

Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2024 – 10:11 AM EDT

:	8U9L
:	Crystal Structure of RelA-cRel chimera complex with DNA
:	Chang, A.; Wu, Y.; Li, S.X.; Smale, S.; Chen, L.
:	2023-09-19
:	3.09 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
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 3.09 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.



Matria	Whole archive	Similar resolution		
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R _{free}	164625	1351 (3.10-3.10)		
Clashscore	180529	1454 (3.10-3.10)		
Ramachandran outliers	177936	1391 (3.10-3.10)		
Sidechain outliers	177891	1391 (3.10-3.10)		
RSRZ outliers	164620	1351 (3.10-3.10)		

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	С	20	30%	65%	5%
1	Е	20	25%	65%	10%
1	Ι	20	5% 45%	50%	
1	М	20	50%	50%	
2	D	20	25%	60%	15%



Mol	Chain	Length		Qu	ality of chain		
2	F	20	15%		60%	25%	
2	J	20	30)%	70%		
2	Ν	20	10%	30%	60%		
3	А	277		68%		28%	·
3	В	277		68%		26%	5%•
3	G	277		70%		25%	•
3	Н	277		71%		21%	6% •
3	Κ	277		69%		29%	•
3	L	277		62%		30%	6% •
3	Ο	277		69%		27%	•
3	Р	277		65%		29%	5% •



$\mathbf{2}$ Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20864 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 DNA chain called DNA (5'-D(P*TP*TP*GP*AP*TP*GP*GP*GP*AP*AP *TP*TP*TP*CP*CP*GP*AP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	20	Total	С	Ν	Ο	Р	0	0	0
1	Ľ	20	412	197	70	125	20	0	0	0
1	С	20	Total	С	Ν	Ο	Р	0	0	0
1	U	20	412	197	70	125	20		0	
1	т	20	Total	С	Ν	Ο	Р	0	0	0
1	1		412	197	70	125	20		0	
1	1 M	20	Total	С	Ν	0	Р	0	0	0
			412	197	70	125	20	U	U	U

• Molecule 2 is a DNA chain called DNA (5'-D(P*GP*AP*AP*TP*CP*GP*GP*AP*AP*AP *TP*TP*CP*CP*CP*AP*TP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	Б	20	Total	С	Ν	0	Р	0	0	0
	Г	20	410	195	78	117	20	0	0	0
0	П	20	Total	С	Ν	0	Р	0	0	0
	D	20	410	195	78	117	20	0		0
0	т	20	Total	С	Ν	0	Р	0	0	0
	J		410	195	78	117	20			0
0	O N	20	Total	С	Ν	0	Р	0	0	0
	20	410	195	78	117	20	0		0	

• Molecule 3 is a protein called Transcription factor p65,Proto-oncogene c-Rel chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3		276	Total	С	Ν	Ο	\mathbf{S}	0	0	0
5	Л	270	2203	1388	394	410	11	0	0	
2	В	274	Total	С	Ν	0	S	0	0	0
J	D	214	2191	1382	391	407	11			
9	С	276	Total	С	Ν	0	S	0	0	0
3	3 G	270	2203	1388	394	410	11	0	0	0



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	Ц	274	Total	С	Ν	Ο	\mathbf{S}	0	0	0
5	11	214	2191	1382	391	407	11	0	0	0
2	K	276	Total	С	Ν	Ο	S	0	0	0
5	Γ	270	2203	1388	394	410	11	0	0	
2	т	274	Total	С	Ν	0	S	0	0	0
5			2191	1382	391	407	11			
2	0	276	Total	С	Ν	0	S	0	0	0
5	3 0	270	2203	1388	394	410	11	0	0	0
2	3 P	274	Total	С	Ν	0	S	0	0	0
J			2191	1382	391	407	11	0		U

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There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP Q04207
А	111	GLU	GLY	conflict	UNP P15307
А	127	PRO	GLY	conflict	UNP P15307
А	144	LEU	CYS	conflict	UNP P15307
А	145	CYS	VAL	conflict	UNP P15307
А	147	GLN	MET	conflict	UNP P15307
А	148	VAL	PHE	conflict	UNP P15307
А	154	HIS	ASP	conflict	UNP P15307
А	171	ASP	-	linker	UNP P15307
А	172	ASN	-	linker	UNP P15307
А	173	ARG	-	linker	UNP P15307
А	174	ALA	-	linker	UNP P15307
А	175	PRO	-	linker	UNP P15307
А	176	ASN	-	linker	UNP P15307
В	1	MET	-	initiating methionine	UNP Q04207
В	111	GLU	GLY	conflict	UNP P15307
В	127	PRO	GLY	conflict	UNP P15307
В	144	LEU	CYS	conflict	UNP P15307
В	145	CYS	VAL	conflict	UNP P15307
В	147	GLN	MET	conflict	UNP P15307
В	148	VAL	PHE	conflict	UNP P15307
В	154	HIS	ASP	conflict	UNP P15307
В	171	ASP	-	linker	UNP P15307
В	172	ASN	-	linker	UNP P15307
В	173	ARG	-	linker	UNP P15307
B	174	ALA	-	linker	UNP P15307
В	175	PRO	-	linker	UNP P15307
В	176	ASN	-	linker	UNP P15307
G	1	MET	-	initiating methionine	UNP Q04207



Chain	Residue	Modelled	Actual	Comment	Reference
G	111	GLU	GLY	conflict	UNP P15307
G	127	PRO	GLY	conflict	UNP P15307
G	144	LEU	CYS	conflict	UNP P15307
G	145	CYS	VAL	conflict	UNP P15307
G	147	GLN	MET	conflict	UNP P15307
G	148	VAL	PHE	conflict	UNP P15307
G	154	HIS	ASP	conflict	UNP P15307
G	171	ASP	-	linker	UNP P15307
G	172	ASN	-	linker	UNP P15307
G	173	ARG	-	linker	UNP P15307
G	174	ALA	-	linker	UNP P15307
G	175	PRO	-	linker	UNP P15307
G	176	ASN	-	linker	UNP P15307
Н	1	MET	-	initiating methionine	UNP Q04207
Н	111	GLU	GLY	conflict	UNP P15307
Н	127	PRO	GLY	conflict	UNP P15307
Н	144	LEU	CYS	conflict	UNP P15307
Н	145	CYS	VAL	conflict	UNP P15307
Н	147	GLN	MET	conflict	UNP P15307
Н	148	VAL	PHE	conflict	UNP P15307
Н	154	HIS	ASP	conflict	UNP P15307
Н	171	ASP	-	linker	UNP P15307
Н	172	ASN	-	linker	UNP P15307
Н	173	ARG	-	linker	UNP P15307
Н	174	ALA	-	linker	UNP P15307
Н	175	PRO	-	linker	UNP P15307
Н	176	ASN	-	linker	UNP P15307
K	1	MET	-	initiating methionine	UNP Q04207
K	111	GLU	GLY	conflict	UNP P15307
K	127	PRO	GLY	conflict	UNP P15307
K	144	LEU	CYS	conflict	UNP P15307
K	145	CYS	VAL	conflict	UNP P15307
K	147	GLN	MET	conflict	UNP P15307
K	148	VAL	PHE	conflict	UNP P15307
K	154	HIS	ASP	conflict	UNP P15307
K	171	ASP	-	linker	UNP P15307
K	172	ASN	-	linker	UNP P15307
K	173	ARG	-	linker	UNP P15307
K	174	ALA	-	linker	UNP P15307
K	175	PRO	-	linker	UNP P15307
K	176	ASN	-	linker	UNP P15307
L	1	MET	-	initiating methionine	UNP Q04207



Chain	Residue	Modelled	Actual	Comment	Reference
L	111	GLU	GLY	conflict	UNP P15307
L	127	PRO	GLY	conflict	UNP P15307
L	144	LEU	CYS	CYS conflict	
L	145	CYS	VAL	conflict	UNP P15307
L	147	GLN	MET	conflict	UNP P15307
L	148	VAL	PHE	conflict	UNP P15307
L	154	HIS	ASP	conflict	UNP P15307
L	171	ASP	-	linker	UNP P15307
L	172	ASN	-	linker	UNP P15307
L	173	ARG	-	linker	UNP P15307
L	174	ALA	-	linker	UNP P15307
L	175	PRO	-	linker	UNP P15307
L	176	ASN	-	linker	UNP P15307
0	1	MET	-	initiating methionine	UNP Q04207
0	111	GLU	GLY	conflict	UNP P15307
0	127	PRO	GLY	conflict	UNP P15307
0	144	LEU	CYS	conflict	UNP P15307
0	145	CYS	VAL	conflict	UNP P15307
0	147	GLN	MET	conflict	UNP P15307
0	148	VAL	PHE	conflict	UNP P15307
0	154	HIS	ASP	conflict	UNP P15307
0	171	ASP	-	linker	UNP P15307
0	172	ASN	-	linker	UNP P15307
0	173	ARG	-	linker	UNP P15307
0	174	ALA	-	linker	UNP P15307
0	175	PRO	-	linker	UNP P15307
0	176	ASN	-	linker	UNP P15307
Р	1	MET	-	initiating methionine	UNP Q04207
Р	111	GLU	GLY	conflict	UNP P15307
Р	127	PRO	GLY	conflict	UNP P15307
Р	144	LEU	CYS	conflict	UNP P15307
Р	145	CYS	VAL	conflict	UNP P15307
Р	147	GLN	MET	conflict	UNP P15307
Р	148	VAL	PHE	conflict	UNP P15307
Р	154	HIS	ASP	conflict	UNP P15307
Р	171	ASP	-	linker	UNP P15307
Р	172	ASN	-	linker	UNP P15307
Р	173	ARG	-	linker	UNP P15307
Р	174	ALA	-	linker	UNP P15307
Р	175	PRO	-	linker	UNP P15307
Р	176	ASN	_	linker	UNP P15307



