Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 04:58 PM EDT

PDB ID	:	6CQ6
Title	:	K2P2.1(TREK-1) apo structure
Authors	:	Lolicato, M.; Minor, D.L.
Deposited on	:	2018-03-14
Resolution	:	3.10 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:

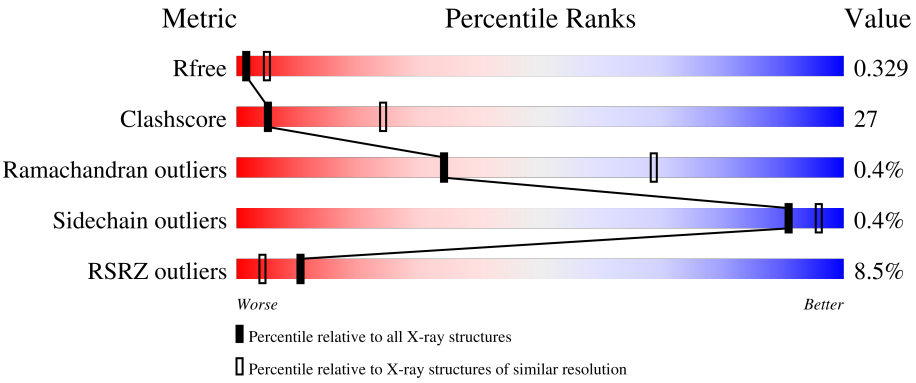
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	312	8% 44% 42% 14%
1	B	312	7% 46% 43% · 10%

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
3	K	A	402	-	-	-	X
3	K	A	406	-	-	-	X
4	D10	A	407	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4490 atoms, of which 127 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2103	1405	332	362	4			
1	B	282	Total	C	N	O	S	0	0	0
			2186	1455	346	380	5			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	LEU	initiating methionine	UNP P97438
A	84	ARG	LYS	engineered mutation	UNP P97438
A	85	GLU	GLN	engineered mutation	UNP P97438
A	86	LYS	THR	engineered mutation	UNP P97438
A	88	LEU	ILE	engineered mutation	UNP P97438
A	89	ARG	ALA	engineered mutation	UNP P97438
A	90	ALA	GLN	engineered mutation	UNP P97438
A	92	PRO	ALA	engineered mutation	UNP P97438
A	95	SER	ASN	engineered mutation	UNP P97438
A	96	ASP	SER	engineered mutation	UNP P97438
A	97	GLN	THR	engineered mutation	UNP P97438
A	119	ALA	ASN	engineered mutation	UNP P97438
A	300	ALA	SER	engineered mutation	UNP P97438
A	306	ALA	GLU	engineered mutation	UNP P97438
A	323	SER	ALA	engineered mutation	UNP P97438
A	324	ASN	GLU	engineered mutation	UNP P97438
A	325	SER	-	expression tag	UNP P97438
A	326	LEU	-	expression tag	UNP P97438
A	327	GLU	-	expression tag	UNP P97438
A	328	VAL	-	expression tag	UNP P97438
A	329	LEU	-	expression tag	UNP P97438
A	330	PHE	-	expression tag	UNP P97438
A	331	GLN	-	expression tag	UNP P97438
B	20	MET	LEU	initiating methionine	UNP P97438
B	84	ARG	LYS	engineered mutation	UNP P97438

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Chain	Residue	Modelled	Actual	Comment	Reference
B	85	GLU	GLN	engineered mutation	UNP P97438
B	86	LYS	THR	engineered mutation	UNP P97438
B	88	LEU	ILE	engineered mutation	UNP P97438
B	89	ARG	ALA	engineered mutation	UNP P97438
B	90	ALA	GLN	engineered mutation	UNP P97438
B	92	PRO	ALA	engineered mutation	UNP P97438
B	95	SER	ASN	engineered mutation	UNP P97438
B	96	ASP	SER	engineered mutation	UNP P97438
B	97	GLN	THR	engineered mutation	UNP P97438
B	119	ALA	ASN	engineered mutation	UNP P97438
B	300	ALA	SER	engineered mutation	UNP P97438
B	306	ALA	GLU	engineered mutation	UNP P97438
B	323	SER	ALA	engineered mutation	UNP P97438
B	324	ASN	GLU	engineered mutation	UNP P97438
B	325	SER	-	expression tag	UNP P97438
B	326	LEU	-	expression tag	UNP P97438
B	327	GLU	-	expression tag	UNP P97438
B	328	VAL	-	expression tag	UNP P97438
B	329	LEU	-	expression tag	UNP P97438
B	330	PHE	-	expression tag	UNP P97438
B	331	GLN	-	expression tag	UNP P97438

