



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:46 PM UTC

PDB ID : 6PIS / pdb_00006pis
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:

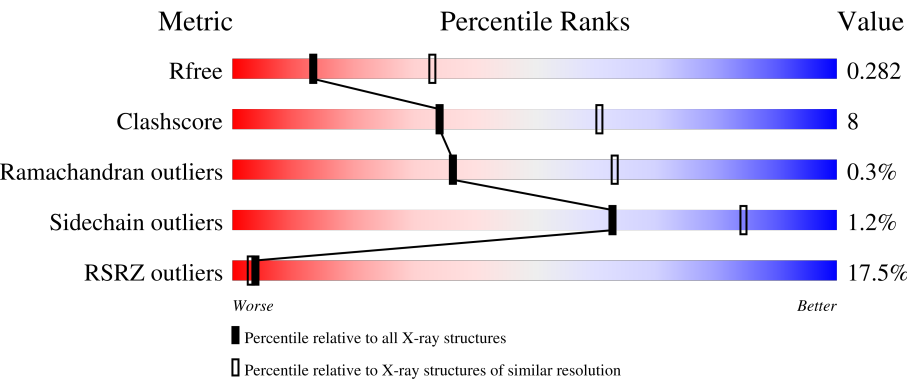
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (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 $\leq 5\%$. 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	310	19% 65%11%24%
1	B	310	22% 65%11%23%
2	L	213	9% 79%20%
2	M	213	13% 82%17%
3	H	224	9% 79%16%

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Mol	Chain	Length	Quality of chain
3	I	224	17% 76% 18% • •

2 Entry composition

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			

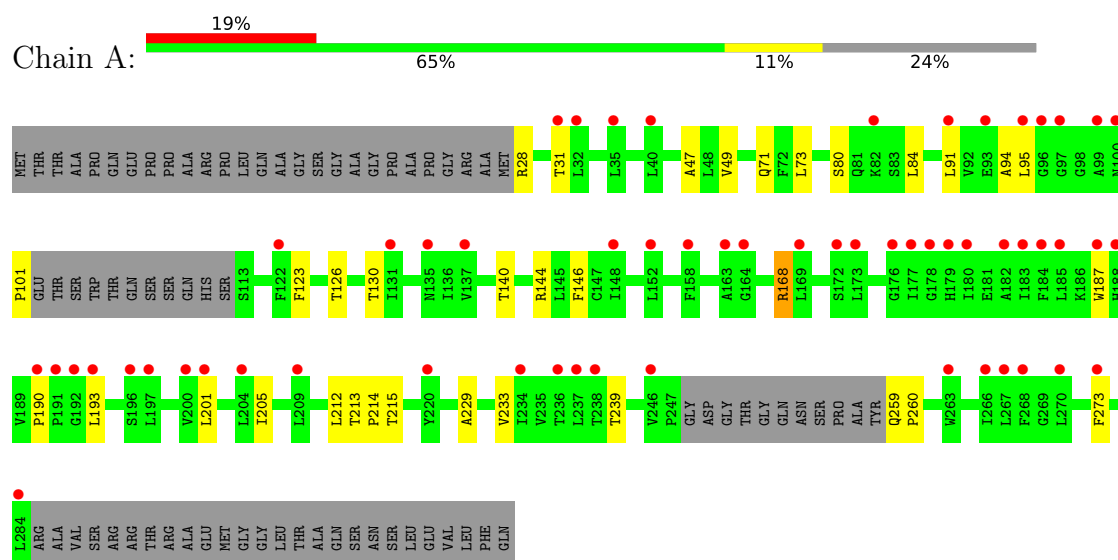
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

