

wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 04:38 am BST

PDB ID 4C3J

> Title Structure of 14-subunit RNA polymerase I at 3.35 A resolution, crystal form

Authors : Fernandez-Tornero, C.; Moreno-Morcillo, M.; Rashid, U.J.; Taylor, N.M.I.;

Ruiz, F.M.; Gruene, T.; Legrand, P.; Steuerwald, U.; Muller, C.W.

Deposited on 2013-08-24

Resolution 3.35 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-467MolProbity Xtriage (Phenix) 1.13

EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove) Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

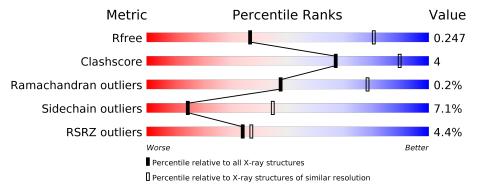
Validation Pipeline (wwPDB-VP) 2.11

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 3.35 Å.

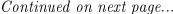
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
Wiethe	$(\# {\rm Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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% 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		Qua	ality of chain				
-1	٨	1004	2%						
1	A	1664		77%			14%	•	8%
2	В	1203	3%	81%				15%	
_			2%	0170			-		
3	С	335		74%			16%	•	9%
4	D	107	%						
4	D	137	35%	8%		57%			
F	17.	015	2%						
5	Е	215			91%				9%
6	${ m F}$	155		56%	8%		35%		_





Continued from previous page...

Mol	Chain	Length		Qua	ality of chain				
7	G	326	6%	68%		11%	• 21	%	_
8	Н	146	8%	79%			12%	8%	-
9	I	125	13%	77%			22%		
10	J	70		77%			13%	9%	.
11	K	142	%	58%	12%	•	27%		-
12	L	70	%	56%	9%		36%		_
13	M	415	21%		75%				_
14	N	233	13%	53%	6%	40	0%		-



2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 34552 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 DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190.

$oxed{N}$	/Iol	Chain	Residues		\mathbf{A}	\mathbf{toms}		ZeroOcc	AltConf	Trace	
	1	A	1523	Total 12019	C 7577	N 2086	O 2292	S 64	0	0	0

• Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues		\mathbf{A}	toms		ZeroOcc	$\mathbf{AltConf}$	Trace	
2	В	1176	Total 9322	C 5898	N 1629	O 1745	S 50	0	0	0

• Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues		\mathbf{At}	oms		ZeroOcc	AltConf	Trace	
3	С	304	Total	С	N	O	S	0	0	0
		00-	2418	1536	414	460	8			

• Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues		Aton	ıs		ZeroOcc	AltConf	Trace
4	D	59	Total 466	C 292	N 80	O 94	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chai	n Residue	Modelled	Actual	Comment	Reference
D	12	SER	THR	conflict	UNP P50106

• Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC1.



Mol	Chain	Residues		Atoms					AltConf	Trace
5	E	215	Total	С	N	О	S	0	0	0
		210	1759	1116	310	321	12			

• Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC2.

Mol	Chain	Residues		Atoms					AltConf	Trace
6	F	100	Total	C	N	0	S	0	0	0
			823	522	144	154	3			

• Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	G	259	Total 2052	C 1301	N 348	O 398	S 5	0	0	0

• Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUB-UNIT RPABC3.

Mol	Chain	Residues		Atoms					AltConf	Trace
8	Н	134	Total 1072	C 676	N 181	O 211	S 4	0	0	0

• Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	I	124	Total 942	C 584	N 160	O 189	S 9	0	0	0

• Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
10	J	69	Total 569	C 362	N 101	O 100	S 6	0	0	0

• Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUB-UNIT RPAC2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
11	К	103	Total 810	C 506	N 132	O 167	S 5	0	0	0



• Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
12	L	45	Total 359	C 221	N 71	O 63	S 4	0	0	0

• Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
13	М	105	Total 831	C 528	N 137	O 166	0	0	0

• Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
14	N	139	Total 1103	C 706	N 179	O 214	S 4	0	0	0

• Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

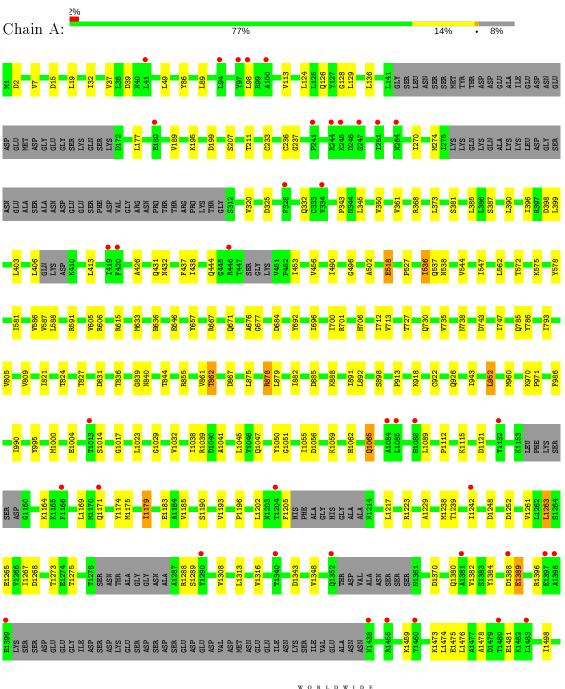
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	В	1	Total Zn 1 1	0	0
15	A	2	Total Zn 2 2	0	0
15	L	1	Total Zn 1 1	0	0
15	J	1	Total Zn 1 1	0	0
15	I	2	Total Zn 2 2	0	0



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 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.

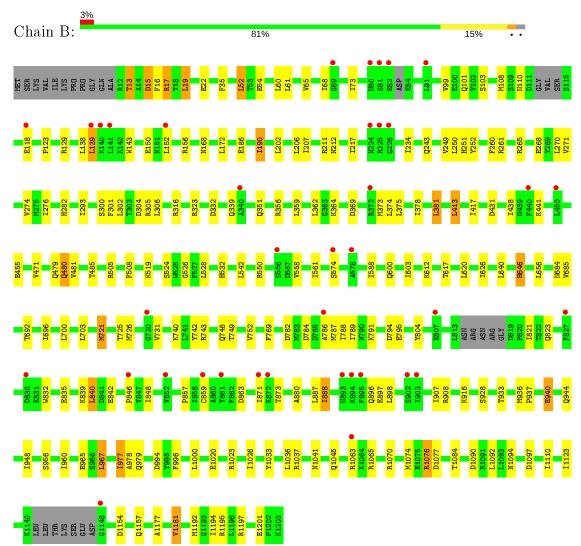
• Molecule 1: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190



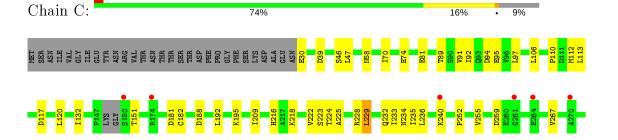




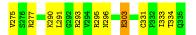
• Molecule 2: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135



• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1







• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

Chain D: 35% 8% 57%

• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain E: 91% 9%



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

Chain F: 56% 8% 35%

• Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

Chain G: 68% 11% · 21%

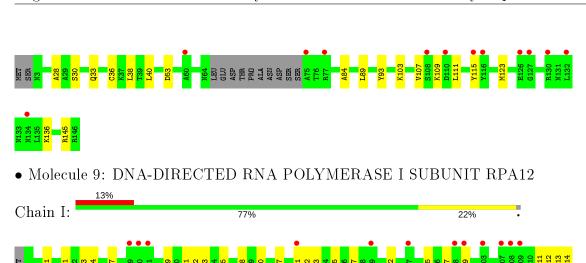
| MET | MET

##25 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 | 12.28 |

• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

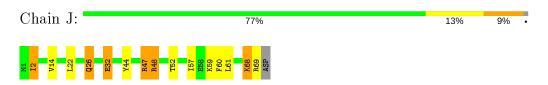
Chain H: 79% 12% 8%



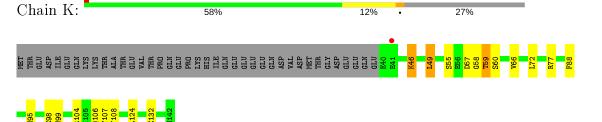




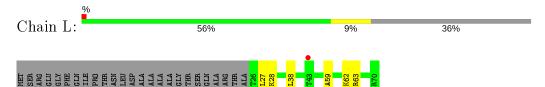
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



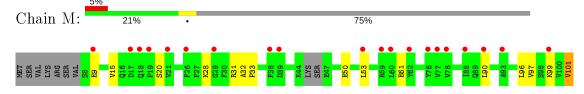
• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2



