



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:55 PM UTC

PDB ID : 4WFH / pdb_00004wfh
Title : Human TRAAK K⁺ channel in a Tl⁺ 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

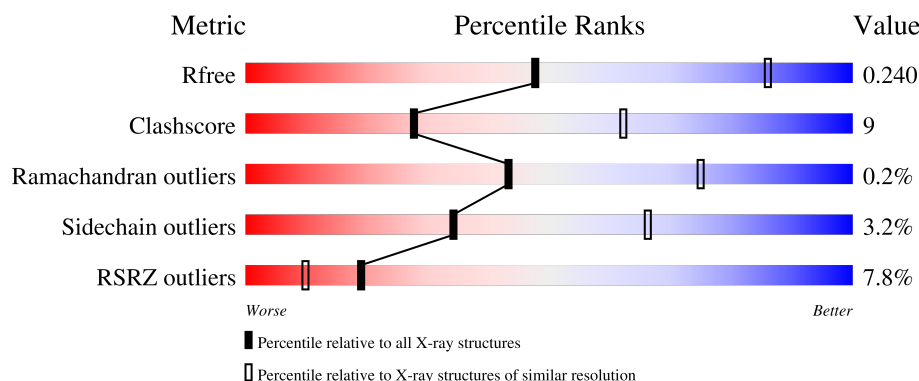
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (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 ≥ 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	10% 67% 17% 15%
1	B	299	8% 67% 13% 19%
2	D	211	6% 82% 17%
2	F	211	5% 82% 16%
3	E	217	7% 76% 20%

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Mol	Chain	Length	Quality of chain
3	G	217	7% 76% 20% ••

2 Entry composition

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
1	A	253	Total	C	N	O	S	0	0	0
			1963	1299	318	340	6			
1	B	243	Total	C	N	O	S	0	0	0
			1888	1246	306	330	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLN	ASN	engineered mutation	UNP Q9NYG8
A	108	GLN	ASN	engineered mutation	UNP Q9NYG8
A	291	SER	-	expression tag	UNP Q9NYG8
A	292	ASN	-	expression tag	UNP Q9NYG8
A	293	SER	-	expression tag	UNP Q9NYG8
A	294	LEU	-	expression tag	UNP Q9NYG8
A	295	GLU	-	expression tag	UNP Q9NYG8
A	296	VAL	-	expression tag	UNP Q9NYG8
A	297	LEU	-	expression tag	UNP Q9NYG8
A	298	PHE	-	expression tag	UNP Q9NYG8
A	299	GLN	-	expression tag	UNP Q9NYG8
B	104	GLN	ASN	engineered mutation	UNP Q9NYG8
B	108	GLN	ASN	engineered mutation	UNP Q9NYG8
B	291	SER	-	expression tag	UNP Q9NYG8
B	292	ASN	-	expression tag	UNP Q9NYG8
B	293	SER	-	expression tag	UNP Q9NYG8
B	294	LEU	-	expression tag	UNP Q9NYG8
B	295	GLU	-	expression tag	UNP Q9NYG8
B	296	VAL	-	expression tag	UNP Q9NYG8
B	297	LEU	-	expression tag	UNP Q9NYG8
B	298	PHE	-	expression tag	UNP Q9NYG8
B	299	GLN	-	expression tag	UNP Q9NYG8

- Molecule 2 is a protein called ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	211	Total	C	N	O	S	0	0	0
			1616	1003	271	333	9			
2	F	211	Total	C	N	O	S	0	0	0
			1616	1003	271	333	9			

- Molecule 3 is a protein called ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	211	Total	C	N	O	S	0	0	0
			1614	1026	261	319	8			
3	G	210	Total	C	N	O	S	0	0	0
			1605	1022	260	315	8			

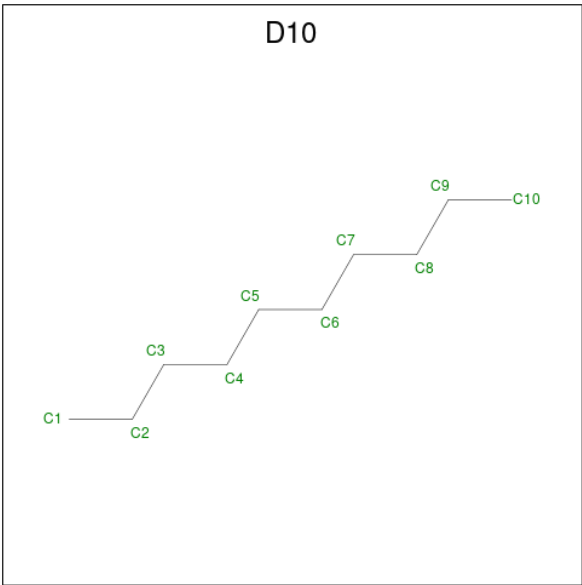
- Molecule 4 is THALLIUM (I) ION (CCD ID: TL) (formula: Tl).

