Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 10:22 AM EDT

PDB ID	:	6PIS
Title	:	Mouse two pore domain K+ channel TRAAK (K2P4.1) - Fab complex structure
Authors	:	Brohawn, S.G.
Deposited on	:	2019-06-27
Resolution	:	2.77 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:

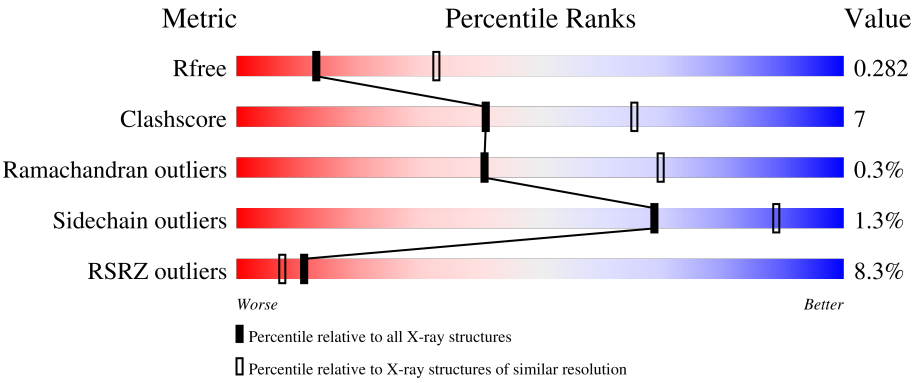
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	310	11% 66% 9% 24%
1	B	310	12% 67% 9% 23%
2	L	213	4% 78% 20%
2	M	213	3% 82% 17%
3	H	224	4% 79% 15%

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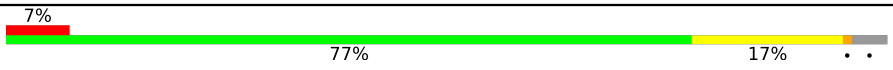
Mol	Chain	Length	Quality of chain
3	I	224	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10250 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	235	Total	C	N	O	S	0	0	0
			1838	1227	295	310	6			
1	B	239	Total	C	N	O	S	0	0	0
			1868	1247	299	316	6			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O88454
A	2	THR	-	expression tag	UNP O88454
A	3	THR	-	expression tag	UNP O88454
A	4	ALA	-	expression tag	UNP O88454
A	5	PRO	-	expression tag	UNP O88454
A	6	GLN	-	expression tag	UNP O88454
A	7	GLU	-	expression tag	UNP O88454
A	8	PRO	-	expression tag	UNP O88454
A	9	PRO	-	expression tag	UNP O88454
A	10	ALA	-	expression tag	UNP O88454
A	11	ARG	-	expression tag	UNP O88454
A	12	PRO	-	expression tag	UNP O88454
A	13	LEU	-	expression tag	UNP O88454
A	14	GLN	-	expression tag	UNP O88454
A	15	ALA	-	expression tag	UNP O88454
A	16	GLY	-	expression tag	UNP O88454
A	17	SER	-	expression tag	UNP O88454
A	18	GLY	-	expression tag	UNP O88454
A	19	ALA	-	expression tag	UNP O88454
A	20	GLY	-	expression tag	UNP O88454
A	21	PRO	-	expression tag	UNP O88454
A	22	ALA	-	expression tag	UNP O88454
A	23	PRO	-	expression tag	UNP O88454
A	24	GLY	-	expression tag	UNP O88454
A	25	ARG	-	expression tag	UNP O88454

