

wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 03:20 AM JST

PDB ID	:	7EH2
Title	:	Thermus thermophilus transcription initiation complex containing a template-
		strand pyrimidine at position TSS-2 and GpG RNA primer
Authors	:	Li, L.; Zhang, Y.
Deposited on	:	2021-03-27
Resolution	:	3.34 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	:	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 3.34 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.



]	Percentile	relative	to	X-ray	structures	of	similar	resolution	

Motria	Whole archive	Similar resolution			
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$			
R_{free}	130704	1060 (3.38-3.30)			
Clashscore	141614	1111 (3.38-3.30)			
Ramachandran outliers	138981	1090 (3.38-3.30)			
Sidechain outliers	138945	1089 (3.38-3.30)			
RSRZ outliers	127900	1028 (3.38-3.30)			
RNA backbone	3102	1129 (3.78-2.90)			

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	Qua	lity of chain	
1	А	315	3% 52%	20% •	27%
1	В	315	5%	16% ·	30%
1	K	315	<mark>6%</mark> 54%	16% •	28%
1	L	315	53%	17% •	29%



Mol	Chain	Length	Quality of chain						
2	С	1119	77%		21% •••				
2	М	1119	74%		23% ••				
3	D	1524	77%		18% ••				
3	Ν	1524	4% 75%		21% ••				
4	Е	99	72%		22% • 5%				
4	0	99	2% – 76%		19% 5%				
5	F	443	4% 65%	12% •	22%				
5	Р	443	6% 63%	15%	22%				
6	G	27	44%	48%	7%				
6	J	27	33%	59%	7%				
7	Н	19	37%	53%	11%				
7	Ω	19	42%	47%	11%				
8	T	2		100%					
8	R	2		100%					



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 56841 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		Ate	oms			ZeroOcc	AltConf	Trace
1	Δ	220	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	229	1777	1136	306	333	2	0	0	0
1	В	າາາ	Total	С	Ν	0	S	0	0	0
	D		1750	1118	304	326	2	0	0	0
1	K	К 227	Total	С	Ν	0	S	0	0	0
1	Γ		1781	1138	308	333	2	0		0
1	т	225	Total	С	Ν	0	S	0	0	0
	Ц	220	1773	1133	308	330	2		0	0

• Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

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

Mol	Chain	Residues		Atoms					AltConf	Trace
2	С	1111	Total 8742	C 5534	N 1552	O 1632	S 24	0	0	0
2	М	1111	Total 8724	C 5520	N 1551	O 1629	S 24	0	0	0

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

Mol	Chain	Residues		Atoms					AltConf	Trace
3	D	1486	Total	С	Ν	0	S	0	0	0
			11680	7405	2051	2189	35	Ŭ		
3	N	1486	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
3	IN	1480	11675	7402	2047	2191	35	0		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Е	94	Total 761	C 486	N 132	O 139	S 4	0	0	0
4	О	94	Total 761	C 486	N 132	0 139	${S \atop 4}$	0	0	0





• Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
5	F	346	Total	С	Ν	0	S	0	0	0
5	I.		2803	1768	509	522	4	0		
5	D	247	Total	С	Ν	0	S	0	0	0
D	Р	347	2757	1738	490	525	4		U	U

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1
Р	-19	MET	-	expression tag	UNP Q5SKW1
Р	-18	GLY	-	expression tag	UNP Q5SKW1
Р	-17	SER	-	expression tag	UNP Q5SKW1
Р	-16	SER	-	expression tag	UNP Q5SKW1
Р	-15	HIS	-	expression tag	UNP Q5SKW1
Р	-14	HIS	-	expression tag	UNP Q5SKW1
Р	-13	HIS	-	expression tag	UNP Q5SKW1
Р	-12	HIS	-	expression tag	UNP Q5SKW1
Р	-11	HIS	-	expression tag	UNP Q5SKW1
Р	-10	HIS	-	expression tag	UNP Q5SKW1
Р	-9	SER	-	expression tag	UNP Q5SKW1
Р	-8	SER	-	expression tag	UNP Q5SKW1
Р	-7	GLY	-	expression tag	UNP Q5SKW1
Р	-6	LEU	-	expression tag	UNP Q5SKW1



