



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:00 PM UTC

PDB ID : 4WFF / pdb_00004wff
Title : Human TRAAK K⁺ channel in a K⁺ bound nonconductive 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

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
Mogul : 2022.3.0, CSD as543be (2022)
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

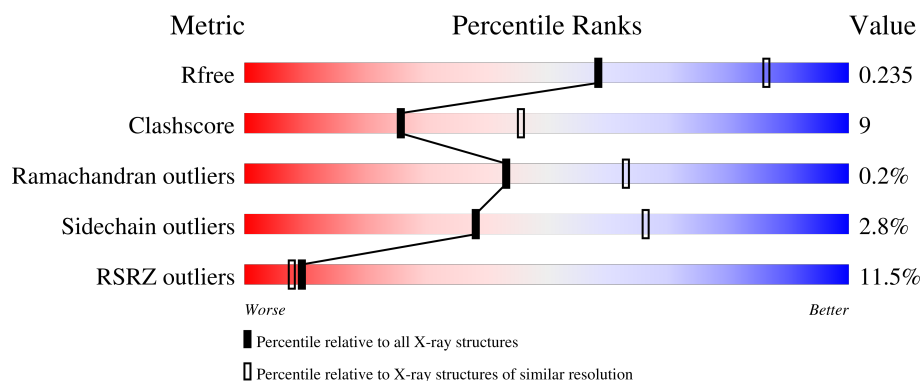
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	13% 67% 17% 15%
1	B	299	19% 66% 17% 15%
2	D	211	7% 83% 15% .
2	F	211	9% 84% 14% .
3	E	217	5% 77% 18% ..

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Mol	Chain	Length	Quality of chain
3	G	217	5% 76% 19% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10585 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	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			

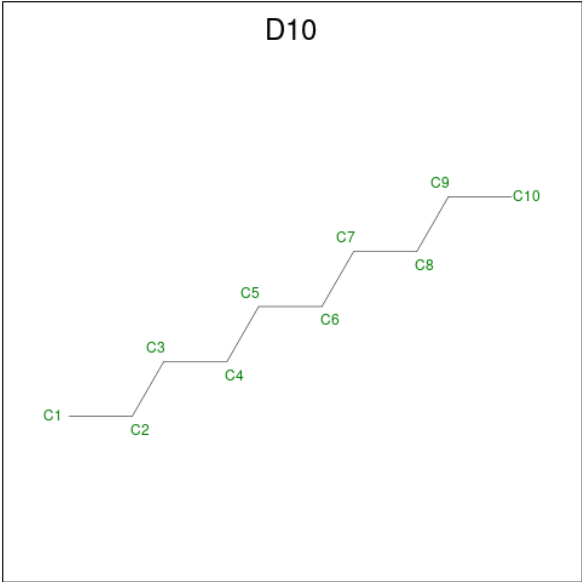
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	K	0	0
			4	4		
4	B	1	Total	K	0	0
			1	1		

- 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 DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	C	0	0
			10	10		

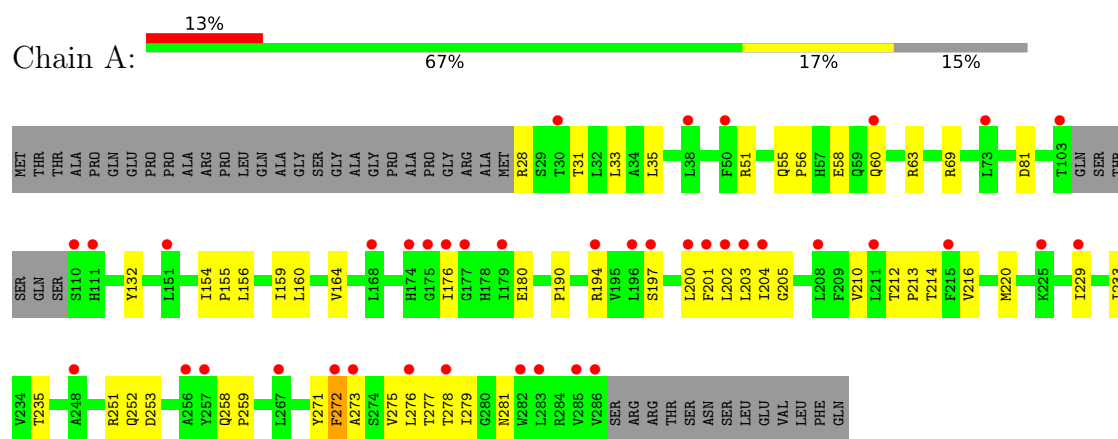
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	24	Total	O	0	0
			24	24		
7	B	20	Total	O	0	0
			20	20		
7	D	24	Total	O	0	0
			24	24		
7	E	50	Total	O	0	0
			50	50		
7	F	33	Total	O	0	0
			33	33		
7	G	32	Total	O	0	0
			32	32		

