



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:00 PM GMT

PDB ID : 4WFG
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

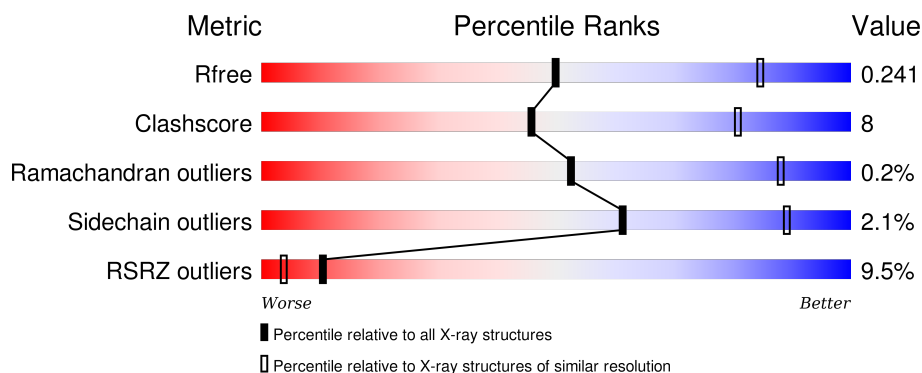
1 Overall quality at a glance

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.



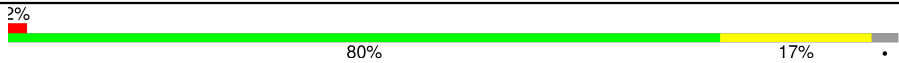
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>10%</div> <div>66%</div> <div>18%</div> <div>15%</div> </div>
1	B	299	<div> <div>23%</div> <div>69%</div> <div>16%</div> <div>15%</div> </div>
2	D	211	<div> <div>2%</div> <div>83%</div> <div>16%</div> <div>•</div> </div>
2	F	211	<div> <div>4%</div> <div>85%</div> <div>14%</div> <div>•</div> </div>
3	E	217	<div> <div>5%</div> <div>82%</div> <div>15%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	217	 A horizontal bar chart showing the quality of chain G. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '80%', a yellow segment labeled '17%', and a small grey segment at the end. A small black dot is located at the far right end of the bar.

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 (three-letter code: TL) (formula: Tl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Tl	0	0
			3	3		
4	A	5	Total	Tl	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	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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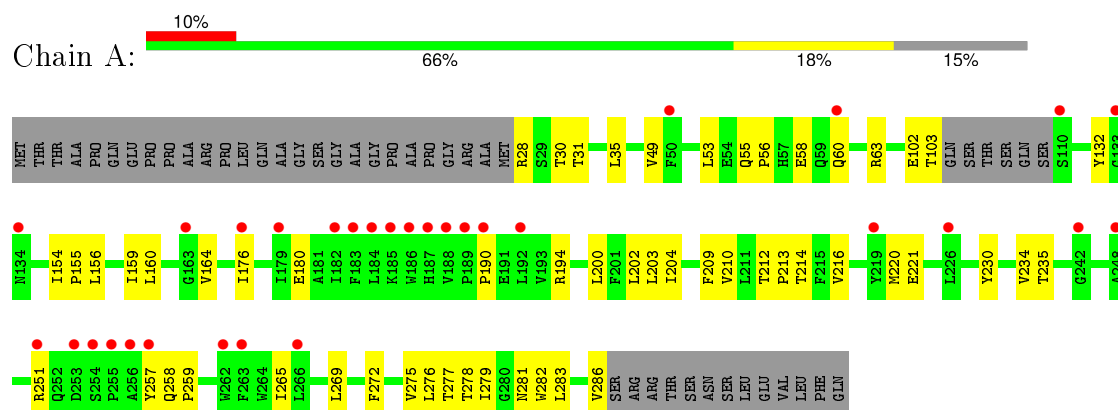
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	35	Total	O	0	0
			35	35		

