



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 07:41 AM EDT

PDB ID : 3UM7  
Title : Crystal structure of the human two pore domain K<sup>+</sup> ion channel TRAAK (K2P4.1)  
Authors : Brohawn, S.G.; MacKinnon, R.  
Deposited on : 2011-11-12  
Resolution : 3.31 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 : 4.02b-467  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

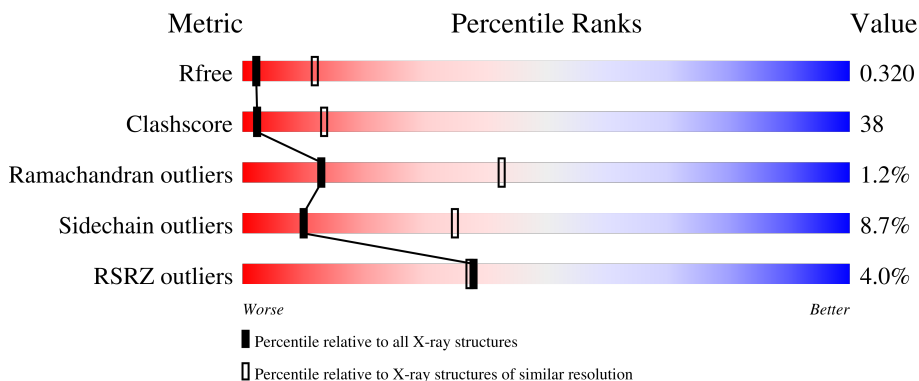
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	A	309	
1	B	309	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 3745 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 Potassium channel subfamily K member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	259	Total 1935	C 1277	N 312	O 339	S 7	0	0	0
1	B	244	Total 1805	C 1197	N 286	O 316	S 6	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLN	ASN	ENGINEERED MUTATION	UNP Q9NYG8
A	108	GLN	ASN	ENGINEERED MUTATION	UNP Q9NYG8
A	301	SER	-	EXPRESSION TAG	UNP Q9NYG8
A	302	ASN	-	EXPRESSION TAG	UNP Q9NYG8
A	303	SER	-	EXPRESSION TAG	UNP Q9NYG8
A	304	LEU	-	EXPRESSION TAG	UNP Q9NYG8
A	305	GLU	-	EXPRESSION TAG	UNP Q9NYG8
A	306	VAL	-	EXPRESSION TAG	UNP Q9NYG8
A	307	LEU	-	EXPRESSION TAG	UNP Q9NYG8
A	308	PHE	-	EXPRESSION TAG	UNP Q9NYG8
A	309	GLN	-	EXPRESSION TAG	UNP Q9NYG8
B	104	GLN	ASN	ENGINEERED MUTATION	UNP Q9NYG8
B	108	GLN	ASN	ENGINEERED MUTATION	UNP Q9NYG8
B	301	SER	-	EXPRESSION TAG	UNP Q9NYG8
B	302	ASN	-	EXPRESSION TAG	UNP Q9NYG8
B	303	SER	-	EXPRESSION TAG	UNP Q9NYG8
B	304	LEU	-	EXPRESSION TAG	UNP Q9NYG8
B	305	GLU	-	EXPRESSION TAG	UNP Q9NYG8
B	306	VAL	-	EXPRESSION TAG	UNP Q9NYG8
B	307	LEU	-	EXPRESSION TAG	UNP Q9NYG8
B	308	PHE	-	EXPRESSION TAG	UNP Q9NYG8
B	309	GLN	-	EXPRESSION TAG	UNP Q9NYG8

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total K 5 5	0	0



MET  
GLY  
GLY  
LEU  
THR  
ALA  
GLN  
SER  
SER  
ASN  
SER  
LEU  
LEU  
GLU  
VAL  
LEU  
PHE  
GLN

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.94Å 130.85Å 132.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.20 – 3.31 31.07 – 3.31	Depositor EDS
% Data completeness (in resolution range)	75.4 (31.20-3.31) 75.7 (31.07-3.31)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.31Å)	Xtrriage
Refinement program	REFMAC refmac_5.6.0117	Depositor
R, $R_{free}$	0.317 , 0.323 0.315 , 0.320	Depositor DCC
$R_{free}$ test set	882 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	109.0	Xtrriage
Anisotropy	0.024	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 152.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.028 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	3745	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	175.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
K

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	0.56	2/1980 (0.1%)	0.64	1/2704 (0.0%)
1	B	0.53	0/1848	0.60	0/2528
All	All	0.55	2/3828 (0.1%)	0.62	1/5232 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	TRP	CD2-CE2	5.16	1.47	1.41
1	A	114	TRP	CD2-CE2	5.00	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LEU	CA-CB-CG	-5.18	103.38	115.30

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	A	1935	0	1908	152	0
1	B	1805	0	1762	152	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3745	0	3670	282	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 38.

