



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:17 am BST

PDB ID : 4WFE  
Title : Human TRAAK K<sup>+</sup> channel in a K<sup>+</sup> bound conductive conformation  
Authors : Brohawn, S.G.; MacKinnon, R.  
Deposited on : 2014-09-15  
Resolution : 2.50 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

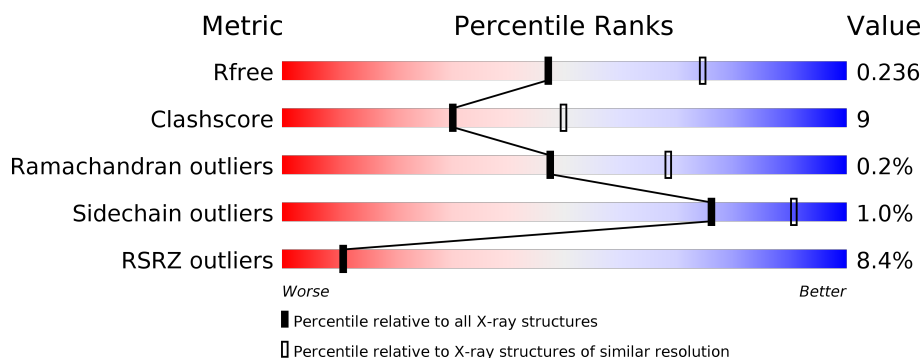
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	299	<div> <div>12%</div> <div>64%</div> <div>21%</div> <div>15%</div> </div>
1	B	299	<div> <div>20%</div> <div>65%</div> <div>21%</div> <div>15%</div> </div>
2	D	211	<div> <div>%</div> <div>85%</div> <div>14%</div> </div>
2	F	211	<div> <div>5%</div> <div>83%</div> <div>17%</div> </div>
3	E	217	<div> <div>%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>
3	G	217	<div> <div>%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10598 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	255	Total	C	N	O	S	0	0	0
			1984	1310	323	345	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	291	SER	-	expression tag	UNP Q9NYG8
A	292	ASN	-	expression tag	UNP Q9NYG8
A	293	SER	-	expression tag	UNP Q9NYG8
A	294	LEU	-	expression tag	UNP Q9NYG8
A	295	GLU	-	expression tag	UNP Q9NYG8
A	296	VAL	-	expression tag	UNP Q9NYG8
A	297	LEU	-	expression tag	UNP Q9NYG8
A	298	PHE	-	expression tag	UNP Q9NYG8
A	299	GLN	-	expression tag	UNP Q9NYG8
B	104	GLN	ASN	engineered mutation	UNP Q9NYG8
B	108	GLN	ASN	engineered mutation	UNP Q9NYG8
B	291	SER	-	expression tag	UNP Q9NYG8
B	292	ASN	-	expression tag	UNP Q9NYG8
B	293	SER	-	expression tag	UNP Q9NYG8
B	294	LEU	-	expression tag	UNP Q9NYG8
B	295	GLU	-	expression tag	UNP Q9NYG8
B	296	VAL	-	expression tag	UNP Q9NYG8
B	297	LEU	-	expression tag	UNP Q9NYG8
B	298	PHE	-	expression tag	UNP Q9NYG8
B	299	GLN	-	expression tag	UNP Q9NYG8

- Molecule 2 is a protein called ANTI-TRAAK ANTIBODY 13E9 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 ANTI-TRAAK ANTIBODY 13E9 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	1	Total	K	0	0
			1	1		
4	A	5	Total	K	0	0
			5	5		

- 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	2	Total	Ca	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	25	Total	O	0	0
			25	25		
6	D	22	Total	O	0	0
			22	22		
6	E	57	Total	O	0	0
			57	57		
6	F	29	Total	O	0	0
			29	29		