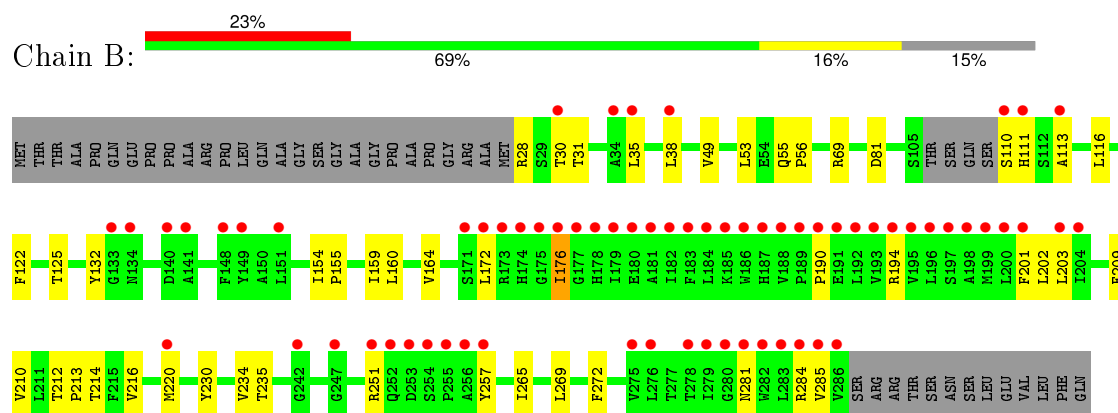
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

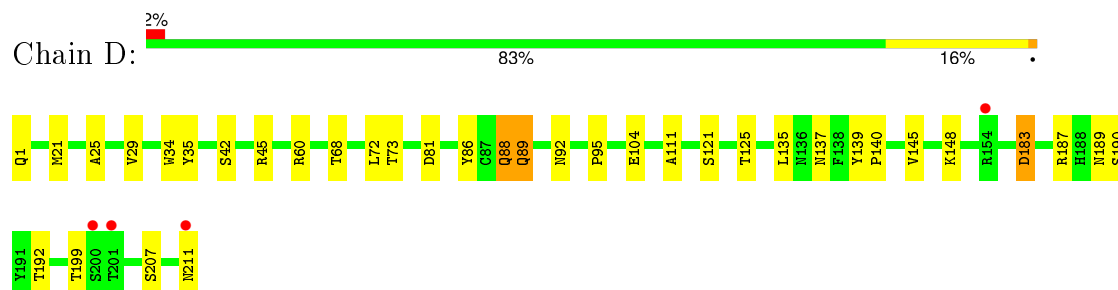
- Molecule 1: Potassium channel subfamily K member 4



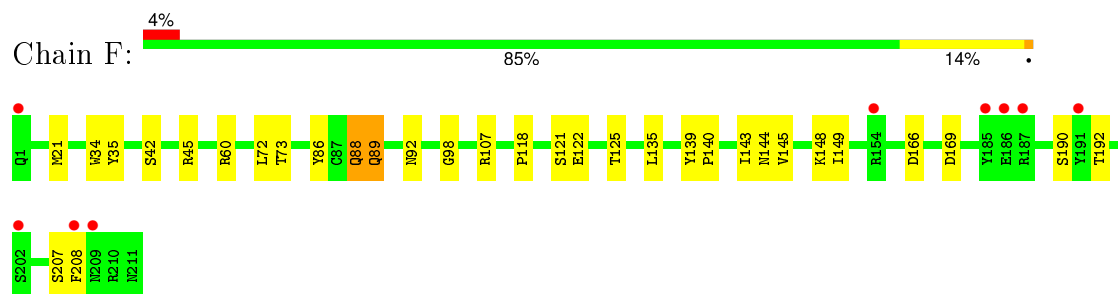
- Molecule 1: Potassium channel subfamily K member 4



