

wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2023 – 07:19 pm BST

PDB ID	:	8ASC
Title	:	$\mathrm{Ku70}/\mathrm{80}$ binds to the Ku-binding motif of PAXX
Authors	:	Seif El Dahan, M.; Ropars, V.; Charbonnier, J.B.
Deposited on	:	2022-08-19
Resolution	:	2.95 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 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
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
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)	:	2.33

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 2.95 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	3104 (3.00-2.92)		
Clashscore	141614	3462 (3.00-2.92)		
Ramachandran outliers	138981	3340 (3.00-2.92)		
Sidechain outliers	138945	3343 (3.00-2.92)		
RSRZ outliers	127900	2986 (3.00-2.92)		

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 cha	in	
1	А	544	64%	27%	• 8%
1	Е	544	% 60%	30%	• 9%
1	K	544	61%	30%	• 8%
1	О	544	61%	30%	• 8%
2	В	572	<u>5%</u> 65%	27%	• 7%



Mol	Chain	Length	Quality of chain							
2	F	572	^{2%} 67%		26%	• 6%				
2	L	572	66%	26%	• 7%					
2	Р	572	63%		29%	• 7%				
3	С	30	33%	30%	37%					
3	G	30	47%	20%	33%					
3	М	30	33%	30%	37%					
3	Q	30	47% 20		33%					
4	D	15	40%		53%	7%				
4	Н	15	60%		33%	7%				
4	Ν	15	47%		47%	7%				
4	R	15	60%		40%					
5	J	28	64%		36%					
5	Т	28	4%	%	29%					



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 36383 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	Atoms					ZeroOcc	AltConf	Trace
1	Δ	400	Total	С	Ν	0	\mathbf{S}	0	0	0
	I A	499	4027	2576	681	752	18	0	0	0
1	F	407	Total	С	C N O S	0	0	0		
	Ľ	497	4015	2569	683	745	18	0	0	U
1	K	502	Total	С	Ν	0	S	0	0	0
		302	4052	2590	686	758	18	0		0
1	1 0	408	Total	С	Ν	0	S	0	0	0
	498	4023	2575	684	746	18	0	0	U	

• Molecule 1 is a protein called X-ray repair cross-complementing protein 6.

• Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	9 D	521	Total	С	Ν	Ο	S	0	0 0	0
	D		4248	2720	715	790	23	0		0
0	Б	537	Total	С	Ν	0	S	0	0	0
	Г		4282	2736	720	803	23			0
0	т	520	Total	С	Ν	0	S	0	0	0
	550	4238	2712	715	788	23	0	0		
0	9 D	521	Total	С	Ν	0	S	0	0	0
2 P	551	4242	2714	713	792	23	U	0	0	

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-16	MET	-	initiating methionine	UNP P13010
В	-15	HIS	-	expression tag	UNP P13010
В	-14	HIS	-	expression tag	UNP P13010
В	-13	HIS	-	expression tag	UNP P13010
В	-12	HIS	-	expression tag	UNP P13010
В	-11	HIS	-	expression tag	UNP P13010
В	-10	HIS	-	expression tag	UNP P13010
В	-9	HIS	-	expression tag	UNP P13010



Chain В

В

В

В

В

В

В

В

В

В

F

F

F

F

F

F

F

F

F

F

F

F

F

F

F

F

F

F

L

L

L

L

L

L

L

 \mathbf{L}

L

L

L

L

L

L

Residue	Modelled	Actual	Comment	Reference
-8	HIS	-	expression tag	UNP P13010
-7	HIS	-	expression tag	UNP P13010
-6	HIS	-	expression tag	UNP P13010
-5	GLU	-	expression tag	UNP P13010
-4	ASN	-	expression tag	UNP P13010
-3	LEU	-	expression tag	UNP P13010
-2	TYR	-	expression tag	UNP P13010
-1	PHE	-	expression tag	UNP P13010
0	GLN	-	expression tag	UNP P13010
1	GLY	-	expression tag	UNP P13010
-16	MET	-	initiating methionine	UNP P13010
-15	HIS	-	expression tag	UNP P13010
-14	HIS	-	expression tag	UNP P13010
-13	HIS	-	expression tag	UNP P13010
-12	HIS	-	expression tag	UNP P13010
-11	HIS	-	expression tag	UNP P13010
-10	HIS	-	expression tag	UNP P13010
-9	HIS	-	expression tag	UNP P13010
-8	HIS	-	expression tag	UNP P13010
-7	HIS	-	expression tag	UNP P13010
-6	HIS	-	expression tag	UNP P13010
-5	GLU	-	expression tag	UNP P13010
-4	ASN	-	expression tag	UNP P13010
-3	LEU	-	expression tag	UNP P13010
-2	TYR	-	expression tag	UNP P13010
-1	PHE	-	expression tag	UNP P13010
0	GLN	-	expression tag	UNP P13010
1	GLY	-	expression tag	UNP P13010
-16	MET	-	initiating methionine	UNP P13010
-15	HIS	-	expression tag	UNP P13010

