

wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 10:13 am BST

PDB ID : 3PJS

Title: Mechanism of Activation Gating in the Full-Length KcsA K+ Channel

Authors: Uysal, S.; Cuello, L.G.; Kossiakoff, A.; Perozo, E.

Deposited on : 2010-11-10

Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} Mol Probity & : & 4.02 \, b\text{-}467 \\ Xtriage & (Phenix) & : & 1.13 \end{array}$

EDS: 2.11

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)

al geometry (DNA, RNA) : Parkinson et al. (1996)

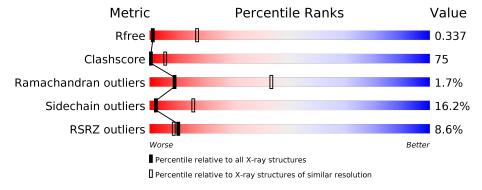
Ideal geometry (DNA, RNA) : Parkin Validation Pipeline (wwPDB-VP) : 2.11

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 3.80 Å.

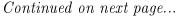
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 on 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	215	27%	53%		17%	<u>-</u>
			<u>%</u>	5573		27,70	
1	С	215	28%	53%		17%	·
2	В	224	31%	51%	_	13%	• •
2	D	224	30%	52%	_	13%	•
3	K	166	21%	54%	8% •	16%	_
3	L	166	18%	58%	8%	16%	_





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Mol	Chain	Length		Quality of chain		
			20%			
3	M	166	22%	55%	7%	16%
			15%			
3	N	166	23%	54%	7%	16%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10982 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 FAB light chain.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Λ	A 215	Total	С	N	О	S	0	0	0
1	1 A		1658	1038	276	339	5	0		
1	С	215	Total	С	N	О	S	0	0	0
1		215	1658	1038	276	339	5	0	U	

• Molecule 2 is a protein called FAB heavy chain.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
9	D	В 219	Total	С	N	О	S	0	0	0
	2 D		1653	1050	272	325	6	0		
9	D	219	Total	С	N	О	S	0	0	0
	ש	219	1653	1050	272	325	6	U		

• Molecule 3 is a protein called Voltage-gated potassium channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3 K	139	Total	С	N	О	S	0	0	0
3	IX		1090	697	195	196	2	U	0	U
2	Ŧ	139	Total	С	N	О	S	0	0	0
3	3 L	139	1090	697	195	196	2			
3	M	M 120	Total	С	N	О	S	0	0	0
3	IVI	139	1090	697	195	196	2	0		0
2	3 N	139	Total	С	N	О	S	0	0	0
3			1090	697	195	196	2		0	

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-5	MET	-	EXPRESSION TAG	UNP P0A334
K	-4	HIS	-	EXPRESSION TAG	UNP P0A334
K	-3	HIS	-	EXPRESSION TAG	UNP P0A334
K	-2	HIS	-	EXPRESSION TAG	UNP P0A334



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Chain	Residue	$oxed{f Modelled}$	Actual	Comment	Reference
K	-1	HIS	-	EXPRESSION TAG	UNP P0A334
K	0	HIS	-	EXPRESSION TAG	UNP P0A334
K	1	HIS	-	EXPRESSION TAG	UNP P0A334
K	2	PRO	_	EXPRESSION TAG	UNP P0A334
K	3	PRO	-	EXPRESSION TAG	UNP P0A334
K	4	MET	-	EXPRESSION TAG	UNP P0A334
K	5	LEU	-	EXPRESSION TAG	UNP P0A334
K	6	SER	-	EXPRESSION TAG	UNP P0A334
K	7	GLY	-	EXPRESSION TAG	UNP P0A334
K	8	LEU	-	EXPRESSION TAG	UNP P0A334
K	9	LEU	-	EXPRESSION TAG	UNP P0A334
K	10	ALA	_	EXPRESSION TAG	UNP P0A334
K	11	ARG	_	EXPRESSION TAG	UNP P0A334
K	12	LEU	-	EXPRESSION TAG	UNP P0A334
K	13	VAL	-	EXPRESSION TAG	UNP P0A334
K	14	LYS	-	EXPRESSION TAG	UNP P0A334
K	15	LEU	-	EXPRESSION TAG	UNP P0A334
K	16	LEU	-	EXPRESSION TAG	UNP P0A334
K	17	LEU	-	EXPRESSION TAG	UNP P0A334
K	18	GLY	-	EXPRESSION TAG	UNP P0A334
K	19	ARG	-	EXPRESSION TAG	UNP P0A334
K	20	HIS	-	EXPRESSION TAG	UNP P0A334
K	21	GLY	-	EXPRESSION TAG	UNP P0A334
K	25	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
K	117	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
K	120	GLN	GLU	ENGINEERED MUTATION	UNP P0A334
K	121	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
K	122	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
K	123	GLN	GLY	ENGINEERED MUTATION	UNP P0A334
K	124	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
L	-5	MET	-	EXPRESSION TAG	UNP P0A334
L	-4	HIS	-	EXPRESSION TAG	UNP P0A334
L	-3	HIS	-	EXPRESSION TAG	UNP P0A334
L	-2	HIS	-	EXPRESSION TAG	UNP P0A334
L	-1	HIS	-	EXPRESSION TAG	UNP P0A334
L	0	HIS	-	EXPRESSION TAG	UNP P0A334
L	1	HIS	-	EXPRESSION TAG	UNP P0A334
L	2	PRO	-	EXPRESSION TAG	UNP P0A334
L	3	PRO	-	EXPRESSION TAG	UNP P0A334
L	4	MET	-	EXPRESSION TAG	UNP P0A334
L	5	LEU	-	EXPRESSION TAG	UNP P0A334
L	6	SER	-	EXPRESSION TAG	UNP P0A334