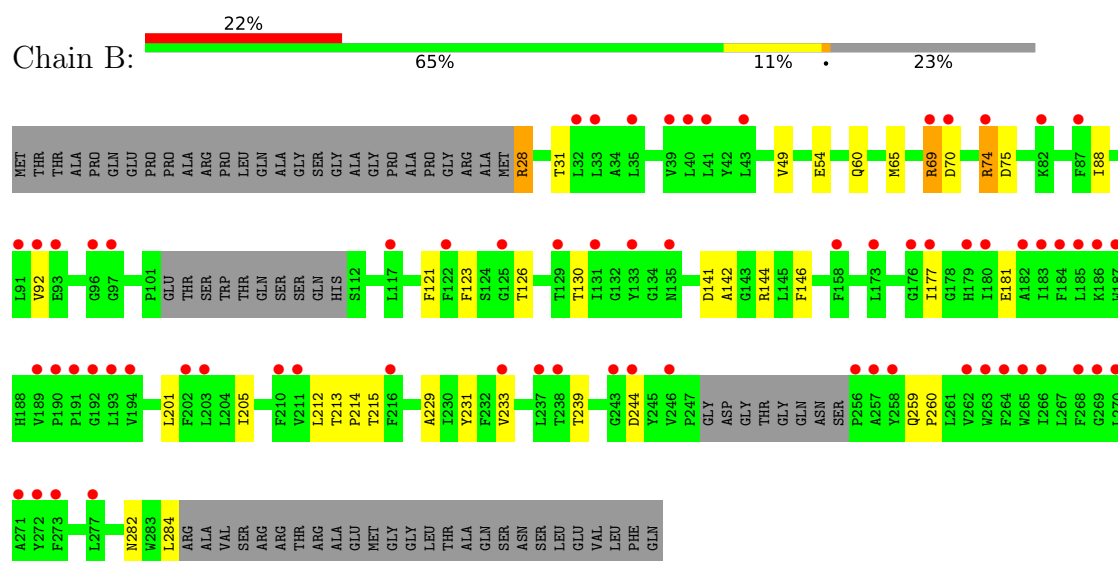
3 Residue-property plots

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.

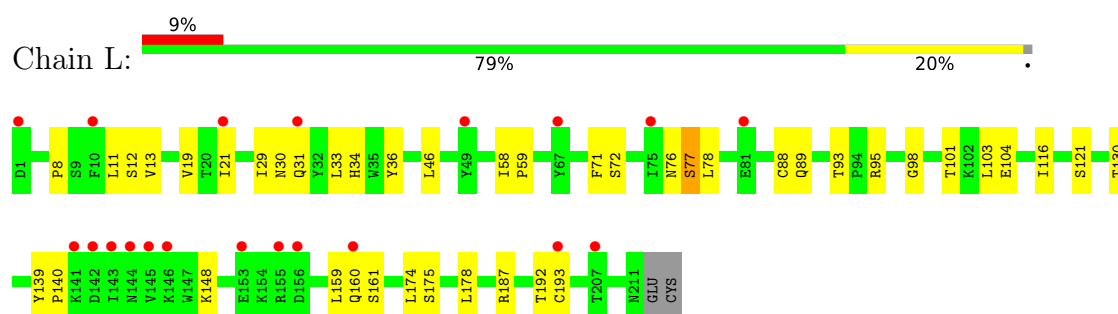
- Molecule 1: Potassium channel subfamily K member 4



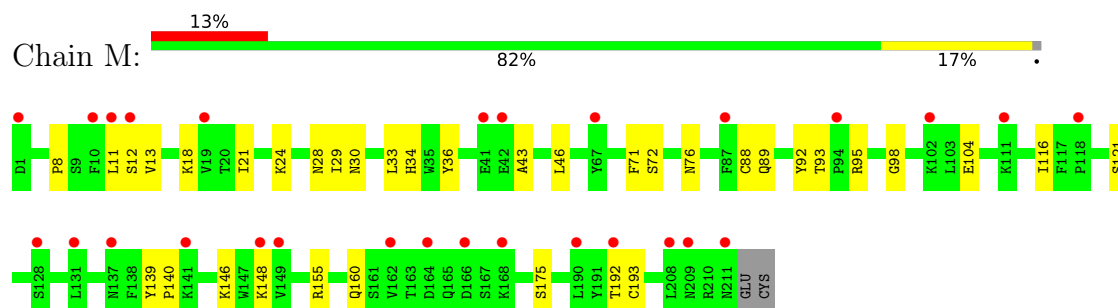
- Molecule 1: Potassium channel subfamily K member 4