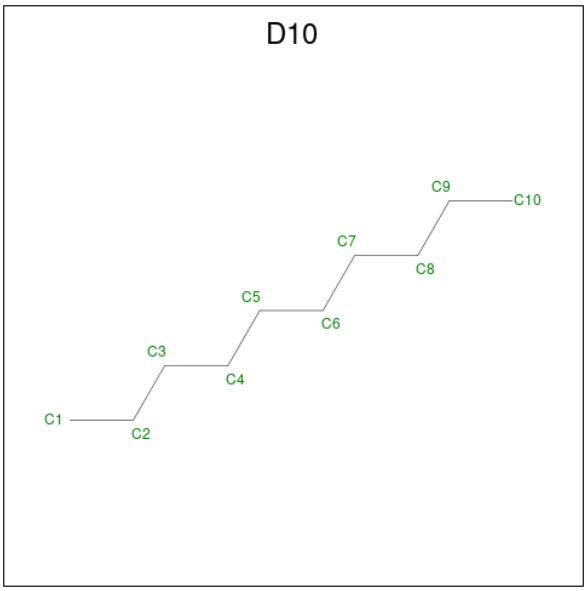
- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cd 1 1	0	0
2	B	2	Total Cd 2 2	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total K 5 5	0	0
3	B	1	Total K 1 1	0	0

- Molecule 4 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).

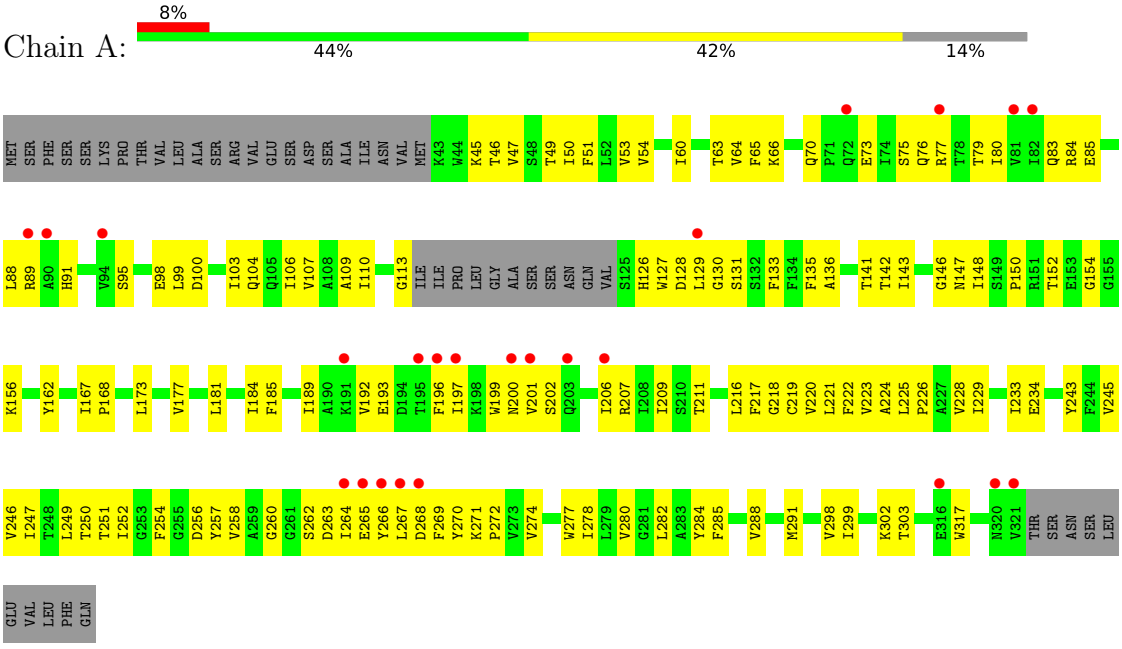


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H 14 5 9	0	0
4	A	1	Total C H 14 5 9	0	0
4	A	1	Total C H 30 10 20	0	0
4	A	1	Total C H 30 10 20	0	0
4	A	1	Total C H 30 10 20	0	0
4	B	1	Total C H 14 5 9	0	0
4	B	1	Total C H 30 10 20	0	0
4	B	1	Total C H 30 10 20	0	0

