Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 11:53 AM BST

PDB ID	:	3WPF
Title	:	Crystal structure of mouse TLR9 (unliganded form)
Authors	:	Ohto, U.; Shimizu, T.
Deposited on	:	2014-01-11
Resolution	:	1.96 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
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:

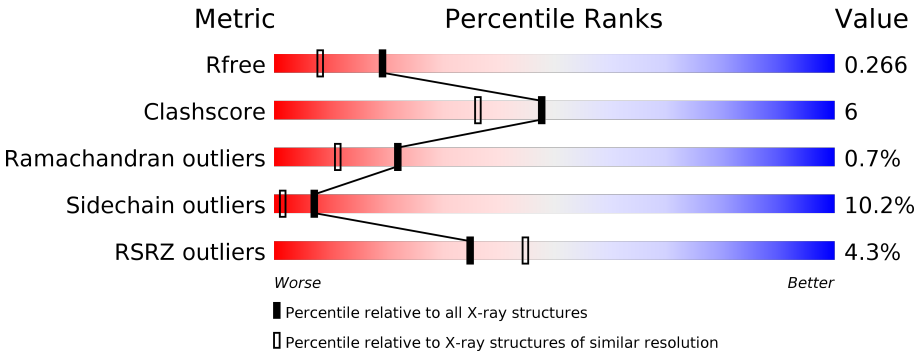
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.96 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 respectively. 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	803	4% 73% 17% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6196 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.

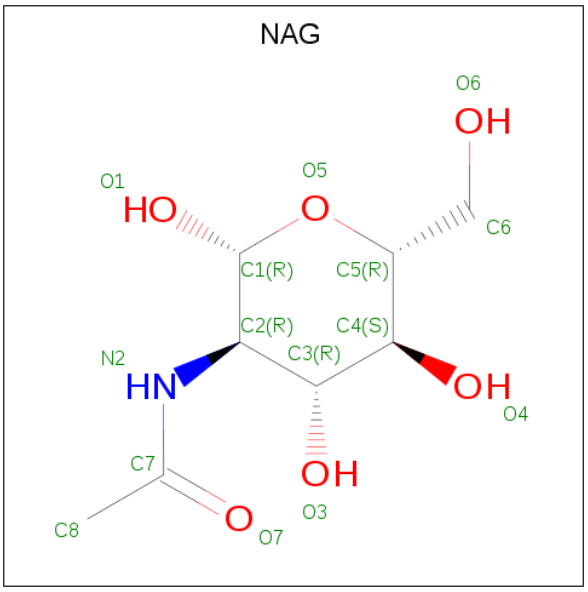
- Molecule 1 is a protein called Toll-like receptor 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5858	3746	1031	1052	29			

There are 17 discrepancies between the modelled and reference sequences:

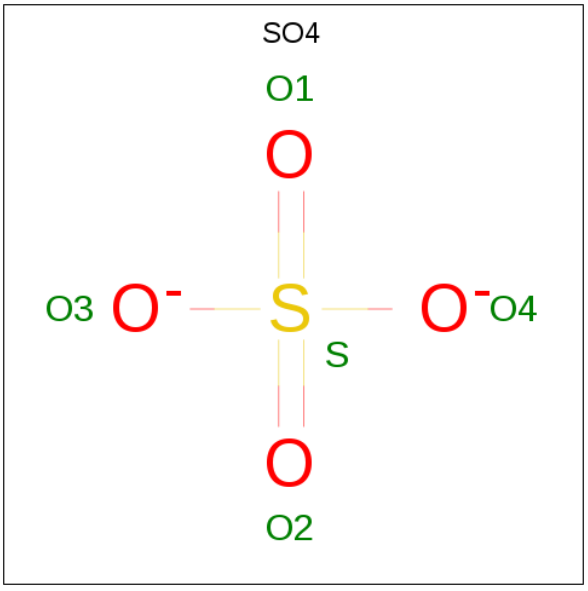
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	-	expression tag	UNP Q9EQU3
A	23	SER	-	expression tag	UNP Q9EQU3
A	24	PRO	-	expression tag	UNP Q9EQU3
A	25	TRP	-	expression tag	UNP Q9EQU3
A	200	GLN	ASN	engineered mutation	UNP Q9EQU3
A	242	GLN	ASN	engineered mutation	UNP Q9EQU3
A	309	GLN	ASN	engineered mutation	UNP Q9EQU3
A	495	GLN	ASN	engineered mutation	UNP Q9EQU3
A	568	GLN	ASN	engineered mutation	UNP Q9EQU3
A	695	GLN	ASN	engineered mutation	UNP Q9EQU3
A	752	GLN	ASN	engineered mutation	UNP Q9EQU3
A	819	GLU	-	expression tag	UNP Q9EQU3
A	820	PHE	-	expression tag	UNP Q9EQU3
A	821	LEU	-	expression tag	UNP Q9EQU3
A	822	VAL	-	expression tag	UNP Q9EQU3
A	823	PRO	-	expression tag	UNP Q9EQU3
A	824	ARG	-	expression tag	UNP Q9EQU3

