



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:03 PM UTC

PDB ID : 4WFG / pdb_00004wfg
Title : Human TRAAK K⁺ channel in a Tl⁺ bound conductive conformation
Authors : Brohawn, S.G.; MacKinnon, R.
Deposited on : 2014-09-15
Resolution : 3.00 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

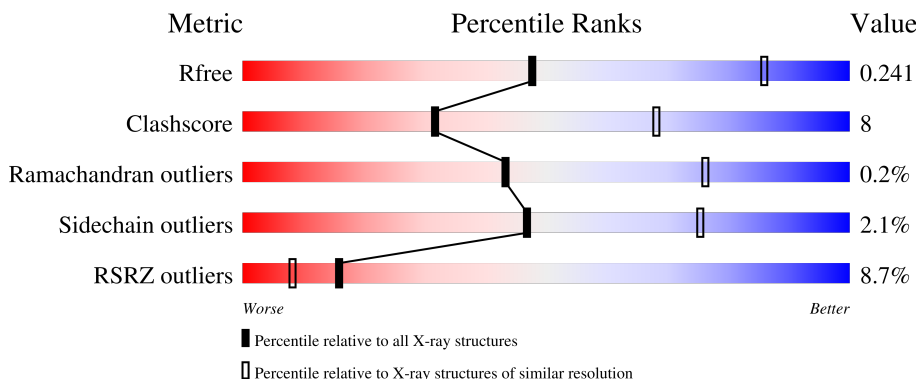
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	299	11% 66% 19% 15%
1	B	299	13% 69% 16% 15%
2	D	211	7% 82% 17% •
2	F	211	5% 85% 14% •
3	E	217	6% 80% 16% ••

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Mol	Chain	Length	Quality of chain
3	G	217	5% 79% 18%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10599 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 THALLIUM (I) ION (CCD ID: TL) (formula: Tl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Tl	0	0
			5	5		
4	B	3	Total	Tl	0	0
			3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	G	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	22	Total	O	0	0
			22	22		
6	B	24	Total	O	0	0
			24	24		
6	D	19	Total	O	0	0
			19	19		
6	E	57	Total	O	0	0
			57	57		
6	F	33	Total	O	0	0
			33	33		

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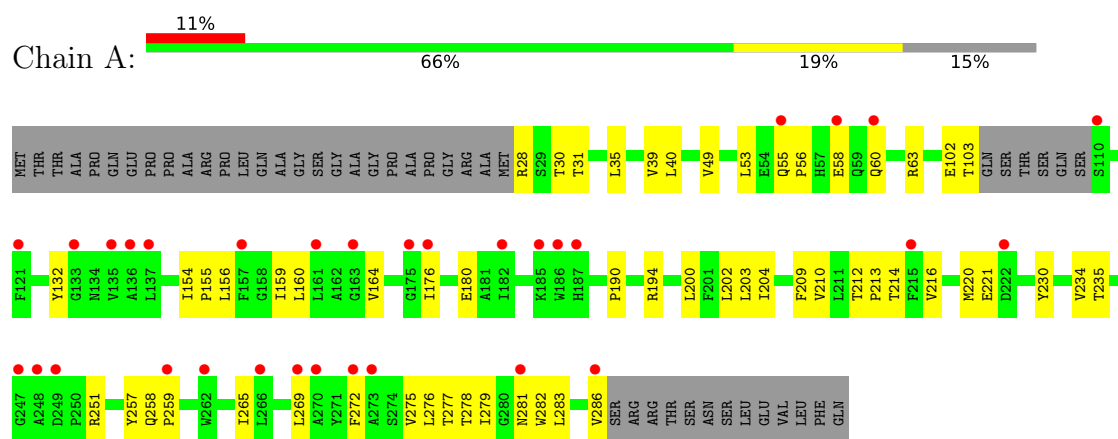
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	35	Total	O	0	0
			35	35		