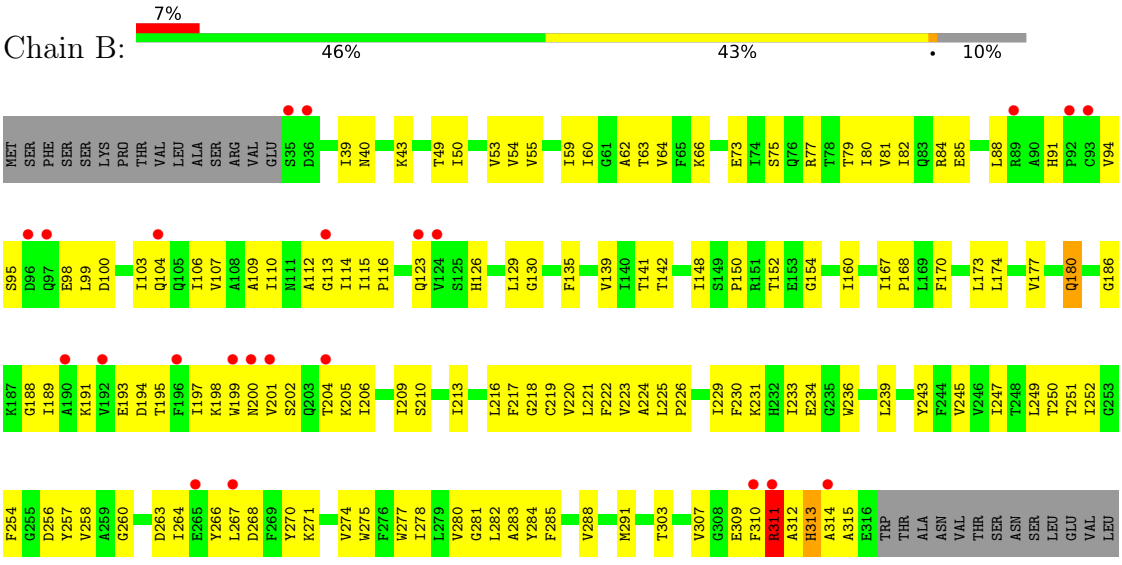
3 Residue-property plots (i)

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 2



• Molecule 1: Potassium channel subfamily K member 2



PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.72Å 120.42Å 126.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.96 – 3.10 45.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (14.96-3.10) 99.8 (45.89-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.260 , 0.302 0.278 , 0.329	Depositor DCC
R_{free} test set	938 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	123.1	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 128.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4490	wwPDB-VP
Average B, all atoms (Å^2)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CD, D10, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	1/2156 (0.0%)	0.39	0/2932
1	B	0.27	0/2239	0.45	3/3046 (0.1%)
All	All	0.27	1/4395 (0.0%)	0.42	3/5978 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	TRP	CB-CG	-5.48	1.40	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	311	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	311	ARG	CG-CD-NE	5.78	123.94	111.80
1	B	180	GLN	CA-CB-CG	5.62	125.77	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	ASP	Peptide
1	B	263	ASP	Peptide

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	2103	0	2153	123	0
1	B	2186	0	2241	135	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	0	0
3	B	1	0	0	0	0
4	A	40	78	84	0	0
4	B	25	49	53	0	0
All	All	4363	127	4531	238	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 27.