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (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		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 4 is water.

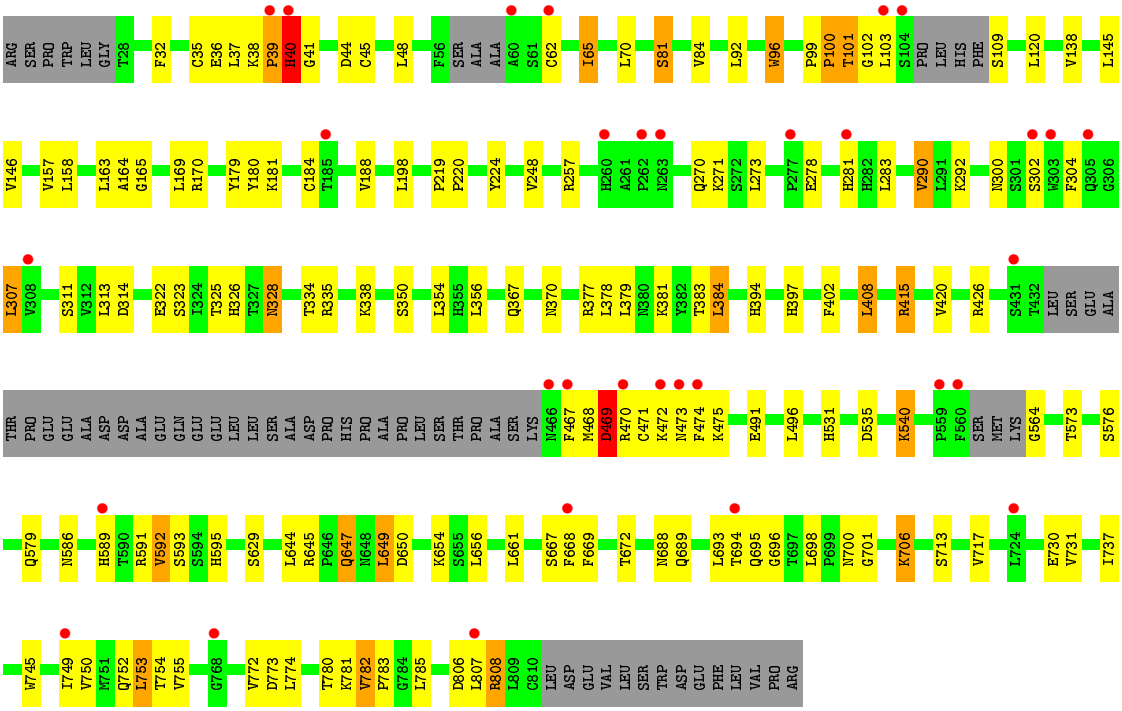
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	236	Total O 236 236	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 9

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.26Å 119.28Å 130.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.61 – 1.96 44.61 – 1.96	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.61-1.96) 97.8 (44.61-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.226 , 0.265 0.227 , 0.266	Depositor DCC
R_{free} test set	3971 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6196	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, 0.333 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: 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	0.33	0/5987	0.57	1/8124 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	165	GLY	N-CA-C	-6.08	97.90	113.10