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 (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	G	1	Total	Ca	0	0
			1	1		

- Molecule 6 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



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

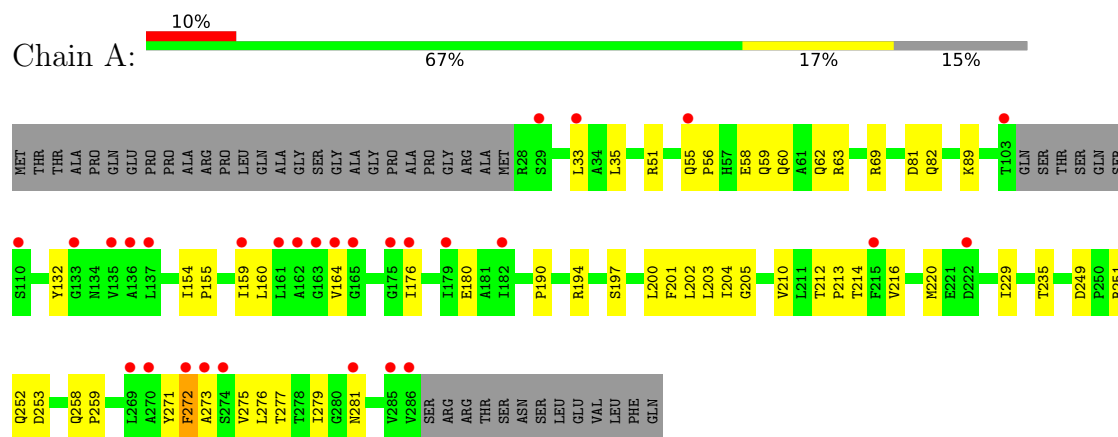
- Molecule 7 is water.

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

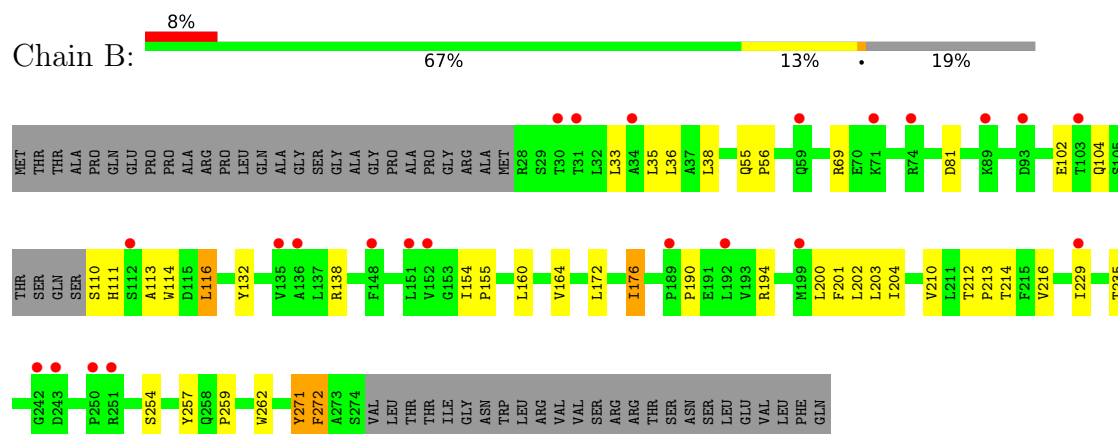
3 Residue-property plots [i](#)

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.