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 (5'-D(P*TP*TP*GP*AP*TP*GP*GP*GP*AP*AP*TP*TP*TP*CP*CP*G P*AP*TP*TP*C)-3')



• Molecule 1: DNA (5'-D(P*TP*TP*GP*AP*TP*GP*GP*GP*AP*AP*TP*TP*TP*CP*CP*G P*AP*TP*TP*C)-3')



• Molecule 1: DNA (5'-D(P*TP*TP*GP*AP*TP*GP*GP*GP*AP*AP*TP*TP*TP*CP*CP*G P*AP*TP*TP*C)-3')

• Molecule 1: DNA (5'-D(P*TP*TP*GP*AP*TP*GP*GP*GP*AP*AP*TP*TP*TP*CP*CP*G P*AP*TP*TP*C)-3')



• Molecule 2: DNA (5'-D(P*GP*AP*AP*TP*CP*GP*GP*AP*AP*AP*TP*TP*CP*CP*CP*AP*AP*AP)-3')

Chain F:	15%	60%	25%
G1 A2 A3 C5 C5 G6	A9 A10 T11 T12 C13 C13 C13 C13 A16 C14 C15 C15 C18 C18 A19 A20		
		WORLDWIDE	

• Molecule 2: DNA (5'-D(P*GP*AP*AP*TP*CP*GP*GP*AP*AP*AP*TP*TP*CP*CP*CP*A P*TP*CP*AP*A)-3')

Chain D:	25%	60%	15%
61 A2 A2 C5 G5 G5 G7 A9 A10	T11 C14 C15 A16 A19 A20		

• Molecule 2: DNA (5'-D(P*GP*AP*AP*TP*CP*GP*GP*AP*AP*AP*TP*TP*CP*CP*CP*AP*AP*A)-3')

С	h	ai	in	ι,	J:	•								3()%	5				70%	
G1	A2	A3 	T4	ស	66	G7	A8	A9	A10	T11	T10	211	C13	C14	C15	A16	T 1 7		ALS		

• Molecule 2: DNA (5'-D(P*GP*AP*AP*TP*CP*GP*GP*AP*AP*AP*TP*TP*CP*CP*CP*AP*AP*A)-3')

|--|

• Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera

Chain A:		68%	28%	•
MET P2 R16 R18 R18 K20	228 129 138 138 138 138 138 138	P52 P52 153 154 155 155 155 155 165 163 163 166 166 166 166	H69 H69 L73 R84 R84 R84 R85 F87 R83 F88 F88 F89 F89 F89 F98 F96 F96 F96	(197 (198 (199 (110) (110) (111) (111) (112)
1113 1114 1115 1117 1117 1117 1126 1127	L132 D133 T134 E135 C137 C137 D138 D138	V148 F149 L150 P151 P151 P153 E153 E153 F157 T158 A160 A160 A161 A161 A173	N176 T177 T177 R184 N186 R187 R187 R187 R187 R187 R199 F199 F199 F199 V205	E208 D209 V212 E220 A221 R222
G223 S224 F225 S226 S226 H231 H231 R233	V234 A235 L239 L248 R253 R253	2202 1263 1204 1204 1271 1271 1271		

• Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera





• Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera



• Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera



• Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera



• Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera





• Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera



• Molecule 3: Transcription factor p65,Proto-oncogene c-Rel chimera





4 Data and refinement statistics (i)

Property	Value	Source			
Space group	P 1	Depositor			
Cell constants	65.91Å 110.46Å 1 62.84 Å	Deperitor			
a, b, c, α , β , γ	82.20° 77.98° 72.81°	Depositor			
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	47.92 - 3.09	Depositor			
Resolution (A)	47.92 - 3.09	EDS			
% Data completeness	96.0 (47.92-3.09)	Depositor			
(in resolution range)	94.6 (47.92-3.09)	EDS			
R _{merge}	0.09	Depositor			
R _{sym}	(Not available)	Depositor			
$< I/\sigma(I) > 1$	$1.59 (at 3.07 \text{\AA})$	Xtriage			
Refinement program	PHENIX (1.16_3549: ???)	Depositor			
D D.	0.277 , 0.329	Depositor			
Π, Π_{free}	0.278 , 0.331	DCC			
R_{free} test set	73196 reflections (2.65%)	wwPDB-VP			
Wilson B-factor $(Å^2)$	79.3	Xtriage			
Anisotropy	0.399	Xtriage			
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.29 , 72.3	EDS			
L-test for twinning ²	$< L >=0.45, < L^2>=0.28$	Xtriage			
Estimated twinning fraction	0.038 for h,h-k,h-l	Xtriage			
F_o, F_c correlation	0.96	EDS			
Total number of atoms	20864	wwPDB-VP			
Average B, all atoms $(Å^2)$	85.0	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 79.65 % 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 5.3229e-07. 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)

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	Bo	ond lengths	В	ond angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	С	1.36	1/460~(0.2%)	1.25	2/707~(0.3%)
1	Ε	1.27	2/460~(0.4%)	1.12	1/707~(0.1%)
1	Ι	1.68	9/460~(2.0%)	1.40	7/707~(1.0%)
1	М	1.72	6/460~(1.3%)	1.46	8/707~(1.1%)
2	D	1.33	2/460~(0.4%)	1.21	3/705~(0.4%)
2	F	1.33	4/460~(0.9%)	1.14	2/705~(0.3%)
2	J	1.79	10/460~(2.2%)	1.78	13/705~(1.8%)
2	Ν	1.94	15/460~(3.3%)	1.67	13/705~(1.8%)
3	А	0.44	0/2258	0.68	1/3061~(0.0%)
3	В	0.43	0/2245	0.64	0/3042
3	G	0.45	0/2258	0.69	0/3061
3	Н	0.45	0/2245	0.67	0/3042
3	Κ	0.47	0/2258	0.70	0/3061
3	L	0.46	0/2245	0.69	0/3042
3	0	0.50	2/2258~(0.1%)	0.72	1/3061~(0.0%)
3	Р	0.47	0/2245	0.67	0/3042
All	All	0.77	51/21692~(0.2%)	0.86	51/30060~(0.2%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Ν	19	DA	N9-C4	-11.79	1.30	1.37
2	J	1	DG	OP3-P	-10.69	1.48	1.61
1	С	1	DT	OP3-P	-10.66	1.48	1.61
2	F	1	DG	OP3-P	-10.62	1.48	1.61
2	D	1	DG	OP3-P	-10.50	1.48	1.61
1	М	1	DT	OP3-P	-10.47	1.48	1.61
2	Ν	1	DG	OP3-P	-10.44	1.48	1.61
1	Ι	1	DT	OP3-P	-10.02	1.49	1.61
1	Е	1	DT	OP3-P	-10.01	1.49	1.61
2	J	8	DA	N7-C5	7.54	1.43	1.39
2	J	15	DC	C1'-N1	7.34	1.58	1.49
2	Ν	12	DT	C1'-N1	7.14	1.58	1.49



