



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:44 pm GMT

PDB ID : 2DWE  
Title : Crystal structure of KcsA-FAB-TBA complex in Rb+  
Authors : Yohannan, S.; Zhou, Y.  
Deposited on : 2006-08-10  
Resolution : 2.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

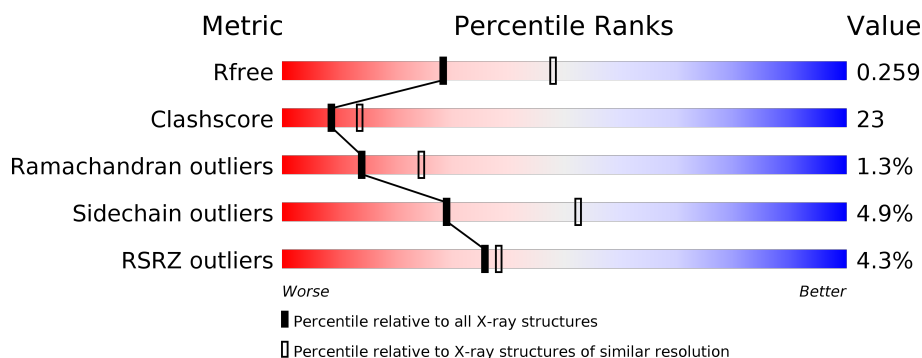
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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  $\geq 3$ , 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	219	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>5%</div> </div> </div>
2	B	212	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>33%</div> <div>• •</div> </div> </div>
3	C	103	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>27%</div> </div> </div>

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
5	L2C	C	201	X	-	-	X
6	F09	C	202	-	-	-	X
7	TBA	C	4001	-	-	X	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4223 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 ANTIBODY FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1641	1039	274	322	6			

- Molecule 2 is a protein called ANTIBODY FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1649	1023	283	338	5			

- Molecule 3 is a protein called Voltage-gated potassium channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	S	0	0	0
			777	507	135	133	2			

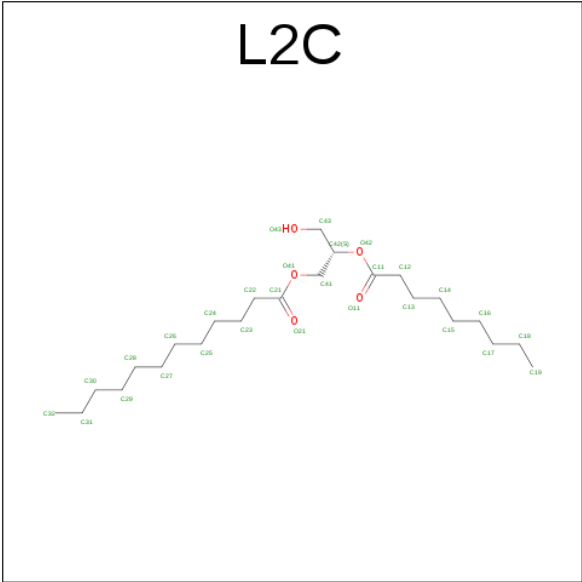
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	90	CYS	LEU	ENGINEERED	UNP P0A334

- Molecule 4 is RUBIDIUM ION (three-letter code: RB) (formula: Rb).

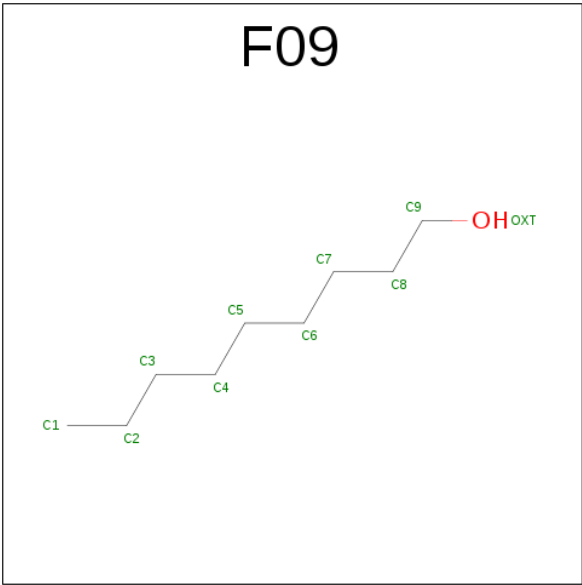
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total	Rb	0	0
			3	3		

- Molecule 5 is (2S)-3-HYDROXY-2-(NONANOYLOXY)PROPYL LAURATE (three-letter code: L2C) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>5</sub>).