	<i>v</i> 1	1 0			
Chain	Residue	Modelled	Actual	Comment	Reference
Р	-5	VAL	-	expression tag	UNP Q5SKW1
Р	-4	PRO	-	expression tag	UNP Q5SKW1
Р	-3	ARG	-	expression tag	UNP Q5SKW1
Р	-2	GLY	-	expression tag	UNP Q5SKW1
Р	-1	SER	-	expression tag	UNP Q5SKW1
Р	0	HIS	-	expression tag	UNP Q5SKW1

• Molecule 6 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
6	С	25	Total	С	Ν	Ο	Р	0	0	0
0	G	20	516	246	99	147	24	0	0	
6	т	25	Total	С	Ν	0	Р	0	0	0
0	1	2.0	516	246	99	147	24	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
7	Ц	17	Total	С	Ν	0	Р	0	0	0
1	11	17	345	165	63	101	16	0	0	0
7	0	17	Total	С	Ν	0	Р	0	0	0
'	V V	11	345	165	63	101	16	0		U

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
0	т	2	Total	С	Ν	Ο	Р	0	0	0
0	1	2	43	20	10	12	1	0	0	0
0	D	0	Total	С	Ν	Ο	Р	0	0	0
0	n	2	43	20	10	12	1	0	0	0

• 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
9	N	2	Total Zn 2 2	0	0

• 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
10	L	1	Total Mg 1 1	0	0
10	Ν	1	Total Mg 1 1	0	0

• Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	А	4	Total O 4 4	0	0
11	В	4	Total O 4 4	0	0
11	С	5	Total O 5 5	0	0
11	D	10	Total O 10 10	0	0
11	Ε	2	Total O 2 2	0	0
11	F	1	Total O 1 1	0	0
11	К	2	Total O 2 2	0	0
11	L	1	Total O 1 1	0	0
11	М	1	Total O 1 1	0	0
11	Ν	9	Total O 9 9	0	0
11	О	2	Total O 2 2	0	0
11	G	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 1: DNA-directed RNA polymerase subunit alpha







• Molecule 2: DNA-directed RNA polymerase subunit beta





L717

• Molecule 2: DNA-directed RNA polymerase subunit beta Chain M: 74% 23% •• GLU GLY GLY GLY GLY GLY D1058 D1059 11060 A11 S11 K11 ARG