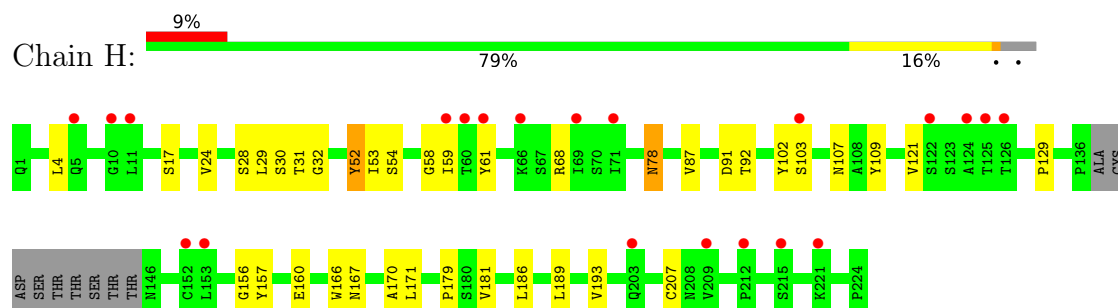
- Molecule 2: ANTIBODY FAB FRAGMENT LIGHT CHAIN



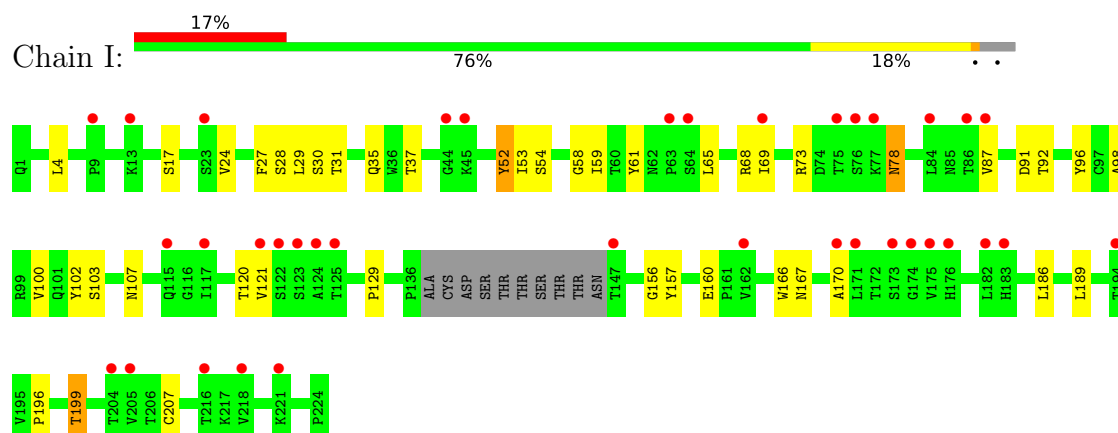
• Molecule 2: ANTIBODY FAB FRAGMENT LIGHT CHAIN



• Molecule 3: ANTIBODY FAB FRAGMENT HEAVY CHAIN



• Molecule 3: ANTIBODY FAB FRAGMENT HEAVY CHAIN



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (4.90%)	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)	0.31 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	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.*

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

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	0.61	0/1888	1.06	0/2569
1	B	0.60	0/1920	1.07	0/2613
2	L	0.60	0/1674	0.85	0/2275
2	M	0.61	0/1674	0.84	0/2275
3	H	0.66	0/1680	0.84	0/2301
3	I	0.64	0/1672	0.84	0/2290
All	All	0.62	0/10508	0.93	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	Sidechain,Peptide
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

