

Full wwPDB X-ray Structure Validation Report (i)

Mar 12, 2024 – 12:28 pm GMT

PDB ID	:	8PNM
Title	:	Structure of human KCTD15 BTB domain mutant G88D crystal form 2
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Deposited on	:	2023-06-30
Resolution	:	1.94 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.94 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	А	116	78%	10%	• 10%
1	В	116	% • 83%	•	16%
1	С	116	^{2%} 77%	5%	18%
1	D	116	84%	•	11%
1	Е	116	4%	8%	14%



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Mol	Chain	Length	Quality of chain				
1	F	116	3% 73%	8% • 18%			
1	G	116	2% 	•• 9%			
1	Н	116	3% 77%	10% • 12%			
1	Ι	116	5%	7% • 12%			
1	J	116	3% 82%	9% • 7%			
1	К	116	2% 73%	9% 18%			
1	L	116	3% 85%	7% 8%			





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2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9618 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	C	05	Total	С	Ν	0	S	0	0	0
1	U	95	776	501	125	148	2	0	0	0
1	Δ	104	Total	С	Ν	0	S	0	0	0
1	A	104	814	527	132	153	2	0	0	0
1	С	105	Total	С	Ν	0	S	0	0	0
1	G	105	816	528	134	152	2	0	0	0
1	F	100	Total	С	Ν	0	S	0	0	0
1	Ľ	100	781	507	125	147	2	0	0	0
1	т	108	Total	С	Ν	0	S	0	0	0
1	1	108	811	522	135	153	1	0		
1	П	102	Total	С	Ν	0	S	0	0	0
1	D	105	797	516	132	147	2	0	0	0
1	В	08	Total	С	Ν	0	S	0	0	0
1	D	90	775	502	124	147	2	0	0	0
1	т	102	Total	С	Ν	0	S	0	0	0
1	1	102	785	510	128	146	1	0	0	U
1	Ц	102	Total	С	Ν	0	S	0	0	0
1	11	102	779	505	127	145	2	0	0	U
1	K	05	Total	С	Ν	0	S	0	0	0
1	Γ	90	735	473	121	139	2	0	0	0
1	1 E	05	Total	С	Ν	0	S	0	0	0
	Г	90	743	480	121	140	2	0	0	U
1	Т	107	Tota	l C	Ν	0		0	0	0
		107	760	49	1 122	2 14	7	0	U	U

• Molecule 1 is a protein called BTB/POZ domain-containing protein KCTD15.

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	1	SER	-	expression tag	UNP Q96SI1
С	2	MET	-	expression tag	UNP Q96SI1
С	39	ASP	GLY	engineered mutation	UNP Q96SI1
А	1	SER	-	expression tag	UNP Q96SI1
А	2	MET	-	expression tag	UNP Q96SI1



Chain	Residue	Modelled	Actual	Comment	Reference
А	39	ASP	GLY	engineered mutation	UNP Q96SI1
G	1	SER	-	expression tag	UNP Q96SI1
G	2	MET	-	expression tag	UNP Q96SI1
G	39	ASP	GLY	engineered mutation	UNP Q96SI1
Е	1	SER	-	expression tag	UNP Q96SI1
Е	2	MET	-	expression tag	UNP Q96SI1
Е	39	ASP	GLY	engineered mutation	UNP Q96SI1
J	1	SER	-	expression tag	UNP Q96SI1
J	2	MET	-	expression tag	UNP Q96SI1
J	39	ASP	GLY	engineered mutation	UNP Q96SI1
D	1	SER	-	expression tag	UNP Q96SI1
D	2	MET	-	expression tag	UNP Q96SI1
D	39	ASP	GLY	engineered mutation	UNP Q96SI1
В	1	SER	_	expression tag	UNP Q96SI1
В	2	MET	-	expression tag	UNP Q96SI1
В	39	ASP	GLY	engineered mutation	UNP Q96SI1
Ι	1	SER	-	expression tag	UNP Q96SI1
Ι	2	MET	_	expression tag	UNP Q96SI1
Ι	39	ASP	GLY	engineered mutation	UNP Q96SI1
Н	1	SER	_	expression tag	UNP Q96SI1
Н	2	MET	-	expression tag	UNP Q96SI1
Н	39	ASP	GLY	engineered mutation	UNP Q96SI1
K	1	SER	-	expression tag	UNP Q96SI1
K	2	MET	-	expression tag	UNP Q96SI1
K	39	ASP	GLY	engineered mutation	UNP Q96SI1
F	1	SER	-	expression tag	UNP Q96SI1
F	2	MET	-	expression tag	UNP Q96SI1
F	39	ASP	GLY	engineered mutation	UNP Q96SI1
L	1	SER	-	expression tag	UNP Q96SI1
L	2	MET	-	expression tag	UNP Q96SI1
L	39	ASP	GLY	engineered mutation	UNP Q96SI1