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	5858	0	5908	72	0
2	A	42	0	39	0	0
3	A	60	0	0	2	0
4	A	236	0	0	5	1
All	All	6196	0	5947	72	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 (72) 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:426:ARG:NH1	3:A:911:SO4:O3	2.21	0.73
1:A:36:GLU:HG2	1:A:44:ASP:HB3	1.71	0.72
1:A:782:VAL:HG22	1:A:785:LEU:HB2	1.74	0.68
1:A:164:ALA:O	4:A:1185:HOH:O	2.11	0.67
1:A:328:ASN:OD1	1:A:328:ASN:N	2.27	0.66
1:A:472:LYS:O	1:A:474:PHE:N	2.23	0.66
1:A:470:ARG:NE	1:A:472:LYS:HB3	2.15	0.61
1:A:706:LYS:HB2	1:A:730:GLU:HB2	1.82	0.60
1:A:304:PHE:HA	1:A:307:LEU:HD22	1.83	0.59
1:A:379:LEU:HD11	1:A:384:LEU:HD22	1.86	0.57
1:A:808:ARG:NH2	3:A:913:SO4:O2	2.38	0.57
1:A:224:TYR:CD2	1:A:248:VAL:HB	2.40	0.57
1:A:300:ASN:OD1	1:A:302:SER:OG	2.20	0.57
1:A:146:VAL:HG13	1:A:170:ARG:HD2	1.88	0.56
1:A:323:SER:HA	1:A:326:HIS:CE1	2.42	0.55
1:A:322:GLU:O	1:A:325:THR:OG1	2.19	0.55
1:A:589:HIS:O	1:A:592:VAL:HG22	2.09	0.52
1:A:593:SER:OG	1:A:595:HIS:O	2.28	0.52
1:A:772:VAL:HG21	1:A:807:LEU:HB2	1.92	0.51
1:A:470:ARG:HD3	1:A:472:LYS:H	1.78	0.49
1:A:754:THR:O	1:A:781:LYS:HG3	2.12	0.49
1:A:96:TRP:HD1	1:A:99:PRO:HG3	1.78	0.49
1:A:564:GLY:O	1:A:591:ARG:NH1	2.47	0.48
1:A:470:ARG:HD2	1:A:472:LYS:HE2	1.94	0.48
1:A:408:LEU:HB3	1:A:496:LEU:HD11	1.95	0.48
1:A:180:TYR:CE2	1:A:181:LYS:HG3	2.49	0.48
1:A:367:GLN:HB3	1:A:394:HIS:NE2	2.29	0.48
1:A:470:ARG:CZ	1:A:472:LYS:HB3	2.45	0.47
1:A:749:ILE:O	1:A:752:GLN:HG2	2.15	0.47
1:A:278:GLU:HG2	1:A:281:HIS:CE1	2.50	0.47
1:A:650:ASP:O	1:A:654:LYS:NZ	2.47	0.47
1:A:695:GLN:N	1:A:696:GLY:HA3	2.30	0.47
1:A:644:LEU:HA	1:A:644:LEU:HD12	1.79	0.46
1:A:45:CYS:HB2	1:A:70:LEU:HD23	1.97	0.46
1:A:32:PHE:O	1:A:35:CYS:N	2.48	0.46
1:A:383:THR:HG22	1:A:384:LEU:HD13	1.98	0.46
1:A:468:MET:O	1:A:470:ARG:N	2.45	0.46
1:A:469:ASP:C	1:A:471:CYS:HB2	2.37	0.46