expression tag

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-14

-13

-12

-11

-10

-9

-8

-7

-6

-5

-4

-3

HIS

HIS

HIS

HIS

HIS

HIS

HIS

HIS

HIS

GLU

ASN

LEU

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UNP P13010



Chain	Residue	Modelled	Actual Comment		Reference
L	-2	TYR	-	expression tag	UNP P13010
L	-1	PHE	-	expression tag	UNP P13010
L	0	GLN	-	expression tag	UNP P13010
L	1	GLY	-	expression tag	UNP P13010
Р	-16	MET	-	initiating methionine	UNP P13010
Р	-15	HIS	-	expression tag	UNP P13010
Р	-14	HIS	-	expression tag	UNP P13010
Р	-13	HIS	-	expression tag	UNP P13010
Р	-12	HIS	-	expression tag	UNP P13010
Р	-11	HIS	-	expression tag	UNP P13010
Р	-10	HIS	-	expression tag	UNP P13010
Р	-9	HIS	-	expression tag	UNP P13010
Р	-8	HIS	-	expression tag	UNP P13010
Р	-7	HIS	-	expression tag	UNP P13010
Р	-6	HIS	-	expression tag	UNP P13010
Р	-5	GLU	-	expression tag	UNP P13010
Р	-4	ASN	-	expression tag	UNP P13010
Р	-3	LEU	-	expression tag	UNP P13010
Р	-2	TYR	-	expression tag	UNP P13010
Р	-1	PHE	-	expression tag	UNP P13010
Р	0	GLN	-	expression tag	UNP P13010
Р	1	GLY	-	expression tag	UNP P13010

• Molecule 3 is a DNA chain called DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*G P*GP*CP*CP*CP*GP*AP*TP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	С	Ν	0	Р	0	0	0
0	C	19	393	185	76	113	19	0	0	0
2	3 G	20	Total	С	Ν	0	Р	0	0	0
0		20	412	194	79	119	20			0
2	М	<u>الم</u>	Total	С	Ν	0	Р	0	0	0
3 1/1	19	393	185	76	113	19	0	0	0	
3 Q	20	Total	С	Ν	0	Р	0	0	0	
		412	194	79	119	20	0		U	

• Molecule 4 is a DNA chain called DNA (5'-D(P*GP*GP*CP*CP*CP*CP*CP*CP*GP*AP *TP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	14	Total 285	C 134	N 52	O 85	Р 14	0	0	0



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	п	15	Total	С	Ν	0	Р	0	0	0
4 П	11	10	304	143	55	91	15	0	0	0
4	4 N	14	Total	С	Ν	0	Р	0	0	0
4			285	134	52	85	14			
A D		15	Total	С	Ν	0	Р	0	0	0
4	n	K 15	304	143	55	91	15	0	U	U

• Molecule 5 is a protein called Protein PAXX.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
5	5 J	28	Total	С	Ν	0	S	0	0	0
5			214	132	41	40	1			
5	5 T	T 28	Total	С	Ν	0	S	0	0	0
Э			214	132	41	40	1	0	0	0

• Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	K	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	Р	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	Total O 1 1	0	0
7	Е	6	Total O 6 6	0	0
7	F	3	Total O 3 3	0	0
7	K	4	Total O 4 4	0	0
7	L	2	Total O 2 2	0	0
7	Ν	1	Total O 1 1	0	0
7	О	3	Total O 3 3	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: X-ray repair cross-complementing protein 6









LE518 V414 A280 LE51 P415 P283 V522 E418 P283 V523 E524 P283 V529 P436 F281 V531 E534 P283 V532 E418 P283 V533 F436 F283 V539 P430 F310 V531 F436 F336 V533 P447 T334 F10 P443 T332 F10 P446 T334 F10 P446 T334 F446 F446 T334 F446 F446 T334 F446 F446 T336 F446 F446 T344 <t

