

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 21, 2023 – 12:17 AM EDT

PDB ID	:	5IG3
Title	:	Crystal structure of the human CaMKII-alpha hub
Authors	:	McSpadden, E.; Cao, Y.M.; Bhattacharyya, M.; Gee, C.L.; Barros, T.;
		Kuriyan, J.
Deposited on	:	2016-02-26
Resolution	:	2.75  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	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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 <sub>free</sub>	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	153	5% 82%		11% • 6%
		100	3%		
1	В	153	72%	11%	17%
1	$\mathbf{C}$	153	70%	16%	• 14%
1	D	153	8%	10% •	17%
1	Е	153	67%	14%	18%



Mol	Chain	Length	Quality of chain					
			9%					
1	F	153	69%	12%	20%			



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6312 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 Calcium/calmodulin-dependent protein kinase type II subunit alpha.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	1.4.4	Total	С	Ν	0	S	0	0 0	0
	A	144	1168	738	212	212	6	0	0	0
1	р	197	Total	С	Ν	0	S	0	0	0
	D	127	1031	655	182	188	6	0	0	0
1	C	120	Total	С	Ν	0	S	0	0	0
		132	1066	673	191	196	6	0	0	0
1	П	197	Total	С	Ν	0	S	0	0	0
	D	121	1024	647	182	189	6			0
1	F	195	Total	С	Ν	0	S	0	0	0
		120	1012	641	180	185	6	0	0	0
1	F	193	Total	С	Ν	0	S	0	0	0
	L,	120	996	630	177	183	6			U

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference			
А	323	GLY	-	expression tag	UNP Q9UQM7			
А	324	SER	-	expression tag	UNP Q9UQM7			
А	325	SER	-	expression tag	UNP Q9UQM7			
А	326	HIS	-	expression tag	UNP Q9UQM7			
А	327	HIS	-	expression tag	UNP Q9UQM7			
А	328	HIS	-	expression tag	UNP Q9UQM7			
А	329	HIS	-	expression tag	UNP Q9UQM7			
А	330	HIS	-	expression tag	UNP Q9UQM7			
А	331	HIS	-	expression tag	UNP Q9UQM7			
А	332	SER	-	expression tag	UNP Q9UQM7			
А	333	SER	-	expression tag	UNP Q9UQM7			
А	334	GLY	-	expression tag	UNP Q9UQM7			
А	335	LEU	-	expression tag	UNP Q9UQM7			
А	336	GLU	-	expression tag	UNP Q9UQM7			
А	337	VAL	-	expression tag	UNP Q9UQM7			
А	338	LEU	-	expression tag	UNP Q9UQM7			
	Continued on next page							

