



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 10:48 AM EST

PDB ID : 4WFH  
Title : Human TRAAK K<sup>+</sup> channel in a Tl<sup>+</sup> bound nonconductive conformation  
Authors : Brohawn, S.G.; MacKinnon, R.  
Deposited on : 2014-09-15  
Resolution : 3.01 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

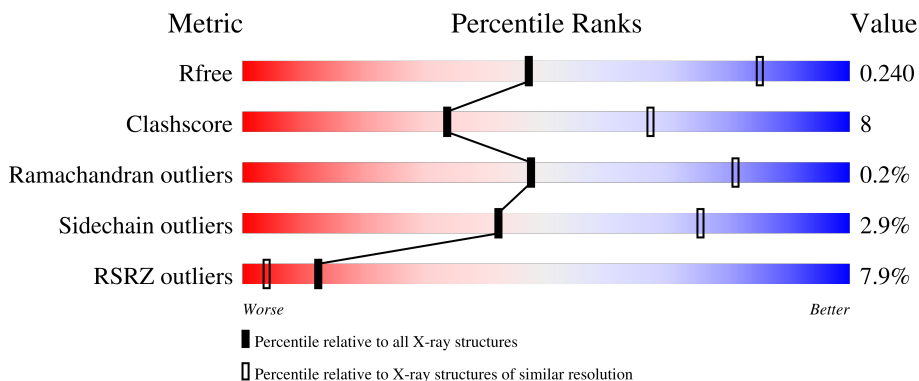
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; 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: 17%; 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: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></div> </div>
2	D	211	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; 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: 1%; height: 10px; background-color: grey;"></div> </div>
2	F	211	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; 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: 0%; height: 10px; background-color: grey;"></div> </div>
3	E	217	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; 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: 6%; 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
6	D10	B	303	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10506 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	243	Total 1888	C 1246	N 306	O 330	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			

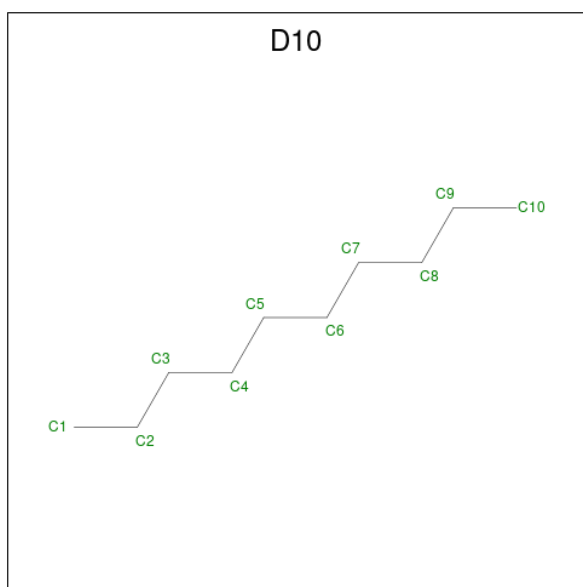
- Molecule 4 is THALLIUM (I) ION (three-letter code: TL) (formula: Tl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Tl	0	0
			5	5		
4	B	2	Total	Tl	0	0
			2	2		

- 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: C<sub>10</sub>H<sub>22</sub>).



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

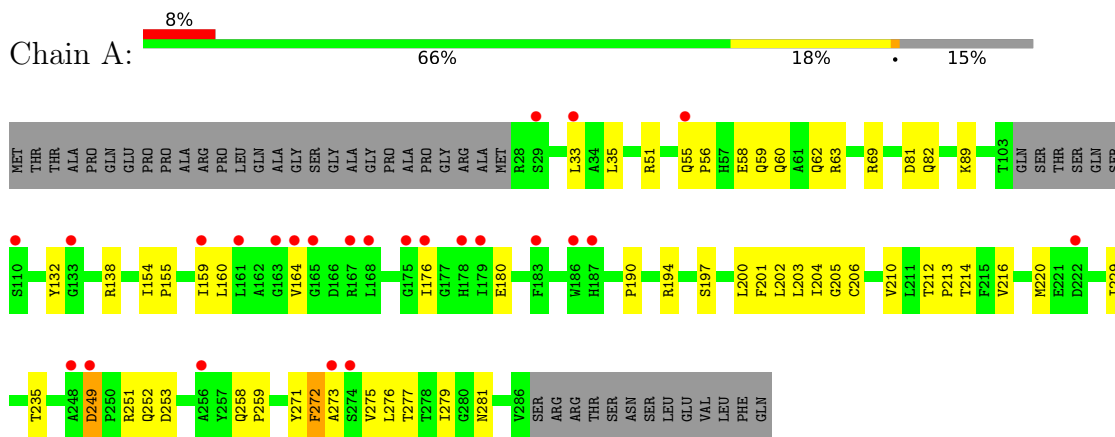
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	25	Total O 25 25	0	0
7	B	21	Total O 21 21	0	0
7	D	23	Total O 23 23	0	0
7	E	51	Total O 51 51	0	0
7	F	33	Total O 33 33	0	0
7	G	31	Total O 31 31	0	0

