



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 05:17 AM EDT

PDB ID : 4WFF
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

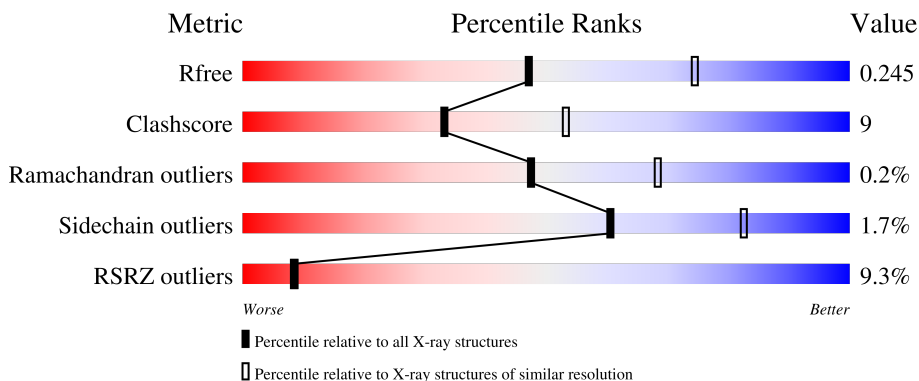
1 Overall quality at a glance i

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.



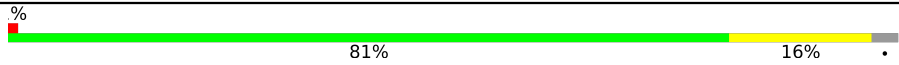
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>
1	B	299	<div style="display: flex; align-items: center;"> <div style="width: 20%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>
2	D	211	<div style="display: flex; align-items: center;"> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
2	F	211	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
3	E	217	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	G	217	

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
4	K	B	301	-	-	-	X
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
			Total	C	N	O	S			
1	A	253	Total 1963	C 1299	N 318	O 340	S 6	0	0	0
1	B	253	Total 1970	C 1300	N 321	O 343	S 6	0	0	0

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	A	4	Total	K	0	0
			4	4		
4	B	1	Total	K	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: 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 (three-letter code: D10) (formula: C₁₀H₂₂).



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

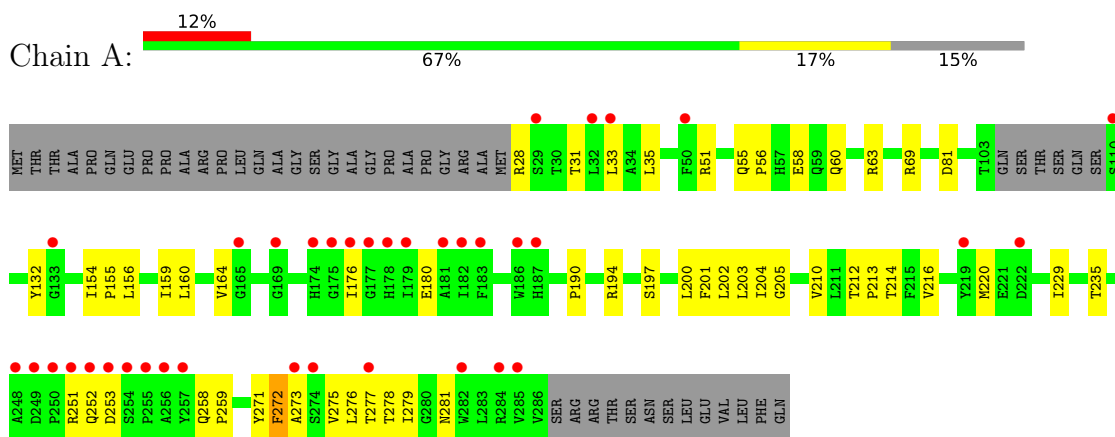
- Molecule 7 is water.

