



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:07 am BST

PDB ID : 4I9W  
Title : Human two pore domain K<sup>+</sup> channel TRAAK (K2P4.1) - Fab complex structure  
Authors : Brohawn, S.G.; Mackinnon, R.  
Deposited on : 2012-12-05  
Resolution : 2.75 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.

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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)	:	1.13
EDS	:	2.11
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)	:	2.11

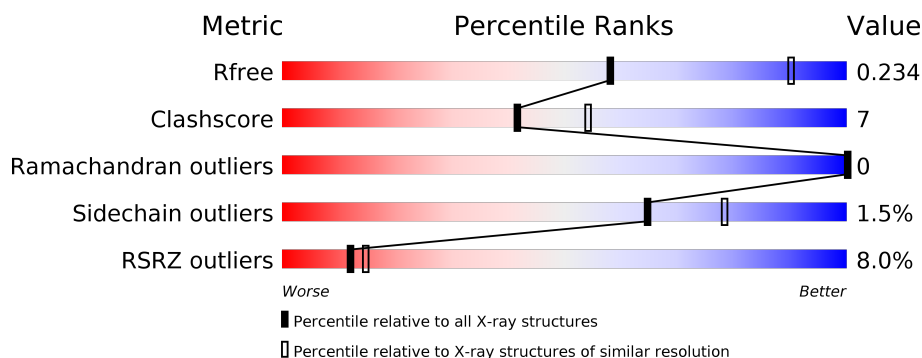
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>9%</div> <div>65% 17% 18%</div> </div>
1	B	309	<div> <div>17%</div> <div>68% 14% 18%</div> </div>
2	D	211	<div> <div>%</div> <div>86% 13% .</div> </div>
2	F	211	<div> <div>9%</div> <div>87% 11% .</div> </div>
3	E	217	<div> <div>2%</div> <div>83% 13% .</div> </div>
3	G	217	<div> <div>%</div> <div>84% 12% .</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10544 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
1	A	253	Total	C	N	O	S	0	0	0
			1963	1299	318	340	6			
1	B	253	Total	C	N	O	S	0	0	0
			1970	1300	321	343	6			

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 a protein called ANTIBODY FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	211	Total	C	N	O	S	0	0	0
			1616	1003	271	333	9			
2	F	211	Total	C	N	O	S	0	0	0
			1616	1003	271	333	9			

- Molecule 3 is a protein called ANTIBODY FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	211	Total	C	N	O	S	0	0	0
			1614	1026	261	319	8			
3	G	210	Total	C	N	O	S	0	0	0
			1605	1022	260	315	8			

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	K	0	0
			3	3		
4	A	2	Total	K	0	0
			2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total	O	0	0
			17	17		
6	B	19	Total	O	0	0
			19	19		
6	D	20	Total	O	0	0
			20	20		
6	E	40	Total	O	0	0
			40	40		
6	F	27	Total	O	0	0
			27	27		

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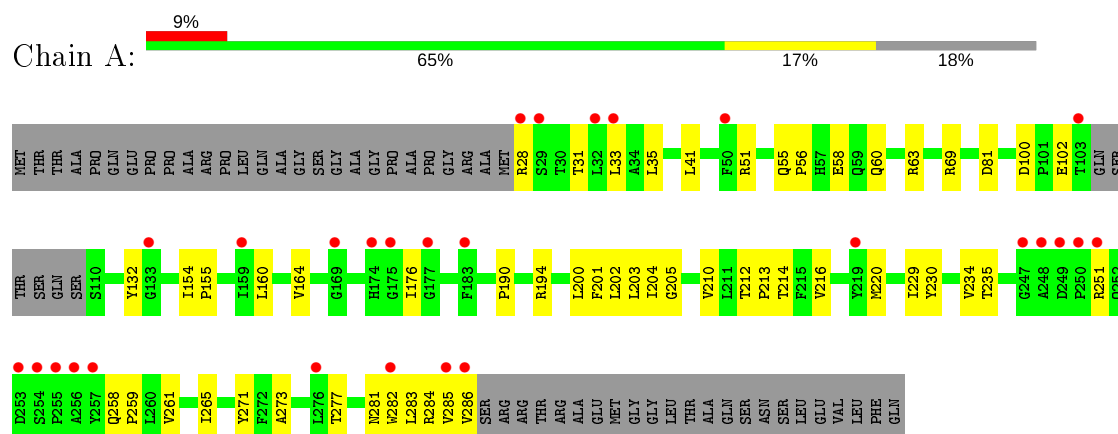
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	30	Total	O	0	0
			30	30		