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ALA	-	expression tag	UNP O88454
A	107	GLN	ASN	engineered mutation	UNP O88454
A	110	GLN	ASN	engineered mutation	UNP O88454
A	302	SER	-	expression tag	UNP O88454
A	303	ASN	-	expression tag	UNP O88454
A	304	SER	-	expression tag	UNP O88454
A	305	LEU	-	expression tag	UNP O88454
A	306	GLU	-	expression tag	UNP O88454
A	307	VAL	-	expression tag	UNP O88454
A	308	LEU	-	expression tag	UNP O88454
A	309	PHE	-	expression tag	UNP O88454
A	310	GLN	-	expression tag	UNP O88454
B	1	MET	-	expression tag	UNP O88454
B	2	THR	-	expression tag	UNP O88454
B	3	THR	-	expression tag	UNP O88454
B	4	ALA	-	expression tag	UNP O88454
B	5	PRO	-	expression tag	UNP O88454
B	6	GLN	-	expression tag	UNP O88454
B	7	GLU	-	expression tag	UNP O88454
B	8	PRO	-	expression tag	UNP O88454
B	9	PRO	-	expression tag	UNP O88454
B	10	ALA	-	expression tag	UNP O88454
B	11	ARG	-	expression tag	UNP O88454
B	12	PRO	-	expression tag	UNP O88454
B	13	LEU	-	expression tag	UNP O88454
B	14	GLN	-	expression tag	UNP O88454
B	15	ALA	-	expression tag	UNP O88454
B	16	GLY	-	expression tag	UNP O88454
B	17	SER	-	expression tag	UNP O88454
B	18	GLY	-	expression tag	UNP O88454
B	19	ALA	-	expression tag	UNP O88454
B	20	GLY	-	expression tag	UNP O88454
B	21	PRO	-	expression tag	UNP O88454
B	22	ALA	-	expression tag	UNP O88454
B	23	PRO	-	expression tag	UNP O88454
B	24	GLY	-	expression tag	UNP O88454
B	25	ARG	-	expression tag	UNP O88454
B	26	ALA	-	expression tag	UNP O88454
B	107	GLN	ASN	engineered mutation	UNP O88454
B	110	GLN	ASN	engineered mutation	UNP O88454
B	302	SER	-	expression tag	UNP O88454
B	303	ASN	-	expression tag	UNP O88454

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Chain	Residue	Modelled	Actual	Comment	Reference
B	304	SER	-	expression tag	UNP O88454
B	305	LEU	-	expression tag	UNP O88454
B	306	GLU	-	expression tag	UNP O88454
B	307	VAL	-	expression tag	UNP O88454
B	308	LEU	-	expression tag	UNP O88454
B	309	PHE	-	expression tag	UNP O88454
B	310	GLN	-	expression tag	UNP O88454

- Molecule 2 is a protein called ANTIBODY FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1639	1030	274	331	4			
2	M	211	Total	C	N	O	S	0	0	0
			1639	1030	274	331	4			

- Molecule 3 is a protein called ANTIBODY FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	215	Total	C	N	O	S	0	0	0
			1634	1044	269	316	5			
3	I	214	Total	C	N	O	S	0	0	0
			1626	1040	267	314	5			

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

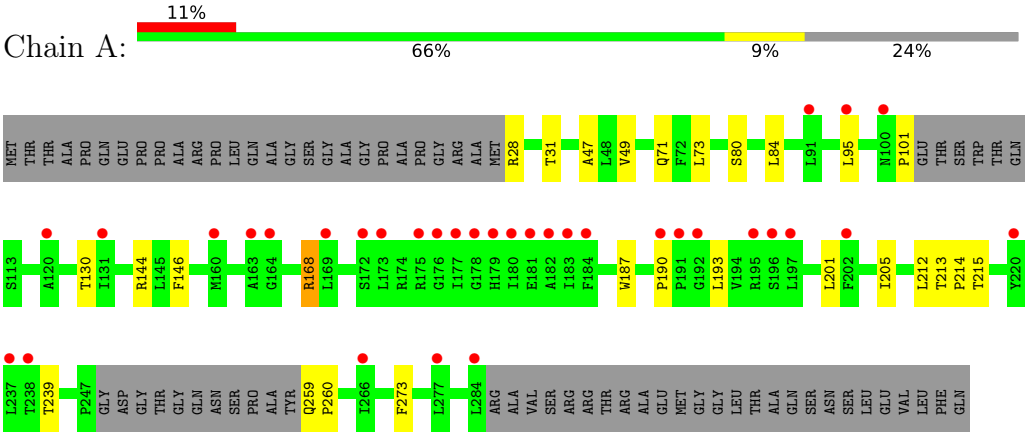
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	K	0	0
			5	5		
4	B	1	Total	K	0	0
			1	1		

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.

