,14,15	0.82	0	15,19,21	0.82	0
6	NAG	C	915	1	14,14,15	0.60	0	15,19,21	1.02	0
6	NAG	C	916	1	14,14,15	0.70	0	15,19,21	2.02	4 (26%)
2	URI	D	901	-	12,18,18	0.97	1 (8%)	15,26,26	2.30	3 (20%)
3	UCG	D	902	-	39,52,52	1.41	8 (20%)	48,82,82	1.97	14 (29%)
6	NAG	D	909	1	14,14,15	0.62	0	15,19,21	1.70	1 (6%)
6	NAG	D	912	1	14,14,15	0.92	1 (7%)	15,19,21	1.34	3 (20%)
6	NAG	D	913	1	14,14,15	0.57	0	15,19,21	1.81	4 (26%)
6	NAG	D	914	1	14,14,15	0.72	0	15,19,21	1.89	3 (20%)

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	URI	A	901	-	-	0/2/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UCG	A	902	-	-	0/17/67/67	0/6/6/6
6	NAG	A	910	1	-	0/6/23/26	0/1/1/1
6	NAG	A	913	1	-	0/6/23/26	0/1/1/1
6	NAG	A	914	1	-	0/6/23/26	0/1/1/1
6	NAG	A	915	1	-	0/6/23/26	0/1/1/1
6	NAG	A	916	1	-	0/6/23/26	0/1/1/1
2	URI	B	901	-	-	0/2/22/22	0/2/2/2
3	UCG	B	902	-	-	0/17/67/67	0/6/6/6
6	NAG	B	909	1	-	0/6/23/26	0/1/1/1
6	NAG	B	912	1	-	0/6/23/26	0/1/1/1
6	NAG	B	913	1	-	0/6/23/26	0/1/1/1
6	NAG	B	914	1	-	0/6/23/26	0/1/1/1
6	NAG	B	915	1	-	0/6/23/26	0/1/1/1
2	URI	C	901	-	-	0/2/22/22	0/2/2/2
3	UCG	C	902	-	-	0/17/67/67	0/6/6/6
6	NAG	C	910	1	-	0/6/23/26	0/1/1/1
6	NAG	C	914	1	-	0/6/23/26	0/1/1/1
6	NAG	C	915	1	-	0/6/23/26	0/1/1/1
6	NAG	C	916	1	-	0/6/23/26	0/1/1/1
2	URI	D	901	-	-	0/2/22/22	0/2/2/2
3	UCG	D	902	-	-	0/17/67/67	0/6/6/6
6	NAG	D	909	1	-	0/6/23/26	0/1/1/1
6	NAG	D	912	1	-	0/6/23/26	0/1/1/1
6	NAG	D	913	1	-	0/6/23/26	0/1/1/1
6	NAG	D	914	1	-	0/6/23/26	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	UCG	P1-O15	-3.14	1.41	1.54
3	C	902	UCG	O12-C15	-3.01	1.38	1.45
3	D	902	UCG	P2-O17	-2.93	1.42	1.54
3	C	902	UCG	P2-O17	-2.91	1.42	1.54
3	B	902	UCG	C6-N	-2.86	1.31	1.35
3	A	902	UCG	O12-C15	-2.86	1.38	1.45
3	A	902	UCG	P2-O17	-2.78	1.43	1.54
3	C	902	UCG	P-O6	-2.65	1.45	1.54
3	A	902	UCG	P1-O15	-2.61	1.43	1.54
2	B	901	URI	C6-N1	-2.57	1.32	1.35
3	D	902	UCG	P1-O15	-2.54	1.44	1.54
3	D	902	UCG	C6-N	-2.50	1.32	1.35
3	B	902	UCG	P2-O17	-2.49	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	UCG	O13-C16	-2.44	1.39	1.45
3	B	902	UCG	O13-C16	-2.37	1.39	1.45
3	A	902	UCG	P-O6	-2.33	1.46	1.54
3	A	902	UCG	O13-C16	-2.32	1.40	1.45
3	D	902	UCG	P-O6	-2.32	1.46	1.54
3	B	902	UCG	P-O6	-2.27	1.46	1.54
