



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:08 PM UTC

PDB ID : 3EFD / pdb\_00003efd  
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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

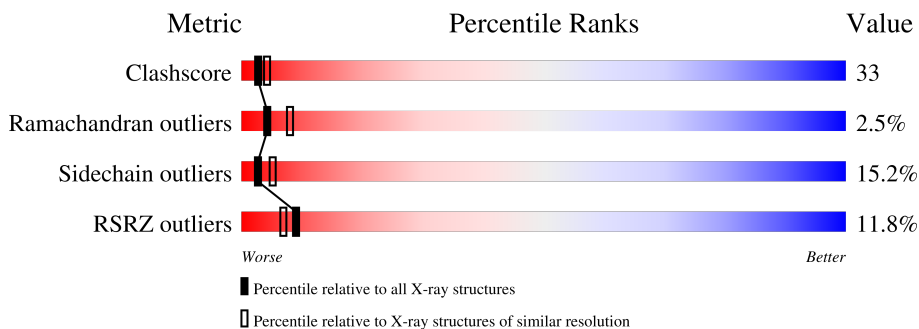
# 1 Overall quality at a glance

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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	
2	H	222	
3	K	30	

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	L	211	1615	1012	268	330	5	0	0	0

- Molecule 2 is a protein called FabH.

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

- Molecule 3 is a protein called KcsA.

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

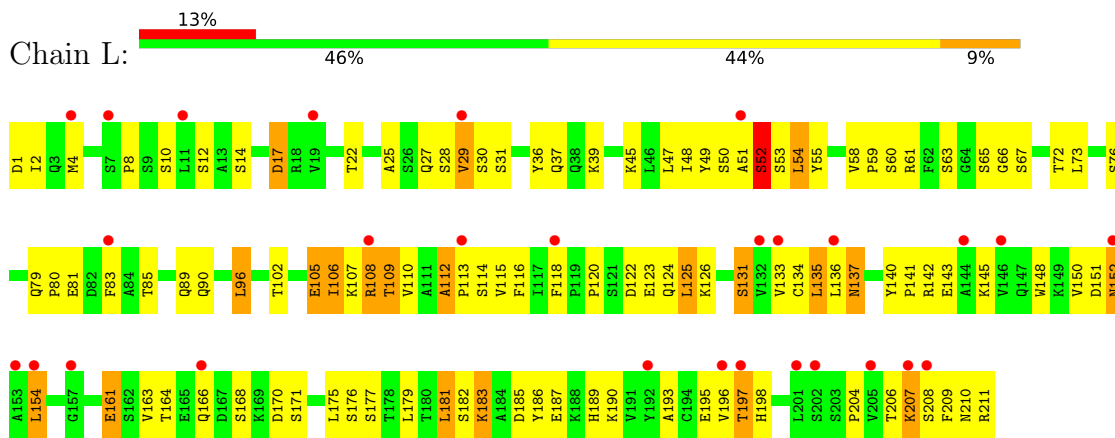
- Molecule 4 is water.

