



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2016 – 02:16 PM EDT

PDB ID : 5GMH
Title : Crystal structure of monkey TLR7 in complex with R848
Authors : Zhang, Z.; Ohto, U.; Shimizu, T.
Deposited on : 2016-07-14
Resolution : 2.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

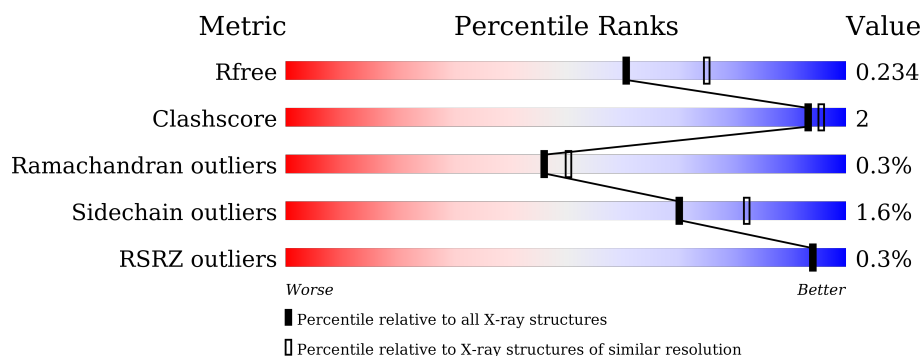
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	817	 88% 7% 6%
1	B	817	 87% 8% 6%

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
4	SO4	A	911	-	-	-	X
4	SO4	A	915	-	-	-	X
4	SO4	A	920	-	-	-	X
4	SO4	A	924	-	-	-	X
4	SO4	B	916	-	-	-	X
4	SO4	B	918	-	-	-	X
4	SO4	B	919	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13621 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.

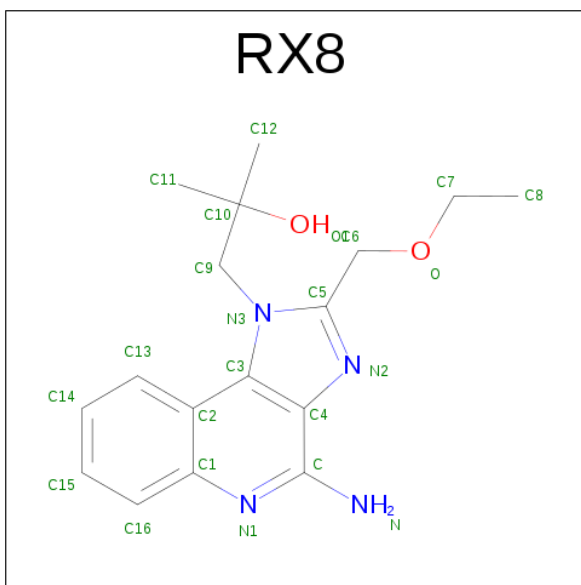
- Molecule 1 is a protein called Toll-like receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	0	1	0
			6258	4010	1066	1152	30			
1	B	772	Total	C	N	O	S	0	3	0
			6272	4017	1068	1157	30			

There are 16 discrepancies between the modelled and reference sequences:

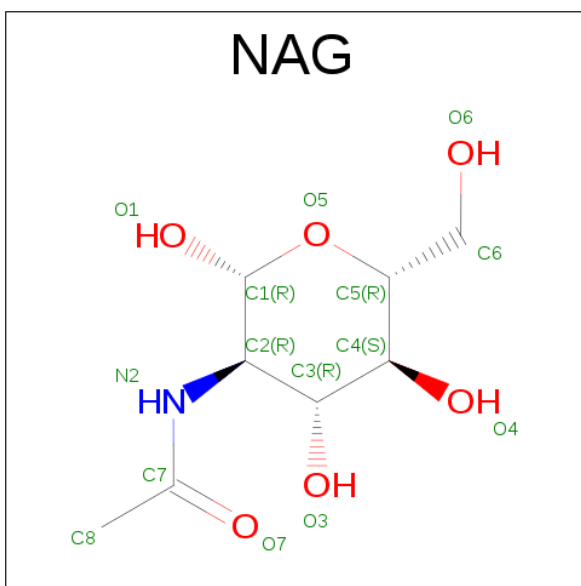
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP B3Y653
A	24	SER	-	expression tag	UNP B3Y653
A	25	PRO	-	expression tag	UNP B3Y653
A	26	TRP	-	expression tag	UNP B3Y653
A	167	GLN	ASN	engineered mutation	UNP B3Y653
A	389	GLN	ASN	engineered mutation	UNP B3Y653
A	488	GLN	ASN	engineered mutation	UNP B3Y653
A	799	GLN	ASN	engineered mutation	UNP B3Y653
B	23	ARG	-	expression tag	UNP B3Y653
B	24	SER	-	expression tag	UNP B3Y653
B	25	PRO	-	expression tag	UNP B3Y653
B	26	TRP	-	expression tag	UNP B3Y653
B	167	GLN	ASN	engineered mutation	UNP B3Y653
B	389	GLN	ASN	engineered mutation	UNP B3Y653
B	488	GLN	ASN	engineered mutation	UNP B3Y653
B	799	GLN	ASN	engineered mutation	UNP B3Y653