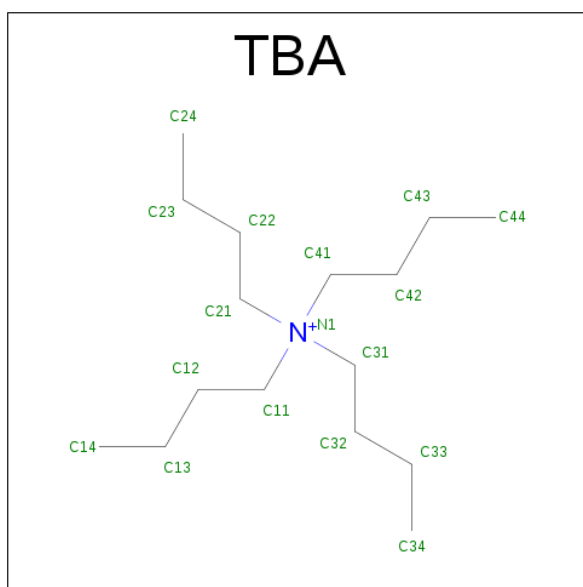
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			29	24	5		

- Molecule 6 is NONAN-1-OL (three-letter code: F09) (formula: C<sub>9</sub>H<sub>20</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			10	9	1		

- Molecule 7 is TETRABUTYLAMMONIUM ION (three-letter code: TBA) (formula: C<sub>16</sub>H<sub>36</sub>N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	C N	0	0
			17	16 1		

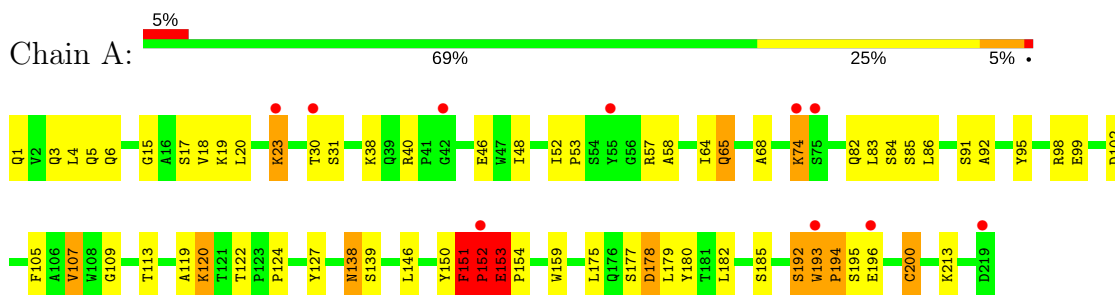
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	33	Total	O	0	0
			33	33		
8	B	50	Total	O	0	0
			50	50		
8	C	14	Total	O	0	0
			14	14		

