



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:54 PM GMT

PDB ID : 4WFF  
Title : Human TRAAK K<sup>+</sup> channel in a K<sup>+</sup> 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](mailto: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.

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

MolProbity : 4.02b-467  
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

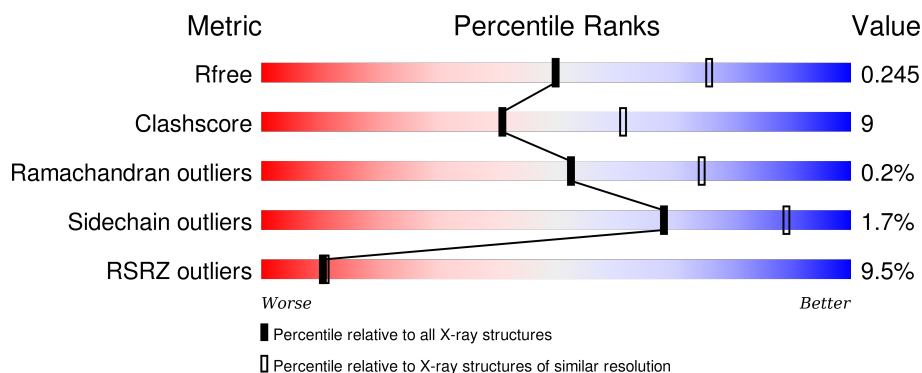
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>13%</div> <div>67% 17% 15%</div> </div>
1	B	299	<div> <div>20%</div> <div>68% 16% 15%</div> </div>
2	D	211	<div> <div>%</div> <div>84% 15%</div> </div>
2	F	211	<div> <div>9%</div> <div>86% 13%</div> </div>
3	E	217	<div> <div>3%</div> <div>80% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	217	 <div>81%16%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	D10	B	302	-	-	-	X

## 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			

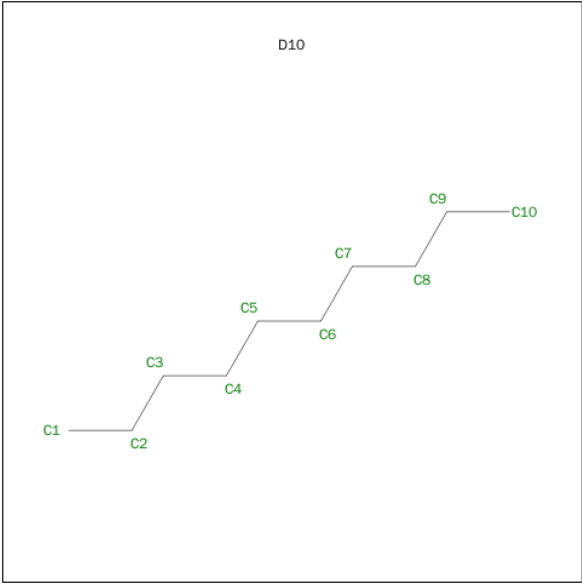
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- 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 DECANE (three-letter code: D10) (formula: C<sub>10</sub>H<sub>22</sub>).



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

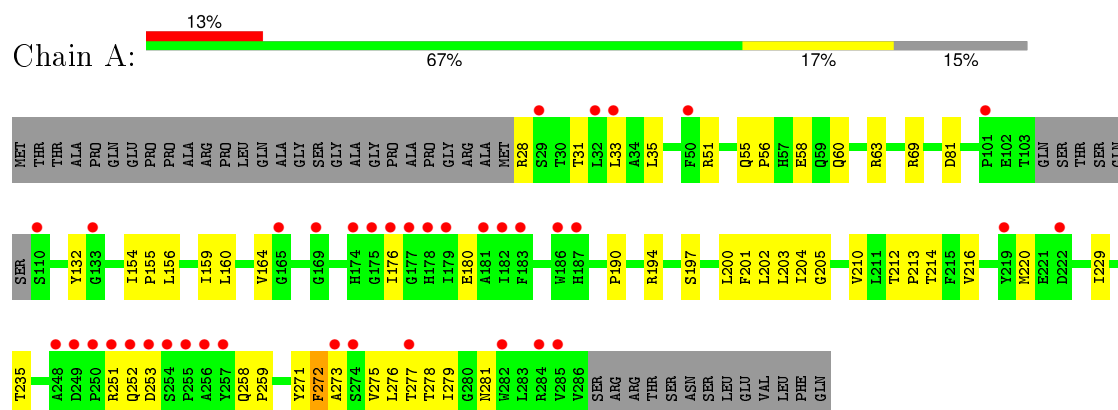
- Molecule 7 is water.