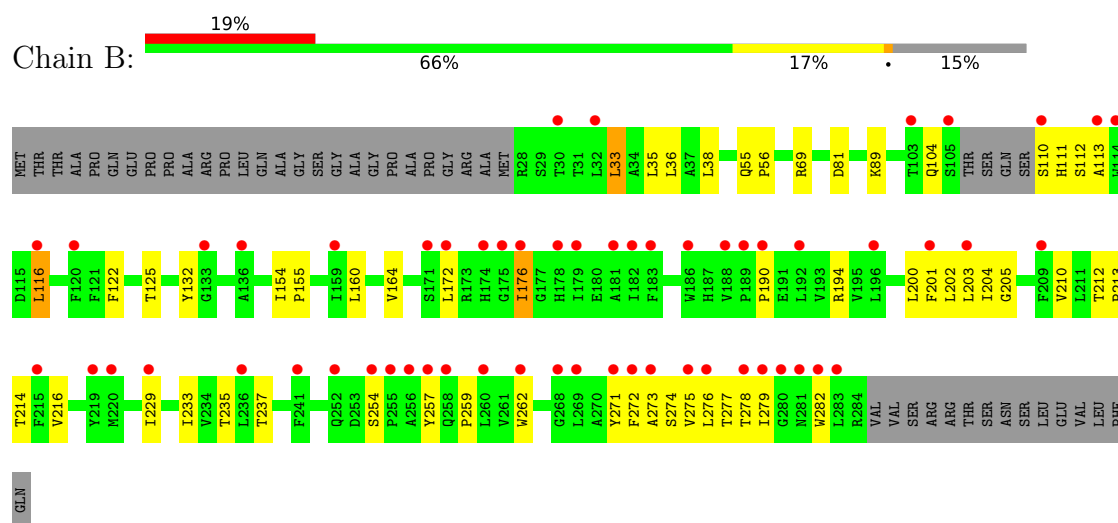
3 Residue-property plots [i](#)

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.

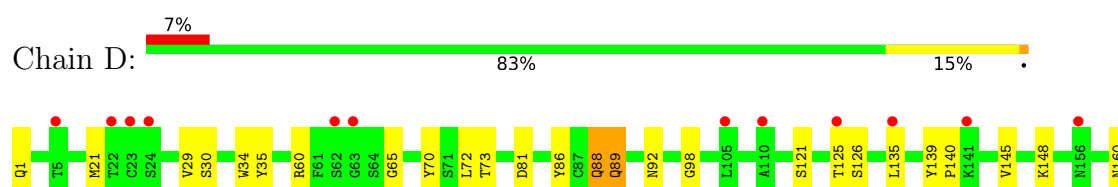
- Molecule 1: Potassium channel subfamily K member 4



- Molecule 1: Potassium channel subfamily K member 4

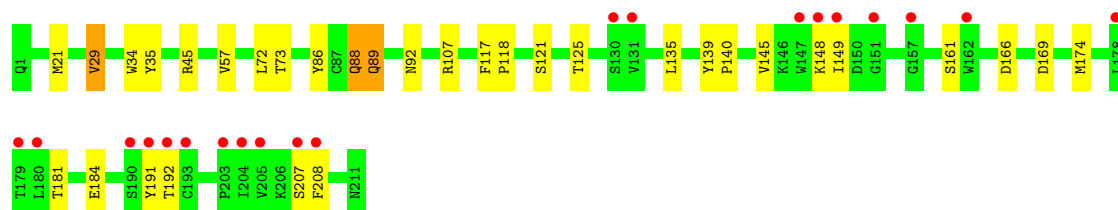
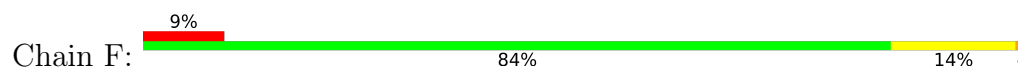


- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN

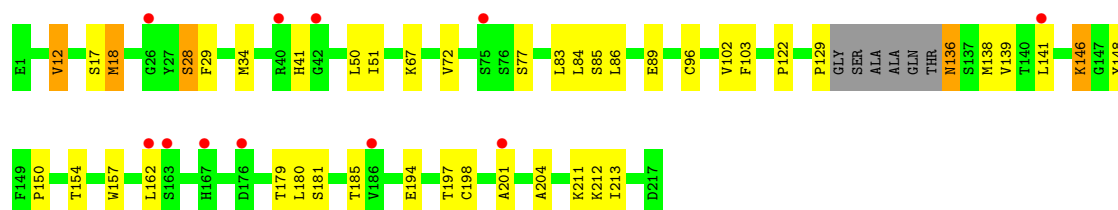
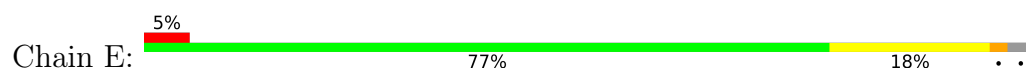