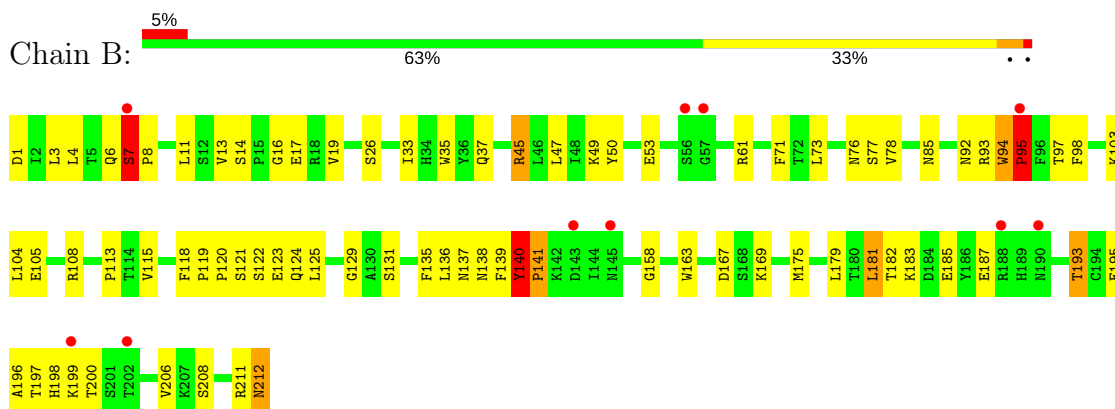
### 3 Residue-property plots [i](#)

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

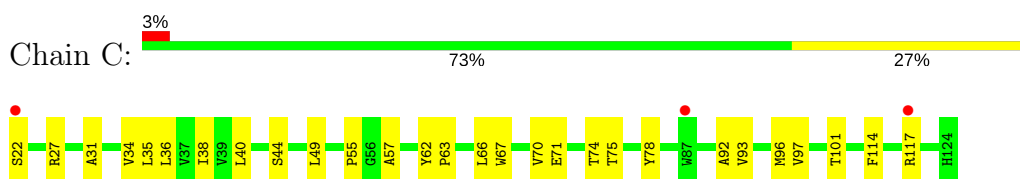
#### • Molecule 1: ANTIBODY FAB HEAVY CHAIN



#### • Molecule 2: ANTIBODY FAB LIGHT CHAIN



#### • Molecule 3: Voltage-gated potassium channel



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.56Å 154.56Å 75.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.84 – 2.50 26.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.84-2.50) 97.9 (26.84-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.24 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.266 0.225 , 0.259	Depositor DCC
$R_{free}$ test set	1527 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.2	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4223	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TBA, L2C, F09, RB

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	0.37	0/1685	0.72	1/2303 (0.0%)
2	B	0.43	0/1686	0.95	7/2287 (0.3%)
3	C	0.43	0/797	0.64	0/1093
All	All	0.41	0/4168	0.81	8/5683 (0.1%)

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
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	94	TRP	C-N-CD	-19.32	78.08	120.60
2	B	94	TRP	C-N-CA	13.59	179.09	122.00
2	B	140	TYR	C-N-CD	10.83	151.15	128.40
2	B	140	TYR	C-N-CA	-10.31	78.71	122.00
2	B	141	PRO	N-CA-C	-9.62	87.08	112.10
2	B	140	TYR	N-CA-C	6.83	129.43	111.00
2	B	95	PRO	CA-N-CD	-6.44	102.49	111.50
1	A	152	PRO	N-CA-C	-5.60	97.54	112.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	PHE	Sidechain
2	B	140	TYR	Sidechain

## 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	1641	0	1608	77	0
2	B	1649	0	1576	77	0
3	C	777	0	789	33	0
4	C	3	0	0	0	0
5	C	29	0	45	1	0
6	C	10	0	19	0	0
7	C	17	0	36	11	0
8	A	33	0	0	2	0
8	B	50	0	0	2	0
8	C	14	0	0	1	0
All	All	4223	0	4073	186	0

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 23.