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

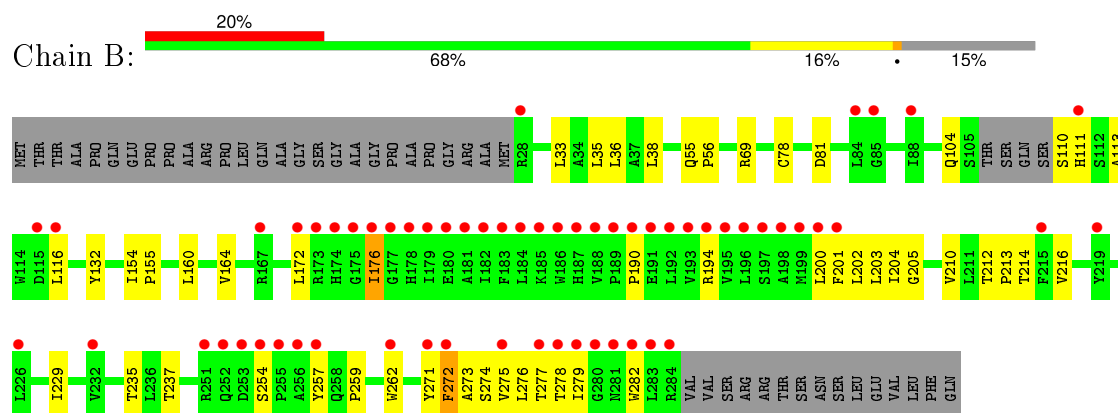
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

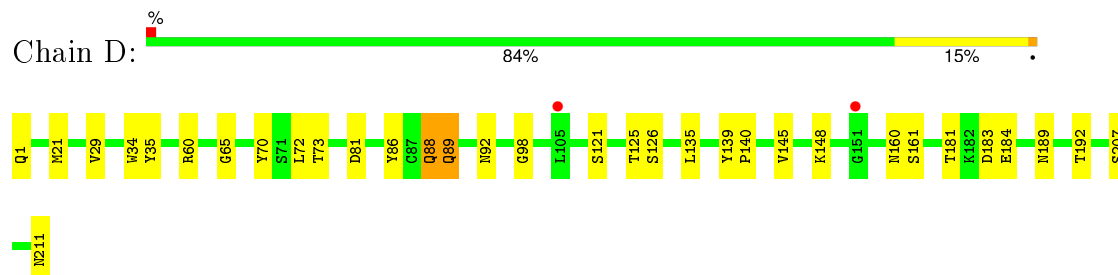
- Molecule 1: Potassium channel subfamily K member 4



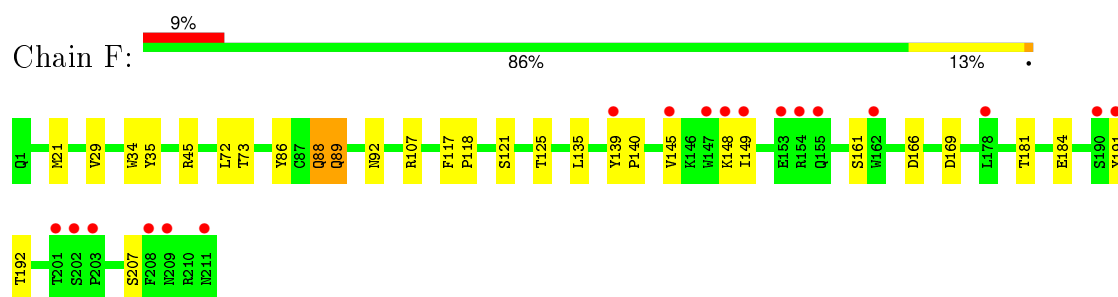
- Molecule 1: Potassium channel subfamily K member 4