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	34	$\begin{array}{cc} \text{Total} & \text{O} \\ 34 & 34 \end{array}$	0	0
2	А	29	Total O 29 29	0	0
2	G	11	Total O 11 11	0	0
2	Ε	27	$\begin{array}{cc} \text{Total} & \text{O} \\ 27 & 27 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	15	Total O 15 15	0	0
2	D	14	Total O 14 14	0	0
2	В	28	TotalO2828	0	0
2	Ι	13	Total O 13 13	0	0
2	Н	17	Total O 17 17	0	0
2	К	22	Total O 22 22	0	0
2	F	22	$\begin{array}{cc} \text{Total} & \text{O} \\ 22 & 22 \end{array}$	0	0
2	L	14	Total O 14 14	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: BTB/POZ domain-containing protein KCTD15





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	71.26Å 72.09 Å 94.41 Å	Deperitor
a, b, c, α , β , γ	89.63° 77.08° 60.50°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	61.31 - 1.94	Depositor
Resolution (A)	61.31 - 1.94	EDS
% Data completeness	65.1 (61.31-1.94)	Depositor
(in resolution range)	$65.1 \ (61.31 - 1.94)$	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.03 (at 1.94 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.236 , 0.273	Depositor
Π, Π_{free}	0.235 , 0.270	DCC
R_{free} test set	3779 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	44.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 39.2	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	0.007 for -h+k,k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9618	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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).