- Molecule 2 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
2	A	1	Total	C	N	O	0	0
			23	17	4	2		
2	B	1	Total	C	N	O	0	0
			23	17	4	2		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



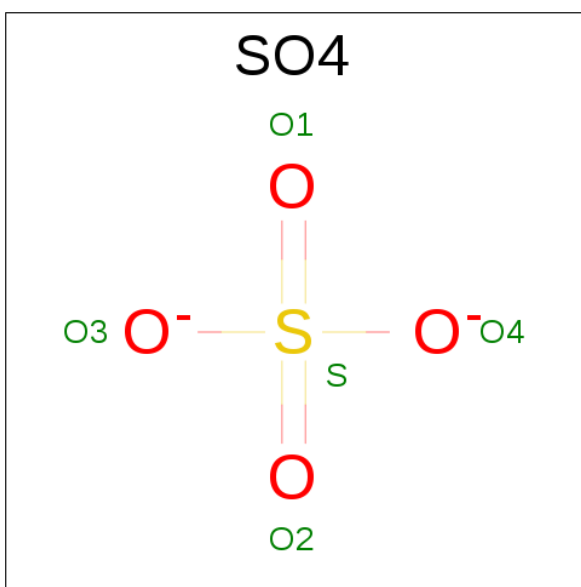
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

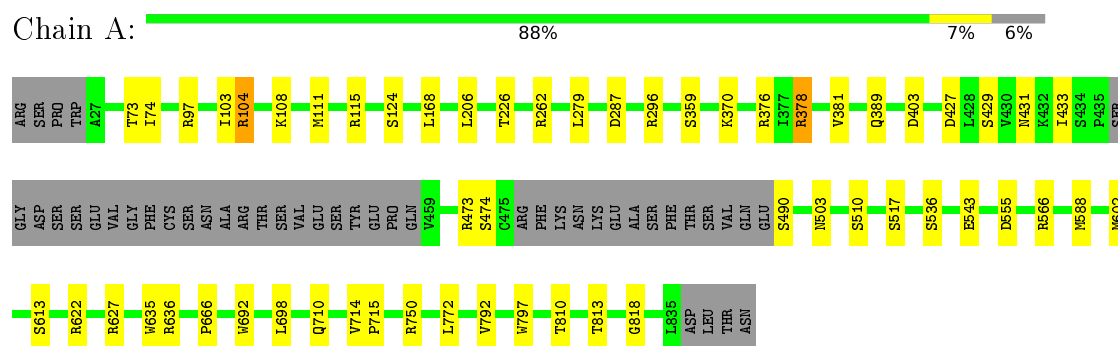
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	397	Total 397	O 397	0	0
5	B	256	Total 256	O 256	0	0

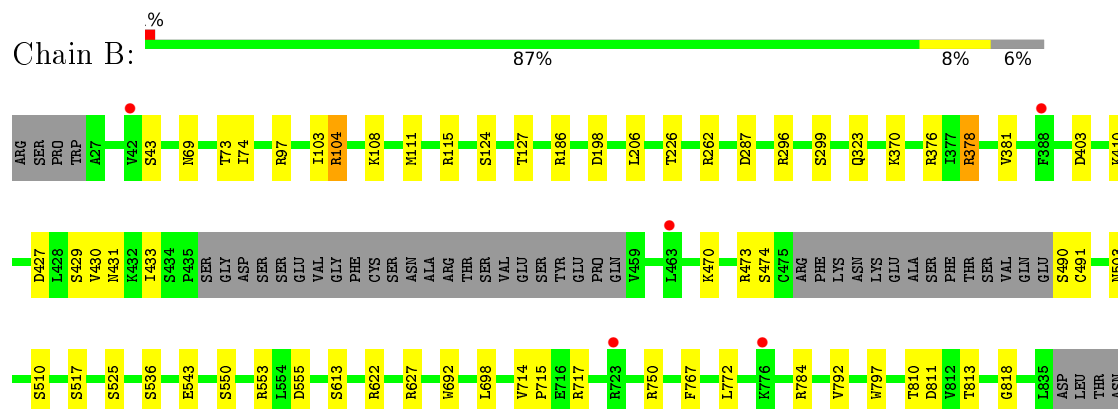
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 7