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	3	DA	N9-C4	-7.08	1.33	1.37
2	Ν	5	DC	C3'-O3'	-6.96	1.34	1.44
2	Ν	5	DC	N3-C4	6.91	1.38	1.33
1	Ι	13	DT	C1'-N1	6.83	1.58	1.49
1	Ι	2	DT	C1'-N1	6.57	1.57	1.49
2	F	16	DA	N7-C5	-6.48	1.35	1.39
2	Ν	16	DA	C3'-O3'	-6.45	1.35	1.44
1	Ι	18	DT	N1-C2	6.40	1.43	1.38
2	Ν	19	DA	N3-C4	-6.40	1.31	1.34
2	Ν	14	DC	C3'-O3'	-6.08	1.36	1.44
1	М	4	DA	C3'-O3'	-6.07	1.36	1.44
1	Ι	9	DA	C3'-O3'	-5.91	1.36	1.44
2	J	19	DA	C3'-O3'	-5.85	1.36	1.44
1	Ι	13	DT	N1-C2	5.85	1.42	1.38
2	F	14	DC	C3'-O3'	-5.76	1.36	1.44
2	Ν	4	DT	C1'-N1	5.72	1.56	1.49
1	Ι	19	DT	C1'-N1	5.71	1.56	1.49
2	J	12	DT	C1'-N1	5.65	1.56	1.49
1	Ι	18	DT	C1'-N1	5.61	1.56	1.49
1	М	18	DT	P-O5'	-5.56	1.54	1.59
1	М	17	DA	N9-C4	-5.54	1.34	1.37
2	J	10	DA	C3'-O3'	-5.51	1.36	1.44
2	J	7	DG	C8-N7	-5.49	1.27	1.30
1	М	1	DT	N1-C2	-5.46	1.33	1.38
2	J	8	DA	N9-C4	-5.43	1.34	1.37
2	Ν	18	DC	N1-C2	-5.42	1.34	1.40
3	0	78	CYS	CB-SG	-5.40	1.73	1.81
1	Ε	6	DG	C3'-O3'	-5.39	1.36	1.44
3	0	183	CYS	CB-SG	-5.38	1.73	1.81
1	М	8	DG	C3'-O3'	-5.35	1.36	1.44
2	F	16	DA	C3'-O3'	-5.33	1.37	1.44
2	Ν	19	DA	C2-N3	-5.32	1.28	1.33
2	Ν	19	DA	N7-C5	-5.17	1.36	1.39
2	Ν	14	DC	C4-C5	-5.14	1.38	1.43
2	Ν	5	DC	C1'-N1	5.07	1.55	1.49
2	Ν	6	DG	C5'-C4'	5.07	1.56	1.51
1	Ι	10	DA	N9-C4	5.06	1.40	1.37
2	J	14	DC	P-O5'	-5.04	1.54	1.59
2	D	8	DA	N9-C4	-5.02	1.34	1.37

All (51) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	J	14	DC	O5'-P-OP2	-19.59	87.19	110.70
2	J	10	DA	O5'-P-OP2	-12.82	94.16	105.70
2	Ν	4	DT	O5'-P-OP2	-12.65	94.31	105.70
2	Ν	9	DA	O5'-P-OP1	-9.29	97.33	105.70
1	М	3	DG	O5'-P-OP1	-8.56	97.99	105.70
2	Ν	12	DT	OP2-P-O3'	8.26	123.38	105.20
1	Ι	14	DC	O5'-P-OP1	-8.11	98.40	105.70
2	J	18	DC	O4'-C1'-N1	7.86	113.50	108.00
1	М	5	DT	O4'-C1'-N1	-7.78	102.55	108.00
2	Ν	11	DT	O5'-P-OP2	-7.59	98.87	105.70
2	J	9	DA	OP2-P-O3'	7.09	120.80	105.20
1	С	9	DA	O5'-P-OP1	-7.08	99.33	105.70
2	J	8	DA	O5'-P-OP2	-6.63	99.74	105.70
2	J	14	DC	O4'-C1'-N1	6.54	112.58	108.00
2	D	9	DA	05'-P-OP2	-6.44	99.91	105.70
2	D	10	DA	O5'-P-OP2	-6.34	100.00	105.70
1	М	14	DC	O5'-P-OP2	-6.31	100.03	105.70
1	Ι	2	DT	N3-C4-O4	6.26	123.66	119.90
1	Ι	17	DA	O4'-C1'-N9	-5.93	103.85	108.00
1	М	5	DT	N3-C4-O4	5.93	123.46	119.90
1	Ι	8	DG	O5'-P-OP1	-5.82	100.46	105.70
2	Ν	12	DT	N3-C4-O4	5.80	123.38	119.90
2	Ν	4	DT	N3-C4-O4	5.80	123.38	119.90
2	F	12	DT	N3-C4-O4	5.71	123.33	119.90
2	Ν	18	DC	O4'-C1'-N1	-5.66	104.03	108.00
2	Ν	11	DT	N3-C4-O4	5.64	123.28	119.90
1	М	12	DT	N3-C4-O4	5.45	123.17	119.90
2	J	13	DC	OP2-P-O3'	5.37	117.02	105.20
2	J	18	DC	C3'-C2'-C1'	-5.37	96.06	102.50
3	0	201	LEU	CA-CB-CG	5.36	127.63	115.30
2	J	10	DA	OP1-P-OP2	5.36	127.63	119.60
1	Ι	13	DT	N3-C4-O4	5.35	123.11	119.90
1	М	19	DT	N3-C4-O4	5.30	123.08	119.90
2	D	7	DG	05'-P-OP2	-5.27	100.96	105.70
1	М	5	DT	C5-C4-O4	-5.24	121.23	124.90
1	Ι	16	DG	04'-C1'-N9	-5.23	104.34	108.00
2	J	11	DT	OP1-P-OP2	5.21	127.41	119.60
2	J	8	DA	C3'-C2'-C1'	-5.21	96.25	102.50
1	М	12	DT	O5'-P-OP2	-5.20	101.02	105.70
2	N	13	DC	05'-P-OP1	-5.18	101.03	105.70
2	N	4	DT	C5-C4-O4	-5.16	121.29	124.90
2	F	11	DT	OP1-P-OP2	5.15	127.32	119.60
2	Ν	13	DC	OP2-P-O3'	5.11	116.44	105.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Е	18	DT	N3-C4-O4	5.09	122.96	119.90
2	J	7	DG	OP2-P-O3'	5.09	116.41	105.20
2	Ν	16	DA	O4'-C1'-N9	-5.09	104.44	108.00
1	Ι	11	DT	N3-C4-O4	5.07	122.94	119.90
2	N	5	DC	O4'-C1'-N1	5.07	111.55	108.00
2	J	4	DT	N3-C4-O4	5.06	122.94	119.90
1	С	5	DT	N3-C4-O4	5.02	122.91	119.90
3	А	132	LEU	CA-CB-CG	5.01	126.83	115.30

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	С	412	0	229	16	0
1	Е	412	0	229	20	0
1	Ι	412	0	229	29	0
1	М	412	0	229	44	0
2	D	410	0	225	22	0
2	F	410	0	225	26	0
2	J	410	0	225	56	0
2	N	410	0	225	65	0
3	А	2203	0	2175	43	0
3	В	2191	0	2165	57	0
3	G	2203	0	2175	38	0
3	Н	2191	0	2165	46	0
3	K	2203	0	2175	43	0
3	L	2191	0	2165	62	0
3	0	2203	0	2175	49	0
3	Р	2191	0	2165	55	0
All	All	20864	0	19176	559	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 14.

All (559) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:M:3:DG:N1	2:N:18:DC:O2	1.86	1.06
1:M:2:DT:N3	2:N:19:DA:N1	2.06	1.04
1:M:12:DT:OP2	3:P:19:TYR:OH	1.78	1.01
1:M:17:DA:N1	2:N:4:DT:N3	2.09	1.00
1:I:8:DG:N1	2:J:13:DC:N3	2.09	0.99
2:J:5:DC:H41	3:L:24:ARG:HH22	1.12	0.98
1:M:18:DT:N3	2:N:3:DA:N1	2.13	0.97
1:M:16:DG:O6	2:N:5:DC:N4	1.98	0.96
1:M:16:DG:N1	2:N:5:DC:N3	2.14	0.95
2:N:17:DT:H2"	2:N:18:DC:C5	2.02	0.94
2:D:1:DG:H2'	2:D:2:DA:C8	2.02	0.94
1:I:8:DG:N2	2:J:13:DC:O2	1.99	0.94
1:I:8:DG:O6	2:J:13:DC:N4	2.00	0.93
3:L:9:GLN:HG3	3:L:10:PRO:HD2	1.50	0.93
1:C:6:DG:N2	2:D:15:DC:O2	2.00	0.93
3:P:9:GLN:HG3	3:P:10:PRO:HD2	1.50	0.93
1:I:9:DA:N1	2:J:12:DT:N3	2.15	0.93
1:I:7:DG:N1	2:J:14:DC:N3	2.16	0.92
1:I:7:DG:N2	2:J:14:DC:O2	2.03	0.91
2:J:15:DC:H2"	2:J:16:DA:C8	2.06	0.91
3:P:18:ARG:NH1	3:P:22:GLU:OE2	2.06	0.89
2:N:15:DC:H2"	2:N:16:DA:C8	2.09	0.88
2:N:15:DC:H2"	2:N:16:DA:N7	1.89	0.86
1:M:7:DG:O6	3:O:18:ARG:NH2	2.09	0.86
2:J:5:DC:H41	3:L:24:ARG:NH2	1.74	0.85
2:D:5:DC:H41	3:H:24:ARG:HH22	1.22	0.85
3:H:9:GLN:HG3	3:H:10:PRO:HD2	1.59	0.84
2:J:17:DT:H4'	2:J:18:DC:H5'	1.58	0.84
2:N:1:DG:H2'	2:N:2:DA:C8	2.14	0.83
2:J:1:DG:H2'	2:J:2:DA:C8	2.14	0.83
3:B:117:ILE:HG21	3:B:131:LEU:HD11	1.60	0.83
1:I:6:DG:N1	2:J:15:DC:N3	2.26	0.82
1:E:3:DG:N2	2:F:18:DC:O2	2.12	0.82
1:E:17:DA:N6	2:F:4:DT:O4	2.10	0.81
3:G:73:LEU:HD22	3:G:99:LEU:HD22	1.61	0.81
1:M:15:DC:N4	2:N:6:DG:O6	2.11	0.81
2:J:10:DA:H2"	2:J:11:DT:H5"	1.63	0.80
1:I:6:DG:N2	2:J:15:DC:O2	2.14	0.80
2:F:1:DG:H2'	2:F:2:DA:C8	2.18	0.79
1:C:7:DG:N1	2:D:14:DC:N3	2.25	0.79
3:O:28:SER:HA	3:O:99:LEU:O	1.83	0.79