• Molecule 2: X-ray repair cross-complementing protein 5 5% Chain B: 65% 27% • 7% GLY ARG 321 1393 1394 ASP GLU A542 K543 K544 LYS ASP GLN VAL THR ALA GLN GLN CLU TLE PHE CLN (532 (533 L536 F537 P538 L539 L539 **4527** 1528 P529 L530 • Molecule 2: X-ray repair cross-complementing protein 5 Chain F: 67% 26% • 6%

 3175
 T78
 T78
 MET

 ARG
 AS
 HS
 HS

 ARG
 B99
 HS
 HS

 ARG
 B99
 HS
 HS

 ARG
 B99
 HS
 HS

 F133
 B93
 HS
 HS

 F137
 B93
 HS
 HS

 F137
 B93
 HS
 HS

 F137
 B93
 HS
 HS

 F137
 B93
 HS
 HS

 F237
 B100
 G101
 HS

 K203
 B100
 G101
 HS

 K238
 B116
 G10
 MI

 K238
 B113
 MI
 M

 K238
 B113
 MI
 M

 K244
 MI
 MI
 M

 K238
 MI
 MI
 M

 K242
 MI
 M
 M

 K243
 MI
 M
 M

 K244
 MI
 M
 M







D386 K246 V390 L266 V390 L266 V393 L266 V3394 L267 V3395 L267 V3395 L267 V300 L268 V301 L267 V302 L269 V407 L284 K399 K274 K407 L297 K417 L297 K418 L311 K465 V321 K466 V321 K466 V332 K466 V331



• Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*A P*TP*AP*T)-3')

Chain C:	33%	30%	37%
C C C C C C C C	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		

• Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*A P*TP*AP*T)-3')

Chain G:	47%	20%	33%
C0 14 87 69 69 610 C11 C12	11 11 12 13 14 14 15 15 15 15 15 15 15 15 15 15 15 15 15		

• Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*A P*TP*AP*T)-3')

Chain M:	33%	30%	37%
60 61 61 61 61 61 61 61 61 61 61 61 61 61	Git 4 11 11 11 11 11 11 11 11 11 11 11 11 11	DD	

• Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*AP*TP*AP*T)-3')

Chain Q:	47%	20%	33%	
00 14 010 011 011 012	11 11 11 11 11 11 11 11 11 11 11 11 11			
• Molecule)	4: DNA (5'-D(P*GP*GP	*GP*CP*CP*C	P*TP*CP*GP*A	P*TP*CP*CP*G)-3'

Chain D:	40%	53%	7%



DC G16 C19 C19 C23 G24 A25 C27 C27 C27 C27 C28	0.00 0.00		
• Molecule 4: D	NA (5'-D(P*GP*GP*GP	*CP*CP*CP*TP*CP*GP	*AP*TP*CP*CP*G)-3'
Chain H:	60%	33%	7%
C15 616 C20 C21 C27 C27 C27 C27 C27 C27 C27			
• Molecule 4: D	NA (5'-D(P*GP*GP*GP	*CP*CP*CP*TP*CP*GP	*AP*TP*CP*CP*G)-3'
Chain N:	47%	47%	7%
DC 616 617 122 122 624 624 624 624 624 726	0250		
• Molecule 4: D	NA (5'-D(P*GP*GP*GP	*CP*CP*CP*TP*CP*GP	*AP*TP*CP*CP*G)-3'
Chain R:	60%	40%	_
C15 617 617 617 620 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2			
• Molecule 5: Pr	otein PAXX		
Chain J:	64%	36%	
R177 8184 8184 1186 1186 1186 8198 8192 8192 8192 8192 8192	E208		
• Molecule 5: Pr	otein PAXX		
Chain T:	71%	29%	_
8177 8184 8184 8184 8190 8193 8193 8194 9195	E 2202 1204 €		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	85.02Å 428.57Å 96.06Å	Deperitor
a, b, c, α , β , γ	90.00° 90.01° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	45.32 - 2.95	Depositor
Resolution (A)	47.73 - 2.95	EDS
% Data completeness	23.9 (45.32-2.95)	Depositor
(in resolution range)	21.9(47.73-2.95)	EDS
R _{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.47 (at 2.96 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
P.P.	0.252 , 0.298	Depositor
n, n_{free}	0.253 , 0.296	DCC
R_{free} test set	2001 reflections (5.85%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	1.703	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.28 , 36.8	EDS
L-test for twinning ²	$< L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.358 for h,-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	36383	wwPDB-VP
Average B, all atoms $(Å^2)$	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.10% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	ond lengths	Bond angles		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.37	0/4105	0.75	4/5529~(0.1%)	
1	Е	0.33	0/4093	0.71	0/5512	
1	Κ	0.37	0/4129	0.75	3/5561~(0.1%)	
1	0	0.37	1/4101~(0.0%)	0.74	1/5523~(0.0%)	
2	В	0.34	0/4334	0.70	4/5842~(0.1%)	
2	F	0.33	0/4369	0.70	2/5892~(0.0%)	
2	L	0.35	1/4324~(0.0%)	0.68	3/5831~(0.1%)	
2	Р	0.32	0/4329	0.69	1/5840~(0.0%)	
3	С	0.50	0/441	0.84	0/679	
3	G	0.55	0/462	0.83	0/711	
3	М	0.51	0/441	0.86	0/679	
3	Q	0.54	0/462	0.84	0/711	
4	D	0.56	0/318	0.88	0/488	
4	Н	0.59	0/339	0.94	1/520~(0.2%)	
4	N	0.56	0/318	0.86	0/488	
4	R	0.62	0/339	0.92	0/520	
5	J	0.25	0/218	0.59	0/290	
5	Т	0.27	0/218	0.58	0/290	
All	All	0.37	2/37340~(0.0%)	0.73	19/50906~(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
2	F	0	1