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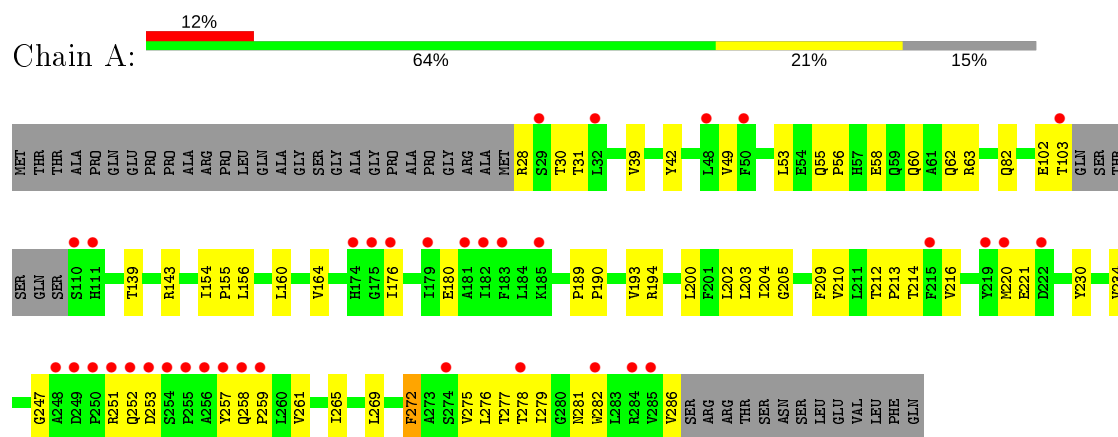
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	38	Total	O	0	0
			38	38		

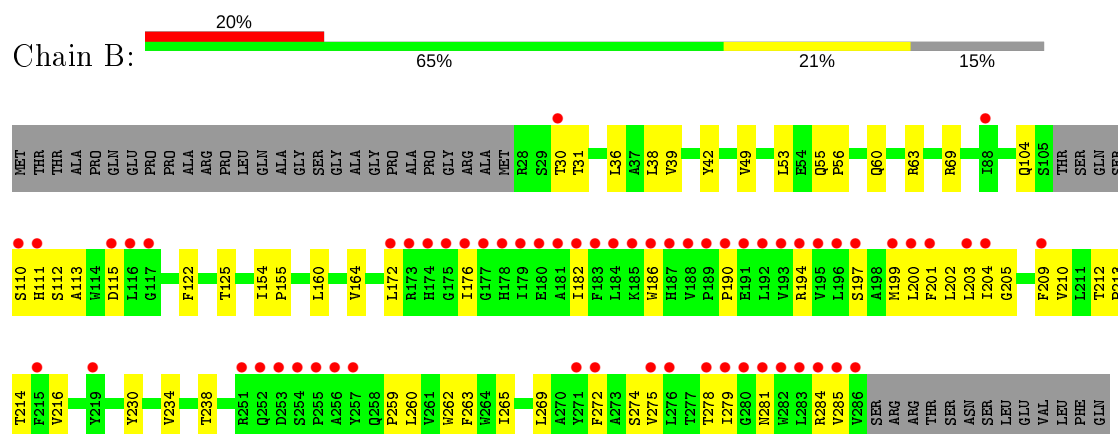
### 3 Residue-property plots

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.

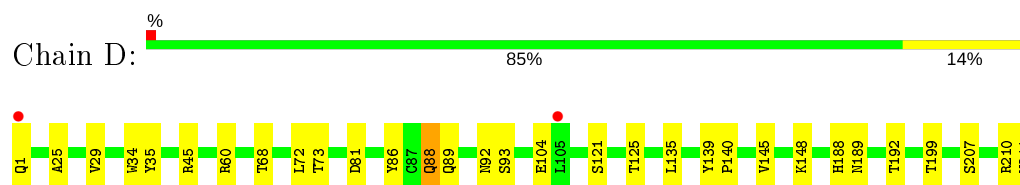
- Molecule 1: Potassium channel subfamily K member 4



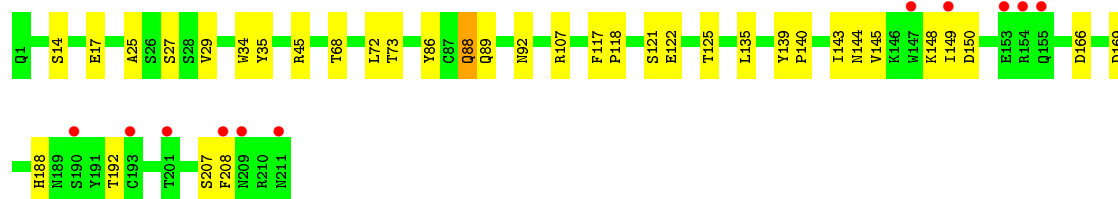
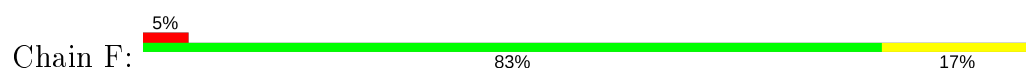
- Molecule 1: Potassium channel subfamily K member 4