Mal	Chain	Boi	nd lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.31	0/836	0.56	0/1141	
1	В	0.29	0/795	0.52	0/1082	
1	С	0.43	1/796~(0.1%)	0.64	1/1080~(0.1%)	
1	D	0.31	0/818	0.56	0/1116	
1	Ε	0.30	0/802	0.51	0/1095	
1	F	0.30	0/763	0.53	0/1040	
1	G	0.28	0/837	0.51	0/1141	
1	Н	0.44	1/799~(0.1%)	1.36	3/1091~(0.3%)	
1	Ι	0.33	0/806	0.61	0/1100	
1	J	0.33	0/832	0.97	7/1138~(0.6%)	
1	Κ	0.29	0/753	0.54	0/1026	
1	L	0.28	0/781	0.45	0/1076	
All	All	0.33	2/9618~(0.0%)	0.70	11/13126~(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	Ι	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	С	59	GLU	CD-OE1	-6.44	1.18	1.25
1	Н	98	VAL	CB-CG1	-6.08	1.40	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Н	36	LEU	CB-CG-CD2	-30.94	58.40	111.00
1	Н	36	LEU	CB-CG-CD1	23.75	151.37	111.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	J	94	LEU	CB-CG-CD2	-15.05	85.42	111.00
1	J	94	LEU	CB-CG-CD1	13.99	134.78	111.00
1	J	94	LEU	CA-CB-CG	9.75	137.72	115.30
1	J	98	VAL	CG1-CB-CG2	8.48	124.47	110.90
1	С	59	GLU	CA-CB-CG	6.69	128.12	113.40
1	J	94	LEU	CD1-CG-CD2	-6.55	90.84	110.50
1	Н	98	VAL	CG1-CB-CG2	5.50	119.70	110.90
1	J	68	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	J	29	PRO	N-CD-CG	-5.18	95.43	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Ι	90	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	А	814	0	741	10	0
1	В	775	0	703	2	0
1	С	776	0	715	5	0
1	D	797	0	708	3	0
1	Е	781	0	702	7	0
1	F	743	0	658	7	0
1	G	816	0	730	2	0
1	Н	779	0	685	8	0
1	Ι	785	0	698	7	0
1	J	811	0	700	10	0
1	Κ	735	0	667	5	0
1	L	760	0	609	4	0
2	А	29	0	0	3	0
2	В	28	0	0	2	0
2	C	$\overline{34}$	0	0	1	0
2	D	14	0	0	0	0
2	E	$\overline{27}$	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	22	0	0	0	0
2	G	11	0	0	1	0
2	Н	17	0	0	0	0
2	Ι	13	0	0	1	0
2	J	15	0	0	0	0
2	Κ	22	0	0	0	0
2	L	14	0	0	0	0
All	All	9618	0	8316	67	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 4.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:89:ALA:O	2:A:201:HOH:O	1.90	0.88
1:I:56:ARG:NH1	2:I:201:HOH:O	2.13	0.81
1:J:95:GLN:HA	1:J:98:VAL:HG22	1.62	0.80
1:J:44:VAL:HG12	1:J:50:GLN:HG3	1.65	0.78
1:A:93:GLN:N	2:A:201:HOH:O	2.18	0.76
1:E:11:ILE:HD11	1:E:25:LEU:HD11	1.74	0.69
1:A:100:GLU:OE1	1:A:103:ARG:NH2	2.27	0.68
1:A:5:SER:N	2:A:202:HOH:O	2.27	0.67
1:D:74:LEU:HD11	1:F:84:LEU:HD22	1.76	0.66
1:B:14:GLY:O	2:B:201:HOH:O	2.13	0.65
1:G:88:GLU:OE2	2:G:201:HOH:O	2.15	0.64
1:G:59:GLU:O	1:G:62:ARG:HG2	1.98	0.64
1:E:36:LEU:O	1:E:40:THR:HG22	1.99	0.62
1:K:3:THR:HG23	1:K:6:ASN:HB2	1.82	0.61
1:L:70:THR:O	1:L:72:LYS:N	2.37	0.57
1:K:60:ILE:HG21	1:K:88:GLU:HG3	1.88	0.56
1:F:36:LEU:O	1:F:40:THR:HG22	2.05	0.56
1:I:54:ILE:HG22	1:I:56:ARG:HB2	1.88	0.56
1:I:56:ARG:HG3	1:I:88:GLU:OE1	2.06	0.55
1:C:11:ILE:HD11	1:C:25:LEU:HD11	1.87	0.55
1:D:36:LEU:O	1:D:40:THR:HB	2.08	0.53
1:J:28:TYR:CE2	1:J:96:PRO:HG2	2.44	0.52
1:H:95:GLN:HA	1:H:98:VAL:HG13	1.92	0.52
1:B:40:THR:O	2:B:202:HOH:O	2.19	0.52
1:C:87:GLU:OE1	1:I:72:LYS:HE2	2.11	0.51
1:K:56:ARG:HD2	1:K:91:TYR:CE2	2.46	0.51