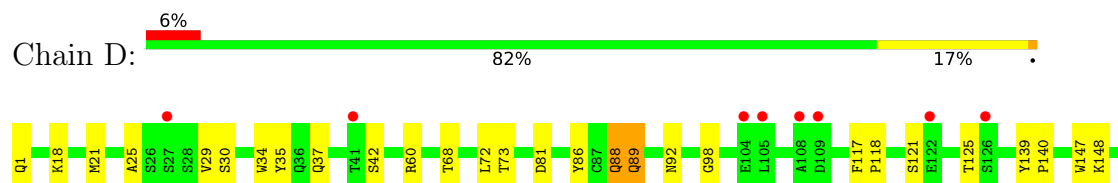
- Molecule 1: Potassium channel subfamily K member 4

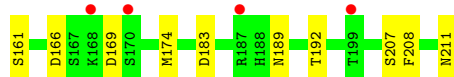


- Molecule 1: Potassium channel subfamily K member 4

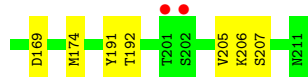
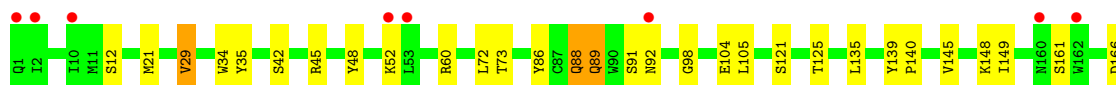
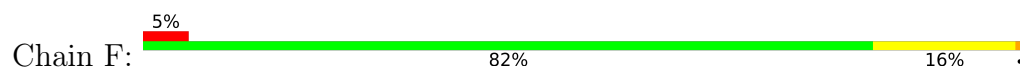


- Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN

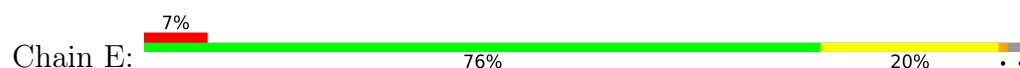




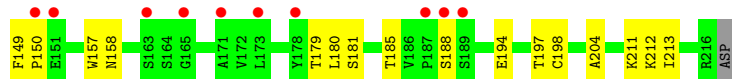
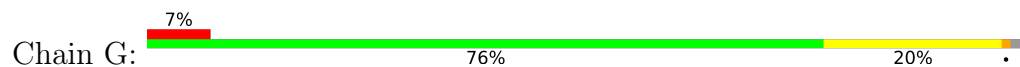
● Molecule 2: ANTI-TRAAK ANTIBODY 13E9 FAB FRAGMENT LIGHT CHAIN



● 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	80.97Å 138.75Å 96.76Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	48.20 – 3.01 48.20 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.20-3.01) 99.0 (48.20-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.203 , 0.238 0.207 , 0.240	Depositor DCC
R_{free} test set	2098 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	81.5	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10506	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D10, CA, 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	0.45	0/2013	0.74	0/2745
1	B	0.90	1/1937 (0.1%)	0.74	2/2638 (0.1%)
2	D	0.48	0/1655	0.70	0/2247
2	F	0.51	0/1655	0.71	0/2247
3	E	0.55	0/1656	0.75	0/2260
3	G	0.55	0/1647	0.75	0/2249
All	All	0.60	1/10563 (0.0%)	0.73	2/14386 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	TYR	C-N	34.01	1.79	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	TYR	CA-C-N	5.68	128.46	120.28
1	B	271	TYR	C-N-CA	5.68	128.46	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1963	0	1985	44	0
1	B	1888	0	1899	32	0
2	D	1616	0	1542	25	0
2	F	1616	0	1542	27	0
3	E	1614	0	1586	30	0
3	G	1605	0	1582	34	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	184	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 9.