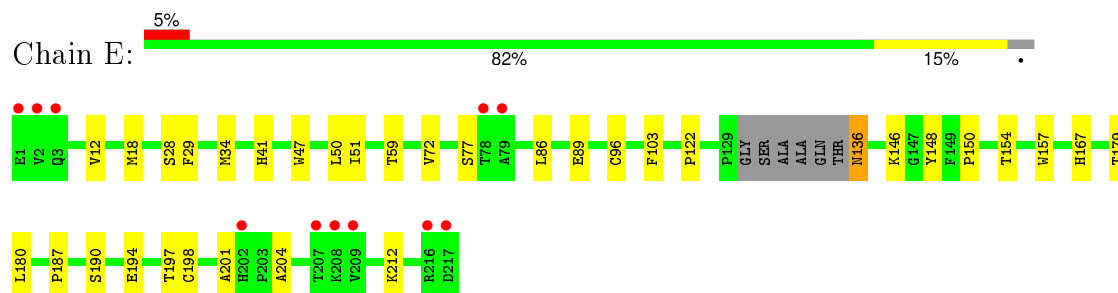
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



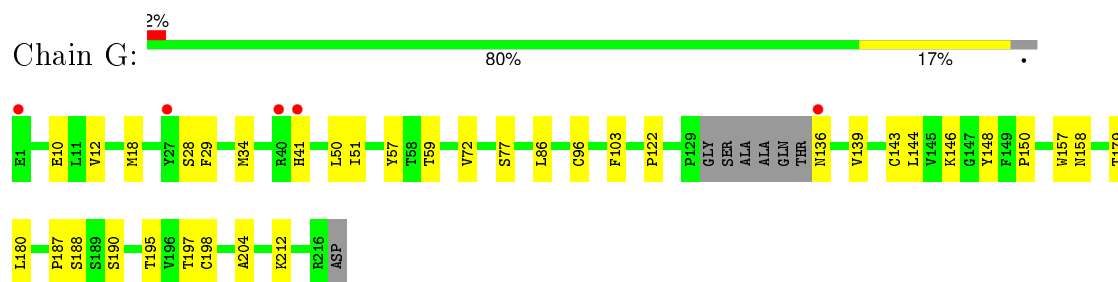
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



