



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:33 am GMT

PDB ID : 3EFD
Title : The crystal structure of the cytoplasmic domain of KcsA
Authors : Uysal, S.; Vasquez, V.; Tereshko, V.; Esaki, K.; Fellouse, F.A.; Sidhu, S.S.; Koide, S.; Perozo, E.; Kossiakoff, A.
Deposited on : 2008-09-08
Resolution : 2.60 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
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

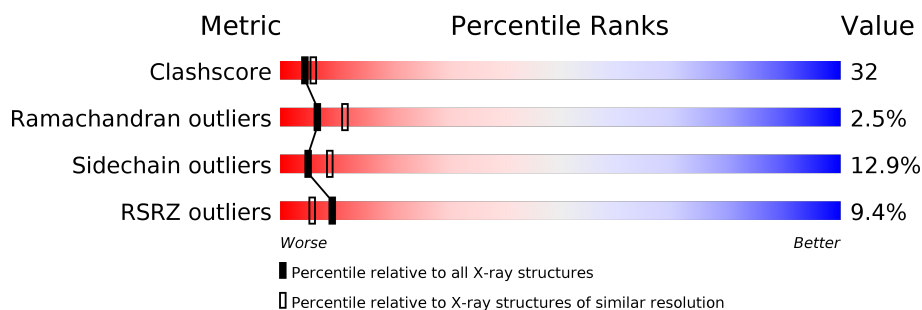
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	L	211	<div> <div>10%</div> <div>49%</div> <div>44%</div> <div>7%</div> </div>
2	H	222	<div> <div>8%</div> <div>49%</div> <div>40%</div> <div>8%</div> <div>...</div> </div>
3	K	30	<div> <div>17%</div> <div>63%</div> <div>27%</div> <div>10%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3553 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 FabL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1615	1012	268	330	5			

- Molecule 2 is a protein called FabH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1625	1031	269	318	7			

- Molecule 3 is a protein called KcsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	30	Total	C	N	O	S	0	0	0
			254	151	49	53	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	23	Total O 23 23	0	0
4	K	6	Total O 6 6	0	0
4	L	30	Total O 30 30	0	0

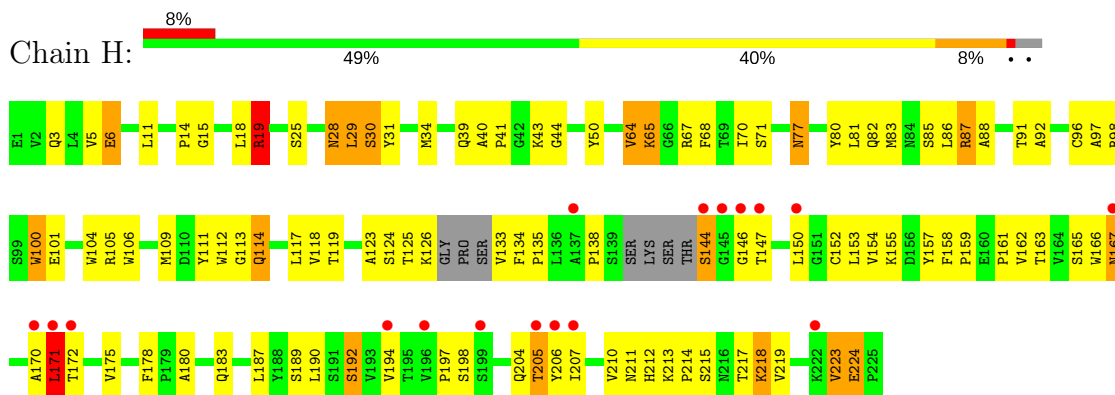
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