6	B	912	NAG	O5-C1	-2.22	1.40	1.43
3	C	902	UCG	C6-N	-2.21	1.32	1.35
6	D	912	NAG	O5-C1	-2.20	1.40	1.43
6	B	909	NAG	O5-C1	-2.20	1.40	1.43
3	A	902	UCG	C6-N	-2.17	1.32	1.35
3	D	902	UCG	O12-C15	-2.16	1.40	1.45
6	B	915	NAG	C2-N2	-2.13	1.42	1.46
3	C	902	UCG	C10-N2	-2.07	1.32	1.35
3	C	902	UCG	O-C3	-2.07	1.40	1.45
3	D	902	UCG	O13-C16	-2.06	1.40	1.45
3	B	902	UCG	P1-O15	-2.05	1.46	1.54
3	D	902	UCG	C11-C9	2.18	1.45	1.41
3	B	902	UCG	C11-C9	2.20	1.45	1.41
2	B	901	URI	O4'-C1'	2.31	1.44	1.41
2	A	901	URI	O4'-C1'	2.44	1.44	1.41
3	C	902	UCG	C11-C9	2.58	1.46	1.41
3	A	902	UCG	P-O8	2.67	1.59	1.51
3	B	902	UCG	P-O8	2.73	1.60	1.51
3	D	902	UCG	P-O8	2.79	1.60	1.51
2	D	901	URI	O4'-C1'	2.81	1.44	1.41

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	902	UCG	C9-C11-N3	-4.80	117.03	123.59
3	B	902	UCG	C9-C11-N3	-4.43	117.53	123.59
3	D	902	UCG	C9-C11-N3	-4.24	117.80	123.59
3	A	902	UCG	C9-C11-N3	-3.94	118.20	123.59
6	A	914	NAG	C1-O5-C5	-3.93	107.26	112.25
3	B	902	UCG	N2-C12-N3	-3.83	121.62	127.44
3	A	902	UCG	N2-C12-N3	-3.57	122.01	127.44
6	B	915	NAG	C2-N2-C7	-3.42	118.64	123.04
3	D	902	UCG	N2-C12-N3	-3.32	122.39	127.44
6	D	914	NAG	C6-C5-C4	-3.27	104.94	113.02
6	D	914	NAG	C3-C2-N2	-3.23	102.82	110.56
6	D	913	NAG	C4-C3-C2	-3.14	106.34	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	910	NAG	C6-C5-C4	-3.13	105.30	113.02
3	B	902	UCG	C11-C9-C10	-3.08	117.22	120.90
6	A	916	NAG	C4-C3-C2	-3.06	106.47	111.23
3	A	902	UCG	C11-C9-C10	-3.00	117.31	120.90
2	C	901	URI	C5'-C4'-C3'	-2.97	108.06	115.08
3	D	902	UCG	C11-C9-C10	-2.85	117.49	120.90
3	C	902	UCG	C10-C9-N5	-2.81	106.90	109.48
3	C	902	UCG	N2-C12-N3	-2.77	123.23	127.44
3	B	902	UCG	O2-C1-C2	-2.75	103.22	111.16
6	A	916	NAG	C6-C5-C4	-2.75	106.24	113.02
6	D	913	NAG	O7-C7-C8	-2.74	117.04	122.06
3	C	902	UCG	C11-C9-C10	-2.67	117.70	120.90
6	C	910	NAG	C3-C2-N2	-2.65	104.20	110.56
6	B	913	NAG	C6-C5-C4	-2.65	106.48	113.02
2	D	901	URI	C5'-C4'-C3'	-2.63	108.86	115.08
6	C	916	NAG	C6-C5-C4	-2.63	106.53	113.02
3	D	902	UCG	C10-C9-N5	-2.63	107.06	109.48
6	D	912	NAG	O4-C4-C3	-2.54	104.63	110.34
6	B	914	NAG	C6-C5-C4	-2.48	106.90	113.02
3	B	902	UCG	C6-N-C8	-2.46	117.29	121.28
2	D	901	URI	C4'-O4'-C1'	-2.44	107.04	109.72