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:L:248:LEU:HD21	3:L:252:VAL:HG22	1.65	0.78
1:C:7:DG:N2	2:D:14:DC:O2	2.11	0.78
3:B:9:GLN:HG3	3:B:10:PRO:HD2	1.66	0.77
3:P:248:LEU:HD21	3:P:252:VAL:HG22	1.67	0.77
1:M:8:DG:O6	3:O:16:ARG:NH2	2.18	0.77
2:J:6:DG:N7	3:L:18:ARG:NH2	2.34	0.76
3:G:150:LEU:HD22	3:G:161:LEU:HD11	1.66	0.76
1:M:17:DA:N6	2:N:4:DT:O4	2.15	0.76
3:H:128:GLU:HG2	3:O:117:ILE:HG13	1.69	0.76
3:B:128:GLU:HG2	3:K:117:ILE:HG13	1.69	0.75
3:P:150:LEU:HD22	3:P:161:LEU:HD21	1.69	0.75
3:O:55:VAL:HG12	3:O:148:VAL:HG22	1.67	0.75
3:H:8:GLU:HB2	3:H:43:THR:HG22	1.69	0.74
3:A:253:ARG:NH2	3:A:271:GLU:OE1	2.21	0.74
3:P:62:LYS:HD2	3:P:141:VAL:HG11	1.68	0.73
1:M:1:DT:N3	2:N:20:DA:C2	2.57	0.73
3:L:209:ASP:OD2	3:L:262:SER:OG	2.08	0.72
3:P:59:LEU:HD11	3:P:101:ILE:HG12	1.70	0.72
3:G:28:SER:HA	3:G:99:LEU:O	1.89	0.72
3:A:73:LEU:HD22	3:A:99:LEU:HD22	1.70	0.72
3:A:28:SER:HA	3:A:99:LEU:O	1.90	0.72
1:I:5:DT:H3	2:J:16:DA:H61	1.35	0.72
1:C:6:DG:N2	2:D:15:DC:C2	2.54	0.71
3:L:62:LYS:HD2	3:L:141:VAL:HG11	1.73	0.71
1:M:2:DT:N3	2:N:19:DA:C2	2.59	0.71
3:A:55:VAL:HG12	3:A:148:VAL:HG22	1.72	0.70
1:M:2:DT:C2	2:N:19:DA:C2	2.79	0.70
3:O:186:ASN:HB2	3:O:199:PHE:H	1.56	0.70
2:J:18:DC:H2"	2:J:19:DA:OP2	1.91	0.70
3:K:28:SER:HA	3:K:99:LEU:O	1.90	0.69
1:I:11:DT:H1'	1:I:12:DT:H5"	1.74	0.69
3:G:55:VAL:HG12	3:G:148:VAL:HG22	1.73	0.69
3:K:69:HIS:NE2	3:K:138:ASP:O	2.16	0.69
3:A:69:HIS:NE2	3:A:138:ASP:O	2.16	0.69
2:J:15:DC:H2"	2:J:16:DA:H8	1.55	0.69
2:N:19:DA:H8	2:N:19:DA:OP2	1.74	0.69
3:A:150:LEU:HD22	3:A:161:LEU:HD11	1.75	0.69
3:A:117:ILE:HG13	3:L:128:GLU:HG2	1.75	0.69
1:M:16:DG:N2	2:N:5:DC:O2	2.20	0.69
3:H:248:LEU:HD21	3:H:252:VAL:HG22	1.74	0.68
3:H:18:ARG:NH1	3:H:22:GLU:OE2	2.26	0.68