All (186) 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)
2:B:7:SER:HB3	2:B:8:PRO:HD3	1.36	1.07
2:B:141:PRO:HD2	2:B:198:HIS:CE1	1.91	1.04
2:B:141:PRO:HD2	2:B:198:HIS:NE2	1.75	1.00
7:C:4001:TBA:H131	7:C:4001:TBA:H411	1.42	1.00
2:B:7:SER:HB3	2:B:8:PRO:CD	1.93	0.95
1:A:5:GLN:HB2	1:A:23:LYS:HG3	1.47	0.93
2:B:95:PRO:HD2	8:B:250:HOH:O	1.74	0.88
1:A:151:PHE:HB3	1:A:152:PRO:HD2	1.59	0.85
2:B:104:LEU:HD12	2:B:105:GLU:H	1.43	0.84
3:C:31:ALA:O	3:C:35:LEU:HG	1.78	0.82
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.61	0.81
1:A:74:LYS:HA	1:A:74:LYS:HZ1	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:PHE:CD2	1:A:152:PRO:HD3	2.15	0.80
2:B:140:TYR:CG	2:B:140:TYR:O	2.35	0.79
2:B:61:ARG:HG2	2:B:76:ASN:O	1.83	0.78
3:C:117:ARG:CZ	3:C:117:ARG:HB3	2.13	0.78
2:B:136:LEU:HD11	2:B:196:ALA:HB2	1.65	0.78
1:A:151:PHE:O	1:A:152:PRO:C	2.21	0.77
1:A:151:PHE:CD2	1:A:152:PRO:CD	2.69	0.76
1:A:74:LYS:HA	1:A:74:LYS:NZ	2.01	0.75
1:A:151:PHE:CB	1:A:152:PRO:HD2	2.16	0.75
2:B:179:LEU:HG	2:B:181:LEU:HD11	1.69	0.74
3:C:34:VAL:O	3:C:38:ILE:HG12	1.87	0.74
1:A:40:ARG:NH1	1:A:91:SER:O	2.20	0.74
2:B:7:SER:CB	2:B:8:PRO:HD3	2.16	0.73
3:C:22:SER:OG	3:C:27:ARG:NE	2.21	0.73
1:A:151:PHE:C	1:A:152:PRO:O	2.27	0.72
1:A:119:ALA:HB3	1:A:151:PHE:CE2	2.26	0.70
1:A:46:GLU:OE2	1:A:64:ILE:HG21	1.92	0.70
2:B:13:VAL:HG11	2:B:19:VAL:CG2	2.22	0.70
2:B:13:VAL:HG11	2:B:19:VAL:HG23	1.74	0.69
2:B:141:PRO:HG3	2:B:199:LYS:CD	2.22	0.69
1:A:151:PHE:CG	1:A:152:PRO:CD	2.77	0.67
2:B:7:SER:O	2:B:8:PRO:C	2.31	0.67
3:C:75:THR:OG1	7:C:4001:TBA:H432	1.96	0.66
2:B:141:PRO:HD2	2:B:198:HIS:HE2	1.61	0.65
2:B:212:ASN:HD22	2:B:212:ASN:C	1.98	0.65
2:B:181:LEU:HD23	2:B:185:GLU:HG3	1.77	0.65
2:B:211:ARG:HG2	2:B:211:ARG:HH11	1.61	0.65
2:B:104:LEU:HD12	2:B:105:GLU:N	2.10	0.65
2:B:7:SER:CB	2:B:8:PRO:CD	2.71	0.65
2:B:1:ASP:CG	2:B:95:PRO:HG2	2.17	0.64
1:A:17:SER:HB2	1:A:83:LEU:O	1.97	0.64
2:B:193:THR:HB	2:B:208:SER:HB3	1.80	0.63
3:C:93:VAL:HG21	5:C:201:L2C:H192	1.79	0.63
2:B:140:TYR:O	2:B:140:TYR:CD2	2.52	0.63
2:B:33:ILE:HG21	2:B:71:PHE:CD2	2.34	0.63
2:B:187:GLU:HA	2:B:187:GLU:OE2	2.00	0.61
2:B:137:ASN:HB3	2:B:138:ASN:HD22	1.65	0.61
2:B:141:PRO:CD	2:B:198:HIS:CE1	2.76	0.61
1:A:17:SER:HB2	1:A:84:SER:HA	1.82	0.61
1:A:178:ASP:O	1:A:179:LEU:HD23	2.01	0.61
1:A:31:SER:HB2	3:C:62:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:THR:CB	2:B:208:SER:HB3	2.31	0.61
2:B:61:ARG:HD3	2:B:77:SER:O	2.01	0.60
2:B:76:ASN:O	2:B:77:SER:HB3	1.99	0.60
3:C:117:ARG:NH1	3:C:117:ARG:HB3	2.16	0.60
7:C:4001:TBA:C13	7:C:4001:TBA:H411	2.23	0.60
1:A:192:SER:HB2	1:A:196:GLU:OE2	2.02	0.60
1:A:3:GLN:HB2	1:A:107:VAL:HG21	1.84	0.60