All (184) 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	1.40
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
3:E:180:LEU:C	3:E:180:LEU:HD12	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:180:LEU:HD12	3:G:180:LEU:C	2.19	0.68
1:A:58:GLU:OE2	1:B:113:ALA:N	2.27	0.68
3:E:55:THR:C	7:E:344:HOH:O	2.37	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
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
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:E:136:ASN:N	3:E:136:ASN:ND2	2.42	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: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
3:G:50:LEU:C	3:G:50:LEU:HD12	2.29	0.58
1:A:212:THR:O	1:A:216:VAL:HG23	2.04	0.58
1:B:38:LEU:C	1:B:38:LEU:HD23	2.30	0.57
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
3:E:50:LEU:C	3:E:50:LEU:HD12	2.31	0.56
1:A:55:GLN:N	1:A:56:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:214:THR:HG21	1:A:229:ILE:HG12	1.89	0.54
3:E:29:PHE:CD2	3:E:77:SER:HA	2.43	0.54
3:E:191:TRP:C	7:E:314:HOH:O	2.50	0.54
1:A:69:ARG:CZ	1:B:104:GLN:HE21	2.21	0.53
2:D:1:GLN:HA	2:D:1:GLN:OE1	2.08	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: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
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
2:F:192:THR:HG22	2:F:207:SER:HG	1.77	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:84:LEU:O	3:G:85:SER:C	2.55	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:B:201:PHE:CD1	1:B:201:PHE:C	2.92	0.47
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
1:B:254:SER:HB3	1:B:257:TYR:CB	2.44	0.47
3:E:138:MET:HE3	3:E:185:THR:HG22	1.97	0.47
1:A:200:LEU:O	1:A:204:ILE:HG22	2.15	0.47
2:F:72:LEU:HD23	2:F:72:LEU:C	2.39	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:84:LEU:O	3:E:85:SER:C	2.56	0.47
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
3:G:138:MET:HE3	3:G:185:THR:HG22	1.99	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
3:G:180:LEU:C	3:G:180:LEU:CD1	2.87	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
3:E:76:SER:O	3:E:77:SER:C	2.60	0.44
3:G:76:SER:O	3:G:77:SER:C	2.60	0.44
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	1.82	0.44
3:E:73:ASP:OD1	3:E:73:ASP:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:D:208:PHE:CD1	2:D:208:PHE:C	2.98	0.42
3:E:141:LEU:HD22	3:E:213:ILE:HG21	2.01	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
3:E:180:LEU:C	3:E:180:LEU:CD1	2.88	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
3:G:34:MET:HE1	3:G:96:CYS:HB2	2.03	0.41
1:A:160:LEU:CD1	1:B:36:LEU:HA	2.50	0.41
2:D:192:THR:HG22	2:D:207:SER:HG	1.84	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
3:G:64:PHE:O	3:G:65:LYS:C	2.64	0.41
2:D:72:LEU:HD23	2:D:72:LEU:C	2.45	0.40
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
3:E:174:GLN:O	3:E:175:SER:C	2.64	0.40
2:F:135:LEU:HD21	2:F:145:VAL:HG22	2.03	0.40
3:G:3:GLN:C	3:G:4:LEU:HD12	2.45	0.40
2:D:117:PHE:HA	2:D:118:PRO:HD3	1.81	0.40
2:F:72:LEU:C	2:F:72:LEU:CD2	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24	59
3	G	206/217 (95%)	200 (97%)	4 (2%)	2 (1%)	12	43
All	All	1319/1454 (91%)	1273 (96%)	43 (3%)	3 (0%)	43	75

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%)	202 (99%)	2 (1%)	68	83
1	B	197/242 (81%)	193 (98%)	4 (2%)	48	75
2	D	184/184 (100%)	175 (95%)	9 (5%)	22	55
2	F	184/184 (100%)	176 (96%)	8 (4%)	26	59
3	E	187/190 (98%)	180 (96%)	7 (4%)	30	63
3	G	186/190 (98%)	180 (97%)	6 (3%)	34	66
All	All	1142/1232 (93%)	1106 (97%)	36 (3%)	34	66

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	272	PHE
1	B	33	LEU
1	B	116	LEU
1	B	176	ILE
1	B	272	PHE
2	D	18	LYS
2	D	21	MET
2	D	30	SER
2	D	42	SER
2	D	88	GLN
2	D	89	GLN
2	D	161	SER
2	D	174	MET
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
3	E	211	LYS
2	F	21	MET
2	F	29	VAL
2	F	42	SER
2	F	88	GLN
2	F	89	GLN