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

Chain D: 77% 18%



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Chain F:	65%	12%	22%
	メルンししのンれる下のの丸ののの人人がよ		
9 5 8 8 H H H H H H H H H	SEE SEE SEE SEE SEE SEE SEE SEE SEE SEE	5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	LE AS PR CLE
GLU ASP PRO ASP ASP LEU LEU GLU ASP	LEU ASP ASP ASP ASP CLU CLU CLU ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	LVS LVS LVS LVS LVS LVS LVS LVS LVS LVS	E10 K10 T12 C12 C12 E12 C13 C13 C13 C13 C13 C13 C13 C13 C13 C13
813 8140 8144 8144 9144 115 115 115 115 115 115 115 115 115	116 116 117 117 117 117 117 117 117 117	118 118 118 120 120 1210 1210 1210 1210	F23 F23 F23 G25 G25 G25 G25 G25 G28 G28 G28 G28 G28 G28 G28 G26 G28 G26 G26 G26 G26 G26 G26 G26 G27 G26 G27 G27 G27 G27 G27 G27 G27 G27 G27 G27
05 26 61 62 62 7 65 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9	5 5 5 5 5 5 5 6 6 6 6 6 6 6 6 6 7 7 7 7 7 7 7 7 7 7	
		12 14 14 14 14	
• Molecule 5:	RNA polymerase sigma facto	or SigA	
Chain P:	63%	15%	22%
MET GLY SER HIS HIS HIS HIS HIS HIS	SER GLY VAL LEU VAL LEU ARO GLY SER MET LYS SER LYS SER ARG CLY SARA AASN AASN AASN AASN AASN AASN AASN	GLN GLU GLU GLU GLU GLU VAL LEU LLEU GLU GLU GLU GLU GLU	GLU PRO GLU GLU GLU GLU PRO GLU PRO ASP PRO ASP
GLU ASP PRO ASP ASP LEU GLU ASP ASP	LEU ASP PRO GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU	LLE PRO LLYS SER Y84 G89 G89 G89 C132 L122 L122	1127 1127 1127 1132 1136 1136 1136 1137 1138 1139 1141 1141 1142
D152 P153 L163 L163 L173 H175	R178 1192 1192 1193 1193 1193 1193 1193 1193	A239 W242 1244 R244 R273 R273 Q277 L278 T287 T287	E318 E318 E318 E318 E318 E318
K325 ● D326 ● F332 F332 F332 ● F341 - F354 ●	L356 2362 8362 8364 8365 8365 8365 8365 8366 1376 1376 1376 1376 1376 1376 1376 1	A388 6399 1339 1339 1400 6401 1400 6401 1400 8403 8401 1400 8403 8403 8403 8403 8403 8403 8403 8	A404 R406 R406 E412 E412 R419 R419 P423
• Moleculo 6:	DNA (97 MED)		
• Molecule 0:	DNA (27-MER)		
Chain G:	44%	48%	7%
• Molecule 6:	DNA (27-MER)		
Chain J:	33%	59%	7%
• Molecule 7: TP*AP*G)-3 ⁷	DNA $(5'-D(*CP*C*TP*GP))$	*CP*AP*TP*CP*C	P*GP*TP*GP*A





• Molecule 7: DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*CP*CP* TP*AP*G)-3')

Chain Q:	42%	47%	11%
DC DC CC CC A6 C0 C0 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	C16 117 A18 G19		
• Molecule 8: R	1 NA (5'-R(*GP*G)-3)	')	
Chain I:		100%	
There are no ou	tlier residues recorde	d for this chain.	
• Molecule 8: R	LNA (5'-R(*GP*G)-3	')	
Chain R:		100%	

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	184.85Å 104.20Å 296.65Å	Depositor
a, b, c, α , β , γ	90.00° 98.42° 90.00°	Depositor
Bosolution (Å)	97.82 - 3.34	Depositor
Resolution (A)	123.62 - 3.34	EDS
% Data completeness	99.3 (97.82-3.34)	Depositor
(in resolution range)	$99.6\ (123.62-3.34)$	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.35 (at 3.33 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
D D .	0.201 , 0.247	Depositor
n, n_{free}	0.201 , 0.246	DCC
R_{free} test set	8256 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	88.8	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.29, 59.4	EDS
L-test for $twinning^2$	$ L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	56841	wwPDB-VP
Average B, all atoms $(Å^2)$	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 38.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8581e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: MG, 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).

Mal	Chain	Bond	lengths	Bo	ond angles
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/1809	0.46	0/2464
1	В	0.25	0/1782	0.45	0/2424
1	Κ	0.26	0/1813	0.47	0/2466
1	L	0.26	0/1805	0.47	0/2454
2	С	0.26	0/8909	0.44	0/12054
2	М	0.26	0/8890	0.45	1/12030~(0.0%)
3	D	0.25	0/11885	0.44	0/16081
3	Ν	0.25	0/11880	0.44	0/16074
4	Е	0.24	0/775	0.41	0/1045
4	0	0.25	0/775	0.40	0/1045
5	F	0.25	0/2848	0.41	0/3832
5	Р	0.25	0/2800	0.41	0/3777
6	G	0.54	0/580	0.93	0/895
6	J	0.55	0/580	0.95	0/895
7	Н	0.56	0/386	0.92	0/594
7	Q	0.54	0/386	0.90	0/594
8	Ι	0.30	0/48	0.92	0/74
8	R	0.35	0/48	1.06	0/74
All	All	0.27	0/57999	0.47	1/78872~(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
3	D	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	М	211	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	274	ARG	Peptide
3	D	276	ASP	Peptide

