



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:12 AM UTC

PDB ID : 4I9W / pdb_00004i9w
Title : Human two pore domain K⁺ 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

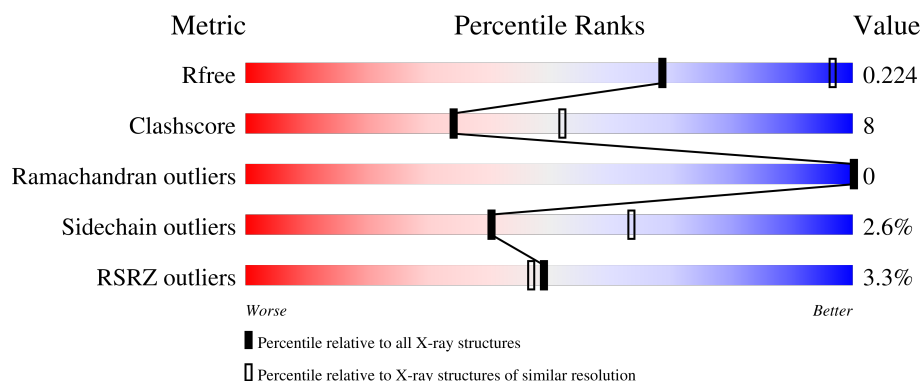
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 ≥ 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	5% 64% 17% 18%
1	B	309	5% 66% 15% 18%
2	D	211	% 86% 13% .
2	F	211	3% 86% 12% .
3	E	217	3% 80% 16% ..

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Mol	Chain	Length	Quality of chain
3	G	217	 81% 15% ..

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 (CCD ID: K) (formula: K).

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

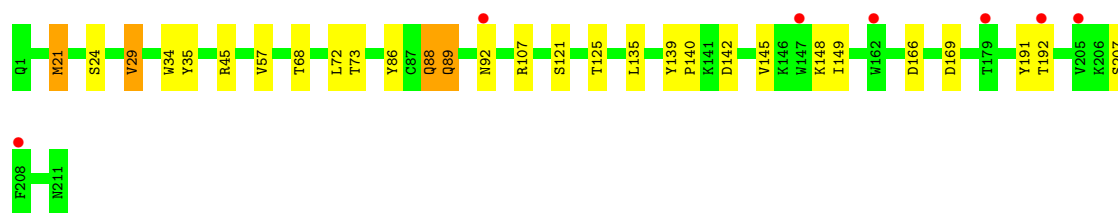
- Molecule 6 is water.

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		

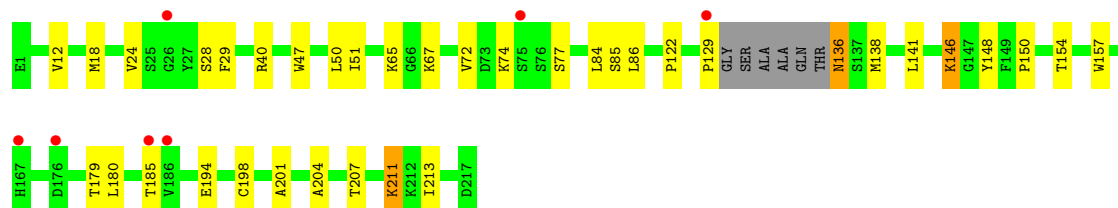
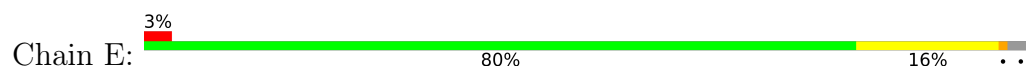
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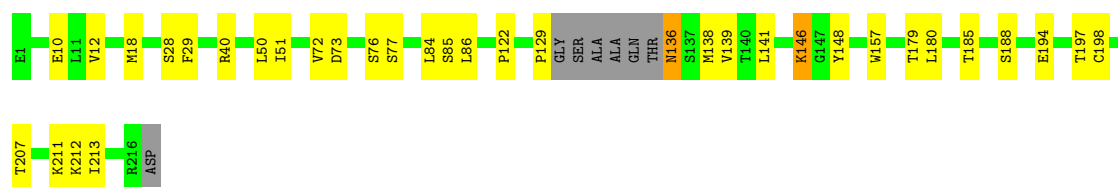
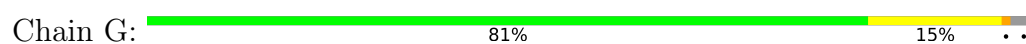
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	30	Total	O	0	0
			30	30		