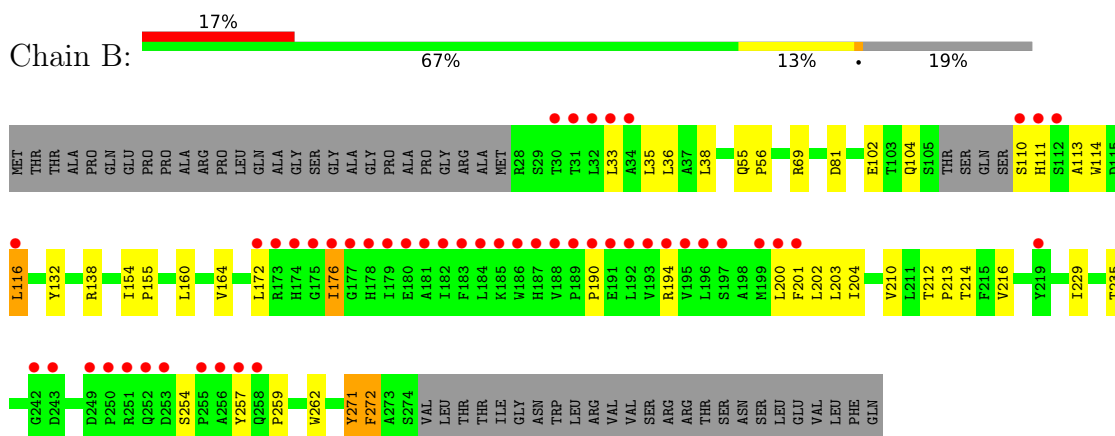
### 3 Residue-property plots [i](#)

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.

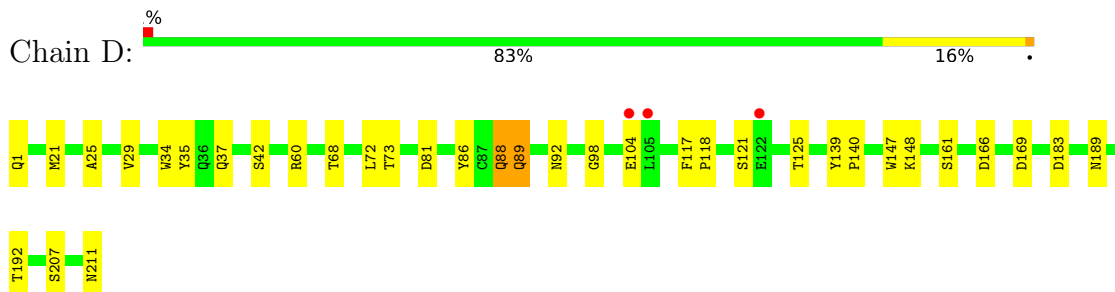
- Molecule 1: Potassium channel subfamily K member 4



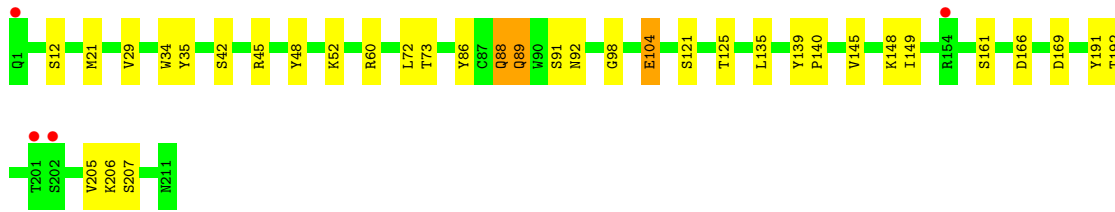
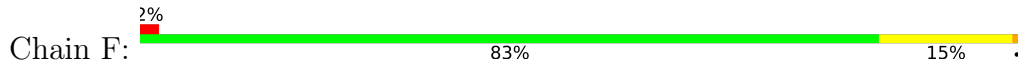
- Molecule 1: Potassium channel subfamily K member 4