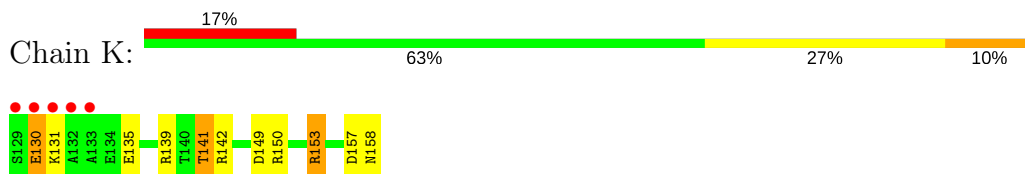
• Molecule 1: FabL



• Molecule 2: FabH



• Molecule 3: KcsA



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	115.50Å 115.50Å 76.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 38.41 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.60) 97.9 (38.41-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.225 , 0.276 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 77.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3553	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 [i](#)

5.1 Standard geometry [i](#)

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	L	0.57	0/1649	0.71	0/2238
2	H	0.60	0/1668	0.72	0/2274
3	K	0.60	0/256	0.84	0/340
All	All	0.59	0/3573	0.72	0/4852

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 [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	L	1615	0	1576	100	0
2	H	1625	0	1565	107	0
3	K	254	0	238	17	0
4	H	23	0	0	1	0
4	K	6	0	0	5	0
4	L	30	0	0	1	0
All	All	3553	0	3379	218	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 32.