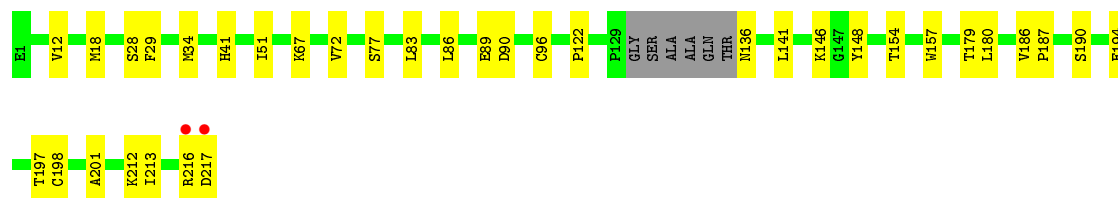
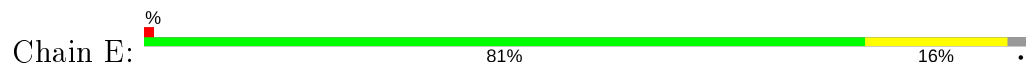
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



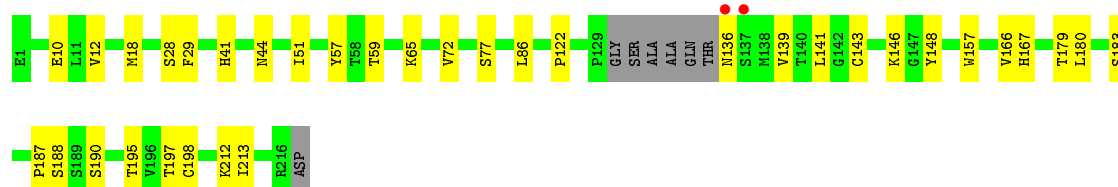
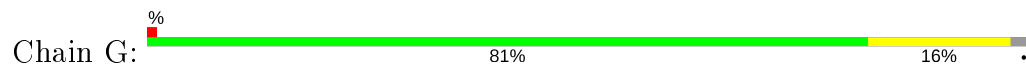
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



- Molecule 3: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN



- Molecule 3: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.80 Å 138.52 Å 96.84 Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	48.20 – 2.50 48.23 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.20-2.50) 99.6 (48.23-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.199 , 0.234 0.202 , 0.236	Depositor DCC
$R_{free}$ test set	3686 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.4	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 57.0	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	0.95	EDS
Total number of atoms	10598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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, 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	0.36	0/2013	0.47	0/2745
1	B	0.37	0/2035	0.49	0/2774
2	D	0.45	0/1655	0.57	0/2247
2	F	0.45	0/1655	0.57	0/2247
3	E	0.49	0/1656	0.60	0/2260
3	G	0.47	0/1647	0.61	0/2249
All	All	0.43	0/10661	0.55	0/14522

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	A	1963	0	1985	52	0
1	B	1984	0	2006	48	0
2	D	1616	0	1542	25	0
2	F	1616	0	1542	26	0
3	E	1614	0	1586	22	1
3	G	1605	0	1582	25	1
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	G	1	0	0	0	0
6	A	20	0	0	0	0
6	B	25	0	0	1	0
6	D	22	0	0	2	0
6	E	57	0	0	1	0
6	F	29	0	0	3	0
6	G	38	0	0	4	0
All	All	10598	0	10243	191	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 9.