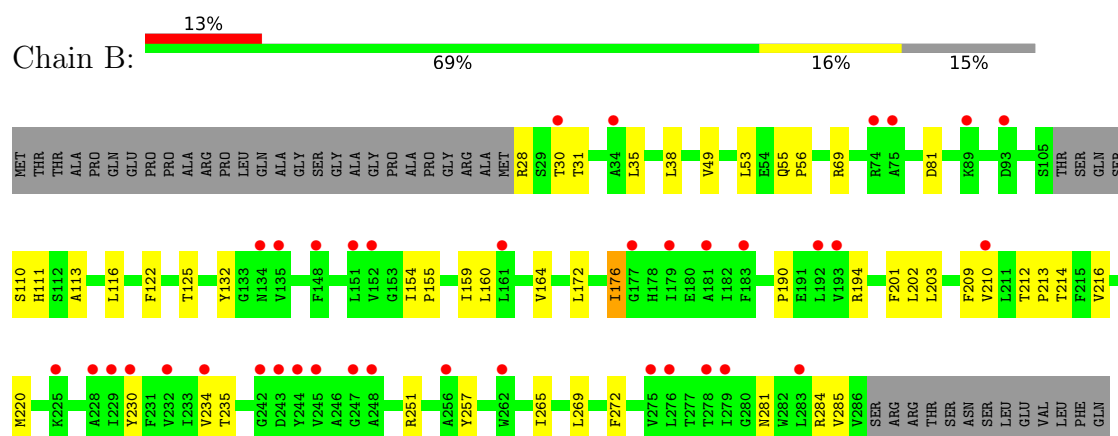
3 Residue-property plots [i](#)

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

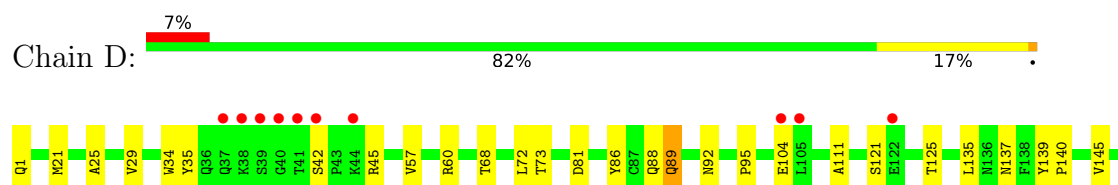
- Molecule 1: Potassium channel subfamily K member 4

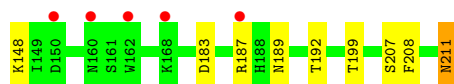


- Molecule 1: Potassium channel subfamily K member 4

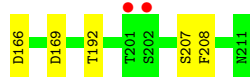
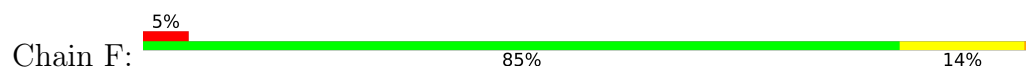


- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN

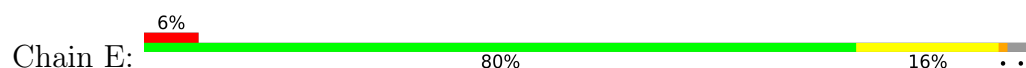




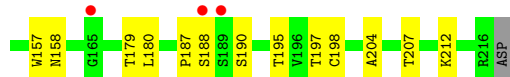
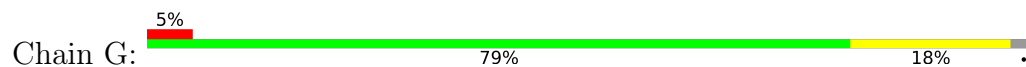
• Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



• 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, α , β , γ	80.80Å 138.76Å 96.32Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	48.00 – 3.00 48.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.00-3.00) 99.5 (48.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.202 , 0.236 0.209 , 0.241	Depositor DCC
R_{free} test set	2131 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	84.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10599	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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, TL