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Chain	Residue	Modelled	Actual	${f Comment}$	Reference
L	7	GLY	-	EXPRESSION TAG	UNP P0A334
L	8	LEU	-	EXPRESSION TAG	UNP P0A334
L	9	LEU	-	EXPRESSION TAG	UNP P0A334
L	10	ALA	-	EXPRESSION TAG	UNP P0A334
L	11	ARG	-	EXPRESSION TAG	UNP P0A334
L	12	LEU	-	EXPRESSION TAG	UNP P0A334
L	13	VAL	-	EXPRESSION TAG	UNP P0A334
L	14	LYS	-	EXPRESSION TAG	UNP P0A334
L	15	LEU	-	EXPRESSION TAG	UNP P0A334
L	16	LEU	-	EXPRESSION TAG	UNP P0A334
L	17	LEU	-	EXPRESSION TAG	UNP P0A334
L	18	GLY	-	EXPRESSION TAG	UNP P0A334
L	19	ARG	-	EXPRESSION TAG	UNP P0A334
L	20	HIS	-	EXPRESSION TAG	UNP P0A334
L	21	GLY	-	EXPRESSION TAG	UNP P0A334
L	25	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
L	117	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
L	120	GLN	GLU	ENGINEERED MUTATION	UNP P0A334
L	121	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
L	122	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
L	123	GLN	GLY	ENGINEERED MUTATION	UNP P0A334
L	124	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
M	-5	MET	-	EXPRESSION TAG	UNP P0A334
M	-4	HIS	-	EXPRESSION TAG	UNP P0A334
M	-3	HIS	_	EXPRESSION TAG	UNP P0A334
M	-2	HIS	-	EXPRESSION TAG	UNP P0A334
M	-1	HIS	_	EXPRESSION TAG	UNP P0A334
M	0	HIS	-	EXPRESSION TAG	UNP P0A334
M	1	HIS	_	EXPRESSION TAG	UNP P0A334
M	2	PRO	_	EXPRESSION TAG	UNP P0A334
M	3	PRO	_	EXPRESSION TAG	UNP P0A334
M	4	MET	_	EXPRESSION TAG	UNP P0A334
M	5	LEU	-	EXPRESSION TAG	UNP P0A334
M	6	SER	-	EXPRESSION TAG	UNP P0A334
M	7	GLY		EXPRESSION TAG	UNP P0A334
M	8	LEU	-	EXPRESSION TAG	UNP P0A334
M	9	LEU	-	EXPRESSION TAG	UNP P0A334
M	10	ALA	-	EXPRESSION TAG	UNP P0A334
M	11	ARG	-	EXPRESSION TAG	UNP P0A334
M	12	LEU	-	EXPRESSION TAG	UNP P0A334
M	13	VAL	-	EXPRESSION TAG	UNP P0A334
M	14	LYS	-	EXPRESSION TAG	UNP P0A334



