Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 05:08 PM EDT

PDB ID	:	3FB8
Title	:	KcsA Potassium channel in the open-conductive state with 20 A opening at T112 in the presence of Rb+ ion
Authors	:	Cuello, L.G.; Jogini, V.; Cortes, D.M.; Perozo, E.
Deposited on	:	2008-11-18
Resolution	:	3.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

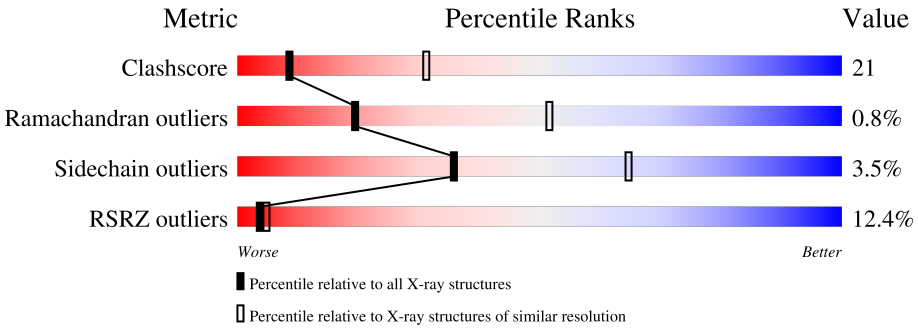
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.40 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))
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 of 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	219	14% 78% 21% .
2	B	212	16% 70% 30%
3	C	104	30% 49% 5% 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3915 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 fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1648	1042	275	325	6			

- Molecule 2 is a protein called antibody fab fragment 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	87	Total	C	N	O	S	0	0	0
			610	400	100	108	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	25	GLN	HIS	engineered mutation	UNP P0A334
C	90	CYS	LEU	engineered mutation	UNP P0A334
C	117	GLN	ARG	engineered mutation	UNP P0A334
C	120	GLN	GLU	engineered mutation	UNP P0A334
C	121	GLN	ARG	engineered mutation	UNP P0A334
C	122	GLN	ARG	engineered mutation	UNP P0A334
C	124	GLN	HIS	engineered mutation	UNP P0A334

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

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

- Molecule 5 is water.

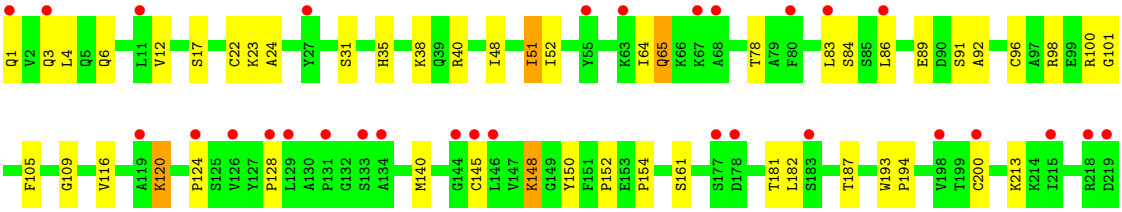
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total O 3 3	0	0
5	D	1	Total O 1 1	0	0

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.

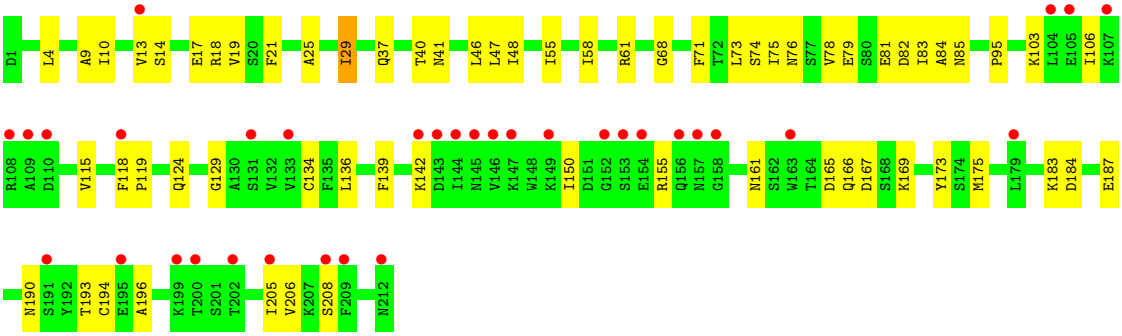
• Molecule 1: antibody fab fragment heavy chain