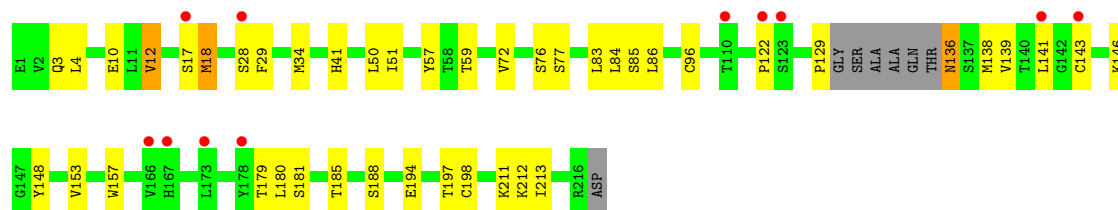
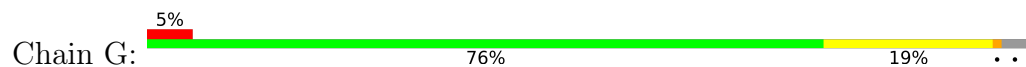
● Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



● 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	80.67Å 138.89Å 96.53Å 90.00° 95.15° 90.00°	Depositor
Resolution (Å)	48.10 – 2.50 48.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.10-2.50) 99.2 (48.10-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.213 , 0.245 (Not available) , 0.235	Depositor DCC
R_{free} test set	3632 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10585	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D10, 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	0.54	0/2013	0.75	0/2745
1	B	0.54	0/2021	0.75	1/2754 (0.0%)
2	D	0.56	0/1655	0.76	0/2247
2	F	0.58	0/1655	0.74	1/2247 (0.0%)
3	E	0.67	0/1656	0.78	1/2260 (0.0%)
3	G	0.64	0/1647	0.78	0/2249
All	All	0.59	0/10647	0.76	3/14502 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	146	LYS	N-CA-C	5.51	118.21	109.50
1	B	89	LYS	N-CA-C	-5.36	105.44	111.28
2	F	57	VAL	N-CA-C	5.21	113.11	108.63