• Molecule 1: Toll-like receptor 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.10Å 140.09Å 151.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.20 47.08 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.01-2.20) 98.7 (47.08-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.185 , 0.225 0.192 , 0.234	Depositor DCC
R_{free} test set	5212 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13621	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 4.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RX8, 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	0.85	0/6389	0.94	19/8657 (0.2%)
1	B	0.81	0/6403	0.92	21/8676 (0.2%)
All	All	0.83	0/12792	0.93	40/17333 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	B	378	ARG	NE-CZ-NH1	9.97	125.28	120.30
1	A	622	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	B	115	ARG	NE-CZ-NH2	9.24	124.92	120.30
1	A	115	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	A	622	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	A	378	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	376	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	B	296	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	B	115	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	A	115	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	B	627	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	376	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	622	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	B	378	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	B	811	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	262	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	750	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	602	MET	CG-SD-CE	-6.09	90.46	100.20
1	B	296	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	627	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	473	ARG	NE-CZ-NH1	-5.78	117.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	750	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	287	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	784	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	B	473	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	B	767	PHE	CB-CG-CD1	-5.41	117.01	120.80
1	B	287	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	376	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	566	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	376	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	296	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	262	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	636	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	186	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	104	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	296	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	553	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	104	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	198	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	6258	0	6301	21	0
1	B	6272	0	6309	23	0
2	A	23	0	22	4	0
2	B	23	0	22	2	0
3	A	126	0	116	1	0
3	B	126	0	115	2	0
4	A	85	0	0	1	0
4	B	55	0	0	0	0
5	A	397	0	0	4	1
5	B	256	0	0	4	0
All	All	13621	0	12885	49	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 2.

All (49) 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:279:LEU:HA	5:A:1198:HOH:O	1.62	0.99
4:A:920:SO4:O2	5:A:1001:HOH:O	1.87	0.93
1:A:431:ASN:HB2	1:A:503:ASN:HD21	1.58	0.69
1:B:431:ASN:HB2	1:B:503:ASN:HD21	1.58	0.68
1:B:206:LEU:O	1:B:226:THR:HG23	1.97	0.65
1:B:410:LYS:NZ	5:B:1002:HOH:O	2.31	0.64
1:A:206:LEU:O	1:A:226:THR:HG23	1.98	0.62
1:B:517:SER:O	1:B:543:GLU:HG3	1.99	0.61
1:A:517:SER:O	1:A:543:GLU:HG3	2.02	0.60
1:A:433:ILE:H	1:A:503:ASN:HD22	1.50	0.59
1:A:772:LEU:HD13	1:A:797:TRP:CZ2	2.38	0.57
1:B:433:ILE:H	1:B:503:ASN:HD22	1.55	0.55
2:A:901:RX8:C11	2:A:901:RX8:H11	2.38	0.54
1:B:510:SER:OG	1:B:536:SER:O	2.26	0.53
1:A:510:SER:OG	1:A:536:SER:O	2.24	0.53
2:B:901:RX8:H19	2:B:901:RX8:H9	1.92	0.52
1:B:714:VAL:HB	1:B:715:PRO:HD2	1.90	0.52
2:A:901:RX8:H2	2:A:901:RX8:H11	1.94	0.49
1:A:714:VAL:HB	1:A:715:PRO:HD2	1.95	0.49
1:A:431:ASN:CB	1:A:503:ASN:HD21	2.26	0.47
1:B:127:THR:HB	5:B:1134:HOH:O	2.14	0.47
1:B:470:LYS:NZ	5:B:1011:HOH:O	2.47	0.47
1:A:97:ARG:NH2	1:A:474:SER:O	2.49	0.45
1:B:555:ASP:OD2	2:B:901:RX8:N1	2.49	0.45
1:B:431:ASN:CB	1:B:503:ASN:HD21	2.26	0.45
1:A:103:ILE:HD12	5:A:1217:HOH:O	2.15	0.45
1:A:279:LEU:CA	5:A:1198:HOH:O	2.38	0.45
1:A:73:THR:HG22	1:A:74:ILE:HG13	1.99	0.44
1:B:717:ARG:NE	5:B:1003:HOH:O	2.40	0.44
1:B:103:ILE:HD11	1:B:111:MET:SD	2.58	0.43
1:B:73:THR:HG22	1:B:74:ILE:HG13	2.01	0.43
1:B:97:ARG:NH2	1:B:474:SER:O	2.52	0.43
1:B:525:SER:HA	1:B:550:SER:O	2.20	0.42
2:A:901:RX8:H9	2:A:901:RX8:H19	2.01	0.42
1:A:555:ASP:OD2	2:A:901:RX8:N1	2.53	0.42
1:A:378:ARG:HD2	1:A:403:ASP:OD2	2.20	0.42
1:B:69:ASN:HD22	3:B:905:NAG:H83	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:SER:HB2	1:A:389:GLN:NE2	2.35	0.41
1:A:427:ASP:OD2	1:A:429:SER:HB2	2.20	0.41
1:A:588:MET:HE3	3:A:906:NAG:O5	2.19	0.41
1:B:299:SER:HA	1:B:323:GLN:O	2.20	0.41
1:A:103:ILE:HD11	1:A:111:MET:SD	2.61	0.41
1:A:692:TRP:CE2	1:A:715:PRO:HD3	2.55	0.41
1:B:378:ARG:HD2	1:B:403:ASP:OD2	2.21	0.41
1:B:692:TRP:CE2	1:B:715:PRO:HD3	2.56	0.41
1:B:491:CYS:HB3	3:B:902:NAG:H81	2.03	0.40
1:B:772:LEU:HD13	1:B:797:TRP:CZ2	2.57	0.40
1:A:635:TRP:HB3	1:A:666:PRO:HG2	2.04	0.40
1:B:427:ASP:OD2	1:B:429:SER:HB2	2.22	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)
5:A:1362:HOH:O	5:A:1380:HOH:O[2_555]	2.15	0.05