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	26	0
1	B	1868	0	1898	32	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	29	0
4	A	5	0	0	0	0
4	B	1	0	0	0	0
All	All	10250	0	10169	155	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 (155) 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:91:LEU:HD23	1:B:65:MET:HE1	1.76	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:11:LEU:C	2:L:11:LEU:HD12	2.26	0.61
2:L:33:LEU:HD11	2:L:88:CYS:HB2	1.83	0.60
2:M:11:LEU:HD12	2:M:11:LEU:C	2.27	0.59
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
1:B:28:ARG:O	1:B:31:THR:OG1	2.22	0.57
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
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:94:ALA:CB	1:B:65:MET:HE2	2.36	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
1:A:94:ALA:HB3	1:B:65:MET:HE2	1.89	0.55
1:A:28:ARG:O	1:A:31:THR:OG1	2.23	0.54
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:L:76:ASN:O	2:L:77:SER:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:59:ILE:HG21	3:I:61:TYR:CZ	2.48	0.48
1:B:123:PHE:O	1:B:126:THR:OG1	2.29	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
1:A:123:PHE:O	1:A:126:THR:OG1	2.29	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
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
3:H:189:LEU:C	3:H:189:LEU:HD12	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:91:LEU:HA	1:B:65:MET:HE1	2.00	0.43
3:I:189:LEU:HD12	3:I:189:LEU:C	2.43	0.43
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:140:THR:OG1	1:B:54:GLU:OE2	2.37	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
3:I:35:GLN:CD	3:I:35:GLN:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:B:141:ASP:O	1:B:142:ALA:C	2.65	0.40
1:B:231:TYR:OH	1:B:244:ASP:OD2	2.38	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%)	12	35
2	M	209/213 (98%)	200 (96%)	9 (4%)	0	100	100
3	H	211/224 (94%)	202 (96%)	8 (4%)	1 (0%)	24	52
3	I	210/224 (94%)	199 (95%)	10 (5%)	1 (0%)	24	52
All	All	1301/1494 (87%)	1245 (96%)	52 (4%)	4 (0%)	36	63

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 ⓘ

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%)	57	81
1	B	198/251 (79%)	196 (99%)	2 (1%)	68	86
2	L	188/190 (99%)	187 (100%)	1 (0%)	81	92
2	M	188/190 (99%)	186 (99%)	2 (1%)	65	85
3	H	186/194 (96%)	183 (98%)	3 (2%)	55	81
3	I	185/194 (95%)	182 (98%)	3 (2%)	55	81
All	All	1140/1270 (90%)	1126 (99%)	14 (1%)	63	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	THR

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Mol	Chain	Res	Type
1	A	239	THR
1	A	273	PHE
1	B	130	THR
1	B	239	THR
2	L	121	SER
3	H	17	SER
3	H	30	SER
3	H	52	TYR
3	I	17	SER
3	I	30	SER
3	I	199	THR
2	M	24	LYS
2	M	121	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	60	GLN
1	A	179	HIS
1	B	55	GLN
1	B	60	GLN
2	L	37	GLN
2	L	38	GLN
2	L	89	GLN
2	L	188	HIS
2	L	189	ASN
2	L	211	ASN
3	H	5	GLN
3	H	41	GLN
3	H	183	HIS
3	I	3	GLN
3	I	41	GLN
3	I	176	HIS
3	I	183	HIS
2	M	3	GLN
2	M	27	GLN
2	M	28	ASN
2	M	37	GLN
2	M	38	GLN
2	M	137	ASN
2	M	189	ASN

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Mol	Chain	Res	Type
2	M	211	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 [i](#)