3	D	902	UCG	C6-N-C8	-2.43	117.34	121.28
6	A	910	NAG	C2-N2-C7	-2.43	119.92	123.04
3	A	902	UCG	C6-N-C8	-2.38	117.43	121.28
2	C	901	URI	O4'-C4'-C5'	-2.37	104.03	109.17
3	A	902	UCG	C10-C9-N5	-2.33	107.33	109.48
3	A	902	UCG	O2-C1-C2	-2.29	104.53	111.16
6	A	916	NAG	O3-C3-C4	-2.26	105.25	110.34
3	B	902	UCG	C1-C2-C3	-2.23	99.11	103.29
2	A	901	URI	C6-N1-C2	-2.22	117.68	121.28
3	A	902	UCG	O10-C14-C15	-2.20	102.63	106.60
6	D	912	NAG	C3-C2-N2	-2.19	105.32	110.56
6	A	915	NAG	O4-C4-C3	-2.15	105.49	110.34
6	C	916	NAG	O4-C4-C3	-2.14	105.51	110.34
3	D	902	UCG	C17-O10-C14	-2.14	107.36	109.72
6	A	913	NAG	O4-C4-C3	-2.05	105.72	110.34
6	C	916	NAG	O3-C3-C4	-2.04	105.74	110.34
6	B	914	NAG	O3-C3-C4	-2.00	105.83	110.34
3	D	902	UCG	C6-C5-C7	2.13	121.27	117.28
6	A	915	NAG	O5-C5-C6	2.16	112.02	107.35
6	B	913	NAG	O5-C5-C6	2.18	112.07	107.35
3	B	902	UCG	O7-P-O1	2.24	113.00	106.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	912	NAG	C4-C3-C2	2.24	114.71	111.23
3	B	902	UCG	O-C-N	2.25	112.83	108.08
3	D	902	UCG	O10-C14-N4	2.34	113.01	108.10
3	D	902	UCG	C2-C1-C	2.37	105.67	99.98
6	B	912	NAG	C4-C3-C2	2.38	114.93	111.23
3	A	902	UCG	C2-C1-C	2.47	105.91	99.98
3	D	902	UCG	O-C-N	2.49	113.34	108.08
3	A	902	UCG	O-C-N	2.50	113.36	108.08
6	A	915	NAG	C2-N2-C7	2.72	126.54	123.04
6	B	914	NAG	C3-C4-C5	2.75	115.00	110.20
3	A	902	UCG	O17-P2-O12	2.95	113.74	108.46
3	C	902	UCG	O17-P2-O12	3.04	113.89	108.46
3	A	902	UCG	O17-P2-O13	3.09	113.98	108.46
6	D	913	NAG	C8-C7-N2	3.16	122.15	116.11
3	B	902	UCG	C2-C1-C	3.25	107.77	99.98
6	B	913	NAG	C1-O5-C5	3.28	116.41	112.25
6	C	910	NAG	C1-O5-C5	3.33	116.47	112.25
6	D	913	NAG	C1-O5-C5	3.41	116.57	112.25
3	D	902	UCG	O17-P2-O13	3.88	115.41	108.46
3	D	902	UCG	O17-P2-O12	4.05	115.70	108.46
3	B	902	UCG	O17-P2-O13	4.17	115.92	108.46
6	B	915	NAG	C1-O5-C5	4.32	117.73	112.25
6	A	910	NAG	C1-O5-C5	4.59	118.07	112.25
3	C	902	UCG	C11-N3-C12	4.60	122.33	115.94
6	D	914	NAG	C1-O5-C5	4.73	118.25	112.25
3	D	902	UCG	C11-N3-C12	4.85	122.67	115.94
3	A	902	UCG	C11-N3-C12	4.86	122.69	115.94
6	B	914	NAG	C1-O5-C5	5.50	119.23	112.25
3	A	902	UCG	C7-N1-C8	5.52	119.61	114.14
3	D	902	UCG	C7-N1-C8	5.56	119.65	114.14
6	D	909	NAG	C1-O5-C5	5.64	119.40	112.25