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	1777	0	1812	42	0
1	В	1750	0	1797	31	0
1	K	1781	0	1828	32	0
1	L	1773	0	1826	35	0
2	С	8742	0	8826	138	0
2	М	8724	0	8795	165	0
3	D	11680	0	11864	187	0
3	N	11675	0	11851	203	0
4	Е	761	0	778	14	0
4	0	761	0	778	12	0
5	F	2803	0	2878	39	0
5	Р	2757	0	2780	47	0
6	G	516	0	283	10	0
6	J	516	0	283	15	0
7	Н	345	0	193	9	0
7	Q	345	0	193	10	0
8	Ι	43	0	23	0	0
8	R	43	0	23	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	1	0	0	0	0
10	L	1	0	0	0	0
10	Ν	1	0	0	0	0
11	А	4	0	0	0	0
11	В	4	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
11	С	5	0	0	0	0		
11	D	10	0	0	0	0		
11	Е	2	0	0	0	0		
11	F	1	0	0	0	0		
11	G	1	0	0	0	0		
11	Κ	2	0	0	0	0		
11	L	1	0	0	0	0		
11	М	1	0	0	0	0		
11	Ν	9	0	0	3	0		
11	0	2	0	0	0	0		
All	All	56841	0	56811	882	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 8.

The worst 5 of 882 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:M:462:ASP:HB3	2:M:468:ARG:HD2	1.58	0.84
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.62	0.81
2:M:683:ASN:HB3	2:M:872:ASN:HB2	1.61	0.81
5:P:408:LEU:O	5:P:412:GLU:HB2	1.83	0.77
3:N:60:CYS:SG	11:N:1702:HOH:O	2.43	0.76

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	227/315~(72%)	220 (97%)	7(3%)	0	100	100
1	В	220/315~(70%)	214 (97%)	6 (3%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	Κ	225/315~(71%)	219~(97%)	6 (3%)	0	100	100
1	L	223/315~(71%)	219 (98%)	4 (2%)	0	100	100
2	С	$1107/1119 \ (99\%)$	1082 (98%)	25~(2%)	0	100	100
2	М	1107/1119 (99%)	1077 (97%)	30 (3%)	0	100	100
3	D	1482/1524~(97%)	1447 (98%)	35~(2%)	0	100	100
3	Ν	1482/1524~(97%)	1446 (98%)	36 (2%)	0	100	100
4	Е	92/99~(93%)	90 (98%)	2 (2%)	0	100	100
4	Ο	92/99~(93%)	91 (99%)	1 (1%)	0	100	100
5	F	344/443~(78%)	342 (99%)	2 (1%)	0	100	100
5	Р	345/443~(78%)	334 (97%)	11 (3%)	0	100	100
All	All	6946/7630 ($91%$)	6781 (98%)	165 (2%)	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	Perce	ntiles
1	А	195/273~(71%)	185~(95%)	10~(5%)	24	57
1	В	195/273~(71%)	179~(92%)	16 (8%)	11	39
1	Κ	198/273~(72%)	182 (92%)	16 (8%)	11	39
1	L	198/273~(72%)	188~(95%)	10 (5%)	24	57
2	С	931/941~(99%)	879~(94%)	52~(6%)	21	54
2	М	927/941~(98%)	879~(95%)	48~(5%)	23	56
3	D	1241/1279~(97%)	1175~(95%)	66~(5%)	22	56
3	Ν	1240/1279~(97%)	1181 (95%)	59~(5%)	25	59
4	Ε	83/88~(94%)	79~(95%)	4(5%)	25	59
4	Ο	83/88~(94%)	81 (98%)	2(2%)	49	75
5	F	300/388~(77%)	289~(96%)	11 (4%)	34	64