- 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	80.80 Å 138.76 Å 96.32 Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	48.00 – 3.00 48.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.00-3.00) 99.2 (48.01-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.01 Å)	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	2130 reflections (5.31%)	DCC
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 , 54.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 42275 reflections	Xtriage
F_o, F_c correlation	0.91	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.30	0/2013	0.43	0/2745
1	B	0.31	0/2035	0.44	0/2774
2	D	0.36	0/1655	0.50	0/2247
2	F	0.37	0/1655	0.51	0/2247
3	E	0.40	0/1656	0.54	0/2260
3	G	0.39	0/1647	0.56	0/2249
All	All	0.35	0/10661	0.50	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	37	0
1	B	1984	0	2005	33	0
2	D	1616	0	1542	27	0
2	F	1616	0	1542	23	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	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	158	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 (158) 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: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
1:B:38:LEU:HD23	1:B:38:LEU:C	2.17	0.65
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
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:180:LEU:C	3:E:180:LEU:HD12	2.21	0.61
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:THR:O	1:A:216:VAL:HG23	2.01	0.60
3:G:146:LYS:HB3	3:G:179:THR:HG23	1.83	0.60
3:E:146:LYS:HB3	3:E: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
3:G:180:LEU:HD12	3:G:180:LEU:C	2.24	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:NH1	1:B:251:ARG:HG2	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
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.34	0.57
2:D:192:THR:HG22	2:D:207:SER:OG	2.05	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
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:D:139:TYR:CG	2:D:140:PRO:HA	2.44	0.53
2:D:35:TYR:HH	3:E:103:PHE:HD2	1.57	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:209:PHE:O	1:A:213:PRO:HG2	2.11	0.51
1:A:176:ILE:HG22	1:A:180:GLU:OE2	2.11	0.51
2:F:121:SER:O	2:F:125:THR:HG23	2.11	0.50
1:B:209:PHE:O	1:B:213:PRO:HG2	2.12	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	1.93	0.50
3:G:122:PRO:HB3	3:G:148:TYR:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:199:THR:O	2:D:199:THR:HG22	2.13	0.49
1:A:210:VAL:O	1:A:214:THR:HG23	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
2:F:72:LEU:HD23	2:F:72:LEU:C	2.34	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
2:F:35:TYR:HH	3:G:103:PHE:HD2	1.62	0.48
1:B:281:ASN:O	1:B:285:VAL:HG23	2.14	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
3:G:197:THR:HG23	6:G:401:HOH:O	2.14	0.47
1:A:55:GLN:N	1:A:56:PRO:HD2	2.29	0.47
3:E:150:PRO:HD2	3:E:204:ALA:CB	2.45	0.47
2:D:211:ASN:OD1	2:D:211:ASN:N	2.35	0.47
1:A:200:LEU:O	1:A:204:ILE:HG22	2.15	0.47
3:G:57:TYR:CZ	3:G:59:THR:HG23	2.49	0.47
2:D:1:GLN:HA	2:D:1:GLN:OE1	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:E:34:MET:HE1	3:E:96:CYS:HB2	1.98	0.46
3:G:50:LEU:C	3:G:50:LEU:HD12	2.36	0.46
3:G:29:PHE:CD1	3:G:77:SER:HA	2.51	0.46
2:D:89:GLN:NE2	2:D:92:ASN:H	2.14	0.46
1:B:49:VAL:HG12	1:B:53:LEU:HD12	1.98	0.46
2:F:45:ARG:NE	6:F:306:HOH:O	2.46	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
3:E:89:GLU:HA	3:E:89:GLU:OE2	2.17	0.44
2:D:45:ARG:NH1	6:D:318:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:149:ILE:HG13	2:F:149:ILE:O	2.17	0.44
1:A:49:VAL:HG12	1:A:53:LEU:HD12	1.99	0.44
3:E:89:GLU:HG2	6:E:304:HOH:O	2.18	0.44
3:E:50:LEU:HD12	3:E:50:LEU:C	2.37	0.44
3:G:150:PRO:HD2	3:G:204:ALA:CB	2.47	0.44
1:B:220:MET:HG3	1:B:257:TYR:CE1	2.52	0.44
1:A:230:TYR:O	1:A:234:VAL:HG23	2.18	0.43
3:G:34:MET:CE	3:G:96:CYS:HB2	2.48	0.43
2:D:199:THR:O	2:D:199:THR:CG2	2.66	0.43
3:G:158:ASN:OD1	6:G:401:HOH:O	2.21	0.43
1:A:278:THR:O	1:A:281:ASN:HB3	2.18	0.43
2:F:135:LEU:HD21	2:F:145:VAL:HG22	2.01	0.43
2:F:34:TRP:HA	2:F:86:TYR:O	2.18	0.43
3:G:187:PRO:O	3:G:190:SER:HB2	2.18	0.43
1:B:122:PHE:O	1:B:125:THR:OG1	2.22	0.43
1:A:282:TRP:O	1:A:286:VAL:HG23	2.18	0.43
2:D:72:LEU:C	2:D:72:LEU:HD23	2.38	0.43
3:G:34:MET:HE1	3:G:96:CYS:HB2	2.00	0.43
3:G:57:TYR:OH	3:G:59:THR:HG23	2.19	0.42
1:B:201:PHE:C	1:B:201:PHE:CD2	2.92	0.42
2:D:135:LEU:HD21	2:D:145:VAL:HG22	2.01	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
3:G:57:TYR:OH	3:G:59:THR:CG2	2.68	0.42
1:B:30:THR:HG23	1:B:31:THR:N	2.35	0.42
1:B:38:LEU:CD2	1:B:38:LEU:C	2.88	0.42
2:F:45:ARG:NH2	6:F:306:HOH:O	2.51	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:F:89:GLN:NE2	2:F:92:ASN:H	2.15	0.41
3:G:72:VAL:N	6:G:425:HOH:O	2.33	0.41
1:B:28:ARG:HB2	1:B:31:THR:OG1	2.21	0.41
1:A:275:VAL:O	1:A:279:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HA	1:A:35:LEU:HD12	1.90	0.41
2:D:111:ALA:HB2	2:D:199:THR:HG21	2.02	0.41
1:B:202:LEU:HD12	1:B:202:LEU:C	2.41	0.41
2:D:137:ASN:ND2	3:E:167:HIS:HE1	2.18	0.41
1:A:30:THR:HG23	1:A:31:THR:N	2.36	0.41
1:B:35:LEU:HA	1:B:35:LEU:HD12	1.88	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
1:A:202:LEU:C	1:A:202:LEU:HD12	2.41	0.40
2:D:25:ALA:O	2:D:68:THR:OG1	2.39	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 ⓘ