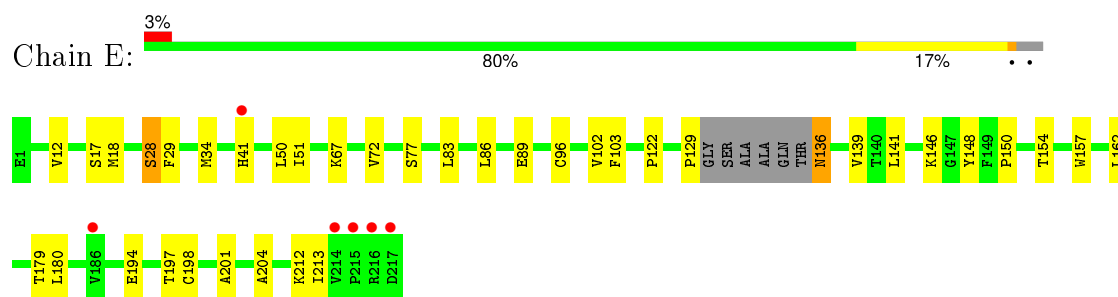
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



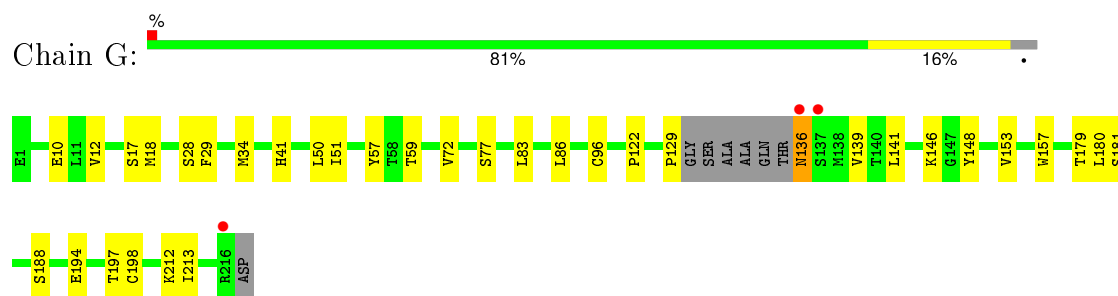
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.67Å 138.89Å 96.53Å 90.00° 95.15° 90.00°	Depositor
Resolution (Å)	48.10 – 2.50 48.07 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.10-2.50) 98.9 (48.07-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.213 , 0.245 0.215 , 0.245	Depositor DCC
$R_{free}$ test set	3632 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 72628 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: K, D10, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/2013	0.49	0/2745
1	B	0.38	0/2021	0.48	1/2754 (0.0%)
2	D	0.43	0/1655	0.54	0/2247
2	F	0.45	0/1655	0.55	0/2247
3	E	0.50	0/1656	0.60	0/2260
3	G	0.49	0/1647	0.60	0/2249
All	All	0.44	0/10647	0.54	1/14502 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	CYS	CA-CB-SG	5.39	123.70	114.00