1:A:377:ARG:NH1	1:A:402:PHE:O	2.47	0.45
1:A:700:ASN:HA	1:A:701:GLY:HA2	1.71	0.45
1:A:713:SER:O	1:A:737:ILE:HD11	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ARG:HB3	1:A:415:ARG:HE	1.49	0.45
1:A:717:VAL:HB	1:A:745:TRP:CE2	2.52	0.45
1:A:645:ARG:HB3	1:A:647:GLN:OE1	2.17	0.44
1:A:38:LYS:O	1:A:40:HIS:N	2.51	0.44
1:A:782:VAL:HA	1:A:783:PRO:HD3	1.73	0.44
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.89	0.44
1:A:644:LEU:HG	1:A:649:LEU:HD13	2.00	0.44
1:A:806:ASP:OD1	1:A:808:ARG:HD3	2.18	0.44
1:A:290:VAL:HB	1:A:314:ASP:HB3	1.99	0.44
1:A:370:ASN:HA	1:A:397:HIS:HB2	1.98	0.44
1:A:669:PHE:O	1:A:695:GLN:HG3	2.18	0.44
1:A:158:LEU:HD22	1:A:163:LEU:HD11	1.99	0.43
1:A:101:THR:HA	1:A:102:GLY:HA3	1.38	0.43
1:A:749:ILE:HD12	1:A:752:GLN:NE2	2.33	0.43
1:A:367:GLN:HB3	1:A:394:HIS:CD2	2.54	0.43
1:A:470:ARG:N	1:A:471:CYS:HB2	2.34	0.42
1:A:219:PRO:HA	1:A:220:PRO:HD3	1.91	0.42
1:A:753:LEU:O	1:A:781:LYS:HG2	2.20	0.41
1:A:338:LYS:HB3	1:A:338:LYS:HE2	1.74	0.41
1:A:531:HIS:HD2	4:A:1096:HOH:O	2.02	0.41
1:A:39:PRO:C	1:A:41:GLY:H	2.23	0.41
1:A:100:PRO:O	1:A:102:GLY:HA3	2.20	0.41
1:A:157:VAL:HG23	4:A:1176:HOH:O	2.20	0.41
1:A:688:ASN:HB3	1:A:689:GLN:H	1.75	0.41
1:A:531:HIS:HE1	4:A:1063:HOH:O	2.04	0.41
1:A:62:CYS:O	1:A:65:ILE:HG23	2.21	0.41
1:A:472:LYS:O	1:A:474:PHE:HD1	2.04	0.40
1:A:38:LYS:HB3	1:A:40:HIS:NE2	2.37	0.40
1:A:540:LYS:HE2	4:A:1223:HOH:O	2.20	0.40
1:A:667:SER:HG	1:A:668:PHE:HD1	1.63	0.40
1:A:81:SER:HA	1:A:84:VAL:HG23	2.03	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)
4:A:1191:HOH:O	4:A:1214:HOH:O[2_455]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	730/803 (91%)	675 (92%)	50 (7%)	5 (1%)	22 11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	469	ASP
1	A	473	ASN
1	A	100	PRO
1	A	39	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	674/728 (93%)	605 (90%)	69 (10%)	7 1