2:B:195:GLU:HG2	2:B:206:VAL:HG12	1.85	0.59
2:B:141:PRO:HG3	2:B:199:LYS:HD3	1.85	0.58
1:A:153:GLU:O	1:A:154:PRO:C	2.39	0.58
1:A:23:LYS:NZ	1:A:23:LYS:HB3	2.18	0.58
1:A:138:ASN:CG	1:A:139:SER:N	2.57	0.58
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.85	0.57
3:C:75:THR:CG2	7:C:4001:TBA:H432	2.33	0.57
3:C:117:ARG:NH1	3:C:117:ARG:CB	2.68	0.57
2:B:16:GLY:O	2:B:77:SER:HA	2.04	0.57
2:B:183:LYS:O	2:B:187:GLU:HG2	2.05	0.57
7:C:4001:TBA:H131	7:C:4001:TBA:C41	2.28	0.56
1:A:193:TRP:O	1:A:194:PRO:C	2.43	0.56
3:C:74:THR:O	7:C:4001:TBA:H431	2.05	0.56
1:A:193:TRP:CG	1:A:194:PRO:N	2.74	0.55
3:C:22:SER:OG	3:C:27:ARG:CD	2.54	0.55
1:A:5:GLN:HE21	1:A:23:LYS:CD	2.19	0.55
1:A:153:GLU:HB3	8:A:228:HOH:O	2.06	0.55
1:A:17:SER:CB	1:A:84:SER:HA	2.38	0.54
1:A:182:LEU:HD12	1:A:182:LEU:C	2.28	0.54
2:B:193:THR:HA	2:B:208:SER:HB3	1.90	0.54
3:C:36:LEU:O	3:C:40:LEU:HG	2.08	0.53
3:C:75:THR:HG23	7:C:4001:TBA:H432	1.91	0.53
3:C:44:SER:OG	3:C:66:LEU:HA	2.09	0.53
2:B:181:LEU:HD12	2:B:181:LEU:N	2.24	0.52
1:A:151:PHE:O	1:A:152:PRO:O	2.26	0.52
3:C:22:SER:HG	3:C:27:ARG:HE	1.55	0.52
1:A:175:LEU:HB2	1:A:180:TYR:CE2	2.44	0.52
1:A:1:GLN:N	1:A:1:GLN:OE1	2.38	0.52
2:B:94:TRP:O	3:C:55:PRO:HA	2.09	0.52
1:A:193:TRP:O	1:A:195:SER:N	2.43	0.51
2:B:167:ASP:OD2	2:B:169:LYS:HB2	2.10	0.51
1:A:91:SER:O	1:A:92:ALA:HB2	2.11	0.51
2:B:95:PRO:O	2:B:97:THR:HG23	2.10	0.51
3:C:117:ARG:CB	3:C:117:ARG:CZ	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HB3	1:A:86:LEU:HD21	1.93	0.51
2:B:115:VAL:HG22	2:B:136:LEU:HD13	1.92	0.51
3:C:74:THR:O	7:C:4001:TBA:C43	2.59	0.51
3:C:67:TRP:O	3:C:71:GLU:HG2	2.11	0.50
1:A:6:GLN:HE22	1:A:95:TYR:HA	1.77	0.50
1:A:53:PRO:HB3	1:A:74:LYS:HZ3	1.77	0.50
1:A:159:TRP:CZ3	1:A:200:CYS:HB3	2.47	0.50
2:B:115:VAL:HG22	2:B:136:LEU:CD1	2.42	0.50
3:C:97:VAL:O	3:C:101:THR:HB	2.12	0.50
1:A:52:ILE:O	1:A:52:ILE:HG23	2.12	0.50
1:A:5:GLN:CB	1:A:23:LYS:HG3	2.33	0.49
3:C:75:THR:OG1	7:C:4001:TBA:C43	2.59	0.49
1:A:120:LYS:O	1:A:120:LYS:HD2	2.12	0.49
1:A:193:TRP:HB3	1:A:194:PRO:HD3	1.94	0.49
2:B:179:LEU:CG	2:B:181:LEU:HD11	2.41	0.49
2:B:122:SER:HA	2:B:125:LEU:HD12	1.95	0.49
2:B:6:GLN:O	2:B:7:SER:O	2.31	0.49
2:B:136:LEU:CD1	2:B:196:ALA:HB2	2.39	0.49
1:A:151:PHE:CB	1:A:152:PRO:CD	2.83	0.48
1:A:151:PHE:CG	1:A:152:PRO:N	2.82	0.48
1:A:18:VAL:HG22	1:A:19:LYS:N	2.28	0.48
2:B:140:TYR:O	2:B:140:TYR:CD1	2.65	0.48
3:C:92:ALA:O	3:C:96:MET:HG3	2.13	0.48
2:B:193:THR:CA	2:B:208:SER:HB3	2.44	0.48
1:A:20:LEU:HB3	8:A:240:HOH:O	2.14	0.47
1:A:193:TRP:O	1:A:196:GLU:O	2.31	0.47
1:A:15:GLY:O	1:A:85:SER:HA	2.14	0.47
1:A:3:GLN:HE21	1:A:98:ARG:HH12	1.61	0.47
1:A:122:THR:O	1:A:150:TYR:HA	2.15	0.47