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (\AA)
1:C:7:DG:O6	2:D:14:DC:N4	2.21	0.67
3:K:73:LEU:HD22	3:K:99:LEU:HD22	1.75	0.67
1:E:2:DT:N3	2:F:19:DA:C2	2.63	0.66
3:B:248:LEU:HD21	3:B:252:VAL:HG22	1.77	0.66
3:L:9:GLN:HG2	3:L:167:ASN:ND2	2.10	0.66
1:M:2:DT:O2	2:N:19:DA:C2	2.48	0.66
3:G:54:THR:HG22	3:G:85:ALA:HA	1.78	0.66
2:F:17:DT:H2"	2:F:18:DC:C5	2.31	0.65
3:H:9:GLN:OE1	3:H:167:ASN:N	2.30	0.65
2:J:19:DA:OP2	2:J:19:DA:C4	2.50	0.65
1:E:8:DG:O6	3:A:16:ARG:NH2	2.30	0.64
3:K:69:HIS:O	3:K:116:ARG:NH1	2.30	0.64
3:B:8:GLU:HB2	3:B:43:THR:HG22	1.78	0.64
3:L:91:ARG:HG3	3:L:93:PRO:HA	1.79	0.64
1:I:5:DT:H3	2:J:16:DA:N6	1.96	0.64
1:E:1:DT:N3	2:F:20:DA:H2	1.96	0.63
2:J:19:DA:H1'	2:J:20:DA:O4'	1.99	0.63
3:O:209:ASP:OD2	3:O:262:SER:OG	2.16	0.63
2:N:19:DA:H2"	2:N:20:DA:C8	2.34	0.62
3:B:163:PRO:O	3:P:48:GLY:HA2	1.99	0.62
3:L:18:ARG:NH1	3:L:22:GLU:OE2	2.32	0.62
1:I:7:DG:O6	2:J:14:DC:N4	2.22	0.62
3:H:195:GLY:O	3:H:239:ARG:NH1	2.29	0.62
3:H:28:SER:HA	3:H:99:LEU:O	2.00	0.62
3:K:64:PRO:HB2	3:K:65:PRO:HD3	1.82	0.62
2:N:14:DC:H2"	2:N:15:DC:C5	2.35	0.62
1:E:12:DT:OP2	3:B:19:TYR:OH	2.12	0.61
3:H:259:ARG:NH1	3:H:264:ARG:HG2	2.16	0.61
3:A:186:ASN:HB2	3:A:199:PHE:H	1.66	0.61
3:B:62:LYS:HD2	3:B:141:VAL:HG11	1.82	0.61
3:L:66:HIS:CD2	3:L:165:VAL:HG11	2.36	0.61
3:B:91:ARG:HG3	3:B:93:PRO:HA	1.81	0.60
2:N:11:DT:H2'	2:N:12:DT:H71	1.81	0.60
2:J:5:DC:H2"	2:J:6:DG:C8	2.36	0.60
3:H:192:CYS:HB3	3:H:248:LEU:HD22	1.84	0.60
2:N:13:DC:H2"	2:N:14:DC:H6	1.65	0.60
3:O:54:THR:HG22	3:O:85:ALA:HA	1.83	0.60
3:O:150:LEU:HD22	3:O:161:LEU:HD11	1.84	0.60
1:I:9:DA:OP1	3:L:207:LYS:NZ	2.24	0.60
3:O:64:PRO:HB2	3:O:65:PRO:HD3	1.83	0.60
3:K:55:VAL:HG12	3:K:148:VAL:HG22	1.84	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:M:4:DA:H61	2:N:17:DT:H3	1.49	0.59
3:L:61:THR:HG22	3:L:63:ASP:H	1.68	0.59
3:L:150:LEU:HD22	3:L:161:LEU:HD21	1.83	0.59
2:F:9:DA:OP2	3:A:233:GLN:NE2	2.32	0.59
2:D:10:DA:H2"	2:D:11:DT:H5"	1.84	0.59
3:B:9:GLN:OE1	3:B:167:ASN:N	2.36	0.59
1:M:1:DT:C2	2:N:20:DA:C2	2.91	0.59
2:N:9:DA:OP2	3:O:233:GLN:NE2	2.30	0.59
3:O:192:CYS:HA	3:O:274:TYR:CD2	2.37	0.59
1:M:1:DT:C2	2:N:20:DA:H2	2.20	0.59
2:N:17:DT:H2"	2:N:18:DC:C4	2.38	0.58
3:O:113:ILE:HD13	3:O:134:ILE:HD12	1.84	0.58
3:P:53:GLY:O	3:P:87:PHE:HB3	2.03	0.58
2:N:13:DC:H2"	2:N:14:DC:C6	2.38	0.58
3:O:30:PRO:HB3	3:O:39:LYS:HE2	1.86	0.58
2:F:11:DT:H72	3:A:173:ARG:HD3	1.86	0.58
3:H:150:LEU:HD22	3:H:161:LEU:HD21	1.86	0.58
3:A:113:ILE:HD13	3:A:134:ILE:HD12	1.86	0.58
2:N:12:DT:H2"	2:N:13:DC:H6	1.69	0.58
3:K:43:THR:HG23	3:K:95:PHE:HB3	1.86	0.57
2:N:7:DG:P	3:O:232:ARG:HH12	2.27	0.57
1:I:6:DG:H1	2:J:15:DC:N4	2.02	0.57
3:H:248:LEU:HB3	3:H:276:PRO:HA	1.87	0.57
3:L:192:CYS:HA	3:L:274:TYR:HD2	1.69	0.57
2:F:19:DA:OP2	2:F:19:DA:H8	1.87	0.57
2:F:15:DC:H2"	2:F:16:DA:C8	2.39	0.57
1:I:6:DG:N2	2:J:15:DC:C2	2.58	0.57
3:B:195:GLY:O	3:B:239:ARG:NH1	2.37	0.56
2:J:10:DA:C2'	2:J:11:DT:H5"	2.34	0.56
3:K:150:LEU:HD22	3:K:161:LEU:HD11	1.86	0.56
1:M:4:DA:N6	2:N:17:DT:H3	2.04	0.56
3:H:63:ASP:O	3:H:66:HIS:ND1	2.39	0.56
3:A:231:HIS:HB3	3:A:235:ALA:HB3	1.86	0.56
3:H:209:ASP:OD2	3:H:262:SER:OG	2.21	0.56
3:K:259:ARG:NH1	3:K:264:ARG:HG2	2.21	0.56
1:M:3:DG:C2	2:N:18:DC:O2	2.58	0.56
3:O:69:HIS:O	3:O:116:ARG:NH1	2.38	0.56
3:P:61:THR:HG22	3:P:63:ASP:H	1.71	0.56
1:I:13:DT:H2'	3:L:21:CYS:SG	2.45	0.55
1:C:13:DT:H2"	1:C:14:DC:H5'	1.87	0.55
3:B:29:ILE:HD11	3:B:101:ILE:HG13	1.88	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:G:64:PRO:HB2	3:G:65:PRO:HD3	1.88	0.55
3:G:43:THR:HG23	3:G:95:PHE:HB3	1.88	0.55
3:B:16:ARG:HH21	3:B:173:ARG:NH2	2.04	0.55
1:I:6:DG:C2	2:J:15:DC:N3	2.75	0.55
3:K:113:ILE:HD13	3:K:134:ILE:HD12	1.88	0.55
2:J:5:DC:N4	3:L:24:ARG:HH22	1.94	0.55
3:K:175:PRO:HG3	3:K:204:LYS:HE3	1.88	0.55
3:P:195:GLY:O	3:P:239:ARG:NH1	2.39	0.54
1:I:6:DG:O6	2:J:15:DC:N4	2.38	0.54
2:N:14:DC:H2"	2:N:15:DC:C6	2.43	0.54
1:M:17:DA:C2	1:M:18:DT:C2	2.96	0.54
3:G:52:PRO:HG2	3:G:151:PRO:HG3	1.90	0.54
2:J:15:DC:C2'	2:J:16:DA:C8	2.84	0.54
3:L:122:ASN:HD21	3:L:126:VAL:HG22	1.73	0.54
1:C:6:DG:N1	2:D:15:DC:N3	2.53	0.53
3:H:136:ASP:O	3:H:137:CYS:HB2	2.08	0.53
2:J:11:DT:OP2	3:K:19:TYR:OH	2.13	0.53
3:H:53:GLY:O	3:H:87:PHE:HB3	2.08	0.53
3:B:122:ASN:HD21	3:B:126:VAL:HG22	1.72	0.53
1:C:11:DT:H1'	1:C:12:DT:H5"	1.90	0.53
3:G:69:HIS:NE2	3:G:138:ASP:O	2.26	0.53
2:J:11:DT:H72	3:K:173:ARG:HD3	1.90	0.53
2:J:14:DC:H2"	2:J:15:DC:C5	2.44	0.53
3:L:192:CYS:HA	3:L:274:TYR:CD2	2.43	0.53
3:L:253:ARG:HG2	3:L:271:GLU:HG3	1.89	0.53
2:D:11:DT:OP1	3:G:106:LYS:HB2	2.08	0.53
3:O:4:VAL:HB	3:O:164:ILE:HD11	1.91	0.53
3:H:138:ASP:O	3:H:139:LEU:HB2	2.09	0.52
3:K:186:ASN:HB2	3:K:199:PHE:H	1.74	0.52
3:L:259:ARG:NH1	3:L:264:ARG:HG2	2.24	0.52
2:F:3:DA:C8	2:F:4:DT:H72	2.44	0.52
3:A:64:PRO:HB2	3:A:65:PRO:HD3	1.90	0.52
2:N:15:DC:C2'	2:N:16:DA:N7	2.69	0.52
3:P:253:ARG:HG2	3:P:271:GLU:HG3	1.91	0.52
3:A:149:PHE:HD1	3:A:160:ALA:HA	1.74	0.52
3:O:150:LEU:HD22	3:O:161:LEU:HD21	1.91	0.52
3:H:91:ARG:HG3	3:H:93:PRO:HA	1.91	0.52
2:J:9:DA:C2	2:J:10:DA:C4	2.97	0.52
1:M:8:DG:C2	1:M:9:DA:C4	2.98	0.52
1:E:1:DT:N3	2:F:20:DA:C2	2.68	0.52
1:E:7:DG:O6	3:A:18:ARG:NH2	2.43	0.52