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	Р	291/388~(75%)	281 (97%)	10 (3%)	37 67
All	All	5882/6484~(91%)	5578 (95%)	304 (5%)	23 56

5 of 304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	М	939	ARG
3	Ν	1413	THR
3	Ν	142	LEU
3	Ν	686	GLU
5	Р	376	ILE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such side chains are listed below:

Mol	Chain	Res	Type
2	С	704	HIS
3	D	973	GLN
2	М	141	HIS
2	М	704	HIS
3	Ν	994	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	Ι	1/2~(50%)	0	0
8	R	1/2~(50%)	0	0
All	All	2/4~(50%)	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 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)

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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$Q{<}0.9$
1	А	229/315~(72%)	0.39	10 (4%) 34 35	63, 82, 107, 131	0
1	В	222/315~(70%)	0.55	16 (7%) 15 16	66, 96, 127, 148	0
1	K	227/315~(72%)	0.55	20 (8%) 10 10	70, 92, 113, 130	0
1	L	225/315~(71%)	0.47	18 (8%) 12 12	68, 99, 133, 152	0
2	С	$1111/1119 \ (99\%)$	0.17	5 (0%) 91 91	46, 80, 132, 163	0
2	М	$1111/1119 \ (99\%)$	0.28	20 (1%) 68 67	51, 100, 161, 179	0
3	D	1486/1524~(97%)	0.32	53 (3%) 42 41	48, 83, 143, 186	1 (0%)
3	N	1486/1524~(97%)	0.34	62 (4%) 36 36	52, 90, 142, 196	1 (0%)
4	Е	94/99~(94%)	0.23	0 100 100	63, 85, 122, 130	0
4	Ο	94/99~(94%)	0.14	2 (2%) 63 63	71, 100, 137, 144	0
5	F	346/443~(78%)	0.35	16 (4%) 32 33	58, 91, 135, 158	0
5	Р	347/443~(78%)	0.53	26 (7%) 14 14	70, 108, 173, 191	0
6	G	25/27~(92%)	-0.08	0 100 100	87, 128, 187, 196	0
6	J	25/27~(92%)	0.13	0 100 100	90, 134, 190, 196	0
7	Н	17/19~(89%)	0.04	0 100 100	77, 110, 182, 190	0
7	Q	17/19~(89%)	0.04	0 100 100	93, 122, 186, 189	0
8	Ι	2/2~(100%)	0.75	0 100 100	79, 79, 79, 85	2 (100%)
8	R	2/2~(100%)	0.30	0 100 100	88, 88, 88, 93	2 (100%)
All	All	7066/7726~(91%)	0.32	248 (3%) 44 43	46, 91, 148, 196	6 (0%)

The worst 5 of 248 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	Р	392	VAL	8.5
1	В	138	LEU	5.2
5	Р	391	GLY	5.1



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Mol	Chain	\mathbf{Res}	Type	RSRZ
3	Ν	394	LEU	4.8
5	Р	389	PHE	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
10	MG	L	401	1/1	0.77	0.17	77,77,77,77	0
9	ZN	Ν	1601	1/1	0.95	0.24	93,93,93,93	0
10	MG	N	1603	1/1	0.98	0.23	61,61,61,61	0
10	MG	D	2003	1/1	0.99	0.24	54,54,54,54	0
9	ZN	D	2001	1/1	0.99	0.23	78,78,78,78	0
9	ZN	N	1602	1/1	0.99	0.15	129,129,129,129	0
9	ZN	D	2002	1/1	1.00	0.17	95,95,95,95	0

6.5 Other polymers (i)

There are no such residues in this entry.