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

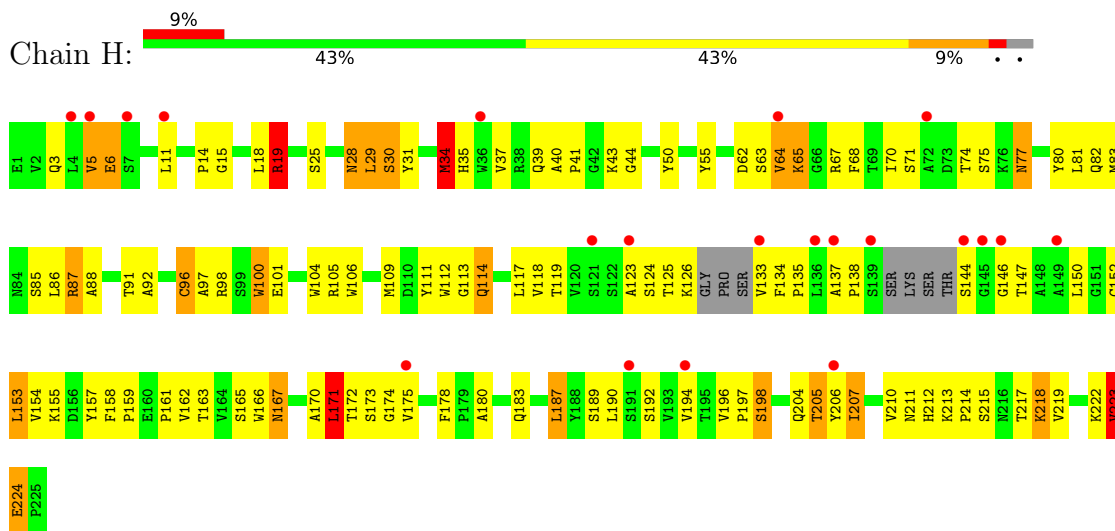
### 3 Residue-property plots

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.

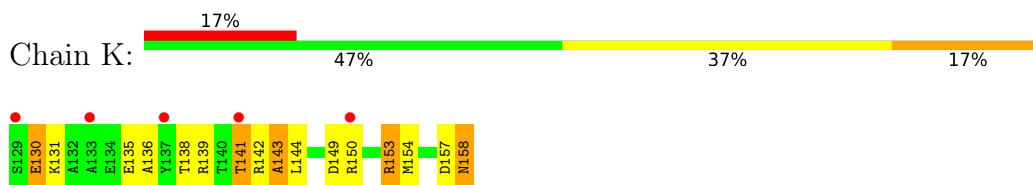
- Molecule 1: FabL



- Molecule 2: FabH



- Molecule 3: KcsA



## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.50Å 115.50Å 76.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.60) 98.0 (50.00-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.61Å)	Xtrriage
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.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.9	Xtrriage
Anisotropy	0.022	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 84.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.034 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3553	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage'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.*

<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 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	0.74	1/1649 (0.1%)	1.03	5/2238 (0.2%)
2	H	0.73	0/1668	1.06	13/2274 (0.6%)
3	K	0.73	0/256	0.99	1/340 (0.3%)
All	All	0.73	1/3573 (0.0%)	1.04	19/4852 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	52	SER	C-N	-5.09	1.26	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	29	VAL	N-CA-C	-7.30	106.02	113.10
2	H	34	MET	N-CA-C	6.97	119.76	109.24
1	L	112	ALA	CA-C-N	6.67	126.59	119.85
1	L	112	ALA	C-N-CA	6.67	126.59	119.85
2	H	55	TYR	N-CA-C	-6.21	105.35	113.17
2	H	196	VAL	CA-C-N	6.01	127.35	119.84
2	H	196	VAL	C-N-CA	6.01	127.35	119.84
1	L	137	ASN	N-CA-C	5.98	118.99	109.24
2	H	137	ALA	CA-C-N	5.77	125.75	120.21
2	H	137	ALA	C-N-CA	5.77	125.75	120.21
2	H	207	ILE	N-CA-C	5.51	115.93	107.77
2	H	63	SER	N-CA-C	-5.36	106.72	113.20
2	H	198	SER	N-CA-C	5.26	117.09	111.36
2	H	96	CYS	CB-CA-C	-5.24	100.65	109.50
1	L	112	ALA	N-CA-C	5.23	117.19	110.39
2	H	174	GLY	N-CA-C	-5.22	106.52	115.08
3	K	143	ALA	N-CA-C	-5.17	105.34	110.97
2	H	223	VAL	N-CA-C	5.14	115.13	108.35
2	H	37	VAL	N-CA-C	-5.06	100.60	108.95

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	L	1615	0	1576	102	0
2	H	1625	0	1565	112	0
3	K	254	0	238	20	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	228	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 33.