All (218) 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:L:4:MET:HE2	1:L:25:ALA:HA	1.30	1.09
1:L:4:MET:HE2	1:L:25:ALA:CA	1.83	1.07
1:L:136:LEU:HD11	1:L:196:VAL:HG21	1.38	1.05
1:L:123:GLU:O	1:L:126:LYS:HG2	1.58	1.04
1:L:4:MET:CE	1:L:25:ALA:CB	2.35	1.04
1:L:4:MET:CE	1:L:25:ALA:HA	1.87	1.03
3:K:150:ARG:HA	3:K:153:ARG:HH12	1.26	0.99
1:L:4:MET:HE1	1:L:25:ALA:CB	1.94	0.98
2:H:19:ARG:HG2	2:H:82:GLN:HG2	1.44	0.96
2:H:223:VAL:O	2:H:224:GLU:HB2	1.66	0.93
1:L:4:MET:HE2	1:L:25:ALA:CB	1.99	0.92
2:H:64:VAL:O	2:H:65:LYS:O	1.88	0.92
1:L:124:GLN:HE22	1:L:131:SER:HB2	1.35	0.90
2:H:29:LEU:HB2	2:H:77:ASN:ND2	1.87	0.87
1:L:4:MET:CE	1:L:25:ALA:HB2	2.05	0.86
1:L:197:THR:HG23	1:L:204:PRO:HG3	1.59	0.84
1:L:136:LEU:HD11	1:L:196:VAL:CG2	2.07	0.84
1:L:4:MET:HE1	1:L:25:ALA:HB1	1.59	0.82
3:K:150:ARG:HA	3:K:153:ARG:NH1	1.94	0.82
1:L:4:MET:CE	1:L:25:ALA:CA	2.50	0.81
2:H:98:ARG:HH21	2:H:100:TRP:HB3	1.46	0.80
1:L:110:VAL:O	1:L:110:VAL:HG12	1.83	0.77
2:H:175:VAL:HG22	2:H:194:VAL:HG23	1.67	0.74
1:L:30:SER:HB3	3:K:157:ASP:OD1	1.87	0.74
2:H:163:THR:HB	2:H:211:ASN:HB3	1.69	0.71
2:H:64:VAL:HG11	2:H:68:PHE:HB2	1.71	0.71
1:L:8:PRO:O	1:L:102:THR:HG23	1.91	0.71
1:L:22:THR:HG22	1:L:72:THR:HG22	1.71	0.70
3:K:157:ASP:C	3:K:158:ASN:HD22	1.95	0.70
2:H:180:ALA:HA	2:H:190:LEU:HB3	1.74	0.70
1:L:4:MET:HE2	1:L:25:ALA:HB2	1.69	0.69
2:H:153:LEU:CD2	2:H:155:LYS:HB2	2.23	0.69
2:H:167:ASN:HD22	2:H:167:ASN:N	1.91	0.69
2:H:6:GLU:OE2	2:H:96:CYS:HB2	1.93	0.69
1:L:190:LYS:O	1:L:210:ASN:HA	1.92	0.68
1:L:154:LEU:HD23	1:L:154:LEU:H	1.57	0.68
2:H:29:LEU:HB2	2:H:77:ASN:HD21	1.59	0.68
2:H:29:LEU:HD21	2:H:34:MET:HG3	1.77	0.67
2:H:19:ARG:CG	2:H:82:GLN:HG2	2.21	0.67
1:L:186:TYR:CZ	1:L:211:ARG:HD3	2.30	0.67
2:H:125:THR:O	2:H:187:LEU:HD11	1.95	0.66
1:L:79:GLN:HB3	1:L:80:PRO:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:195:GLU:HB3	4:L:229:HOH:O	1.96	0.65
1:L:49:TYR:O	1:L:53:SER:HB2	1.96	0.65
1:L:125:LEU:HD12	1:L:183:LYS:HG3	1.77	0.65
1:L:190:LYS:HB2	1:L:210:ASN:ND2	2.10	0.65
2:H:213:LYS:HB3	2:H:214:PRO:HD3	1.78	0.65
1:L:115:VAL:H	2:H:144:SER:CB	2.10	0.65
1:L:55:TYR:HB3	1:L:58:VAL:HG21	1.78	0.65
1:L:193:ALA:HB2	1:L:208:SER:HB3	1.78	0.64
1:L:186:TYR:CE2	1:L:211:ARG:HD3	2.33	0.64
2:H:147:THR:HB	2:H:197:PRO:HA	1.79	0.64
2:H:5:VAL:HA	2:H:114:GLN:NE2	2.13	0.64
1:L:136:LEU:CD1	1:L:196:VAL:HG21	2.22	0.63
1:L:55:TYR:HB3	1:L:58:VAL:CG2	2.27	0.63
1:L:36:TYR:HE1	1:L:89:GLN:HE21	1.47	0.63
3:K:158:ASN:HD22	3:K:158:ASN:N	1.94	0.63
3:K:153:ARG:NH2	4:K:39:HOH:O	2.32	0.62
1:L:115:VAL:H	2:H:144:SER:HB3	1.63	0.62
2:H:159:PRO:HD2	2:H:214:PRO:HG2	1.81	0.62
2:H:104:TRP:CZ3	2:H:105:ARG:HG3	2.35	0.62
2:H:167:ASN:HD21	2:H:207:ILE:H	1.48	0.62
1:L:115:VAL:HA	1:L:135:LEU:O	2.01	0.61
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.83	0.61
2:H:153:LEU:HD21	2:H:155:LYS:HB2	1.81	0.61
2:H:6:GLU:CD	2:H:113:GLY:HA3	2.21	0.61
3:K:131:LYS:O	3:K:135:GLU:HB2	2.02	0.60
1:L:96:LEU:HD23	1:L:96:LEU:N	2.16	0.60
2:H:97:ALA:HA	2:H:111:TYR:O	2.03	0.59
2:H:64:VAL:O	2:H:65:LYS:C	2.41	0.59
2:H:153:LEU:C	2:H:153:LEU:HD23	2.23	0.59
2:H:64:VAL:HG11	2:H:68:PHE:CB	2.32	0.59
1:L:65:SER:HB3	1:L:72:THR:OG1	2.03	0.58
2:H:6:GLU:H	2:H:114:GLN:HE22	1.51	0.58
2:H:3:GLN:HG2	2:H:25:SER:OG	2.04	0.58