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	1984	45	0
1	B	1970	0	1988	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1616	0	1542	27	0
2	F	1616	0	1542	27	0
3	E	1614	0	1586	29	1
3	G	1605	0	1582	32	1
4	A	4	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	G	1	0	0	0	0
6	B	10	0	22	6	0
7	A	24	0	0	1	0
7	B	20	0	0	1	0
7	D	24	0	0	3	0
7	E	50	0	0	3	0
7	F	33	0	0	4	0
7	G	32	0	0	3	0
All	All	10585	0	10246	196	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 (196) 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)
1:B:272:PHE:CD2	6:B:302:D10:H92	1.97	0.99
2:F:35:TYR:HE1	2:F:88:GLN:HG2	1.32	0.94
2:D:35:TYR:HE2	2:D:88:GLN:HG2	1.37	0.90
3:E:89:GLU:HG2	7:E:303:HOH:O	1.77	0.83
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.61	0.80
1:B:272:PHE:HD2	6:B:302:D10:H92	1.43	0.79
2:F:35:TYR:CE1	2:F:88:GLN:HG2	2.18	0.78
2:D:72:LEU:HD23	2:D:73:THR:N	1.99	0.77
6:B:302:D10:H12	6:B:302:D10:H52	1.66	0.75
2:F:72:LEU:HD23	2:F:73:THR:N	2.01	0.74
2:D:35:TYR:CE2	2:D:88:GLN:HG2	2.20	0.74
1:A:60:GLN:OE1	1:A:63:ARG:NH2	2.21	0.73
1:B:69:ARG:NH1	1:B:81:ASP:OD1	2.20	0.72
1:A:58:GLU:OE2	1:B:113:ALA:N	2.22	0.72
1:A:212:THR:HB	1:A:213:PRO:HD3	1.71	0.72
1:B:212:THR:HB	1:B:213:PRO:HD3	1.71	0.71
3:G:197:THR:HG22	3:G:212:LYS:HA	1.72	0.71
2:D:189:ASN:ND2	2:D:211:ASN:OD1	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:MET:O	1:A:251:ARG:NH2	2.25	0.69
3:E:51:ILE:HD13	3:E:72:VAL:HG13	1.74	0.69
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.26	0.69
3:E:157:TRP:CZ3	3:E:198:CYS:HB3	2.29	0.67
3:G:139:VAL:CG2	3:G:188:SER:HB3	2.25	0.67
6:B:302:D10:H12	6:B:302:D10:C5	2.24	0.66
3:G:180:LEU:HD12	3:G:180:LEU:C	2.20	0.66
1:A:202:LEU:O	1:A:271:TYR:OH	2.14	0.66
2:D:1:GLN:HA	2:D:1:GLN:OE1	1.96	0.66
3:G:51:ILE:HD13	3:G:72:VAL:HG13	1.76	0.66
2:D:98:GLY:O	7:D:321:HOH:O	2.12	0.66
3:E:28:SER:HB3	3:G:28:SER:HB3	1.76	0.65
3:G:157:TRP:CZ3	3:G:198:CYS:HB3	2.33	0.64
2:F:148:LYS:HB2	2:F:192:THR:OG1	1.97	0.64
3:G:139:VAL:HG23	3:G:188:SER:HB3	1.79	0.64
3:E:180:LEU:C	3:E:180:LEU:HD12	2.23	0.64
2:D:148:LYS:HB2	2:D:192:THR:OG1	1.97	0.63
2:F:89:GLN:HE21	2:F:92:ASN:H	1.45	0.63
3:G:146:LYS:HB3	3:G:179:THR:HG23	1.81	0.63
1:A:276:LEU:HA	1:A:279:ILE:HG22	1.80	0.62
2:D:89:GLN:HE21	2:D:92:ASN:H	1.47	0.62
2:F:121:SER:O	2:F:125:THR:HG23	2.00	0.62
1:A:69:ARG:NH1	1:A:81:ASP:OD1	2.32	0.61
3:E:154:THR:OG1	3:E:201:ALA:HB3	1.99	0.61
3:E:146:LYS:HB3	3:E:179:THR:HG23	1.81	0.61
1:B:190:PRO:O	1:B:194:ARG:HG2	2.00	0.60
2:D:121:SER:O	2:D:125:THR:HG23	2.01	0.60
2:D:126:SER:OG	7:D:315:HOH:O	2.16	0.60
1:B:202:LEU:HA	1:B:271:TYR:OH	2.02	0.60
1:A:205:GLY:HA3	1:A:271:TYR:CE1	2.36	0.60
1:B:38:LEU:C	1:B:38:LEU:HD23	2.27	0.59
1:B:172:LEU:O	1:B:176:ILE:HD12	2.02	0.59
1:A:190:PRO:O	1:A:194:ARG:HG2	2.02	0.59
1:B:212:THR:O	1:B:216:VAL:HG23	2.02	0.59
2:F:166:ASP:HB3	2:F:169:ASP:OD1	2.03	0.59
1:B:69:ARG:HD3	7:B:401:HOH:O	2.02	0.58
2:D:192:THR:HG22	2:D:207:SER:OG	2.03	0.58
2:F:192:THR:HG22	2:F:207:SER:OG	2.04	0.58
1:A:159:ILE:HG22	1:B:35:LEU:HD21	1.85	0.58