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Chain	Residue	Modelled	Actual	Comment	Reference
А	339	PHE	-	expression tag	UNP Q9UQM7
A	340	GLN	-	expression tag	UNP Q9UQM7
А	341	GLY	-	expression tag	UNP Q9UQM7
А	342	PRO	-	expression tag	UNP Q9UQM7
А	343	HIS	-	expression tag	UNP Q9UQM7
А	344	MET	-	expression tag	UNP Q9UQM7
В	323	GLY	-	expression tag	UNP Q9UQM7
В	324	SER	-	expression tag	UNP Q9UQM7
В	325	SER	-	expression tag	UNP Q9UQM7
В	326	HIS	-	expression tag	UNP Q9UQM7
В	327	HIS	-	expression tag	UNP Q9UQM7
В	328	HIS	-	expression tag	UNP Q9UQM7
В	329	HIS	-	expression tag	UNP Q9UQM7
В	330	HIS	-	expression tag	UNP Q9UQM7
В	331	HIS	-	expression tag	UNP Q9UQM7
В	332	SER	-	expression tag	UNP Q9UQM7
В	333	SER	-	expression tag	UNP Q9UQM7
В	334	GLY	-	expression tag	UNP Q9UQM7
В	335	LEU	-	expression tag	UNP Q9UQM7
В	336	GLU	-	expression tag	UNP Q9UQM7
В	337	VAL	-	expression tag	UNP Q9UQM7
В	338	LEU	-	expression tag	UNP Q9UQM7
В	339	PHE	-	expression tag	UNP Q9UQM7
В	340	GLN	-	expression tag	UNP Q9UQM7
В	341	GLY	-	expression tag	UNP Q9UQM7
В	342	PRO	-	expression tag	UNP Q9UQM7
В	343	HIS	-	expression tag	UNP Q9UQM7
В	344	MET	-	expression tag	UNP Q9UQM7
С	323	GLY	-	expression tag	UNP Q9UQM7
С	324	SER	-	expression tag	UNP Q9UQM7
С	325	SER	-	expression tag	UNP Q9UQM7
С	326	HIS	-	expression tag	UNP Q9UQM7
С	327	HIS	-	expression tag	UNP Q9UQM7
С	328	HIS	-	expression tag	UNP Q9UQM7
С	329	HIS	-	expression tag	UNP Q9UQM7
C	330	HIS	-	expression tag	UNP $Q9UQM7$
C	331	HIS	-	expression tag	UNP Q9UQM7
C	332	SER	-	expression tag	UNP Q9UQM7
C	333	SER	-	expression tag	UNP Q9UQM7
С	334	GLY	-	expression tag	UNP Q9UQM7
C	335	LEU	-	expression tag	UNP Q9UQM7
С	336	GLU	-	expression tag	UNP Q9UQM7



Chain	Residue	Modelled	Actual Comment		Reference
С	337	VAL	-	expression tag	UNP O9UOM7
	338	LEU	_	expression tag	UNP O9UOM7
	339	PHE	_	expression tag	UNP O9UOM7
	340	GLN		expression tag	UNP O9UOM7
	341	GLN	_	expression tag	UNP Q9UQM7
C	342	PRO	_	expression tag	UNP Q9UQM7
C	343	HIS	_	expression tag	UNP O9UOM7
	344	MET	_	expression tag	UNP O9UOM7
D	323	GLY	_	expression tag	UNP Q9UQM7
D	324	SEB	_	expression tag	UNP Q9UQM7
D	325	SER	_	expression tag	UNP Q9UQM7
D	326	HIS	_	expression tag	UNP Q9UQM7
D	327	HIS	_	expression tag	UNP Q9UQM7
D	328	HIS		expression tag	UNP O9UOM7
D	329	HIS	_	expression tag	UNP Q9UQM7
D	330	HIS	_	expression tag	UNP Q9UQM7
D	331	HIS	_	expression tag	UNP Q9UQM7
D	332	SEB	_	expression tag	UNP Q9UQM7
D	333	SER	_	expression tag	UNP Q9UQM7
D	334	GLY	_	expression tag	UNP Q9UQM7
D	335	LEU	_	expression tag	UNP Q9UQM7
D	336	GLU	_	expression tag	UNP Q9UQM7
D	337	VAL	_	expression tag	UNP Q9UQM7
D	338	LEU	_	expression tag	UNP Q9UQM7
D	339	PHE	_	expression tag	UNP Q9UQM7
D	340	GLN	_	expression tag	UNP Q9UQM7
D	341	GLY	_	expression tag	UNP Q9UQM7
D	342	PRO	_	expression tag	UNP Q9UQM7
D	343	HIS	_	expression tag	UNP Q9UQM7
D	344	MET	_	expression tag	UNP Q9UQM7
E	323	GLY	_	expression tag	UNP Q9UQM7
E	324	SER	_	expression tag	UNP Q9UQM7
E	325	SER	_	expression tag	UNP Q9UQM7
E	326	HIS	-	expression tag	UNP Q9UQM7
E	327	HIS	_	expression tag	UNP Q9UQM7
Е	328	HIS	-	expression tag	UNP Q9UQM7
Е	329	HIS	-	expression tag	UNP Q9UQM7
Е	330	HIS	-	expression tag	UNP Q9UQM7
Е	331	HIS	-	expression tag	UNP Q9UQM7
Е	332	SER	-	expression tag	UNP Q9UQM7
Е	333	SER	-	expression tag	UNP Q9UQM7
Е	334	GLY	-	expression tag	UNP Q9UQM7



