

wwPDB X-ray Structure Validation Summary Report (i)

May 17, 2020 - 01:52 am BST

PDB ID	:	6HC2
Title	:	Crystal structure of NuMA/LGN hetero-hexamers
Authors	:	Pasqualato, S.; Culurgioni, S.; Foadi, J.; Alfieri, A.; Mapelli, M.
Deposited on	:	2018-08-13
Resolution	:	4.31 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:

:	4.02b-467
:	1.13
:	2.11
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	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 4.31 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)

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%

Mol	Chain	Length	Quality of chain		
1	А	367	79%	19%	••
1	С	367	86%	12%	·
1	Е	367	89%	9%	•
1	G	367	91%	8%	·
1	Ι	367	89%	11%	
1	К	367	88%	11%	•
1	М	367	90%	9%	•



Mol	Chain	Length	Quality of chain	
1	0	367	89%	10% ••
1	Q	367	88%	11% •
1	S	367	90%	8% ••
1	U	367	89%	10% •
1	W	367	87%	12% •
2	В	71	44% 18% • 37%	
2	D	71	35% 13% • 49%	
2	F	71	31% 17% •• 48%	
2	Н	71	30% 15% 6% 49%	
2	J	71	37% 13% 7% 44%	
2	L	71	38% 17% 6% • 38%	
2	N	71	41% 14% 45%	
2	Р	71	45% 10% • 3 9%	
2	R	71	25% 23% 7% • 44%	
2	Т	71	34% 23% 7% 37%	
2	V	71	41% 11% . 45%	
2	x	71	2004 2004 706 4404	
-	~ ~ ~	11		





2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 37558 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	Δ	265	Total	С	Ν	Ο	S	0	0	0
	A	300	2834	1778	497	548	11	0	0	0
1	C	267	Total	С	Ν	Ο	S	0	0	0
	U	307	2847	1783	500	552	12	0	0	0
1	F	266	Total	С	Ν	Ο	S	0	0	0
		300	2798	1750	494	545	9	0	0	0
1	C	267	Total	С	Ν	Ο	S	0	0	0
	G	307	2815	1759	499	547	10	0	0	0
1	т	267	Total	С	Ν	Ο	S	0	0	0
	1	307	2820	1768	497	546	9	0	0	0
1	V	266	Total	С	Ν	Ο	S	0	0	0
		300	2828	1772	497	547	12	0	0	0
1	М	266	Total	С	Ν	Ο	S	0	0	0
	IVI	300	2820	1767	499	544	10	0	0	0
1	0	365	Total	С	Ν	Ο	S	0	0	0
		000	2821	1767	496	547	11	0	0	0
1	0	367	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	V V	307	2831	1773	500	547	11	0	0	0
1	C	360	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	L D	302	2800	1753	496	541	10	0	0	0
1	I	366	Total	С	Ν	Ο	S	0	0	0
		500	2823	1767	499	547	10	0	0	0
1	W	366	Total	С	Ν	Ο	S	0	0	0
	v v	500	2817	1763	499	545	10	0	0	0

• Molecule 1 is a protein called G-protein-signaling modulator 2.

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	GLY	-	expression tag	UNP P81274
А	2	PRO	-	expression tag	UNP P81274
А	3	LEU	-	expression tag	UNP P81274
А	4	GLY	-	expression tag	UNP P81274
А	5	SER	-	expression tag	UNP P81274