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (\AA)
2:N:11:DT:OP1	3:O:106:LYS:HB2	2.09	0.52
3:O:170:TYR:HB3	3:O:177:THR:HB	1.91	0.52
3:O:192:CYS:HA	3:O:274:TYR:HD2	1.75	0.52
3:G:2:PRO:HG3	3:G:49:TYR:HB2	1.92	0.52
3:L:28:SER:HB2	3:L:97:GLN:O	2.10	0.52
3:P:192:CYS:SG	3:P:248:LEU:HB2	2.50	0.52
3:H:53:GLY:C	3:H:87:PHE:HB3	2.30	0.52
3:K:62:LYS:HD2	3:K:141:VAL:HG11	1.91	0.52
3:L:53:GLY:C	3:L:87:PHE:HB3	2.30	0.52
1:M:13:DT:H2"	1:M:14:DC:H5'	1.92	0.52
2:D:15:DC:H2"	2:D:16:DA:C8	2.45	0.52
1:E:13:DT:H2"	1:E:14:DC:H5'	1.92	0.51
3:O:67:ARG:HB3	3:O:134:ILE:HD11	1.92	0.51
3:G:149:PHE:HD1	3:G:160:ALA:HA	1.75	0.51
2:J:18:DC:C2'	2:J:19:DA:OP2	2.58	0.51
2:D:5:DC:N4	3:H:24:ARG:HH22	1.99	0.51
1:E:3:DG:C2	2:F:19:DA:C2	2.99	0.51
3:H:105:LYS:HB2	3:H:108:GLU:HG3	1.93	0.51
1:M:3:DG:C4	2:N:19:DA:C2	2.99	0.51
3:A:62:LYS:HD2	3:A:141:VAL:HG11	1.93	0.51
3:O:251:PRO:HB3	3:O:275:LEU:HD23	1.93	0.51
3:B:18:ARG:NH1	3:B:22:GLU:OE2	2.43	0.51
3:G:136:ASP:OD1	3:G:138:ASP:HB2	2.12	0.51
1:I:1:DT:C2'	1:I:2:DT:H71	2.41	0.51
3:L:138:ASP:O	3:L:139:LEU:HB2	2.10	0.51
3:L:187:ARG:NH1	3:L:196:ASP:HB3	2.26	0.51
1:M:1:DT:O2	2:N:20:DA:C2	2.64	0.51
3:O:56:ARG:HD3	3:O:121:ILE:HD12	1.93	0.50
2:N:5:DC:H41	3:P:24:ARG:HH22	1.59	0.50
1:E:1:DT:H3	2:F:20:DA:H2	1.45	0.50
2:F:17:DT:H2"	2:F:18:DC:C6	2.47	0.50
1:I:18:DT:H2'	1:I:19:DT:H72	1.92	0.50
2:J:6:DG:C2	2:J:7:DG:C5	2.99	0.50
3:K:59:LEU:HD13	3:K:73:LEU:HG	1.93	0.50
3:A:136:ASP:OD1	3:A:138:ASP:HB2	2.12	0.50
1:I:15:DC:H2"	1:I:16:DG:C8	2.46	0.50
3:K:56:ARG:HD3	3:K:121:ILE:HD12	1.94	0.50
1:M:4:DA:H1'	1:M:5:DT:H5'	1.92	0.50
2:N:14:DC:C2	2:N:15:DC:C4	3.00	0.50
3:B:8:GLU:HB2	3:B:43:THR:CG2	2.41	0.50
3:B:56:ARG:HG2	3:B:83:TYR:O	2.11	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:L:73:LEU:HD22	3:L:99:LEU:HD22	1.93	0.50
1:M:1:DT:O2	2:N:20:DA:H2	1.94	0.50
2:N:19:DA:OP2	2:N:19:DA:C8	2.60	0.50
3:G:56:ARG:HA	3:G:83:TYR:O	2.12	0.50
3:P:68:PRO:HG2	3:P:131:LEU:HD21	1.93	0.50
3:O:204:LYS:HE3	3:O:233:GLN:OE1	2.12	0.50
3:P:53:GLY:C	3:P:87:PHE:HB3	2.32	0.50
3:G:92:ARG:N	3:G:93:PRO:HD2	2.26	0.50
3:K:30:PRO:HB3	3:K:39:LYS:HE2	1.94	0.50
3:A:30:PRO:HB3	3:A:39:LYS:HE2	1.94	0.49
3:G:113:ILE:HD13	3:G:134:ILE:HD12	1.94	0.49
2:N:16:DA:C4	2:N:17:DT:C5	2.99	0.49
3:B:28:SER:HA	3:B:99:LEU:O	2.11	0.49
3:O:73:LEU:HD22	3:O:99:LEU:HD22	1.94	0.49
3:P:91:ARG:HG3	3:P:93:PRO:HA	1.94	0.49
3:P:138:ASP:O	3:P:139:LEU:HB2	2.12	0.49
3:K:56:ARG:HA	3:K:83:TYR:O	2.12	0.49
3:O:8:GLU:O	3:O:42:PRO:HA	2.12	0.49
3:P:248:LEU:HB3	3:P:276:PRO:HA	1.94	0.49
3:O:62:LYS:HD2	3:O:141:VAL:HG11	1.93	0.49
1:I:8:DG:C6	2:J:13:DC:N3	2.79	0.49
3:A:259:ARG:NH1	3:A:264:ARG:HG2	2.27	0.49
3:K:35:THR:OG1	3:K:37:THR:HG22	2.12	0.49
3:L:53:GLY:O	3:L:87:PHE:HB3	2.13	0.49
3:A:192:CYS:HA	3:A:274:TYR:CD2	2.48	0.49
3:B:28:SER:HB2	3:B:97:GLN:O	2.13	0.49
3:B:61:THR:HG22	3:B:63:ASP:H	1.77	0.49
1:M:5:DT:P	3:O:27:GLY:HA2	2.53	0.49
3:P:28:SER:HA	3:P:99:LEU:O	2.13	0.48
3:P:243:TYR:CE1	3:P:252:VAL:HG21	2.48	0.48
3:H:151:PRO:O	3:H:152:ASP:HB2	2.13	0.48
3:P:97:GLN:HG2	3:P:98:ASN:H	1.78	0.48
3:L:97:GLN:HG2	3:L:98:ASN:H	1.77	0.48
3:L:243:TYR:CE1	3:L:252:VAL:HG21	2.48	0.48
1:M:5:DT:H2"	1:M:6:DG:C8	2.47	0.48
2:N:3:DA:C8	2:N:4:DT:H72	2.49	0.48
2:N:15:DC:C2	2:N:16:DA:C6	3.01	0.48
3:A:56:ARG:HA	3:A:83:TYR:O	2.14	0.48
1:M:18:DT:O2	2:N:3:DA:C2	2.66	0.48
3:A:209:ASP:OD2	3:A:262:SER:OG	2.26	0.48
3:K:92:ARG:N	3:K:93:PRO:HD2	2.28	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:L:28:SER:HA	3:L:99:LEU:O	2.14	0.48
3:L:63:ASP:O	3:L:66:HIS:ND1	2.40	0.48
3:H:3:TYR:N	3:H:3:TYR:HD2	2.12	0.48
2:J:8:DA:C2	2:J:9:DA:C4	3.02	0.48
3:L:16:ARG:HH21	3:L:173:ARG:NH2	2.11	0.48
3:H:97:GLN:HG2	3:H:98:ASN:H	1.78	0.48
3:B:136:ASP:O	3:B:137:CYS:HB2	2.14	0.48
3:O:63:ASP:HB3	3:O:64:PRO:HD2	1.96	0.48
1:E:11:DT:H1'	1:E:12:DT:H5"	1.95	0.48
1:M:2:DT:C2	2:N:19:DA:H2	2.29	0.48
3:P:111:GLU:O	3:P:115:LEU:HB2	2.14	0.48
3:H:192:CYS:HA	3:H:274:TYR:CD2	2.49	0.48
3:L:205:VAL:O	3:L:233:GLN:NE2	2.43	0.48
3:K:205:VAL:O	3:K:233:GLN:NE2	2.45	0.47
3:P:259:ARG:NH1	3:P:264:ARG:HG2	2.29	0.47
3:G:212:VAL:O	3:G:223:GLY:N	2.47	0.47
3:H:24:ARG:HG3	3:H:25:SER:O	2.15	0.47
2:J:12:DT:H1'	2:J:13:DC:H5'	1.96	0.47
3:K:203:ASP:O	3:K:205:VAL:HG13	2.14	0.47
1:M:10:DA:H1'	1:M:11:DT:H5'	1.96	0.47
2:N:11:DT:H2"	2:N:12:DT:C5'	2.44	0.47
3:G:192:CYS:HA	3:G:274:TYR:CD2	2.50	0.47
3:H:209:ASP:CG	3:H:262:SER:OG	2.53	0.47
3:L:53:GLY:HA2	3:L:157:PHE:CD2	2.50	0.47
3:L:116:ARG:HD2	3:L:121:ILE:HB	1.95	0.47
3:O:156:ASN:O	3:O:158:THR:N	2.47	0.47
1:C:12:DT:H72	3:H:173:ARG:HD3	1.97	0.47
1:I:3:DG:H2"	1:I:4:DA:C8	2.50	0.47
3:K:265:GLU:O	3:K:266:LEU:HD12	2.14	0.47
3:A:111:GLU:HG3	3:L:114:ILE:HD13	1.96	0.47
3:B:97:GLN:HG2	3:B:98:ASN:H	1.79	0.47
1:C:9:DA:H2"	1:C:10:DA:H8	1.78	0.47
3:G:59:LEU:HD13	3:G:73:LEU:HG	1.96	0.47
3:O:62:LYS:HA	3:O:143:ARG:HE	1.79	0.47
3:O:204:LYS:HA	3:O:233:GLN:O	2.14	0.47
3:P:23:GLY:C	3:P:24:ARG:HG2	2.35	0.47
3:A:69:HIS:O	3:A:116:ARG:NH1	2.48	0.47
3:A:133:ASP:O	3:A:134:ILE:HB	2.15	0.47
2:J:14:DC:H2"	2:J:15:DC:H5	1.80	0.47
3:K:136:ASP:OD1	3:K:138:ASP:HB2	2.14	0.47
3:H:8:GLU:CB	3:H:43:THR:HG22	2.43	0.47