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, 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	235/310 (75%)	1.33	58 (24%)	2 1	40, 97, 218, 254	0
1	B	239/310 (77%)	1.60	68 (28%)	1 1	41, 94, 185, 220	0
2	L	211/213 (99%)	0.84	20 (9%)	14 11	47, 72, 99, 118	0
2	M	211/213 (99%)	0.99	28 (13%)	7 6	42, 70, 91, 106	0
3	H	215/224 (95%)	0.65	21 (9%)	13 10	39, 65, 102, 128	0
3	I	214/224 (95%)	1.08	37 (17%)	4 3	34, 68, 134, 172	0
All	All	1325/1494 (88%)	1.10	232 (17%)	4 3	34, 77, 158, 254	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	LEU	11.0
2	L	142	ASP	10.4
3	I	123	SER	9.5
1	B	135	ASN	8.9
3	I	122	SER	8.2
1	A	266	ILE	7.5
1	A	180	ILE	7.3
1	A	173	LEU	7.0
1	B	273	PHE	6.8
1	B	265	TRP	6.7
1	B	177	ILE	6.6
2	M	11	LEU	6.5
1	A	177	ILE	6.5
2	M	137	ASN	6.4
2	M	1	ASP	6.4
1	A	176	GLY	6.4
1	B	266	ILE	5.9
1	A	95	LEU	5.8
3	I	45	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
2	M	209	ASN	5.7
1	B	270	LEU	5.7
3	H	66	LYS	5.7
1	A	238	THR	5.7
3	I	125	THR	5.7
2	M	102	LYS	5.5
2	L	153	GLU	5.4
3	I	147	THR	5.3
2	L	156	ASP	5.3
1	B	191	PRO	5.3
2	L	155	ARG	5.2
3	H	61	TYR	5.2
1	B	176	GLY	5.2
1	B	92	VAL	5.2
1	B	96	GLY	5.1
1	A	172	SER	5.1
1	B	262	VAL	5.1
1	B	246	VAL	5.0
1	A	236	THR	4.9
1	B	194	VAL	4.9
1	B	183	ILE	4.7
3	I	76	SER	4.7
3	H	59	ILE	4.6
1	A	169	LEU	4.6
1	A	237	LEU	4.5
3	I	174	GLY	4.5
1	A	135	ASN	4.5
1	B	129	THR	4.4
1	B	122	PHE	4.4
2	L	141	LYS	4.4
2	L	143	ILE	4.4
1	B	193	LEU	4.4
1	B	190	PRO	4.4
2	M	208	LEU	4.2
3	I	124	ALA	4.2
1	B	180	ILE	4.2
3	I	176	HIS	4.1
1	B	182	ALA	4.1
1	A	91	LEU	4.1
3	H	124	ALA	4.1
2	L	67	TYR	4.0
3	H	212	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
2	L	207	THR	3.9
2	M	12	SER	3.9
1	A	187	TRP	3.9
3	I	221	LYS	3.9
2	M	10	PHE	3.8
1	B	185	LEU	3.8
1	A	220	TYR	3.8
3	I	115	GLN	3.7
1	B	187	TRP	3.7
2	M	164	ASP	3.6
1	B	184	PHE	3.6
1	A	100	ASN	3.6
1	A	270	LEU	3.6
1	A	201	LEU	3.5
3	H	126	THR	3.5
3	H	11	LEU	3.5
1	A	267	LEU	3.4
2	L	10	PHE	3.4
1	B	189	VAL	3.4
1	A	191	PRO	3.4
3	H	125	THR	3.4
2	L	144	ASN	3.4
1	B	97	GLY	3.3
1	B	133	TYR	3.3
1	A	183	ILE	3.3
1	A	204	LEU	3.3
1	A	182	ALA	3.3
2	M	141	LYS	3.2
3	I	194	THR	3.2
2	M	19	VAL	3.2
2	M	118	PRO	3.2
2	M	42	GLU	3.1
1	B	243	GLY	3.1
1	B	264	PHE	3.1
3	I	173	SER	3.1
1	A	152	LEU	3.1
1	B	192	GLY	3.1
1	A	184	PHE	3.1
1	B	39	VAL	3.1
1	B	263	TRP	3.1
3	I	204	THR	3.0
1	B	268	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	179	HIS	3.0
1	A	131	ILE	3.0
1	B	69	ARG	3.0
1	B	91	LEU	2.9
1	B	258	TYR	2.9