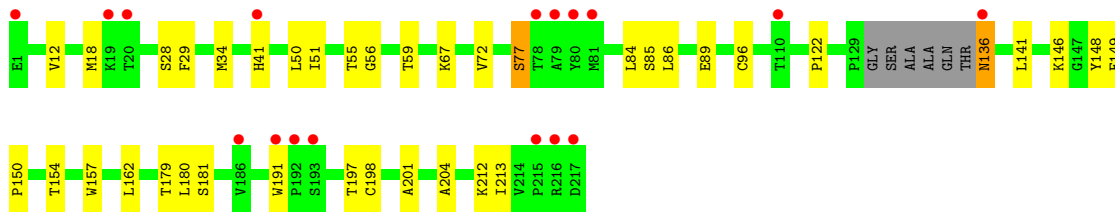
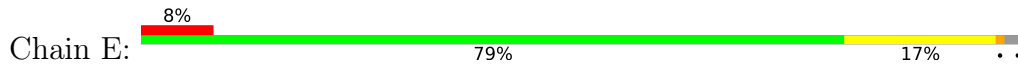
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



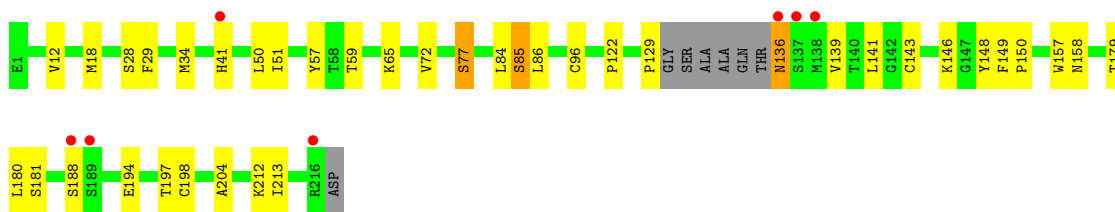
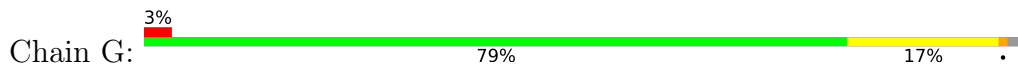
- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



- 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, $\alpha$ , $\beta$ , $\gamma$	80.97Å 138.75Å 96.76Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	48.20 – 3.01 48.22 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.20-3.01) 99.1 (48.22-3.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.203 , 0.238 0.208 , 0.240	Depositor DCC
$R_{free}$ test set	2098 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.5	Xtrriage
Anisotropy	0.551	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 58.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D10, 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	0.32	0/2013	0.44	0/2745
1	B	0.55	1/1937 (0.1%)	0.45	0/2638
2	D	0.38	0/1655	0.49	0/2247
2	F	0.40	0/1655	0.52	0/2247
3	E	0.43	0/1656	0.56	0/2260
3	G	0.44	0/1647	0.57	0/2249
All	All	0.43	1/10563 (0.0%)	0.50	0/14386

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	TYR	C-N	19.78	1.79	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1963	0	1985	45	0
1	B	1888	0	1899	32	0
2	D	1616	0	1542	22	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	27	0
3	G	1605	0	1582	30	0
4	A	5	0	0	0	0
4	B	2	0	0	0	0
5	A	2	0	0	0	0
5	G	1	0	0	0	0
6	B	10	0	22	2	0
7	A	25	0	0	2	0
7	B	21	0	0	2	0
7	D	23	0	0	4	0
7	E	51	0	0	5	0
7	F	33	0	0	3	0
7	G	31	0	0	5	0
All	All	10506	0	10158	173	0