3	B	902	UCG	C11-N3-C12	5.72	123.88	115.94
3	C	902	UCG	C7-N1-C8	6.09	120.17	114.14
6	C	916	NAG	C1-O5-C5	6.10	119.99	112.25
3	B	902	UCG	C7-N1-C8	6.29	120.37	114.14
2	C	901	URI	C4-N3-C2	6.49	120.56	114.14
6	A	916	NAG	C1-O5-C5	6.72	120.78	112.25
2	D	901	URI	C4-N3-C2	7.43	121.50	114.14
2	B	901	URI	C4-N3-C2	7.92	121.99	114.14
2	A	901	URI	C4-N3-C2	8.41	122.47	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	URI	1	0
3	A	902	UCG	4	0
2	B	901	URI	1	0
3	B	902	UCG	6	0
6	B	914	NAG	1	0
2	C	901	URI	1	0
3	C	902	UCG	5	0
2	D	901	URI	1	0
3	D	902	UCG	1	0
6	D	909	NAG	1	0
6	D	913	NAG	1	0

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, 95^{th} 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	747/811 (92%)	-0.08	19 (2%)	61	61	18, 32, 62, 90	0
1	B	738/811 (90%)	0.08	25 (3%)	49	50	19, 37, 70, 94	0
1	C	738/811 (90%)	0.31	53 (7%)	18	20	19, 43, 78, 112	0
1	D	735/811 (90%)	0.24	49 (6%)	21	22	21, 41, 86, 104	0
All	All	2958/3244 (91%)	0.13	146 (4%)	33	35	18, 38, 76, 112	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	TYR	8.4
1	C	761	THR	8.2
1	B	817	LEU	7.3
1	C	733	SER	6.7
1	D	64	TYR	6.4
1	C	458	ASP	6.2
1	D	807	GLY	5.5
1	D	817	LEU	5.4
1	A	64	TYR	5.4
1	D	818	GLU	5.3
1	C	760	THR	5.0
1	D	776	CYS	5.0
1	B	64	TYR	5.0
1	D	783	PHE	4.9
1	D	786	TRP	4.9
1	C	780	ILE	4.7
1	D	789	GLU	4.6
1	D	805	SER	4.6
1	D	810	ARG	4.5
1	C	806	PRO	4.4
1	C	807	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	112	ASN	4.4
1	D	88	ASN	4.2
1	C	779	ASP	4.2
1	D	808	ASP	4.0
1	C	45	VAL	4.0
1	C	808	ASP	4.0
1	A	761	THR	4.0
1	B	46	ILE	4.0
1	C	459	PHE	3.9
1	C	814	ILE	3.8
1	C	74	PHE	3.8
1	D	751	ILE	3.8
1	A	100	VAL	3.8
1	C	125	LYS	3.7
1	B	808	ASP	3.6
1	C	84	GLN	3.6
1	B	780	ILE	3.6
1	A	778	CYS	3.5
1	D	65	VAL	3.5
1	B	778	CYS	3.5
1	D	752	ASN	3.5
1	D	84	GLN	3.5
1	D	774	PHE	3.5
1	D	809	GLN	3.5
1	C	805	SER	3.4
1	C	273	GLY	3.4
1	D	792	ASN	3.4
1	C	87	GLN	3.4
1	D	87	GLN	3.4
1	C	66	THR	3.3
1	B	38	LYS	3.2
1	D	780	ILE	3.2
1	D	804	ALA	3.2
1	D	806	PRO	3.2
1	C	76	THR	3.2
1	D	38	LYS	3.2
1	D	793	VAL	3.1
1	D	227	LEU	3.1
1	D	678	PHE	3.1
1	C	752	ASN	3.0
1	B	63	LYS	3.0
1	C	735	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	790	HIS	3.0
1	B	112	ASN	3.0
1	B	807	GLY	2.9
1	A	458	ASP	2.9