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	767/817 (94%)	721 (94%)	44 (6%)	2 (0%)	46	50
1	B	769/817 (94%)	724 (94%)	42 (6%)	3 (0%)	39	42
All	All	1536/1634 (94%)	1445 (94%)	86 (6%)	5 (0%)	46	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	GLY

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Mol	Chain	Res	Type
1	B	818	GLY
1	A	381	VAL
1	B	381	VAL
1	B	430	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	726/768 (94%)	714 (98%)	12 (2%)	68	81
1	B	728/768 (95%)	717 (98%)	11 (2%)	72	84
All	All	1454/1536 (95%)	1431 (98%)	23 (2%)	70	82

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	108	LYS
1	A	124	SER
1	A	168	LEU
1	A	370	LYS
1	A	490	SER
1	A	613	SER
1	A	698	LEU
1	A	710	GLN
1	A	792	VAL
1	A	810	THR
1	A	813	THR
1	B	43	SER
1	B	104	ARG
1	B	108	LYS
1	B	124	SER
1	B	370	LYS
1	B	490	SER
1	B	613	SER

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Mol	Chain	Res	Type
1	B	698	LEU
1	B	792	VAL
1	B	810	THR
1	B	813	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	181	GLN
1	A	241	GLN
1	A	503	ASN
1	A	587	HIS
1	A	708	HIS
1	A	734	GLN
1	A	748	GLN
1	A	800	HIS
1	B	66	ASN
1	B	173	ASN
1	B	503	ASN
1	B	587	HIS
1	B	820	HIS

5.3.3 RNA [i](#)

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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