2:H:165:SER:C	2:H:166:TRP:CD1	2.78	0.57
2:H:18:LEU:HB3	2:H:83:MET:HE3	1.84	0.57
1:L:141:PRO:O	1:L:198:HIS:CE1	2.57	0.57
2:H:29:LEU:H	2:H:77:ASN:HD21	1.52	0.57
2:H:28:ASN:HD22	2:H:30:SER:H	1.53	0.57
2:H:5:VAL:HA	2:H:114:GLN:HE22	1.69	0.57
2:H:88:ALA:O	2:H:91:THR:HB	2.06	0.56
1:L:4:MET:HE1	1:L:25:ALA:HB2	1.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:162:VAL:HG22	2:H:190:LEU:HD21	1.88	0.56
2:H:180:ALA:HB2	2:H:190:LEU:HD23	1.89	0.55
1:L:63:SER:O	1:L:73:LEU:HD12	2.07	0.55
2:H:71:SER:OG	2:H:80:TYR:HB2	2.07	0.54
1:L:120:PRO:HG3	1:L:186:TYR:CZ	2.42	0.54
3:K:153:ARG:NE	4:K:39:HOH:O	2.39	0.54
3:K:142:ARG:HD3	4:K:4:HOH:O	2.08	0.54
1:L:166:GLN:HG2	1:L:171:SER:HB2	1.89	0.54
1:L:114:SER:HB3	1:L:116:PHE:CE1	2.42	0.54
1:L:141:PRO:O	1:L:198:HIS:HE1	1.90	0.53
3:K:153:ARG:CZ	4:K:39:HOH:O	2.57	0.53
2:H:44:GLY:HA3	4:H:227:HOH:O	2.09	0.53
2:H:166:TRP:O	2:H:167:ASN:HB2	2.09	0.52
2:H:187:LEU:HD22	2:H:187:LEU:N	2.24	0.52
2:H:212:HIS:O	2:H:215:SER:O	2.27	0.52
2:H:39:GLN:HG3	2:H:44:GLY:O	2.10	0.52
1:L:80:PRO:O	1:L:83:PHE:HD1	1.93	0.52
2:H:134:PHE:HB3	2:H:135:PRO:HD2	1.92	0.52
2:H:153:LEU:HD21	2:H:155:LYS:HD2	1.93	0.51
1:L:30:SER:O	1:L:31:SER:HB2	2.10	0.51
1:L:49:TYR:N	1:L:49:TYR:CD1	2.78	0.51
2:H:11:LEU:HA	2:H:119:THR:O	2.11	0.51
1:L:113:PRO:HD3	1:L:198:HIS:HD2	1.76	0.51
1:L:123:GLU:O	1:L:126:LYS:CG	2.46	0.51
2:H:88:ALA:O	2:H:91:THR:CB	2.59	0.50
2:H:97:ALA:HB2	2:H:112:TRP:CD2	2.46	0.50
2:H:165:SER:O	2:H:166:TRP:CD1	2.65	0.50
2:H:175:VAL:HG22	2:H:194:VAL:CG2	2.37	0.50
1:L:110:VAL:O	1:L:110:VAL:CG1	2.54	0.50
1:L:163:VAL:HG12	1:L:164:THR:O	2.10	0.50
2:H:64:VAL:HG12	2:H:65:LYS:N	2.25	0.49
1:L:4:MET:HE3	1:L:25:ALA:HA	1.87	0.49
2:H:166:TRP:HZ2	2:H:192:SER:HG	1.59	0.49
2:H:123:ALA:HB1	2:H:125:THR:HG22	1.94	0.49
1:L:114:SER:HB3	1:L:116:PHE:CZ	2.47	0.49
2:H:147:THR:HA	2:H:198:SER:HB2	1.94	0.49
1:L:186:TYR:CE2	1:L:211:ARG:CD	2.95	0.49
3:K:158:ASN:ND2	3:K:158:ASN:N	2.61	0.49
1:L:106:ILE:HG23	1:L:166:GLN:CD	2.32	0.49
2:H:150:LEU:HD13	2:H:223:VAL:HG21	1.95	0.49
3:K:153:ARG:HB2	3:K:153:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:27:GLN:O	1:L:28:SER:C	2.52	0.48
1:L:79:GLN:HB3	1:L:80:PRO:CD	2.43	0.48
2:H:91:THR:O	2:H:92:ALA:HB2	2.13	0.48
1:L:54:LEU:HD11	1:L:60:SER:HA	1.95	0.48
1:L:115:VAL:N	2:H:144:SER:HB3	2.27	0.48
2:H:14:PRO:HA	2:H:86:LEU:O	2.13	0.48
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.14	0.48
2:H:64:VAL:CG1	2:H:68:PHE:H	2.27	0.47
2:H:210:VAL:HG12	2:H:211:ASN:N	2.29	0.47
2:H:34:MET:O	2:H:50:TYR:HA	2.14	0.47
1:L:181:LEU:HD22	1:L:185:ASP:HB3	1.96	0.47
3:K:131:LYS:HB2	3:K:135:GLU:OE1	2.14	0.47
1:L:114:SER:HB2	1:L:137:ASN:HB3	1.96	0.47
1:L:187:GLU:HA	1:L:211:ARG:HH21	1.78	0.47
2:H:150:LEU:HD12	2:H:150:LEU:C	2.35	0.47
2:H:217:THR:HG23	2:H:219:VAL:HG23	1.95	0.47
1:L:197:THR:CG2	1:L:204:PRO:HG3	2.39	0.47
1:L:89:GLN:HG2	1:L:90:GLN:N	2.28	0.47
2:H:114:GLN:H	2:H:114:GLN:CD	2.17	0.47
2:H:210:VAL:CG1	2:H:211:ASN:N	2.77	0.47
1:L:124:GLN:NE2	1:L:131:SER:HB2	2.17	0.47
1:L:133:VAL:O	1:L:148:TRP:HH2	1.97	0.47
1:L:148:TRP:HZ2	1:L:177:SER:O	1.98	0.46
2:H:183:GLN:HE21	2:H:189:SER:HB2	1.80	0.46
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.50	0.46
1:L:48:ILE:HG21	1:L:52:SER:HA	1.96	0.46
2:H:101:GLU:HG2	2:H:106:TRP:HB2	1.96	0.46