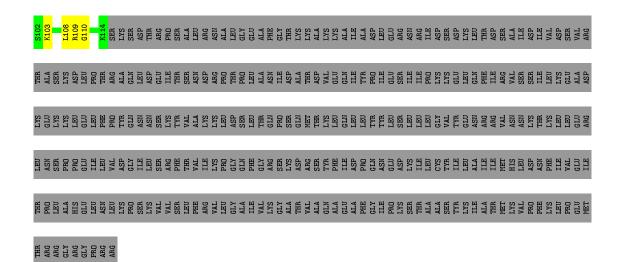
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4



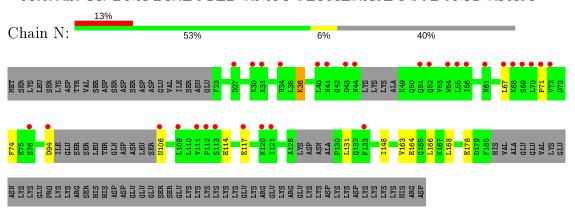
• Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49







• Molecule 14: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	401.02Å 139.84Å 140.94Å	Donositor
a, b, c, α , β , γ	90.00° 90.39° 90.00°	Depositor
Resolution (Å)	49.05 - 3.35	Depositor
Resolution (A)	48.66 - 3.35	EDS
% Data completeness	99.5 (49.05-3.35)	Depositor
(in resolution range)	99.6 (48.66-3.35)	EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.47 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
D D.	0.213 , 0.220	Depositor
R, R_{free}	0.237 , 0.247	DCC
R_{free} test set	5612 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.27 , 76.1	EDS
L-test for twinning ²	$< L >=0.43, < L^2>=0.25$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34552	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ 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: ZN

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
WIOI	Chain	RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/12233	0.58	0/16523
2	В	0.39	0/9527	0.59	0/12879
3	С	0.39	0/2469	0.60	0/3347
4	D	0.40	0/472	0.52	0/639
5	Е	0.39	0/1795	0.55	0/2416
6	F	0.38	0/838	0.54	0/1129
7	G	0.38	0/2094	0.57	0/2843
8	Н	0.38	0/1090	0.57	0/1476
9	I	0.39	0/954	0.57	0/1285
10	J	0.41	0/578	0.61	0/775
11	K	0.39	0/821	0.59	0/1108
12	L	0.38	0/361	0.60	0/478
13	М	0.38	0/846	0.53	0/1136
14	N	0.38	0/1124	0.52	0/1512
All	All	0.39	0/35202	0.58	0/47546

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	A	12019	0	12051	118	0
2	В	9322	0	9187	90	0
3	С	2418	0	2401	22	0
4	D	466	0	466	4	0
5	Ε	1759	0	1788	9	0
6	F	823	0	841	7	0
7	G	2052	0	2016	14	0
8	Н	1072	0	1042	6	0
9	I	942	0	933	13	0
10	J	569	0	585	13	0
11	K	810	0	801	12	0
12	L	359	0	381	1	0
13	M	831	0	820	12	0
14	N	1103	0	1106	6	0
15	A	2	0	0	0	0
15	В	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	34552	0	34418	269	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 269 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
7100111 1	7100H1 2	${f distance} ({f A})$	$ \text{overlap } (\text{\AA})$
11:K:59:THR:HG22	11:K:107:THR:OG1	1.46	1.13
11:K:60:SER:OG	11:K:106:GLN:HG2	1.63	0.97
2:B:99:VAL:HG21	2:B:417:ILE:HD11	1.58	0.84
1:A:1382:VAL:HA	2:B:1070:ARG:NH1	1.94	0.81
3:C:222:VAL:HG21	3:C:225:ALA:HB2	1.68	0.75

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	A	1503/1664~(90%)	1422 (95%)	79 (5%)	2 (0%)	51	82
2	В	$1166/1203 \ (97\%)$	1094 (94%)	68 (6%)	4 (0%)	41	73
3	С	300/335~(90%)	283 (94%)	17 (6%)	0	100	100
4	D	55/137~(40%)	52 (94%)	3 (6%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	98/155~(63%)	95 (97%)	3 (3%)	0	100	100
7	G	251/326 (77%)	232 (92%)	17 (7%)	2 (1%)	19	53
8	Н	130/146 (89%)	119 (92%)	10 (8%)	1 (1%)	19	53
9	I	120/125~(96%)	108 (90%)	12 (10%)	0	100	100
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	101/142 (71%)	95 (94%)	5 (5%)	1 (1%)	15	49
12	L	43/70 (61%)	40 (93%)	3 (7%)	0	100	100
13	М	101/415 (24%)	94 (93%)	7 (7%)	0	100	100
14	N	131/233 (56%)	122 (93%)	9 (7%)	0	100	100
All	All	4279/5236 (82%)	4020 (94%)	249 (6%)	10 (0%)	47	78