1:A:212:THR:O	1:A:216:VAL:HG23	2.04	0.58
3:G:194:GLU:HG2	7:G:404:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:57:TYR:CE1	3:G:59:THR:HG23	2.40	0.57
1:B:273:ALA:O	1:B:277:THR:HG23	2.04	0.57
3:E:136:ASN:N	3:E:136:ASN:HD22	2.03	0.56
2:F:29:VAL:HG21	2:F:89:GLN:HG3	1.88	0.56
3:G:197:THR:HG23	7:G:407:HOH:O	2.05	0.56
1:B:278:THR:O	1:B:282:TRP:CD1	2.58	0.56
1:B:55:GLN:N	1:B:56:PRO:CD	2.69	0.56
3:E:136:ASN:N	3:E:136:ASN:ND2	2.52	0.56
1:A:202:LEU:HA	1:A:271:TYR:OH	2.07	0.55
1:B:274:SER:O	1:B:278:THR:HG23	2.06	0.55
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.88	0.55
3:G:12:VAL:HG21	3:G:86:LEU:HD12	1.89	0.54
2:F:135:LEU:HD21	2:F:145:VAL:HG22	1.89	0.54
3:G:50:LEU:C	3:G:50:LEU:HD12	2.31	0.54
1:A:154:ILE:N	1:A:155:PRO:HD2	2.22	0.54
2:D:135:LEU:HD21	2:D:145:VAL:HG22	1.90	0.54
1:A:55:GLN:N	1:A:56:PRO:CD	2.71	0.54
2:D:139:TYR:CG	2:D:140:PRO:HA	2.43	0.54
2:F:139:TYR:CG	2:F:140:PRO:HA	2.43	0.53
1:B:154:ILE:N	1:B:155:PRO:HD2	2.22	0.53
1:A:132:TYR:OH	1:A:235:THR:HG23	2.08	0.53
3:E:122:PRO:HB3	3:E:148:TYR:HB3	1.91	0.52
3:G:122:PRO:HB3	3:G:148:TYR:HB3	1.90	0.52
1:B:214:THR:HG21	1:B:229:ILE:HG12	1.91	0.52
1:A:275:VAL:O	1:A:279:ILE:HG22	2.10	0.51
3:E:138:MET:HE3	3:E:185:THR:HG22	1.93	0.51
3:G:136:ASN:N	3:G:136:ASN:ND2	2.57	0.51
2:F:149:ILE:HG22	2:F:191:TYR:CE1	2.45	0.51
1:A:214:THR:HG21	1:A:229:ILE:HG12	1.91	0.51
3:E:50:LEU:C	3:E:50:LEU:HD12	2.35	0.51
1:A:273:ALA:O	1:A:277:THR:HG23	2.11	0.50
1:B:202:LEU:HD12	1:B:203:LEU:N	2.27	0.50
3:G:29:PHE:CD2	3:G:77:SER:HA	2.47	0.50
1:A:69:ARG:HD2	7:A:402:HOH:O	2.12	0.50
3:G:138:MET:HE3	3:G:185:THR:HG22	1.93	0.49
1:A:200:LEU:O	1:A:204:ILE:HG22	2.13	0.49
3:G:57:TYR:OH	3:G:59:THR:CG2	2.61	0.49
3:G:197:THR:HG22	3:G:212:LYS:CA	2.42	0.49
3:E:29:PHE:CD2	3:E:77:SER:HA	2.48	0.49
1:B:132:TYR:OH	1:B:235:THR:HG23	2.13	0.48
2:D:29:VAL:CG1	2:D:89:GLN:HG3	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:57:TYR:CZ	3:G:59:THR:HG23	2.48	0.48
1:B:205:GLY:HA3	1:B:271:TYR:CZ	2.48	0.48
2:D:192:THR:HG22	2:D:207:SER:CB	2.44	0.48
1:A:202:LEU:HD12	1:A:203:LEU:N	2.29	0.48
1:B:254:SER:HB3	1:B:257:TYR:CB	2.44	0.48
2:F:192:THR:HG22	2:F:207:SER:CB	2.44	0.48
1:A:258:GLN:N	1:A:259:PRO:HD2	2.29	0.47
1:B:160:LEU:O	1:B:164:VAL:HG23	2.14	0.47
2:F:192:THR:HG22	2:F:207:SER:HG	1.79	0.47
2:F:45:ARG:NE	7:F:304:HOH:O	2.47	0.47
1:B:201:PHE:CD1	1:B:201:PHE:C	2.92	0.47
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.44	0.47
1:A:277:THR:O	1:A:281:ASN:N	2.47	0.47
1:B:259:PRO:O	1:B:262:TRP:HB3	2.14	0.47
1:A:272:PHE:O	1:A:276:LEU:HD23	2.15	0.47
1:A:160:LEU:O	1:A:164:VAL:HG23	2.14	0.47
1:A:176:ILE:HG22	1:A:180:GLU:OE2	2.15	0.47
2:D:211:ASN:OD1	2:D:211:ASN:N	2.36	0.47
3:E:129:PRO:HD3	3:E:141:LEU:HD23	1.96	0.46
1:B:110:SER:O	1:B:111:HIS:HB3	2.15	0.46
1:B:200:LEU:O	1:B:204:ILE:HG22	2.16	0.46
2:F:72:LEU:HD23	2:F:72:LEU:C	2.41	0.46
3:G:136:ASN:N	3:G:136:ASN:HD22	2.14	0.46
1:A:160:LEU:CD1	1:B:36:LEU:HA	2.46	0.46
1:B:272:PHE:O	1:B:276:LEU:HG	2.16	0.45
1:A:210:VAL:O	1:A:214:THR:HG23	2.16	0.45
