

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 02:32 AM EST

PDB ID	:	4J4A
Title	:	Crystal Structure of Engineered Trimeric Cortexillin-1 Coiled-Coil Variant
Authors	:	Bjelic, S.; Steinmetz, M.O.; Kammerer, R.A.
Deposited on		
Resolution	:	1.65 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:

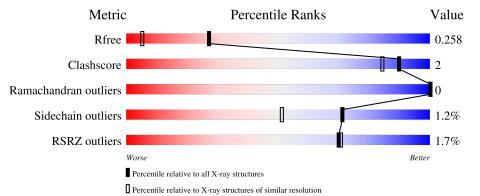
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.65 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3122(1.66-1.62)
Clashscore	141614	3268(1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	27	93%		7%
1	В	27	7%	15%	7%
1	С	27	4% 85%	7%	7%
1	D	27	96%		•
1	Е	27	89%		11%



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Mol	Chain	Length	Quality of chain	
1	F	27	85%	15%
1	G	27	4% 67% 19%	15%
1	Н	27	4% 67% 15%	19%
1	Ι	27	78%	19%
1	J	27	96%	·
1	K	27	89%	• 7%
1	L	27	78%	22%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2524 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		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
1	А	27	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	21	218	139	39	39	1	0	0	0
1	В	25	Total	С	Ν	0	S	0	0	0
	D	20	197	126	36	34	1	0	0	0
1	С	25	Total	С	Ν	0	S	0	0	0
	U	20	208	134	37	36	1	0	0	0
1	D	27	Total	С	Ν	0	S	0	0	0
1	D	21	218	139	39	39	1	0	0	0
1	Е	24	Total	С	Ν	Ο	\mathbf{S}	0	0	0
L	Ľ	24	190	121	33	35	1	0	0	0
1	F	23	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	Ľ	20	178	114	31	32	1	0	0	0
1	G	23	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	ŭ	20	188	120	35	32	1	0	0	0
1	Н	22	Total	С	Ν	Ο	S	1	1 0	0
1	11		174	110	30	33	1	1	0	
1	Ι	22	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	I		180	116	31	32	1	0	0	0
1	J	27	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	5	21	214	136	38	39	1	U	0	0
1	Κ	25	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	17	20	197	124	36	36	1	0	U	0
1	L	21	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	Ц	41	168	108	29	30	1		U	0

• Molecule 1 is a protein called Cortexillin-1.

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	GLY	-	expression tag	UNP Q54HG2
А	0	SER	ASN	conflict	UNP Q54HG2
А	4	ILE	GLU	conflict	UNP Q54HG2
А	7	ARG	ALA	conflict	UNP Q54HG2
А	8	ILE	ARG	conflict	UNP Q54HG2