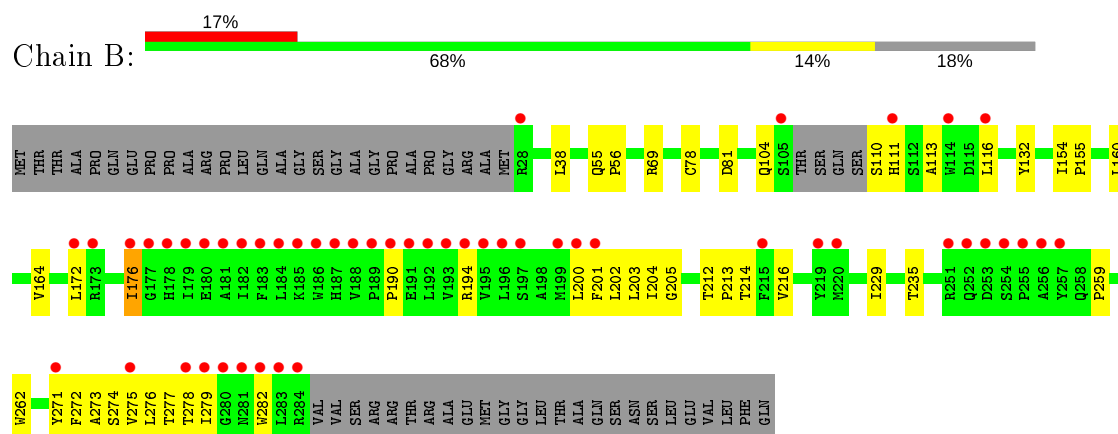
### 3 Residue-property plots [i](#)

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

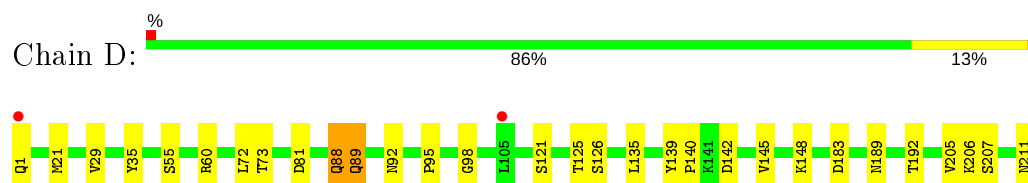
- Molecule 1: Potassium channel subfamily K member 4



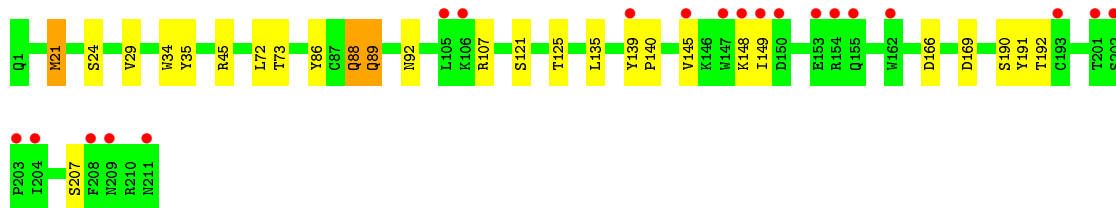
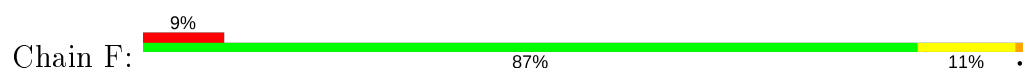
- Molecule 1: Potassium channel subfamily K member 4