All (282) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLN:HG3	1:A:100:ASP:HB3	1.25	1.09
1:A:214:THR:CB	1:A:229:ILE:HD13	1.86	1.04
1:A:214:THR:HB	1:A:229:ILE:HD13	1.38	1.04
1:A:78:CYS:SG	1:A:79:VAL:HG23	2.03	0.99
1:B:138:ARG:HH11	1:B:138:ARG:CG	1.81	0.93
1:A:54:GLU:CD	1:A:139:THR:HG23	1.91	0.90
1:A:142:GLY:O	1:A:146:CYS:HB2	1.73	0.88
1:A:134:ASN:HD22	1:A:245:VAL:HG11	1.39	0.87
1:B:54:GLU:CB	1:B:114:TRP:CZ2	2.57	0.86
1:B:214:THR:HG21	1:B:229:ILE:HD13	1.58	0.86
1:A:221:GLU:OE1	1:A:246:ALA:HA	1.77	0.85
1:A:54:GLU:OE2	1:A:139:THR:HG23	1.78	0.83
1:A:214:THR:CG2	1:A:229:ILE:HD13	2.07	0.83
1:B:53:LEU:O	1:B:139:THR:HG21	1.80	0.81
1:A:39:VAL:HG11	1:A:160:LEU:HD11	1.61	0.81
1:A:76:HIS:ND1	1:B:79:VAL:HA	1.97	0.80
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.45	0.80
1:B:95:LEU:HD12	1:B:99:ALA:HB3	1.64	0.80
1:B:100:ASP:OD1	1:B:101:PRO:HD2	1.82	0.80
1:A:79:VAL:HG22	1:B:76:HIS:HB3	1.64	0.79
1:B:54:GLU:HG3	1:B:114:TRP:HZ2	1.48	0.78
1:A:91:VAL:O	1:A:95:LEU:HB2	1.83	0.77
1:B:134:ASN:OD1	1:B:135:VAL:N	2.18	0.77
1:A:237:THR:OG1	1:A:239:VAL:HG23	1.84	0.77
1:B:201:PHE:HA	1:B:204:ILE:HD12	1.67	0.76
1:A:79:VAL:HG13	1:B:76:HIS:ND1	2.00	0.75
1:B:54:GLU:HG3	1:B:114:TRP:CZ2	2.22	0.74
1:A:114:TRP:CZ3	1:A:135:VAL:HG21	2.23	0.73
1:A:265:ILE:O	1:A:269:LEU:HB2	1.88	0.72
1:A:214:THR:HB	1:A:229:ILE:CD1	2.17	0.72
1:A:274:SER:O	1:A:278:THR:HG23	1.90	0.72
1:B:54:GLU:HB3	1:B:114:TRP:CE2	2.25	0.71
1:B:123:SER:HA	1:B:126:ILE:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLN:O	1:B:261:VAL:HG12	1.90	0.71
1:B:54:GLU:CB	1:B:114:TRP:HZ2	2.01	0.71
1:B:54:GLU:CG	1:B:114:TRP:HZ2	2.04	0.70
1:A:36:LEU:HA	1:A:160:LEU:HD21	1.72	0.70
1:A:130:ILE:HG22	1:A:240:GLY:HA3	1.73	0.70
1:A:35:LEU:O	1:A:39:VAL:HG23	1.91	0.70
1:B:134:ASN:HD22	1:B:245:VAL:HG11	1.56	0.70
1:B:154:ILE:N	1:B:155:PRO:HD2	2.06	0.70
1:A:37:ALA:O	1:A:41:LEU:HG	1.92	0.70
1:A:73:LEU:O	1:A:76:HIS:CD2	2.45	0.69
1:B:88:ILE:O	1:B:91:VAL:HG12	1.93	0.69
1:B:127:ILE:HA	1:B:154:ILE:HG12	1.75	0.69
1:B:114:TRP:CG	1:B:114:TRP:O	2.46	0.69