All (238) 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:311:ARG:HD2	1:B:311:ARG:C	1.68	1.13
1:A:73:GLU:HG2	1:A:77:ARG:HD2	1.21	1.11
1:B:311:ARG:HD2	1:B:311:ARG:O	1.64	0.98
1:A:88:LEU:HD11	1:A:99:LEU:HD13	1.51	0.93
1:A:77:ARG:NH2	1:B:123:GLN:HB2	1.93	0.83
1:B:95:SER:HB3	1:B:98:GLU:HB2	1.60	0.83
1:B:107:VAL:HA	1:B:110:ILE:HD12	1.60	0.82
1:A:73:GLU:CG	1:A:77:ARG:HD2	2.08	0.81
1:A:91:HIS:NE2	1:B:95:SER:OG	2.13	0.81
1:B:152:THR:HG22	1:B:154:GLY:H	1.48	0.77
1:A:73:GLU:HG2	1:A:77:ARG:CD	2.09	0.76
1:B:109:ALA:HB1	1:B:114:ILE:HG21	1.67	0.75
1:A:202:SER:O	1:A:206:ILE:HG12	1.85	0.75
1:A:152:THR:HG22	1:A:154:GLY:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:HB	1:B:251:THR:HG23	1.68	0.74
1:A:73:GLU:O	1:A:77:ARG:HG3	1.87	0.74
1:B:95:SER:O	1:B:98:GLU:N	2.21	0.74
1:A:63:THR:HA	1:A:66:LYS:NZ	2.03	0.74
1:B:194:ASP:HA	1:B:197:ILE:HG12	1.70	0.74
1:A:197:ILE:HD12	1:A:206:ILE:HG21	1.71	0.72
1:A:260:GLY:O	1:A:266:TYR:OH	2.07	0.70
1:B:202:SER:OG	1:B:205:LYS:HB2	1.92	0.70
1:A:141:THR:O	1:A:142:THR:OG1	2.11	0.68
1:A:167:ILE:HB	1:A:168:PRO:HD3	1.75	0.68
1:B:94:VAL:HG22	1:B:95:SER:H	1.58	0.68
1:A:193:GLU:HA	1:A:197:ILE:HG13	1.76	0.68
1:B:106:ILE:O	1:B:110:ILE:HG13	1.94	0.68
1:A:245:VAL:HG13	1:A:277:TRP:HZ2	1.59	0.68
1:A:271:LYS:CG	1:A:272:PRO:HD3	2.24	0.67
1:B:275:TRP:HA	1:B:278:ILE:HD12	1.75	0.67
1:A:95:SER:OG	1:A:98:GLU:OE1	2.11	0.67
1:B:194:ASP:HA	1:B:197:ILE:CG1	2.25	0.67
1:A:219:CYS:O	1:A:223:VAL:HB	1.95	0.67
1:B:193:GLU:O	1:B:197:ILE:HG12	1.95	0.66
1:B:167:ILE:HB	1:B:168:PRO:HD3	1.77	0.66
1:B:198:LYS:O	1:B:201:VAL:HG13	1.95	0.66
1:B:245:VAL:HG13	1:B:277:TRP:HZ2	1.62	0.65
1:A:126:HIS:N	1:B:73:GLU:OE2	2.27	0.65
1:A:265:GLU:O	1:A:266:TYR:HB3	1.96	0.65
1:A:234:GLU:OE2	1:A:262:SER:OG	2.15	0.64
1:B:206:ILE:HA	1:B:209:ILE:HD13	1.78	0.64
1:A:63:THR:HA	1:A:66:LYS:HZ2	1.61	0.64
1:A:79:THR:O	1:A:83:GLN:HG3	1.98	0.64
1:A:84:ARG:NH1	1:B:116:PRO:HA	2.13	0.64
1:A:109:ALA:O	1:A:113:GLY:N	2.31	0.63
1:B:201:VAL:HB	1:B:206:ILE:HD11	1.79	0.63
1:B:221:LEU:HA	1:B:225:LEU:HD12	1.81	0.63
1:A:271:LYS:HG2	1:A:272:PRO:HD3	1.81	0.63
1:B:107:VAL:HA	1:B:110:ILE:CD1	2.29	0.63
1:A:218:GLY:HA3	1:A:284:TYR:CE1	2.34	0.63
1:B:107:VAL:HG22	1:B:110:ILE:HD12	1.79	0.63
1:B:218:GLY:HA3	1:B:284:TYR:CE1	2.34	0.62
1:A:143:ILE:HG12	1:A:251:THR:HA	1.80	0.62
1:A:217:PHE:CZ	1:A:221:LEU:HD11	2.35	0.62
1:B:191:LYS:O	1:B:195:THR:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:CG2	1:A:233:ILE:HD12	2.30	0.61
1:B:245:VAL:HG13	1:B:277:TRP:CZ2	2.35	0.61
1:B:91:HIS:O	1:B:94:VAL:HG12	2.00	0.61
1:B:198:LYS:H	1:B:201:VAL:CG1	2.14	0.60
1:A:247:ILE:HD12	1:A:254:PHE:HE2	1.67	0.60