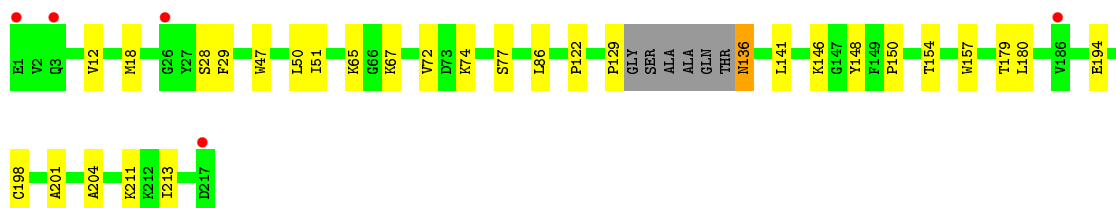
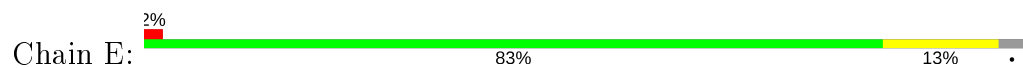
- Molecule 2: ANTIBODY FAB FRAGMENT LIGHT CHAIN



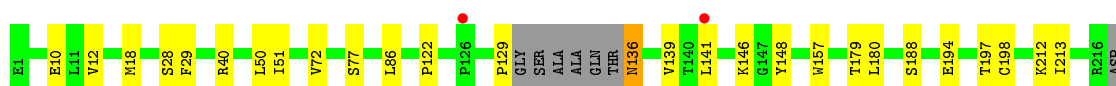
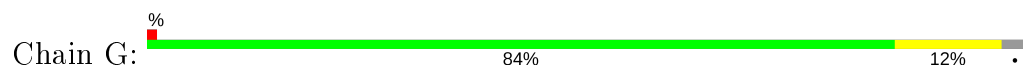
- Molecule 2: ANTIBODY FAB FRAGMENT LIGHT CHAIN



• Molecule 3: ANTIBODY FAB FRAGMENT HEAVY CHAIN



• Molecule 3: ANTIBODY FAB FRAGMENT HEAVY CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.89Å 138.91Å 97.46Å 90.00° 94.87° 90.00°	Depositor
Resolution (Å)	48.60 – 2.75 48.55 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.60-2.75) 99.3 (48.55-2.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.201 , 0.236 0.199 , 0.234	Depositor DCC
$R_{free}$ test set	2797 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.7	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 66.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	0/2013	0.47	0/2745
1	B	0.36	0/2021	0.48	1/2754 (0.0%)
2	D	0.41	0/1655	0.54	0/2247
2	F	0.42	0/1655	0.54	0/2247
3	E	0.47	0/1656	0.59	0/2260
3	G	0.47	0/1647	0.59	0/2249
All	All	0.42	0/10647	0.53	1/14502 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	78	CYS	CA-CB-SG	5.92	124.65	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	40	ARG	Peptide

## 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	1963	0	1985	36	0
1	B	1970	0	1988	29	0
2	D	1616	0	1542	21	0
2	F	1616	0	1542	21	0
3	E	1614	0	1586	21	1
3	G	1605	0	1582	22	1
4	A	2	0	0	0	0
4	B	3	0	0	0	0
5	A	1	0	0	0	0
5	G	1	0	0	0	0
6	A	17	0	0	1	0
6	B	19	0	0	1	0
6	D	20	0	0	2	0
6	E	40	0	0	2	0
6	F	27	0	0	3	0
6	G	30	0	0	3	0
All	All	10544	0	10225	145	1

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 7.