48 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	RX8	A	901	-	22,25,25	1.45	4 (18%)	23,37,37	2.36	4 (17%)
3	NAG	A	902	1	14,14,15	1.34	2 (14%)	15,19,21	1.96	6 (40%)
3	NAG	A	903	1,3	14,14,15	0.66	0	15,19,21	0.96	1 (6%)
3	NAG	A	904	3	14,14,15	0.61	0	15,19,21	1.44	1 (6%)
3	NAG	A	905	1	14,14,15	0.98	0	15,19,21	1.36	1 (6%)
3	NAG	A	906	1	14,14,15	0.73	0	15,19,21	2.24	4 (26%)
3	NAG	A	907	1	14,14,15	0.95	1 (7%)	15,19,21	1.48	3 (20%)
3	NAG	A	908	1	14,14,15	0.54	0	15,19,21	1.34	1 (6%)
3	NAG	A	909	1	14,14,15	0.48	0	15,19,21	1.39	2 (13%)
3	NAG	A	910	1	14,14,15	0.56	0	15,19,21	3.24	2 (13%)
4	SO4	A	911	-	4,4,4	0.79	0	6,6,6	0.37	0
4	SO4	A	912	-	4,4,4	0.80	0	6,6,6	0.78	0
4	SO4	A	913	-	4,4,4	0.56	0	6,6,6	0.43	0
4	SO4	A	914	-	4,4,4	0.92	0	6,6,6	1.26	1 (16%)
4	SO4	A	915	-	4,4,4	0.86	0	6,6,6	0.23	0
4	SO4	A	916	-	4,4,4	0.69	0	6,6,6	0.74	0
4	SO4	A	917	-	4,4,4	1.02	0	6,6,6	0.66	0
4	SO4	A	918	-	4,4,4	0.59	0	6,6,6	0.36	0
4	SO4	A	919	-	4,4,4	1.18	0	6,6,6	1.21	1 (16%)
4	SO4	A	920	-	4,4,4	0.88	0	6,6,6	0.42	0
4	SO4	A	921	-	4,4,4	0.66	0	6,6,6	0.94	1 (16%)
4	SO4	A	922	-	4,4,4	0.94	0	6,6,6	0.77	0
4	SO4	A	923	-	4,4,4	0.66	0	6,6,6	0.46	0
4	SO4	A	924	-	4,4,4	0.46	0	6,6,6	0.31	0
4	SO4	A	925	-	4,4,4	0.75	0	6,6,6	0.62	0
4	SO4	A	926	-	4,4,4	0.72	0	6,6,6	0.75	0
4	SO4	A	927	-	4,4,4	0.48	0	6,6,6	0.13	0
2	RX8	B	901	-	22,25,25	1.57	3 (13%)	23,37,37	2.34	5 (21%)
3	NAG	B	902	1	14,14,15	1.21	1 (7%)	15,19,21	1.75	4 (26%)
3	NAG	B	903	1,3	14,14,15	0.69	0	15,19,21	1.08	1 (6%)
3	NAG	B	904	3	14,14,15	0.92	1 (7%)	15,19,21	1.84	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	905	1,3	14,14,15	0.70	0	15,19,21	2.08	5 (33%)
3	NAG	B	906	3	14,14,15	1.06	1 (7%)	15,19,21	2.50	6 (40%)
3	NAG	B	907	1	14,14,15	0.51	0	15,19,21	2.26	3 (20%)
3	NAG	B	908	1	14,14,15	0.53	0	15,19,21	1.69	5 (33%)
3	NAG	B	909	1	14,14,15	0.38	0	15,19,21	1.48	3 (20%)
3	NAG	B	910	1	14,14,15	0.49	0	15,19,21	1.63	1 (6%)
4	SO4	B	911	-	4,4,4	0.66	0	6,6,6	0.73	0
4	SO4	B	912	-	4,4,4	1.01	0	6,6,6	0.29	0
4	SO4	B	913	-	4,4,4	0.65	0	6,6,6	0.48	0
4	SO4	B	914	-	4,4,4	0.58	0	6,6,6	1.10	1 (16%)
4	SO4	B	915	-	4,4,4	1.04	0	6,6,6	0.42	0
4	SO4	B	916	-	4,4,4	0.62	0	6,6,6	0.37	0
4	SO4	B	917	-	4,4,4	0.69	0	6,6,6	0.29	0
4	SO4	B	918	-	4,4,4	0.70	0	6,6,6	0.28	0
4	SO4	B	919	-	4,4,4	0.52	0	6,6,6	0.33	0
4	SO4	B	920	-	4,4,4	0.73	0	6,6,6	0.44	0