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	43	0
1	B	1970	0	1988	38	0
2	D	1616	0	1542	23	0
2	F	1616	0	1542	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1614	0	1586	24	1
3	G	1605	0	1582	28	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	177	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 (177) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C5	6:B:302:D10:H12	2.24	0.66
1:A:202:LEU:O	1:A:271:TYR:OH	2.14	0.66
2:D:1:GLN:OE1	2:D:1:GLN:HA	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
3:G:139:VAL:HG23	3:G:188:SER:HB3	1.79	0.64
2:F:148:LYS:HB2	2:F:192:THR:OG1	1.97	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
3:G:180:LEU:C	3:G:180:LEU:HD12	2.20	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:172:LEU:O	1:B:176:ILE:HD12	2.02	0.59
1:B:212:THR:O	1:B:216:VAL:HG23	2.02	0.59
1:A:190:PRO:O	1:A:194:ARG:HG2	2.02	0.59
3:E:180:LEU:HD12	3:E:180:LEU:C	2.23	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:212:THR:O	1:A:216:VAL:HG23	2.04	0.58
1:A:159:ILE:HG22	1:B:35:LEU:HD21	1.85	0.58
3:G:194:GLU:HG2	7:G:404:HOH:O	2.02	0.58
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:HD22	3:E:136:ASN:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:38:LEU:HD23	1:B:38:LEU:C	2.27	0.54
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
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
2:D:139:TYR:CG	2:D:140:PRO:HA	2.43	0.54
1:A:55:GLN:N	1:A:56:PRO:CD	2.71	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:G:122:PRO:HB3	3:G:148:TYR:HB3	1.90	0.52
3:E:122:PRO:HB3	3:E:148:TYR:HB3	1.91	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:G:136:ASN:ND2	3:G:136:ASN:N	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
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:273:ALA:O	1:A:277:THR:HG23	2.11	0.50
1:A:69:ARG:HD2	7:A:402:HOH:O	2.12	0.50
3:G:50:LEU:C	3:G:50:LEU:HD12	2.31	0.50
1:A:200:LEU:O	1:A:204:ILE:HG22	2.13	0.49
3:G:197:THR:HG22	3:G:212:LYS:CA	2.42	0.49
3:G:57:TYR:OH	3:G:59:THR:CG2	2.61	0.49
3:E:29:PHE:CD2	3:E:77:SER:HA	2.48	0.49
2:D:29:VAL:CG1	2:D:89:GLN:HG3	2.38	0.48
3:G:57:TYR:CZ	3:G:59:THR:HG23	2.48	0.48
1:B:132:TYR:OH	1:B:235:THR:HG23	2.13	0.48
2:D:192:THR:HG22	2:D:207:SER:CB	2.44	0.48
1:B:205:GLY:HA3	1:B:271:TYR:CZ	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:45:ARG:NE	7:F:304:HOH:O	2.47	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
2:D:211:ASN:OD1	2:D:211:ASN:N	2.36	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
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
3:E:50:LEU:HD12	3:E:50:LEU:C	2.35	0.46
3:G:136:ASN:HD22	3:G:136:ASN:N	2.14	0.46
1:B:200:LEU:O	1:B:204:ILE:HG22	2.16	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
2:F:29:VAL:CG2	2:F:89:GLN:HG3	2.45	0.45
1:A:210:VAL:O	1:A:214:THR:HG23	2.16	0.45
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.46	0.45
1:A:176:ILE:HD11	1:A:201:PHE:HA	1.98	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
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: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
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:302:D10:C5	6:B:302:D10:C1	2.93	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:B:201:PHE:CD1	1:B:201:PHE:C	2.92	0.42
1:A:33:LEU:HD23	1:A:33:LEU:O	2.19	0.42
2:F:45:ARG:NH2	7:F:332:HOH:O	2.49	0.42
1:A:28:ARG:HB2	1:A:31:THR:HG23	2.02	0.42
2:D:34:TRP:HA	2:D:86:TYR:O	2.20	0.42
1:A:202:LEU:CA	1:A:271:TYR:OH	2.68	0.42
1:A:55:GLN:N	1:A:56:PRO:HD2	2.34	0.42
3:E:150:PRO:HD2	3:E:204:ALA:CB	2.50	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
2:F:72:LEU:HD23	2:F:72:LEU:C	2.41	0.41
3:E:139:VAL:HA	7:E:346:HOH:O	2.20	0.41
3:G:198:CYS:C	7:G:429:HOH:O	2.58	0.41
3:G:34:MET:CE	3:G:96:CYS:HB2	2.50	0.41
3:G:180:LEU:C	3:G:180:LEU:CD1	2.89	0.41
3:E:34:MET:CE	3:E:96:CYS:HB2	2.51	0.41
3:G:148:TYR:CE2	3:G:153:VAL:HG13	2.55	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
2:F:166:ASP:OD1	7:F:326:HOH:O	2.22	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
1:A:51:ARG:HE	1:B:116:LEU:HD23	1.86	0.40
2:F:181:THR:HG23	2:F:184:GLU:H	1.85	0.40
3:E:162:LEU:HA	7:E:337:HOH:O	2.20	0.40
1:B:210:VAL:O	1:B:214:THR:HG23	2.21	0.40
2:D:72:LEU:HD23	2:D:73:THR:H	1.77	0.40
1:A:69:ARG:CZ	1:B:104:GLN:HE21	2.34	0.40
1:A:35:LEU:HA	1:A:35:LEU:HD12	1.92	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%)	34	55
3	G	206/217 (95%)	202 (98%)	3 (2%)	1 (0%)	34	55
All	All	1329/1454 (91%)	1291 (97%)	36 (3%)	2 (0%)	52	75