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	0.44	0/2013	0.73	0/2745
1	B	0.46	0/2035	0.73	0/2774
2	D	0.45	0/1655	0.70	1/2247 (0.0%)
2	F	0.47	0/1655	0.70	1/2247 (0.0%)
3	E	0.50	0/1656	0.74	1/2260 (0.0%)
3	G	0.50	0/1647	0.73	0/2249
All	All	0.47	0/10661	0.72	3/14522 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	57	VAL	N-CA-C	6.11	113.88	108.63
2	D	57	VAL	N-CA-C	5.17	113.07	108.63
3	E	146	LYS	N-CA-C	5.14	117.63	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1963	0	1985	39	0
1	B	1984	0	2005	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1616	0	1542	29	0
2	F	1616	0	1542	26	0
3	E	1614	0	1586	23	1
3	G	1605	0	1582	26	1
4	A	5	0	0	0	0
4	B	3	0	0	0	0
5	A	2	0	0	0	0
5	G	1	0	0	0	0
6	A	22	0	0	0	0
6	B	24	0	0	0	0
6	D	19	0	0	1	0
6	E	57	0	0	1	0
6	F	33	0	0	5	0
6	G	35	0	0	4	0
All	All	10599	0	10242	167	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 (167) 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	0.92
2:D:35:TYR:HE2	2:D:88:GLN:HG2	1.39	0.88
2:D:189:ASN:ND2	2:D:211:ASN:OD1	2.09	0.81
2:F:35:TYR:CE1	2:F:88:GLN:HG2	2.17	0.79
2:F:72:LEU:HD23	2:F:73:THR:N	2.01	0.75
1:A:60:GLN:OE1	1:A:63:ARG:NH2	2.20	0.74
1:B:251:ARG:HH11	1:B:251:ARG:HG2	1.53	0.74
2:D:35:TYR:CE2	2:D:88:GLN:HG2	2.22	0.73
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.71	0.71
2:D:72:LEU:HD23	2:D:73:THR:N	2.07	0.70
1:B:38:LEU:C	1:B:38:LEU:HD23	2.17	0.70
1:B:281:ASN:O	1:B:284:ARG:HG2	1.92	0.70
1:A:212:THR:HB	1:A:213:PRO:HD3	1.74	0.70
1:A:58:GLU:OE2	1:B:113:ALA:N	2.26	0.69
1:B:212:THR:HB	1:B:213:PRO:HD3	1.74	0.68
2:F:98:GLY:O	6:F:305:HOH:O	2.13	0.67
3:E:180:LEU:C	3:E:180:LEU:HD12	2.21	0.66
1:B:69:ARG:NH1	1:B:81:ASP:OD1	2.29	0.65
2:D:89:GLN:HE21	2:D:92:ASN:H	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:180:LEU:HD12	3:G:180:LEU:C	2.24	0.63
2:F:89:GLN:HE21	2:F:92:ASN:H	1.47	0.63
1:A:276:LEU:HA	1:A:279:ILE:HG22	1.81	0.62
1:B:190:PRO:O	1:B:194:ARG:HG2	1.99	0.62
3:G:12:VAL:HG21	3:G:86:LEU:HD12	1.81	0.62
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.81	0.60
1:A:212:THR:O	1:A:216:VAL:HG23	2.01	0.60
3:E:146:LYS:HB3	3:E:179:THR:HG23	1.83	0.60
3:G:146:LYS:HB3	3:G:179:THR:HG23	1.83	0.60
1:B:212:THR:O	1:B:216:VAL:HG23	2.00	0.60
3:G:51:ILE:HD13	3:G:72:VAL:HG13	1.84	0.60
3:E:51:ILE:HD13	3:E:72:VAL:HG13	1.84	0.58
1:A:220:MET:O	1:A:251:ARG:NH2	2.36	0.58
2:F:166:ASP:HB3	2:F:169:ASP:OD2	2.03	0.58
1:B:251:ARG:HG2	1:B:251:ARG:NH1	2.18	0.58
2:D:148:LYS:HB2	2:D:192:THR:OG1	2.04	0.58
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.34	0.58
2:F:192:THR:HG22	2:F:207:SER:OG	2.04	0.58
1:B:202:LEU:HD12	1:B:203:LEU:N	2.19	0.57
2:F:148:LYS:HB2	2:F:192:THR:OG1	2.03	0.57
3:G:195:THR:HG22	6:G:401:HOH:O	2.03	0.57