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

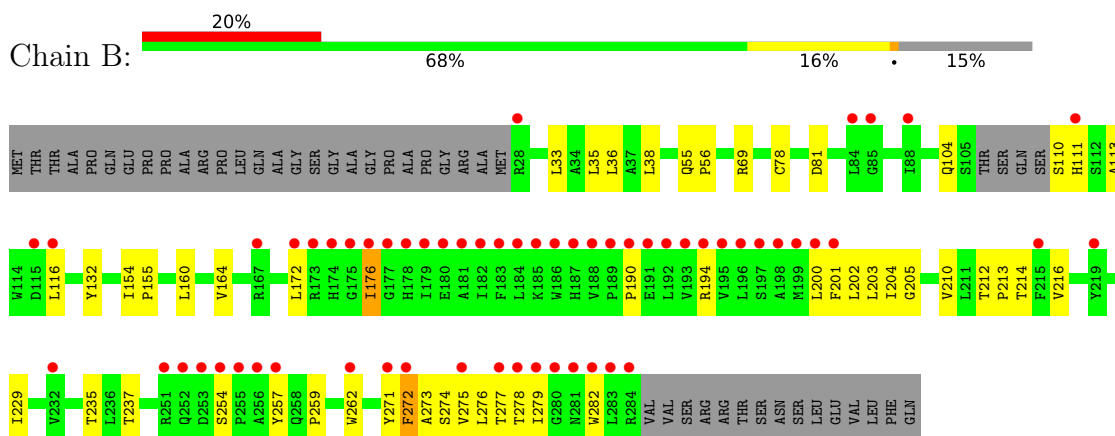
3 Residue-property plots [i](#)

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.

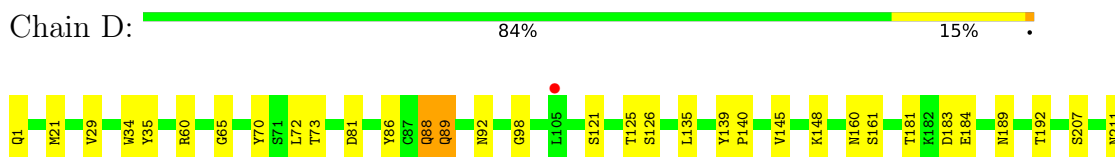
- Molecule 1: Potassium channel subfamily K member 4



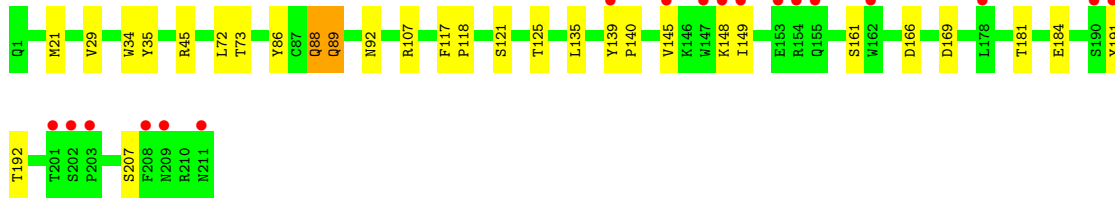
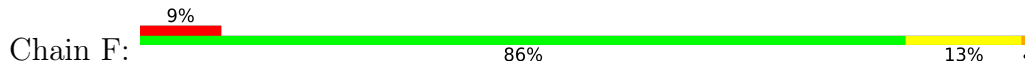
- Molecule 1: Potassium channel subfamily K member 4



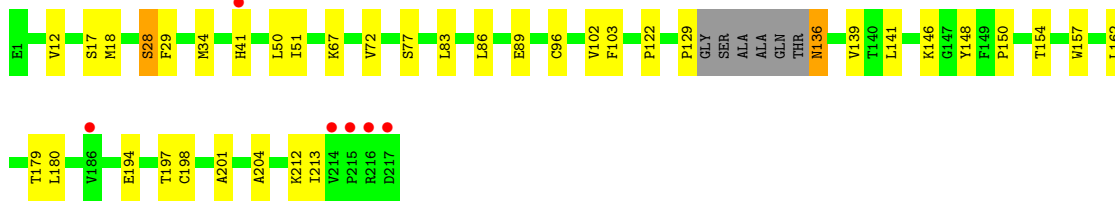
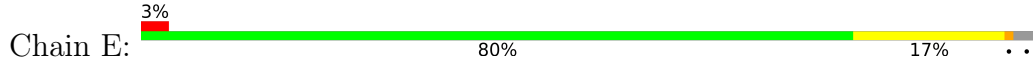
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