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	206/242 (85%)	204 (99%)	2 (1%)	82	95
2	D	184/184 (100%)	179 (97%)	5 (3%)	52	79
2	F	184/184 (100%)	180 (98%)	4 (2%)	60	84
3	E	187/190 (98%)	183 (98%)	4 (2%)	61	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	186/190 (98%)	183 (98%)	3 (2%)	70	90
All	All	1151/1232 (93%)	1132 (98%)	19 (2%)	68	89

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	PHE
1	B	176	ILE
1	B	272	PHE
2	D	21	MET
2	D	88	GLN
2	D	89	GLN
2	D	161	SER
2	D	183	ASP
3	E	18	MET
3	E	28	SER
3	E	67	LYS
3	E	136	ASN
2	F	21	MET
2	F	88	GLN
2	F	89	GLN
2	F	161	SER
3	G	18	MET
3	G	136	ASN
3	G	181	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	88	GLN
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 carbohydrates 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	0.30	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	-	-	0/7/7/7	0/0/0/0

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.

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	253/299 (84%)	0.81	38 (15%) 3 3	52, 111, 167, 193	0
1	B	253/299 (84%)	1.42	61 (24%) 1 1	49, 118, 238, 288	0
2	D	211/211 (100%)	0.12	2 (0%) 85 88	59, 87, 121, 136	0
2	F	211/211 (100%)	0.31	18 (8%) 13 14	50, 85, 144, 165	0
3	E	211/217 (97%)	0.18	6 (2%) 56 61	50, 74, 110, 149	0
3	G	210/217 (96%)	0.13	3 (1%) 78 80	50, 84, 118, 165	0
All	All	1349/1454 (92%)	0.54	128 (9%) 10 11	49, 89, 169, 288	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	ALA	12.9
1	B	183	PHE	9.8
1	B	251	ARG	9.4
1	B	279	ILE	9.1
1	B	184	LEU	8.5
1	B	189	PRO	8.5
1	B	284	ARG	8.0
1	B	179	ILE	7.9
1	B	176	ILE	7.9
2	F	154	ARG	7.1
1	B	190	PRO	7.1
2	F	155	GLN	7.1
1	A	255	PRO	7.0
1	B	281	ASN	6.8
2	F	208	PHE	6.7
1	B	192	LEU	6.6
1	B	252	GLN	5.9
1	B	283	LEU	5.9
1	B	116	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	180	GLU	5.8
1	B	188	VAL	5.7
1	B	282	TRP	5.6
1	B	187	HIS	5.5
1	B	280	GLY	5.5
1	B	256	ALA	5.5
1	B	186	TRP	5.4
1	B	172	LEU	5.3
1	B	178	HIS	5.2
1	B	185	LYS	5.2
2	D	105	LEU	5.0
1	B	193	VAL	5.0
1	A	253	ASP	5.0
1	A	183	PHE	4.9
1	B	201	PHE	4.9
2	F	147	TRP	4.9
1	A	257	TYR	4.8
1	B	219	TYR	4.8
1	B	271	TYR	4.7