Chain A:



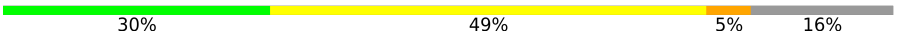
• Molecule 2: antibody fab fragment light chain

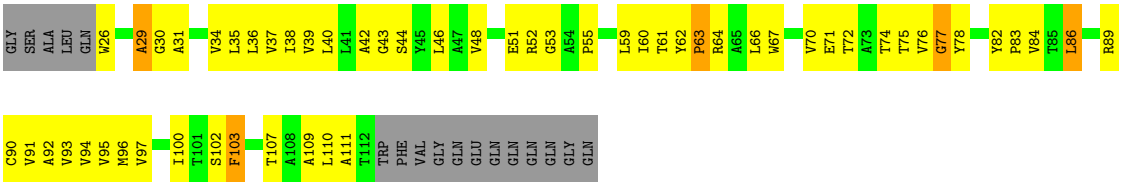
Chain B:



• Molecule 3: Voltage-gated potassium channel

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	155.64Å 155.64Å 73.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 42.29 – 3.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.40) 86.9 (42.29-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.284 , 0.304 0.287 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	88.6	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.045 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	3915	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: 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	0.34	0/1692	0.66	0/2312
2	B	0.34	0/1686	0.64	0/2287
3	C	0.42	0/623	0.69	0/860
All	All	0.36	0/4001	0.66	0/5459

There are no bond length outliers.

There are no bond angle outliers.

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	1648	0	1620	40	6
2	B	1649	0	1580	73	5
3	C	610	0	608	48	0
4	C	4	0	0	0	0
5	B	3	0	0	0	0
5	D	1	0	0	0	0
All	All	3915	0	3808	157	6

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 21.