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Chain	Residue	Modelled	Actual	${f Comment}$	Reference
M	15	LEU	-	EXPRESSION TAG	UNP P0A334
M	16	LEU	_	EXPRESSION TAG	UNP P0A334
M	17	LEU	-	EXPRESSION TAG	UNP P0A334
M	18	GLY	_	EXPRESSION TAG	UNP P0A334
M	19	ARG	-	EXPRESSION TAG	UNP P0A334
M	20	HIS	_	EXPRESSION TAG	UNP P0A334
M	21	GLY	-	EXPRESSION TAG	UNP P0A334
M	25	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
M	117	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
M	120	GLN	GLU	ENGINEERED MUTATION	UNP P0A334
M	121	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
M	122	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
M	123	GLN	GLY	ENGINEERED MUTATION	UNP P0A334
M	124	GLN	HIS	ENGINEERED MUTATION	UNP P0A334
N	-5	MET	-	EXPRESSION TAG	UNP P0A334
N	-4	HIS	-	EXPRESSION TAG	UNP P0A334
N	-3	HIS	-	EXPRESSION TAG	UNP P0A334
N	-2	HIS	-	EXPRESSION TAG	UNP P0A334
N	-1	HIS	-	EXPRESSION TAG	UNP P0A334
N	0	HIS	_	EXPRESSION TAG	UNP P0A334
N	1	HIS	-	EXPRESSION TAG	UNP P0A334
N	2	PRO	-	EXPRESSION TAG	UNP P0A334
N	3	PRO	_	EXPRESSION TAG	UNP P0A334
N	4	MET	-	EXPRESSION TAG	UNP P0A334
N	5	LEU	_	EXPRESSION TAG	UNP P0A334
N	6	SER	_	EXPRESSION TAG	UNP P0A334
N	7	GLY	-	EXPRESSION TAG	UNP P0A334
N	8	LEU	_	EXPRESSION TAG	UNP P0A334
N	9	LEU	-	EXPRESSION TAG	UNP P0A334
N	10	ALA	_	EXPRESSION TAG	UNP P0A334
N	11	ARG	_	EXPRESSION TAG	UNP P0A334
N	12	LEU	-	EXPRESSION TAG	UNP P0A334
N	13	VAL	-	EXPRESSION TAG	UNP P0A334
N	14	LYS	-	EXPRESSION TAG	UNP P0A334
N	15	LEU	-	EXPRESSION TAG	UNP P0A334
N	16	LEU	-	EXPRESSION TAG	UNP P0A334
N	17	LEU	-	EXPRESSION TAG	UNP P0A334
N	18	GLY	-	EXPRESSION TAG	UNP P0A334
N	19	ARG	-	EXPRESSION TAG	UNP P0A334
N	20	HIS	-	EXPRESSION TAG	UNP P0A334
N	21	GLY	-	EXPRESSION TAG	UNP P0A334
N	25	GLN	HIS	ENGINEERED MUTATION	UNP P0A334



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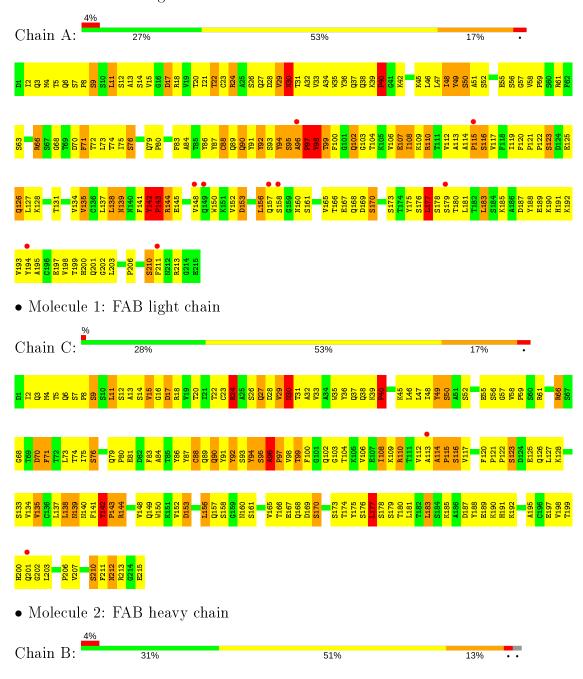
Chain	Residue	Modelled	Actual	Comment	Reference
N	117	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
N	120	GLN	GLU	ENGINEERED MUTATION	UNP P0A334
N	121	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
N	122	GLN	ARG	ENGINEERED MUTATION	UNP P0A334
N	123	GLN	GLY	ENGINEERED MUTATION	UNP P0A334
N	124	GLN	HIS	ENGINEERED MUTATION	UNP P0A334



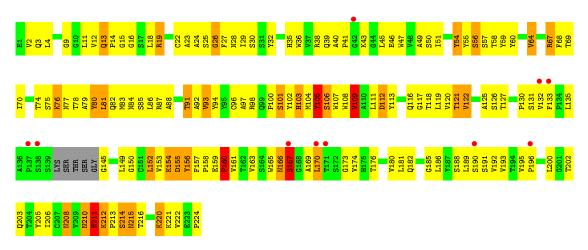
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