All (228) 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:HE1	1:L:25:ALA:CB	1.54	1.38
1:L:4:MET:HE2	1:L:25:ALA:HA	1.28	1.12
1:L:4:MET:HE1	1:L:25:ALA:HB2	1.11	1.08
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
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
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
1:L:4:MET:CE	1:L:25:ALA:CA	2.50	0.89
2:H:29:LEU:HB2	2:H:77:ASN:ND2	1.87	0.87
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
3:K:150:ARG:HA	3:K:153:ARG:NH1	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:ARG:HH21	2:H:100:TRP:HB3	1.46	0.80
1:L:4:MET:HE1	1:L:25:ALA:HB1	1.64	0.79
1:L:110:VAL:HG12	1:L:110:VAL:O	1.83	0.77
1:L:4:MET:CE	1:L:25:ALA:HB2	2.05	0.76
3:K:157:ASP:C	3:K:158:ASN:HD22	1.95	0.75
1:L:30:SER:HB3	3:K:157:ASP:OD1	1.87	0.74
2:H:175:VAL:HG22	2:H:194:VAL:HG23	1.67	0.74
1:L:4:MET:HE1	1:L:25:ALA:CA	2.15	0.71
2:H:163:THR:HB	2:H:211:ASN:HB3	1.69	0.71
1:L:8:PRO:O	1:L:102:THR:HG23	1.91	0.71
2:H:64:VAL:HG11	2:H:68:PHE:HB2	1.71	0.71
1:L:22:THR:HG22	1:L:72:THR:HG22	1.71	0.70
2:H:180:ALA:HA	2:H:190:LEU:HB3	1.74	0.70
2:H:6:GLU:OE2	2:H:96:CYS:HB2	1.93	0.69
2:H:153:LEU:CD2	2:H:155:LYS:HB2	2.23	0.69
2:H:167:ASN:N	2:H:167:ASN:HD22	1.91	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
3:K:150:ARG:HG3	3:K:154:MET:HE3	1.76	0.66
1:L:79:GLN:HB3	1:L:80:PRO:HD2	1.78	0.66
1:L:4:MET:HE2	1:L:25:ALA:CA	2.13	0.66
1:L:49:TYR:O	1:L:53:SER:HB2	1.96	0.65
1:L:195:GLU:HB3	4:L:229:HOH:O	1.96	0.65
2:H:6:GLU:CD	2:H:113:GLY:HA3	2.21	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:55:TYR:HB3	1:L:58:VAL:HG21	1.78	0.65
1:L:115:VAL:H	2:H:144:SER:CB	2.10	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:64:VAL:O	2:H:65:LYS:C	2.41	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
2:H:153:LEU:HD23	2:H:153:LEU:C	2.23	0.64
1:L:136:LEU:CD1	1:L:196:VAL:HG21	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:55:TYR:HB3	1:L:58:VAL:CG2	2.27	0.63
2:H:100:TRP:CD1	2:H:100:TRP:H	2.14	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
2:H:165:SER:C	2:H:166:TRP:CD1	2.78	0.62
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
3:K:131:LYS:O	3:K:135:GLU:HB2	2.02	0.60
1:L:96:LEU:N	1:L:96:LEU:HD23	2.16	0.60
2:H:97:ALA:HA	2:H:111:TYR:O	2.03	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
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
2:H:162:VAL:HG22	2:H:190:LEU:HD21	1.88	0.56
1:L:63:SER:O	1:L:73:LEU:HD12	2.07	0.55
2:H:180:ALA:HB2	2:H:190:LEU:HD23	1.89	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:106:ILE:HG23	1:L:166:GLN:CD	2.32	0.54