1:B:212:THR:HB	1:B:213:PRO:HD3	1.73	0.69
1:A:214:THR:HG21	1:A:229:ILE:HD13	1.73	0.69
1:A:258:GLN:HB2	1:A:259:PRO:HD3	1.75	0.69
1:A:28:ARG:HB2	1:A:31:THR:OG1	1.93	0.68
1:A:147:ILE:HG23	1:B:233:ILE:HD12	1.75	0.68
1:B:54:GLU:CG	1:B:114:TRP:CZ2	2.76	0.68
1:B:76:HIS:N	1:B:77:PRO:HD3	2.08	0.68
1:A:147:ILE:HG12	1:B:233:ILE:HD12	1.75	0.68
1:A:154:ILE:HB	1:A:155:PRO:HD3	1.74	0.68
1:B:249:ASP:OD1	1:B:250:PRO:HD2	1.93	0.67
1:B:138:ARG:HH11	1:B:138:ARG:HG2	1.58	0.66
1:A:84:LEU:HA	1:A:87:LEU:HD12	1.77	0.66
1:A:95:LEU:HA	1:A:99:ALA:HB3	1.77	0.66
1:B:54:GLU:HB3	1:B:114:TRP:CZ2	2.30	0.66
1:B:228:ALA:O	1:B:232:VAL:HG23	1.96	0.66
1:A:258:GLN:O	1:A:261:VAL:HG22	1.95	0.66
1:A:49:VAL:HG11	1:A:145:PHE:CE1	2.32	0.65
1:B:279:ILE:HD12	1:B:283:LEU:HD12	1.79	0.65
1:B:35:LEU:HB3	1:B:160:LEU:HD21	1.78	0.64
1:B:205:GLY:HA3	1:B:271:TYR:CZ	2.32	0.64
1:A:95:LEU:HA	1:A:99:ALA:CB	2.27	0.64
1:B:86:LEU:O	1:B:90:GLU:HB2	1.97	0.64
1:A:285:VAL:HA	1:A:288:ARG:HD3	1.79	0.64
1:B:167:ARG:HA	1:B:167:ARG:HH11	1.63	0.64
1:B:233:ILE:O	1:B:237:THR:HG23	1.97	0.64
1:A:154:ILE:HD13	1:B:237:THR:HB	1.80	0.64
1:A:210:VAL:O	1:A:214:THR:HG23	1.97	0.64
1:B:204:ILE:O	1:B:208:LEU:HG	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:TRP:O	1:A:114:TRP:CD1	2.52	0.62
1:B:49:VAL:O	1:B:53:LEU:HB2	1.99	0.62
1:B:139:THR:O	1:B:143:ARG:HG3	1.99	0.62
1:B:138:ARG:CG	1:B:138:ARG:NH1	2.51	0.62
1:A:100:ASP:HB2	1:A:101:PRO:HD2	1.80	0.62
1:B:54:GLU:CB	1:B:114:TRP:CE2	2.82	0.62
1:B:54:GLU:HB2	1:B:114:TRP:CZ2	2.33	0.61
1:A:39:VAL:HG11	1:A:160:LEU:CD1	2.31	0.61
1:A:32:LEU:HD12	1:A:33:LEU:HD23	1.83	0.61
1:B:58:GLU:HG2	1:B:114:TRP:HB3	1.83	0.61
1:A:86:LEU:HD12	1:A:87:LEU:N	2.14	0.61
1:A:128:THR:HG21	1:A:265:ILE:HD11	1.81	0.60
1:A:266:LEU:HD23	1:A:267:LEU:HD23	1.83	0.60
1:A:261:VAL:O	1:A:265:ILE:HG23	2.01	0.60
1:A:262:TRP:O	1:A:265:ILE:HG12	2.02	0.60
1:B:54:GLU:HB3	1:B:114:TRP:NE1	2.17	0.60
1:A:272:PHE:O	1:A:275:VAL:HG22	2.02	0.59
1:B:200:LEU:HD12	1:B:201:PHE:N	2.17	0.59
1:A:147:ILE:HG23	1:B:233:ILE:CD1	2.33	0.59