	lovo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:11:ILE:HD11	1:C:25:LEU:CD1	2.40	0.51
1:J:68:LEU:HD21	1:J:94:LEU:CD1	2.41	0.51
1:J:95:GLN:HA	1:J:98:VAL:CG2	2.35	0.50
1:H:94:LEU:O	1:H:98:VAL:HG12	2.13	0.49
1:H:41:GLU:O	1:H:41:GLU:HG2	2.13	0.49
1:F:95:GLN:O	1:F:98:VAL:HG22	2.14	0.48
1:C:12:ASP:OD2	2:C:201:HOH:O	2.20	0.48
1:A:42:PRO:HD3	1:A:52:TYR:CZ	2.49	0.47
1:C:25:LEU:HD13	1:C:37:PHE:CZ	2.50	0.46
1:L:70:THR:C	1:L:72:LYS:H	2.17	0.46
1:J:68:LEU:HA	1:J:68:LEU:HD23	1.70	0.45
1:F:95:GLN:HA	1:F:98:VAL:HG22	1.99	0.45
1:I:84:LEU:HD22	1:I:84:LEU:H	1.82	0.45
1:A:94:LEU:O	1:A:98:VAL:HG23	2.16	0.45
1:E:25:LEU:HD13	1:E:37:PHE:CZ	2.52	0.44
1:A:43:ILE:HG22	1:A:44:VAL:HG13	1.99	0.44
1:K:67:PHE:CD2	1:K:97:MET:HB2	2.52	0.44
1:L:28:TYR:CE1	1:L:96:PRO:HG2	2.53	0.44
1:D:35:ARG:HG2	1:D:39:ASP:OD2	2.18	0.43
1:I:42:PRO:HB3	1:I:52:TYR:CE1	2.53	0.43
1:H:59:GLU:O	1:H:62:ARG:NH1	2.52	0.43
1:F:40:THR:OG1	1:F:41:GLU:N	2.51	0.43
1:E:11:ILE:HG12	1:E:37:PHE:CZ	2.53	0.43
1:J:94:LEU:HA	1:J:94:LEU:HD22	1.86	0.43
1:F:56:ARG:HD2	1:F:91:TYR:CE2	2.53	0.43
1:E:60:ILE:HD13	1:E:84:LEU:HD23	2.01	0.42
1:H:56:ARG:HA	1:H:56:ARG:HD2	1.93	0.42
1:A:100:GLU:OE1	1:A:103:ARG:CZ	2.67	0.42
1:L:6:ASN:HA	1:L:21:SER:HB2	2.02	0.42
1:I:86:TYR:CE1	1:I:90:ARG:HD3	2.55	0.41
1:E:25:LEU:HD13	1:E:37:PHE:CE1	2.55	0.41
1:A:42:PRO:HD3	1:A:52:TYR:OH	2.20	0.41
1:H:11:ILE:HD11	1:H:25:LEU:HD11	2.02	0.41
1:H:22:LEU:HD23	1:H:22:LEU:HA	1.86	0.41
1:H:84:LEU:H	1:H:84:LEU:HD22	1.85	0.41
1:J:95:GLN:CA	1:J:98:VAL:HG22	2.44	0.41
1:A:33:ILE:HG13	1:A:92:TYR:CD1	2.56	0.41
1:E:11:ILE:HG12	1:E:37:PHE:HZ	1.84	0.41
1:K:82:PHE:C	1:K:82:PHE:CD1	2.94	0.40
1:J:56:ARG:NH2	1:J:88:GLU:OE2	2.48	0.40
1:J:14:GLY:HA2	1:F:19:THR:O	2.22	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	Percer	ntiles
1	А	102/116~(88%)	97~(95%)	4 (4%)	1 (1%)	15	6
1	В	94/116~(81%)	90~(96%)	4 (4%)	0	100	100
1	С	91/116~(78%)	88~(97%)	3(3%)	0	100	100
1	D	99/116~(85%)	94 (95%)	5 (5%)	0	100	100
1	Е	96/116~(83%)	92~(96%)	4 (4%)	0	100	100
1	F	91/116 (78%)	86 (94%)	4 (4%)	1 (1%)	14	5
1	G	101/116~(87%)	97~(96%)	4 (4%)	0	100	100
1	Н	98/116~(84%)	90~(92%)	7~(7%)	1 (1%)	15	6
1	Ι	98/116~(84%)	94~(96%)	4 (4%)	0	100	100
1	J	104/116~(90%)	100 (96%)	4 (4%)	0	100	100
1	K	91/116~(78%)	87~(96%)	4 (4%)	0	100	100
1	L	103/116~(89%)	98~(95%)	4 (4%)	1 (1%)	15	6
All	All	1168/1392 (84%)	1113 (95%)	51 (4%)	4 (0%)	41	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	71	SER
1	Н	42	PRO
1	F	41	GLU
1	А	43	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	А	83/109~(76%)	83~(100%)	0	100	100
1	В	79/109~(72%)	79~(100%)	0	100	100
1	С	82/109~(75%)	82~(100%)	0	100	100
1	D	77/109~(71%)	77~(100%)	0	100	100
1	Ε	79/109~(72%)	77~(98%)	2(2%)	47	35
1	F	74/109~(68%)	73~(99%)	1 (1%)	67	58
1	G	80/109~(73%)	79~(99%)	1 (1%)	69	62
1	Н	74/109~(68%)	73~(99%)	1 (1%)	67	58
1	Ι	76/109~(70%)	74 (97%)	2(3%)	46	32
1	J	76/109~(70%)	74 (97%)	2(3%)	46	32
1	Κ	75/109~(69%)	74~(99%)	1 (1%)	69	62
1	L	65/109~(60%)	64 (98%)	1 (2%)	65	56
All	All	920/1308~(70%)	909~(99%)	11 (1%)	71	64