All (157) 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:55:ILE:HB	2:B:58:ILE:HD12	1.35	1.05
2:B:47:LEU:HA	2:B:58:ILE:HD13	1.51	0.90
3:C:51:GLU:HG3	3:C:59:LEU:HB3	1.54	0.90
2:B:29:ILE:HD13	2:B:68:GLY:O	1.71	0.89
3:C:74:THR:HG22	3:C:103:PHE:HE1	1.36	0.89
2:B:78:VAL:HG11	2:B:106:ILE:HD11	1.55	0.88
2:B:167:ASP:OD2	2:B:169:LYS:HB2	1.79	0.83
3:C:74:THR:HG22	3:C:103:PHE:CE1	2.15	0.81
2:B:55:ILE:HB	2:B:58:ILE:CD1	2.10	0.81
1:A:65:GLN:NE2	1:A:65:GLN:H	1.79	0.80
1:A:120:LYS:H	1:A:120:LYS:HE3	1.49	0.78
1:A:22:CYS:HG	1:A:96:CYS:HG	0.88	0.78
2:B:134:CYS:HG	2:B:194:CYS:HG	0.77	0.76
2:B:25:ALA:CB	2:B:29:ILE:HD12	2.16	0.75
3:C:42:ALA:O	3:C:46:LEU:HD13	1.86	0.75
1:A:31:SER:HB2	3:C:62:TYR:CE1	2.22	0.74
2:B:47:LEU:HA	2:B:58:ILE:CD1	2.19	0.72
2:B:29:ILE:HD13	2:B:29:ILE:H	1.54	0.72
3:C:89:ARG:O	3:C:93:VAL:HG23	1.90	0.72
2:B:21:PHE:HE1	2:B:75:ILE:HD13	1.56	0.70
2:B:183:LYS:O	2:B:187:GLU:HG2	1.91	0.70
2:B:74:SER:C	2:B:75:ILE:HD12	2.13	0.69
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.73	0.68
1:A:101:GLY:HA3	3:C:62:TYR:CE1	2.29	0.68
3:C:26:TRP:HA	3:C:29:ALA:HB3	1.77	0.68
3:C:36:LEU:O	3:C:40:LEU:HD23	1.95	0.67
3:C:93:VAL:O	3:C:97:VAL:HG23	1.94	0.67
2:B:29:ILE:HD11	2:B:71:PHE:HE1	1.59	0.66
3:C:44:SER:OG	3:C:66:LEU:HA	1.96	0.66
2:B:183:LYS:HB3	2:B:183:LYS:NZ	2.11	0.65
2:B:61:ARG:HG3	2:B:76:ASN:O	1.96	0.64
3:C:86:LEU:HD12	3:C:86:LEU:O	1.97	0.64
3:C:53:GLY:O	3:C:55:PRO:HD3	1.98	0.64
1:A:148:LYS:HB3	1:A:181:THR:HG23	1.79	0.64
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.79	0.63
2:B:47:LEU:C	2:B:48:ILE:HD12	2.20	0.63
1:A:120:LYS:HE3	1:A:120:LYS:N	2.14	0.62
3:C:62:TYR:HB2	3:C:63:PRO:HD3	1.82	0.61
1:A:51:ILE:HD13	1:A:52:ILE:C	2.21	0.61
2:B:21:PHE:HE1	2:B:75:ILE:CD1	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:LEU:HB3	2:B:48:ILE:HD12	1.83	0.61
1:A:120:LYS:H	1:A:120:LYS:CE	2.13	0.60
3:C:86:LEU:HD12	3:C:86:LEU:C	2.23	0.59
3:C:34:VAL:O	3:C:38:ILE:HG12	2.03	0.59
1:A:38:LYS:HB2	1:A:48:ILE:HD11	1.85	0.59
2:B:75:ILE:HD12	2:B:75:ILE:N	2.18	0.59
3:C:71:GLU:OE2	3:C:78:TYR:HD1	1.86	0.59
2:B:13:VAL:CG2	2:B:17:GLU:HB3	2.32	0.59
3:C:36:LEU:HD12	3:C:102:SER:HB2	1.85	0.58
3:C:91:VAL:O	3:C:95:VAL:HG23	2.04	0.58
2:B:29:ILE:HD13	2:B:29:ILE:N	2.17	0.58
2:B:47:LEU:CA	2:B:58:ILE:HD13	2.29	0.58
2:B:29:ILE:CD1	2:B:68:GLY:O	2.47	0.58
1:A:6:GLN:HE21	1:A:109:GLY:HA3	1.69	0.57
3:C:84:VAL:HG22	3:C:84:VAL:O	2.05	0.57