All (191) 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:D:189:ASN:ND2	2:D:211:ASN:OD1	2.07	0.86
2:F:35:TYR:HE1	2:F:88:GLN:HG2	1.44	0.83
1:B:281:ASN:O	1:B:284:ARG:HG2	1.83	0.78
1:B:122:PHE:O	1:B:125:THR:OG1	2.02	0.77
2:F:35:TYR:CE1	2:F:88:GLN:HG2	2.21	0.75
1:A:202:LEU:HD12	1:A:203:LEU:N	2.03	0.73
3:E:51:ILE:HD13	3:E:72:VAL:HG13	1.71	0.72
1:A:58:GLU:OE2	1:B:113:ALA:N	2.23	0.71
1:A:60:GLN:OE1	1:A:63:ARG:NH2	2.24	0.71
2:D:35:TYR:HE2	2:D:88:GLN:HG2	1.55	0.70
3:G:51:ILE:HD13	3:G:72:VAL:HG13	1.72	0.70
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.74	0.69
1:A:28:ARG:HB2	1:A:31:THR:HG23	1.75	0.68
1:B:110:SER:O	1:B:111:HIS:HB3	1.94	0.67
1:B:212:THR:HB	1:B:213:PRO:HD3	1.75	0.67
3:E:89:GLU:HG2	6:E:303:HOH:O	1.92	0.67
2:F:72:LEU:HD23	2:F:73:THR:N	2.09	0.67
1:A:212:THR:HB	1:A:213:PRO:HD3	1.77	0.67
1:B:38:LEU:HD23	1:B:38:LEU:C	2.15	0.67
3:G:57:TYR:CE1	3:G:59:THR:HG23	2.29	0.67
1:B:202:LEU:HD12	1:B:203:LEU:N	2.11	0.66
1:B:38:LEU:HD23	1:B:39:VAL:N	2.11	0.66
3:E:141:LEU:HD22	3:E:213:ILE:HG21	1.79	0.65
2:D:35:TYR:CE2	2:D:88:GLN:HG2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ILE:HG22	1:B:269:LEU:HD12	1.79	0.64
1:B:212:THR:O	1:B:216:VAL:HG23	1.96	0.64
3:E:146:LYS:HB3	3:E:179:THR:HG23	1.80	0.64
3:E:157:TRP:CZ3	3:E:198:CYS:HB3	2.32	0.64
1:A:102:GLU:O	1:A:103:THR:HG23	1.99	0.63
2:D:72:LEU:HD23	2:D:73:THR:N	2.14	0.63
3:G:146:LYS:HB3	3:G:179:THR:HG23	1.80	0.62
1:B:190:PRO:O	1:B:194:ARG:HG2	1.99	0.62
2:D:211:ASN:OD1	2:D:211:ASN:N	2.31	0.62
3:G:57:TYR:OH	3:G:59:THR:CG2	2.48	0.61
1:A:276:LEU:HA	1:A:279:ILE:HG22	1.81	0.61
2:F:118:PRO:HB3	2:F:208:PHE:CZ	2.36	0.61
2:D:199:THR:HG22	2:D:199:THR:O	2.00	0.61
3:G:141:LEU:HD22	3:G:213:ILE:HG21	1.80	0.61
2:F:107:ARG:HB2	6:F:329:HOH:O	2.01	0.61
1:A:212:THR:O	1:A:216:VAL:HG23	2.01	0.60
1:A:265:ILE:HG22	1:A:269:LEU:HD12	1.83	0.60
3:G:57:TYR:CZ	3:G:59:THR:HG23	2.37	0.60
1:B:160:LEU:O	1:B:164:VAL:HG23	2.02	0.59
2:D:89:GLN:HE21	2:D:92:ASN:H	1.50	0.59
1:B:260:LEU:O	1:B:263:PHE:HB2	2.02	0.59
1:A:160:LEU:O	1:A:164:VAL:HG23	2.02	0.59
3:G:12:VAL:HG21	3:G:86:LEU:HD12	1.83	0.59
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.84	0.57
3:E:67:LYS:HE2	3:E:90:ASP:OD1	2.05	0.57
1:A:28:ARG:HB2	1:A:31:THR:CG2	2.35	0.57
3:E:180:LEU:HD12	3:E:180:LEU:C	2.25	0.57
2:F:89:GLN:HE21	2:F:92:ASN:H	1.52	0.56
1:A:277:THR:O	1:A:281:ASN:N	2.37	0.56
1:A:39:VAL:O	1:A:42:TYR:N	2.38	0.56
2:D:148:LYS:HB2	2:D:192:THR:OG1	2.05	0.56
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.38	0.56
1:A:154:ILE:N	1:A:155:PRO:HD2	2.20	0.56
1:A:209:PHE:O	1:A:213:PRO:HG2	2.04	0.56
2:F:148:LYS:HB2	2:F:192:THR:OG1	2.05	0.56
3:G:44:ASN:HB2	6:G:412:HOH:O	2.06	0.55
3:G:44:ASN:CB	6:G:412:HOH:O	2.54	0.55
1:A:156:LEU:HD21	1:B:38:LEU:HD21	1.89	0.55