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	62	ARG
1	Е	51	HIS
1	Е	62	ARG
1	J	78	ASP
1	J	98	VAL
1	Ι	38	ASN
1	Ι	56	ARG
1	Н	98	VAL
1	K	51	HIS
1	F	87	GLU
1	L	51	HIS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:



Mol	Chain	Res	Type
1	Е	38	ASN
1	D	51	HIS
1	Κ	6	ASN
1	L	51	HIS

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)

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	104/116~(89%)	0.29	3 (2%) 51 59	29, 44, 75, 104	0
1	В	98/116~(84%)	0.16	1 (1%) 82 86	34, 48, 70, 89	0
1	С	95/116~(81%)	0.28	2 (2%) 63 70	28, 38, 74, 91	0
1	D	103/116~(88%)	0.33	4 (3%) 39 47	35, 50, 81, 92	0
1	Ε	100/116~(86%)	0.33	5 (5%) 28 36	30, 43, 72, 88	0
1	F	95/116 (81%)	0.40	4 (4%) 36 43	33, 42, 67, 83	0
1	G	105/116~(90%)	0.33	2 (1%) 66 72	37, 54, 80, 85	0
1	Н	102/116~(87%)	0.42	4 (3%) 39 47	36, 50, 80, 109	0
1	Ι	102/116~(87%)	0.38	6 (5%) 22 28	34, 49, 75, 91	0
1	J	108/116~(93%)	0.31	4 (3%) 41 49	38, 59, 79, 104	0
1	Κ	95/116~(81%)	0.25	2 (2%) 63 70	35, 44, 71, 85	0
1	L	107/116~(92%)	0.34	3 (2%) 53 60	37, 58, 78, 86	0
All	All	1214/1392~(87%)	0.32	40 (3%) 46 54	28, 48, 78, 109	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	45	LEU	5.3
1	Е	42	PRO	5.1
1	С	38	ASN	4.9
1	G	48	LEU	4.7
1	F	104	TRP	4.4
1	Н	49	LYS	3.8
1	L	3	THR	3.7
1	J	98	VAL	3.2
1	J	86	TYR	3.0
1	L	70	THR	3.0
1	Н	36	LEU	2.9



8PNM

Mol	Chain	Res	Type	RSRZ
1	F	82	PHE	2.9
1	Е	40	THR	2.8
1	Н	41	GLU	2.8
1	Ι	77	ASP	2.8
1	Κ	82	PHE	2.8
1	J	104	TRP	2.6
1	А	43	ILE	2.6
1	G	75	LEU	2.5
1	F	73	LEU	2.5
1	Ι	43	ILE	2.5
1	Е	37	PHE	2.4
1	Ι	78	ASP	2.4
1	Е	78	ASP	2.4
1	F	42	PRO	2.4
1	В	104	TRP	2.3
1	С	78	ASP	2.3
1	D	75	LEU	2.3
1	D	79	PHE	2.2
1	Κ	73	LEU	2.2
1	А	47	SER	2.2
1	Е	41	GLU	2.2
1	J	44	VAL	2.2
1	L	77	ASP	2.2
1	D	110	GLN	2.2
1	Н	50	GLN	2.2
1	Ι	22	LEU	2.1
1	Ι	101	LEU	2.1
1	Ι	42	PRO	2.1
1	D	78	ASP	2.1

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)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