2:B:124:GLN:HG2	2:B:129:GLY:O	2.05	0.57
1:A:23:LYS:HD3	1:A:78:THR:CG2	2.35	0.57
3:C:64:ARG:O	3:C:67:TRP:N	2.38	0.56
2:B:29:ILE:HD11	2:B:71:PHE:CE1	2.39	0.56
1:A:64:ILE:HD12	1:A:65:GLN:O	2.06	0.56
2:B:25:ALA:HB3	2:B:29:ILE:HD12	1.88	0.56
2:B:47:LEU:CB	2:B:48:ILE:HD12	2.36	0.55
2:B:85:ASN:ND2	2:B:103:LYS:HD3	2.22	0.55
2:B:21:PHE:CE1	2:B:75:ILE:HD13	2.41	0.54
3:C:39:VAL:O	3:C:43:GLY:N	2.34	0.54
3:C:89:ARG:O	3:C:92:ALA:HB3	2.06	0.54
2:B:78:VAL:CG1	2:B:106:ILE:HD11	2.33	0.54
3:C:109:ALA:C	3:C:111:ALA:H	2.11	0.54
3:C:107:THR:C	3:C:109:ALA:H	2.11	0.54
1:A:1:GLN:OE1	1:A:1:GLN:N	2.42	0.53
2:B:19:VAL:HG12	2:B:75:ILE:HB	1.91	0.53
1:A:182:LEU:C	1:A:182:LEU:HD12	2.29	0.53
2:B:46:LEU:O	2:B:58:ILE:HD11	2.09	0.53
1:A:101:GLY:HA3	3:C:62:TYR:HE1	1.75	0.53
1:A:51:ILE:HD13	1:A:52:ILE:N	2.24	0.52
1:A:83:LEU:HB3	1:A:86:LEU:HD21	1.92	0.52
1:A:140:MET:HE3	1:A:187:THR:HG22	1.90	0.52
2:B:18:ARG:NH1	2:B:76:ASN:OD1	2.43	0.52
3:C:36:LEU:HD12	3:C:102:SER:CB	2.39	0.51
3:C:109:ALA:C	3:C:111:ALA:N	2.63	0.51
3:C:60:ILE:O	3:C:61:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ALA:HB3	2:B:10:ILE:HD12	1.92	0.51
2:B:13:VAL:HG13	2:B:106:ILE:HD13	1.93	0.51
3:C:100:ILE:O	3:C:100:ILE:HG22	2.11	0.51
3:C:109:ALA:O	3:C:111:ALA:N	2.44	0.51
2:B:9:ALA:C	2:B:10:ILE:HD12	2.31	0.51
1:A:23:LYS:HD3	1:A:78:THR:HG23	1.94	0.50
1:A:65:GLN:H	1:A:65:GLN:HE21	1.58	0.50
2:B:13:VAL:CG1	2:B:106:ILE:HD13	2.42	0.50
1:A:17:SER:CB	1:A:84:SER:HA	2.42	0.50
1:A:101:GLY:HA3	3:C:62:TYR:CD1	2.47	0.49
2:B:79:GLU:HG3	2:B:81:GLU:HG2	1.95	0.49
2:B:10:ILE:HD12	2:B:10:ILE:N	2.28	0.49
2:B:161:ASN:HB3	2:B:175:MET:HE3	1.95	0.49
2:B:115:VAL:HG22	2:B:136:LEU:CD1	2.43	0.49
3:C:74:THR:O	3:C:75:THR:OG1	2.27	0.49
2:B:13:VAL:HG13	2:B:106:ILE:CD1	2.42	0.49
2:B:205:ILE:N	2:B:205:ILE:HD12	2.29	0.48
3:C:35:LEU:O	3:C:38:ILE:HB	2.13	0.48
2:B:142:LYS:HB3	2:B:173:TYR:CG	2.49	0.48
1:A:148:LYS:HB2	1:A:148:LYS:NZ	2.29	0.47
2:B:136:LEU:HD22	2:B:136:LEU:N	2.29	0.47
3:C:48:VAL:O	3:C:52:ARG:HG3	2.13	0.47
2:B:13:VAL:HG22	2:B:14:SER:N	2.29	0.47
2:B:150:ILE:HD12	2:B:155:ARG:HH11	1.78	0.47
3:C:37:VAL:O	3:C:37:VAL:HG12	2.15	0.47
2:B:48:ILE:HD13	2:B:73:LEU:CD1	2.45	0.47
3:C:82:TYR:HB2	3:C:83:PRO:HD2	1.96	0.47
2:B:25:ALA:CB	2:B:29:ILE:CD1	2.91	0.46
3:C:48:VAL:HG13	3:C:60:ILE:C	2.35	0.46
1:A:12:VAL:O	1:A:116:VAL:HA	2.15	0.46
2:B:142:LYS:HD3	2:B:173:TYR:CE2	2.50	0.46
1:A:145:CYS:HG	1:A:200:CYS:HG	1.64	0.46