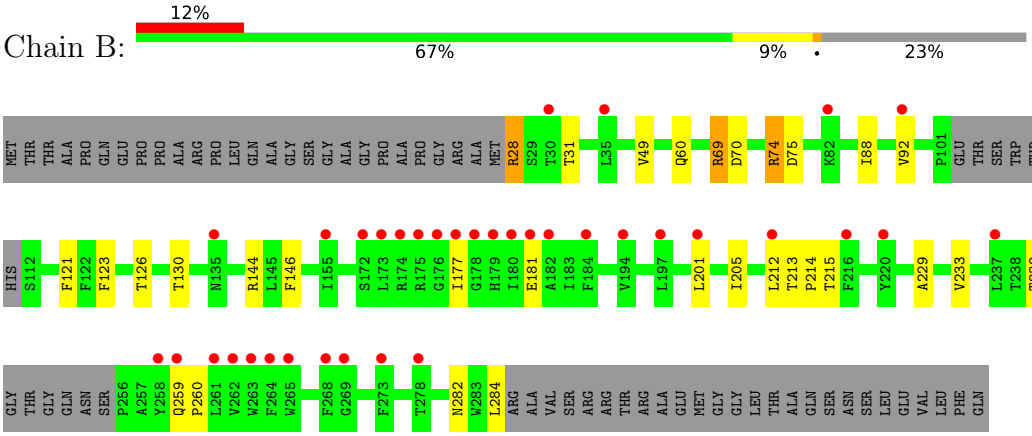
• Molecule 1: Potassium channel subfamily K member 4

Chain A:



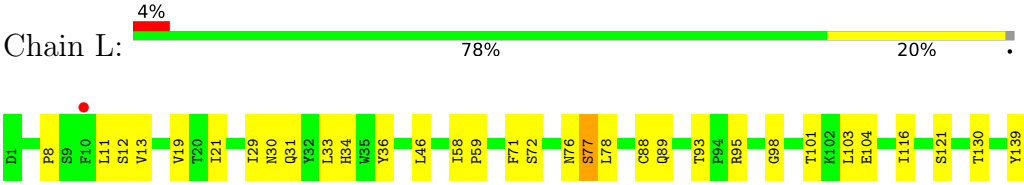
• Molecule 1: Potassium channel subfamily K member 4

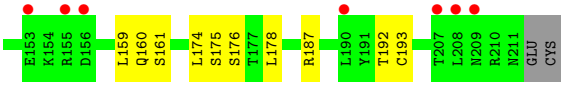
Chain B:



• Molecule 2: ANTIBODY FAB FRAGMENT LIGHT CHAIN

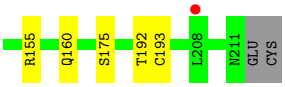
Chain L:





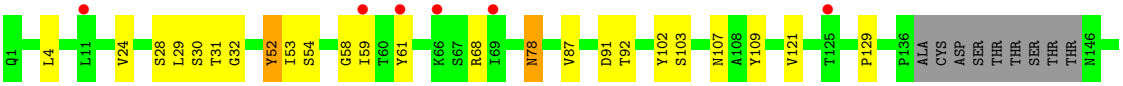
• Molecule 2: ANTIBODY FAB FRAGMENT LIGHT CHAIN

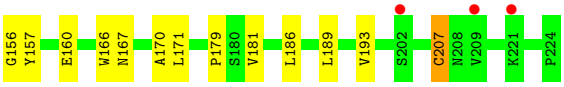
Chain M:



• Molecule 3: ANTIBODY FAB FRAGMENT HEAVY CHAIN

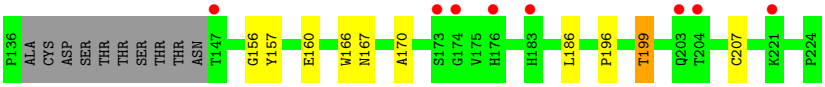
Chain H:





• Molecule 3: ANTIBODY FAB FRAGMENT HEAVY CHAIN

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.45Å 154.51Å 202.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.91 – 2.77 122.91 – 2.77	Depositor EDS
% Data completeness (in resolution range)	44.6 (122.91-2.77) 44.6 (122.91-2.77)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.248 , 0.286 0.252 , 0.282	Depositor DCC
R_{free} test set	1287 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	65.7	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	10250	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: 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	0.36	0/1888	0.49	0/2569
1	B	0.36	0/1920	0.50	0/2613
2	L	0.37	0/1674	0.58	0/2275
2	M	0.39	0/1674	0.58	0/2275
3	H	0.41	0/1680	0.62	0/2301
3	I	0.40	0/1672	0.61	0/2290
All	All	0.38	0/10508	0.56	0/14323

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	2
1	B	0	5
2	L	0	1
3	H	0	2
3	I	0	3
All	All	0	13

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain
1	A	168	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	144	ARG	Sidechain
1	B	28	ARG	Peptide,Sidechain
1	B	69	ARG	Sidechain
1	B	74	ARG	Sidechain
3	H	160	GLU	Peptide
3	H	52	TYR	Sidechain
3	I	160	GLU	Peptide
3	I	52	TYR	Sidechain
3	I	73	ARG	Sidechain
2	L	187	ARG	Sidechain

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	1838	0	1871	20	0
1	B	1868	0	1898	25	0
2	L	1639	0	1604	36	0
2	M	1639	0	1604	27	0
3	H	1634	0	1599	29	0
3	I	1626	0	1593	27	0
4	A	5	0	0	0	0
4	B	1	0	0	0	0
All	All	10250	0	10169	145	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 7.