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 (173) 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:271:TYR:C	1:B:272:PHE:N	1.79	1.35
2:F:35:TYR:HE1	2:F:88:GLN:HG2	1.39	0.88
2:D:35:TYR:HE2	2:D:88:GLN:HG2	1.38	0.86
1:A:249:ASP:HB2	7:A:411:HOH:O	1.78	0.83
3:E:136:ASN:N	3:E:136:ASN:HD22	1.81	0.78
2:F:35:TYR:CE1	2:F:88:GLN:HG2	2.21	0.75
2:F:72:LEU:HD23	2:F:73:THR:N	2.00	0.74
1:A:60:GLN:OE1	1:A:63:ARG:NH2	2.22	0.73
2:D:35:TYR:CE2	2:D:88:GLN:HG2	2.24	0.72
1:A:212:THR:HB	1:A:213:PRO:HD3	1.72	0.71
1:B:212:THR:HB	1:B:213:PRO:HD3	1.71	0.71
1:B:69:ARG:NH1	1:B:81:ASP:OD1	2.25	0.70
2:D:29:VAL:HG11	2:D:89:GLN:HG3	1.72	0.70
1:B:202:LEU:HA	1:B:271:TYR:OH	1.92	0.70
2:F:98:GLY:O	7:F:329:HOH:O	2.11	0.69
3:E:28:SER:HB3	3:G:28:SER:HB3	1.75	0.68
1:A:58:GLU:OE2	1:B:113:ALA:N	2.27	0.68
3:E:136:ASN:N	3:E:136:ASN:ND2	2.42	0.67
2:D:72:LEU:HD23	2:D:73:THR:N	2.09	0.67
2:D:60:ARG:NH1	2:D:81:ASP:OD1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:MET:O	1:A:251:ARG:NH2	2.30	0.65
2:D:148:LYS:HB2	2:D:192:THR:OG1	1.97	0.64
1:A:202:LEU:O	1:A:271:TYR:OH	2.16	0.64
3:E:154:THR:OG1	3:E:201:ALA:HB3	1.97	0.63
3:E:180:LEU:C	3:E:180:LEU:HD12	2.19	0.63
1:A:69:ARG:NH1	1:A:81:ASP:OD1	2.32	0.63
3:E:51:ILE:HD13	3:E:72:VAL:HG13	1.80	0.63
3:G:180:LEU:HD12	3:G:180:LEU:C	2.19	0.63
2:F:192:THR:HG22	2:F:207:SER:OG	1.99	0.62
2:F:148:LYS:HB2	2:F:192:THR:OG1	1.98	0.62
3:G:51:ILE:HD13	3:G:72:VAL:HG13	1.80	0.62
2:D:192:THR:HG22	2:D:207:SER:OG	1.99	0.62
3:E:55:THR:C	7:E:344:HOH:O	2.37	0.62
3:E:157:TRP:CZ3	3:E:198:CYS:HB3	2.35	0.62
1:B:69:ARG:CD	7:B:407:HOH:O	2.50	0.60
3:G:194:GLU:HG2	7:G:402:HOH:O	2.01	0.60
3:G:197:THR:HG22	3:G:212:LYS:HA	1.84	0.60
2:F:89:GLN:HE21	2:F:92:ASN:H	1.48	0.60
1:A:276:LEU:HA	1:A:279:ILE:HG22	1.83	0.60
2:F:121:SER:O	2:F:125:THR:HG23	2.02	0.59
3:E:122:PRO:HB3	3:E:148:TYR:HB3	1.85	0.59
1:A:190:PRO:O	1:A:194:ARG:HG2	2.03	0.58
2:D:121:SER:O	2:D:125:THR:HG23	2.03	0.58
1:B:212:THR:O	1:B:216:VAL:HG23	2.03	0.58
1:B:190:PRO:O	1:B:194:ARG:HG2	2.02	0.58
1:A:212:THR:O	1:A:216:VAL:HG23	2.04	0.58
1:B:172:LEU:O	1:B:176:ILE:HD12	2.05	0.57
1:A:69:ARG:NH2	1:B:104:GLN:HE21	2.03	0.57
3:G:122:PRO:HB3	3:G:148:TYR:HB3	1.85	0.57
2:D:89:GLN:HE21	2:D:92:ASN:H	1.52	0.57
3:E:56:GLY:N	7:E:344:HOH:O	2.37	0.57
3:G:157:TRP:CZ3	3:G:198:CYS:HB3	2.40	0.56
3:G:139:VAL:HG23	3:G:188:SER:HB3	1.87	0.56
1:A:132:TYR:OH	1:A:235:THR:HG23	2.06	0.56
1:A:55:GLN:N	1:A:56:PRO:CD	2.69	0.55
3:E:162:LEU:HA	7:E:338:HOH:O	2.06	0.55