2:D:192:THR:HG22	2:D:207:SER:OG	2.05	0.57
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.34	0.57
1:A:202:LEU:HD12	1:A:203:LEU:N	2.20	0.57
2:F:60:ARG:HB3	6:F:320:HOH:O	2.04	0.56
1:A:154:ILE:N	1:A:155:PRO:HD2	2.20	0.56
1:A:102:GLU:O	1:A:103:THR:HG23	2.07	0.55
1:B:122:PHE:O	1:B:125:THR:OG1	2.22	0.55
3:E:29:PHE:CD2	3:E:77:SER:HA	2.41	0.55
1:B:154:ILE:N	1:B:155:PRO:HD2	2.21	0.55
1:B:172:LEU:O	1:B:176:ILE:HD12	2.06	0.55
1:A:28:ARG:HB2	1:A:31:THR:HG23	1.89	0.54
2:F:72:LEU:HD23	2:F:72:LEU:C	2.34	0.53
2:D:139:TYR:CG	2:D:140:PRO:HA	2.44	0.53
2:F:139:TYR:CG	2:F:140:PRO:HA	2.44	0.52
1:A:190:PRO:O	1:A:194:ARG:HG2	2.08	0.52
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.42	0.52
3:E:157:TRP:CZ3	3:E:198:CYS:HB3	2.44	0.52
2:F:143:ILE:HG13	2:F:144:ASN:N	2.24	0.51
1:B:160:LEU:O	1:B:164:VAL:HG23	2.11	0.51
1:A:176:ILE:HG22	1:A:180:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PHE:O	1:A:213:PRO:HG2	2.11	0.51
3:G:50:LEU:C	3:G:50:LEU:HD12	2.36	0.51
2:F:121:SER:O	2:F:125:THR:HG23	2.11	0.50
1:B:55:GLN:N	1:B:56:PRO:CD	2.75	0.50
1:B:209:PHE:O	1:B:213:PRO:HG2	2.12	0.50
3:E:122:PRO:HB3	3:E:148:TYR:HB3	1.93	0.50
3:G:122:PRO:HB3	3:G:148:TYR:HB3	1.93	0.50
1:A:265:ILE:HG22	1:A:269:LEU:HD12	1.94	0.49
1:A:160:LEU:O	1:A:164:VAL:HG23	2.12	0.49
2:D:121:SER:O	2:D:125:THR:HG23	2.13	0.49
1:A:159:ILE:HG22	1:B:35:LEU:HD21	1.94	0.49
3:E:136:ASN:N	3:E:136:ASN:OD1	2.45	0.49
1:A:210:VAL:O	1:A:214:THR:HG23	2.13	0.49
2:D:199:THR:HG22	2:D:199:THR:O	2.13	0.49
3:G:157:TRP:CZ3	3:G:198:CYS:HB3	2.48	0.48
3:G:139:VAL:CG2	3:G:188:SER:HB3	2.42	0.48
3:E:50:LEU:C	3:E:50:LEU:HD12	2.37	0.48
1:B:265:ILE:HG22	1:B:269:LEU:HD12	1.95	0.48
1:A:221:GLU:OE2	1:A:257:TYR:OH	2.27	0.48
2:F:107:ARG:HB2	6:F:333:HOH:O	2.14	0.48
1:B:281:ASN:O	1:B:285:VAL:HG23	2.14	0.47
2:D:72:LEU:HD23	2:D:72:LEU:C	2.38	0.47
2:F:192:THR:HG22	2:F:207:SER:CB	2.44	0.47
1:B:210:VAL:O	1:B:214:THR:HG23	2.14	0.47
2:D:192:THR:HG22	2:D:207:SER:CB	2.44	0.47
1:A:55:GLN:N	1:A:56:PRO:HD2	2.29	0.47
1:B:201:PHE:CD2	1:B:201:PHE:C	2.92	0.47
3:G:197:THR:HG23	6:G:401:HOH:O	2.14	0.47
3:E:150:PRO:HD2	3:E:204:ALA:CB	2.45	0.47
1:A:200:LEU:O	1:A:204:ILE:HG22	2.15	0.47
2:D:211:ASN:OD1	2:D:211:ASN:N	2.35	0.47
3:G:57:TYR:CZ	3:G:59:THR:HG23	2.49	0.47
1:B:38:LEU:C	1:B:38:LEU:CD2	2.88	0.47
2:D:1:GLN:OE1	2:D:1:GLN:HA	2.15	0.47
3:G:197:THR:HG22	3:G:212:LYS:HA	1.96	0.46
1:B:110:SER:O	1:B:111:HIS:HB2	2.15	0.46
3:E:187:PRO:O	3:E:190:SER:HB2	2.16	0.46
3:G:139:VAL:HG23	3:G:188:SER:HB3	1.97	0.46
3:G:29:PHE:CD1	3:G:77:SER:HA	2.51	0.46
1:B:49:VAL:HG12	1:B:53:LEU:HD12	1.98	0.46
2:D:89:GLN:NE2	2:D:92:ASN:H	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HD12	1:B:202:LEU:C	2.41	0.46
2:F:45:ARG:NE	6:F:306:HOH:O	2.46	0.45