1:A:221:GLU:CD	1:A:246:ALA:O	2.41	0.58
1:A:32:LEU:CD1	1:A:33:LEU:HD23	2.33	0.58
1:A:233:ILE:CD1	1:B:147:ILE:HG23	2.34	0.58
1:B:259:PRO:O	1:B:263:PHE:HB3	2.03	0.58
1:A:69:ARG:HG3	1:B:88:ILE:HD11	1.84	0.58
1:B:70:GLU:HA	1:B:73:LEU:HB3	1.84	0.58
1:A:64:GLU:O	1:A:68:VAL:HG23	2.03	0.58
1:A:53:LEU:O	1:A:139:THR:HG21	2.04	0.57
1:B:79:VAL:HG12	1:B:79:VAL:O	2.03	0.57
1:B:43:LEU:HD21	1:B:262:TRP:CH2	2.39	0.57
1:B:41:LEU:O	1:B:45:SER:N	2.35	0.57
1:B:114:TRP:O	1:B:114:TRP:CD1	2.58	0.57
1:A:203:LEU:O	1:A:207:LEU:HG	2.05	0.57
1:B:100:ASP:CG	1:B:101:PRO:HD2	2.25	0.57
1:B:54:GLU:CB	1:B:114:TRP:NE1	2.68	0.57
1:B:123:SER:O	1:B:126:ILE:HB	2.04	0.57
1:A:88:ILE:HD12	1:B:69:ARG:NH1	2.20	0.56
1:A:265:ILE:HG13	1:A:266:LEU:N	2.19	0.56
1:B:138:ARG:HG3	1:B:138:ARG:NH1	2.19	0.56
1:B:54:GLU:OE2	1:B:139:THR:HG23	2.06	0.56
1:A:221:GLU:OE2	1:A:246:ALA:O	2.24	0.56
1:A:271:TYR:CE2	1:A:275:VAL:HG11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:VAL:CG1	1:B:241:PHE:H	2.19	0.56
1:A:51:ARG:O	1:A:55:GLN:HB2	2.07	0.55
1:B:35:LEU:CB	1:B:160:LEU:HD21	2.37	0.55
1:B:67:GLU:HG3	1:B:68:VAL:N	2.21	0.55
1:A:140:ASP:HA	1:A:143:ARG:HD3	1.89	0.55
1:B:36:LEU:O	1:B:40:LEU:HB2	2.07	0.55
1:B:44:VAL:O	1:B:48:LEU:HG	2.05	0.55
1:B:48:LEU:HD23	1:B:116:LEU:HD22	1.88	0.55
1:A:76:HIS:N	1:A:77:PRO:HD3	2.22	0.55
1:B:137:LEU:HD13	1:B:143:ARG:HA	1.89	0.55
1:A:180:GLU:HB2	1:A:193:VAL:HG11	1.89	0.54
1:B:43:LEU:HD11	1:B:127:ILE:CD1	2.38	0.54
1:A:85:GLY:HA2	1:B:69:ARG:HH12	1.72	0.54
1:A:55:GLN:N	1:A:56:PRO:HD2	2.23	0.54
1:B:53:LEU:HD13	1:B:142:GLY:HA2	1.90	0.54
1:B:49:VAL:HG12	1:B:53:LEU:HD12	1.90	0.54
1:B:121:PHE:O	1:B:125:THR:HG23	2.07	0.54
1:B:138:ARG:N	1:B:138:ARG:HD2	2.23	0.54
1:B:203:LEU:O	1:B:207:LEU:HG	2.08	0.54
1:A:212:THR:O	1:A:216:VAL:HG23	2.07	0.54
1:A:214:THR:CB	1:A:229:ILE:CD1	2.75	0.54
1:B:124:GLY:O	1:B:128:THR:HG23	2.08	0.53
1:A:212:THR:HB	1:A:213:PRO:HD3	1.89	0.53
1:B:206:CYS:HA	1:B:210:VAL:HB	1.89	0.53
1:A:49:VAL:O	1:A:53:LEU:HB2	2.09	0.53
1:B:137:LEU:C	1:B:138:ARG:HD2	2.29	0.53