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Chain	Residue	Modelled	Actual	Comment	Reference			
А	6	MET	-	expression tag	UNP P81274			
С	1	GLY	-	expression tag	UNP P81274			
С	2	PRO	-	expression tag	UNP P81274			
С	3	LEU	-	expression tag	UNP P81274			
С	4	GLY	-	expression tag	UNP P81274			
С	5	SER	-	expression tag	UNP P81274			
С	6	MET	-	expression tag	UNP P81274			
E	1	GLY	-	expression tag	UNP P81274			
Е	2	PRO	-	expression tag	UNP P81274			
Е	3	LEU	-	expression tag	UNP P81274			
Е	4	GLY	-	expression tag	UNP P81274			
Е	5	SER	-	expression tag	UNP P81274			
Е	6	MET	_	expression tag	UNP P81274			
G	1	GLY	-	expression tag	UNP P81274			
G	2	PRO	_	expression tag	UNP P81274			
G	3	LEU	-	expression tag	UNP P81274			
G	4	GLY	_	expression tag	UNP P81274			
G	5	SER	-	expression tag	UNP P81274			
G	6	MET	-	expression tag	UNP P81274			
Ι	1	GLY	-	expression tag	UNP P81274			
Ι	2	PRO	-	expression tag	UNP P81274			
Ι	3	LEU	-	expression tag	UNP P81274			
Ι	4	GLY	-	expression tag	UNP P81274			
Ι	5	SER	-	expression tag	UNP P81274			
Ι	6	MET	-	expression tag	UNP P81274			
K	1	GLY	-	expression tag	UNP P81274			
K	2	PRO	-	expression tag	UNP P81274			
K	3	LEU	-	expression tag	UNP P81274			
K	4	GLY	-	expression tag	UNP P81274			
K	5	SER	-	expression tag	UNP P81274			
K	6	MET	-	expression tag	UNP P81274			
М	1	GLY	-	expression tag	UNP P81274			
М	2	PRO	-	expression tag	UNP P81274			
М	3	LEU	-	expression tag	UNP P81274			
М	4	GLY	-	expression tag	UNP P81274			
М	5	SER	-	expression tag	UNP P81274			
М	6	MET	-	expression tag	UNP P81274			
0	1	GLY	-	expression tag	UNP P81274			
0	2	PRO	-	expression tag	UNP P81274			
0	3	LEU	-	expression tag	UNP P81274			
0	4	GLY	-	expression tag	UNP P81274			
0	5	SER	-	expression tag	UNP P81274			

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Chain	Residue	Modelled	Actual	Comment	Reference
0	6	MET	-	expression tag	UNP P81274
Q	1	GLY	-	expression tag	UNP P81274
Q	2	PRO	-	expression tag	UNP P81274
Q	3	LEU	-	expression tag	UNP P81274
Q	4	GLY	-	expression tag	UNP P81274
Q	5	SER	-	expression tag	UNP P81274
Q	6	MET	-	expression tag	UNP P81274
S	1	GLY	-	expression tag	UNP P81274
S	2	PRO	-	expression tag	UNP P81274
S	3	LEU	-	expression tag	UNP P81274
S	4	GLY	-	expression tag	UNP P81274
S	5	SER	-	expression tag	UNP P81274
S	6	MET	-	expression tag	UNP P81274
U	1	GLY	-	expression tag	UNP P81274
U	2	PRO	-	expression tag	UNP P81274
U	3	LEU	-	expression tag	UNP P81274
U	4	GLY	-	expression tag	UNP P81274
U	5	SER	-	expression tag	UNP P81274
U	6	MET	-	expression tag	UNP P81274
W	1	GLY	-	expression tag	UNP P81274
W	2	PRO	-	expression tag	UNP P81274
W	3	LEU	-	expression tag	UNP P81274
W	4	GLY	-	expression tag	UNP P81274
W	5	SER	-	expression tag	UNP P81274
W	6	MET	-	expression tag	UNP P81274

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• Molecule 2 is a protein called Nuclear mitotic apparatus protein 1.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
0	р	4 5	Total	С	Ν	Ο	S	0	0	0
	D	40	329	206	53	68	2	0	0	0
0	р	26	Total	С	Ν	Ο	S	0	0	0
	D		280	177	44	57	2	0	0	0
<u></u>	F	37	Total	С	Ν	Ο	S	0	0	0
	Ľ	57	288	182	46	58	2	0	0	0
0	и	26	Total	С	Ν	Ο	S	0	0	0
	11	50	284	180	44	58	2	0	0	0
<u></u>	т	40	Total	С	Ν	Ο	S	0	0	0
	1	40	307	192	49	64	2	0	0	U
0	т	4.4	Total	С	Ν	Ο	S	0	0	0
	44	341	210	58	71	2	0	0	0	
9	N	30	Total	С	Ν	Ο	S	0	0	0
	1	39	305	191	49	63	2	U	U	



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
	D	43	Total	С	Ν	Ο	S	0	0	0
	1	40	320	200	52	66	2	0	0	0
9	D	40	Total	С	Ν	Ο	S	0	0	0
	π	40	312	195	50	65	2	0	0	0
	т	Г 45	Total	С	Ν	Ο	S	0	0	0
	1		337	209	55	71	2	0	0	0
9	V	20	Total	С	Ν	Ο	S	0	0	0
			301	187	49	63	2	0	0	0
9	v	40	Total	С	Ν	Ο	S	0	0	0
	2 X	40	300	187	49	62	2	0	0	0