1:B:188:GLY:HA2	1:B:191:LYS:NZ	2.16	0.60
1:A:267:LEU:CD1	1:A:269:PHE:HB3	2.33	0.59
1:B:258:VAL:HG12	1:B:260:GLY:H	1.65	0.59
1:A:249:LEU:HB2	1:A:285:PHE:CE2	2.38	0.59
1:A:135:PHE:CZ	1:A:150:PRO:HD3	2.38	0.58
1:B:222:PHE:CE1	1:B:280:VAL:HG12	2.38	0.58
1:A:200:ASN:OD1	1:A:201:VAL:N	2.36	0.58
1:A:197:ILE:HD12	1:A:206:ILE:CG2	2.32	0.58
1:B:39:ILE:HD13	1:B:43:LYS:HE3	1.86	0.58
1:A:246:VAL:HG11	1:B:160:ILE:HG23	1.87	0.57
1:A:270:TYR:O	1:A:274:VAL:HG23	2.05	0.57
1:B:250:THR:O	1:B:251:THR:HG22	2.05	0.57
1:B:266:TYR:HB3	1:B:271:LYS:NZ	2.20	0.57
1:A:133:PHE:HA	1:B:62:ALA:HB2	1.87	0.57
1:B:278:ILE:O	1:B:282:LEU:HG	2.05	0.57
1:A:75:SER:O	1:A:79:THR:HG23	2.04	0.57
1:A:76:GLN:O	1:A:80:ILE:HG13	2.04	0.56
1:A:278:ILE:O	1:A:282:LEU:HG	2.04	0.56
1:B:213:ILE:HD11	1:B:217:PHE:HE2	1.70	0.56
1:B:213:ILE:HD11	1:B:217:PHE:CE2	2.40	0.56
1:B:141:THR:HG22	1:B:170:PHE:CZ	2.41	0.56
1:B:311:ARG:C	1:B:311:ARG:CD	2.60	0.56
1:A:76:GLN:HA	1:A:79:THR:OG1	2.06	0.56
1:B:95:SER:O	1:B:99:LEU:N	2.39	0.55
1:B:218:GLY:HA3	1:B:284:TYR:CZ	2.41	0.55
1:B:135:PHE:CZ	1:B:150:PRO:HD3	2.41	0.55
1:B:216:LEU:O	1:B:220:VAL:HG23	2.07	0.55
1:A:103:ILE:O	1:A:107:VAL:HG23	2.06	0.55
1:B:210:SER:O	1:B:213:ILE:HG22	2.06	0.55
1:B:229:ILE:HG22	1:B:233:ILE:HD12	1.88	0.54
1:B:202:SER:O	1:B:206:ILE:HG13	2.07	0.54
1:A:250:THR:O	1:A:251:THR:OG1	2.26	0.54
1:B:84:ARG:HG2	1:B:88:LEU:CD1	2.37	0.54
1:B:180:GLN:HA	1:B:180:GLN:NE2	2.22	0.54
1:B:270:TYR:O	1:B:274:VAL:HG23	2.07	0.54
1:B:49:THR:O	1:B:53:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASP:OD1	1:A:131:SER:N	2.37	0.54
1:B:209:ILE:HD12	1:B:209:ILE:H	1.73	0.54
1:B:75:SER:O	1:B:79:THR:HG23	2.08	0.54
1:B:113:GLY:HA3	1:B:126:HIS:CD2	2.43	0.53
1:B:220:VAL:HA	1:B:224:ALA:HB3	1.90	0.53
1:B:39:ILE:HD12	1:B:40:ASN:N	2.23	0.53
1:B:81:VAL:O	1:B:85:GLU:HG3	2.08	0.53
1:A:207:ARG:O	1:A:211:THR:HG23	2.09	0.53
1:B:60:ILE:O	1:B:64:VAL:HG23	2.09	0.53
1:A:221:LEU:O	1:A:226:PRO:HD3	2.07	0.53
1:B:229:ILE:CG2	1:B:233:ILE:HD12	2.37	0.53
1:B:141:THR:HG22	1:B:170:PHE:CE2	2.43	0.53
1:A:222:PHE:CE1	1:A:280:VAL:HG12	2.44	0.53
1:B:129:LEU:HD12	1:B:130:GLY:N	2.24	0.52
1:A:63:THR:HA	1:A:66:LYS:HZ3	1.75	0.52
1:B:256:ASP:OD1	1:B:257:TYR:N	2.42	0.52
1:A:285:PHE:HA	1:A:288:VAL:HB	1.90	0.52
1:A:100:ASP:O	1:A:104:GLN:HG3	2.09	0.52
1:A:192:VAL:HG13	1:A:196:PHE:HE1	1.75	0.52
1:B:141:THR:O	1:B:142:THR:OG1	2.27	0.52
1:A:181:LEU:HA	1:A:184:ILE:HD12	1.92	0.52
1:B:62:ALA:O	1:B:66:LYS:HG2	2.11	0.51
1:A:147:ASN:ND2	1:A:258:VAL:HG21	2.26	0.51
1:B:107:VAL:HA	1:B:110:ILE:CG1	2.40	0.51
1:B:77:ARG:O	1:B:80:ILE:HG22	2.10	0.51
1:A:298:VAL:O	1:A:302:LYS:HG2	2.09	0.51