Chain	Residue	Modelled	Actual	Comment	Reference
Е	335	LEU	-	expression tag	UNP Q9UQM7
Е	336	GLU	-	expression tag	UNP Q9UQM7
Е	337	VAL	-	expression tag	UNP Q9UQM7
Е	338	LEU	-	expression tag	UNP Q9UQM7
Е	339	PHE	-	expression tag	UNP Q9UQM7
Е	340	GLN	-	expression tag	UNP Q9UQM7
Е	341	GLY	-	expression tag	UNP Q9UQM7
Е	342	PRO	-	expression tag	UNP Q9UQM7
Е	343	HIS	-	expression tag	UNP Q9UQM7
Е	344	MET	-	expression tag	UNP Q9UQM7
F	323	GLY	-	expression tag	UNP Q9UQM7
F	324	SER	-	expression tag	UNP Q9UQM7
F	325	SER	-	expression tag	UNP Q9UQM7
F	326	HIS	-	expression tag	UNP Q9UQM7
F	327	HIS	-	expression tag	UNP Q9UQM7
F	328	HIS	-	expression tag	UNP Q9UQM7
F	329	HIS	-	expression tag	UNP Q9UQM7
F	330	HIS	-	expression tag	UNP Q9UQM7
F	331	HIS	-	expression tag	UNP Q9UQM7
F	332	SER	-	expression tag	UNP Q9UQM7
F	333	SER	-	expression tag	UNP Q9UQM7
F	334	GLY	-	expression tag	UNP Q9UQM7
F	335	LEU	-	expression tag	UNP Q9UQM7
F	336	GLU	-	expression tag	UNP Q9UQM7
F	337	VAL	-	expression tag	UNP Q9UQM7
F	338	LEU	-	expression tag	UNP Q9UQM7
F	339	PHE	-	expression tag	UNP Q9UQM7
F	340	GLN	-	expression tag	UNP Q9UQM7
F	341	GLY	-	expression tag	UNP Q9UQM7
F	342	PRO	-	expression tag	UNP Q9UQM7
F	343	HIS	-	expression tag	UNP Q9UQM7
F	344	MET	-	expression tag	UNP Q9UQM7

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	3	Total O 3 3	0	0
2	В	6	Total O 6 6	0	0
2	С	2	Total O 2 2	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total O 2 2	0	0
2	Е	1	Total O 1 1	0	0
2	F	1	Total O 1 1	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: Calcium/calmodulin-dependent protein kinase type II subunit alpha







 $\bullet$  Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha



• Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha $_{9\%}$ 

С	ha	ai	n	F	:														6	99	%												•	1	.29	%					20	%							
GLY	SER	NEK	SIH	SIH	SIH	STH	SER	SER	GLY	LEU	GLU	VAL	LEU	РПЕ	GLN GLN	PRO	HIS	M344	V345	R346	K347	Q348	T351	L357	I358	C373	D374	P375	G376	M377	T378	L392	D393	F394		1330 F399	E400	N401	LEU	SER	ARG	ASN	SER	K408	T414	L415	N416	P417	H418
I419		D424	I 429		I434	D430	A440	G441	G442	I443	P444	11 40 4	K461	101	1464 V465	H466	F467	╞	A472	PRO	SER	VAL																											