1:A:202:LEU:HD12	1:A:202:LEU:C	2.41	0.45
1:A:277:THR:O	1:A:281:ASN:N	2.48	0.45
1:A:132:TYR:OH	1:A:235:THR:HG23	2.17	0.45
1:B:132:TYR:OH	1:B:235:THR:HG23	2.17	0.45
3:E:154:THR:OG1	3:E:201:ALA:HB3	2.16	0.45
2:D:45:ARG:NH1	6:D:318:HOH:O	2.49	0.44
3:E:34:MET:CE	3:E:96:CYS:HB2	2.48	0.44
3:E:197:THR:HG22	3:E:212:LYS:HA	2.00	0.44
1:A:49:VAL:HG12	1:A:53:LEU:HD12	1.99	0.44
2:F:149:ILE:HG13	2:F:149:ILE:O	2.17	0.44
3:E:89:GLU:HG2	6:E:304:HOH:O	2.18	0.44
1:B:220:MET:HG3	1:B:257:TYR:CE1	2.52	0.44
3:E:180:LEU:C	3:E:180:LEU:CD1	2.91	0.44
3:G:150:PRO:HD2	3:G:204:ALA:CB	2.47	0.44
1:A:230:TYR:O	1:A:234:VAL:HG23	2.18	0.43
3:E:89:GLU:OE2	3:E:89:GLU:HA	2.17	0.43
3:G:34:MET:CE	3:G:96:CYS:HB2	2.48	0.43
2:D:35:TYR:HH	3:E:103:PHE:HD2	1.66	0.43
2:D:199:THR:O	2:D:199:THR:CG2	2.66	0.43
1:A:39:VAL:O	1:A:40:LEU:C	2.62	0.43
1:A:278:THR:O	1:A:281:ASN:HB3	2.18	0.43
2:F:34:TRP:HA	2:F:86:TYR:O	2.18	0.43
2:F:135:LEU:HD21	2:F:145:VAL:HG22	2.01	0.43
3:G:158:ASN:OD1	6:G:401:HOH:O	2.21	0.43
3:G:187:PRO:O	3:G:190:SER:HB2	2.18	0.43
3:G:3:GLN:C	3:G:4:LEU:HD12	2.43	0.43
1:A:282:TRP:O	1:A:286:VAL:HG23	2.18	0.43
3:G:57:TYR:OH	3:G:59:THR:HG23	2.19	0.42
2:F:192:THR:HG22	2:F:207:SER:HG	1.84	0.42
2:D:135:LEU:HD21	2:D:145:VAL:HG22	2.01	0.42
1:A:160:LEU:C	1:A:160:LEU:HD23	2.45	0.42
2:D:34:TRP:HA	2:D:86:TYR:O	2.19	0.42
2:D:95:PRO:HG2	3:E:47:TRP:CG	2.55	0.42
1:B:230:TYR:O	1:B:234:VAL:HG23	2.20	0.42
1:A:154:ILE:N	1:A:155:PRO:CD	2.82	0.42
1:B:30:THR:HG23	1:B:31:THR:N	2.35	0.42
3:G:57:TYR:OH	3:G:59:THR:CG2	2.68	0.42
2:F:35:TYR:HH	3:G:103:PHE:HD2	1.67	0.42
2:F:45:ARG:NH2	6:F:306:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:180:LEU:C	3:G:180:LEU:CD1	2.92	0.42
1:A:276:LEU:HA	1:A:279:ILE:CG2	2.48	0.42
1:A:28:ARG:HB2	1:A:31:THR:CG2	2.49	0.41
1:A:156:LEU:HD21	1:B:38:LEU:CD2	2.50	0.41
1:A:258:GLN:N	1:A:259:PRO:HD2	2.34	0.41
1:A:283:LEU:HB2	1:B:159:ILE:HD11	2.01	0.41
3:E:28:SER:HB2	3:G:28:SER:HB2	2.01	0.41
2:D:192:THR:HG22	2:D:207:SER:HG	1.84	0.41
2:F:89:GLN:NE2	2:F:92:ASN:H	2.15	0.41
1:B:28:ARG:HB2	1:B:31:THR:OG1	2.21	0.41
3:G:72:VAL:N	6:G:425:HOH:O	2.33	0.41
1:A:35:LEU:HD12	1:A:35:LEU:HA	1.90	0.41
1:A:275:VAL:O	1:A:279:ILE:HG22	2.21	0.41
2:D:111:ALA:HB2	2:D:199:THR:HG21	2.02	0.41
2:D:208:PHE:CD1	2:D:208:PHE:C	2.99	0.41
2:D:137:ASN:ND2	3:E:167:HIS:HE1	2.18	0.41
2:F:208:PHE:CD1	2:F:208:PHE:C	2.98	0.41
1:A:30:THR:HG23	1:A:31:THR:N	2.36	0.41
1:B:35:LEU:HD12	1:B:35:LEU:HA	1.88	0.41
2:F:72:LEU:C	2:F:72:LEU:CD2	2.94	0.41
1:A:55:GLN:N	1:A:56:PRO:CD	2.84	0.40
2:F:118:PRO:HB3	2:F:208:PHE:CZ	2.56	0.40
2:D:25:ALA:O	2:D:68:THR:OG1	2.39	0.40
3:E:76:SER:O	3:E:77:SER:C	2.64	0.40
2:D:183:ASP:O	2:D:187:ARG:HG3	2.21	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]	2.14	0.06