1:A:88:ILE:HA	1:A:91:VAL:HG12	1.90	0.53
1:B:54:GLU:CB	1:B:114:TRP:HE1	2.21	0.53
1:A:233:ILE:O	1:A:237:THR:HG23	2.08	0.53
1:A:45:SER:O	1:A:49:VAL:HG23	2.09	0.52
1:A:114:TRP:O	1:A:114:TRP:CG	2.61	0.52
1:A:134:ASN:OD1	1:A:135:VAL:HG12	2.09	0.52
1:A:76:HIS:CE1	1:B:79:VAL:HG13	2.45	0.52
1:A:114:TRP:CE3	1:A:135:VAL:HG21	2.45	0.52
1:A:178:HIS:O	1:A:182:ILE:HG12	2.10	0.52
1:A:233:ILE:HD13	1:B:147:ILE:HG23	1.91	0.52
1:B:144:LEU:HA	1:B:147:ILE:HD12	1.91	0.52
1:A:128:THR:HG21	1:A:265:ILE:CD1	2.40	0.52
1:A:221:GLU:CD	1:A:246:ALA:HA	2.30	0.51
1:B:28:ARG:H	1:B:28:ARG:HD3	1.75	0.51
1:A:35:LEU:O	1:A:38:LEU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:O	1:A:42:TYR:HB3	2.11	0.51
1:A:245:VAL:CG1	1:A:248:ALA:HB3	2.41	0.51
1:A:247:GLY:HA3	1:A:258:GLN:HG2	1.92	0.51
1:B:214:THR:HA	1:B:228:ALA:HB1	1.93	0.51
1:A:79:VAL:HG12	1:A:79:VAL:O	2.11	0.51
1:A:246:ALA:O	1:A:257:TYR:OH	2.23	0.51
1:A:214:THR:HG22	1:A:229:ILE:HA	1.93	0.50
1:A:147:ILE:HG22	1:A:148:PHE:CD2	2.46	0.50
1:A:164:VAL:O	1:A:168:LEU:HB3	2.12	0.49
1:A:86:LEU:HD12	1:A:87:LEU:H	1.77	0.49
1:B:54:GLU:CD	1:B:139:THR:HG23	2.32	0.49
1:B:200:LEU:O	1:B:204:ILE:HG13	2.12	0.49
1:A:59:GLN:OE1	1:A:61:ALA:HB2	2.12	0.49
1:A:53:LEU:HD11	1:A:141:ALA:HB3	1.93	0.49
1:A:32:LEU:HA	1:A:35:LEU:HB3	1.94	0.49
1:A:225:LYS:O	1:A:229:ILE:HG12	2.12	0.49
1:B:54:GLU:HB2	1:B:114:TRP:HZ2	1.71	0.49
1:B:43:LEU:HD11	1:B:127:ILE:HD13	1.94	0.49
1:A:143:ARG:HB3	1:B:226:LEU:HD21	1.95	0.49
1:A:114:TRP:CZ3	1:A:135:VAL:CG2	2.93	0.48
1:A:271:TYR:CD2	1:A:271:TYR:C	2.86	0.48
1:A:276:LEU:HD23	1:A:279:ILE:HD11	1.93	0.48
1:A:236:LEU:C	1:A:238:THR:H	2.15	0.48
1:A:257:TYR:O	1:A:261:VAL:HG13	2.14	0.48
1:B:35:LEU:O	1:B:39:VAL:N	2.43	0.48
1:B:236:LEU:C	1:B:238:THR:H	2.17	0.48
1:A:80:SER:OG	1:A:83:GLU:HG3	2.13	0.48
1:A:101:PRO:HG2	1:A:104:GLN:HG2	1.94	0.48
1:A:239:VAL:HG12	1:B:131:GLY:HA3	1.94	0.48
1:B:113:ALA:O	1:B:114:TRP:HB3	2.13	0.48
1:B:229:ILE:O	1:B:233:ILE:HG13	2.14	0.48
1:A:151:LEU:HD11	1:B:233:ILE:HD13	1.96	0.48