2:F:149:ILE:HG13	2:F:149:ILE:O	2.07	0.55
1:A:202:LEU:HD12	1:A:202:LEU:C	2.27	0.54
3:G:157:TRP:CZ3	3:G:198:CYS:HB3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:ASP:HB3	2:F:169:ASP:OD2	2.08	0.54
1:B:281:ASN:O	1:B:285:VAL:HG23	2.07	0.54
1:A:160:LEU:HD11	1:B:36:LEU:HD12	1.89	0.54
1:B:209:PHE:O	1:B:213:PRO:HG2	2.08	0.54
1:A:176:ILE:HG22	1:A:180:GLU:OE2	2.08	0.54
2:F:118:PRO:HB3	2:F:208:PHE:CE1	2.43	0.53
3:G:180:LEU:C	3:G:180:LEU:HD12	2.28	0.53
1:A:156:LEU:HD21	1:B:38:LEU:CD2	2.39	0.53
1:A:102:GLU:O	1:A:103:THR:CG2	2.57	0.53
3:G:195:THR:HG22	6:G:401:HOH:O	2.07	0.53
1:B:30:THR:HG23	1:B:31:THR:N	2.24	0.53
2:D:188:HIS:O	2:D:210:ARG:NE	2.32	0.53
1:B:172:LEU:O	1:B:176:ILE:HD12	2.09	0.52
1:B:49:VAL:HG12	1:B:53:LEU:HD12	1.91	0.52
1:B:154:ILE:N	1:B:155:PRO:HD2	2.23	0.52
1:A:221:GLU:OE2	1:A:257:TYR:OH	2.23	0.51
3:E:28:SER:HB2	3:G:28:SER:HB2	1.93	0.51
3:E:89:GLU:HA	3:E:89:GLU:OE2	2.11	0.51
1:A:49:VAL:HG12	1:A:53:LEU:HD12	1.93	0.51
1:B:259:PRO:O	1:B:262:TRP:HB3	2.10	0.51
1:B:182:ILE:O	1:B:186:TRP:HD1	1.93	0.50
2:D:192:THR:HG22	2:D:207:SER:CB	2.41	0.50
2:D:199:THR:O	2:D:199:THR:CG2	2.59	0.50
2:F:192:THR:HG22	2:F:207:SER:CB	2.41	0.50
2:D:192:THR:HG22	2:D:207:SER:OG	2.12	0.50
2:F:192:THR:HG22	2:F:207:SER:OG	2.12	0.50
1:A:139:THR:O	1:A:143:ARG:HD2	2.11	0.50
1:A:190:PRO:O	1:A:194:ARG:HG2	2.11	0.50
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.41	0.50
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.42	0.49
1:A:261:VAL:O	1:A:265:ILE:HG13	2.13	0.49
1:A:210:VAL:O	1:A:214:THR:HG23	2.12	0.49
3:E:187:PRO:O	3:E:190:SER:HB2	2.13	0.49
1:B:199:MET:O	1:B:203:LEU:HB2	2.12	0.49
3:G:29:PHE:HB2	3:G:77:SER:HB2	1.94	0.49
3:E:216:ARG:O	3:E:217:ASP:C	2.51	0.49
1:A:282:TRP:O	1:A:286:VAL:HG23	2.13	0.48
1:A:220:MET:O	1:A:251:ARG:NH2	2.46	0.48
3:G:57:TYR:OH	3:G:59:THR:HG21	2.13	0.48
2:F:121:SER:O	2:F:125:THR:HG23	2.13	0.48
2:F:143:ILE:HG13	2:F:144:ASN:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:ARG:NH2	6:F:304:HOH:O	2.43	0.48
2:D:45:ARG:NE	6:D:318:HOH:O	2.37	0.48
3:E:29:PHE:CD2	3:E:77:SER:HA	2.49	0.48
1:A:55:GLN:N	1:A:56:PRO:HD2	2.29	0.47
1:A:82:GLN:OE1	1:A:82:GLN:N	2.42	0.47
1:B:172:LEU:O	1:B:176:ILE:CD1	2.62	0.47
2:F:25:ALA:O	2:F:68:THR:OG1	2.32	0.47
3:E:29:PHE:HB2	3:E:77:SER:HB2	1.95	0.47
1:A:230:TYR:O	1:A:234:VAL:HG23	2.15	0.47
2:F:150:ASP:OD2	2:F:188:HIS:ND1	2.42	0.47
2:D:121:SER:O	2:D:125:THR:HG23	2.15	0.47
1:B:112:SER:HB3	1:B:115:ASP:HB3	1.96	0.47
1:B:210:VAL:O	1:B:214:THR:HG23	2.15	0.47
3:G:29:PHE:CD1	3:G:77:SER:HA	2.50	0.47
2:F:139:TYR:CG	2:F:140:PRO:HA	2.51	0.46
1:B:238:THR:HG22	1:B:269:LEU:HD21	1.96	0.46
3:G:197:THR:HG22	3:G:212:LYS:HA	1.97	0.46
3:E:217:ASP:CG	3:E:217:ASP:OXT	2.53	0.46
1:A:275:VAL:O	1:A:279:ILE:HG22	2.16	0.46
1:B:230:TYR:O	1:B:234:VAL:HG23	2.16	0.46