3:C:70:VAL:O	3:C:74:THR:HG23	2.16	0.46
2:B:183:LYS:HB3	2:B:183:LYS:HZ3	1.79	0.46
2:B:25:ALA:HB3	2:B:29:ILE:CD1	2.47	0.45
2:B:13:VAL:HG22	2:B:17:GLU:HB3	1.99	0.44
1:A:120:LYS:H	1:A:120:LYS:CD	2.29	0.44
1:A:98:ARG:HD3	1:A:100:ARG:CZ	2.48	0.44
3:C:51:GLU:OE1	3:C:84:VAL:HG12	2.17	0.44
2:B:40:THR:HG22	2:B:41:ASN:ND2	2.33	0.44
1:A:3:GLN:O	1:A:24:ALA:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ALA:O	2:B:103:LYS:HD2	2.17	0.43
1:A:3:GLN:O	1:A:4:LEU:HD12	2.18	0.43
2:B:193:THR:HG22	2:B:208:SER:HB3	1.99	0.43
3:C:30:GLY:O	3:C:34:VAL:HG23	2.19	0.43
1:A:124:PRO:CB	1:A:150:TYR:HB3	2.46	0.43
2:B:193:THR:HG22	2:B:208:SER:CB	2.49	0.43
1:A:52:ILE:O	1:A:52:ILE:HG23	2.18	0.43
2:B:118:PHE:HA	2:B:119:PRO:HD3	1.87	0.43
3:C:100:ILE:O	3:C:100:ILE:CG2	2.66	0.43
1:A:35:HIS:CG	1:A:105:PHE:HE2	2.37	0.42
1:A:140:MET:CE	1:A:187:THR:HG22	2.48	0.42
2:B:55:ILE:CB	2:B:58:ILE:HD12	2.27	0.42
2:B:75:ILE:CD1	2:B:75:ILE:N	2.81	0.42
2:B:139:PHE:HE1	2:B:142:LYS:HA	1.83	0.42
2:B:61:ARG:NH1	2:B:82:ASP:OD1	2.53	0.42
2:B:21:PHE:CE1	2:B:75:ILE:CD1	2.99	0.42
3:C:72:THR:HG22	3:C:96:MET:HG2	2.00	0.42
2:B:83:ILE:HD13	2:B:166:GLN:HG2	2.01	0.42
1:A:1:GLN:N	1:A:1:GLN:CD	2.73	0.42
1:A:128:PRO:HG3	1:A:213:LYS:HD2	2.01	0.42
3:C:76:VAL:O	3:C:77:GLY:O	2.38	0.42
3:C:90:CYS:O	3:C:94:VAL:HG23	2.20	0.42
2:B:47:LEU:O	2:B:58:ILE:CD1	2.68	0.41
1:A:23:LYS:HD3	1:A:78:THR:OG1	2.20	0.41
3:C:60:ILE:C	3:C:61:THR:CG2	2.88	0.41
2:B:136:LEU:CD1	2:B:196:ALA:HB2	2.51	0.41
3:C:36:LEU:C	3:C:38:ILE:H	2.24	0.41
2:B:47:LEU:O	2:B:58:ILE:HD13	2.20	0.41
2:B:48:ILE:HD13	2:B:73:LEU:HD13	2.02	0.41
1:A:40:ARG:NH2	1:A:89:GLU:HB3	2.36	0.41
1:A:91:SER:O	1:A:92:ALA:HB2	2.21	0.41
2:B:13:VAL:HG23	2:B:17:GLU:CD	2.41	0.41
2:B:9:ALA:CB	2:B:10:ILE:HD12	2.51	0.40
2:B:85:ASN:ND2	2:B:103:LYS:CD	2.84	0.40
3:C:29:ALA:C	3:C:31:ALA:N	2.75	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:OE1	2:B:18:ARG:NE[3_755]	1.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:OE1	2:B:18:ARG:CZ[3_755]	1.69	0.51
1:A:1:GLN:OE1	1:A:193:TRP:CZ3[6_664]	1.92	0.28
1:A:65:GLN:OE1	2:B:18:ARG:CD[3_755]	1.97	0.23
1:A:65:GLN:OE1	2:B:18:ARG:NH1[3_755]	2.10	0.10
1:A:161:SER:CB	2:B:206:VAL:CG2[6_664]	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	217/219 (99%)	212 (98%)	5 (2%)	0	100 100
2	B	210/212 (99%)	203 (97%)	7 (3%)	0	100 100
3	C	85/104 (82%)	68 (80%)	13 (15%)	4 (5%)	2 15