1:A:205:GLY:HA3	1:A:271:TYR:CE1	2.42	0.54
2:F:166:ASP:HB3	2:F:169:ASP:OD1	2.07	0.54
1:B:55:GLN:N	1:B:56:PRO:CD	2.71	0.54
2:D:1:GLN:HA	2:D:1:GLN:OE1	2.08	0.54
1:A:214:THR:HG21	1:A:229:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:29:PHE:CD2	3:E:77:SER:HA	2.43	0.54
1:A:69:ARG:CZ	1:B:104:GLN:HE21	2.21	0.53
3:G:50:LEU:C	3:G:50:LEU:HD12	2.29	0.53
3:G:139:VAL:CG2	3:G:188:SER:HB3	2.38	0.53
1:B:132:TYR:OH	1:B:235:THR:HG23	2.09	0.53
1:A:154:ILE:N	1:A:155:PRO:HD2	2.24	0.53
2:D:211:ASN:OD1	2:D:211:ASN:N	2.41	0.53
3:E:197:THR:HG22	3:E:212:LYS:HA	1.90	0.53
1:B:38:LEU:C	1:B:38:LEU:HD23	2.30	0.53
1:B:214:THR:HG21	1:B:229:ILE:HG12	1.90	0.52
1:A:59:GLN:HB2	7:A:420:HOH:O	2.09	0.52
3:G:29:PHE:CD2	3:G:77:SER:HA	2.45	0.52
1:A:159:ILE:HG22	1:B:35:LEU:HD21	1.92	0.52
2:D:189:ASN:ND2	2:D:211:ASN:OD1	2.32	0.52
3:E:146:LYS:HB3	3:E:179:THR:HG23	1.91	0.51
2:F:29:VAL:HG21	2:F:89:GLN:HG3	1.92	0.51
1:A:275:VAL:O	1:A:279:ILE:HG22	2.10	0.51
6:B:303:D10:H61	6:B:303:D10:H103	1.91	0.51
2:F:149:ILE:HG22	2:F:191:TYR:CE1	2.45	0.51
3:E:50:LEU:C	3:E:50:LEU:HD12	2.31	0.51
1:A:202:LEU:HA	1:A:271:TYR:OH	2.11	0.51
3:G:146:LYS:HB3	3:G:179:THR:HG23	1.92	0.50
1:B:154:ILE:N	1:B:155:PRO:HD2	2.25	0.50
3:E:12:VAL:HG21	3:E:86:LEU:HD12	1.93	0.50
3:G:12:VAL:HG21	3:G:86:LEU:HD12	1.92	0.50
2:F:139:TYR:CG	2:F:140:PRO:HA	2.47	0.49
2:D:147:TRP:N	7:D:301:HOH:O	2.44	0.49
3:G:57:TYR:CZ	3:G:59:THR:HG23	2.46	0.49
3:E:12:VAL:HG21	3:E:86:LEU:CD1	2.43	0.49
3:E:191:TRP:C	7:E:314:HOH:O	2.50	0.49
3:G:12:VAL:HG21	3:G:86:LEU:CD1	2.42	0.49
3:G:136:ASN:N	3:G:136:ASN:ND2	2.58	0.49
2:F:60:ARG:HB3	7:F:318:HOH:O	2.12	0.49
2:D:98:GLY:O	7:D:320:HOH:O	2.20	0.48
3:G:197:THR:HG23	7:G:401:HOH:O	2.14	0.48
2:D:37:GLN:HA	7:D:312:HOH:O	2.13	0.48
2:D:139:TYR:CG	2:D:140:PRO:HA	2.48	0.48
1:A:58:GLU:HG3	1:B:114:TRP:HD1	1.79	0.48
1:A:277:THR:O	1:A:281:ASN:HB2	2.14	0.48
1:A:252:GLN:O	1:A:253:ASP:HB2	2.14	0.47
2:D:192:THR:HG22	2:D:207:SER:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:SER:HB3	1:B:257:TYR:CB	2.44	0.47
1:A:200:LEU:O	1:A:204:ILE:HG22	2.15	0.47
2:F:89:GLN:HG2	2:F:91:SER:H	1.78	0.47
2:F:192:THR:HG22	2:F:207:SER:CB	2.45	0.47
3:E:34:MET:HE1	3:E:96:CYS:HB2	1.98	0.46
3:G:34:MET:HE1	3:G:96:CYS:HB2	1.97	0.46
3:E:34:MET:CE	3:E:96:CYS:HB2	2.46	0.46
3:G:34:MET:CE	3:G:96:CYS:HB2	2.46	0.46
3:E:89:GLU:HG2	7:E:302:HOH:O	2.15	0.46
3:E:150:PRO:HD2	3:E:204:ALA:CB	2.46	0.46
6:B:303:D10:H61	6:B:303:D10:C10	2.46	0.46
1:A:176:ILE:HG22	1:A:180:GLU:OE2	2.16	0.46