1:L:114:SER:HB3	1:L:116:PHE:CE1	2.42	0.54
1:L:27:GLN:O	1:L:28:SER:C	2.52	0.53
1:L:4:MET:CE	1:L:25:ALA:HB1	2.28	0.53
1:L:141:PRO:O	1:L:198:HIS:HE1	1.90	0.53
2:H:18:LEU:HB3	2:H:83:MET:HE3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:LEU:HD12	2:H:150:LEU:C	2.35	0.52
2:H:166:TRP:O	2:H:167:ASN:HB2	2.09	0.52
2:H:187:LEU:N	2:H:187:LEU:HD22	2.24	0.52
2:H:39:GLN:HG3	2:H:44:GLY:O	2.10	0.52
2:H:212:HIS:O	2:H:215:SER:O	2.27	0.52
1:L:80:PRO:O	1:L:83:PHE:HD1	1.93	0.52
2:H:114:GLN:H	2:H:114:GLN:CD	2.17	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:CD1	1:L:49:TYR:N	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
1:L:81:GLU:H	1:L:81:GLU:CD	2.17	0.50
2:H:64:VAL:HG12	2:H:65:LYS:N	2.25	0.49
2:H:165:SER:C	2:H:166:TRP:HD1	2.20	0.49
1:L:114:SER:HB3	1:L:116:PHE:CZ	2.47	0.49
2:H:123:ALA:HB1	2:H:125:THR:HG22	1.94	0.49
1:L:186:TYR:CE2	1:L:211:ARG:CD	2.95	0.49
2:H:147:THR:HA	2:H:198:SER:HB2	1.94	0.49
3:K:158:ASN:N	3:K:158:ASN:ND2	2.61	0.49
2:H:150:LEU:HD13	2:H:223:VAL:HG21	1.95	0.49
2:H:153:LEU:CD2	2:H:153:LEU:C	2.85	0.49
3:K:153:ARG:HB2	3:K:153:ARG:HH11	1.77	0.49
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
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.14	0.48
2:H:14:PRO:HA	2:H:86:LEU:O	2.13	0.48
2:H:64:VAL:CG1	2:H:68:PHE:H	2.27	0.47
2:H:34:MET:O	2:H:50:TYR:HA	2.14	0.47
2:H:210:VAL:HG12	2:H:211:ASN:N	2.29	0.47
1:L:181:LEU:HD22	1:L:185:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:K:131:LYS:HB2	3:K:135:GLU:OE1	2.14	0.47
1:L:89:GLN:HG2	1:L:90:GLN:N	2.28	0.47
1:L:197:THR:CG2	1:L:204:PRO:HG3	2.39	0.47
2:H:217:THR:HG23	2:H:219:VAL:HG23	1.95	0.47
2:H:40:ALA:O	2:H:41:PRO:C	2.57	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
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.50	0.46
2:H:183:GLN:HE21	2:H:189:SER:HB2	1.80	0.46
2:H:213:LYS:O	2:H:214:PRO:C	2.58	0.46
1:L:48:ILE:HG21	1:L:52:SER:HA	1.96	0.46
2:H:34:MET:HB3	2:H:34:MET:HE3	1.53	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
1:L:170:ASP:O	1:L:171:SER:C	2.59	0.46
1:L:133:VAL:C	1:L:148:TRP:HH2	2.24	0.46
2:H:77:ASN:HD22	2:H:77:ASN:HA	1.52	0.46
3:K:149:ASP:O	3:K:150:ARG:C	2.56	0.46
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.98	0.46
2:H:87:ARG:HH11	2:H:87:ARG:CG	2.30	0.45
2:H:204:GLN:O	2:H:205:THR:HG23	2.15	0.45
1:L:193:ALA:HB2	1:L:208:SER:CB	2.44	0.45
3:K:141:THR:HG22	3:K:142:ARG:N	2.32	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