4	SO4	B	921	-	4,4,4	0.57	0	6,6,6	0.64	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	RX8	A	901	-	-	0/5/9/9	0/3/3/3
3	NAG	A	902	1	-	0/6/23/26	0/1/1/1
3	NAG	A	903	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	904	3	-	0/6/23/26	0/1/1/1
3	NAG	A	905	1	-	0/6/23/26	0/1/1/1
3	NAG	A	906	1	-	0/6/23/26	0/1/1/1
3	NAG	A	907	1	-	0/6/23/26	0/1/1/1
3	NAG	A	908	1	-	0/6/23/26	0/1/1/1
3	NAG	A	909	1	-	0/6/23/26	0/1/1/1
3	NAG	A	910	1	-	0/6/23/26	0/1/1/1
4	SO4	A	911	-	-	0/0/0/0	0/0/0/0
4	SO4	A	912	-	-	0/0/0/0	0/0/0/0
4	SO4	A	913	-	-	0/0/0/0	0/0/0/0
4	SO4	A	914	-	-	0/0/0/0	0/0/0/0
4	SO4	A	915	-	-	0/0/0/0	0/0/0/0
4	SO4	A	916	-	-	0/0/0/0	0/0/0/0
4	SO4	A	917	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	918	-	-	0/0/0/0	0/0/0/0
4	SO4	A	919	-	-	0/0/0/0	0/0/0/0
4	SO4	A	920	-	-	0/0/0/0	0/0/0/0
4	SO4	A	921	-	-	0/0/0/0	0/0/0/0
4	SO4	A	922	-	-	0/0/0/0	0/0/0/0
4	SO4	A	923	-	-	0/0/0/0	0/0/0/0
4	SO4	A	924	-	-	0/0/0/0	0/0/0/0
4	SO4	A	925	-	-	0/0/0/0	0/0/0/0
4	SO4	A	926	-	-	0/0/0/0	0/0/0/0
4	SO4	A	927	-	-	0/0/0/0	0/0/0/0
2	RX8	B	901	-	-	0/5/9/9	0/3/3/3
3	NAG	B	902	1	-	0/6/23/26	0/1/1/1
3	NAG	B	903	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	904	3	-	0/6/23/26	0/1/1/1
3	NAG	B	905	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	906	3	-	0/6/23/26	0/1/1/1
3	NAG	B	907	1	-	0/6/23/26	0/1/1/1
3	NAG	B	908	1	-	0/6/23/26	0/1/1/1
3	NAG	B	909	1	-	0/6/23/26	0/1/1/1
3	NAG	B	910	1	-	0/6/23/26	0/1/1/1
4	SO4	B	911	-	-	0/0/0/0	0/0/0/0
4	SO4	B	912	-	-	0/0/0/0	0/0/0/0
4	SO4	B	913	-	-	0/0/0/0	0/0/0/0
4	SO4	B	914	-	-	0/0/0/0	0/0/0/0
4	SO4	B	915	-	-	0/0/0/0	0/0/0/0
4	SO4	B	916	-	-	0/0/0/0	0/0/0/0
4	SO4	B	917	-	-	0/0/0/0	0/0/0/0
4	SO4	B	918	-	-	0/0/0/0	0/0/0/0
4	SO4	B	919	-	-	0/0/0/0	0/0/0/0
4	SO4	B	920	-	-	0/0/0/0	0/0/0/0
4	SO4	B	921	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	NAG	O7-C7	-2.60	1.17	1.23
2	B	901	RX8	O1-C10	-2.54	1.37	1.44
3	B	902	NAG	C1-C2	-2.48	1.48	1.52
3	A	902	NAG	O5-C1	-2.42	1.39	1.43
3	A	907	NAG	O5-C1	2.03	1.47	1.43
3	B	906	NAG	C1-C2	2.06	1.55	1.52
3	B	904	NAG	O5-C5	2.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	RX8	C15-C16	2.13	1.41	1.36
2	B	901	RX8	C2-C3	2.27	1.44	1.40
2	A	901	RX8	C1-N1	2.38	1.41	1.37
2	A	901	RX8	C2-C3	3.24	1.46	1.40
2	A	901	RX8	C9-C10	3.40	1.58	1.54
2	B	901	RX8	C9-C10	5.05	1.60	1.54