2:F:48:TYR:O	2:F:52:LYS:HB2	2.16	0.46
1:B:259:PRO:O	1:B:262:TRP:HB3	2.16	0.45
1:A:210:VAL:O	1:A:214:THR:HG23	2.16	0.45
2:F:72:LEU:HD23	2:F:73:THR:H	1.80	0.45
1:A:176:ILE:HD11	1:A:201:PHE:HA	1.98	0.45
1:B:69:ARG:NE	7:B:407:HOH:O	2.48	0.45
2:F:29:VAL:CG2	2:F:89:GLN:HG3	2.46	0.45
1:A:252:GLN:O	1:A:253:ASP:CB	2.65	0.45
1:B:160:LEU:O	1:B:164:VAL:HG23	2.17	0.45
1:A:258:GLN:N	1:A:259:PRO:HD2	2.32	0.45
1:B:110:SER:O	1:B:111:HIS:HB3	2.15	0.45
1:A:277:THR:O	1:A:281:ASN:N	2.49	0.44
1:B:200:LEU:O	1:B:204:ILE:HG22	2.18	0.44
3:G:136:ASN:N	3:G:136:ASN:HD22	2.16	0.44
3:E:154:THR:HG1	3:E:201:ALA:HB3	1.83	0.44
1:B:210:VAL:O	1:B:214:THR:HG23	2.17	0.44
2:F:34:TRP:HA	2:F:86:TYR:O	2.18	0.44
2:F:45:ARG:NH2	7:F:304:HOH:O	2.51	0.44
1:A:89:LYS:HE2	1:B:102:GLU:OE1	2.19	0.43
1:A:176:ILE:HG21	1:A:197:SER:HB2	1.99	0.43
1:A:160:LEU:O	1:A:164:VAL:HG23	2.18	0.43
3:G:84:LEU:O	3:G:85:SER:C	2.55	0.43
1:A:132:TYR:OH	1:A:235:THR:CG2	2.66	0.43
3:G:150:PRO:HD2	3:G:204:ALA:CB	2.48	0.43
3:G:157:TRP:N	7:G:427:HOH:O	2.25	0.43
1:B:201:PHE:CD1	1:B:201:PHE:C	2.92	0.43
3:E:149:PHE:HA	3:E:150:PRO:HA	1.84	0.43
1:A:273:ALA:O	1:A:277:THR:HG23	2.19	0.42
2:D:34:TRP:HA	2:D:86:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:84:LEU:O	3:E:85:SER:C	2.56	0.42
3:G:180:LEU:C	3:G:180:LEU:CD1	2.87	0.42
3:E:141:LEU:HD22	3:E:213:ILE:HG21	2.01	0.42
2:F:72:LEU:HD23	2:F:72:LEU:C	2.39	0.42
3:G:158:ASN:OD1	7:G:401:HOH:O	2.22	0.42
1:A:60:GLN:HB3	1:B:138:ARG:NH2	2.35	0.42
2:D:166:ASP:HB3	2:D:169:ASP:OD1	2.20	0.42
1:B:132:TYR:OH	1:B:235:THR:CG2	2.67	0.42
1:B:202:LEU:HD12	1:B:203:LEU:N	2.35	0.42
3:G:149:PHE:HA	3:G:150:PRO:HA	1.86	0.42
1:A:272:PHE:O	1:A:276:LEU:HD23	2.19	0.41
3:G:57:TYR:OH	3:G:59:THR:CG2	2.67	0.41
3:G:129:PRO:HD3	3:G:141:LEU:HD23	2.02	0.41
3:G:141:LEU:HD22	3:G:213:ILE:HG21	2.02	0.41
1:A:33:LEU:O	1:A:33:LEU:HD23	2.20	0.41
2:D:192:THR:HG23	7:D:314:HOH:O	2.21	0.41
1:A:160:LEU:CD1	1:B:36:LEU:HA	2.50	0.41
3:E:180:LEU:C	3:E:180:LEU:CD1	2.88	0.41
1:A:35:LEU:HD12	1:A:35:LEU:HA	1.92	0.41
1:A:82:GLN:OE1	1:A:82:GLN:N	2.48	0.41
2:D:25:ALA:O	2:D:68:THR:OG1	2.39	0.41
2:F:12:SER:CB	2:F:104:GLU:HG3	2.51	0.40
2:F:149:ILE:O	2:F:149:ILE:HG13	2.21	0.40
1:A:51:ARG:HE	1:B:116:LEU:HD23	1.87	0.40
2:F:135:LEU:HD21	2:F:145:VAL:HG22	2.03	0.40
2:D:117:PHE:HA	2:D:118:PRO:HD3	1.81	0.40
1:A:206:CYS:H	1:A:271:TYR:HH	1.69	0.40
1:A:202:LEU:HD12	1:A:203:LEU:N	2.37	0.40
2:F:205:VAL:O	2:F:206:LYS:HD3	2.22	0.40
3:G:194:GLU:CG	7:G:402:HOH:O	2.67	0.40