1	C	59	GLN	2.9
1	C	65	VAL	2.9
1	D	811	GLY	2.9
1	B	810	ARG	2.9
1	C	100	VAL	2.9
1	C	186	VAL	2.8
1	B	762	THR	2.8
1	D	737	SER	2.8
1	C	726	HIS	2.8
1	A	46	ILE	2.8
1	C	778	CYS	2.8
1	C	791	LEU	2.8
1	C	272	GLY	2.7
1	D	785	ARG	2.7
1	B	113	GLY	2.7
1	C	817	LEU	2.7
1	D	791	LEU	2.7
1	B	735	VAL	2.7
1	D	779	ASP	2.7
1	C	53	ARG	2.6
1	D	729	SER	2.6
1	B	753	LYS	2.6
1	B	806	PRO	2.6
1	D	243	LYS	2.6
1	D	750	THR	2.6
1	B	273	GLY	2.6
1	C	126	ASN	2.5
1	A	807	GLY	2.5
1	D	59	GLN	2.5
1	C	63	LYS	2.5
1	D	803	CYS	2.5
1	C	762	THR	2.5
1	C	777	THR	2.5
1	A	806	PRO	2.4
1	B	100	VAL	2.4
1	A	206	LEU	2.4
1	C	206	LEU	2.4
1	D	272	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	274	ALA	2.4
1	D	739	LYS	2.4
1	D	726	HIS	2.4
1	C	55	GLN	2.4
1	C	86	LEU	2.4
1	C	80	ASN	2.4
1	B	779	ASP	2.3
1	D	100	VAL	2.3
1	C	785	ARG	2.3
1	D	775	GLU	2.3
1	A	45	VAL	2.3
1	B	458	ASP	2.3
1	A	488	LEU	2.3
1	D	228	PHE	2.3
1	C	46	ILE	2.3
1	C	678	PHE	2.3
1	D	701	LEU	2.3
1	C	61	VAL	2.2
1	A	228	PHE	2.2
1	D	74	PHE	2.2
1	C	425	LEU	2.2
1	A	762	THR	2.2
1	D	794	LYS	2.2
1	A	782	ASP	2.2
1	C	70	LEU	2.2
1	C	188	GLU	2.2
1	C	401	LEU	2.1
1	A	758	THR	2.1
1	D	781	GLY	2.1
1	C	81	GLU	2.1
1	A	63	LYS	2.1
1	C	56	GLU	2.1
1	B	122	LEU	2.1
1	B	777	THR	2.1
1	A	779	ASP	2.1
1	B	65	VAL	2.1
1	C	734	GLU	2.0
1	A	208	LEU	2.0
1	B	130	LEU	2.0
1	D	778	CYS	2.0
1	B	246	ILE	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	NAG	B	903	14/15	0.97	0.15	1.12	26,30,36,52	0
4	NAG	A	903	14/15	0.97	0.17	1.02	19,21,25,29	0
4	NAG	C	903	14/15	0.97	0.14	0.37	28,31,36,46	0
8	NAG	D	903	14/15	0.97	0.15	0.09	24,26,31,35	0
7	NAG	B	910	14/15	0.96	0.13	-0.22	21,22,29,31	0
4	NAG	A	904	14/15	0.97	0.12	-0.38	24,28,34,38	0
8	NAG	D	906	14/15	0.97	0.09	-0.63	27,31,33,35	0
7	NAG	D	910	14/15	0.94	0.10	-0.69	27,30,35,49	0
7	NAG	A	911	14/15	0.96	0.09	-1.12	21,23,26,26	0
8	NAG	C	907	14/15	0.97	0.08	-1.13	22,24,26,26	0
8	NAG	D	904	14/15	0.97	0.07	-1.25	28,32,41,41	0
8	NAG	C	911	14/15	0.97	0.08	-1.34	24,26,29,32	0
4	NAG	C	904	14/15	0.94	0.09	-1.62	34,39,48,48	0
8	NAG	B	904	14/15	0.96	0.07	-1.65	31,35,41,42	0
8	NAG	B	906	14/15	0.98	0.07	-2.02	19,22,23,23	0
5	NAG	A	908	14/15	0.97	0.07	-2.23	20,23,25,26	0
7	NAG	B	911	14/15	0.96	0.09	-	32,36,40,48	0