● 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, α , β , γ	80.89Å 138.91Å 97.46Å 90.00° 94.87° 90.00°	Depositor
Resolution (Å)	48.60 – 2.75 48.60 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.60-2.75) 99.3 (48.60-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.201 , 0.236 (Not available) , 0.224	Depositor DCC
R_{free} test set	2798 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10544	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.52	0/2013	0.74	0/2745
1	B	0.52	0/2021	0.73	0/2754
2	D	0.54	0/1655	0.73	0/2247
2	F	0.55	0/1655	0.75	1/2247 (0.0%)
3	E	0.63	0/1656	0.81	2/2260 (0.1%)
3	G	0.62	0/1647	0.80	1/2249 (0.0%)
All	All	0.56	0/10647	0.76	4/14502 (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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	146	LYS	N-CA-C	5.79	118.64	109.50
3	G	146	LYS	N-CA-C	5.32	117.91	109.50
2	F	57	VAL	N-CA-C	5.21	113.11	108.63
3	E	40	ARG	N-CA-C	-5.03	103.04	110.48

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	37	0
1	B	1970	0	1988	31	0
2	D	1616	0	1542	23	0
2	F	1616	0	1542	21	0
3	E	1614	0	1586	24	1
3	G	1605	0	1582	26	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	157	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 8.

All (157) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:180:LEU:HD12	3:G:180:LEU:C	2.22	0.65
3:G:197:THR:HG22	3:G:212:LYS:CA	2.28	0.63
3:E:180:LEU:C	3:E:180:LEU:HD12	2.24	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:198:CYS:C	6:G:426:HOH:O	2.42	0.63
3:G:194:GLU:HG2	6:G:425:HOH:O	1.98	0.62
1:B:38:LEU:C	1:B:38:LEU:HD23	2.25	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
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
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
2:D:192:THR:HG22	2:D:207:SER:OG	2.04	0.57
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.85	0.57
3:E:129:PRO:HD3	3:E:141:LEU:HD23	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:50:LEU:C	3:G:50:LEU:HD12	2.31	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:N	3:E:136:ASN:HD22	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:138:MET:HE3	3:E:185:THR:HG22	1.91	0.53
3:G:138:MET:HE3	3:G:185:THR:HG22	1.91	0.53
3:E:154:THR:OG1	3:E:201:ALA:HB3	2.08	0.52
3:E:50:LEU:C	3:E:50:LEU:HD12	2.34	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:N	3:G:136:ASN:ND2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	3:G:136:ASN:HD22	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
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: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:201:PHE:CD2	1:B:201:PHE:C	2.93	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:72:LEU:HD23	2:F:72:LEU:C	2.42	0.45
2:F:149:ILE:HG13	2:F:149:ILE:O	2.17	0.45
1:A:55:GLN:N	1:A:56:PRO:HD2	2.32	0.45
1:A:258:GLN:N	1:A:259:PRO:HD2	2.31	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:202:LEU:HD12	1:B:202:LEU:C	2.44	0.43
3:G:73:ASP:C	3:G:73:ASP:OD1	2.61	0.43
1:B:205:GLY:HA3	1:B:271:TYR:CZ	2.53	0.43
2:D:192:THR:HG22	2:D:207:SER:HG	1.82	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:B:122:PHE:O	1:B:125:THR:OG1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:THR:HG21	1:A:229:ILE:HG12	2.00	0.42
1:A:51:ARG:HE	1:B:116:LEU:HD23	1.84	0.42
1:A:282:TRP:CH2	1:A:286:VAL:HG21	2.54	0.42
1:B:214:THR:HG21	1:B:229:ILE:HG12	2.02	0.42
3:E:84:LEU:O	3:E:85:SER:C	2.62	0.42
1:A:202:LEU:HD12	1:A:202:LEU:C	2.44	0.41
3:G:76:SER:O	3:G:77:SER:C	2.62	0.41
1:A:69:ARG:CZ	1:B:104:GLN:HE21	2.33	0.41
3:E:180:LEU:C	3:E:180:LEU:CD1	2.93	0.41
1:A:100:ASP:O	1:A:102:GLU:HG2	2.20	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:HD12	1:A:35:LEU:HA	1.92	0.41
3:E:65:LYS:HE2	3:E:65:LYS:HB2	1.92	0.41
1:A:176:ILE:HD11	1:A:201:PHE:HA	2.03	0.41
1:A:210:VAL:O	1:A:214:THR:HG23	2.21	0.41
1:A:33:LEU:O	1:A:33:LEU:HD23	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
3:G:84:LEU:O	3:G:85:SER:C	2.63	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:D:72:LEU:HD23	2:D:72:LEU:C	2.45	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%)	203 (100%)	1 (0%)	81	89
1	B	206/248 (83%)	201 (98%)	5 (2%)	43	65
2	D	184/184 (100%)	177 (96%)	7 (4%)	29	52
2	F	184/184 (100%)	177 (96%)	7 (4%)	29	52
3	E	187/190 (98%)	181 (97%)	6 (3%)	34	58
3	G	186/190 (98%)	182 (98%)	4 (2%)	45	67
All	All	1151/1244 (92%)	1121 (97%)	30 (3%)	40	63