2:F:29:VAL:CG2	2:F:89:GLN:HG3	2.45	0.45
3:G:198:CYS:C	7:G:429:HOH:O	2.58	0.45
1:A:176:ILE:HD11	1:A:201:PHE:HA	1.98	0.45
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.46	0.45
1:A:278:THR:O	1:A:281:ASN:HB3	2.16	0.45
3:G:129:PRO:HD3	3:G:141:LEU:HD23	1.97	0.45
2:D:192:THR:HG22	2:D:207:SER:HG	1.80	0.45
3:E:84:LEU:O	3:E:85:SER:C	2.59	0.44
3:E:197:THR:HG22	3:E:212:LYS:HA	1.98	0.44
3:E:83:LEU:HB3	3:E:86:LEU:HD21	1.99	0.44
3:E:18:MET:C	3:E:18:MET:SD	3.01	0.44
3:E:141:LEU:HD22	3:E:213:ILE:HG21	1.99	0.44
3:G:17:SER:HB2	3:G:83:LEU:O	2.17	0.44
2:F:72:LEU:HD23	2:F:73:THR:H	1.82	0.44
2:F:89:GLN:NE2	2:F:92:ASN:H	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:ILE:HG13	2:F:149:ILE:O	2.18	0.44
1:B:55:GLN:N	1:B:56:PRO:HD2	2.33	0.44
1:A:202:LEU:C	1:A:271:TYR:HH	2.23	0.44
1:B:237:THR:HA	6:B:302:D10:H91	1.99	0.44
2:F:107:ARG:HB2	7:F:325:HOH:O	2.17	0.44
2:F:117:PHE:HA	2:F:118:PRO:HD3	1.89	0.43
1:B:122:PHE:O	1:B:125:THR:OG1	2.31	0.43
3:G:141:LEU:HD22	3:G:213:ILE:HG21	1.99	0.43
1:A:252:GLN:O	1:A:253:ASP:CB	2.67	0.43
2:D:60:ARG:HH11	2:D:81:ASP:CG	2.27	0.43
2:F:34:TRP:HA	2:F:86:TYR:O	2.19	0.43
3:E:17:SER:HB2	3:E:83:LEU:O	2.19	0.43
1:A:277:THR:O	1:A:281:ASN:HB2	2.19	0.43
2:D:65:GLY:HA3	2:D:70:TYR:HA	2.00	0.43
6:B:302:D10:C5	6:B:302:D10:C1	2.93	0.43
3:G:76:SER:O	3:G:77:SER:C	2.62	0.43
1:A:252:GLN:O	1:A:253:ASP:HB2	2.19	0.43
1:B:275:VAL:O	1:B:279:ILE:HG13	2.18	0.43
1:A:33:LEU:O	1:A:33:LEU:HD23	2.19	0.42
2:D:72:LEU:HD23	2:D:72:LEU:C	2.44	0.42
1:A:28:ARG:HB2	1:A:31:THR:HG23	2.02	0.42
2:F:45:ARG:NH2	7:F:332:HOH:O	2.49	0.42
3:G:3:GLN:C	3:G:4:LEU:HD12	2.44	0.42
2:D:34:TRP:HA	2:D:86:TYR:O	2.20	0.42
3:G:18:MET:SD	3:G:18:MET:C	3.03	0.42
1:A:55:GLN:N	1:A:56:PRO:HD2	2.34	0.42
1:A:202:LEU:CA	1:A:271:TYR:OH	2.68	0.42
3:E:150:PRO:HD2	3:E:204:ALA:CB	2.50	0.42
3:G:84:LEU:O	3:G:85:SER:C	2.62	0.42
1:B:201:PHE:HE1	1:B:275:VAL:HG22	1.85	0.41
3:E:102:VAL:HG22	3:E:103:PHE:N	2.35	0.41
1:A:276:LEU:HA	1:A:279:ILE:CG2	2.48	0.41
1:B:202:LEU:HD12	1:B:202:LEU:C	2.46	0.41
3:E:180:LEU:C	3:E:180:LEU:CD1	2.93	0.41
3:E:139:VAL:HA	7:E:346:HOH:O	2.20	0.41
2:F:208:PHE:CD1	2:F:208:PHE:C	2.98	0.41
3:G:34:MET:CE	3:G:96:CYS:HB2	2.50	0.41
2:D:208:PHE:CD1	2:D:208:PHE:C	2.99	0.41
3:E:34:MET:CE	3:E:96:CYS:HB2	2.51	0.41
1:A:176:ILE:HG21	1:A:197:SER:HB2	2.02	0.41
2:D:160:ASN:N	7:D:308:HOH:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:148:TYR:CE2	3:G:153:VAL:HG13	2.55	0.41
1:A:58:GLU:CD	1:B:112:SER:HG	2.28	0.40
1:A:156:LEU:HD21	1:B:38:LEU:CD2	2.50	0.40
1:B:33:LEU:HD13	1:B:33:LEU:HA	1.88	0.40
2:F:166:ASP:OD1	7:F:326:HOH:O	2.22	0.40
1:A:51:ARG:HE	1:B:116:LEU:HD23	1.86	0.40
3:E:154:THR:HG1	3:E:201:ALA:HB3	1.86	0.40
3:E:162:LEU:HA	7:E:337:HOH:O	2.20	0.40
2:F:181:THR:HG23	2:F:184:GLU:H	1.85	0.40
1:B:210:VAL:O	1:B:214:THR:HG23	2.21	0.40
1:A:35:LEU:HD12	1:A:35:LEU:HA	1.92	0.40
1:A:69:ARG:CZ	1:B:104:GLN:HE21	2.34	0.40
2:D:72:LEU:HD23	2:D:73:THR:H	1.77	0.40
2:D:181:THR:HG23	2:D:184:GLU:H	1.85	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]	2.16	0.04