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There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	1858	GLY	-	expression tag	UNP Q14980
В	1859	PRO	-	expression tag	UNP Q14980
D	1858	GLY	-	expression tag	UNP Q14980
D	1859	PRO	-	expression tag	UNP Q14980
F	1858	GLY	-	expression tag	UNP Q14980
F	1859	PRO	-	expression tag	UNP Q14980
Н	1858	GLY	-	expression tag	UNP Q14980
Н	1859	PRO	-	expression tag	UNP Q14980
J	1858	GLY	-	expression tag	UNP Q14980
J	1859	PRO	-	expression tag	UNP Q14980
L	1858	GLY	-	expression tag	UNP Q14980
L	1859	PRO	-	expression tag	UNP Q14980
N	1858	GLY	-	expression tag	UNP Q14980
N	1859	PRO	-	expression tag	UNP Q14980
Р	1858	GLY	-	expression tag	UNP Q14980
Р	1859	PRO	-	expression tag	UNP Q14980
R	1858	GLY	-	expression tag	UNP Q14980
R	1859	PRO	-	expression tag	UNP Q14980
Т	1858	GLY	-	expression tag	UNP Q14980
Т	1859	PRO	-	expression tag	UNP Q14980
V	1858	GLY	-	expression tag	UNP Q14980
V	1859	PRO	-	expression tag	UNP Q14980
Х	1858	GLY	-	expression tag	UNP Q14980
Х	1859	PRO	-	expression tag	UNP Q14980



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. 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. 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: G-protein-signaling modulator 2

• Molecule 1: G-protein-signaling modulator 2

Chain G:



8%

G1 G1 1363 64 15 71 15 15 15 15 15 15 15 15 16 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15 15

• Molecule 1: G-protein-signaling modulator 2



• Molecule 1: G-protein-signaling modulator 2





 \bullet Molecule 1: G-protein-signaling modulator 2

Chain M:	90% ·	
CLY CLY 55 64 64 64 71 816 816 816 816 849 849 849 849 849 849 849 849 849 849	Y65 E76 E76 H80 K16 F111 T115 H121 H121 K131 V144 V144 V144 Q159 Q159 Q194 Q194	Y279 R316
N3 67 19333 19333 19333 19333 1933 1932 1932		

• Molecule 1: G-protein-signaling modulator 2



• Molecule 1: G-protein-signaling modulator 2

Chain Q:



11%

Q19.4 Q1 N32.3 N32.3 N32.3 S5 N32.3 N1 N33.3 N1 N36.0 N3 N36.0 N4 N36.0 N4 N4 N4 N14 N4 N4</td

 \bullet Molecule 1: G-protein-signaling modulator 2



• Molecule 1: G-protein-signaling modulator 2

Chain	U:											89%	Ď										10%	•		
GLY P2 S5	H8 V9	R12	M13 E14	L20	R34	F40	T53	157	L61	Y65	T87	K96	F111	1115	H121	N140	V144	E162 F163	V167 R168	V185	L188	<mark>գ194</mark>	1246	R316	W319	N323

1326 1328 1328 1328 1356 1356 1356 1356 1360 1363 1360 1363

 \bullet Molecule 1: G-protein-signaling modulator 2

Chain	W	/: '													8	7%)										12	%	·		
GLY P2 64	F7	H8 V9	R10	Y11 R12	A15			R26	K29	F40	4	L51 K52	T53	L54 S55	A56	157	q60 L61	Y65	D90	L92	F111	1115	H121	N140	V144	K150	C154	P157	V185	<mark>q194</mark>	620 <mark>9</mark>
N210 F211 R235	1264	R316	-	W319	N323	1328	H331	D332		S352	<mark>T356</mark>	N360		D363	M366	V367															

• Molecule 2: Nuclear mitotic apparatus protein 1

Chain B:	44%	18% •	37%
GLY PRO LEU GLY SER PRO D1864 V1865 C1866 G1866	L1870 L1871 L1871 L1871 L1875 T1876 T1879 T1879 ARG SER ARG SER ARG CLN ALA ARG	GLY VAL SER SER SER GLY ALA PRO P1897 F1902 F1902 Y1903	M1904 M1908 D1908 D1909 E1910 F1911 P1911 A1919 GLN ARG GLN ARG ARG