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1389	GLU
1	A	237	GLY
2	В	532	HIS
2	В	1154	ASP
11	K	46	LYS

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	Percentiles
1	A	$1343/1465 \ (92\%)$	1268 (94%)	75 (6%)	21 53
2	В	$1024/1053 \ (97\%)$	928 (91%)	96 (9%)	8 31
3	С	$269/296 \ (91\%)$	243 (90%)	26 (10%)	8 30
4	D	56/116 (48%)	50 (89%)	6 (11%)	6 25
5	E	197/197 (100%)	192 (98%)	5 (2%)	47 73
6	F	90/137 (66%)	86 (96%)	4 (4%)	28 59
7	G	$234/291 \ (80\%)$	219 (94%)	15 (6%)	17 48
8	Н	116/128 (91%)	111 (96%)	5 (4%)	29 60
9	I	109/110 (99%)	100 (92%)	9 (8%)	11 37
10	J	64/65 (98%)	56 (88%)	8 (12%)	4 18
11	K	93/130 (72%)	86 (92%)	7 (8%)	13 42
12	L	40/57 (70%)	36 (90%)	4 (10%)	7 29
13	M	94/371 (25%)	90 (96%)	4 (4%)	29 60
14	N	128/220 (58%)	117 (91%)	11 (9%)	10 36
All	All	3857/4636 (83%)	3582 (93%)	275 (7%)	14 45

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	${f Res}$	\mathbf{Type}
2	В	550	ARG
2	В	944	GLN
11	K	124	LEU
2	В	646	HIS
2	В	832	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	${f Res}$	Type
2	В	351	GLN
2	В	724	GLN
9	I	100	GLN
2	В	361	HIS
2	В	646	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)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	1

All chain breaks are listed below:

Mode	l Chain	Residue-1	Atom-1	Residue-2	Atom-2	$oxed{f Distance (\AA)}$
1	I	79:GLY	С	80:ALA	N	4.36



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>	# RSRZ > 2	$\mathrm{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	1523/1664 (91%)	0.16	40 (2%) 56 58	82, 114, 166, 248	0
2	В	1176/1203 (97%)	0.30	38 (3%) 47 50	80, 119, 170, 238	0
3	С	304/335 (90%)	0.11	6 (1%) 65 68	108, 134, 171, 191	0
4	D	59/137 (43%)	0.32	1 (1%) 70 73	114, 157, 188, 193	0
5	E	$215/215 \; (100\%)$	0.06	5 (2%) 60 63	95, 143, 193, 201	0
6	F	100/155 (64%)	-0.13	0 100 100	88, 115, 156, 167	0
7	G	259/326 (79%)	0.43	19 (7%) 15 17	102, 167, 256, 274	0
8	Н	134/146 (91%)	0.48	12 (8%) 9 11	114, 141, 173, 184	0
9	I	124/125 (99%)	0.58	16 (12%) 3 4	105, 177, 215, 229	0
10	J	69/70 (98%)	0.29	0 100 100	105, 124, 150, 176	0
11	K	103/142 (72%)	-0.03	1 (0%) 82 86	101, 125, 165, 206	0
12	L	45/70~(64%)	0.15	1 (2%) 62 65	130, 156, 183, 191	0
13	M	105/415~(25%)	1.11	20 (19%) 1 1	161, 209, 254, 264	0
14	N	139/233~(59%)	0.97	31 (22%) 0 0	113, 211, 252, 271	0
All	All	$4355/5236 \ (83\%)$	0.27	190 (4%) 34 37	80, 126, 209, 274	0

The worst 5 of 190 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1340	THR	6.9
13	M	17	ASP	5.3
9	I	103	SER	5.2
9	I	41	GLN	5.2
14	N	54	TRP	5.2



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 carbohydrates 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
15	ZN	I	1127	1/1	0.93	0.10	$156,\!156,\!156,\!156$	0
15	ZN	A	2665	1/1	0.99	0.13	111,111,111,111	0
15	ZN	В	2204	1/1	0.99	0.18	109,109,109,109	0
15	ZN	L	1071	1/1	0.99	0.11	136,136,136,136	0
15	ZN	J	1070	1/1	0.99	0.24	111,111,111,111	0
15	ZN	I	1126	1/1	0.99	0.15	151,151,151,151	0
15	ZN	A	2664	1/1	0.99	0.08	122,122,122,122	0

6.5 Other polymers (i)

There are no such residues in this entry.