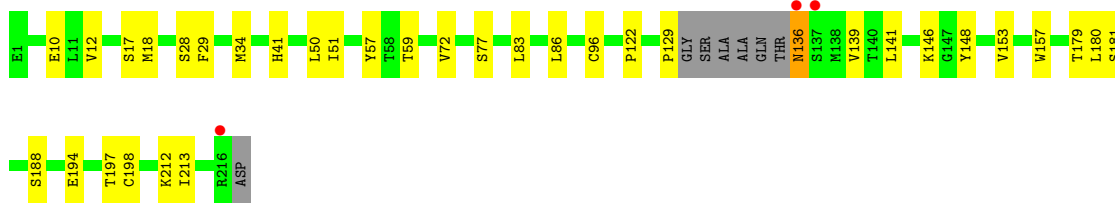
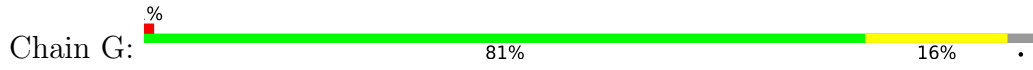
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



• 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 48.07 – 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
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.213 , 0.245 0.215 , 0.245	Depositor DCC
R_{free} test set	3631 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtrriage
Anisotropy	0.325	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: K, CA, D10

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:H12	6:B:302:D10:C5	2.24	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
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:HD12	3:G:180:LEU:C	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: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
3:E:180:LEU:C	3:E:180:LEU:HD12	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: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
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

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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:C	1:B:38:LEU:HD23	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
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: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
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: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: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
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

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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
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
3:E:50:LEU:C	3:E:50:LEU:HD12	2.35	0.46
1:B:200:LEU:O	1:B:204:ILE:HG22	2.16	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
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
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:O	1:A:33:LEU:HD23	2.19	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
2:D:34:TRP:HA	2:D:86:TYR:O	2.20	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
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
3:E:139:VAL:HA	7:E:346:HOH:O	2.20	0.41
2:F:72:LEU:HD23	2:F:72:LEU:C	2.41	0.41
3:G:34:MET:CE	3:G:96:CYS:HB2	2.50	0.41
3:G:198:CYS:C	7:G:429:HOH:O	2.58	0.41
3:E:34:MET:CE	3:E:96:CYS:HB2	2.51	0.41
3:G:180:LEU:C	3:G:180:LEU:CD1	2.89	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
3:G:148:TYR:CE2	3:G:153:VAL:HG13	2.55	0.41
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: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 [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	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%)	29	48
3	G	206/217 (95%)	202 (98%)	3 (2%)	1 (0%)	29	48
All	All	1329/1454 (91%)	1291 (97%)	36 (3%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	41	HIS
3	G	41	HIS

5.3.2 Protein sidechains [i](#)

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%)	88	96
1	B	206/242 (85%)	204 (99%)	2 (1%)	76	90
2	D	184/184 (100%)	179 (97%)	5 (3%)	44	71
2	F	184/184 (100%)	180 (98%)	4 (2%)	52	77
3	E	187/190 (98%)	183 (98%)	4 (2%)	53	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	186/190 (98%)	183 (98%)	3 (2%)	62	84
All	All	1151/1232 (93%)	1132 (98%)	19 (2%)	60	82

