

wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2023 – 02:49 PM JST

PDB ID : 6JCY

Title: Mycobacterium tuberculosis RNA polymerase transcription initiation open

complex with a chimeric ECF sigma factor sigH/E

Authors : Li, L.; Zhang, Y.

Deposited on : 2019-01-30

Resolution : 3.11 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

Xtriage (Phenix) : 1.13 EDS : 2.36

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

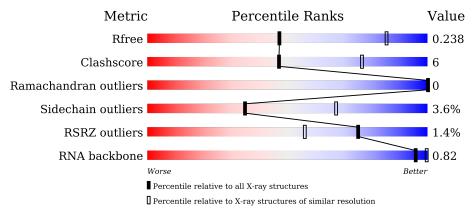
Validation Pipeline (wwPDB-VP) : 2.36

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 3.11 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
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	A	368	50%	10%	40%
1	В	368	50%	12%	37%
2	С	1174	.%	81%	15% • •
3	D	1317	.%	79%	16% • •

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Mol	Chain	Length	C	Quality of chain
4	Б	110	3%	
4	Е	110	3%	9% • 31%
5	F	209	63%	14% • 22%
6	G	23	30%	70%
7	Н	20	45%	55%
8	I	6		100%



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 24729 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 subunit alpha.

\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms		ZeroOcc	AltConf	Trace	
1	А	221	Total		- '	О	S	0	0	0
1	71	221	1673	1054	288	329	2		O	
1	D	231	Total	С	N	O	S	0	0	0
1	Б	231	1719	1085	293	338	3	0	U	

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET			UNP P9WGZ1
			-	initiating methionine	
A	-19	GLY	-	expression tag	UNP P9WGZ1
A	-18	HIS	-	expression tag	UNP P9WGZ1
A	-17	HIS	-	expression tag	UNP P9WGZ1
A	-16	HIS	-	expression tag	UNP P9WGZ1
A	-15	HIS	-	expression tag	UNP P9WGZ1
A	-14	HIS	-	expression tag	UNP P9WGZ1
A	-13	HIS	-	expression tag	UNP P9WGZ1
A	-12	HIS	-	expression tag	UNP P9WGZ1
A	-11	HIS	-	expression tag	UNP P9WGZ1
A	-10	HIS	_	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	SER	-	expression tag	UNP P9WGZ1
A	-7	SER	-	expression tag	UNP P9WGZ1
A	-6	GLY	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	ILE	-	expression tag	UNP P9WGZ1
A	-3	GLU	-	expression tag	UNP P9WGZ1
A	-2	GLY	-	expression tag	UNP P9WGZ1
A	-1	ARG	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
В	-20	MET	-	initiating methionine	UNP P9WGZ1
В	-19	GLY	-	expression tag	UNP P9WGZ1
В	-18	HIS	-	expression tag	UNP P9WGZ1
В	-17	HIS	-	expression tag	UNP P9WGZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-16	HIS	-	expression tag	UNP P9WGZ1
В	-15	HIS	-	expression tag	UNP P9WGZ1
В	-14	HIS	-	expression tag	UNP P9WGZ1
В	-13	HIS	-	expression tag	UNP P9WGZ1
В	-12	HIS	-	expression tag	UNP P9WGZ1
В	-11	HIS	-	expression tag	UNP P9WGZ1
В	-10	HIS	-	expression tag	UNP P9WGZ1
В	-9	HIS	-	expression tag	UNP P9WGZ1
В	-8	SER	-	expression tag	UNP P9WGZ1
В	-7	SER	-	expression tag	UNP P9WGZ1
В	-6	GLY	-	expression tag	UNP P9WGZ1
В	-5	HIS	-	expression tag	UNP P9WGZ1
В	-4	ILE	-	expression tag	UNP P9WGZ1
В	-3	GLU		expression tag	UNP P9WGZ1
В	-2	GLY	-	expression tag	UNP P9WGZ1
В	-1	ARG	-	expression tag	UNP P9WGZ1
В	0	HIS	-	expression tag	UNP P9WGZ1

• Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
2	С	1139	Total 8572	C 5364	N 1504	O 1665	S 39	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	5	MET	-	initiating methionine	UNP P9WGY9
С	6	VAL	-	expression tag	UNP P9WGY9

• Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues		A	toms		ZeroOcc	AltConf	Trace	
3	D	1260	Total 9802	C 6141	N 1774	O 1847	S 40	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P9WGY7
D	1	VAL	-	expression tag	UNP P9WGY7



• Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
4	Е	76	Total 594	C 379	N 101	O 114	0	0	0

• Molecule 5 is a protein called ECF RNA polymerase sigma factor SigH,ECF RNA polymerase sigma factor SigE,ECF RNA polymerase sigma factor SigH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	164	Total 1238	C 774	N 221	O 238	S 5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P9WGH9
F	0	ALA	-	expression tag	UNP P9WGH9

• Molecule 6 is a DNA chain called DNA (5'-D(*TP*TP*GP*TP*GP*GP*GP*AP*GP*CP* TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*A)-3').

Mo	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
6	C	23	Total	С	N	О	Р	0	0	0
0	G	20	464	221	84	137	22	U	0	U

• Molecule 7 is a DNA chain called DNA (5'-D(*TP*GP*CP*AP*TP*CP*GP*TP*GP* AP*GP*TP*CP*GP*AP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
7	Н	20	Total 412	C 196	N 77	O 120	P 19	0	0	0

• Molecule 8 is a RNA chain called RNA (5'-R(*CP*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
Q	Т	6	Total	С	N	О	Р	0	0	0
0	1	0	122	56	21	40	5	U		U

• Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	Total Zn 2 2	0	0

 \bullet Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total Mg 1 1	0	0

• Molecule 11 is water.

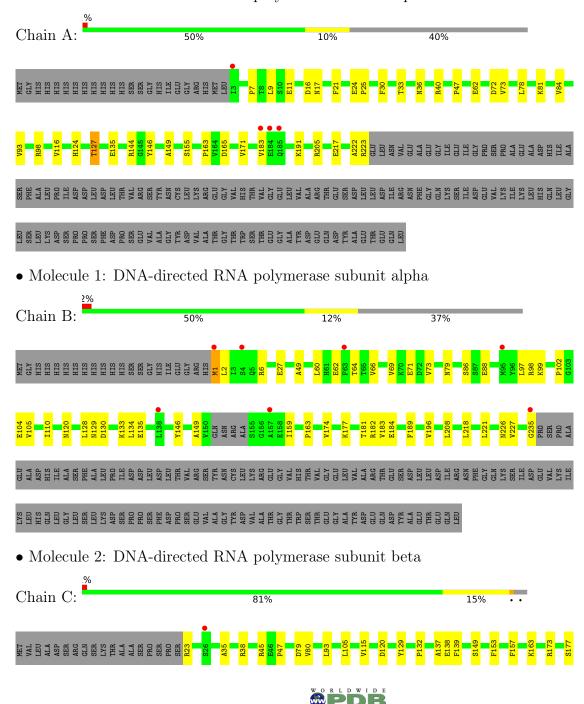
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	11	Total O 11 11	0	0
11	В	9	Total O 9 9	0	0
11	С	37	Total O 37 37	0	0
11	D	58	Total O 58 58	0	0
11	E	2	Total O 2 2	0	0
11	F	5	Total O 5 5	0	0
11	G	1	Total O 1 1	0	0
11	Н	6	Total O 6 6	0	0
11	I	1	Total O 1 1	0	0