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%)	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%)	34	76
3	G	206/217 (95%)	200 (97%)	5 (2%)	1 (0%)	34	76
All	All	1331/1454 (92%)	1296 (97%)	33 (2%)	2 (0%)	52	88

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%)	92	98
1	B	208/242 (86%)	205 (99%)	3 (1%)	74	93
2	D	184/184 (100%)	177 (96%)	7 (4%)	40	78
2	F	184/184 (100%)	178 (97%)	6 (3%)	45	82
3	E	187/190 (98%)	184 (98%)	3 (2%)	70	92
3	G	186/190 (98%)	182 (98%)	4 (2%)	60	88
All	All	1153/1232 (94%)	1129 (98%)	24 (2%)	61	89

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	88	GLN
2	D	89	GLN
2	D	104	GLU
2	D	183	ASP
2	D	190	SER
3	E	18	MET
3	E	59	THR
3	E	136	ASN
2	F	21	MET

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Mol	Chain	Res	Type
2	F	42	SER
2	F	88	GLN
2	F	89	GLN
2	F	122	GLU
2	F	190	SER
3	G	18	MET
3	G	136	ASN
3	G	143	CYS
3	G	144	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.43	31 (12%) 5 2	66, 130, 185, 197	0
1	B	255/299 (85%)	1.68	68 (26%) 1 0	63, 132, 227, 242	0
2	D	211/211 (100%)	-0.32	4 (1%) 70 41	64, 96, 136, 153	0
2	F	211/211 (100%)	-0.20	9 (4%) 39 16	59, 95, 160, 175	0
3	E	211/217 (97%)	0.18	11 (5%) 31 12	55, 83, 116, 168	0
3	G	210/217 (96%)	-0.14	5 (2%) 62 32	57, 89, 128, 191	0
All	All	1351/1454 (92%)	0.32	128 (9%) 10 4	55, 99, 183, 242	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	ILE	20.8
1	B	181	ALA	17.9
1	B	183	PHE	16.6
1	B	180	GLU	16.3
1	B	182	ILE	12.8
1	B	176	ILE	11.8
1	B	178	HIS	10.8
1	B	186	TRP	10.3
1	B	184	LEU	10.2
1	B	193	VAL	9.7
1	B	197	SER	9.3
1	B	286	VAL	9.1
1	B	177	GLY	8.9
1	B	200	LEU	8.7
1	B	256	ALA	8.6
1	B	194	ARG	8.1
1	B	285	VAL	8.1
1	B	282	TRP	8.0
1	B	283	LEU	8.0