All (145) 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)
3:H:92:THR:HG22	3:H:121:VAL:H	1.43	0.81
1:B:60:GLN:HE21	2:L:30:ASN:HD22	1.29	0.81
3:H:103:SER:OG	3:H:107:ASN:ND2	2.19	0.74
2:L:33:LEU:HD23	2:L:71:PHE:CD2	2.26	0.70
3:I:28:SER:O	3:I:31:THR:HG22	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:33:LEU:HD23	2:M:71:PHE:CD2	2.28	0.68
2:M:28:ASN:ND2	2:M:30:ASN:OD1	2.28	0.67
3:H:92:THR:HG22	3:H:121:VAL:N	2.10	0.66
1:A:213:THR:HB	1:A:214:PRO:HD3	1.79	0.64
1:B:213:THR:HB	1:B:214:PRO:HD3	1.81	0.62
2:M:33:LEU:HD11	2:M:88:CYS:HB2	1.81	0.61
2:L:33:LEU:HD11	2:L:88:CYS:HB2	1.83	0.60
2:M:36:TYR:HD1	2:M:46:LEU:HA	1.67	0.59
1:A:49:VAL:HG11	1:B:146:PHE:CE1	2.38	0.58
2:L:36:TYR:HD1	2:L:46:LEU:HA	1.69	0.58
2:M:148:LYS:HB2	2:M:192:THR:HB	1.86	0.57
1:B:60:GLN:NE2	2:L:30:ASN:HD22	2.00	0.57
2:L:19:VAL:HG21	2:L:78:LEU:HD11	1.86	0.56
2:L:11:LEU:C	2:L:11:LEU:HD12	2.26	0.56
3:I:156:GLY:CA	3:I:186:LEU:HD13	2.36	0.56
1:B:69:ARG:NH2	1:B:70:ASP:OD1	2.38	0.56
3:I:166:TRP:CZ3	3:I:207:CYS:HB3	2.41	0.56
1:A:146:PHE:CE1	1:B:49:VAL:HG11	2.40	0.56
3:H:166:TRP:CZ3	3:H:207:CYS:HB3	2.41	0.55
2:M:11:LEU:HD12	2:M:11:LEU:C	2.27	0.55
3:H:156:GLY:CA	3:H:186:LEU:HD13	2.37	0.54
2:L:11:LEU:HD13	2:L:13:VAL:HG23	1.90	0.53
3:H:92:THR:CG2	3:H:121:VAL:H	2.19	0.52
3:I:54:SER:OG	3:I:58:GLY:N	2.41	0.52
2:L:148:LYS:HB2	2:L:192:THR:HB	1.91	0.52
2:M:36:TYR:CE2	2:M:89:GLN:HG2	2.45	0.52
3:I:196:PRO:O	3:I:199:THR:HG22	2.10	0.51
2:L:36:TYR:CE2	2:L:89:GLN:HG2	2.45	0.50
3:H:103:SER:HG	3:H:107:ASN:ND2	2.08	0.50
2:M:12:SER:HA	2:M:104:GLU:O	2.12	0.50
2:L:33:LEU:HD12	2:L:34:HIS:H	1.76	0.50
2:M:146:LYS:HG2	2:M:155:ARG:HH11	1.75	0.50
3:I:207:CYS:SG	3:I:207:CYS:O	2.70	0.50
2:L:8:PRO:HG2	2:L:11:LEU:HD23	1.93	0.50
2:L:159:LEU:HB3	3:H:181:VAL:HG11	1.93	0.49
2:M:88:CYS:O	2:M:98:GLY:N	2.45	0.49
2:L:116:ILE:HD12	2:L:193:CYS:HB2	1.93	0.49
3:I:52:TYR:HE2	3:I:100:VAL:HG11	1.77	0.49
2:M:160:GLN:HA	2:M:175:SER:O	2.13	0.49
1:A:146:PHE:CD1	1:B:49:VAL:HG11	2.48	0.49
1:A:95:LEU:HD11	1:B:92:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:59:ILE:HG21	3:I:61:TYR:CZ	2.48	0.48
1:B:28:ARG:O	1:B:31:THR:OG1	2.22	0.48
3:I:65:LEU:CD2	3:I:69:ILE:HD11	2.44	0.48
2:M:36:TYR:CD1	2:M:46:LEU:HA	2.48	0.48
2:L:12:SER:HA	2:L:104:GLU:O	2.13	0.48