2:H:159:PRO:HD2	2:H:214:PRO:CG	2.43	0.46
2:H:167:ASN:ND2	2:H:167:ASN:N	2.62	0.46
2:H:77:ASN:HD22	2:H:77:ASN:HA	1.52	0.46
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.98	0.46
2:H:204:GLN:O	2:H:205:THR:HG23	2.15	0.45
2:H:87:ARG:CG	2:H:87:ARG:HH11	2.30	0.45
1:L:81:GLU:CD	1:L:81:GLU:H	2.17	0.45
3:K:141:THR:HG22	3:K:142:ARG:N	2.32	0.45
1:L:193:ALA:HB2	1:L:208:SER:CB	2.44	0.45
2:H:158:PHE:CE2	2:H:159:PRO:HB3	2.52	0.45
2:H:138:PRO:HB3	2:H:150:LEU:HB3	1.99	0.45
2:H:98:ARG:NH2	2:H:100:TRP:HB3	2.23	0.45
2:H:19:ARG:HG2	2:H:82:GLN:CG	2.30	0.45
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:117:LEU:HD12	2:H:118:VAL:N	2.31	0.45
1:L:124:GLN:HE22	1:L:131:SER:CB	2.18	0.45
1:L:131:SER:HA	1:L:179:LEU:O	2.17	0.45
2:H:153:LEU:CD2	2:H:153:LEU:C	2.85	0.44
2:H:165:SER:C	2:H:166:TRP:HD1	2.20	0.44
2:H:70:ILE:HG23	2:H:70:ILE:O	2.18	0.44
2:H:97:ALA:HB1	2:H:109:MET:HB3	2.00	0.44
1:L:59:PRO:HB2	1:L:61:ARG:HG2	2.00	0.44
2:H:15:GLY:N	2:H:86:LEU:O	2.44	0.43
1:L:112:ALA:HA	1:L:113:PRO:HD3	1.78	0.43
1:L:193:ALA:CB	1:L:208:SER:HB3	2.47	0.43
2:H:170:ALA:O	2:H:171:LEU:HB2	2.18	0.43
1:L:107:LYS:HA	1:L:140:TYR:OH	2.18	0.43
2:H:29:LEU:N	2:H:77:ASN:HD21	2.16	0.43
1:L:207:LYS:HD3	1:L:207:LYS:HA	1.82	0.43
1:L:54:LEU:HA	1:L:54:LEU:HD23	1.77	0.43
3:K:130:GLU:HB2	3:K:131:LYS:H	1.39	0.43
1:L:163:VAL:HG22	1:L:175:LEU:HD12	2.00	0.43
1:L:27:GLN:O	1:L:29:VAL:HG13	2.18	0.43
1:L:182:SER:HB3	1:L:185:ASP:H	1.84	0.43
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.89	0.43
1:L:190:LYS:HB2	1:L:210:ASN:HD21	1.84	0.43
2:H:29:LEU:CB	2:H:77:ASN:ND2	2.70	0.42
2:H:40:ALA:O	2:H:41:PRO:C	2.57	0.42
2:H:172:THR:HG23	2:H:175:VAL:HG21	2.02	0.42
2:H:183:GLN:NE2	2:H:189:SER:HB2	2.33	0.42
2:H:64:VAL:HG13	2:H:67:ARG:HB2	2.00	0.42
2:H:126:LYS:HE3	2:H:126:LYS:HB2	1.93	0.42
2:H:133:VAL:N	2:H:154:VAL:HA	2.35	0.42
2:H:41:PRO:O	2:H:43:LYS:HG2	2.19	0.42
2:H:19:ARG:HA	2:H:81:LEU:O	2.20	0.42
1:L:108:ARG:HH21	1:L:170:ASP:HB2	1.85	0.42
1:L:176:SER:HB2	2:H:178:PHE:CE2	2.55	0.41
2:H:213:LYS:O	2:H:214:PRO:C	2.58	0.41
2:H:210:VAL:O	2:H:218:LYS:HA	2.20	0.41
3:K:150:ARG:HB3	4:K:1:HOH:O	2.20	0.41
2:H:40:ALA:HB3	2:H:43:LYS:HG3	2.03	0.41
1:L:152:ASN:HD22	1:L:152:ASN:HA	1.64	0.41
1:L:170:ASP:O	1:L:171:SER:C	2.59	0.41
1:L:195:GLU:OE1	1:L:206:THR:OG1	2.36	0.41
1:L:51:ALA:O	1:L:52:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14:SER:O	1:L:17:ASP:HB2	2.21	0.41
1:L:55:TYR:HB3	1:L:58:VAL:HG23	2.01	0.41
2:H:31:TYR:CD2	2:H:31:TYR:N	2.88	0.41
2:H:126:LYS:HB2	2:H:157:TYR:HA	2.03	0.41
2:H:218:LYS:HB2	2:H:218:LYS:HE2	1.80	0.41
3:K:149:ASP:O	3:K:150:ARG:C	2.56	0.41
1:L:118:PHE:CE1	2:H:150:LEU:HA	2.55	0.41
1:L:133:VAL:C	1:L:148:TRP:HH2	2.24	0.41
2:H:87:ARG:HG3	2:H:87:ARG:NH1	2.35	0.41
2:H:138:PRO:HG2	2:H:224:GLU:HG3	2.02	0.40
1:L:136:LEU:HB2	1:L:175:LEU:HB3	2.02	0.40
1:L:161:GLU:OE1	1:L:175:LEU:HD21	2.22	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	L	209/211 (99%)	185 (88%)	21 (10%)	3 (1%)	13	26
2	H	209/222 (94%)	180 (86%)	21 (10%)	8 (4%)	4	5
3	K	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
All	All	446/463 (96%)	388 (87%)	47 (10%)	11 (2%)	6	11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	52	SER
2	H	65	LYS
2	H	152	CYS
2	H	161	PRO
2	H	224	GLU