ChainResidueModelledActualCommentReferenceA11ILELEUconflictUNP Q54HG2A118ILETHRconflictUNP Q54HG2B-1GLY-expression tagUNP Q54HG2B0SERASNconflictUNP Q54HG2B0SERASNconflictUNP Q54HG2B14ILEGLUconflictUNP Q54HG2B7ARGALAconflictUNP Q54HG2B8ILEARGconflictUNP Q54HG2B11ILELEUconflictUNP Q54HG2B18ILETHRconflictUNP Q54HG2C-1GLY-expression tagUNP Q54HG2C-1GLY-expression tagUNP Q54HG2C-1GLY-expression tagUNP Q54HG2C4ILEGLUconflictUNP Q54HG2C7ARGALAconflictUNP Q54HG2C11ILELEUconflictUNP Q54HG2C18ILETHRconflictUNP Q54HG2C18ILETHRconflictUNP Q54HG2C19-1GLY-expression tagUNP Q54HG210-1GLY-expression tagD-1GLY-expression tagUNP Q54HG2D11<		Continued from previous page							
A15ILELEUconflictUNP Q54HG2A18ILETHRconflictUNP Q54HG2B-1GLY-expression tagUNP Q54HG2B0SERASNconflictUNP Q54HG2B4ILEGLUconflictUNP Q54HG2B7ARGALAconflictUNP Q54HG2B8ILEARGconflictUNP Q54HG2B11ILELEUconflictUNP Q54HG2B15ILELEUconflictUNP Q54HG2C-1GLY-expression tagUNP Q54HG2C0SERASNconflictUNP Q54HG2C-1GLY-expression tagUNP Q54HG2C0SERASNconflictUNP Q54HG2C11ILEGLUconflictUNP Q54HG2C11ILELEUconflictUNP Q54HG2C13ILETHRconflictUNP Q54HG2C14ILELEUconflictUNP Q54HG2D-1GLY-expression tagUNP Q54HG2D0SERASNconflictUNP Q54HG2D0SERASNconflictUNP Q54HG2D0SERASNconflictUNP Q54HG2D11ILEGLUconflictUNP Q54HG2D14ILEGLU<	Chain	Residue	Modelled	Actual	Comment	Reference			
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E15ILELEUconflictUNP Q54HG2E18ILETHRconflictUNP Q54HG2F-1GLY-expression tagUNP Q54HG2F0SERASNconflictUNP Q54HG2F4ILEGLUconflictUNP Q54HG2F7ARGALAconflictUNP Q54HG2F8ILEARGconflictUNP Q54HG2F11ILELEUconflictUNP Q54HG2	Е	8	ILE	ARG	conflict	UNP Q54HG2			
E18ILETHRconflictUNP Q54HG2F-1GLY-expression tagUNP Q54HG2F0SERASNconflictUNP Q54HG2F4ILEGLUconflictUNP Q54HG2F7ARGALAconflictUNP Q54HG2F8ILEARGconflictUNP Q54HG2F11ILELEUconflictUNP Q54HG2	Е	11	ILE	LEU	conflict	UNP Q54HG2			
F-1GLY-expression tagUNP Q54HG2F0SERASNconflictUNP Q54HG2F4ILEGLUconflictUNP Q54HG2F7ARGALAconflictUNP Q54HG2F8ILEARGconflictUNP Q54HG2F11ILELEUconflictUNP Q54HG2	Е	15	ILE	LEU	conflict	UNP Q54HG2			
F0SERASNconflictUNP Q54HG2F4ILEGLUconflictUNP Q54HG2F7ARGALAconflictUNP Q54HG2F8ILEARGconflictUNP Q54HG2F11ILELEUconflictUNP Q54HG2	Е	18	ILE	THR	conflict	UNP Q54HG2			
F4ILEGLUconflictUNP Q54HG2F7ARGALAconflictUNP Q54HG2F8ILEARGconflictUNP Q54HG2F11ILELEUconflictUNP Q54HG2	F	-1	GLY	-	expression tag	UNP Q54HG2			
F7ARGALAconflictUNP Q54HG2F8ILEARGconflictUNP Q54HG2F11ILELEUconflictUNP Q54HG2	F	0	SER	ASN	conflict	UNP Q54HG2			
F8ILEARGconflictUNP Q54HG2F11ILELEUconflictUNP Q54HG2	F	4	ILE	GLU	conflict	UNP Q54HG2			
F 11 ILE LEU conflict UNP Q54HG2	F	7	ARG	ALA	conflict	UNP Q54HG2			
	F	8	ILE	ARG	conflict	UNP Q54HG2			
F15ILELEUconflictUNP Q54HG2	F	11	ILE	LEU	conflict	UNP Q54HG2			
	F	15	ILE	LEU	conflict	UNP Q54HG2			