1:A:75:ALA:C	1:A:77:PRO:HD3	2.34	0.47
1:A:195:VAL:O	1:A:199:MET:HG2	2.14	0.47
1:A:231:PHE:HE1	1:A:245:VAL:HA	1.80	0.47
1:B:76:HIS:N	1:B:77:PRO:CD	2.76	0.47
1:B:127:ILE:C	1:B:129:THR:H	2.16	0.47
1:A:127:ILE:HD12	1:A:157:PHE:CD1	2.49	0.47
1:A:167:ARG:HA	1:A:167:ARG:NE	2.29	0.47
1:B:135:VAL:HG13	1:B:135:VAL:O	2.14	0.47
1:B:265:ILE:O	1:B:269:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD23	1:A:226:LEU:C	2.35	0.47
1:B:127:ILE:HG22	1:B:154:ILE:HA	1.95	0.47
1:A:72:PHE:CE1	1:A:87:LEU:HD11	2.50	0.47
1:B:55:GLN:HA	1:B:58:GLU:HB3	1.97	0.46
1:A:94:ALA:O	1:A:99:ALA:HB2	2.16	0.46
1:B:149:TYR:O	1:B:153:GLY:HA3	2.16	0.46
1:A:160:LEU:O	1:A:164:VAL:HG23	2.16	0.46
1:B:129:THR:HG22	1:B:154:ILE:HD13	1.96	0.46
1:A:70:GLU:CD	1:A:74:ARG:HE	2.18	0.46
1:A:100:ASP:C	1:A:102:GLU:H	2.19	0.46
1:B:28:ARG:HD3	1:B:28:ARG:N	2.29	0.46
1:B:140:ASP:HA	1:B:143:ARG:HD2	1.97	0.46
1:B:195:VAL:O	1:B:199:MET:HG2	2.16	0.46
1:A:235:THR:HG21	1:A:264:TRP:CZ3	2.51	0.46
1:A:127:ILE:HG13	1:A:128:THR:N	2.30	0.46
1:A:256:ALA:O	1:A:259:PRO:HD2	2.16	0.46
1:A:233:ILE:HD12	1:B:147:ILE:HG23	1.99	0.45
1:B:154:ILE:N	1:B:155:PRO:CD	2.77	0.45
1:B:261:VAL:O	1:B:264:TRP:HB3	2.16	0.45
1:A:49:VAL:HG11	1:A:145:PHE:CD1	2.51	0.45
1:B:199:MET:O	1:B:203:LEU:HG	2.16	0.45
1:A:154:ILE:CD1	1:B:237:THR:HB	2.45	0.45
1:A:220:MET:HE3	1:A:257:TYR:HE1	1.81	0.45
1:A:209:PHE:CE1	1:A:267:LEU:HB3	2.52	0.45
1:B:164:VAL:O	1:B:168:LEU:HG	2.18	0.44
1:B:75:ALA:C	1:B:77:PRO:HD3	2.38	0.44
1:A:28:ARG:HD2	1:A:31:THR:OG1	2.17	0.44
1:B:138:ARG:HG2	1:B:138:ARG:NH1	2.24	0.44
1:A:216:VAL:HG12	1:A:220:MET:HE2	2.00	0.43
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.73	0.43
1:A:245:VAL:HG11	1:A:248:ALA:HB3	2.00	0.43
1:A:240:GLY:O	1:A:241:PHE:C	2.53	0.43
1:A:253:ASP:O	1:A:255:PRO:HD3	2.18	0.43
1:B:214:THR:CG2	1:B:229:ILE:HD13	2.37	0.43
1:A:95:LEU:HD13	1:B:95:LEU:HD23	2.00	0.43
1:A:157:PHE:O	1:A:160:LEU:N	2.51	0.43
1:A:271:TYR:CZ	1:A:275:VAL:HG11	2.53	0.43
1:A:186:TRP:O	1:A:187:HIS:CB	2.66	0.43
1:A:214:THR:HG21	1:A:229:ILE:CD1	2.46	0.43