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LEU
1	B	33	LEU
1	B	116	LEU

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Mol	Chain	Res	Type
1	B	176	ILE
1	B	211	LEU
1	B	238	THR
2	D	21	MET
2	D	55	SER
2	D	88	GLN
2	D	89	GLN
2	D	142	ASP
2	D	183	ASP
2	D	211	ASN
3	E	18	MET
3	E	24	VAL
3	E	67	LYS
3	E	136	ASN
3	E	207	THR
3	E	211	LYS
2	F	21	MET
2	F	24	SER
2	F	29	VAL
2	F	68	THR
2	F	88	GLN
2	F	89	GLN
2	F	142	ASP
3	G	18	MET
3	G	136	ASN
3	G	207	THR
3	G	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	B	55	GLN
2	D	88	GLN
2	D	136	ASN
2	D	137	ASN
2	D	209	ASN
2	F	88	GLN
2	F	92	ASN
2	F	209	ASN
3	G	136	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](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	253/309 (81%)	0.44	15 (5%)	28 28	63, 129, 196, 260	0
1	B	253/309 (81%)	0.41	14 (5%)	30 30	59, 127, 257, 269	0
2	D	211/211 (100%)	0.13	2 (0%)	81 81	68, 96, 134, 160	0
2	F	211/211 (100%)	0.09	7 (3%)	49 47	57, 96, 188, 250	0
3	E	211/217 (97%)	0.01	7 (3%)	49 47	60, 82, 117, 178	0
3	G	210/217 (96%)	-0.08	0	100 100	57, 93, 141, 194	0
All	All	1349/1474 (91%)	0.18	45 (3%)	49 47	57, 98, 195, 269	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	22	THR	5.8
3	E	176	ASP	4.0
1	A	256	ALA	3.7
2	D	7	SER	3.6
3	E	26	GLY	3.5
1	B	272	PHE	3.5
1	B	220	MET	3.5
1	B	279	ILE	3.4
1	A	110	SER	3.3
3	E	186	VAL	3.0
1	B	275	VAL	2.9
2	F	205	VAL	2.8
1	A	151	LEU	2.8
1	A	248	ALA	2.8
2	F	179	THR	2.8
1	A	276	LEU	2.7
1	A	177	GLY	2.7
1	A	175	GLY	2.7
2	F	162	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	75	SER	2.7
1	B	136	ALA	2.7
2	F	208	PHE	2.6
1	B	196	LEU	2.5
1	A	200	LEU	2.4
1	B	164	VAL	2.4
1	B	182	ILE	2.4
1	B	105	SER	2.4
1	A	159	ILE	2.4
3	E	185	THR	2.3
1	B	229	ILE	2.3
1	B	114	TRP	2.3
1	A	203	LEU	2.3
1	A	50	PHE	2.3
2	F	147	TRP	2.3
1	B	282	TRP	2.2
1	A	176	ILE	2.2
1	B	183	PHE	2.2
2	F	192	THR	2.2
1	A	257	TYR	2.2
1	A	41	LEU	2.2
2	F	92	ASN	2.1
3	E	129	PRO	2.1
3	E	167	HIS	2.1
1	A	278	THR	2.0
1	B	116	LEU	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 [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, 95th 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($\text{\AA}^2$)	Q<0.9
4	K	B	401	1/1	0.85	0.31	125,125,125,125	0
4	K	B	402	1/1	0.96	0.07	81,81,81,81	0
5	CA	G	301	1/1	0.96	0.07	113,113,113,113	0
4	K	A	402	1/1	0.97	0.05	96,96,96,96	0
4	K	B	403	1/1	0.99	0.03	83,83,83,83	0
5	CA	A	403	1/1	0.99	0.02	104,104,104,104	0
4	K	A	401	1/1	0.99	0.03	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.