2:L:88:CYS:O	2:L:98:GLY:N	2.44	0.48
3:I:65:LEU:HD23	3:I:69:ILE:HD11	1.96	0.47
1:B:69:ARG:CZ	1:B:69:ARG:HB3	2.45	0.47
3:H:171:LEU:HD21	3:H:193:VAL:HG21	1.96	0.47
2:L:76:ASN:O	2:L:77:SER:C	2.53	0.47
1:B:28:ARG:HB3	1:B:31:THR:OG1	2.15	0.47
1:B:75:ASP:OD2	3:H:102:TYR:OH	2.33	0.47
2:M:8:PRO:HG2	2:M:11:LEU:HD23	1.97	0.47
3:H:129:PRO:HB3	3:H:157:TYR:HB3	1.96	0.47
2:L:36:TYR:CD1	2:L:46:LEU:HA	2.50	0.46
3:H:53:ILE:HD12	3:H:59:ILE:HD11	1.97	0.46
1:A:201:LEU:O	1:A:205:ILE:HG22	2.15	0.46
2:M:33:LEU:HD12	2:M:34:HIS:H	1.79	0.46
3:H:54:SER:OG	3:H:58:GLY:N	2.41	0.46
3:H:167:ASN:HB2	3:H:170:ALA:HB3	1.98	0.46
1:B:123:PHE:O	1:B:126:THR:OG1	2.29	0.46
2:L:11:LEU:HD11	2:L:103:LEU:HD13	1.98	0.46
3:I:53:ILE:HD12	3:I:59:ILE:HD11	1.98	0.46
2:L:21:ILE:O	2:L:72:SER:HA	2.15	0.46
2:L:93:THR:HG22	2:L:95:ARG:NE	2.31	0.46
2:M:21:ILE:O	2:M:72:SER:HA	2.16	0.46
1:B:201:LEU:O	1:B:205:ILE:HG22	2.16	0.45
3:H:207:CYS:SG	3:H:207:CYS:O	2.73	0.45
1:A:212:LEU:O	1:A:215:THR:OG1	2.33	0.45
1:A:259:GLN:HB2	1:A:260:PRO:CD	2.47	0.45
3:I:129:PRO:HB3	3:I:157:TYR:HB3	1.98	0.45
3:I:167:ASN:HB2	3:I:170:ALA:HB3	1.98	0.45
1:B:212:LEU:O	1:B:215:THR:OG1	2.33	0.45
3:I:87:VAL:HG12	3:I:121:VAL:HG11	1.99	0.45
3:I:166:TRP:CH2	3:I:207:CYS:HB3	2.50	0.45
3:I:156:GLY:HA2	3:I:186:LEU:HD13	1.98	0.45
3:I:96:TYR:CE1	2:M:43:ALA:HB2	2.51	0.45
2:L:12:SER:HB3	2:L:104:GLU:HB2	1.98	0.45
2:L:160:GLN:HA	2:L:175:SER:O	2.17	0.45
3:H:87:VAL:HG12	3:H:121:VAL:HG11	1.98	0.45
2:M:33:LEU:HD23	2:M:71:PHE:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:8:PRO:CG	2:M:11:LEU:HD23	2.46	0.44
1:A:71:GLN:NE2	3:I:52:TYR:HE1	2.15	0.44
1:A:101:PRO:CB	1:B:88:ILE:HG21	2.47	0.44
3:H:166:TRP:CH2	3:H:207:CYS:HB3	2.53	0.44
2:L:33:LEU:HD23	2:L:71:PHE:CG	2.53	0.44
2:M:93:THR:HG22	2:M:95:ARG:NE	2.33	0.44
2:L:33:LEU:HD12	2:L:34:HIS:N	2.33	0.44
1:B:282:ASN:O	1:B:284:LEU:O	2.35	0.44
3:H:171:LEU:CD2	3:H:193:VAL:HG21	2.47	0.44
3:I:52:TYR:OH	3:I:102:TYR:OH	2.31	0.44
2:L:11:LEU:CD1	2:L:13:VAL:HG23	2.47	0.44
2:L:8:PRO:CG	2:L:11:LEU:HD23	2.48	0.43
3:H:29:LEU:HD23	3:H:78:ASN:OD1	2.18	0.43
3:I:27:PHE:CE1	3:I:31:THR:HG21	2.53	0.43
3:H:156:GLY:HA2	3:H:186:LEU:HD13	2.00	0.43
3:H:59:ILE:HG21	3:H:61:TYR:CZ	2.53	0.43
2:M:139:TYR:CG	2:M:140:PRO:HA	2.53	0.43