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	249/299 (83%)	243 (98%)	6 (2%)	0	100	100
1	B	251/299 (84%)	244 (97%)	7 (3%)	0	100	100
2	D	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
2	F	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
3	E	207/217 (95%)	202 (98%)	4 (2%)	1 (0%)	24	60
3	G	206/217 (95%)	200 (97%)	5 (2%)	1 (0%)	24	60
All	All	1331/1454 (92%)	1296 (97%)	33 (2%)	2 (0%)	43	76

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%)	81	89
1	B	208/242 (86%)	205 (99%)	3 (1%)	59	80
2	D	184/184 (100%)	179 (97%)	5 (3%)	39	71
2	F	184/184 (100%)	179 (97%)	5 (3%)	39	71
3	E	187/190 (98%)	182 (97%)	5 (3%)	39	71
3	G	186/190 (98%)	181 (97%)	5 (3%)	39	71
All	All	1153/1232 (94%)	1129 (98%)	24 (2%)	47	75

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	PHE
1	B	116	LEU
1	B	176	ILE
1	B	272	PHE
2	D	21	MET
2	D	42	SER
2	D	89	GLN
2	D	104	GLU
2	D	211	ASN
3	E	18	MET
3	E	59	THR
3	E	136	ASN
3	E	143	CYS
3	E	207	THR
2	F	21	MET
2	F	42	SER
2	F	89	GLN
2	F	122	GLU
2	F	143	ILE
3	G	18	MET
3	G	136	ASN
3	G	143	CYS
3	G	144	LEU
3	G	207	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	B	59	GLN
2	D	88	GLN
2	D	137	ASN
2	D	209	ASN
3	E	136	ASN
3	E	167	HIS
2	F	88	GLN
3	G	136	ASN