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	L	400	ARG	CB-CG	-5.52	1.37	1.52
1	0	525	PHE	CE2-CZ	5.30	1.47	1.37

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	495	LEU	CB-CG-CD2	8.39	125.27	111.00
2	F	339	CYS	CA-CB-SG	8.08	128.54	114.00
2	Р	339	CYS	CA-CB-SG	7.54	127.58	114.00
1	Κ	258	ARG	CG-CD-NE	7.42	127.37	111.80
2	L	400	ARG	NE-CZ-NH2	-6.73	116.94	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	65	ASP	Mainchain

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	4027	0	4101	148	0
1	Е	4015	0	4099	156	0
1	K	4052	0	4128	166	0
1	0	4023	0	4110	163	0
2	В	4248	0	4299	125	0
2	F	4282	0	4312	127	0
2	L	4238	0	4281	121	0
2	Р	4242	0	4278	133	0
3	С	393	0	213	13	0
3	G	412	0	224	11	0
3	М	393	0	213	18	0
3	Q	412	0	224	10	0
4	D	285	0	157	10	0
4	Н	304	0	168	10	0
4	N	285	0	157	8	0
4	R	304	0	168	8	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	214	0	212	11	0
5	Т	214	0	212	9	0
6	А	5	0	0	0	0
6	F	5	0	0	0	0
6	Κ	5	0	0	0	0
6	Р	5	0	0	0	0
7	В	1	0	0	0	0
7	Ε	6	0	0	0	0
7	F	3	0	0	0	0
7	Κ	4	0	0	1	0
7	L	2	0	0	0	0
7	Ν	1	0	0	0	0
7	0	3	0	0	0	0
All	All	36383	0	35556	1063	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 15.

The worst 5 of 1063 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)
2:F:250:ARG:HD3	2:F:258:SER:HB3	1.37	1.06
2:L:400:ARG:NH2	3:M:10:DG:O3'	1.93	1.02
1:O:339:ARG:HA	1:O:405:ASN:HA	1.44	0.99
1:A:207:LYS:HD2	1:A:208:PRO:HD2	1.48	0.96
1:A:493:LEU:HD13	2:B:321:VAL:HG11	1.46	0.96

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	А	495/544~(91%)	478 (97%)	15 (3%)	2~(0%)	34	69
1	Ε	493/544~(91%)	474 (96%)	16 (3%)	3~(1%)	25	60
1	Κ	498/544~(92%)	484 (97%)	13 (3%)	1 (0%)	47	79
1	Ο	494/544~(91%)	472 (96%)	21 (4%)	1 (0%)	47	79
2	В	525/572~(92%)	513 (98%)	11 (2%)	1 (0%)	47	79
2	F	533/572~(93%)	517 (97%)	14 (3%)	2~(0%)	34	69
2	L	524/572~(92%)	507~(97%)	15 (3%)	2~(0%)	34	69
2	Р	527/572~(92%)	506 (96%)	18 (3%)	3 (1%)	25	60
5	J	26/28~(93%)	24 (92%)	2(8%)	0	100	100
5	Т	26/28~(93%)	23 (88%)	3 (12%)	0	100	100
All	All	4141/4520 (92%)	3998 (96%)	128 (3%)	15 (0%)	34	69