1	B	253	ASP	4.7
1	A	256	ALA	4.7
2	F	201	THR	4.6
1	A	248	ALA	4.4
1	B	196	LEU	4.3
1	A	219	TYR	4.2
1	A	178	HIS	4.2
1	B	197	SER	4.2
3	E	217	ASP	4.2
1	B	182	ILE	4.0
2	F	211	ASN	4.0
1	B	278	THR	3.8
1	A	110	SER	3.8
1	A	254	SER	3.8
1	A	176	ILE	3.8
1	A	285	VAL	3.8
3	E	216	ARG	3.7
1	A	277	THR	3.6
1	B	174	HIS	3.6
1	A	284	ARG	3.5
1	B	200	LEU	3.5
3	G	136	ASN	3.4
1	B	255	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	29	SER	3.4
1	B	177	GLY	3.4
1	B	194	ARG	3.4
1	B	199	MET	3.4
2	F	149	ILE	3.4
1	A	181	ALA	3.3
1	A	251	ARG	3.3
1	A	274	SER	3.2
1	A	174	HIS	3.2
1	A	165	GLY	3.2
1	B	215	PHE	3.2
1	B	111	HIS	3.1
1	B	275	VAL	3.0
1	A	186	TRP	3.0
2	F	139	TYR	3.0
3	E	186	VAL	3.0
1	A	133	GLY	3.0
1	A	177	GLY	2.9
1	B	277	THR	2.9
1	A	249	ASP	2.9
3	G	137	SER	2.8
1	B	173	ARG	2.8
1	B	257	TYR	2.8
1	B	191	GLU	2.8
2	F	162	TRP	2.8
1	A	252	GLN	2.7
1	A	282	TRP	2.7
3	E	41	HIS	2.7
2	F	153	GLU	2.7
1	A	169	GLY	2.7
2	F	190	SER	2.6
3	G	216	ARG	2.6
1	B	254	SER	2.6
1	A	32	LEU	2.6
1	A	182	ILE	2.6
2	F	202	SER	2.5
2	F	209	ASN	2.5
2	F	178	LEU	2.5
2	F	203	PRO	2.5
3	E	215	PRO	2.4
1	A	33	LEU	2.4
2	F	148	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	88	ILE	2.4
1	B	167	ARG	2.4
1	A	250	PRO	2.4
1	B	175	GLY	2.4
3	E	214	VAL	2.4
2	F	191	TYR	2.4
1	A	179	ILE	2.4
1	B	262	TRP	2.3
1	B	115	ASP	2.3
2	F	145	VAL	2.3
1	A	273	ALA	2.3
1	B	232	VAL	2.3
1	B	85	GLY	2.2
1	B	272	PHE	2.2
1	A	222	ASP	2.2
1	B	28	ARG	2.2
1	B	198	ALA	2.2
1	A	175	GLY	2.2
1	B	84	LEU	2.2
1	B	195	VAL	2.2
1	A	50	PHE	2.1
1	A	187	HIS	2.1
1	B	226	LEU	2.1
1	A	101	PRO	2.0
2	D	151	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, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	D10	B	302	10/10	0.79	0.50	5.86	90,99,108,112	0
4	K	A	306	1/1	0.87	0.11	-0.78	87,87,87,87	0
4	K	A	302	1/1	0.97	0.13	-0.84	86,86,86,86	0
4	K	A	303	1/1	0.94	0.12	-1.06	91,91,91,91	0
5	CA	A	304	1/1	0.95	0.10	-1.23	102,102,102,102	0
4	K	A	301	1/1	0.94	0.07	-1.66	80,80,80,80	0
5	CA	A	305	1/1	0.97	0.08	-2.15	93,93,93,93	0
4	K	B	301	1/1	0.73	0.79	-	121,121,121,121	0
5	CA	G	301	1/1	0.92	0.12	-	113,113,113,113	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.