8	BMA	D	905	11/12	0.90	0.10	-	40,48,56,56	0
8	BMA	B	908	11/12	0.93	0.17	-	39,45,54,61	0
8	NAG	B	907	14/15	0.97	0.09	-	23,26,33,42	0
4	MAN	C	906	11/12	0.89	0.22	-	60,70,80,95	0
7	NAG	A	912	14/15	0.92	0.15	-	29,36,42,52	0
5	NAG	A	909	14/15	0.94	0.12	-	26,30,34,36	0
8	BMA	C	913	11/12	0.83	0.30	-	57,64,72,75	0
8	BMA	D	908	11/12	0.88	0.32	-	47,57,62,64	0
8	NAG	D	907	14/15	0.96	0.14	-	31,36,44,52	0
8	BMA	C	909	11/12	0.93	0.30	-	41,47,51,57	0
4	MAN	A	906	11/12	0.88	0.15	-	34,44,49,53	0
4	BMA	C	905	11/12	0.89	0.15	-	44,50,64,65	0
8	NAG	C	908	14/15	0.94	0.13	-	25,30,35,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	BMA	A	907	11/12	0.91	0.28	-	40,46,54,56	0
8	BMA	B	905	11/12	0.83	0.12	-	41,50,53,59	0
7	NAG	D	911	14/15	0.93	0.11	-	33,39,45,49	0
4	BMA	A	905	11/12	0.90	0.10	-	36,42,49,51	0
8	NAG	C	912	14/15	0.93	0.17	-	34,40,46,47	0

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NAG	C	915	14/15	0.95	0.17	5.68	33,46,55,57	0
6	NAG	C	910	14/15	0.94	0.17	2.85	43,51,60,64	0
3	UCG	A	902	47/47	0.90	0.15	1.81	26,41,85,94	0
6	NAG	A	916	14/15	0.94	0.18	1.64	35,46,57,58	0
3	UCG	B	902	47/47	0.85	0.20	1.50	31,51,91,100	0
6	NAG	D	913	14/15	0.86	0.15	1.26	50,58,70,72	0
6	NAG	D	912	14/15	0.89	0.12	0.53	43,54,65,68	0
6	NAG	B	914	14/15	0.95	0.11	0.29	34,41,44,57	0
6	NAG	A	910	14/15	0.97	0.11	0.19	35,39,42,48	0
3	UCG	D	902	47/47	0.89	0.14	0.03	33,48,79,96	0
2	URI	D	901	17/17	0.98	0.10	-0.21	21,24,31,31	0
2	URI	C	901	17/17	0.97	0.10	-0.51	26,33,42,44	0
2	URI	A	901	17/17	0.98	0.10	-0.55	19,22,29,31	0
6	NAG	D	909	14/15	0.98	0.08	-0.81	31,39,51,56	0
3	UCG	C	902	47/47	0.94	0.10	-0.91	34,42,61,70	0
6	NAG	B	913	14/15	0.94	0.08	-1.11	42,49,60,62	0
2	URI	B	901	17/17	0.98	0.07	-1.24	18,22,36,37	0
6	NAG	B	912	14/15	0.91	0.21	-	43,56,64,69	0
6	NAG	C	916	14/15	0.91	0.12	-	49,55,65,65	0
6	NAG	A	915	14/15	0.90	0.11	-	45,52,61,66	0
6	NAG	B	915	14/15	0.90	0.18	-	43,49,61,64	0
6	NAG	B	909	14/15	0.84	0.26	-	51,71,83,93	0
6	NAG	A	913	14/15	0.92	0.13	-	40,49,56,61	0
6	NAG	D	914	14/15	0.94	0.15	-	48,57,62,64	0
6	NAG	C	914	14/15	0.96	0.20	-	41,50,66,73	0
6	NAG	A	914	14/15	0.92	0.18	-	48,58,67,68	0

6.5 Other polymers (i)

There are no such residues in this entry.