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

Sometimes 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 monosaccharides 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%)	0.74	37 (14%) 2 2	52, 111, 167, 193	0
1	B	253/299 (84%)	1.32	60 (23%) 0 0	49, 118, 238, 288	0
2	D	211/211 (100%)	0.06	1 (0%) 91 91	59, 87, 121, 136	0
2	F	211/211 (100%)	0.25	18 (8%) 10 10	50, 85, 144, 165	0
3	E	211/217 (97%)	0.13	6 (2%) 53 56	50, 74, 110, 149	0
3	G	210/217 (96%)	0.08	3 (1%) 75 77	50, 84, 118, 165	0
All	All	1349/1454 (92%)	0.47	125 (9%) 8 8	49, 89, 169, 288	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	ALA	12.4
1	B	183	PHE	9.6
1	B	251	ARG	9.2
1	B	279	ILE	8.8
1	B	184	LEU	8.2
1	B	189	PRO	8.1
1	B	284	ARG	7.8
1	B	179	ILE	7.6
1	B	176	ILE	7.6
2	F	154	ARG	6.9
2	F	155	GLN	6.9
1	B	190	PRO	6.8
1	A	255	PRO	6.7
1	B	281	ASN	6.6
2	F	208	PHE	6.5
1	B	192	LEU	6.4
1	B	252	GLN	5.7
1	B	283	LEU	5.6
1	B	116	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	180	GLU	5.5
1	B	188	VAL	5.5
1	B	282	TRP	5.4
1	B	280	GLY	5.3
1	B	187	HIS	5.3
1	B	186	TRP	5.3
1	B	256	ALA	5.2
1	B	172	LEU	5.1
1	B	185	LYS	5.1
1	B	178	HIS	5.0
2	D	105	LEU	4.8
1	B	193	VAL	4.8
1	A	183	PHE	4.8
1	A	253	ASP	4.8
2	F	147	TRP	4.7
1	B	201	PHE	4.7
1	A	257	TYR	4.6
1	B	219	TYR	4.6
1	B	271	TYR	4.5
2	F	201	THR	4.5
1	A	256	ALA	4.5
1	B	253	ASP	4.5
1	A	248	ALA	4.2
1	B	196	LEU	4.1
1	A	219	TYR	4.1
1	A	178	HIS	4.1
1	B	197	SER	4.0
3	E	217	ASP	4.0
2	F	211	ASN	3.9
1	B	182	ILE	3.8
1	A	110	SER	3.8
1	B	278	THR	3.7
1	A	254	SER	3.7
1	A	176	ILE	3.7
1	A	285	VAL	3.6
3	E	216	ARG	3.6
1	A	277	THR	3.5
1	B	174	HIS	3.5
1	A	284	ARG	3.4
1	A	29	SER	3.4
3	G	136	ASN	3.4
1	B	200	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	255	PRO	3.3
1	B	194	ARG	3.3
1	B	177	GLY	3.2
2	F	149	ILE	3.2
1	B	199	MET	3.2
1	A	274	SER	3.2
1	A	251	ARG	3.2
1	A	174	HIS	3.1
1	A	181	ALA	3.1
1	B	215	PHE	3.1
1	A	165	GLY	3.0
1	B	111	HIS	2.9
1	A	186	TRP	2.9
2	F	139	TYR	2.9
1	B	275	VAL	2.8
1	A	133	GLY	2.8
3	E	186	VAL	2.8
1	A	249	ASP	2.8
1	A	177	GLY	2.7
3	G	137	SER	2.7
1	B	277	THR	2.7
1	B	257	TYR	2.7
1	B	173	ARG	2.7
1	B	191	GLU	2.7
2	F	162	TRP	2.6
1	A	252	GLN	2.6
1	A	282	TRP	2.6
1	A	169	GLY	2.6
3	E	41	HIS	2.6
2	F	153	GLU	2.5
2	F	190	SER	2.5
3	G	216	ARG	2.5
1	B	254	SER	2.5
1	A	32	LEU	2.5
1	A	182	ILE	2.4
2	F	202	SER	2.4
2	F	209	ASN	2.4
2	F	178	LEU	2.4
1	B	167	ARG	2.3
1	A	33	LEU	2.3
2	F	203	PRO	2.3
3	E	215	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	148	LYS	2.3
1	A	250	PRO	2.3
1	B	88	ILE	2.3
3	E	214	VAL	2.3
1	A	179	ILE	2.3
2	F	191	TYR	2.2
1	B	262	TRP	2.2
1	B	175	GLY	2.2
1	B	115	ASP	2.2
2	F	145	VAL	2.1
1	B	232	VAL	2.1
1	A	273	ALA	2.1
1	B	272	PHE	2.1
1	B	28	ARG	2.1
1	B	85	GLY	2.1
1	A	222	ASP	2.1
1	B	84	LEU	2.1
1	A	175	GLY	2.1
1	B	198	ALA	2.0
1	A	187	HIS	2.0
1	B	195	VAL	2.0
1	A	50	PHE	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 monosaccharides 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	0.73	0.79	121,121,121,121	0

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

6.5 Other polymers [i](#)

There are no such residues in this entry.