5.3.3 RNA ⓘ

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 11 ligands modelled in this entry, 11 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	253/299 (84%)	0.58	32 (12%) 8 5	66, 130, 185, 197	0
1	B	255/299 (85%)	0.81	38 (14%) 5 3	63, 132, 227, 242	0
2	D	211/211 (100%)	0.03	15 (7%) 22 11	64, 96, 136, 153	0
2	F	211/211 (100%)	-0.01	11 (5%) 33 17	59, 95, 160, 175	0
3	E	211/217 (97%)	0.06	12 (5%) 29 15	55, 83, 116, 168	0
3	G	210/217 (96%)	0.02	10 (4%) 35 19	57, 89, 128, 191	0
All	All	1351/1454 (92%)	0.28	118 (8%) 16 8	55, 99, 183, 242	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	201	THR	8.0
3	G	41	HIS	7.5
1	B	278	THR	6.8
3	E	41	HIS	6.4
1	B	148	PHE	6.2
1	A	248	ALA	6.1
2	D	41	THR	5.6
1	B	275	VAL	5.5
1	B	151	LEU	5.4
1	B	152	VAL	5.4
2	F	1	GLN	5.4
2	F	202	SER	5.3
1	A	222	ASP	5.3
1	A	269	LEU	5.1
3	E	42	GLY	4.9
1	A	185	LYS	4.9
3	G	189	SER	4.7
1	A	262	TRP	4.6
3	G	136	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
2	D	40	GLY	4.6
1	B	276	LEU	4.5
2	F	162	TRP	4.5
3	E	1	GLU	4.4
1	B	243	ASP	4.1
2	D	105	LEU	4.1
1	B	89	LYS	4.0
1	A	136	ALA	4.0
1	A	135	VAL	4.0
2	D	42	SER	4.0
1	B	93	ASP	3.8
1	B	34	ALA	3.7
2	F	55	SER	3.7
1	A	273	ALA	3.7
1	B	242	GLY	3.6
2	D	39	SER	3.5
3	E	165	GLY	3.4
1	B	229	ILE	3.4
3	G	188	SER	3.4
1	B	279	ILE	3.4
3	E	183	SER	3.3
2	D	37	GLN	3.3
1	A	270	ALA	3.3
1	A	55	GLN	3.3
3	E	167	HIS	3.2
2	F	160	ASN	3.2
2	F	53	LEU	3.1
1	A	163	GLY	3.1
2	D	104	GLU	3.1
1	A	266	LEU	3.1
1	A	247	GLY	3.1
1	B	183	PHE	3.0
1	A	249	ASP	3.0
1	A	133	GLY	3.0
1	B	244	TYR	2.9
1	B	134	ASN	2.9
3	G	42	GLY	2.9
2	D	150	ASP	2.9
1	B	75	ALA	2.9
3	E	26	GLY	2.9
1	A	137	LEU	2.9
1	A	259	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	111	THR	2.8
3	E	2	VAL	2.8
3	G	137	SER	2.8
2	F	164	ASP	2.8
3	E	166	VAL	2.7
1	B	179	ILE	2.7
1	B	228	ALA	2.7
1	B	234	VAL	2.7
3	G	40	ARG	2.6
2	F	52	LYS	2.6
3	G	151	GLU	2.6
1	A	58	GLU	2.6
1	A	286	VAL	2.6
1	B	181	ALA	2.6
1	B	232	VAL	2.6
1	A	60	GLN	2.5
1	B	192	LEU	2.5
1	A	121	PHE	2.5
2	D	162	TRP	2.5
2	F	59	ALA	2.4
3	E	209	VAL	2.4
1	A	182	ILE	2.4
1	A	161	LEU	2.4
1	B	248	ALA	2.4
1	B	256	ALA	2.3
3	E	162	LEU	2.3
1	B	193	VAL	2.3
1	A	110	SER	2.3
1	A	186	TRP	2.3
1	B	74	ARG	2.3
2	D	187	ARG	2.3
2	D	122	GLU	2.3
1	A	187	HIS	2.3
2	F	161	SER	2.3
3	G	165	GLY	2.2
1	A	176	ILE	2.2
3	G	138	MET	2.2
1	B	135	VAL	2.2
1	B	283	LEU	2.2
1	B	30	THR	2.2
1	B	245	VAL	2.2
1	B	161	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	177	GLY	2.1
1	A	157	PHE	2.1
1	B	247	GLY	2.1
1	A	281	ASN	2.1
1	B	225	LYS	2.1
1	B	230	TYR	2.1
1	A	175	GLY	2.1
1	B	210	VAL	2.0
2	D	44	LYS	2.0
2	D	160	ASN	2.0
1	A	215	PHE	2.0
1	A	272	PHE	2.0
2	D	38	LYS	2.0
1	B	262	TRP	2.0
2	D	168	LYS	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	TL	B	301	1/1	0.88	0.11	164,164,164,164	0
4	TL	B	302	1/1	0.90	0.11	164,164,164,164	0
4	TL	A	304	1/1	0.94	0.29	164,164,164,164	0
4	TL	B	303	1/1	0.94	0.21	164,164,164,164	0
5	CA	G	301	1/1	0.98	0.06	106,106,106,106	0
4	TL	A	301	1/1	0.99	0.02	106,106,106,106	0
5	CA	A	305	1/1	0.99	0.05	108,108,108,108	0
5	CA	A	306	1/1	0.99	0.04	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TL	A	307	1/1	0.99	0.02	103,103,103,103	0
4	TL	A	302	1/1	1.00	0.04	109,109,109,109	0
4	TL	A	303	1/1	1.00	0.06	118,118,118,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.