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Mol	Chain	Res	Type	RSRZ
3	E	217	ASP	7.9
1	B	190	PRO	7.7
1	A	183	PHE	7.4
1	B	278	THR	7.4
1	B	185	LYS	7.1
1	B	201	PHE	7.0
1	B	279	ILE	6.8
1	B	275	VAL	6.6
3	E	1	GLU	6.1
1	B	172	LEU	6.0
1	B	192	LEU	6.0
1	B	255	PRO	6.0
1	A	188	VAL	5.9
1	B	253	ASP	5.8
1	B	187	HIS	5.6
1	B	188	VAL	5.5
1	B	195	VAL	5.1
1	B	254	SER	4.9
1	B	199	MET	4.8
1	A	184	LEU	4.8
1	B	280	GLY	4.7
1	A	187	HIS	4.7
1	B	257	TYR	4.6
1	A	189	PRO	4.6
1	B	175	GLY	4.6
3	G	1	GLU	4.5
1	B	196	LEU	4.4
1	B	191	GLU	4.3
3	G	41	HIS	4.3
3	E	216	ARG	4.2
1	B	173	ARG	4.2
2	F	208	PHE	4.2
1	B	204	ILE	4.2
1	A	186	TRP	4.0
1	B	189	PRO	4.0
3	G	136	ASN	4.0
1	B	174	HIS	3.8
1	B	34	ALA	3.7
3	E	3	GLN	3.7
1	A	253	ASP	3.6
1	B	171	SER	3.5
2	F	186	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	140	ASP	3.5
1	B	284	ARG	3.4
1	A	179	ILE	3.4
2	F	209	ASN	3.4
1	A	257	TYR	3.4
1	B	198	ALA	3.3
1	B	242	GLY	3.3
2	F	185	TYR	3.3
1	A	134	ASN	3.2
1	A	110	SER	3.2
1	A	60	GLN	3.2
1	A	251	ARG	3.1
2	F	154	ARG	3.0
1	A	133	GLY	3.0
3	E	209	VAL	3.0
1	B	281	ASN	2.9
1	A	190	PRO	2.9
1	B	111	HIS	2.9
1	B	276	LEU	2.9
3	E	79	ALA	2.8
1	A	50	PHE	2.8
2	D	201	THR	2.8
1	A	185	LYS	2.8
1	A	182	ILE	2.7
1	A	219	TYR	2.7
1	B	30	THR	2.7
1	B	38	LEU	2.6
1	B	148	PHE	2.6
2	D	154	ARG	2.5
1	A	226	LEU	2.5
2	D	200	SER	2.5
2	F	187	ARG	2.5
2	F	191	TYR	2.5
1	B	220	MET	2.5
1	A	263	PHE	2.4
1	B	134	ASN	2.4
3	E	202	HIS	2.4
1	A	256	ALA	2.3
1	B	151	LEU	2.3
1	B	149	TYR	2.3
1	B	252	GLN	2.3
1	B	110	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	78	THR	2.2
2	F	1	GLN	2.2
1	A	255	PRO	2.2
1	B	35	LEU	2.2
3	E	2	VAL	2.2
3	E	208	LYS	2.1
1	A	266	LEU	2.1
1	A	176	ILE	2.1
2	F	202	SER	2.1
1	B	133	GLY	2.1
1	A	192	LEU	2.1
1	B	113	ALA	2.1
1	B	203	LEU	2.1
3	E	207	THR	2.0
1	B	247	GLY	2.0
1	A	248	ALA	2.0
1	A	254	SER	2.0
3	G	40	ARG	2.0
1	A	242	GLY	2.0
1	A	262	TRP	2.0
2	D	211	ASN	2.0
3	G	27	TYR	2.0
1	B	141	ALA	2.0
1	B	251	ARG	2.0
1	A	163	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	A	305	1/1	0.95	0.11	-1.07	108,108,108,108	0
4	TL	A	303	1/1	0.99	0.08	-2.08	118,118,118,118	0
5	CA	A	306	1/1	0.92	0.09	-2.17	111,111,111,111	0
4	TL	A	307	1/1	0.99	0.11	-2.88	103,103,103,103	0
4	TL	A	302	1/1	0.99	0.09	-3.07	109,109,109,109	0
4	TL	A	301	1/1	0.99	0.11	-4.20	106,106,106,106	0
4	TL	B	303	1/1	0.96	0.31	-	164,164,164,164	0
5	CA	G	301	1/1	0.97	0.12	-	106,106,106,106	0
4	TL	B	301	1/1	0.85	0.09	-	164,164,164,164	0
4	TL	B	302	1/1	0.89	0.07	-	164,164,164,164	0
4	TL	A	304	1/1	0.97	0.37	-	164,164,164,164	0

6.5 Other polymers [i](#)

There are no such residues in this entry.