1:A:40:ARG:HD2	1:A:92:ALA:HB2	1.96	0.47
1:A:127:TYR:HD2	1:A:146:LEU:HD23	1.80	0.47
1:A:102:ASP:O	2:B:50:TYR:OH	2.24	0.46
2:B:211:ARG:HG2	2:B:211:ARG:NH1	2.30	0.46
2:B:45:ARG:HH11	2:B:45:ARG:HG3	1.81	0.46
1:A:105:PHE:HE1	2:B:98:PHE:CZ	2.34	0.46
3:C:66:LEU:O	3:C:70:VAL:HG23	2.15	0.46
1:A:151:PHE:CG	1:A:152:PRO:HD2	2.48	0.45
2:B:93:ARG:HA	3:C:57:ALA:O	2.16	0.45
1:A:57:ARG:HD2	1:A:58:ALA:H	1.82	0.45
2:B:158:GLY:O	2:B:179:LEU:HA	2.16	0.45
2:B:11:LEU:O	2:B:104:LEU:HD12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.99	0.45
2:B:212:ASN:ND2	2:B:212:ASN:C	2.70	0.45
7:C:4001:TBA:C13	7:C:4001:TBA:C41	2.91	0.45
1:A:193:TRP:O	1:A:196:GLU:N	2.49	0.45
3:C:71:GLU:OE1	3:C:78:TYR:HD1	1.99	0.45
2:B:121:SER:HB2	2:B:123:GLU:OE1	2.17	0.44
2:B:14:SER:HB2	2:B:17:GLU:OE2	2.17	0.44
2:B:49:LYS:HE3	2:B:53:GLU:OE1	2.17	0.44
2:B:181:LEU:HD23	2:B:185:GLU:CG	2.46	0.44
1:A:177:SER:O	1:A:178:ASP:HB2	2.16	0.44
2:B:198:HIS:CE1	2:B:200:THR:HG23	2.53	0.44
2:B:124:GLN:HG2	2:B:129:GLY:O	2.17	0.44
1:A:5:GLN:HE21	1:A:23:LYS:HD3	1.83	0.43
1:A:53:PRO:CB	1:A:74:LYS:HZ3	2.31	0.43
2:B:3:LEU:HB3	2:B:26:SER:HB3	2.00	0.43
1:A:3:GLN:HE21	1:A:98:ARG:NH1	2.16	0.43
1:A:40:ARG:HD2	1:A:91:SER:O	2.18	0.43
1:A:57:ARG:HD2	1:A:58:ALA:N	2.33	0.43
1:A:138:ASN:CG	1:A:139:SER:H	2.22	0.43
2:B:35:TRP:CD2	2:B:73:LEU:HB2	2.54	0.43
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.92	0.43
3:C:117:ARG:HH11	3:C:117:ARG:HB2	1.84	0.42
1:A:151:PHE:CD2	1:A:152:PRO:HD2	2.54	0.42
2:B:92:ASN:HD22	2:B:93:ARG:HG3	1.84	0.42
1:A:38:LYS:HB2	1:A:48:ILE:HD11	2.01	0.42
1:A:3:GLN:O	1:A:4:LEU:HD12	2.19	0.42
3:C:114:PHE:HA	3:C:117:ARG:HH22	1.84	0.42
1:A:102:ASP:OD1	1:A:102:ASP:N	2.52	0.42
1:A:193:TRP:CB	1:A:194:PRO:HD3	2.49	0.42
3:C:62:TYR:HB2	3:C:63:PRO:HD3	2.02	0.42
1:A:65:GLN:H	1:A:65:GLN:CD	2.12	0.42
2:B:13:VAL:HG21	2:B:78:VAL:HG21	2.02	0.42
2:B:163:TRP:CD1	2:B:175:MET:HG3	2.55	0.42
3:C:114:PHE:HA	3:C:117:ARG:HH12	1.85	0.41
3:C:35:LEU:O	3:C:38:ILE:HB	2.21	0.41
3:C:49:LEU:HB2	8:C:4009:HOH:O	2.19	0.41
2:B:137:ASN:HB3	2:B:138:ASN:ND2	2.32	0.41
1:A:6:GLN:HE21	1:A:109:GLY:HA3	1.86	0.41
1:A:68:ALA:HA	1:A:82:GLN:O	2.19	0.41
1:A:5:GLN:NE2	1:A:23:LYS:HD3	2.36	0.41
1:A:192:SER:O	1:A:196:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:THR:HB	1:A:154:PRO:HG2	2.03	0.41
2:B:92:ASN:ND2	8:B:255:HOH:O	2.53	0.41
3:C:75:THR:OG1	7:C:4001:TBA:H412	2.21	0.41
1:A:193:TRP:C	1:A:193:TRP:CD1	2.94	0.40
1:A:150:TYR:CE1	1:A:153:GLU:O	2.74	0.40
2:B:120:PRO:HB3	2:B:131:SER:H	1.86	0.40
2:B:179:LEU:HG	2:B:181:LEU:CD1	2.43	0.40
2:B:85:ASN:ND2	2:B:103:LYS:HD3	2.36	0.40
2:B:115:VAL:HA	2:B:135:PHE:O	2.21	0.40
2:B:108:ARG:HG3	2:B:140:TYR:CG	2.56	0.40