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	NAG	C6-C5-C4	-4.57	101.54	112.99
3	B	902	NAG	C3-C4-C5	-4.27	102.61	110.23
3	B	904	NAG	C3-C4-C5	-3.65	103.71	110.23
3	A	906	NAG	O4-C4-C3	-3.60	102.24	110.36
3	A	907	NAG	C4-C3-C2	-3.39	106.08	111.34
3	B	905	NAG	O7-C7-C8	-3.13	116.30	122.07
2	A	901	RX8	O1-C10-C11	-2.69	98.13	108.01
3	B	904	NAG	O3-C3-C4	-2.46	104.82	110.36
4	B	914	SO4	O2-S-O1	-2.45	101.41	109.59
3	A	910	NAG	O4-C4-C5	-2.39	102.93	109.23
4	A	914	SO4	O2-S-O1	-2.35	101.72	109.59
3	B	905	NAG	O7-C7-N2	-2.32	117.12	121.84
3	B	907	NAG	O7-C7-C8	-2.32	117.81	122.07
3	B	906	NAG	C3-C4-C5	-2.21	106.29	110.23
3	B	909	NAG	O3-C3-C4	-2.16	105.49	110.36
4	A	921	SO4	O4-S-O3	-2.15	100.41	109.09
2	B	901	RX8	O1-C10-C11	-2.15	100.09	108.01
3	B	902	NAG	O7-C7-C8	-2.15	118.12	122.07
3	A	902	NAG	O6-C6-C5	-2.09	104.33	111.30
3	B	903	NAG	O5-C5-C4	2.03	113.50	110.13
3	B	908	NAG	C1-O5-C5	2.04	115.13	112.14
3	A	907	NAG	O5-C5-C6	2.04	111.71	107.34
2	B	901	RX8	C12-C10-C9	2.04	114.84	109.89
3	B	908	NAG	O5-C5-C6	2.07	111.77	107.34
3	A	902	NAG	O3-C3-C2	2.09	113.84	109.37
3	B	909	NAG	C1-O5-C5	2.09	115.22	112.14
3	B	909	NAG	C2-N2-C7	2.09	125.83	123.11
3	A	903	NAG	O7-C7-N2	2.15	126.22	121.84
3	B	902	NAG	C2-N2-C7	2.17	125.93	123.11
3	A	902	NAG	C1-O5-C5	2.19	115.37	112.14
3	B	905	NAG	C2-N2-C7	2.20	125.97	123.11
2	B	901	RX8	O1-C10-C9	2.24	114.57	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	RX8	C2-C3-N3	2.26	136.58	131.98
3	B	906	NAG	O3-C3-C2	2.28	114.25	109.37
3	B	906	NAG	O4-C4-C5	2.29	115.26	109.23
4	A	919	SO4	O4-S-O3	2.35	118.56	109.09
3	B	906	NAG	O5-C5-C4	2.43	114.15	110.13
3	B	905	NAG	C1-O5-C5	2.51	115.83	112.14
3	A	906	NAG	O5-C5-C4	2.51	114.30	110.13
3	A	906	NAG	C3-C4-C5	2.54	114.75	110.23
3	A	902	NAG	C2-N2-C7	2.54	126.41	123.11
3	A	909	NAG	C3-C4-C5	2.55	114.77	110.23
3	A	909	NAG	C4-C3-C2	2.60	115.37	111.34
3	B	908	NAG	C3-C4-C5	2.62	114.89	110.23
3	A	902	NAG	O5-C5-C4	2.67	114.55	110.13
3	B	902	NAG	O4-C4-C5	2.69	116.30	109.23
3	B	908	NAG	C2-N2-C7	2.69	126.61	123.11
3	B	908	NAG	C4-C3-C2	2.77	115.64	111.34
2	A	901	RX8	C2-C3-N3	2.87	137.82	131.98
3	B	907	NAG	C3-C4-C5	3.00	115.58	110.23
3	A	904	NAG	C1-O5-C5	3.01	116.57	112.14
3	A	907	NAG	C1-O5-C5	3.02	116.58	112.14
3	A	908	NAG	C4-C3-C2	3.07	116.10	111.34
3	B	906	NAG	C2-N2-C7	3.14	127.19	123.11
3	A	905	NAG	O4-C4-C5	3.23	117.74	109.23
3	B	904	NAG	O4-C4-C5	3.36	118.07	109.23
3	B	904	NAG	C1-O5-C5	3.56	117.38	112.14
2	A	901	RX8	C11-C10-C9	4.54	120.91	109.89
3	B	910	NAG	C1-O5-C5	5.09	119.63	112.14
3	B	905	NAG	C8-C7-N2	5.45	126.55	116.10
3	A	906	NAG	C1-O5-C5	6.31	121.42	112.14
3	B	907	NAG	C1-O5-C5	6.78	122.11	112.14
3	B	906	NAG	C1-O5-C5	6.96	122.38	112.14
2	A	901	RX8	C6-O-C7	8.55	126.87	112.63
2	B	901	RX8	C6-O-C7	9.15	127.87	112.63
3	A	910	NAG	C1-O5-C5	11.80	129.50	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	RX8	4	0
3	A	906	NAG	1	0
4	A	920	SO4	1	0
2	B	901	RX8	2	0
3	B	902	NAG	1	0
3	B	905	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	772/817 (94%)	-0.42	0	100 100	20, 35, 58, 98	0
1	B	772/817 (94%)	-0.28	5 (0%)	90 90	26, 44, 69, 99	0
All	All	1544/1634 (94%)	-0.35	5 (0%)	94 94	20, 40, 66, 99	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	PHE	3.5
1	B	723	ARG	2.9
1	B	463	LEU	2.9
1	B	42	VAL	2.7
1	B	776	LYS	2.2