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Mol	Chain	Res	Type
1	L	66	GLY
2	H	171	LEU
1	L	109	THR
2	H	146	GLY
2	H	19	ARG
2	H	64	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	L	185/185 (100%)	158 (85%)	27 (15%)	3	6
2	H	178/184 (97%)	159 (89%)	19 (11%)	8	14
3	K	26/26 (100%)	22 (85%)	4 (15%)	3	5
All	All	389/395 (98%)	339 (87%)	50 (13%)	5	9

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	10	SER
1	L	17	ASP
1	L	39	LYS
1	L	50	SER
1	L	54	LEU
1	L	67	SER
1	L	70	ASP
1	L	76	SER
1	L	85	THR
1	L	105	GLU
1	L	106	ILE
1	L	108	ARG
1	L	109	THR
1	L	122	ASP
1	L	125	LEU

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Mol	Chain	Res	Type
1	L	131	SER
1	L	135	LEU
1	L	145	LYS
1	L	150	VAL
1	L	152	ASN
1	L	154	LEU
1	L	161	GLU
1	L	168	SER
1	L	181	LEU
1	L	197	THR
1	L	207	LYS
2	H	6	GLU
2	H	19	ARG
2	H	28	ASN
2	H	29	LEU
2	H	30	SER
2	H	77	ASN
2	H	85	SER
2	H	87	ARG
2	H	100	TRP
2	H	114	GLN
2	H	124	SER
2	H	144	SER
2	H	167	ASN
2	H	171	LEU
2	H	192	SER
2	H	205	THR
2	H	206	TYR
2	H	218	LYS
2	H	223	VAL
3	K	130	GLU
3	K	139	ARG
3	K	141	THR
3	K	153	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	79	GLN
1	L	89	GLN
1	L	124	GLN
1	L	152	ASN