All (145) 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:F:35:TYR:HE1	2:F:88:GLN:HG2	1.33	0.93
3:G:197:THR:HG22	3:G:212:LYS:HA	1.57	0.86
2:D:35:TYR:HE2	2:D:88:GLN:HG2	1.43	0.83
1:A:60:GLN:OE1	1:A:63:ARG:NH2	2.12	0.81
2:F:35:TYR:CE1	2:F:88:GLN:HG2	2.19	0.77
1:A:282:TRP:O	1:A:286:VAL:HG23	1.84	0.77
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.67	0.76
1:A:281:ASN:OD1	1:A:284:ARG:NH2	2.18	0.75
2:D:189:ASN:ND2	2:D:211:ASN:OD1	2.17	0.75
1:B:212:THR:HB	1:B:213:PRO:HD3	1.70	0.73
1:A:212:THR:HB	1:A:213:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:98:GLY:O	6:D:320:HOH:O	2.06	0.72
2:F:72:LEU:HD23	2:F:73:THR:N	2.03	0.72
3:E:51:ILE:HD13	3:E:72:VAL:HG13	1.73	0.70
1:A:58:GLU:OE2	1:B:113:ALA:N	2.26	0.69
2:D:72:LEU:HD23	2:D:73:THR:N	2.07	0.69
1:B:273:ALA:O	1:B:277:THR:HG23	1.92	0.68
1:B:69:ARG:NH1	1:B:81:ASP:OD1	2.25	0.68
2:D:35:TYR:CE2	2:D:88:GLN:HG2	2.28	0.67
3:G:51:ILE:HD13	3:G:72:VAL:HG13	1.75	0.67
1:A:282:TRP:CZ3	1:A:286:VAL:HG21	2.30	0.66
3:G:197:THR:HG22	3:G:212:LYS:CA	2.28	0.63
3:E:157:TRP:CZ3	3:E:198:CYS:HB3	2.33	0.63
1:B:274:SER:O	1:B:278:THR:HG23	1.98	0.63
1:A:220:MET:O	1:A:251:ARG:NH2	2.32	0.63
3:G:194:GLU:HG2	6:G:425:HOH:O	1.98	0.62
2:D:89:GLN:HE21	2:D:92:ASN:H	1.48	0.61
1:B:172:LEU:O	1:B:176:ILE:HD12	2.00	0.61
3:G:157:TRP:CZ3	3:G:198:CYS:HB3	2.36	0.61
1:B:278:THR:O	1:B:282:TRP:CD1	2.54	0.60
2:F:107:ARG:HB2	6:F:323:HOH:O	2.01	0.59
3:G:180:LEU:C	3:G:180:LEU:HD12	2.22	0.59
2:F:148:LYS:HB2	2:F:192:THR:OG1	2.02	0.59
1:B:190:PRO:O	1:B:194:ARG:HG2	2.02	0.59
2:D:121:SER:O	2:D:125:THR:HG23	2.03	0.59
2:D:148:LYS:HB2	2:D:192:THR:OG1	2.03	0.59
2:F:166:ASP:HB3	2:F:169:ASP:OD2	2.03	0.59
3:E:180:LEU:C	3:E:180:LEU:HD12	2.24	0.58
2:F:121:SER:O	2:F:125:THR:HG23	2.03	0.58
1:B:212:THR:O	1:B:216:VAL:HG23	2.03	0.58
2:F:192:THR:HG22	2:F:207:SER:OG	2.04	0.58
1:B:38:LEU:HD23	1:B:38:LEU:C	2.25	0.57
3:G:198:CYS:C	6:G:426:HOH:O	2.42	0.57
2:D:192:THR:HG22	2:D:207:SER:OG	2.04	0.57
3:E:129:PRO:HD3	3:E:141:LEU:HD23	1.87	0.57
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.85	0.57
1:A:212:THR:O	1:A:216:VAL:HG23	2.05	0.57