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:1:DT:H2"	1:I:2:DT:H71	1.97	0.47
2:N:11:DT:C2'	2:N:12:DT:H71	2.45	0.47
3:H:53:GLY:HA2	3:H:157:PHE:CD2	2.50	0.47
3:B:94:LEU:HA	3:B:94:LEU:HD23	1.54	0.46
3:H:257:GLN:CD	3:H:266:LEU:HD23	2.35	0.46
3:L:94:LEU:HA	3:L:94:LEU:HD23	1.66	0.46
3:L:111:GLU:O	3:L:115:LEU:HB2	2.15	0.46
2:D:10:DA:C2'	2:D:11:DT:H5"	2.45	0.46
3:G:30:PRO:HB3	3:G:39:LYS:HE2	1.98	0.46
3:A:126:VAL:HG12	3:A:127:PRO:HD2	1.97	0.46
3:B:243:TYR:CE1	3:B:252:VAL:HG21	2.51	0.46
3:B:253:ARG:HG2	3:B:271:GLU:HG3	1.97	0.46
1:I:6:DG:H1	2:J:15:DC:H42	1.62	0.46
3:L:8:GLU:HB2	3:L:43:THR:CG2	2.46	0.46
3:L:207:LYS:HG3	3:L:208:GLU:HG3	1.98	0.46
3:O:212:VAL:O	3:O:223:GLY:N	2.45	0.46
3:P:50:THR:HA	3:P:91:ARG:NH2	2.30	0.46
3:A:29:ILE:HD11	3:A:101:ILE:HG13	1.96	0.46
3:A:63:ASP:O	3:A:66:HIS:ND1	2.48	0.46
3:H:3:TYR:N	3:H:3:TYR:CD2	2.83	0.46
3:L:151:PRO:O	3:L:152:ASP:HB2	2.16	0.46
2:N:11:DT:H2"	2:N:12:DT:H5'	1.97	0.46
3:G:186:ASN:HB2	3:G:199:PHE:H	1.80	0.46
1:M:18:DT:O2	2:N:3:DA:H2	1.99	0.46
3:B:53:GLY:HA2	3:B:157:PHE:CD2	2.51	0.46
3:L:97:GLN:HG2	3:L:98:ASN:N	2.31	0.46
1:I:8:DG:N1	2:J:13:DC:C2	2.75	0.46
3:K:239:ARG:HH22	3:L:184:ARG:HH12	1.62	0.46
3:B:132:LEU:HD13	3:B:132:LEU:O	2.15	0.46
3:H:209:ASP:OD1	3:H:262:SER:OG	2.32	0.46
2:J:11:DT:H5'	3:K:19:TYR:CE2	2.51	0.46
2:F:5:DC:H2"	2:F:6:DG:C8	2.51	0.45
1:C:19:DT:H2"	1:C:20:DC:C5	2.51	0.45
3:P:17:PHE:CG	3:P:101:ILE:HD12	2.50	0.45
3:A:92:ARG:N	3:A:93:PRO:HD2	2.32	0.45
3:G:259:ARG:NH1	3:G:264:ARG:HG2	2.30	0.45
3:B:17:PHE:CE1	3:B:171:ASP:HB2	2.52	0.45
3:G:28:SER:HB2	3:G:97:GLN:O	2.16	0.45
2:N:15:DC:C2'	2:N:16:DA:C8	2.92	0.45
3:O:69:HIS:NE2	3:0:138:ASP:O	2.42	0.45
3:O:159:THR:O	3:O:160:ALA:HB3	2.17	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:P:16:ARG:HH21	3:P:173:ARG:NH2	2.15	0.45
3:B:150:LEU:HA	3:B:150:LEU:HD12	1.81	0.45
3:B:151:PRO:O	3:B:152:ASP:HB2	2.16	0.45
3:H:111:GLU:O	3:H:115:LEU:HB2	2.16	0.45
3:G:111:GLU:HG3	3:P:114:ILE:HD13	1.99	0.45
3:A:59:LEU:HD13	3:A:73:LEU:HG	1.99	0.45
2:J:17:DT:C6	2:J:19:DA:N1	2.85	0.45
2:N:13:DC:C2	2:N:14:DC:C5	3.05	0.45
3:B:131:LEU:O	3:B:131:LEU:HD22	2.17	0.45
3:K:251:PRO:HB3	3:K:275:LEU:HD23	1.98	0.45
3:L:219:TRP:CD1	3:L:244:ALA:HB2	2.52	0.45
3:P:9:GLN:HG2	3:P:167:ASN:ND2	2.32	0.45
3:B:44:ILE:O	3:B:94:LEU:HB2	2.17	0.45
3:A:28:SER:HB2	3:A:97:GLN:O	2.17	0.44
3:G:31:GLY:HA3	3:G:40:THR:OG1	2.17	0.44
3:P:72:GLU:HB2	3:P:81:GLY:HA2	1.99	0.44
3:P:170:TYR:HB3	3:P:177:THR:HB	1.97	0.44
1:E:10:DA:H1'	1:E:11:DT:H5'	1.99	0.44
3:B:63:ASP:O	3:B:66:HIS:ND1	2.51	0.44
3:G:90:GLU:OE1	3:G:91:ARG:HG3	2.18	0.44
3:H:187:ARG:HD3	3:H:189:SER:O	2.17	0.44
2:J:7:DG:H1'	2:J:8:DA:H5'	1.97	0.44
1:M:20:DC:O2	2:N:2:DA:C2	2.70	0.44
3:H:3:TYR:HD2	3:H:3:TYR:H	1.64	0.44
3:O:133:ASP:O	3:O:134:ILE:HB	2.17	0.44
3:A:248:LEU:HA	3:A:248:LEU:HD23	1.70	0.44
3:H:44:ILE:O	3:H:94:LEU:HB2	2.16	0.44
3:P:63:ASP:HB3	3:P:64:PRO:HD2	1.99	0.44
3:A:176:ASN:OD1	3:A:177:THR:HG23	2.17	0.44
3:B:8:GLU:OE2	3:B:33:ARG:HG3	2.18	0.44
3:L:203:ASP:O	3:L:205:VAL:HG13	2.18	0.44
3:P:122:ASN:HD21	3:P:126:VAL:HG22	1.82	0.44
3:K:212:VAL:O	3:K:223:GLY:N	2.51	0.44
1:E:8:DG:C2	1:E:9:DA:C4	3.05	0.44
3:B:150:LEU:HD22	3:B:161:LEU:HD21	1.99	0.44
3:B:164:ILE:HA	3:P:48:GLY:HA2	1.98	0.44
3:G:243:TYR:CZ	3:G:252:VAL:HG11	2.53	0.44
3:P:69:HIS:CD2	3:P:142:VAL:HG12	2.53	0.44
2:D:9:DA:C6	2:D:10:DA:C6	3.06	0.43
1:M:18:DT:C2	2:N:3:DA:N1	2.82	0.43
3:O:59:LEU:HD13	3:O:73:LEU:HG	1.99	0.43



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:P:53:GLY:HA2	3:P:157:PHE:CD2	2.53	0.43
3:H:207:LYS:HG3	3:H:208:GLU:HG3	2.00	0.43
3:K:149:PHE:HD1	3:K:160:ALA:HA	1.83	0.43
2:F:13:DC:H2"	2:F:14:DC:C6	2.53	0.43
3:B:69:HIS:CD2	3:B:71:HIS:H	2.36	0.43
3:O:16:ARG:HH21	3:O:173:ARG:HH21	1.66	0.43
3:A:43:THR:HG23	3:A:95:PHE:HB3	1.99	0.43
1:C:3:DG:C2	2:D:19:DA:C2	3.07	0.43
2:D:5:DC:C2	2:D:6:DG:C5	3.06	0.43
3:G:72:GLU:HB2	3:G:81:GLY:HA2	2.00	0.43
2:J:16:DA:H1'	2:J:17:DT:OP2	2.19	0.43
3:K:231:HIS:HB3	3:K:235:ALA:HB3	2.00	0.43
3:P:34:SER:OG	3:P:39:LYS:HA	2.17	0.43
1:E:7:DG:H2"	1:E:8:DG:OP2	2.19	0.43
2:F:19:DA:H2"	2:F:20:DA:C8	2.53	0.43
2:D:10:DA:C8	2:D:11:DT:H72	2.54	0.43
3:L:93:PRO:HB2	3:L:94:LEU:H	1.73	0.43
1:M:12:DT:H72	3:P:173:ARG:HD3	2.00	0.43
1:E:18:DT:H2'	1:E:19:DT:H72	2.00	0.43
3:A:52:PRO:O	3:A:151:PRO:HD3	2.19	0.43
3:B:16:ARG:HG2	3:B:173:ARG:HB2	2.01	0.43
2:N:12:DT:H5'	3:O:21:CYS:SG	2.58	0.43
2:N:12:DT:C2	2:N:13:DC:C5	3.07	0.43
3:B:192:CYS:HA	3:B:274:TYR:CD2	2.54	0.43
3:L:257:GLN:CD	3:L:266:LEU:HD23	2.39	0.43
3:P:189:SER:HA	3:P:273:GLN:O	2.19	0.43
3:B:116:ARG:HB2	3:B:116:ARG:NH1	2.34	0.43
2:N:14:DC:C2	2:N:15:DC:C5	3.06	0.43
2:N:16:DA:C8	2:N:17:DT:C7	3.02	0.43
3:K:248:LEU:HD23	3:K:248:LEU:HA	1.75	0.43
3:A:203:ASP:O	3:A:205:VAL:HG13	2.18	0.42
3:H:8:GLU:OE2	3:H:33:ARG:HG3	2.19	0.42
3:L:209:ASP:CG	3:L:262:SER:OG	2.57	0.42
1:M:13:DT:OP2	3:P:21:CYS:SG	2.69	0.42
2:F:11:DT:C6	2:F:12:DT:H72	2.54	0.42
3:B:29:ILE:HA	3:B:30:PRO:HD3	1.86	0.42
3:G:251:PRO:HB3	3:G:275:LEU:HD23	2.01	0.42
3:L:175:PRO:HB2	3:L:206:GLN:OE1	2.19	0.42
3:O:4:VAL:HB	3:O:164:ILE:CD1	2.49	0.42
3:O:73:LEU:HA	3:O:100:GLY:O	2.19	0.42
1:C:6:DG:H1	2:D:15:DC:H42	1.67	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:O:67:ARG:HD2	3:O:134:ILE:HG12	2.01	0.42
3:P:71:HIS:NE2	3:P:139:LEU:O	2.47	0.42
1:E:2:DT:C2	2:F:19:DA:H2	2.37	0.42
3:H:7:ILE:HG13	3:H:43:THR:HG23	2.02	0.42
3:K:18:ARG:HA	3:K:18:ARG:HD2	1.80	0.42
3:K:152:ASP:OD1	3:P:264:ARG:NH1	2.53	0.42
3:K:232:ARG:HG2	3:L:234:VAL:HG11	2.00	0.42
3:L:50:THR:HA	3:L:91:ARG:NH2	2.33	0.42
3:L:153:GLU:HB3	3:L:154:HIS:H	1.63	0.42
2:F:11:DT:H1'	2:F:12:DT:H5"	2.00	0.42
3:G:69:HIS:O	3:G:116:ARG:NH1	2.52	0.42
3:H:212:VAL:O	3:H:223:GLY:N	2.52	0.42
3:K:133:ASP:O	3:K:134:ILE:HB	2.20	0.42
3:L:143:ARG:NH1	3:L:168:PRO:HD3	2.35	0.42
3:B:7:ILE:HG13	3:B:43:THR:O	2.20	0.42
1:C:12:DT:C6	1:C:13:DT:H72	2.55	0.42
3:G:223:GLY:O	3:G:224:SER:HB3	2.20	0.42
3:H:62:LYS:HD2	3:H:141:VAL:HG11	2.01	0.42
3:L:66:HIS:HD2	3:L:165:VAL:HG11	1.82	0.42
1:E:2:DT:N3	2:F:19:DA:H2	2.17	0.42
2:F:19:DA:OP2	2:F:19:DA:C8	2.68	0.42
3:B:23:GLY:O	3:B:24:ARG:HG2	2.20	0.42
3:P:69:HIS:HD2	3:P:71:HIS:HB2	1.84	0.42
3:P:192:CYS:HA	3:P:274:TYR:CD2	2.55	0.42
3:B:122:ASN:HD21	3:B:126:VAL:CG2	2.32	0.42
3:B:259:ARG:NH1	3:B:264:ARG:HG2	2.35	0.42
3:H:94:LEU:HD23	3:H:94:LEU:HA	1.59	0.42
1:I:9:DA:H2"	1:I:10:DA:H8	1.85	0.42
2:J:1:DG:H2"	2:J:2:DA:H5'	2.01	0.42
2:J:18:DC:H6	2:J:19:DA:H5'	1.85	0.42
1:M:2:DT:H2"	1:M:3:DG:OP2	2.19	0.42
2:N:19:DA:H2"	2:N:20:DA:OP2	2.20	0.42
3:P:141:VAL:HG22	3:P:170:TYR:CD1	2.55	0.42
1:E:18:DT:H3	2:F:3:DA:H61	1.67	0.42
2:F:11:DT:H2"	2:F:12:DT:H5'	2.02	0.42
3:G:127:PRO:HG2	3:G:130:GLN:OE1	2.20	0.42
3:P:209:ASP:OD2	3:P:262:SER:OG	2.34	0.42
2:F:5:DC:H41	3:B:24:ARG:HH22	1.67	0.41
3:B:138:ASP:O	3:B:139:LEU:HB2	2.19	0.41
3:A:54:THR:HG22	3:A:85:ALA:HA	2.01	0.41
2:J:3:DA:H2"	2:J:4:DT:OP2	2.19	0.41