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Continu	Residue	vious page Modelled	Actual	Comment	Reference
F	18	ILE	THR	conflict	UNP Q54HG2
G F	-1	GLY	ΙΠΚ	expression tag	UNP Q54HG2
G	-1	SER	ASN	conflict	UNP Q54HG2
G	4	ILE	GLU	conflict	UNP Q54HG2
G	7	ARG	ALA	conflict	UNP Q54HG2
G	8	ILE	ARG	conflict	UNP Q54HG2
G	11	ILE	LEU	conflict	UNP Q54HG2
G	11	ILE	LEU	conflict	UNP Q54HG2
G	13	ILE	THR	conflict	UNP Q54HG2
H	-1	GLY	11110	expression tag	UNP Q54HG2
 H	-1	SER	ASN	conflict	UNP Q54HG2
 H	4	ILE	GLU	conflict	UNP Q54HG2
 H	4	ARG	ALA	conflict	-
	-				UNP Q54HG2
H	8	ILE	ARG	conflict	UNP Q54HG2
H	11	ILE	LEU	conflict	UNP Q54HG2
H	15	ILE	LEU	conflict	UNP Q54HG2
H	18	ILE	THR	conflict	UNP Q54HG2
I	-1	GLY	-	expression tag	UNP Q54HG2
I	0	SER	ASN	conflict	UNP Q54HG2
Ι	4	ILE	GLU	conflict	UNP Q54HG2
I	7	ARG	ALA	conflict	UNP Q54HG2
Ι	8	ILE	ARG	conflict	UNP Q54HG2
Ι	11	ILE	LEU	conflict	UNP Q54HG2
Ι	15	ILE	LEU	conflict	UNP Q54HG2
Ι	18	ILE	THR	conflict	UNP Q54HG2
J	-1	GLY	-	expression tag	UNP Q54HG2
J	0	SER	ASN	conflict	UNP Q54HG2
J	4	ILE	GLU	conflict	UNP Q54HG2
J	7	ARG	ALA	conflict	UNP Q54HG2
J	8	ILE	ARG	conflict	UNP Q54HG2
J	11	ILE	LEU	conflict	UNP Q54HG2
J	15	ILE	LEU	conflict	UNP Q54HG2
J	18	ILE	THR	conflict	UNP Q54HG2
Κ	-1	GLY	-	expression tag	UNP Q54HG2
Κ	0	SER	ASN	conflict	UNP Q54HG2
Κ	4	ILE	GLU	conflict	UNP Q54HG2
Κ	7	ARG	ALA	conflict	UNP Q54HG2
Κ	8	ILE	ARG	conflict	UNP Q54HG2
К	11	ILE	LEU	conflict	UNP Q54HG2
Κ	15	ILE	LEU	conflict	UNP Q54HG2
Κ	18	ILE	THR	conflict	UNP Q54HG2
L	-1	GLY	-	expression tag	UNP Q54HG2
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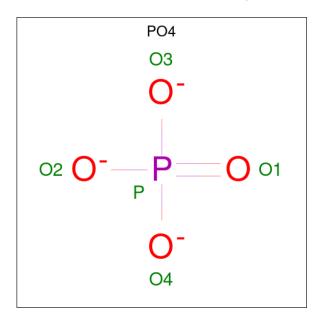
[odelled	Actual	Comment	Reference
SER	ASN	conflict	UNP Q54HG2
ILE	GLU	conflict	UNP Q54HG2
ABC		conflict	UNP O54HC2

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Chain	Residue	Modelled

0

L	4	ILE	GLU	conflict	UNP Q54HG2
L	7	ARG	ALA	conflict	UNP Q54HG2
L	8	ILE	ARG	conflict	UNP Q54HG2
L	11	ILE	LEU	conflict	UNP Q54HG2
L	15	ILE	LEU	conflict	UNP Q54HG2
L	18	ILE	THR	conflict	UNP Q54HG2

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	27	Total O 27 27	0	0
3	В	15	Total O 15 15	0	0
3	С	18	Total O 18 18	0	0
3	D	25	TotalO2525	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Е	20	TotalO2020	0	0
3	F	17	Total O 17 17	0	0
3	G	16	Total O 16 16	0	0
3	Н	11	Total O 11 11	0	0
3	Ι	5	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 5 & 5 \end{array}$	0	0
3	J	4	Total O 4 4	0	0
3	К	13	Total O 13 13	0	0
3	L	13	Total O 13 13	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.

Chain A:	93%	7%
1125 L255		
• Molecule 1: Cortexillin-1		
Chain B:	78%	15% 7%
GLY SER L1 L5 M9 M9 L5 C		
• Molecule 1: Cortexillin-1		
Chain C:	85%	7% 7%
GLY SER 11 12 12		
• Molecule 1: Cortexillin-1		
Chain D:	96%	•
• Molecule 1: Cortexillin-1		
Chain E:	89%	11%
G-1 R.22 ILEU LEU		
• Molecule 1: Cortexillin-1		
Chain F:	85%	15%