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	89.89Å 89.89Å 226.58Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	48.63 - 2.75	Depositor
Resolution (A)	48.63 - 2.75	EDS
% Data completeness	99.9(48.63-2.75)	Depositor
(in resolution range)	99.9(48.63-2.75)	EDS
$R_{merge}$	0.08	Depositor
R <sub>sym</sub>	0.08	Depositor
$< I/\sigma(I) > 1$	1.77 (at 2.77 Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
P. P.	0.220 , $0.268$	Depositor
II, II free	0.228 , $0.275$	DCC
$R_{free}$ test set	1184 reflections $(4.74\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	80.4	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , $62.5$	EDS
L-test for $twinning^2$	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6312	wwPDB-VP
Average B, all atoms $(Å^2)$	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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	Bond angles				
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5			
1	А	0.25	0/1201	0.41	0/1625			
1	В	0.25	0/1058	0.41	0/1431			
1	С	0.25	0/1093	0.42	0/1475			
1	D	0.24	0/1049	0.41	0/1416			
1	Е	0.26	0/1038	0.42	0/1403			
1	F	0.24	0/1020	0.41	0/1377			
All	All	0.25	0/6459	0.41	0/8727			

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1168	0	1117	14	0
1	В	1031	0	994	12	0
1	С	1066	0	1018	14	0
1	D	1024	0	983	9	0
1	Ε	1012	0	974	15	0
1	F	996	0	961	11	0
2	А	3	0	0	0	0
2	В	6	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Е	1	0	0	0	0
2	F	1	0	0	0	0
All	All	6312	0	6047	68	0

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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.

All (68) 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:C:374:ASP:OD2	1:C:458:ARG:NH1	1.90	1.03
1:B:374:ASP:OD1	1:B:458:ARG:NH1	1.93	1.01
1:A:331:HIS:HA	1:A:412:THR:O	1.73	0.88
1:B:393:ASP:OD2	1:E:411:HIS:NE2	2.20	0.74
1:C:346:ARG:NH1	1:C:424:ASP:O	2.24	0.70
1:F:374:ASP:OD2	1:F:376:GLY:N	2.23	0.69
1:A:346:ARG:NH1	1:A:424:ASP:O	2.25	0.69
1:F:439:ASP:O	1:F:441:GLY:N	2.31	0.64
1:B:378:THR:O	1:B:466:HIS:HA	1.99	0.63
1:A:408:LYS:NZ	1:A:439:ASP:O	2.33	0.62
1:B:402:LEU:HD22	1:E:444:PRO:HG3	1.82	0.61
1:F:346:ARG:NH2	1:F:424:ASP:OD1	2.34	0.61
1:F:378:THR:O	1:F:466:HIS:HA	2.00	0.60
1:E:377:MET:O	1:E:391:GLY:N	2.33	0.58
1:C:346:ARG:NH1	1:C:424:ASP:HA	2.18	0.58
1:E:365:ASP:OD2	1:E:368:SER:OG	2.15	0.58
1:A:335:LEU:HD22	1:A:351:ILE:HD13	1.86	0.57
1:A:338:LEU:HD23	1:A:351:ILE:HD11	1.86	0.57
1:D:411:HIS:NE2	1:F:393:ASP:OD2	2.37	0.56
1:E:383:GLU:OE1	1:E:469:ARG:NH2	2.38	0.56
1:C:344:MET:SD	1:C:344:MET:N	2.79	0.55
1:B:373:CYS:HB2	1:B:392:LEU:HD21	1.88	0.55
1:C:393:ASP:OD1	1:C:396:ARG:NH1	2.41	0.55
1:A:346:ARG:NH1	1:A:424:ASP:HA	2.23	0.54
1:B:346:ARG:HD2	1:B:421:LEU:HD13	1.89	0.54
1:C:333:SER:HA	1:C:414:ILE:HB	1.89	0.54
1:B:401:ASN:HB3	1:E:438:LEU:HD11	1.88	0.54
1:C:378:THR:O	1:C:466:HIS:HA	2.08	0.54
1:C:442:GLY:HA2	1:C:443:ILE:HB	1.91	0.52
1:C:382:PRO:HG2	1:C:472:ALA:H	1.74	0.52
1:D:373:CYS:HB2	1:D:392:LEU:HD21	1.92	0.51