There are no symmetry-related clashes.

## 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%)	241 (97%)	8 (3%)	0	100	100
1	B	239/299 (80%)	232 (97%)	7 (3%)	0	100	100
2	D	209/211 (99%)	199 (95%)	10 (5%)	0	100	100
2	F	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
3	E	207/217 (95%)	200 (97%)	6 (3%)	1 (0%)	29	66
3	G	206/217 (95%)	200 (97%)	4 (2%)	2 (1%)	15	50
All	All	1319/1454 (91%)	1273 (96%)	43 (3%)	3 (0%)	47	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	41	HIS
3	G	41	HIS
3	G	85	SER

### 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%)	200 (98%)	4 (2%)	55	82
1	B	197/242 (81%)	193 (98%)	4 (2%)	55	82
2	D	184/184 (100%)	177 (96%)	7 (4%)	33	68
2	F	184/184 (100%)	178 (97%)	6 (3%)	38	72
3	E	187/190 (98%)	181 (97%)	6 (3%)	39	73
3	G	186/190 (98%)	180 (97%)	6 (3%)	39	73
All	All	1142/1232 (93%)	1109 (97%)	33 (3%)	42	75

All (33) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	62	GLN
1	A	138	ARG
1	A	249	ASP
1	A	272	PHE
1	B	33	LEU
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	161	SER
2	D	183	ASP
3	E	18	MET
3	E	59	THR
3	E	67	LYS
3	E	77	SER
3	E	136	ASN
3	E	181	SER
2	F	21	MET
2	F	42	SER
2	F	88	GLN
2	F	89	GLN
2	F	104	GLU
2	F	161	SER
3	G	18	MET
3	G	65	LYS
3	G	77	SER
3	G	136	ASN
3	G	143	CYS
3	G	181	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	B	104	GLN
2	D	88	GLN
2	F	88	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 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	303	-	9,9,9	0.29	0	8,8,8	0.41	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	303	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	303	D10	C2-C3-C4-C5
6	B	303	D10	C3-C4-C5-C6
6	B	303	D10	C6-C7-C8-C9
6	B	303	D10	C5-C6-C7-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	303	D10	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	271:TYR	C	272:PHE	N	1.79