2:L:34:HIS:NE2	3:H:109:TYR:HB3	2.33	0.43
2:L:161:SER:HB2	3:H:179:PRO:HB2	2.00	0.43
3:I:68:ARG:NH2	3:I:91:ASP:OD2	2.51	0.42
2:M:33:LEU:HD12	2:M:89:GLN:O	2.20	0.42
1:A:101:PRO:HB2	1:B:88:ILE:HG21	2.01	0.42
2:L:29:ILE:HG22	2:L:29:ILE:O	2.19	0.42
1:A:28:ARG:O	1:A:31:THR:OG1	2.23	0.42
1:A:47:ALA:HB2	1:B:121:PHE:HA	2.02	0.42
1:B:177:ILE:HG22	1:B:181:GLU:HG3	2.02	0.42
2:L:139:TYR:CG	2:L:140:PRO:HA	2.54	0.42
2:M:29:ILE:HG22	2:M:29:ILE:O	2.20	0.42
1:A:229:ALA:O	1:A:233:VAL:HG23	2.19	0.42
1:B:259:GLN:HB2	1:B:260:PRO:HD3	2.02	0.42
2:L:130:THR:HA	2:L:178:LEU:O	2.20	0.42
3:I:29:LEU:HD23	3:I:78:ASN:OD1	2.20	0.41
1:A:49:VAL:HG11	1:B:146:PHE:CD1	2.54	0.41
3:H:68:ARG:NH2	3:H:91:ASP:OD2	2.53	0.41
2:M:30:ASN:ND2	2:M:92:TYR:OH	2.45	0.41
2:L:160:GLN:OE1	2:L:174:LEU:HD11	2.21	0.41
3:H:189:LEU:HD12	3:H:189:LEU:C	2.41	0.41
1:B:229:ALA:O	1:B:233:VAL:HG23	2.20	0.41
3:H:28:SER:HB3	3:H:31:THR:OG1	2.20	0.41
3:I:92:THR:HG23	3:I:120:THR:HA	2.03	0.41
3:I:103:SER:HB3	3:I:107:ASN:ND2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:8:PRO:O	2:L:101:THR:HG23	2.20	0.41
3:I:53:ILE:HD12	3:I:59:ILE:CD1	2.50	0.41
2:M:33:LEU:HD12	2:M:34:HIS:N	2.36	0.41
2:L:33:LEU:HD12	2:L:89:GLN:O	2.21	0.41
3:I:4:LEU:CD2	3:I:24:VAL:HG22	2.50	0.41
1:B:74:ARG:O	3:H:58:GLY:HA3	2.20	0.41
2:L:58:ILE:HG23	2:L:59:PRO:HD2	2.02	0.41
1:A:80:SER:OG	3:H:32:GLY:HA3	2.22	0.40
1:A:168:ARG:HH21	1:B:28:ARG:HB2	1.86	0.40
2:M:116:ILE:HD12	2:M:193:CYS:HB2	2.03	0.40
1:A:190:PRO:HD2	1:A:193:LEU:HD12	2.03	0.40
1:A:187:TRP:CD1	1:A:187:TRP:O	2.74	0.40
3:I:37:THR:HG22	3:I:98:ALA:O	2.22	0.40
2:M:11:LEU:HD13	2:M:13:VAL:HG23	2.02	0.40
1:A:73:LEU:HD21	1:A:84:LEU:HD23	2.03	0.40
3:H:4:LEU:CD2	3:H:24:VAL:HG22	2.52	0.40
2:M:18:LYS:HG3	2:M:76:ASN:HA	2.03	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	229/310 (74%)	219 (96%)	10 (4%)	0	100	100
1	B	233/310 (75%)	225 (97%)	8 (3%)	0	100	100
2	L	209/213 (98%)	200 (96%)	7 (3%)	2 (1%)	15	41
2	M	209/213 (98%)	200 (96%)	9 (4%)	0	100	100
3	H	211/224 (94%)	202 (96%)	8 (4%)	1 (0%)	29	58
3	I	210/224 (94%)	199 (95%)	10 (5%)	1 (0%)	29	58
All	All	1301/1494 (87%)	1245 (96%)	52 (4%)	4 (0%)	41	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	78	ASN
3	I	78	ASN
2	L	77	SER
2	L	31	GLN