3:G:12:VAL:HG21	3:G:86:LEU:HD12	1.85	0.57
3:G:146:LYS:HB3	3:G:179:THR:HG23	1.87	0.56
2:F:89:GLN:HE21	2:F:92:ASN:H	1.52	0.56
1:A:154:ILE:N	1:A:155:PRO:HD2	2.20	0.56
3:G:129:PRO:HD3	3:G:141:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HA	1:B:271:TYR:OH	2.05	0.56
3:E:146:LYS:HB3	3:E:179:THR:HG23	1.86	0.56
3:G:141:LEU:HD22	3:G:213:ILE:HG21	1.88	0.55
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.37	0.55
3:E:136:ASN:N	3:E:136:ASN:ND2	2.53	0.55
1:B:69:ARG:HD3	6:B:501:HOH:O	2.06	0.55
3:E:29:PHE:CD2	3:E:77:SER:HA	2.42	0.54
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.37	0.54
1:B:154:ILE:N	1:B:155:PRO:HD2	2.22	0.54
2:D:126:SER:OG	6:D:314:HOH:O	2.18	0.54
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.40	0.54
3:E:136:ASN:HD22	3:E:136:ASN:N	2.05	0.54
2:D:1:GLN:HA	2:D:1:GLN:OE1	2.08	0.54
3:E:141:LEU:HD22	3:E:213:ILE:HG21	1.89	0.54
1:B:202:LEU:HD12	1:B:203:LEU:N	2.24	0.53
3:E:154:THR:OG1	3:E:201:ALA:HB3	2.08	0.52
1:A:200:LEU:O	1:A:204:ILE:HG22	2.09	0.52
1:A:69:ARG:HD2	6:A:502:HOH:O	2.10	0.52
1:B:110:SER:O	1:B:111:HIS:HB3	2.09	0.52
3:G:139:VAL:CG2	3:G:188:SER:HB3	2.39	0.52
1:A:202:LEU:HD12	1:A:203:LEU:N	2.26	0.51
1:A:55:GLN:N	1:A:56:PRO:CD	2.74	0.51
3:G:136:ASN:ND2	3:G:136:ASN:N	2.59	0.51
3:G:197:THR:HG23	6:G:430:HOH:O	2.11	0.51
1:A:69:ARG:NH1	1:A:81:ASP:OD2	2.44	0.50
1:B:55:GLN:N	1:B:56:PRO:CD	2.75	0.50
3:E:122:PRO:HB3	3:E:148:TYR:HB3	1.94	0.50
3:G:50:LEU:C	3:G:50:LEU:HD12	2.31	0.50
2:F:29:VAL:HG21	2:F:89:GLN:HG3	1.94	0.50
1:A:261:VAL:O	1:A:265:ILE:HG13	2.12	0.49
1:A:190:PRO:O	1:A:194:ARG:HG2	2.12	0.49
2:D:192:THR:HG22	2:D:207:SER:CB	2.43	0.49
3:G:122:PRO:HB3	3:G:148:TYR:HB3	1.94	0.49
1:A:132:TYR:OH	1:A:235:THR:HG23	2.13	0.49
1:A:281:ASN:O	1:A:285:VAL:HG23	2.13	0.49
2:D:211:ASN:OD1	2:D:211:ASN:N	2.34	0.49
1:B:272:PHE:O	1:B:276:LEU:HG	2.13	0.48
2:F:192:THR:HG22	2:F:207:SER:CB	2.43	0.48
3:G:136:ASN:HD22	3:G:136:ASN:N	2.10	0.48
1:B:160:LEU:O	1:B:164:VAL:HG23	2.13	0.48
3:G:29:PHE:CD1	3:G:77:SER:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:O	1:A:164:VAL:HG23	2.13	0.48
2:D:139:TYR:CG	2:D:140:PRO:HA	2.48	0.48