All	All	512/535 (96%)	483 (94%)	25 (5%)	4 (1%)	19 51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	77	GLY
3	C	29	ALA
3	C	110	LEU
3	C	63	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/185 (100%)	178 (96%)	7 (4%)	33	61
2	B	190/190 (100%)	184 (97%)	6 (3%)	39	67
3	C	55/75 (73%)	53 (96%)	2 (4%)	35	63
All	All	430/450 (96%)	415 (96%)	15 (4%)	36	65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	65	GLN
1	A	120	LYS
1	A	148	LYS
1	A	152	PRO
1	A	154	PRO
1	A	194	PRO
2	B	4	LEU
2	B	29	ILE
2	B	95	PRO
2	B	165	ASP
2	B	184	ASP
2	B	190	ASN
3	C	86	LEU
3	C	103	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	GLN
1	A	6	GLN
1	A	65	GLN
2	B	41	ASN
2	B	85	ASN
2	B	92	ASN
2	B	137	ASN
2	B	190	ASN
2	B	210	ASN
3	C	58	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	219/219 (100%)	0.82	30 (13%) 3 3	83, 136, 162, 192	0
2	B	212/212 (100%)	0.79	34 (16%) 1 2	67, 122, 166, 172	0
3	C	87/104 (83%)	-0.10	0 100 100	49, 67, 145, 156	0
All	All	518/535 (96%)	0.65	64 (12%) 4 5	49, 127, 164, 192	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	157	ASN	6.5
1	A	215	ILE	4.8
2	B	152	GLY	4.8
2	B	145	ASN	4.4
2	B	202	THR	4.3
2	B	199	LYS	4.2
1	A	219	ASP	4.1
2	B	142	LYS	4.0
2	B	153	SER	3.5
1	A	133	SER	3.5
2	B	154	GLU	3.4
2	B	209	PHE	3.4
1	A	83	LEU	3.3
2	B	109	ALA	3.3
1	A	124	PRO	3.3
1	A	134	ALA	3.2
2	B	212	ASN	3.2
2	B	144	ILE	3.2
2	B	191	SER	3.2
2	B	146	VAL	3.1
1	A	27	TYR	3.1
1	A	128	PRO	3.1
1	A	1	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	86	LEU	3.0
1	A	178	ASP	2.9
2	B	143	ASP	2.9
1	A	63	LYS	2.9
2	B	110	ASP	2.8
2	B	131	SER	2.8
1	A	55	TYR	2.7
2	B	158	GLY	2.7
1	A	131	PRO	2.7
2	B	156	GLN	2.7
2	B	179	LEU	2.6
2	B	108	ARG	2.6
2	B	208	SER	2.6
1	A	198	VAL	2.6
2	B	195	GLU	2.5
1	A	218	ARG	2.5
2	B	105	GLU	2.5
2	B	147	LYS	2.5
1	A	129	LEU	2.5
2	B	200	THR	2.4
1	A	146	LEU	2.4
2	B	107	LYS	2.4
2	B	104	LEU	2.4
1	A	145	CYS	2.4
2	B	13	VAL	2.4
1	A	183	SER	2.4
1	A	200	CYS	2.4
2	B	205	ILE	2.4
1	A	126	VAL	2.3
1	A	68	ALA	2.3
2	B	133	VAL	2.3
2	B	163	TRP	2.3
2	B	118	PHE	2.2
1	A	11	LEU	2.2
1	A	80	PHE	2.2
1	A	119	ALA	2.2
1	A	3	GLN	2.2
1	A	144	GLY	2.1
1	A	177	SER	2.1
2	B	149	LYS	2.1
1	A	67	LYS	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
4	RB	C	4	1/1	0.90	0.30	74,74,74,74	1
4	RB	C	1	1/1	0.95	0.23	45,45,45,45	1
4	RB	C	3	1/1	0.99	0.24	91,91,91,91	1
4	RB	C	2	1/1	0.99	0.30	57,57,57,57	1

6.5 Other polymers (i)

There are no such residues in this entry.