1:B:115:ILE:HG22	1:B:115:ILE:O	2.11	0.51
1:A:50:ILE:O	1:A:54:VAL:HG23	2.10	0.51
1:B:247:ILE:HD12	1:B:254:PHE:HE2	1.75	0.51
1:B:188:GLY:HA2	1:B:191:LYS:HZ3	1.72	0.51
1:A:267:LEU:HD23	1:A:267:LEU:H	1.75	0.51
1:A:133:PHE:CA	1:B:62:ALA:HB2	2.41	0.50
1:A:220:VAL:HA	1:A:224:ALA:HB3	1.94	0.50
1:B:173:LEU:O	1:B:177:VAL:HG23	2.11	0.50
1:A:60:ILE:O	1:A:64:VAL:HG23	2.11	0.50
1:B:247:ILE:HD12	1:B:254:PHE:CE2	2.47	0.50
1:A:247:ILE:HG21	1:A:254:PHE:HD2	1.77	0.50
1:B:114:ILE:HB	1:B:116:PRO:HD3	1.93	0.50
1:A:106:ILE:HD11	1:B:103:ILE:HG12	1.92	0.50
1:A:107:VAL:O	1:A:110:ILE:HB	2.12	0.50
1:A:264:ILE:HG22	1:A:264:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:HZ	1:A:150:PRO:HD3	1.77	0.49
1:B:221:LEU:O	1:B:226:PRO:HD3	2.12	0.49
1:A:274:VAL:O	1:A:277:TRP:HB3	2.12	0.49
1:A:249:LEU:HA	1:A:282:LEU:HD23	1.93	0.49
1:B:100:ASP:O	1:B:104:GLN:HG3	2.11	0.49
1:A:256:ASP:OD1	1:A:257:TYR:N	2.45	0.49
1:B:310:PHE:O	1:B:311:ARG:C	2.50	0.49
1:A:189:ILE:O	1:A:193:GLU:HG3	2.13	0.49
1:B:126:HIS:HB3	1:B:148:ILE:HG12	1.95	0.48
1:A:46:THR:O	1:A:46:THR:HG22	2.13	0.48
1:A:245:VAL:HG13	1:A:277:TRP:CZ2	2.45	0.48
1:A:246:VAL:O	1:A:250:THR:HG23	2.13	0.48
1:A:265:GLU:O	1:A:266:TYR:CB	2.59	0.48
1:B:55:VAL:O	1:B:59:ILE:HG13	2.13	0.48
1:B:213:ILE:HD12	1:B:216:LEU:HD23	1.95	0.48
1:A:267:LEU:HD11	1:A:269:PHE:HB3	1.95	0.48
1:A:88:LEU:CD1	1:A:99:LEU:HD13	2.32	0.48
1:A:129:LEU:HD12	1:A:130:GLY:N	2.29	0.48
1:A:209:ILE:HD12	1:A:209:ILE:H	1.79	0.48
1:B:94:VAL:HG22	1:B:95:SER:N	2.27	0.48
1:A:247:ILE:HD12	1:A:254:PHE:CE2	2.47	0.48
1:A:107:VAL:HA	1:A:110:ILE:HD12	1.94	0.47
1:A:129:LEU:HA	1:B:66:LYS:NZ	2.29	0.47
1:A:197:ILE:HG23	1:A:206:ILE:HG13	1.96	0.47
1:B:174:LEU:HD11	1:B:283:ALA:N	2.29	0.47
1:B:314:ALA:O	1:B:315:ALA:HB3	2.14	0.47
1:A:146:GLY:HA2	1:B:254:PHE:HD1	1.79	0.47
1:B:243:TYR:O	1:B:247:ILE:HG12	2.15	0.47
1:B:266:TYR:HB3	1:B:271:LYS:HZ2	1.78	0.47
1:A:147:ASN:OD1	1:A:148:ILE:N	2.48	0.46
1:B:50:ILE:O	1:B:54:VAL:HG23	2.15	0.46
1:B:288:VAL:HA	1:B:291:MET:CE	2.45	0.46
1:A:252:ILE:HG12	1:B:142:THR:HA	1.97	0.46
1:B:249:LEU:HB2	1:B:285:PHE:CE2	2.50	0.46
1:A:216:LEU:O	1:A:220:VAL:HG23	2.15	0.46
1:A:173:LEU:HD22	1:B:54:VAL:HG21	1.97	0.46
1:A:271:LYS:HG3	1:A:272:PRO:HD3	1.96	0.46
1:A:299:ILE:O	1:A:303:THR:HG23	2.15	0.46
1:A:142:THR:HA	1:B:252:ILE:HG12	1.99	0.45
1:A:199:TRP:CG	1:A:200:ASN:N	2.84	0.45
1:B:311:ARG:O	1:B:311:ARG:CD	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HH11	1:B:116:PRO:HA	1.82	0.45
1:A:243:TYR:O	1:A:247:ILE:HG12	2.15	0.45
1:B:230:PHE:O	1:B:234:GLU:HB2	2.17	0.45
1:A:229:ILE:HG23	1:A:233:ILE:HD12	1.98	0.45
1:B:219:CYS:O	1:B:223:VAL:HB	2.17	0.45