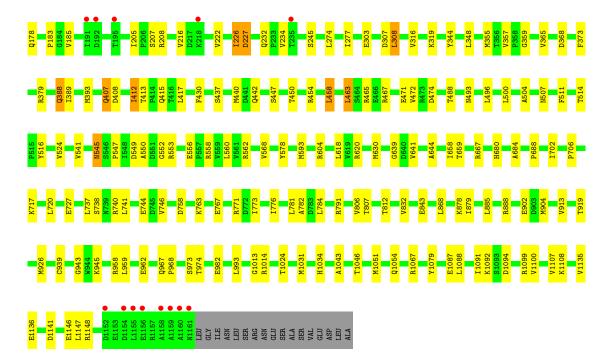


3 Residue-property plots (i)

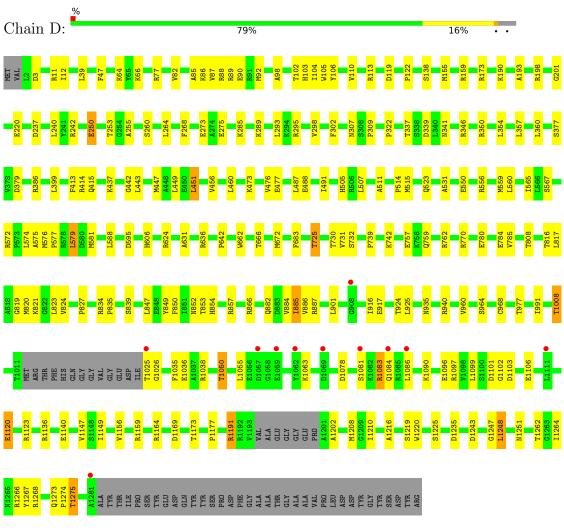
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA-directed RNA polymerase subunit alpha



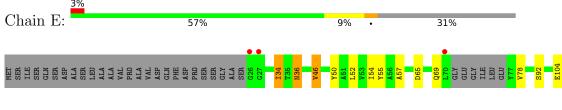


• Molecule 3: DNA-directed RNA polymerase subunit beta'



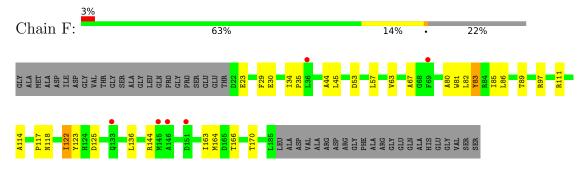


• Molecule 4: DNA-directed RNA polymerase subunit omega





• Molecule 5: ECF RNA polymerase sigma factor SigH,ECF RNA polymerase sigma factor SigE,ECF RNA polymerase sigma factor SigH



• Molecule 6: DNA (5'-D(*TP*TP*GP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*A)-3')



 \bullet Molecule 7: DNA (5'-D(*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP *GP*GP*T)-3')



• Molecule 8: RNA (5'-R(*CP*CP*UP*CP*GP*A)-3')

Chain I:

There are no outlier residues recorded for this chain.



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	128.94Å 163.00Å 129.31Å	Donositon
a, b, c, α , β , γ	90.00° 117.81° 90.00°	Depositor
Resolution (Å)	48.77 - 3.11	Depositor
Resolution (A)	49.05 - 3.11	EDS
% Data completeness	92.5 (48.77-3.11)	Depositor
(in resolution range)	92.6 (49.05-3.11)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\frac{R_{sym}}{\langle I/\sigma(I)\rangle^{-1}}$	1.91 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
D D	0.195 , 0.238	Depositor
R, R_{free}	0.195 , 0.238	DCC
R_{free} test set	2376 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	92.6	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.26 , 46.7	EDS
L-test for twinning ²	$< L > = 0.47, < L^2> = 0.30$	Xtriage
	0.012 for -h-l,k,h	
	0.012 for l,k,-h-l	
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
	0.027 for -h-l,-k,l	
	0.025 for l,-k,h	
F_o, F_c correlation	0.95	EDS
Total number of atoms	24729	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.58% 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, MG

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		RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.26	0/1699	0.47	0/2313
1	В	0.25	0/1744	0.46	0/2375
2	С	0.27	0/8730	0.45	0/11869
3	D	0.26	0/9966	0.43	0/13479
4	Е	0.25	0/605	0.41	0/823
5	F	0.24	0/1263	0.39	0/1722
6	G	0.62	0/520	0.98	0/802
7	Н	0.58	0/462	0.92	0/713
8	I	0.32	0/135	0.88	0/208
All	All	0.28	0/25124	0.48	0/34304