1:A:200:LEU:CD2	1:A:204:ILE:HD11	2.49	0.43
1:A:85:GLY:CA	1:B:69:ARG:HH22	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:CD2	1:A:272:PHE:N	2.87	0.43
1:B:55:GLN:HB3	1:B:56:PRO:HD3	2.01	0.43
1:B:236:LEU:O	1:B:238:THR:HG23	2.19	0.43
1:A:123:SER:O	1:A:126:ILE:HB	2.19	0.42
1:A:276:LEU:O	1:A:279:ILE:HG13	2.19	0.42
1:A:39:VAL:CG1	1:A:160:LEU:HD11	2.40	0.42
1:B:62:GLN:OE1	1:B:100:ASP:HB2	2.19	0.42
1:B:128:THR:HG22	1:B:157:PHE:CZ	2.55	0.42
1:B:243:ASP:OD1	1:B:243:ASP:N	2.51	0.42
1:B:127:ILE:C	1:B:129:THR:N	2.72	0.42
1:A:130:ILE:H	1:A:130:ILE:HG13	1.48	0.42
1:A:271:TYR:HD2	1:A:272:PHE:HD2	1.68	0.42
1:B:32:LEU:HD22	1:B:163:GLY:CA	2.49	0.42
1:A:86:LEU:HD13	1:A:90:GLU:OE2	2.19	0.42
1:B:67:GLU:HG3	1:B:68:VAL:H	1.83	0.42
1:B:36:LEU:O	1:B:36:LEU:HD23	2.19	0.42
1:B:163:GLY:O	1:B:167:ARG:HG2	2.20	0.42
1:B:172:LEU:O	1:B:176:ILE:HB	2.20	0.41
1:B:35:LEU:HA	1:B:38:LEU:HB3	2.02	0.41
1:A:88:ILE:HD12	1:B:69:ARG:HH11	1.85	0.41
1:B:54:GLU:HB2	1:B:114:TRP:HE1	1.82	0.41
1:B:96:GLY:O	1:B:138:ARG:NH1	2.52	0.41
1:B:214:THR:HG22	1:B:232:VAL:HG21	2.01	0.41
1:B:210:VAL:O	1:B:214:THR:HG23	2.21	0.41
1:B:137:LEU:HD11	1:B:146:CYS:HB2	2.01	0.41
1:A:91:VAL:HG11	1:B:91:VAL:HG11	2.01	0.41
1:B:128:THR:OG1	1:B:130:ILE:HG13	2.21	0.41
1:B:156:LEU:O	1:B:159:ILE:HB	2.21	0.41
1:B:236:LEU:C	1:B:238:THR:N	2.74	0.41
1:A:221:GLU:OE1	1:A:246:ALA:CA	2.59	0.41
1:A:226:LEU:HD23	1:A:227:GLU:N	2.36	0.41
1:B:54:GLU:HB2	1:B:114:TRP:NE1	2.36	0.41
1:B:102:GLU:O	1:B:103:THR:HB	2.20	0.41
1:B:201:PHE:O	1:B:204:ILE:HB	2.21	0.41
1:A:245:VAL:HG13	1:A:248:ALA:HB3	2.03	0.41
1:B:232:VAL:O	1:B:235:THR:HB	2.20	0.40
1:B:43:LEU:HD11	1:B:127:ILE:HD11	2.03	0.40
1:B:102:GLU:O	1:B:103:THR:CB	2.67	0.40
1:B:207:LEU:O	1:B:212:THR:OG1	2.39	0.40
1:B:260:LEU:O	1:B:263:PHE:HD2	2.04	0.40
1:A:134:ASN:ND2	1:A:245:VAL:HG11	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TYR:HD2	1:A:272:PHE:N	2.19	0.40
1:B:124:GLY:O	1:B:127:ILE:HG13	2.22	0.40
1:A:265:ILE:O	1:A:269:LEU:CB	2.66	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	A	253/309 (82%)	225 (89%)	26 (10%)	2 (1%)	19	51