2:D:139:TYR:CG	2:D:140:PRO:HA	2.51	0.46
2:D:1:GLN:HA	2:D:1:GLN:OE1	2.16	0.46
1:A:277:THR:O	1:A:281:ASN:HB2	2.16	0.45
3:E:122:PRO:HB3	3:E:148:TYR:HB3	1.98	0.45
3:G:166:VAL:HA	3:G:183:SER:O	2.16	0.45
2:D:135:LEU:HD21	2:D:145:VAL:HG22	1.99	0.45
2:D:192:THR:HG22	2:D:207:SER:HB2	1.99	0.45
2:D:89:GLN:NE2	2:D:92:ASN:H	2.14	0.45
3:G:139:VAL:CG2	3:G:188:SER:HB3	2.47	0.45
2:F:192:THR:HG22	2:F:207:SER:HB2	1.99	0.45
1:B:204:ILE:HG23	1:B:205:GLY:N	2.32	0.45
3:G:187:PRO:O	3:G:190:SER:HB2	2.17	0.45
1:A:49:VAL:O	1:A:53:LEU:HG	2.17	0.44
1:B:182:ILE:O	1:B:186:TRP:CD1	2.70	0.44
1:B:60:GLN:HA	1:B:60:GLN:OE1	2.17	0.44
3:G:65:LYS:HE2	6:G:416:HOH:O	2.17	0.44
1:A:252:GLN:O	1:A:253:ASP:CB	2.66	0.44
1:B:194:ARG:O	1:B:197:SER:OG	2.33	0.44
1:B:55:GLN:N	1:B:56:PRO:CD	2.81	0.44
2:F:135:LEU:HD21	2:F:145:VAL:HG22	1.98	0.44
1:A:200:LEU:O	1:A:204:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:122:PRO:HB3	3:G:148:TYR:HB3	2.00	0.44
1:A:49:VAL:HG12	1:A:53:LEU:CD1	2.48	0.44
2:D:25:ALA:O	2:D:68:THR:OG1	2.35	0.44
3:E:186:VAL:HB	3:E:187:PRO:HD2	2.00	0.44
2:F:45:ARG:NE	6:F:304:HOH:O	2.48	0.44
2:F:89:GLN:NE2	2:F:92:ASN:H	2.16	0.44
3:G:167:HIS:HB2	3:G:183:SER:OG	2.18	0.44
1:A:276:LEU:HA	1:A:279:ILE:CG2	2.46	0.43
1:B:60:GLN:OE1	1:B:63:ARG:NH2	2.47	0.43
1:B:49:VAL:HG12	1:B:53:LEU:CD1	2.48	0.43
3:E:154:THR:OG1	3:E:201:ALA:HB3	2.19	0.43
2:D:34:TRP:HA	2:D:86:TYR:O	2.19	0.42
1:A:30:THR:HG23	1:A:31:THR:N	2.34	0.42
1:A:154:ILE:N	1:A:155:PRO:CD	2.81	0.42
1:A:204:ILE:HG23	1:A:205:GLY:N	2.34	0.42
1:A:258:GLN:N	1:A:259:PRO:HD2	2.35	0.42
1:B:275:VAL:O	1:B:278:THR:OG1	2.26	0.42
2:F:14:SER:N	2:F:17:GLU:OE1	2.48	0.42
1:B:201:PHE:C	1:B:201:PHE:CD2	2.91	0.42
3:G:57:TYR:CZ	3:G:59:THR:CG2	3.02	0.42
1:A:272:PHE:O	1:A:276:LEU:HD23	2.19	0.42
1:A:202:LEU:HD12	1:A:203:LEU:CA	2.50	0.42
1:A:278:THR:HA	1:A:281:ASN:CB	2.50	0.42
2:F:27:SER:O	2:F:29:VAL:HG23	2.20	0.42
2:D:45:ARG:NH2	6:D:318:HOH:O	2.52	0.41
1:B:49:VAL:O	1:B:53:LEU:HG	2.20	0.41
1:B:104:GLN:HE22	2:D:93:SER:H	1.67	0.41
1:B:69:ARG:HD3	6:B:401:HOH:O	2.20	0.41
2:F:34:TRP:HA	2:F:86:TYR:O	2.20	0.41
1:B:200:LEU:O	1:B:204:ILE:HG22	2.20	0.41
1:B:38:LEU:CD2	1:B:38:LEU:C	2.87	0.41
3:E:83:LEU:HB3	3:E:86:LEU:HD21	2.01	0.41
1:A:189:PRO:O	1:A:193:VAL:HG23	2.21	0.41
1:A:62:GLN:O	1:A:63:ARG:C	2.59	0.41
1:B:197:SER:O	1:B:201:PHE:N	2.45	0.41
1:A:155:PRO:HG3	1:B:279:ILE:CG2	2.51	0.41
1:B:39:VAL:O	1:B:42:TYR:N	2.54	0.41
3:E:34:MET:CE	3:E:96:CYS:HB2	2.51	0.41
2:F:117:PHE:HA	2:F:118:PRO:HD3	1.93	0.40
1:B:274:SER:O	1:B:278:THR:HG23	2.20	0.40
1:A:247:GLY:O	1:A:258:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLN:N	1:A:56:PRO:CD	2.84	0.40
1:A:160:LEU:C	1:A:160:LEU:HD23	2.41	0.40
3:E:197:THR:HG22	3:E:212:LYS:HA	2.03	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]	2.05	0.15