1:A:288:VAL:HA	1:A:291:MET:HE3	1.98	0.45
1:A:107:VAL:HA	1:A:110:ILE:CD1	2.47	0.44
1:A:229:ILE:HG22	1:A:233:ILE:HD12	1.99	0.44
1:A:156:LYS:HB2	1:B:239:LEU:HD21	2.00	0.44
1:A:224:ALA:O	1:A:228:VAL:HG23	2.17	0.44
1:A:147:ASN:ND2	1:A:258:VAL:HG11	2.32	0.44
1:A:70:GLN:O	1:A:73:GLU:HB3	2.18	0.44
1:B:309:GLU:O	1:B:312:ALA:N	2.48	0.44
1:B:284:TYR:CE2	1:B:288:VAL:HG21	2.53	0.44
1:A:173:LEU:O	1:A:177:VAL:HG23	2.17	0.43
1:B:114:ILE:C	1:B:116:PRO:HD3	2.39	0.43
1:B:194:ASP:O	1:B:197:ILE:HB	2.18	0.43
1:A:147:ASN:HD21	1:A:258:VAL:HG11	1.83	0.43
1:A:127:TRP:O	1:B:66:LYS:HB2	2.18	0.43
1:B:186:GLY:O	1:B:189:ILE:HG22	2.18	0.43
1:A:147:ASN:CG	1:A:148:ILE:HD12	2.39	0.43
1:B:63:THR:HA	1:B:66:LYS:HE2	2.01	0.43
1:A:147:ASN:OD1	1:A:148:ILE:HD12	2.19	0.43
1:B:135:PHE:O	1:B:139:VAL:HG23	2.19	0.43
1:B:186:GLY:HA2	1:B:189:ILE:HG22	2.00	0.42
1:A:49:THR:O	1:A:53:VAL:HG23	2.19	0.42
1:B:84:ARG:HG2	1:B:88:LEU:HD11	2.01	0.42
1:B:79:THR:HA	1:B:82:ILE:HD12	2.00	0.42
1:B:189:ILE:HD11	1:B:210:SER:HB2	2.00	0.42
1:B:189:ILE:O	1:B:193:GLU:HG3	2.19	0.42
1:B:288:VAL:HA	1:B:291:MET:HE2	2.00	0.42
1:B:231:LYS:HG3	1:B:236:TRP:O	2.20	0.42
1:A:65:PHE:CE1	1:B:135:PHE:HE2	2.38	0.42
1:A:73:GLU:O	1:A:77:ARG:CG	2.63	0.42
1:B:107:VAL:CA	1:B:110:ILE:HD12	2.40	0.42
1:A:185:PHE:CZ	1:A:189:ILE:HG21	2.54	0.42
1:B:249:LEU:HD22	1:B:281:GLY:C	2.40	0.42
1:B:204:THR:HG23	1:B:205:LYS:HG3	2.01	0.41
1:A:136:ALA:HB1	1:A:162:TYR:OH	2.19	0.41
1:A:197:ILE:CD1	1:A:206:ILE:HG21	2.46	0.41
1:B:266:TYR:O	1:B:268:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ARG:HG2	1:B:88:LEU:HG	2.03	0.41
1:A:85:GLU:CG	1:A:89:ARG:HE	2.33	0.41
1:B:199:TRP:CE3	1:B:200:ASN:HB2	2.55	0.41
1:A:268:ASP:HA	1:A:271:LYS:HE2	2.02	0.41
1:B:189:ILE:HD11	1:B:210:SER:CB	2.50	0.41
1:B:225:LEU:HB2	1:B:226:PRO:HD3	2.02	0.41
1:A:45:LYS:HG2	1:A:47:VAL:H	1.84	0.41
1:A:147:ASN:HD22	1:A:258:VAL:HG21	1.86	0.41
1:A:192:VAL:HG13	1:A:196:PHE:CE1	2.55	0.41
1:B:174:LEU:HD11	1:B:283:ALA:CA	2.51	0.41
1:B:194:ASP:HA	1:B:197:ILE:HG13	2.01	0.41
1:B:313:HIS:ND1	1:B:313:HIS:N	2.68	0.41
1:B:303:THR:O	1:B:307:VAL:HG23	2.20	0.40
1:A:225:LEU:N	1:A:226:PRO:HD2	2.37	0.40
1:B:112:ALA:O	1:B:114:ILE:HG23	2.21	0.40
1:B:233:ILE:HD13	1:B:270:TYR:CD1	2.56	0.40
1:A:51:PHE:HA	1:B:173:LEU:HD13	2.03	0.40
1:A:77:ARG:NH2	1:B:123:GLN:CB	2.74	0.40
1:A:271:LYS:N	1:A:272:PRO:CD	2.85	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	264/312 (85%)	253 (96%)	11 (4%)	0	100 100
1	B	280/312 (90%)	263 (94%)	15 (5%)	2 (1%)	22 57
All	All	544/624 (87%)	516 (95%)	26 (5%)	2 (0%)	34 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	LEU
1	B	264	ILE