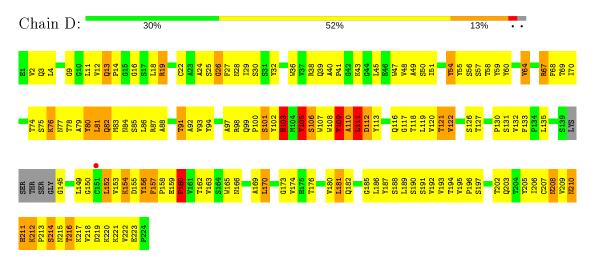
• Molecule 1: FAB light chain



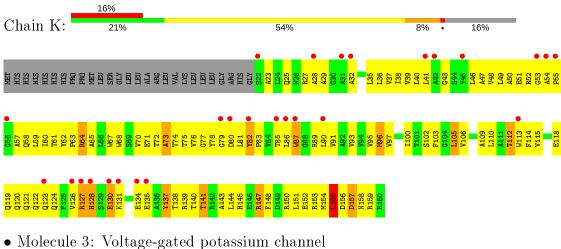




 \bullet Molecule 2: FAB heavy chain

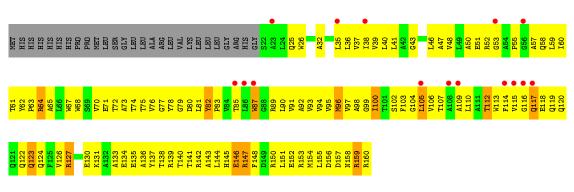


• Molecule 3: Voltage-gated potassium channel

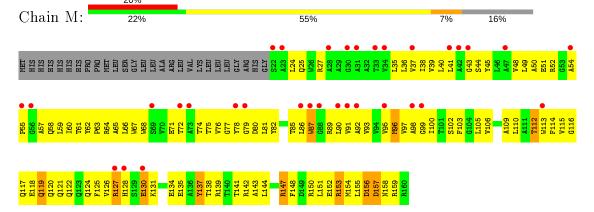




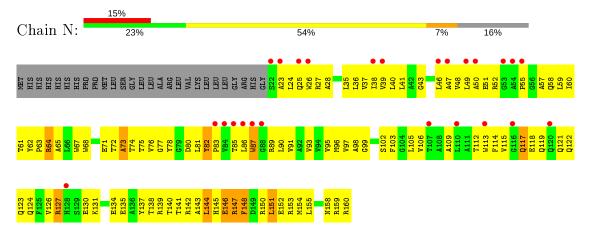




• Molecule 3: Voltage-gated potassium channel



• Molecule 3: Voltage-gated potassium channel





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	118.27Å 176.72Å 340.47Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 - 3.80	Depositor
Resolution (A)	39.17 - 3.70	EDS
% Data completeness	82.4 (40.00-3.80)	Depositor
(in resolution range)	80.9 (39.17-3.70)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.73 (at 3.66Å)	Xtriage
Refinement program	CNS	Depositor
D D.	0.281 , 0.332	Depositor
R, R_{free}	0.289 , 0.337	DCC
R_{free} test set	1513 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	135.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.28 , 163.1	EDS
L-test for twinning ²	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	10982	wwPDB-VP
Average B, all atoms $(Å^2)$	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	Bo	nd lengths	В	ond angles
WIOI	Chain	RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	6/1694~(0.4%)	1.41	$25/2300 \ (1.1\%)$
1	С	0.68	0/1694	1.26	$24/2300 \ (1.0\%)$
2	В	0.78	3/1698~(0.2%)	1.09	$16/2319 \ (0.7\%)$
2	D	0.74	0/1698	1.17	18/2319 (0.8%)
3	K	0.59	0/1113	0.84	3/1517~(0.2%)
3	L	0.63	0/1113	0.75	0/1517
3	M	0.57	0/1113	0.75	$2/1517 \; (0.1\%)$
3	N	0.60	0/1113	0.76	0/1517
All	All	0.69	9/11236 (0.1%)	1.08	88/15306 (0.6%)

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	С	0	1
3	K	0	1
All	All	0	4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	Ideal(A)
1	A	97	PRO	N-CD	-12.23	1.30	1.47
1	A	115	PRO	CA-C	6.68	1.66	1.52
2	В	166	ASN	C-O	-6.56	1.10	1.23
2	В	154	LYS	C-O	-6.42	1.11	1.23
1	A	116	SER	N-CA	5.69	1.57	1.46