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	40	HIS
1	A	48	LEU
1	A	65	ILE
1	A	81	SER
1	A	92	LEU

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Mol	Chain	Res	Type
1	A	96	TRP
1	A	101	THR
1	A	103	LEU
1	A	109	SER
1	A	120	LEU
1	A	138	VAL
1	A	169	LEU
1	A	179	TYR
1	A	184	CYS
1	A	188	VAL
1	A	198	LEU
1	A	257	ARG
1	A	270	GLN
1	A	271	LYS
1	A	273	LEU
1	A	283	LEU
1	A	290	VAL
1	A	292	LYS
1	A	307	LEU
1	A	311	SER
1	A	313	LEU
1	A	328	ASN
1	A	334	THR
1	A	335	ARG
1	A	350	SER
1	A	354	LEU
1	A	356	LEU
1	A	378	LEU
1	A	381	LYS
1	A	384	LEU
1	A	408	LEU
1	A	415	ARG
1	A	420	VAL
1	A	467	PHE
1	A	469	ASP
1	A	475	LYS
1	A	491	GLU
1	A	535	ASP
1	A	540	LYS
1	A	573	THR
1	A	576	SER
1	A	579	GLN

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Mol	Chain	Res	Type
1	A	586	ASN
1	A	592	VAL
1	A	629	SER
1	A	647	GLN
1	A	649	LEU
1	A	656	LEU
1	A	661	LEU
1	A	672	THR
1	A	693	LEU
1	A	694	THR
1	A	698	LEU
1	A	706	LYS
1	A	731	VAL
1	A	750	VAL
1	A	753	LEU
1	A	755	VAL
1	A	773	ASP
1	A	774	LEU
1	A	780	THR
1	A	782	VAL
1	A	808	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
3	SO4	A	905	-	4,4,4	0.12	0	6,6,6	0.10	0
3	SO4	A	914	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	A	904	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	A	909	-	4,4,4	0.13	0	6,6,6	0.11	0
2	NAG	A	902	1	14,14,15	0.45	0	17,19,21	1.20	1 (5%)
3	SO4	A	910	-	4,4,4	0.14	0	6,6,6	0.07	0
2	NAG	A	901	1	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
3	SO4	A	915	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	907	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	A	911	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	A	908	-	4,4,4	0.12	0	6,6,6	0.15	0
3	SO4	A	912	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	A	906	-	4,4,4	0.13	0	6,6,6	0.08	0
2	NAG	A	903	1	14,14,15	0.71	0	17,19,21	1.44	2 (11%)
3	SO4	A	913	-	4,4,4	0.15	0	6,6,6	0.07	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	901	1	-	2/6/23/26	0/1/1/1
2	NAG	A	902	1	-	2/6/23/26	0/1/1/1
2	NAG	A	903	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	903	NAG	C4-C3-C2	4.22	117.20	111.02
2	A	902	NAG	C1-O5-C5	3.22	116.56	112.19
2	A	903	NAG	C3-C4-C5	2.43	114.57	110.24
2	A	901	NAG	C2-N2-C7	-2.11	119.89	122.90

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	903	NAG	C8-C7-N2-C2
2	A	903	NAG	O7-C7-N2-C2
2	A	902	NAG	C8-C7-N2-C2
2	A	902	NAG	O7-C7-N2-C2
2	A	901	NAG	O5-C5-C6-O6
2	A	901	NAG	C4-C5-C6-O6
2	A	903	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	911	SO4	1	0
3	A	913	SO4	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

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	740/803 (92%)	0.25	32 (4%) 35 45	15, 33, 64, 83	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	ASN	6.2
1	A	39	PRO	5.3
1	A	470	ARG	4.0
1	A	472	LYS	3.7
1	A	473	ASN	3.3
1	A	560	PHE	3.2
1	A	308	VAL	3.2
1	A	431	SER	3.2
1	A	40	HIS	3.1
1	A	724	LEU	3.0
1	A	474	PHE	2.9
1	A	467	PHE	2.9
1	A	263	ASN	2.7
1	A	281	HIS	2.7
1	A	104	SER	2.6
1	A	589	HIS	2.5
1	A	60	ALA	2.5
1	A	103	LEU	2.5
1	A	62	CYS	2.5
1	A	305	GLN	2.4
1	A	262	PRO	2.3
1	A	807	LEU	2.3
1	A	302	SER	2.2
1	A	185	THR	2.2
1	A	260	HIS	2.2
1	A	303	TRP	2.1
1	A	559	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	694	THR	2.1
1	A	768	GLY	2.1
1	A	277	PRO	2.0
1	A	749	ILE	2.0
1	A	668	PHE	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)

There are no monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
3	SO4	A	912	5/5	0.73	0.18	81,87,89,92	0
3	SO4	A	907	5/5	0.89	0.17	78,79,80,86	0
2	NAG	A	902	14/15	0.89	0.12	55,62,74,74	0
3	SO4	A	904	5/5	0.90	0.15	95,99,99,101	0
3	SO4	A	914	5/5	0.91	0.23	88,90,91,91	0
2	NAG	A	901	14/15	0.91	0.16	31,38,47,48	0
2	NAG	A	903	14/15	0.91	0.17	50,57,66,67	0
3	SO4	A	915	5/5	0.92	0.13	86,87,89,92	0
3	SO4	A	909	5/5	0.92	0.20	90,91,93,94	0
3	SO4	A	906	5/5	0.93	0.12	90,92,93,94	0
3	SO4	A	910	5/5	0.93	0.12	72,72,75,81	0
3	SO4	A	911	5/5	0.95	0.10	75,77,78,81	0
3	SO4	A	908	5/5	0.96	0.14	43,58,62,62	0
3	SO4	A	905	5/5	0.96	0.14	53,57,66,66	0
3	SO4	A	913	5/5	0.96	0.10	78,81,82,83	0

6.5 Other polymers (i)

There are no such residues in this entry.