2	M	148	LYS	2.9
2	M	168	LYS	2.9
2	L	160	GLN	2.9
1	A	97	GLY	2.9
3	I	170	ALA	2.9
3	I	162	VAL	2.9
3	I	84	LEU	2.9
1	A	82	LYS	2.9
2	M	111	LYS	2.9
3	I	77	LYS	2.9
3	I	69	ILE	2.9
1	B	173	LEU	2.9
1	B	272	TYR	2.8
3	H	221	LYS	2.8
2	L	145	VAL	2.8
3	H	5	GLN	2.8
2	M	211	ASN	2.8
3	I	63	PRO	2.7
2	M	128	SER	2.7
1	B	257	ALA	2.7
1	B	210	PHE	2.7
1	B	117	LEU	2.7
1	A	178	GLY	2.7
1	A	122	PHE	2.7
1	B	271	ALA	2.7
1	B	203	LEU	2.7
1	A	96	GLY	2.7
1	B	87	PHE	2.6
3	I	86	THR	2.6
1	B	74	ARG	2.6
3	H	152	CYS	2.6
1	A	263	TRP	2.6
1	A	268	PHE	2.6
1	B	179	HIS	2.6
3	I	216	THR	2.6
1	A	32	LEU	2.6
1	B	40	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	H	60	THR	2.5
1	B	269	GLY	2.5
1	A	137	VAL	2.5
1	A	200	VAL	2.5
2	M	162	VAL	2.5
1	B	43	LEU	2.5
2	L	31	GLN	2.5
1	A	31	THR	2.5
3	I	23	SER	2.5
1	A	164	GLY	2.5
2	L	146	LYS	2.5
2	L	193	CYS	2.5
1	A	193	LEU	2.5
3	H	153	LEU	2.5
1	B	70	ASP	2.5
3	I	171	LEU	2.4
1	A	192	GLY	2.4
1	A	35	LEU	2.4
1	B	238	THR	2.4
1	B	277	LEU	2.4
2	M	131	LEU	2.4
1	A	163	ALA	2.4
2	L	49	TYR	2.4
1	A	284	LEU	2.4
3	I	13	LYS	2.4
1	B	233	VAL	2.4
1	A	188	HIS	2.3
3	H	103	SER	2.3
1	A	185	LEU	2.3
1	A	197	LEU	2.3
2	M	190	LEU	2.3
3	H	215	SER	2.3
3	H	10	GLY	2.3
1	A	246	VAL	2.3
1	A	158	PHE	2.3
3	I	183	HIS	2.3
2	M	87	PHE	2.3
1	B	186	LYS	2.3
2	M	192	THR	2.3
2	M	41	GLU	2.3
3	I	87	VAL	2.3
3	I	205	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	93	GLU	2.2
3	I	9	PRO	2.2
1	B	211	VAL	2.2
3	I	182	LEU	2.2
1	B	202	PHE	2.2
1	A	93	GLU	2.2
2	M	94	PRO	2.2
1	A	196	SER	2.2
1	A	40	LEU	2.2
1	B	41	LEU	2.2
1	B	158	PHE	2.2
2	M	67	TYR	2.2
1	B	82	LYS	2.2
2	L	1	ASP	2.2
3	I	218	VAL	2.2
1	A	234	ILE	2.2
1	B	131	ILE	2.2
1	B	33	LEU	2.2
1	B	35	LEU	2.2
1	B	125	GLY	2.2
1	A	148	ILE	2.2
1	A	209	LEU	2.1
2	M	149	VAL	2.1
3	H	71	ILE	2.1
3	I	121	VAL	2.1
3	I	175	VAL	2.1
2	L	21	ILE	2.1
3	H	122	SER	2.1
3	I	64	SER	2.1
1	A	99	ALA	2.1
1	B	32	LEU	2.1
1	B	216	PHE	2.1
2	M	166	ASP	2.1
2	L	81	GLU	2.1
1	A	190	PRO	2.1
1	B	256	PRO	2.1
3	H	203	GLN	2.1
3	I	44	GLY	2.1
3	H	69	ILE	2.1
3	H	209	VAL	2.0
1	A	273	PHE	2.0
1	B	244	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
3	I	75	THR	2.0
2	L	75	ILE	2.0
3	I	117	ILE	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	K	B	401	1/1	0.81	0.17	87,87,87,87	0
4	K	A	401	1/1	0.95	0.06	60,60,60,60	0
4	K	A	404	1/1	0.96	0.05	89,89,89,89	0
4	K	A	405	1/1	0.97	0.07	67,67,67,67	0
4	K	A	402	1/1	0.98	0.04	67,67,67,67	0
4	K	A	403	1/1	0.99	0.02	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.