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	195/251 (78%)	192 (98%)	3 (2%)	65	87
1	B	198/251 (79%)	196 (99%)	2 (1%)	76	91
2	L	188/190 (99%)	186 (99%)	2 (1%)	73	90
2	M	188/190 (99%)	185 (98%)	3 (2%)	62	86
3	H	186/194 (96%)	183 (98%)	3 (2%)	62	86
3	I	185/194 (95%)	183 (99%)	2 (1%)	73	90
All	All	1140/1270 (90%)	1125 (99%)	15 (1%)	69	89

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	THR
1	A	239	THR
1	A	273	PHE
1	B	130	THR
1	B	239	THR
2	L	121	SER
2	L	176	SER
3	H	30	SER
3	H	52	TYR
3	H	207	CYS
3	I	30	SER
3	I	199	THR
2	M	24	LYS

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Mol	Chain	Res	Type
2	M	90	GLN
2	M	121	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	B	55	GLN
1	B	60	GLN
3	H	5	GLN
3	I	3	GLN
3	I	176	HIS
2	M	28	ASN
2	M	137	ASN
2	M	188	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	235/310 (75%)	0.97	34 (14%) 2 1	40, 97, 218, 254	0
1	B	239/310 (77%)	0.96	36 (15%) 2 1	41, 94, 185, 220	0
2	L	211/213 (99%)	0.09	9 (4%) 35 30	47, 72, 99, 118	0
2	M	211/213 (99%)	0.19	7 (3%) 46 41	42, 70, 91, 106	0
3	H	215/224 (95%)	0.14	9 (4%) 36 30	39, 65, 102, 128	0
3	I	214/224 (95%)	0.46	15 (7%) 16 11	34, 68, 134, 172	0
All	All	1325/1494 (88%)	0.49	110 (8%) 11 7	34, 77, 158, 254	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	LEU	17.7
1	B	176	GLY	13.3
1	A	180	ILE	12.5
1	A	179	HIS	12.0
1	B	177	ILE	11.5
1	A	177	ILE	10.6
1	A	195	ARG	9.9
1	A	172	SER	9.7
1	B	178	GLY	9.0
1	A	183	ILE	8.1
1	B	258	TYR	7.9
1	A	176	GLY	7.6
1	B	237	LEU	7.5
1	B	180	ILE	6.8
1	B	179	HIS	6.7
1	A	169	LEU	6.6
1	A	191	PRO	6.2
1	A	192	GLY	6.1
1	A	182	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	175	ARG	5.4
1	B	175	ARG	5.3
1	A	178	GLY	4.9
1	B	173	LEU	4.9
3	I	147	THR	4.8
1	B	184	PHE	4.6
3	I	122	SER	4.6
1	A	184	PHE	4.4
2	L	155	ARG	4.3
1	B	182	ALA	4.2
1	B	194	VAL	4.0
3	I	123	SER	3.8
1	B	30	THR	3.7
1	B	273	PHE	3.7
1	B	264	PHE	3.7
1	B	265	TRP	3.7
1	B	262	VAL	3.6
1	A	220	TYR	3.6
1	B	172	SER	3.6
3	H	66	LYS	3.5
2	L	10	PHE	3.5
1	A	181	GLU	3.5
3	I	173	SER	3.5
1	B	263	TRP	3.5
3	I	221	LYS	3.4
2	M	11	LEU	3.3
1	B	201	LEU	3.3
1	B	261	LEU	3.2
1	A	190	PRO	3.2
1	B	259	GLN	3.1
1	A	163	ALA	3.0
1	B	278	THR	2.9
1	A	266	ILE	2.9
3	H	202	SER	2.9
1	B	181	GLU	2.8
3	I	204	THR	2.8
3	I	45	LYS	2.8
3	I	203	GLN	2.8
3	H	221	LYS	2.8
1	A	237	LEU	2.7
3	I	125	THR	2.7
1	B	197	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	190	LEU	2.7
2	M	137	ASN	2.7
1	A	91	LEU	2.6
1	A	196	SER	2.5
2	M	13	VAL	2.5
3	I	77	LYS	2.5
1	A	95	LEU	2.5
2	L	153	GLU	2.4
1	B	269	GLY	2.4
2	L	142	ASP	2.4
1	A	160	MET	2.4
2	M	12	SER	2.4
1	A	238	THR	2.3
1	A	100	ASN	2.3
1	A	284	LEU	2.3
1	B	92	VAL	2.3
2	M	111	LYS	2.3
3	I	176	HIS	2.2
1	B	220	TYR	2.2
3	H	59	ILE	2.2
3	H	61	TYR	2.2
1	A	131	ILE	2.2
3	I	121	VAL	2.2
1	A	164	GLY	2.2
2	M	208	LEU	2.2
3	I	174	GLY	2.2
3	H	125	THR	2.2
1	B	268	PHE	2.2
1	B	135	ASN	2.1
2	L	207	THR	2.1
1	A	277	LEU	2.1
1	B	174	ARG	2.1
1	B	216	PHE	2.1
1	B	155	ILE	2.1
3	H	11	LEU	2.1
3	I	124	ALA	2.1
2	L	209	ASN	2.1
2	L	156	ASP	2.1
1	A	197	LEU	2.1
2	L	208	LEU	2.1
2	M	19	VAL	2.1
1	A	120	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	69	ILE	2.1
3	I	183	HIS	2.1
1	B	82	LYS	2.1
1	A	202	PHE	2.1
3	H	209	VAL	2.0
1	B	212	LEU	2.0
1	B	35	LEU	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	K	A	402	1/1	0.94	0.10	67,67,67,67	0
4	K	A	404	1/1	0.94	0.06	89,89,89,89	0
4	K	B	401	1/1	0.94	0.14	87,87,87,87	0
4	K	A	403	1/1	0.97	0.11	72,72,72,72	0
4	K	A	405	1/1	0.98	0.05	67,67,67,67	0
4	K	A	401	1/1	0.98	0.12	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.