## 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%)	0.21	25 (9%) <b>7</b> <b>2</b>	66, 132, 195, 208	0
1	B	243/299 (81%)	0.87	50 (20%) <b>1</b> <b>0</b>	62, 134, 248, 299	0
2	D	211/211 (100%)	-0.39	3 (1%) <b>75</b> 48	67, 102, 143, 161	0
2	F	211/211 (100%)	-0.37	4 (1%) <b>66</b> <b>37</b>	62, 94, 154, 176	0
3	E	211/217 (97%)	0.15	17 (8%) <b>12</b> <b>3</b>	54, 86, 129, 184	0
3	G	210/217 (96%)	-0.20	7 (3%) 46 <b>20</b>	55, 91, 132, 205	0
All	All	1339/1454 (92%)	0.07	106 (7%) <b>12</b> <b>4</b>	54, 103, 193, 299	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	ILE	11.0
1	B	181	ALA	10.2
1	B	192	LEU	10.2
3	G	136	ASN	10.1
1	B	180	GLU	8.8
3	E	217	ASP	8.8
1	B	183	PHE	8.5
1	B	189	PRO	8.0
1	B	251	ARG	8.0
1	B	193	VAL	7.8
3	G	137	SER	7.8
1	B	178	HIS	7.2
1	B	190	PRO	6.7
1	B	194	ARG	6.5
1	B	250	PRO	6.3
1	B	196	LEU	6.3
1	B	188	VAL	6.2
1	B	176	ILE	5.7
1	B	182	ILE	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	111	HIS	5.6
1	B	195	VAL	5.5
1	B	197	SER	5.5
1	B	184	LEU	5.4
1	B	186	TRP	4.9
1	B	200	LEU	4.8
2	F	201	THR	4.7
1	B	191	GLU	4.6
1	B	177	GLY	4.6
3	E	1	GLU	4.6
1	B	30	THR	4.4
1	B	172	LEU	4.3
1	B	31	THR	4.3
1	B	256	ALA	4.1
1	A	186	TRP	4.0
3	E	20	THR	3.9
1	B	252	GLN	3.8
1	B	34	ALA	3.8
1	B	187	HIS	3.7
1	B	110	SER	3.6
1	A	176	ILE	3.6
1	A	179	ILE	3.6
1	B	253	ASP	3.6
1	A	183	PHE	3.5
1	B	201	PHE	3.5
3	E	193	SER	3.5
3	G	188	SER	3.5
1	B	199	MET	3.5
1	A	163	GLY	3.4
1	A	222	ASP	3.4
3	G	138	MET	3.4
1	A	165	GLY	3.3
1	B	257	TYR	3.3
1	A	110	SER	3.3
1	B	173	ARG	3.2
1	B	116	LEU	3.2
3	E	215	PRO	3.1
3	E	216	ARG	3.1
2	D	105	LEU	3.1
1	B	185	LYS	3.0
1	A	159	ILE	3.0
1	B	255	PRO	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	79	ALA	2.8
3	E	192	PRO	2.8
1	B	242	GLY	2.8
1	A	167	ARG	2.8
1	B	112	SER	2.7
1	A	29	SER	2.7
1	B	33	LEU	2.7
3	E	41	HIS	2.7
1	A	164	VAL	2.7
1	A	249	ASP	2.6
3	G	216	ARG	2.6
1	A	248	ALA	2.6
1	B	258	GLN	2.6
2	D	104	GLU	2.6
1	B	174	HIS	2.5
1	B	175	GLY	2.5
1	B	249	ASP	2.5
3	E	78	THR	2.5
1	A	178	HIS	2.4
2	F	154	ARG	2.4
2	F	202	SER	2.4
3	E	191	TRP	2.4
1	A	187	HIS	2.4
1	A	175	GLY	2.3
1	A	33	LEU	2.3
3	E	186	VAL	2.3
3	E	19	LYS	2.3
3	E	110	THR	2.3
3	E	136	ASN	2.3
1	A	273	ALA	2.3
1	A	55	GLN	2.3
2	D	122	GLU	2.3
3	E	81	MET	2.2
3	E	80	TYR	2.2
1	B	219	TYR	2.2
3	G	41	HIS	2.2
3	G	189	SER	2.2
1	B	32	LEU	2.2
1	A	274	SER	2.1
2	F	1	GLN	2.1
1	A	133	GLY	2.1
1	A	161	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	243	ASP	2.0
1	A	168	LEU	2.0
1	A	256	ALA	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
6	D10	B	303	10/10	0.77	0.90	108,136,140,149	0
4	TL	B	301	1/1	0.78	0.20	240,240,240,240	0
4	TL	B	302	1/1	0.84	0.14	250,250,250,250	0
4	TL	A	301	1/1	0.84	0.23	230,230,230,230	0
5	CA	A	306	1/1	0.91	0.09	117,117,117,117	0
5	CA	G	301	1/1	0.97	0.16	111,111,111,111	0
5	CA	A	305	1/1	0.97	0.05	131,131,131,131	0
4	TL	A	304	1/1	0.98	0.07	117,117,117,117	0
4	TL	A	307	1/1	0.98	0.08	118,118,118,118	0
4	TL	A	302	1/1	0.99	0.07	115,115,115,115	0
4	TL	A	303	1/1	0.99	0.07	112,112,112,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.