There are no symmetry-related clashes.

## 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	217/219 (99%)	198 (91%)	14 (6%)	5 (2%)	7	11
2	B	210/212 (99%)	194 (92%)	14 (7%)	2 (1%)	18	32
3	C	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
All	All	528/534 (99%)	492 (93%)	29 (6%)	7 (1%)	14	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	PRO
1	A	193	TRP
2	B	7	SER
1	A	153	GLU
1	A	151	PHE
2	B	95	PRO
1	A	194	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	183/185 (99%)	169 (92%)	14 (8%)	15	28
2	B	190/190 (100%)	182 (96%)	8 (4%)	34	59
3	C	75/75 (100%)	75 (100%)	0	100	100
All	All	448/450 (100%)	426 (95%)	22 (5%)	29	52

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	30	THR
1	A	65	GLN
1	A	74	LYS
1	A	99	GLU
1	A	107	VAL
1	A	120	LYS
1	A	138	ASN
1	A	153	GLU
1	A	178	ASP
1	A	185	SER
1	A	192	SER
1	A	200	CYS
1	A	213	LYS
2	B	4	LEU
2	B	7	SER
2	B	45	ARG
2	B	181	LEU
2	B	182	THR
2	B	193	THR
2	B	197	THR
2	B	212	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	GLN
1	A	6	GLN
2	B	85	ASN
2	B	92	ASN
2	B	137	ASN
2	B	138	ASN
2	B	212	ASN