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Mol	Chain	Res	Type
1	L	198	HIS
1	L	210	ASN
2	H	28	ASN
2	H	77	ASN
2	H	82	GLN
2	H	114	GLN
2	H	167	ASN
2	H	183	GLN
2	H	209	ASN
2	H	216	ASN
3	K	158	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](#)

There are no ligands in this entry.

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, 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	L	211/211 (100%)	0.58	21 (9%) 8 5	56, 67, 82, 90	0
2	H	215/222 (96%)	0.62	17 (7%) 13 9	54, 71, 84, 85	0
3	K	30/30 (100%)	1.04	5 (16%) 2 1	53, 68, 103, 104	0
All	All	456/463 (98%)	0.63	43 (9%) 9 6	53, 69, 84, 104	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	145	GLY	8.5
2	H	146	GLY	7.2
2	H	206	TYR	6.1
1	L	208	SER	5.6
1	L	153	ALA	5.4
1	L	210	ASN	5.0
1	L	154	LEU	4.5
2	H	196	VAL	4.5
2	H	147	THR	4.2
2	H	207	ILE	4.1
1	L	192	TYR	4.0
2	H	144	SER	3.9
2	H	205	THR	3.8
1	L	199	GLN	3.8
3	K	130	GLU	3.8
2	H	150	LEU	3.5
1	L	191	VAL	3.3
2	H	194	VAL	3.1
1	L	193	ALA	3.1
2	H	171	LEU	3.0
1	L	152	ASN	2.9
2	H	167	ASN	2.8
1	L	196	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	172	THR	2.6
2	H	137	ALA	2.6
3	K	131	LYS	2.5
3	K	132	ALA	2.5
1	L	200	GLY	2.5
1	L	146	VAL	2.5
1	L	133	VAL	2.4
2	H	170	ALA	2.4
1	L	207	LYS	2.4
1	L	108	ARG	2.3
1	L	155	GLN	2.3
2	H	199	SER	2.2
1	L	77	SER	2.2
2	H	222	LYS	2.2
3	K	133	ALA	2.2
3	K	129	SER	2.1
1	L	194	CYS	2.1
1	L	151	ASP	2.0
1	L	116	PHE	2.0
1	L	189	HIS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.