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	220/260 (85%)	220 (100%)	0	100 100
1	B	230/260 (88%)	228 (99%)	2 (1%)	78 91
All	All	450/520 (86%)	448 (100%)	2 (0%)	91 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	311	ARG
1	B	313	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	180	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 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	D10	A	408	-	4,4,9	0.32	0	3,3,8	0.54	0
4	D10	A	409	-	9,9,9	0.31	0	8,8,8	0.77	0
4	D10	B	406	-	9,9,9	0.30	0	8,8,8	0.78	0
4	D10	B	405	-	9,9,9	0.29	0	8,8,8	0.81	0
4	D10	A	410	-	9,9,9	0.30	0	8,8,8	0.79	0
4	D10	B	404	-	4,4,9	0.33	0	3,3,8	0.54	0
4	D10	A	411	-	9,9,9	0.31	0	8,8,8	0.76	0
4	D10	A	407	-	4,4,9	0.32	0	3,3,8	0.53	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
4	D10	A	408	-	-	0/2/2/7	-
4	D10	A	409	-	-	4/7/7/7	-
4	D10	B	406	-	-	3/7/7/7	-
4	D10	B	405	-	-	1/7/7/7	-
4	D10	A	410	-	-	1/7/7/7	-
4	D10	B	404	-	-	0/2/2/7	-
4	D10	A	411	-	-	2/7/7/7	-
4	D10	A	407	-	-	0/2/2/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	411	D10	C4-C5-C6-C7
4	B	405	D10	C6-C7-C8-C9
4	A	409	D10	C6-C7-C8-C9
4	A	411	D10	C6-C7-C8-C9
4	A	410	D10	C7-C8-C9-C10
4	A	409	D10	C2-C3-C4-C5
4	A	409	D10	C4-C5-C6-C7
4	A	409	D10	C5-C6-C7-C8
4	B	406	D10	C2-C3-C4-C5
4	B	406	D10	C4-C5-C6-C7
4	B	406	D10	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	268/312 (85%)	0.48	24 (8%) 9 3	87, 142, 225, 278	0
1	B	282/312 (90%)	0.44	23 (8%) 11 4	87, 143, 228, 284	0
All	All	550/624 (88%)	0.46	47 (8%) 10 4	87, 143, 228, 284	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	GLU	7.5
1	A	264	ILE	6.8
1	B	199	TRP	6.3
1	B	97	GLN	5.6
1	B	200	ASN	5.6
1	B	35	SER	5.3
1	B	265	GLU	5.2
1	B	192	VAL	5.1
1	B	113	GLY	4.9
1	B	123	GLN	4.8
1	A	267	LEU	4.8
1	B	314	ALA	4.8
1	B	92	PRO	4.5
1	A	94	VAL	4.5
1	B	204	THR	4.2
1	A	191	LYS	4.1
1	A	72	GLN	4.0
1	B	93	CYS	4.0
1	B	267	LEU	3.9
1	A	203	GLN	3.9
1	A	82	ILE	3.6
1	A	197	ILE	3.6
1	B	310	PHE	3.5
1	A	90	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	266	TYR	3.3
1	B	36	ASP	3.3
1	A	316	GLU	3.3
1	B	89	ARG	3.2
1	A	200	ASN	3.2
1	A	77	ARG	3.1
1	A	206	ILE	3.1
1	A	81	VAL	3.1
1	A	89	ARG	3.1
1	A	201	VAL	3.0
1	B	104	GLN	2.8
1	B	190	ALA	2.7
1	A	196	PHE	2.5
1	A	321	VAL	2.5
1	A	268	ASP	2.5
1	B	196	PHE	2.3
1	B	311	ARG	2.3
1	A	320	ASN	2.3
1	A	129	LEU	2.3
1	B	201	VAL	2.3
1	B	124	VAL	2.1
1	A	195	THR	2.0
1	B	96	ASP	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^{th} 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K	A	405	1/1	0.56	0.23	104,104,104,104	0
4	D10	B	405	10/10	0.62	0.37	103,142,172,181	0
4	D10	B	404	5/10	0.65	0.23	89,132,170,170	0
3	K	A	402	1/1	0.67	0.84	143,143,143,143	0
3	K	A	406	1/1	0.74	1.04	132,132,132,132	0
4	D10	A	407	5/10	0.74	0.48	102,128,160,161	0
4	D10	A	411	10/10	0.77	0.19	116,164,197,213	0
4	D10	A	410	10/10	0.83	0.26	100,158,178,187	0
4	D10	A	409	10/10	0.83	0.34	106,143,161,176	0
4	D10	A	408	5/10	0.84	0.44	146,176,189,189	0
3	K	A	404	1/1	0.92	0.05	117,117,117,117	0
2	CD	B	402	1/1	0.92	0.11	159,159,159,159	0
4	D10	B	406	10/10	0.92	0.24	100,134,169,180	0
3	K	A	403	1/1	0.94	0.06	127,127,127,127	0
2	CD	B	403	1/1	0.94	0.25	209,209,209,209	0
3	K	B	401	1/1	0.95	0.35	107,107,107,107	0
2	CD	A	401	1/1	0.97	0.08	377,377,377,377	0

6.5 Other polymers (i)

There are no such residues in this entry.