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	249/299 (83%)	243 (98%)	6 (2%)	0	100	100
2	D	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
2	F	209/211 (99%)	200 (96%)	9 (4%)	0	100	100
3	E	207/217 (95%)	202 (98%)	4 (2%)	1 (0%)	24	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	206/217 (95%)	202 (98%)	3 (2%)	1 (0%)	24	43
All	All	1329/1454 (91%)	1291 (97%)	36 (3%)	2 (0%)	43	63

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%)	202 (99%)	2 (1%)	68	86
1	B	206/242 (85%)	202 (98%)	4 (2%)	50	76
2	D	184/184 (100%)	177 (96%)	7 (4%)	29	56
2	F	184/184 (100%)	178 (97%)	6 (3%)	33	61
3	E	187/190 (98%)	180 (96%)	7 (4%)	30	57
3	G	186/190 (98%)	180 (97%)	6 (3%)	34	62
All	All	1151/1232 (93%)	1119 (97%)	32 (3%)	38	66

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	ILE
1	A	272	PHE
1	B	33	LEU
1	B	116	LEU
1	B	176	ILE
1	B	233	ILE
2	D	21	MET
2	D	30	SER
2	D	88	GLN

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Mol	Chain	Res	Type
2	D	89	GLN
2	D	161	SER
2	D	174	MET
2	D	211	ASN
3	E	12	VAL
3	E	18	MET
3	E	28	SER
3	E	67	LYS
3	E	136	ASN
3	E	181	SER
3	E	211	LYS
2	F	21	MET
2	F	29	VAL
2	F	88	GLN
2	F	89	GLN
2	F	161	SER
2	F	174	MET
3	G	12	VAL
3	G	18	MET
3	G	136	ASN
3	G	143	CYS
3	G	181	SER
3	G	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	B	76	HIS
2	D	88	GLN
2	D	137	ASN
2	F	88	GLN
2	F	92	ASN
2	F	209	ASN
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 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	D10	B	302	-	9,9,9	0.31	0	8,8,8	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	D10	B	302	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	302	D10	C4-C5-C6-C7
6	B	302	D10	C2-C3-C4-C5
6	B	302	D10	C7-C8-C9-C10