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	911	5/5	0.81	0.28	8.86	74,83,108,126	0
4	SO4	B	918	5/5	0.82	0.37	5.26	91,98,113,117	0
4	SO4	B	919	5/5	0.87	0.31	5.01	102,104,115,117	0
4	SO4	A	920	5/5	0.89	0.24	3.39	58,62,89,95	0
4	SO4	A	924	5/5	0.95	0.23	2.88	88,93,105,120	0
4	SO4	B	916	5/5	0.84	0.28	2.82	99,102,109,111	0
4	SO4	A	915	5/5	0.92	0.15	2.75	68,83,88,96	0
4	SO4	B	914	5/5	0.96	0.15	1.45	54,56,77,78	0
4	SO4	A	917	5/5	0.93	0.14	1.21	49,68,84,92	0
4	SO4	A	913	5/5	0.87	0.17	1.10	77,85,97,108	0
2	RX8	B	901	23/23	0.97	0.16	0.76	29,33,48,52	0
4	SO4	A	919	5/5	0.91	0.12	0.62	47,54,78,95	0
3	NAG	A	902	14/15	0.97	0.12	0.28	27,31,37,44	0
3	NAG	B	909	14/15	0.92	0.16	-0.02	55,66,71,72	0
3	NAG	A	908	14/15	0.93	0.14	-0.03	48,57,59,67	0
3	NAG	A	910	14/15	0.89	0.12	-0.06	54,68,79,81	0
3	NAG	B	902	14/15	0.94	0.11	-0.16	34,41,45,46	0
2	RX8	A	901	23/23	0.97	0.14	-0.22	31,36,45,51	0
3	NAG	A	907	14/15	0.95	0.10	-0.35	39,41,45,49	0
3	NAG	B	903	14/15	0.97	0.09	-0.42	41,44,49,52	0
3	NAG	B	907	14/15	0.90	0.12	-0.47	58,68,80,83	0
3	NAG	A	906	14/15	0.94	0.11	-0.97	45,54,71,71	0
3	NAG	B	905	14/15	0.96	0.08	-1.05	45,51,60,64	0
3	NAG	A	905	14/15	0.96	0.10	-1.24	35,43,46,52	0
3	NAG	A	903	14/15	0.97	0.07	-1.84	36,42,45,51	0
3	NAG	B	904	14/15	0.91	0.10	-	57,66,72,75	0
3	NAG	A	909	14/15	0.92	0.10	-	60,67,72,80	0
3	NAG	B	910	14/15	0.91	0.24	-	68,83,93,108	0
4	SO4	A	916	5/5	0.89	0.28	-	77,101,114,134	0
4	SO4	A	927	5/5	0.81	0.48	-	117,121,136,153	0
4	SO4	A	914	5/5	0.92	0.14	-	47,69,80,80	0
4	SO4	A	925	5/5	0.71	0.36	-	83,106,114,121	0
4	SO4	B	921	5/5	0.86	0.16	-	79,86,103,114	0
4	SO4	B	920	5/5	0.84	0.23	-	81,86,100,102	0
3	NAG	B	908	14/15	0.89	0.13	-	71,81,91,98	0
3	NAG	B	906	14/15	0.83	0.21	-	69,87,102,104	0
4	SO4	A	922	5/5	0.75	0.40	-	68,75,112,112	0
4	SO4	B	911	5/5	0.81	0.24	-	92,96,101,110	0
3	NAG	A	904	14/15	0.92	0.13	-	58,63,68,71	0
4	SO4	A	923	5/5	0.89	0.12	-	86,87,93,107	0
4	SO4	B	912	5/5	0.77	0.24	-	65,83,97,98	0
4	SO4	A	912	5/5	0.86	0.14	-	67,82,98,103	0
4	SO4	B	915	5/5	0.57	0.29	-	69,92,102,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	926	5/5	0.76	0.27	-	88,91,96,104	0
4	SO4	A	921	5/5	0.87	0.22	-	79,84,98,109	0
4	SO4	B	913	5/5	0.92	0.10	-	64,83,93,97	0
4	SO4	B	917	5/5	0.89	0.28	-	81,93,101,109	0
4	SO4	A	918	5/5	0.89	0.19	-	94,95,107,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.