## 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	249/299 (83%)	242 (97%)	7 (3%)	0	100	100
1	B	251/299 (84%)	242 (96%)	9 (4%)	0	100	100
2	D	209/211 (99%)	198 (95%)	11 (5%)	0	100	100
2	F	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
3	E	207/217 (95%)	203 (98%)	3 (1%)	1 (0%)	29	48
3	G	206/217 (95%)	201 (98%)	4 (2%)	1 (0%)	29	48
All	All	1331/1454 (92%)	1287 (97%)	42 (3%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	41	HIS
3	G	41	HIS

### 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	204/242 (84%)	203 (100%)	1 (0%)	88	96
1	B	208/242 (86%)	207 (100%)	1 (0%)	88	96
2	D	184/184 (100%)	182 (99%)	2 (1%)	73	89
2	F	184/184 (100%)	182 (99%)	2 (1%)	73	89
3	E	187/190 (98%)	185 (99%)	2 (1%)	73	89
3	G	186/190 (98%)	183 (98%)	3 (2%)	62	84
All	All	1153/1232 (94%)	1142 (99%)	11 (1%)	76	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	PHE
1	B	272	PHE
2	D	88	GLN
2	D	104	GLU
3	E	18	MET
3	E	136	ASN
2	F	88	GLN
2	F	122	GLU
3	G	18	MET
3	G	136	ASN
3	G	143	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	59	GLN
2	D	136	ASN
2	D	137	ASN
3	E	167	HIS
3	G	167	HIS