• Molecule 1: Cortexillin-1

G-1 D21 ARG ARA ALA LLEU LLEU			
• Molecule 1: Cortexillin-1			
Chain G:	67%	19%	15%
GLY SER LLD LLD LLD LLD LLD LLD LLD LLD S			
• Molecule 1: Cortexillin-1			
Chain H:	67%	15%	19%
GLY SO L1 L1 K5 M9 M9 A15 A15 A15 LEU LEU			
• Molecule 1: Cortexillin-1			
Chain I:	78%	•	19%
GLY SER L1 L1 E2 A2 ALA ALA ILLE ILLE			
• Molecule 1: Cortexillin-1			
Chain J:	96%		·
• Molecule 1: Cortexillin-1			
Chain K:	89%		• 7%
C-1 E12 ILEU LEU			
• Molecule 1: Cortexillin-1			
Chain L:	78%		22%
G-1 LYS ARSP ALA ILEU LEU			



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	41.88Å 78.05Å 114.98Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.29 - 1.65	Depositor
Resolution (A)	46.29 - 1.65	EDS
% Data completeness	100.0 (46.29-1.65)	Depositor
(in resolution range)	$100.0 \ (46.29 - 1.65)$	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.65 (at 1.65 \text{\AA})$	Xtriage
Refinement program	PHENIX dev_1042	Depositor
D D.	0.213 , 0.258	Depositor
R, R_{free}	0.228 , 0.258	DCC
R_{free} test set	4640 reflections $(10.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	23.1	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 50.4	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2524	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.64% 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: PO4

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	Bond	lengths	Bond angles		
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.75	0/217	0.78	1/285~(0.4%)	
1	В	0.74	0/196	0.69	0/259	
1	С	0.76	0/207	0.85	1/272~(0.4%)	
1	D	0.91	0/217	0.69	0/285	
1	Е	0.82	0/189	0.55	0/249	
1	F	0.84	0/177	0.77	0/234	
1	G	1.05	0/187	0.73	0/245	
1	Н	0.85	0/173	0.62	0/229	
1	Ι	0.67	0/179	0.61	0/236	
1	J	0.76	0/213	0.81	0/281	
1	Κ	0.76	0/196	0.55	0/259	
1	L	0.84	0/167	0.72	0/220	
All	All	0.82	0/2318	0.71	2/3054~(0.1%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	25	LEU	CA-CB-CG	-5.52	102.61	115.30
1	А	25	LEU	CB-CG-CD1	-5.06	102.39	111.00

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	218	0	250	1	0
1	В	197	0	218	2	0
1	С	208	0	242	1	0
1	D	218	0	250	1	0
1	Е	190	0	212	0	0
1	F	178	0	197	0	0
1	G	188	0	213	3	0
1	Н	174	0	187	2	0
1	Ι	180	0	204	0	0
1	J	214	0	239	1	0
1	Κ	197	0	217	1	0
1	L	168	0	193	0	0
2	В	5	0	0	0	0
2	Е	5	0	0	0	0
3	А	27	0	0	0	0
3	В	15	0	0	0	0
3	С	18	0	0	0	0
3	D	25	0	0	0	0
3	Е	20	0	0	0	0
3	F	17	0	0	0	0
3	G	16	0	0	0	0
3	Н	11	0	0	0	0
3	Ι	5	0	0	0	0
3	J	4	0	0	0	0
3	Κ	13	0	0	0	0
3	L	13	0	0	0	0
All	All	2524	0	2622	9	0

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.

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 2.

All (9) 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:G:18:ILE:O	1:G:22:ARG:HG3	1.95	0.65
1:G:17:LYS:HE3	1:G:21:ASP:OD2	1.97	0.65
1:G:11:ILE:HG23	1:H:15:ILE:CD1	2.41	0.50
1:H:1:LEU:HG	1:H:5:LYS:HE3	1.97	0.47
1:J:11:ILE:HD11	1:K:12:GLU:HG3	1.97	0.46



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:15:ILE:CD1	1:C:11:ILE:HG23	2.49	0.42	
1:B:5:LYS:O	1:B:9:MET:HG3	2.20	0.42	
1:D:9:MET:HE3	1:D:9:MET:HB3	1.96	0.41	
1:B:1:LEU:N	1:B:1:LEU:HD12	2.36	0.41	