### 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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z  > 2$
5	L2C	C	201	-	28,28,28	2.46	5 (17%)	30,30,30	4.70	10 (33%)
6	F09	C	202	-	9,9,9	1.39	1 (11%)	8,8,8	0.73	0
7	TBA	C	4001	-	16,16,16	0.82	0	18,18,18	0.60	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
5	L2C	C	201	-	1/1/3/3	0/30/30/30	0/0/0/0
6	F09	C	202	-	-	0/7/7/7	0/0/0/0
7	TBA	C	4001	-	-	0/20/20/20	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	201	L2C	O41-C21	-7.03	1.12	1.33
6	C	202	F09	OXT-C9	-3.93	1.21	1.42
5	C	201	L2C	C23-C22	-2.52	1.42	1.52
5	C	201	L2C	C41-C42	4.90	1.64	1.50
5	C	201	L2C	O42-C42	5.09	1.59	1.46
5	C	201	L2C	O42-C11	6.99	1.54	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	201	L2C	C41-C42-C43	-16.90	74.17	111.87
5	C	201	L2C	O41-C41-C42	-3.73	99.28	108.66
5	C	201	L2C	O41-C21-O21	-2.65	116.97	123.55
5	C	201	L2C	O42-C11-O11	-2.07	118.52	123.68
5	C	201	L2C	C41-O41-C21	2.01	123.19	117.13
5	C	201	L2C	O41-C21-C22	2.09	117.99	111.90
5	C	201	L2C	O42-C42-C41	2.41	117.20	108.44
5	C	201	L2C	O42-C11-C12	3.92	119.69	111.55
5	C	201	L2C	C42-O42-C11	6.69	133.67	117.88
5	C	201	L2C	O42-C42-C43	16.39	167.40	108.39

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	201	L2C	C42

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	201	L2C	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	4001	TBA	11	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	219/219 (100%)	0.27	10 (4%) 33 35	27, 49, 65, 73	0
2	B	212/212 (100%)	0.23	10 (4%) 32 34	22, 46, 66, 78	0
3	C	103/103 (100%)	0.06	3 (2%) 52 55	21, 29, 58, 72	0
All	All	534/534 (100%)	0.21	23 (4%) 36 38	21, 45, 65, 78	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	117	ARG	4.3
1	A	152	PRO	4.1
1	A	75	SER	4.0
2	B	7	SER	3.8
1	A	219	ASP	3.4
1	A	74	LYS	3.3
1	A	23	LYS	3.3
2	B	56	SER	2.9
1	A	42	GLY	2.9
3	C	22	SER	2.8
3	C	87	TRP	2.6
2	B	57	GLY	2.6
2	B	190	ASN	2.5
2	B	143	ASP	2.4
1	A	30	THR	2.3
2	B	199	LYS	2.3
1	A	196	GLU	2.3
1	A	193	TRP	2.3
2	B	188	ARG	2.2
2	B	145	ASN	2.2
1	A	55	TYR	2.1
2	B	202	THR	2.0
2	B	95	PRO	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	L2C	C	201	29/29	0.62	0.47	13.52	82,88,92,93	0
6	F09	C	202	10/10	0.52	0.52	5.36	95,96,97,98	0
7	TBA	C	4001	17/17	0.89	0.25	4.00	20,20,20,20	17
4	RB	C	3001	1/1	0.89	0.11	-	30,30,30,30	1
4	RB	C	3002	1/1	0.96	0.15	-	32,32,32,32	1
4	RB	C	3003	1/1	0.99	0.17	-	36,36,36,36	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.