	loub page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:346:ARG:NH2	1:A:457:ARG:HH22	2.09	0.50
1:F:400:GLU:N	1:F:400:GLU:OE1	2.44	0.50
1:A:402:LEU:HD22	1:F:444:PRO:HG3	1.92	0.50
1:A:449:SER:HA	1:A:470:SER:O	2.11	0.49
1:D:347:LYS:HB3	1:D:419:ILE:HD12	1.95	0.49
1:B:347:LYS:HB3	1:B:419:ILE:HD12	1.95	0.49
1:E:373:CYS:HB2	1:E:392:LEU:HD21	1.95	0.48
1:D:361:ILE:HA	1:D:399:PHE:HE1	1.78	0.48
1:E:346:ARG:HE	1:E:457:ARG:HH22	1.62	0.47
1:F:439:ASP:O	1:F:442:GLY:N	2.39	0.47
1:D:379:ALA:HB3	1:D:389:VAL:HG23	1.97	0.47
1:F:373:CYS:HB2	1:F:392:LEU:HD21	1.96	0.47
1:E:451:GLU:HG2	1:E:469:ARG:HG3	1.97	0.47
1:C:373:CYS:HB2	1:C:392:LEU:HD21	1.97	0.46
1:B:370:THR:HG22	1:B:392:LEU:HD22	1.98	0.45
1:D:377:MET:HA	1:D:465:VAL:O	2.17	0.45
1:D:378:THR:O	1:D:466:HIS:HA	2.16	0.44
1:C:456:HIS:CD2	1:C:458:ARG:HE	2.36	0.44
1:C:438:LEU:HD23	1:C:444:PRO:HA	1.99	0.43
1:E:346:ARG:O	1:E:350:ILE:HG12	2.18	0.43
1:E:467:PHE:CZ	1:E:469:ARG:HB2	2.54	0.43
1:B:393:ASP:OD2	1:E:411:HIS:CE1	2.72	0.43
1:A:346:ARG:HH12	1:A:424:ASP:HA	1.84	0.43
1:B:381:GLU:OE2	1:B:469:ARG:NH2	2.52	0.43
1:A:338:LEU:HD21	1:A:419:ILE:HG13	2.02	0.42
1:D:415:LEU:HB2	1:D:432:ILE:HB	2.02	0.42
1:A:333:SER:HA	1:A:414:ILE:O	2.20	0.42
1:C:453:ARG:HD3	1:C:467:PHE:HB2	2.02	0.41
1:D:467:PHE:CE2	1:D:469:ARG:NH1	2.88	0.41
1:C:449:SER:HB3	1:C:472:ALA:HB2	2.02	0.41
1:A:358:ILE:HD12	1:A:414:ILE:HD11	2.03	0.41
1:E:343:HIS:ND1	1:E:345:VAL:HG22	2.35	0.41
1:F:414:ILE:HG22	1:F:417:PRO:HG3	2.03	0.41
1:E:470:SER:HA	1:E:471:GLY:HA2	1.66	0.41
1:B:383:GLU:O	1:E:446:THR:HG21	2.21	0.40
1:A:338:LEU:HD22	1:A:417:PRO:HB2	2.04	0.40
1:F:416:ASN:N	1:F:417:PRO:HD3	2.36	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	Perce	ntiles
1	А	142/153~(93%)	136~(96%)	6 (4%)	0	100	100
1	В	123/153~(80%)	120 (98%)	3~(2%)	0	100	100
1	С	126/153~(82%)	120 (95%)	6~(5%)	0	100	100
1	D	121/153~(79%)	118 (98%)	3(2%)	0	100	100
1	Ε	121/153~(79%)	118 (98%)	3~(2%)	0	100	100
1	F	119/153~(78%)	118 (99%)	0	1 (1%)	19	34
All	All	752/918~(82%)	730 (97%)	21 (3%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	440	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	ntiles
1	А	125/133~(94%)	124~(99%)	1 (1%)	81	88
1	В	110/133~(83%)	110 (100%)	0	100	100
1	С	114/133~(86%)	111~(97%)	3~(3%)	46	66
1	D	110/133~(83%)	109~(99%)	1 (1%)	78	87
1	Е	108/133~(81%)	107~(99%)	1 (1%)	78	87
1	F	106/133~(80%)	106 (100%)	0	100	100