The worst 5 of 88 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	A	142	TYR	C-N-CD	-26.37	62.58	120.60
1	A	96	ALA	CB-CA-C	-18.99	81.62	110.10
1	A	96	ALA	C-N-CD	-17.89	81.25	120.60
1	A	96	ALA	N-CA-C	16.27	154.93	111.00
1	С	116	SER	N-CA-CB	-16.25	86.13	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	TYR	Mainchain
1	A	92	TYR	Sidechain
1	С	92	TYR	Sidechain
3	K	155	LEU	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	1658	0	1606	299	0
1	С	1658	0	1606	248	0
2	В	1653	0	1597	285	0
2	D	1653	0	1597	274	0
3	K	1090	0	1093	185	0
3	L	1090	0	1093	193	0
3	M	1090	0	1093	181	0
3	N	1090	0	1093	167	0
All	All	10982	0	10778	1632	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 75.

The worst 5 of 1632 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
2:B:165:TRP:HE1	2:B:174:VAL:CG2	1.04	1.58



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Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
2:B:165:TRP:CH2	2:B:193:VAL:HG11	1.39	1.54
2:B:130:PRO:CB	2:B:155:ASP:O	1.64	1.45
1:C:115:PRO:CB	1:C:141:PHE:HB3	1.47	1.45
2:B:165:TRP:CH2	2:B:193:VAL:CG1	1.97	1.43

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	Perce	entiles
1	A	213/215~(99%)	173 (81%)	34 (16%)	6 (3%)	5	35
1	С	213/215~(99%)	177 (83%)	30 (14%)	6 (3%)	5	35
2	В	215/224~(96%)	185 (86%)	28 (13%)	2 (1%)	17	54
2	D	215/224~(96%)	188 (87%)	25 (12%)	2 (1%)	17	54
3	K	137/166 (82%)	116 (85%)	18 (13%)	3 (2%)	6	39
3	L	137/166 (82%)	125 (91%)	10 (7%)	2 (2%)	10	46
3	M	137/166 (82%)	119 (87%)	17 (12%)	1 (1%)	22	60
3	N	137/166 (82%)	116 (85%)	19 (14%)	2 (2%)	10	46
All	All	1404/1542 (91%)	1199 (85%)	181 (13%)	24 (2%)	9	43

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	PRO
1	A	143	PRO
1	С	115	PRO
1	A	40	PRO
1	С	96	ALA



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	Perce	entiles
1	A	189/189~(100%)	155 (82%)	34 (18%)	1	12
1	С	$189/189 \; (100\%)$	155 (82%)	34 (18%)	1	12
2	В	184/188~(98%)	150 (82%)	34 (18%)	1	11
2	D	184/188~(98%)	149 (81%)	35 (19%)	1	10
3	K	108/131~(82%)	94 (87%)	14 (13%)	4	23
3	L	108/131~(82%)	94 (87%)	14 (13%)	4	23
3	M	108/131~(82%)	95 (88%)	13 (12%)	5	25
3	N	$108/131\ (82\%)$	95 (88%)	13 (12%)	5	25
All	All	$1178/1278 \ (92\%)$	987 (84%)	191 (16%)	2	15

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	110	ARG
2	D	58	THR
3	M	153	ARG
1	С	123	SER
1	С	170	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	168	GLN
2	D	39	GLN
3	N	117	GLN
1	С	212	ASN
2	D	82	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	$215/215 \; (100\%)$	0.28	9 (4%) 36 30	98, 197, 222, 222	0
1	С	$215/215 \; (100\%)$	-0.03	2 (0%) 84 79	80, 143, 198, 222	0
2	В	219/224 (97%)	0.14	10 (4%) 32 28	78, 153, 222, 222	0
2	D	219/224 (97%)	-0.09	1 (0%) 91 87	73, 134, 211, 222	0
3	K	139/166 (83%)	0.77	27 (19%) 1 1	78, 222, 222, 222	0
3	L	139/166 (83%)	0.61	15 (10%) 5 5	91, 222, 222, 222	0
3	М	139/166 (83%)	1.09	33 (23%) 0 0	90, 222, 222, 222	0
3	N	139/166 (83%)	0.85	25 (17%) 1 1	106, 222, 222, 222	0
All	All	1424/1542 (92%)	0.37	122 (8%) 10 8	73, 190, 222, 222	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	54	ALA	5.9
3	N	85	THR	5.8
3	L	38	ILE	5.8
3	M	73	ALA	5.7
3	M	79	GLY	5.3

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 carbohydrates in this entry.



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