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.52	0.45
1:L:209:PHE:CD1	1:L:209:PHE:C	2.95	0.45
2:H:19:ARG:HG2	2:H:82:GLN:CG	2.30	0.45
2:H:98:ARG:NH2	2:H:100:TRP:HB3	2.23	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
1:L:142:ARG:O	1:L:143:GLU:C	2.57	0.45
2:H:62:ASP:C	2:H:64:VAL:N	2.75	0.45
2:H:117:LEU:HD12	2:H:118:VAL:N	2.31	0.45
2:H:74:THR:O	2:H:75:SER:C	2.61	0.44
2:H:70:ILE:O	2:H:70:ILE:HG23	2.18	0.44
1:L:59:PRO:HB2	1:L:61:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:ALA:HB1	2:H:109:MET:HB3	2.00	0.44
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:15:GLY:N	2:H:86:LEU:O	2.44	0.43
1:L:107:LYS:HA	1:L:140:TYR:OH	2.18	0.43
2:H:170:ALA:O	2:H:171:LEU:HB2	2.18	0.43
1:L:54:LEU:HD23	1:L:54:LEU:HA	1.77	0.43
1:L:207:LYS:HA	1:L:207:LYS:HD3	1.82	0.43
2:H:29:LEU:N	2:H:77:ASN:HD21	2.16	0.43
1:L:27:GLN:O	1:L:29:VAL:HG13	2.18	0.43
1:L:163:VAL:HG22	1:L:175:LEU:HD12	2.00	0.43
3:K:130:GLU:HB2	3:K:131:LYS:H	1.39	0.43
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.89	0.43
1:L:182:SER:HB3	1:L:185:ASP:H	1.84	0.43
2:H:35:HIS:CG	2:H:109:MET:HE2	2.54	0.43
3:K:136:ALA:C	3:K:138:THR:N	2.77	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: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
1:L:12:SER:OG	1:L:105:GLU:CD	2.62	0.42
2:H:126:LYS:HE3	2:H:126:LYS:HB2	1.93	0.42
2:H:41:PRO:O	2:H:43:LYS:HG2	2.19	0.42
2:H:133:VAL:N	2:H:154:VAL:HA	2.35	0.42
1:L:108:ARG:HH21	1:L:170:ASP:HB2	1.85	0.42
2:H:19:ARG:HA	2:H:81:LEU:O	2.20	0.42
1:L:176:SER:HB2	2:H:178:PHE:CE2	2.55	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
1:L:152:ASN:HD22	1:L:152:ASN:HA	1.64	0.41
2:H:40:ALA:HB3	2:H:43:LYS:HG3	2.03	0.41
1:L:51:ALA:O	1:L:52:SER:HB3	2.20	0.41
1:L:195:GLU:OE1	1:L:206:THR:OG1	2.36	0.41
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:N	2:H:31:TYR:CD2	2.88	0.41
3:K:143:ALA:O	3:K:144:LEU:C	2.64	0.41
1:L:118:PHE:CE1	2:H:150:LEU:HA	2.55	0.41
2:H:18:LEU:HB3	2:H:83:MET:CE	2.51	0.41
2:H:126:LYS:HB2	2:H:157:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:218:LYS:HB2	2:H:218:LYS:HE2	1.80	0.41
2:H:87:ARG:NH1	2:H:87:ARG:HG3	2.35	0.41
2:H:138:PRO:HG2	2:H:224:GLU:HG3	2.02	0.40
2:H:28:ASN:HD22	2:H:28:ASN:C	2.28	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 [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	L	209/211 (99%)	185 (88%)	21 (10%)	3 (1%)	9	19
2	H	209/222 (94%)	180 (86%)	21 (10%)	8 (4%)	2	3
3	K	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
All	All	446/463 (96%)	388 (87%)	47 (10%)	11 (2%)	4	8