3:E:50:LEU:HD12	3:E:50:LEU:C	2.34	0.48
3:G:29:PHE:HB2	3:G:77:SER:HB2	1.96	0.48
1:B:259:PRO:O	1:B:262:TRP:HB3	2.14	0.47
1:B:69:ARG:NH1	1:B:69:ARG:HB3	2.29	0.47
2:F:139:TYR:CG	2:F:140:PRO:HA	2.49	0.47
3:E:211:LYS:NZ	6:E:319:HOH:O	2.47	0.46
1:B:132:TYR:OH	1:B:235:THR:HG23	2.15	0.46
2:F:135:LEU:HD21	2:F:145:VAL:HG22	1.97	0.46
3:G:139:VAL:HG23	3:G:188:SER:HB3	1.98	0.46
1:B:200:LEU:O	1:B:204:ILE:HG22	2.15	0.46
1:B:278:THR:O	1:B:282:TRP:HD1	1.96	0.46
2:D:135:LEU:HD21	2:D:145:VAL:HG22	1.97	0.46
3:E:29:PHE:HB2	3:E:77:SER:HB2	1.97	0.45
1:B:275:VAL:O	1:B:279:ILE:HG13	2.16	0.45
2:F:149:ILE:HG13	2:F:149:ILE:O	2.17	0.45
1:A:258:GLN:N	1:A:259:PRO:HD2	2.31	0.45
1:A:55:GLN:N	1:A:56:PRO:HD2	2.32	0.45
2:F:72:LEU:HD23	2:F:73:THR:H	1.82	0.44
1:A:282:TRP:HE3	1:A:283:LEU:N	2.15	0.44
2:D:89:GLN:NE2	2:D:92:ASN:H	2.15	0.44
3:E:150:PRO:HD2	3:E:204:ALA:CB	2.48	0.44
1:A:28:ARG:HB2	1:A:31:THR:HG23	2.00	0.43
1:B:205:GLY:HA3	1:B:271:TYR:CZ	2.53	0.43
3:E:28:SER:HB3	3:G:28:SER:HB3	2.00	0.43
2:D:95:PRO:HG2	3:E:47:TRP:CG	2.54	0.43
1:A:273:ALA:O	1:A:277:THR:HG23	2.19	0.42
3:E:74:LYS:HE2	6:E:306:HOH:O	2.19	0.42
1:A:214:THR:HG21	1:A:229:ILE:HG12	2.00	0.42
1:A:282:TRP:CH2	1:A:286:VAL:HG21	2.54	0.42
1:A:51:ARG:HE	1:B:116:LEU:HD23	1.84	0.42
1:B:214:THR:HG21	1:B:229:ILE:HG12	2.02	0.42
1:A:69:ARG:CZ	1:B:104:GLN:HE21	2.33	0.41
1:A:100:ASP:O	1:A:102:GLU:HG2	2.20	0.41
1:B:201:PHE:C	1:B:201:PHE:CD2	2.93	0.41
2:D:205:VAL:O	2:D:206:LYS:HD3	2.20	0.41
2:F:149:ILE:HG22	2:F:191:TYR:CE2	2.55	0.41
1:A:35:LEU:HA	1:A:35:LEU:HD12	1.92	0.41
3:E:65:LYS:HB2	3:E:65:LYS:HE2	1.92	0.41
1:A:210:VAL:O	1:A:214:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:HD11	1:A:201:PHE:HA	2.03	0.41
1:A:33:LEU:HD23	1:A:33:LEU:O	2.21	0.41
2:D:88:GLN:HE21	2:D:88:GLN:HB2	1.71	0.40
2:F:29:VAL:CG2	2:F:89:GLN:HG3	2.50	0.40
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.93	0.40
2:F:72:LEU:HD23	2:F:72:LEU:C	2.42	0.40
1:A:230:TYR:O	1:A:234:VAL:HG23	2.22	0.40
2:F:21:MET:HB2	6:F:322:HOH:O	2.21	0.40
2:F:45:ARG:NE	6:F:303:HOH:O	2.55	0.40
1:A:205:GLY:HA3	1:A:271:TYR:CE1	2.55	0.40
2:F:34:TRP:HA	2:F:86:TYR:O	2.22	0.40