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	302	D10	6	0

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%)	1.04	40 (15%) 5 4	52, 111, 167, 193	0
1	B	253/299 (84%)	1.24	58 (22%) 2 1	49, 118, 238, 288	0
2	D	211/211 (100%)	0.84	15 (7%) 22 19	59, 87, 121, 136	0
2	F	211/211 (100%)	0.75	20 (9%) 14 12	50, 85, 144, 165	0
3	E	211/217 (97%)	0.63	11 (5%) 33 29	50, 74, 110, 149	0
3	G	210/217 (96%)	0.69	11 (5%) 33 29	50, 84, 118, 165	0
All	All	1349/1454 (92%)	0.88	155 (11%) 9 8	49, 89, 169, 288	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	208	PHE	5.1
1	B	116	LEU	5.0
1	B	183	PHE	4.9
1	B	279	ILE	4.8
1	B	176	ILE	4.2
1	B	172	LEU	4.1
2	F	162	TRP	3.9
1	B	272	PHE	3.9
1	A	283	LEU	3.7
1	B	201	PHE	3.7
1	B	159	ILE	3.6
1	A	110	SER	3.5
1	B	282	TRP	3.5
2	F	149	ILE	3.5
2	D	105	LEU	3.5
1	B	220	MET	3.4
2	F	190	SER	3.4
2	F	179	THR	3.3
3	G	122	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	196	LEU	3.3
1	B	105	SER	3.2
3	E	26	GLY	3.2
1	B	262	TRP	3.1
2	F	207	SER	3.1
1	A	272	PHE	3.1
1	A	177	GLY	3.1
1	A	201	PHE	3.1
1	B	276	LEU	3.1
1	B	182	ILE	3.1
1	B	175	GLY	3.1
1	B	179	ILE	3.0
1	A	176	ILE	2.9
1	B	241	PHE	2.9
3	E	186	VAL	2.9
2	F	130	SER	2.8
1	B	269	LEU	2.8
2	F	192	THR	2.8
1	B	136	ALA	2.8
1	B	271	TYR	2.8
3	E	40	ARG	2.8
1	B	229	ILE	2.8
2	F	147	TRP	2.7
1	A	208	LEU	2.7
1	B	192	LEU	2.7
1	A	203	LEU	2.7
3	E	42	GLY	2.7
1	A	200	LEU	2.7
2	D	168	LYS	2.7
3	E	176	ASP	2.7
1	A	179	ILE	2.7
1	A	225	LYS	2.7
1	B	178	HIS	2.7
1	B	255	PRO	2.6
1	A	248	ALA	2.6
1	B	174	HIS	2.6
1	A	276	LEU	2.6
1	A	282	TRP	2.6
1	B	260	LEU	2.6
3	G	141	LEU	2.6
2	D	110	ALA	2.6
1	A	257	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	219	TYR	2.6
1	B	283	LEU	2.5
2	D	135	LEU	2.5
1	A	278	THR	2.5
1	B	278	THR	2.5
3	E	75	SER	2.5
1	A	229	ILE	2.5
2	F	148	LYS	2.5
2	D	63	GLY	2.5
1	B	186	TRP	2.5
1	A	168	LEU	2.5
3	G	143	CYS	2.5
1	B	257	TYR	2.5
1	B	120	PHE	2.5
2	F	203	PRO	2.4
1	B	133	GLY	2.4
1	B	258	GLN	2.4
2	F	180	LEU	2.4
3	E	162	LEU	2.4
1	B	273	ALA	2.4
1	B	190	PRO	2.3
3	G	17	SER	2.3
1	A	202	LEU	2.3
2	D	180	LEU	2.3
1	A	103	THR	2.3
2	D	22	THR	2.3
1	A	38	LEU	2.3
3	G	167	HIS	2.3
1	B	188	VAL	2.3
1	B	275	VAL	2.3
1	B	203	LEU	2.3
2	F	191	TYR	2.3
1	B	280	GLY	2.3
1	B	32	LEU	2.3
3	G	173	LEU	2.3
2	D	156	ASN	2.2
2	F	157	GLY	2.2
3	E	141	LEU	2.2
3	G	123	SER	2.2
1	B	209	PHE	2.2
1	A	111	HIS	2.2
1	B	252	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	151	LEU	2.2
1	A	196	LEU	2.2
1	A	197	SER	2.2
1	A	175	GLY	2.2
2	D	24	SER	2.2
3	E	163	SER	2.2
1	A	50	PHE	2.2
1	B	189	PRO	2.2
2	D	141	LYS	2.2
3	E	201	ALA	2.2
1	A	30	THR	2.2
2	D	125	THR	2.2
1	A	267	LEU	2.2
1	B	114	TRP	2.2
2	F	131	VAL	2.1
1	A	60	GLN	2.1
1	A	256	ALA	2.1
1	A	273	ALA	2.1
1	B	113	ALA	2.1
1	A	73	LEU	2.1
2	D	199	THR	2.1
3	G	110	THR	2.1
1	A	204	ILE	2.1
3	G	28	SER	2.1
1	B	215	PHE	2.1
1	A	286	VAL	2.1
1	B	281	ASN	2.1
2	D	23	CYS	2.1
1	B	254	SER	2.1
3	E	167	HIS	2.1
1	A	285	VAL	2.1
1	A	211	LEU	2.1
1	B	30	THR	2.1
2	D	5	THR	2.1
2	F	151	GLY	2.1
2	F	204	ILE	2.1
2	F	205	VAL	2.1
3	G	178	TYR	2.1
2	F	193	CYS	2.1
1	A	215	PHE	2.0
1	B	181	ALA	2.0
1	B	268	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	110	SER	2.0
1	A	194	ARG	2.0
3	G	166	VAL	2.0
1	B	236	LEU	2.0
1	B	256	ALA	2.0
2	F	178	LEU	2.0
1	B	103	THR	2.0
1	A	174	HIS	2.0
1	B	171	SER	2.0
2	D	62	SER	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(Å ²)	Q<0.9
4	K	B	301	1/1	0.70	0.35	121,121,121,121	0
6	D10	B	302	10/10	0.83	0.32	90,99,108,112	0
4	K	A	301	1/1	0.94	0.15	80,80,80,80	0
4	K	A	303	1/1	0.95	0.06	91,91,91,91	0
5	CA	A	305	1/1	0.96	0.07	93,93,93,93	0
5	CA	G	301	1/1	0.96	0.06	113,113,113,113	0
4	K	A	306	1/1	0.96	0.05	87,87,87,87	0
5	CA	A	304	1/1	0.97	0.04	102,102,102,102	0
4	K	A	302	1/1	0.98	0.04	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.