1	B	238/309 (77%)	218 (92%)	16 (7%)	4 (2%)	9	36
All	All	491/618 (79%)	443 (90%)	42 (9%)	6 (1%)	13	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ILE
1	B	114	TRP
1	B	133	GLY
1	A	115	ASP
1	B	103	THR
1	B	79	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	A	192/248 (77%)	174 (91%)	18 (9%)	8	31
1	B	176/248 (71%)	162 (92%)	14 (8%)	12	38
All	All	368/496 (74%)	336 (91%)	32 (9%)	10	35

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	38	LEU
1	A	70	GLU
1	A	86	LEU
1	A	130	ILE
1	A	140	ASP
1	A	144	LEU
1	A	146	CYS
1	A	156	LEU
1	A	168	LEU
1	A	206	CYS
1	A	208	LEU
1	A	257	TYR
1	A	260	LEU
1	A	267	LEU
1	A	272	PHE
1	A	276	LEU
1	A	288	ARG
1	B	28	ARG
1	B	53	LEU
1	B	78	CYS
1	B	83	GLU
1	B	87	LEU
1	B	93	ASP
1	B	138	ARG
1	B	241	PHE
1	B	249	ASP
1	B	257	TYR
1	B	263	PHE
1	B	266	LEU
1	B	279	ILE
1	B	283	LEU

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

Mol	Chain	Res	Type
1	A	60	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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 [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	259/309 (83%)	-0.24	5 (1%) 66 65	69, 157, 249, 297	0
1	B	244/309 (78%)	0.05	15 (6%) 21 21	72, 184, 299, 365	0
All	All	503/618 (81%)	-0.10	20 (3%) 38 37	69, 173, 286, 365	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	SER	5.2
1	B	256	ALA	4.7
1	B	249	ASP	3.4
1	A	106	THR	3.2
1	B	248	ALA	3.2
1	B	283	LEU	3.1
1	B	116	LEU	3.1
1	A	250	PRO	2.9
1	A	27	MET	2.9
1	B	250	PRO	2.9
1	B	194	ARG	2.9
1	B	289	ARG	2.9
1	B	284	ARG	2.8
1	B	286	VAL	2.7
1	B	254	SER	2.6
1	A	134	ASN	2.3
1	B	255	PRO	2.2
1	B	285	VAL	2.1
1	B	29	SER	2.1
1	A	190	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 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
2	K	A	310	1/1	0.83	1.11	133,133,133,133	0
2	K	A	314	1/1	0.93	0.28	21,21,21,21	0
2	K	A	311	1/1	0.97	0.06	30,30,30,30	0
2	K	A	313	1/1	0.98	0.21	21,21,21,21	0
2	K	A	312	1/1	0.99	0.17	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.