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	1673	0	1707	24	0
1	В	1719	0	1737	28	0
2	С	8572	0	8294	113	0
3	D	9802	0	9817	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Ε	594	0	589	9	0
5	F	1238	0	1131	21	0
6	G	464	0	256	16	0
7	Н	412	0	227	8	0
8	I	122	0	66	0	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	A	11	0	0	1	0
11	В	9	0	0	0	0
11	С	37	0	0	1	0
11	D	58	0	0	1	0
11	Ε	2	0	0	0	0
11	F	5	0	0	0	0
11	G	1	0	0	0	0
11	Н	6	0	0	0	0
11	I	1	0	0	0	0
All	All	24729	0	23824	298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 298 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:7:PRO:HA	1:A:25:PRO:HG2	1.55	0.89
1:B:62:GLU:HG3	1:B:64:THR:HG22	1.65	0.78
3:D:882:GLN:HB2	3:D:1248:LEU:HD11	1.67	0.75
3:D:1274:PRO:HG3	4:E:78:VAL:HG11	1.70	0.72
1:A:24:GLU:HG2	1:A:191:LYS:HG3	1.70	0.71

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 r	number of	residues for	which	the	backbone	conformation	was
analysed, and the total number of	residues.						

Mol	Chain	Analysed	ysed Favoured		Outliers	Percen	tiles
1	A	$219/368\ (60\%)$	211 (96%)	8 (4%)	0	100	100
1	В	$227/368\ (62\%)$	213 (94%)	14 (6%)	0	100	100
2	\mathbf{C}	1137/1174~(97%)	1091 (96%)	46 (4%)	0	100	100
3	D	1254/1317~(95%)	1218 (97%)	36 (3%)	0	100	100
4	\mathbf{E}	72/110~(66%)	69 (96%)	3 (4%)	0	100	100
5	F	162/209~(78%)	159 (98%)	3 (2%)	0	100	100
All	All	3071/3546 (87%)	2961 (96%)	110 (4%)	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 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	188/315 (60%)	177 (94%)	11 (6%)	19 50		
1	В	189/315 (60%)	185 (98%)	4 (2%)	53 79		
2	С	897/995 (90%)	863 (96%)	34 (4%)	33 66		
3	D	1032/1096 (94%)	1003 (97%)	29 (3%)	43 73		
4	Е	63/90 (70%)	58 (92%)	5 (8%)	12 40		
5	F	115/167 (69%)	108 (94%)	7 (6%)	18 49		
All	All	2484/2978 (83%)	2394 (96%)	90 (4%)	35 67		

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

Mol	Chain	Res	Type
3	D	443	LEU
3	D	1120	GLU
3	D	505	HIS
3	D	885	ILE
3	D	1248	LEU



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

Mol	Chain	Res	Type
2	С	680	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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)

Of 3 ligands modelled in this entry, 3 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)

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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(m \AA^2)$	Q<0.9
1	A	221/368~(60%)	-0.27	4 (1%) 68 47	66, 83, 133, 168	0
1	В	231/368 (62%)	0.03	7 (3%) 50 27	85, 125, 155, 162	0
2	С	1139/1174 (97%)	-0.16	14 (1%) 79 61	54, 88, 147, 170	0
3	D	1260/1317 (95%)	-0.24	11 (0%) 84 69	59, 95, 146, 178	0
4	E	76/110 (69%)	-0.02	3 (3%) 39 20	90, 117, 139, 145	0
5	F	164/209 (78%)	0.21	6 (3%) 41 21	81, 136, 160, 165	0
6	G	23/23 (100%)	-0.19	0 100 100	93, 134, 158, 165	1 (4%)
7	Н	20/20 (100%)	-0.54	0 100 100	67, 88, 148, 149	0
8	I	6/6 (100%)	-0.35	0 100 100	60, 62, 72, 87	0
All	All	3140/3595 (87%)	-0.17	45 (1%) 75 56	54, 97, 150, 178	1 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	С	1160	ALA	5.7
3	D	1281	ALA	5.6
4	Е	70	LEU	5.5
2	С	1159	ALA	4.7
2	С	1155	LEU	4.4

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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
10	MG	D	2003	1/1	0.89	0.13	59,59,59,59	0
9	ZN	D	2002	1/1	0.98	0.13	123,123,123,123	0
9	ZN	D	2001	1/1	0.99	0.17	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.