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Mol	Chain	Res	Type
2	F	105	LEU
2	F	161	SER
2	F	174	MET
3	G	18	MET
3	G	77	SER
3	G	136	ASN
3	G	143	CYS
3	G	181	SER
3	G	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	B	55	GLN
1	B	76	HIS
1	B	104	GLN
2	D	137	ASN
2	F	88	GLN
2	F	92	ASN
2	F	144	ASN
2	F	209	ASN
3	G	44	ASN
3	G	136	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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, 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%)	0.57	29 (11%)	9 5	66, 132, 195, 208	0
1	B	243/299 (81%)	0.59	23 (9%)	14 7	62, 134, 248, 299	0
2	D	211/211 (100%)	0.11	12 (5%)	29 15	67, 102, 143, 161	0
2	F	211/211 (100%)	0.06	10 (4%)	36 19	62, 94, 154, 176	0
3	E	211/217 (97%)	0.03	15 (7%)	22 11	54, 86, 129, 184	0
3	G	210/217 (96%)	0.10	16 (7%)	20 10	55, 91, 132, 204	0
All	All	1339/1454 (92%)	0.26	105 (7%)	19 10	54, 103, 193, 299	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1	GLN	10.2
1	A	273	ALA	8.5
1	B	152	VAL	8.3
1	B	148	PHE	7.5
2	F	201	THR	7.2
1	B	34	ALA	6.9
1	B	151	LEU	6.4
2	D	105	LEU	6.1
1	A	270	ALA	6.0
3	G	137	SER	5.9
3	G	188	SER	5.8
1	A	163	GLY	5.5
3	G	136	ASN	5.5
2	D	122	GLU	5.4
1	B	192	LEU	5.4
1	A	269	LEU	5.1
1	B	89	LYS	5.0
1	A	161	LEU	5.0
1	A	175	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	250	PRO	4.7
2	D	109	ASP	4.5
3	G	189	SER	4.4
1	A	165	GLY	4.3
2	D	104	GLU	4.3
3	G	151	GLU	4.2
1	A	179	ILE	3.9
1	A	272	PHE	3.9
1	A	159	ILE	3.9
1	A	222	ASP	3.8
1	B	31	THR	3.7
3	E	167	HIS	3.7
3	G	138	MET	3.7
2	F	162	TRP	3.6
3	G	62	GLN	3.6
2	D	168	LYS	3.6
1	B	30	THR	3.5
3	E	192	PRO	3.5
3	E	26	GLY	3.4
3	E	165	GLY	3.4
1	A	135	VAL	3.4
1	A	176	ILE	3.3
1	A	274	SER	3.3
1	B	243	ASP	3.2
1	B	135	VAL	3.2
3	E	2	VAL	3.2
3	G	41	HIS	3.2
1	B	242	GLY	3.1
1	A	55	GLN	3.1
3	E	183	SER	3.1
3	E	188	SER	3.1
3	E	193	SER	3.1
3	E	1	GLU	3.0
1	A	133	GLY	3.0
2	D	108	ALA	2.9
2	F	202	SER	2.9
1	A	136	ALA	2.9
1	B	251	ARG	2.9
2	D	187	ARG	2.8
3	E	123	SER	2.8
3	G	178	TYR	2.8
3	G	173	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	136	ALA	2.8
2	F	160	ASN	2.7
1	A	33	LEU	2.7
3	E	209	VAL	2.7
3	G	63	LYS	2.6
2	D	170	SER	2.6
3	G	171	ALA	2.6
3	E	125	TYR	2.6
1	A	103	THR	2.5
3	E	166	VAL	2.5
1	A	29	SER	2.5
2	F	92	ASN	2.5
1	B	74	ARG	2.4
3	E	42	GLY	2.4
3	E	159	SER	2.4
1	B	229	ILE	2.4
1	A	110	SER	2.4
1	B	112	SER	2.4
2	D	126	SER	2.4
1	B	189	PRO	2.4
1	A	281	ASN	2.3
2	D	27	SER	2.3
1	B	199	MET	2.3
3	G	150	PRO	2.3
2	F	2	ILE	2.3
1	A	137	LEU	2.3
1	A	164	VAL	2.3
1	A	285	VAL	2.3
1	A	286	VAL	2.3
1	A	162	ALA	2.2
2	D	41	THR	2.2
3	G	163	SER	2.2
2	F	52	LYS	2.2
1	A	215	PHE	2.1
1	B	103	THR	2.1
1	A	182	ILE	2.1
2	F	53	LEU	2.1
3	G	187	PRO	2.1
1	B	59	GLN	2.1
1	B	93	ASP	2.1
3	G	165	GLY	2.1
1	B	71	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	10	ILE	2.0
2	D	199	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TL	A	301	1/1	0.91	0.15	230,230,230,230	0
4	TL	B	301	1/1	0.91	0.10	240,240,240,240	0
4	TL	B	302	1/1	0.94	0.08	250,250,250,250	0
6	D10	B	303	10/10	0.94	0.32	108,136,140,149	0
5	CA	A	306	1/1	0.96	0.09	117,117,117,117	0
5	CA	G	301	1/1	0.98	0.04	111,111,111,111	0
5	CA	A	305	1/1	0.98	0.06	131,131,131,131	0
4	TL	A	304	1/1	1.00	0.02	117,117,117,117	0
4	TL	A	307	1/1	1.00	0.02	118,118,118,118	0
4	TL	A	302	1/1	1.00	0.02	115,115,115,115	0
4	TL	A	303	1/1	1.00	0.03	112,112,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.