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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 Allo		Allowed	Outliers	Perce	ntiles
1	А	25/27~(93%)	25~(100%)	0	0	100	100
1	В	23/27~(85%)	23 (100%)	0	0	100	100
1	С	23/27~(85%)	23~(100%)	0	0	100	100
1	D	25/27~(93%)	24 (96%)	1 (4%)	0	100	100
1	Ε	22/27~(82%)	22 (100%)	0	0	100	100
1	\mathbf{F}	21/27~(78%)	21 (100%)	0	0	100	100
1	G	21/27~(78%)	21 (100%)	0	0	100	100
1	Η	20/27~(74%)	20 (100%)	0	0	100	100
1	Ι	20/27~(74%)	20 (100%)	0	0	100	100
1	J	25/27~(93%)	25~(100%)	0	0	100	100
1	Κ	23/27~(85%)	23~(100%)	0	0	100	100
1	L	19/27~(70%)	19 (100%)	0	0	100	100
All	All	267/324 ($82%$)	266 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentile	\mathbf{s}
1	А	23/23~(100%)	23~(100%)	0	100 100	
1	В	19/23~(83%)	18 (95%)	1 (5%)	22 4	
1	С	22/23~(96%)	22~(100%)	0	100 100	
1	D	23/23~(100%)	23 (100%)	0	100 100	
1	Ε	20/23~(87%)	20 (100%)	0	100 100	
1	F	18/23~(78%)	18 (100%)	0	100 100	
1	G	19/23~(83%)	19 (100%)	0	100 100	
1	Н	18/23~(78%)	17 (94%)	1 (6%)	21 3	
1	Ι	19/23~(83%)	18~(95%)	1 (5%)	22 4	
1	J	22/23~(96%)	22 (100%)	0	100 100	
1	Κ	20/23~(87%)	20 (100%)	0	100 100	
1	L	18/23~(78%)	18 (100%)	0	100 100	
All	All	241/276~(87%)	238~(99%)	3 (1%)	71 51	

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	6	LEU
1	Н	0	SER
1	Ι	2	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

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)

2 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	Chain	Dec	Link	Bond lengths			Bond angles			
	Type	Chain	Res		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	PO4	В	101	-	4,4,4	1.68	1 (25%)	$6,\!6,\!6$	0.43	0
2	PO4	Е	101	-	4,4,4	1.79	1 (25%)	$6,\!6,\!6$	0.55	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Е	101	PO4	P-O2	-2.14	1.48	1.54
2	В	101	PO4	P-O2	-2.02	1.48	1.54

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, 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 > 2	$OWAB(Å^2)$	Q<0.9
1	А	27/27~(100%)	-0.13	0 100 100	21, 25, 39, 42	3 (11%)
1	В	25/27~(92%)	0.24	2 (8%) 12 10	24, 33, 46, 54	5 (20%)
1	С	25/27~(92%)	-0.13	1 (4%) 38 36	23, 29, 37, 41	3(12%)
1	D	27/27~(100%)	-0.40	0 100 100	21, 24, 36, 39	2(7%)
1	Ε	24/27~(88%)	-0.22	0 100 100	21, 26, 40, 44	2(8%)
1	F	23/27~(85%)	-0.29	0 100 100	20, 26, 46, 63	2 (8%)
1	G	23/27~(85%)	0.23	1 (4%) 35 32	30, 38, 55, 58	3~(13%)
1	Η	22/27~(81%)	0.17	1 (4%) 33 30	35, 46, 57, 61	2(9%)
1	Ι	22/27~(81%)	-0.07	0 100 100	21, 36, 53, 64	0
1	J	27/27~(100%)	0.08	0 100 100	21, 34, 43, 53	1 (3%)
1	Κ	25/27~(92%)	-0.07	0 100 100	19, 26, 56, 59	2(8%)
1	L	21/27~(77%)	-0.26	0 100 100	17, 22, 39, 43	1 (4%)
All	All	291/324~(89%)	-0.07	5 (1%) 70 71	17, 30, 54, 64	26 (8%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	1	LEU	7.2
1	С	25	LEU	3.2
1	G	3	LEU	2.6
1	Н	9	MET	2.6
1	В	6	LEU	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)

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	PO4	В	101	5/5	0.99	0.07	24,26,26,30	0
2	PO4	Е	101	5/5	0.99	0.10	39,40,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.