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	530	TYR
1	Е	55	ASP
2	L	302	GLU
2	Р	69	SER
2	Р	125	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Percenti	les
1	А	453/492~(92%)	451 (100%)	2~(0%)	91 96	5
1	Ε	452/492~(92%)	446 (99%)	6 (1%)	69 87	7
1	Κ	456/492~(93%)	452 (99%)	4 (1%)	78 91	L
1	Ο	453/492~(92%)	449 (99%)	4 (1%)	78 91	L
2	В	478/513~(93%)	476 (100%)	2~(0%)	91 96	5
2	F	481/513~(94%)	478 (99%)	3~(1%)	86 94	1



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	476/513~(93%)	474 (100%)	2~(0%)	91 96
2	Р	477/513~(93%)	474 (99%)	3 (1%)	86 94
5	J	23/23~(100%)	23~(100%)	0	100 100
5	Т	23/23~(100%)	23~(100%)	0	100 100
All	All	3772/4066~(93%)	3746 (99%)	26(1%)	84 93

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5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	Κ	139	SER
2	L	441	SER
2	Р	441	SER
1	Κ	525	PHE
2	L	539	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
2	L	75	GLN
2	L	514	ASN
2	L	243	HIS
1	0	486	HIS
2	В	514	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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type	Turne	Chain	Dag	Tink	Bond lengths			Bond angles		
	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
6	SO4	F	601	-	4,4,4	0.13	0	$6,\!6,\!6$	0.07	0
6	SO4	Р	601	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
6	SO4	А	601	-	4,4,4	0.14	0	$6,\!6,\!6$	0.06	0
6	SO4	K	601	-	4,4,4	0.15	0	$6,\!6,\!6$	0.07	0

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 (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, 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	А	499/544~(91%)	0.19	36 (7%) 15 8	51, 105, 175, 256	0
1	Е	497/544~(91%)	-0.16	7 (1%) 75 59	46, 80, 134, 187	0
1	K	502/544~(92%)	0.32	43 (8%) 10 6	43, 112, 181, 235	0
1	Ο	498/544~(91%)	-0.12	9 (1%) 68 51	44, 81, 136, 204	0
2	В	531/572~(92%)	0.01	27 (5%) 28 17	44, 92, 161, 227	0
2	F	537/572~(93%)	-0.12	13 (2%) 59 42	47, 84, 145, 208	0
2	L	530/572~(92%)	0.18	43 (8%) 12 6	33, 93, 159, 257	0
2	Р	531/572~(92%)	-0.10	16 (3%) 50 34	45, 83, 137, 194	0
3	С	19/30~(63%)	-0.89	0 100 100	105, 146, 174, 176	0
3	G	20/30~(66%)	-0.90	0 100 100	106, 143, 164, 174	0
3	М	19/30~(63%)	-0.83	0 100 100	102, 148, 184, 186	0
3	Q	20/30~(66%)	-1.00	0 100 100	108, 145, 172, 187	0
4	D	14/15~(93%)	-0.96	0 100 100	130, 154, 191, 201	0
4	Н	15/15~(100%)	-0.75	0 100 100	106, 123, 176, 193	0
4	Ν	14/15~(93%)	-0.72	0 100 100	134, 143, 180, 223	0
4	R	15/15~(100%)	-0.87	0 100 100	114, 131, 185, 213	0
5	J	28/28~(100%)	-0.32	0 100 100	83, 104, 141, 161	0
5	Т	28/28~(100%)	-0.37	1 (3%) 42 28	77, 107, 149, 165	0
All	All	4317/4700 (91%)	-0.01	195 (4%) 33 21	33, 92, 163, 257	0

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	322	PRO	24.4
2	L	321	VAL	12.2
1	Κ	459	VAL	9.6



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Mol	Chain	\mathbf{Res}	Type	RSRZ
1	Κ	131	PHE	9.6
2	L	257	LEU	8.3

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 monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	SO4	K	601	5/5	0.95	0.15	81,82,87,90	0
6	SO4	А	601	5/5	0.97	0.13	98,103,110,110	0
6	SO4	F	601	5/5	0.98	0.13	70,72,77,77	0
6	SO4	Р	601	5/5	0.98	0.12	79,80,84,96	0

6.5 Other polymers (i)

There are no such residues in this entry.