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
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 [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	L	185/185 (100%)	155 (84%)	30 (16%)	2	4
2	H	178/184 (97%)	154 (86%)	24 (14%)	4	7
3	K	26/26 (100%)	21 (81%)	5 (19%)	1	2
All	All	389/395 (98%)	330 (85%)	59 (15%)	3	5

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	2	ILE
1	L	10	SER
1	L	17	ASP
1	L	39	LYS
1	L	45	LYS
1	L	50	SER
1	L	54	LEU
1	L	67	SER
1	L	76	SER
1	L	85	THR
1	L	96	LEU
1	L	105	GLU
1	L	106	ILE
1	L	108	ARG
1	L	109	THR
1	L	122	ASP
1	L	125	LEU
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

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Mol	Chain	Res	Type
1	L	181	LEU
1	L	183	LYS
1	L	197	THR
1	L	207	LYS
2	H	5	VAL
2	H	6	GLU
2	H	19	ARG
2	H	28	ASN
2	H	29	LEU
2	H	30	SER
2	H	34	MET
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	153	LEU
2	H	167	ASN
2	H	171	LEU
2	H	173	SER
2	H	187	LEU
2	H	192	SER
2	H	205	THR
2	H	206	TYR
2	H	218	LYS
2	H	222	LYS
2	H	223	VAL
3	K	130	GLU
3	K	139	ARG
3	K	141	THR
3	K	153	ARG
3	K	158	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	79	GLN
1	L	89	GLN
1	L	124	GLN
1	L	138	ASN

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Mol	Chain	Res	Type
1	L	147	GLN
1	L	152	ASN
1	L	198	HIS
1	L	210	ASN
2	H	13	GLN
2	H	28	ASN
2	H	77	ASN
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 oligosaccharides 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, 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	L	211/211 (100%)	1.05	28 (13%) <b>7</b> <b>5</b>	56, 67, 82, 90	0
2	H	215/222 (96%)	0.94	21 (9%) <b>13</b> <b>10</b>	54, 71, 84, 85	0
3	K	30/30 (100%)	0.89	5 (16%) <b>4</b> <b>3</b>	53, 68, 103, 104	0
All	All	456/463 (98%)	0.99	54 (11%) <b>9</b> <b>7</b>	53, 69, 84, 104	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	145	GLY	6.2
1	L	196	VAL	4.0
1	L	118	PHE	3.8
1	L	201	LEU	3.7
1	L	197	THR	3.5
2	H	136	LEU	3.4
1	L	133	VAL	3.4
2	H	194	VAL	3.3
2	H	146	GLY	3.2
2	H	123	ALA	3.2
1	L	205	VAL	2.8
1	L	207	LYS	2.7
2	H	4	LEU	2.6
1	L	113	PRO	2.6
2	H	11	LEU	2.6
1	L	192	TYR	2.6
2	H	133	VAL	2.5
1	L	153	ALA	2.5
2	H	191	SER	2.5
2	H	137	ALA	2.5
3	K	129	SER	2.5
2	H	206	TYR	2.5
1	L	136	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	208	SER	2.4
1	L	7	SER	2.4
2	H	64	VAL	2.4
3	K	141	THR	2.4
2	H	121	SER	2.4
1	L	51	ALA	2.4
2	H	7	SER	2.3
2	H	139	SER	2.3
2	H	144	SER	2.3
2	H	5	VAL	2.3
2	H	36	TRP	2.3
1	L	83	PHE	2.3
1	L	152	ASN	2.2
1	L	157	GLY	2.2
1	L	4	MET	2.2
1	L	11	LEU	2.2
1	L	154	LEU	2.2
2	H	149	ALA	2.1
1	L	132	VAL	2.1
1	L	146	VAL	2.1
1	L	144	ALA	2.1
2	H	72	ALA	2.1
1	L	166	GLN	2.1
1	L	29	VAL	2.1
2	H	175	VAL	2.1
1	L	108	ARG	2.0
3	K	133	ALA	2.0
1	L	202	SER	2.0
1	L	19	VAL	2.0
3	K	150	ARG	2.0
3	K	137	TYR	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 oligosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.