• Molecule 2: Nuclear mitotic apparatus protein 1

Chain D:	35%	13% •	49%









• Molecule 2: Nuclear mitotic apparatus protein 1



• Molecule 2: Nuclear mitotic apparatus protein 1







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	153.94Å 153.94Å 732.95Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{Bosolution} \left(\overset{\circ}{\mathbf{A}} \right)$	150.65 - 4.31	Depositor
Resolution (A)	183.24 - 4.31	EDS
% Data completeness	$99.8 \ (150.65 - 4.31)$	Depositor
(in resolution range)	$95.8\ (183.24-4.31)$	EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.54 (at 4.30 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
D D.	0.182 , 0.234	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.182 , 0.233	DCC
R_{free} test set	3061 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	212.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.24 , 177.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.45, \langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	37558	wwPDB-VP
Average B, all atoms $(Å^2)$	241.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.82% 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	Bond	lengths	B	ond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.31	0/2885	0.60	5/3892~(0.1%)
1	С	0.31	0/2898	0.57	4/3909~(0.1%)
1	Е	0.29	0/2847	0.52	0/3845
1	G	0.30	0/2865	0.48	0/3868
1	Ι	0.30	0/2872	0.50	0/3881
1	Κ	0.30	0/2880	0.49	0/3887
1	М	0.30	0/2872	0.54	1/3877~(0.0%)
1	0	0.29	0/2872	0.48	0/3876
1	Q	0.30	0/2883	0.51	0/3892
1	S	0.31	0/2851	0.58	2/3847~(0.1%)
1	U	0.32	0/2874	0.53	1/3879~(0.0%)
1	W	0.30	0/2868	0.51	0/3871
2	В	0.46	0/336	0.81	0/458
2	D	0.42	0/286	0.82	0/389
2	F	0.35	0/294	0.85	0/400
2	Η	0.44	0/290	0.83	0/395
2	J	0.47	0/313	0.88	2/426~(0.5%)
2	L	0.52	0/347	0.95	2/470~(0.4%)
2	Ν	0.37	0/311	0.78	0/423
2	Р	0.44	0/326	0.98	3/444~(0.7%)
2	R	0.47	0/318	1.00	2/433~(0.5%)
2	Т	0.40	0/343	0.88	0/467
2	V	0.32	0/306	0.82	0/415
2	X	0.42	0/306	0.82	1/417~(0.2%)
All	All	0.32	0/38243	0.57	$23/\overline{51661}~(0.0\%)$

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	А	0	2



Contr	Jonninueu jiom previous puye												
Mol	Chain	#Chirality outliers	#Planarity outliers										
1	С	0	1										
1	Е	0	1										
1	Ι	0	1										
1	0	0	1										
1	Q	0	2										
1	S	0	1										
1	U	0	1										
1	W	0	1										
2	D	0	1										
2	N	0	1										
2	R	0	1										
2	Т	0	2										
2	Х	0	1										
All	All	0	17										

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There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	S	154	CYS	C-N-CD	-11.86	94.50	120.60
1	С	154	CYS	C-N-CD	-9.94	98.73	120.60
1	М	3	LEU	CB-CG-CD1	8.03	124.65	111.00
1	С	3	LEU	CB-CG-CD2	7.82	124.30	111.00
1	А	236	ARG	NE-CZ-NH2	-7.62	116.49	120.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
1	А	13	MET	Peptide
1	А	153	GLY	Peptide
1	С	154	CYS	Peptide
2	D	1876	TYR	Peptide
1	Е	15	ALA	Peptide

Too-close contacts (i) 5.2

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	2834	0	2726	62	0
1	С	2847	0	2741	46	0
1	Е	2798	0	2657	29	0
1	G	2815	0	2678	21	0
1	Ι	2820	0	2686	32	0
1	K	2828	0	2704	28	0
1	М	2820	0	2688	44	0
1	0	2821	0	2696	31	0
1	Q	2831	0	2707	34	0
1	S	2800	0	2671	31	0
1	U	2823	0	2696	44	0
1	W	2817	0	2685	51	0
2	В	329	0	282	12	0
2	D	280	0	246	8	0
2	F	288	0	248	13	0
2	Н	284	0	255	10	0
2	J	307	0	271	22	0
2	L	341	0	300	16	0
2	Ν	305	0	269	6	0
2	Р	320	0	272	10	0
2	R	312	0	276	17	0
2	Т	337	0	290	14	0
2	V	301	0	260	15	0
2	Х	300	0	258	12	0
All	All	37558	0	35562	453	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 6.