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
All	All	673/798~(84%)	667~(99%)	6 (1%)	78	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	457	ARG
1	С	343	HIS
1	С	344	MET
1	С	380	PHE
1	D	467	PHE
1	Е	424	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	401	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 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	$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9
1	А	144/153~(94%)	0.36	7 (4%) 29 36	52, 78, 140, 186	0
1	В	127/153~(83%)	0.39	5 (3%) 39 46	52, 76, 134, 150	0
1	С	132/153~(86%)	0.63	11 (8%) 11 13	50, 91, 144, 173	0
1	D	127/153~(83%)	0.58	13 (10%) 6 7	53, 94, 136, 164	0
1	Ε	125/153~(81%)	0.79	18 (14%) 2 2	57, 101, 164, 214	0
1	F	123/153~(80%)	0.82	14 (11%) 5 5	58, 100, 155, 193	0
All	All	778/918~(84%)	0.59	68 (8%) 10 12	50, 91, 149, 214	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	390	GLU	7.6
1	Е	369	TYR	6.4
1	F	394	PHE	4.3
1	А	335	LEU	4.3
1	Е	379	ALA	4.2
1	А	472	ALA	4.1
1	Е	357	LEU	3.9
1	С	427	ALA	3.9
1	В	402	LEU	3.9
1	F	344	MET	3.8
1	С	390	GLU	3.8
1	С	472	ALA	3.7
1	Е	392	LEU	3.7
1	С	359	GLU	3.7
1	В	403	TRP	3.6
1	D	396	ARG	3.6
1	С	369	TYR	3.6
1	А	338	LEU	3.5
1	С	421	LEU	3.5



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IVIOI	Unam	nes	туре	nonz
1	D	366	PHE	3.4
1	D	472	ALA	3.4
1	F	348	GLN	3.4
1	С	422	MET	3.4
1	С	402	LEU	3.3
1	F	467	PHE	3.3
1	Е	467	PHE	3.1
1	Е	410	VAL	3.1
1	С	403	TRP	3.1
1	F	419	ILE	2.9
1	F	357	LEU	2.9
1	F	429	ILE	2.8
1	А	337	VAL	2.8
1	С	443	ILE	2.7
1	Е	462	TRP	2.7
1	Е	434	ILE	2.7
1	F	358	ILE	2.7
1	F	434	ILE	2.7
1	С	440	ALA	2.6
1	D	392	LEU	2.6
1	D	361	ILE	2.6
1	А	421	LEU	2.5
1	F	464	ILE	2.4
1	В	398	TYR	2.4
1	А	458	ARG	2.4
1	Е	399	PHE	2.4
1	D	399	PHE	2.3
1	А	405	ARG	2.3
1	Е	464	ILE	2.3
1	Е	391	GLY	2.3
1	Е	421	LEU	2.3
1	F	351	ILE	2.3
1	D	438	LEU	2.3
1	F	398	TYR	2.2
1	Е	455	TRP	2.2
1	Е	466	HIS	2.2
1	F	414	ILE	2.2
1	D	344	MET	2.2
1	D	369	TYR	2.2
1	В	366	PHE	2.2
1	Е	378	THR	2.2
1	D	389	VAL	2.1



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Mol	Chain	Res	Type	RSRZ
1	Ε	472	ALA	2.1
1	D	434	ILE	2.0
1	Е	359	GLU	2.0
1	D	397	PHE	2.0
1	D	401	ASN	2.0
1	F	461	LYS	2.0
1	В	407	SER	2.0

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

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

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 6.4 Ligands (i)

There are no ligands in this entry.

#### 6.5 Other polymers (i)

There are no such residues in this entry.