All (1) 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)
3:E:194:GLU:OE2	3:G:10:GLU:OE1[2_556]	2.13	0.07

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/309 (81%)	241 (97%)	8 (3%)	0	100	100
1	B	249/309 (81%)	242 (97%)	7 (3%)	0	100	100
2	D	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
2	F	209/211 (99%)	199 (95%)	10 (5%)	0	100	100
3	E	207/217 (95%)	201 (97%)	6 (3%)	0	100	100
3	G	206/217 (95%)	201 (98%)	5 (2%)	0	100	100
All	All	1329/1474 (90%)	1284 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/248 (82%)	204 (100%)	0	100	100
1	B	206/248 (83%)	205 (100%)	1 (0%)	88	92
2	D	184/184 (100%)	178 (97%)	6 (3%)	38	58
2	F	184/184 (100%)	179 (97%)	5 (3%)	44	65
3	E	187/190 (98%)	184 (98%)	3 (2%)	62	77
3	G	186/190 (98%)	184 (99%)	2 (1%)	73	84
All	All	1151/1244 (92%)	1134 (98%)	17 (2%)	65	78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	176	ILE
2	D	21	MET
2	D	55	SER
2	D	88	GLN
2	D	89	GLN
2	D	142	ASP
2	D	183	ASP
3	E	18	MET
3	E	67	LYS
3	E	136	ASN
2	F	21	MET
2	F	24	SER
2	F	88	GLN
2	F	89	GLN
2	F	190	SER
3	G	18	MET
3	G	136	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
2	D	88	GLN
2	F	88	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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	253/309 (81%)	0.64	28 (11%) <span>5</span> <span>6</span>	63, 129, 196, 260	0
1	B	253/309 (81%)	1.05	51 (20%) <span>1</span> <span>1</span>	59, 127, 257, 269	0
2	D	211/211 (100%)	0.06	2 (0%) <span>84</span> <span>89</span>	68, 96, 134, 160	0
2	F	211/211 (100%)	0.34	20 (9%) <span>8</span> <span>9</span>	57, 96, 188, 250	0
3	E	211/217 (97%)	0.12	5 (2%) <span>59</span> <span>68</span>	60, 82, 117, 178	0
3	G	210/217 (96%)	0.08	2 (0%) <span>82</span> <span>87</span>	57, 93, 141, 194	0
All	All	1349/1474 (91%)	0.41	108 (8%) <span>12</span> <span>15</span>	57, 98, 195, 269	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	ALA	7.9
1	B	192	LEU	7.8
1	B	176	ILE	7.7
1	B	189	PRO	7.6
1	B	184	LEU	7.3
1	B	279	ILE	6.9
1	B	183	PHE	6.3
1	B	179	ILE	6.2
2	F	201	THR	6.1
1	B	190	PRO	6.0
1	B	180	GLU	5.8
1	A	248	ALA	5.6
1	A	286	VAL	5.6
2	F	147	TRP	5.6
1	B	251	ARG	5.3
1	B	116	LEU	5.3
1	B	275	VAL	5.2
1	A	255	PRO	5.0
1	B	186	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	50	PHE	4.6
1	B	188	VAL	4.6
1	A	253	ASP	4.6
1	A	256	ALA	4.6
1	B	187	HIS	4.6
1	B	282	TRP	4.5
1	B	178	HIS	4.5
1	B	194	ARG	4.5
1	B	177	GLY	4.4
2	F	208	PHE	4.4
2	F	154	ARG	4.3
1	B	256	ALA	4.2
1	B	185	LYS	4.2
1	B	173	ARG	4.1
1	B	253	ASP	4.1
1	A	247	GLY	4.1
2	D	105	LEU	4.1
1	A	29	SER	4.1
3	E	217	ASP	4.0
1	A	257	TYR	4.0
1	B	283	LEU	4.0
1	B	193	VAL	3.9
1	B	201	PHE	3.9
2	F	145	VAL	3.8
2	F	155	GLN	3.8
1	B	281	ASN	3.8
1	B	196	LEU	3.8
1	B	252	GLN	3.8
1	B	114	TRP	3.8
1	B	191	GLU	3.7
1	A	254	SER	3.7
1	B	195	VAL	3.7
1	B	220	MET	3.7
1	B	199	MET	3.3
1	B	255	PRO	3.3
2	F	193	CYS	3.2
1	B	172	LEU	3.1
1	A	32	LEU	3.1
2	F	202	SER	3.1
1	A	282	TRP	3.1
1	B	215	PHE	3.1
1	A	219	TYR	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	200	LEU	3.0
1	B	182	ILE	2.9
2	F	203	PRO	2.8
3	E	186	VAL	2.8
1	B	254	SER	2.8
2	F	204	ILE	2.8
1	B	280	GLY	2.8
1	A	276	LEU	2.7
2	F	153	GLU	2.7
1	B	111	HIS	2.7
2	F	148	LYS	2.7
1	A	249	ASP	2.7
1	B	28	ARG	2.7
1	A	174	HIS	2.6
1	B	257	TYR	2.6
2	F	209	ASN	2.5
1	B	278	THR	2.5
1	A	28	ARG	2.5
1	B	197	SER	2.5
1	A	285	VAL	2.5
1	B	271	TYR	2.5
3	G	141	LEU	2.5
1	A	250	PRO	2.4
1	A	33	LEU	2.4
1	B	219	TYR	2.4
3	E	26	GLY	2.4
2	F	150	ASP	2.4
2	F	211	ASN	2.3
1	B	284	ARG	2.3
1	A	177	GLY	2.3
1	A	133	GLY	2.3
2	F	105	LEU	2.3
2	F	149	ILE	2.3
1	A	103	THR	2.2
1	A	169	GLY	2.2
1	A	175	GLY	2.2
2	D	1	GLN	2.2
1	A	183	PHE	2.2
1	A	251	ARG	2.2
2	F	139	TYR	2.2
2	F	106	LYS	2.1
2	F	162	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	1	GLU	2.1
3	G	126	PRO	2.1
1	B	105	SER	2.0
3	E	3	GLN	2.0
1	A	159	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	K	A	402	1/1	0.91	0.14	96,96,96,96	0
4	K	B	401	1/1	0.93	0.90	125,125,125,125	0
4	K	A	401	1/1	0.95	0.14	87,87,87,87	0
4	K	B	403	1/1	0.96	0.13	83,83,83,83	0
4	K	B	402	1/1	0.97	0.10	81,81,81,81	0
5	CA	A	403	1/1	0.97	0.10	104,104,104,104	0
5	CA	G	301	1/1	0.99	0.18	113,113,113,113	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.