The worst 5 of 453 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4:GLY:H	1:M:6:MET:CE	1.07	1.55
1:M:3:LEU:HD22	1:M:6:MET:CE	1.34	1.54
1:M:4:GLY:N	1:M:6:MET:CE	1.92	1.29
1:M:4:GLY:H	1:M:6:MET:HE1	1.05	1.17
1:M:3:LEU:CD2	1:M:6:MET:CE	2.26	1.14

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	А	363/367~(99%)	352~(97%)	6~(2%)	5(1%)	11 47
1	С	365/367~(100%)	352~(96%)	7(2%)	6(2%)	9 45
1	Ε	364/367~(99%)	349~(96%)	8 (2%)	7(2%)	8 41
1	G	365/367~(100%)	346~(95%)	17~(5%)	2~(0%)	29 68
1	Ι	365/367~(100%)	352~(96%)	13~(4%)	0	100 100
1	K	364/367~(99%)	351~(96%)	10~(3%)	3~(1%)	19 60
1	М	364/367~(99%)	351~(96%)	10 (3%)	3 (1%)	19 60
1	Ο	363/367~(99%)	350~(96%)	12 (3%)	1 (0%)	41 76
1	Q	365/367~(100%)	352 (96%)	10 (3%)	3 (1%)	19 60
1	S	358/367~(98%)	345~(96%)	9 (2%)	4 (1%)	14 52
1	U	364/367~(99%)	351 (96%)	12 (3%)	1 (0%)	41 76
1	W	364/367~(99%)	347 (95%)	14 (4%)	3 (1%)	19 60
2	В	41/71~(58%)	25~(61%)	11 (27%)	5(12%)	0 5
2	D	32/71~(45%)	24~(75%)	6 (19%)	2~(6%)	1 19
2	F	33/71~(46%)	22~(67%)	8 (24%)	3 (9%)	1 12
2	Н	32/71~(45%)	21~(66%)	4 (12%)	7(22%)	0 1
2	J	36/71~(51%)	25~(69%)	7 (19%)	4 (11%)	0 8
2	L	40/71~(56%)	26~(65%)	10 (25%)	4 (10%)	0 10
2	Ν	35/71~(49%)	19 (54%)	14 (40%)	2(6%)	1 20
2	Р	39/71~(55%)	24 (62%)	13 (33%)	2(5%)	2 22
2	R	36/71~(51%)	19(53%)	12 (33%)	5(14%)	0 4
2	Т	41/71~(58%)	27~(66%)	11 (27%)	3 (7%)	1 16
2	V	35/71~(49%)	22~(63%)	10 (29%)	3 (9%)	1 13
2	Х	36/71~(51%)	21 (58%)	9(25%)	6 (17%)	0 3
All	All	4800/5256~(91%)	4473 (93%)	243 (5%)	84 (2%)	8 42



5 of 84 Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	\mathbf{Type}
1	А	14	GLU
1	А	15	ALA
1	С	14	GLU
1	С	155	PRO
1	Е	8	HIS

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	А	285/291~(98%)	276 (97%)	9(3%)	39	62
1	С	287/291~(99%)	280 (98%)	7 (2%)	49	69
1	Е	275/291~(94%)	272 (99%)	3 (1%)	73	85
1	G	278/291~(96%)	271 (98%)	7 (2%)	47	68
1	Ι	279/291~(96%)	275~(99%)	4 (1%)	67	81
1	К	283/291~(97%)	278 (98%)	5 (2%)	59	77
1	М	279/291~(96%)	276 (99%)	3 (1%)	73	85
1	Ο	282/291~(97%)	274 (97%)	8 (3%)	43	65
1	Q	282/291~(97%)	276 (98%)	6 (2%)	53	72
1	S	279/291~(96%)	276 (99%)	3 (1%)	73	85
1	U	281/291~(97%)	275~(98%)	6 (2%)	53	72
1	W	279/291~(96%)	273 (98%)	6 (2%)	52	71
2	В	32/58~(55%)	31 (97%)	1 (3%)	40	63
2	D	29/58~(50%)	27 (93%)	2 (7%)	15	42
2	F	29/58~(50%)	26~(90%)	3~(10%)	7	27
2	Н	30/58~(52%)	29 (97%)	1 (3%)	38	62
2	J	32/58~(55%)	31 (97%)	1 (3%)	40	63
2	L	$\overline{35/58}~(60\%)$	33 (94%)	2 (6%)	20	48
2	N	32/58~(55%)	32 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Р	31/58~(53%)	29~(94%)	2~(6%)	17 44
2	R	33/58~(57%)	28~(85%)	5(15%)	3 16
2	Т	34/58~(59%)	32~(94%)	2~(6%)	19 47
2	V	31/58~(53%)	31~(100%)	0	100 100
2	Х	30/58~(52%)	26~(87%)	4(13%)	4 20
All	All	3747/4188 (90%)	3657~(98%)	90(2%)	49 69

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5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	К	121	HIS
1	0	131	LYS
1	W	121	HIS
1	Κ	163	PHE
1	М	51	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	Ι	360	ASN
1	М	203	ASN
1	W	8	HIS
1	Ι	243	ASN
1	U	8	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 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