### 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 9 ligands modelled in this entry, 9 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	253/299 (84%)	0.69	36 (14%) <b>2</b> <b>2</b>	44, 107, 169, 198	0
1	B	255/299 (85%)	1.31	61 (23%) <b>0</b> <b>0</b>	42, 112, 229, 262	0
2	D	211/211 (100%)	-0.07	2 (0%) <b>84</b> <b>86</b>	47, 73, 107, 121	0
2	F	211/211 (100%)	0.17	11 (5%) <b>27</b> <b>29</b>	43, 73, 135, 163	0
3	E	211/217 (97%)	-0.05	2 (0%) <b>84</b> <b>86</b>	38, 63, 95, 133	0
3	G	210/217 (96%)	0.02	2 (0%) <b>82</b> <b>84</b>	41, 71, 111, 166	0
All	All	1351/1454 (92%)	0.39	114 (8%) <b>11</b> <b>11</b>	38, 78, 166, 262	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	ALA	11.7
1	B	184	LEU	11.0
1	B	183	PHE	10.8
1	B	192	LEU	8.8
1	B	179	ILE	8.3
1	B	189	PRO	8.1
1	B	193	VAL	7.7
1	B	185	LYS	7.3
1	B	187	HIS	7.3
1	B	176	ILE	7.3
1	B	188	VAL	6.7
1	A	255	PRO	6.6
1	B	180	GLU	6.4
1	B	190	PRO	6.2
1	B	286	VAL	6.1
1	A	257	TYR	6.0
1	B	178	HIS	6.0
1	A	256	ALA	5.9
1	A	253	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	282	TRP	5.5
1	B	177	GLY	5.5
1	B	200	LEU	5.4
2	F	208	PHE	5.3
1	A	219	TYR	5.2
1	B	283	LEU	5.1
1	A	254	SER	5.1
1	B	194	ARG	5.1
1	B	256	ALA	5.0
1	B	182	ILE	4.9
1	B	201	PHE	4.9
1	B	172	LEU	4.8
1	B	174	HIS	4.8
1	B	278	THR	4.7
1	B	116	LEU	4.7
1	B	195	VAL	4.7
1	B	196	LEU	4.6
1	A	285	VAL	4.4
1	B	255	PRO	4.3
1	B	285	VAL	4.3
1	B	284	ARG	4.2
1	B	257	TYR	4.2
1	B	271	TYR	4.2
2	F	154	ARG	4.2
1	B	251	ARG	4.1
3	E	216	ARG	4.1
1	A	174	HIS	4.1
1	A	176	ILE	4.0
1	B	199	MET	4.0
1	B	275	VAL	4.0
1	B	186	TRP	4.0
1	B	203	LEU	3.9
1	A	248	ALA	3.9
1	B	219	TYR	3.8
2	F	155	GLN	3.7
3	G	136	ASN	3.7
2	F	201	THR	3.7
2	F	211	ASN	3.6
1	B	280	GLY	3.6
1	B	173	ARG	3.6
1	B	197	SER	3.5
1	B	254	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	276	LEU	3.5
1	B	111	HIS	3.5
1	B	253	ASP	3.4
1	A	183	PHE	3.4
1	A	274	SER	3.3
1	A	215	PHE	3.3
1	A	179	ILE	3.1
1	A	252	GLN	3.1
1	A	110	SER	3.0
1	A	250	PRO	2.9
1	A	284	ARG	2.9
3	E	217	ASP	2.8
2	F	153	GLU	2.8
1	B	115	ASP	2.8
1	B	204	ILE	2.8
1	B	191	GLU	2.7
2	F	147	TRP	2.6
1	A	181	ALA	2.6
1	A	182	ILE	2.6
1	B	272	PHE	2.6
2	F	209	ASN	2.6
1	A	48	LEU	2.5
1	B	215	PHE	2.5
1	A	103	THR	2.5
1	B	281	ASN	2.5
1	A	251	ARG	2.5
1	A	282	TRP	2.5
1	A	258	GLN	2.5
3	G	137	SER	2.4
2	F	149	ILE	2.4
1	A	220	MET	2.4
1	A	32	LEU	2.4
1	B	279	ILE	2.4
1	A	259	PRO	2.4
1	A	50	PHE	2.3
1	A	29	SER	2.3
2	D	1	GLN	2.3
2	F	193	CYS	2.3
1	A	111	HIS	2.2
1	A	175	GLY	2.2
1	A	278	THR	2.2
1	B	110	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	30	THR	2.2
1	B	175	GLY	2.2
2	F	190	SER	2.2
1	B	117	GLY	2.2
1	B	209	PHE	2.1
1	B	88	ILE	2.1
1	B	252	GLN	2.1
1	A	185	LYS	2.1
2	D	105	LEU	2.0
1	A	249	ASP	2.0
1	A	222	ASP	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	304	1/1	0.88	0.49	115,115,115,115	0
4	K	B	301	1/1	0.93	0.67	106,106,106,106	0
4	K	A	303	1/1	0.96	0.12	86,86,86,86	0
4	K	A	307	1/1	0.96	0.08	76,76,76,76	0
4	K	A	302	1/1	0.97	0.10	75,75,75,75	0
5	CA	G	301	1/1	0.97	0.11	84,84,84,84	0
4	K	A	301	1/1	0.98	0.12	70,70,70,70	0
5	CA	A	306	1/1	0.99	0.10	84,84,84,84	0
5	CA	A	305	1/1	0.99	0.13	87,87,87,87	0

## 6.5 Other polymers

There are no such residues in this entry.