	A	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:K:265:GLU:C	3:K:266:LEU:HD12	2.41	0.41	
3:L:63:ASP:HB3	3:L:64:PRO:HD2	2.01	0.41	
1:M:19:DT:O2	2:N:2:DA:C2	2.73	0.41	
3:O:72:GLU:HB2	3:O:81:GLY:CA	2.49	0.41	
3:A:115:LEU:HD12	3:A:115:LEU:HA	1.81	0.41	
1:M:11:DT:H1'	1:M:12:DT:H5"	2.02	0.41	
3:A:212:VAL:O	3:A:223:GLY:N	2.53	0.41	
2:D:9:DA:C2	2:D:10:DA:C4	3.09	0.41	
3:G:148:VAL:HB	3:G:161:LEU:HD22	2.02	0.41	
3:H:132:LEU:HD22	3:H:132:LEU:HA	1.93	0.41	
3:L:231:HIS:HB3	3:L:235:ALA:HB3	2.03	0.41	
3:O:69:HIS:HE1	3:O:71:HIS:CD2	2.39	0.41	
2:D:3:DA:C2'	2:D:4:DT:H71	2.51	0.41	
3:H:69:HIS:CD2	3:H:71:HIS:H	2.39	0.41	
3:K:72:GLU:HB2	3:K:81:GLY:CA	2.51	0.41	
1:M:19:DT:O2	2:N:3:DA:C2	2.74	0.41	
3:B:16:ARG:HH21	3:B:173:ARG:HH22	1.68	0.41	
1:C:3:DG:C2	1:C:4:DA:C4	3.09	0.41	
1:I:10:DA:N1	2:J:11:DT:C2	2.87	0.41	
2:J:6:DG:H2"	2:J:7:DG:OP2	2.21	0.41	
3:K:257:GLN:HB3	3:K:269:PRO:HA	2.02	0.41	
3:0:243:TYR:CG	3:O:244:ALA:N	2.89	0.41	
1:E:17:DA:H2'	1:E:18:DT:H72	2.03	0.41	
2:D:3:DA:H2'	2:D:4:DT:H71	2.02	0.41	
3:K:56:ARG:NH1	3:K:121:ILE:HD13	2.35	0.41	
1:M:2:DT:O2	2:N:19:DA:H2	1.98	0.41	
3:P:94:LEU:HD23	3:P:94:LEU:HA	1.66	0.41	
2:D:11:DT:H5'	3:G:19:TYR:CZ	2.55	0.41	
3:G:72:GLU:HB2	3:G:81:GLY:CA	2.50	0.41	
1:I:1:DT:H2'	1:I:2:DT:H71	2.02	0.41	
2:J:11:DT:H5'	3:K:19:TYR:CZ	2.56	0.41	
3:L:251:PRO:HB3	3:L:275:LEU:HD23	2.02	0.41	
3:L:273:GLN:HE21	3:L:273:GLN:HB2	1.66	0.41	
3:O:88:GLY:H	3:O:89:PRO:HD2	1.86	0.41	
3:B:257:GLN:OE1	3:B:266:LEU:HD23	2.21	0.41	
3:L:105:LYS:HB2	3:L:108:GLU:HG3	2.03	0.41	
3:P:136:ASP:O	3:P:137:CYS:HB2	2.20	0.41	
3:A:196:ASP:O	3:A:239:ARG:HA	2.20	0.40	
3:A:204:LYS:HE3	3:A:233:GLN:OE1	2.20	0.40	
3:G:115:LEU:HD12	3:G:115:LEU:HA	1.90	0.40	
2:J:7:DG:C2	2:J:8:DA:C4	3.09	0.40	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:N:11:DT:H5'	3:O:19:TYR:CE2	2.56	0.40
3:P:212:VAL:HG11	3:P:238:PHE:CZ	2.56	0.40
3:B:182:ILE:HD11	3:B:257:GLN:HA	2.02	0.40
3:B:248:LEU:O	3:B:276:PRO:HB3	2.21	0.40
2:J:11:DT:C2	2:J:12:DT:C5	3.10	0.40
2:J:12:DT:C2	2:J:13:DC:C6	3.10	0.40
3:L:34:SER:OG	3:L:39:LYS:HG3	2.21	0.40
2:N:15:DC:H42	3:O:24:ARG:HH22	1.68	0.40
3:P:72:GLU:HB2	3:P:81:GLY:CA	2.51	0.40
3:B:53:GLY:O	3:B:87:PHE:HB3	2.20	0.40
3:B:67:ARG:NH1	3:B:130:GLN:O	2.54	0.40
1:C:19:DT:H2"	1:C:20:DC:C6	2.57	0.40
3:G:62:LYS:HD2	3:G:141:VAL:HG11	2.02	0.40
3:B:53:GLY:C	3:B:87:PHE:HB3	2.41	0.40
3:B:64:PRO:HB3	3:P:3:TYR:HB3	2.04	0.40
3:B:93:PRO:HB2	3:B:94:LEU:H	1.70	0.40
2:J:4:DT:H2"	2:J:5:DC:OP2	2.20	0.40
3:P:153:GLU:HB3	3:P:154:HIS:H	1.62	0.40
3:P:209:ASP:CG	3:P:262:SER:OG	2.59	0.40
3:P:212:VAL:O	3:P:223:GLY:N	2.54	0.40
3:A:192:CYS:HA	3:A:274:TYR:HD2	1.86	0.40
3:B:248:LEU:HB3	3:B:276:PRO:HA	2.03	0.40
3:G:99:LEU:HA	3:G:99:LEU:HD23	1.86	0.40
3:K:159:THR:O	3:K:160:ALA:HB3	2.21	0.40
3:L:17:PHE:CE2	3:L:101:ILE:HD13	2.57	0.40
1:M:3:DG:C2	2:N:19:DA:C2	3.09	0.40

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	Percentiles
3	А	274/277~(99%)	244 (89%)	20 (7%)	10 (4%)	3 16
3	В	270/277~(98%)	240 (89%)	20~(7%)	10 (4%)	2 16
3	G	274/277~(99%)	242 (88%)	22 (8%)	10 (4%)	3 16
3	Н	270/277~(98%)	240 (89%)	20~(7%)	10 (4%)	2 16
3	Κ	274/277~(99%)	244 (89%)	20 (7%)	10 (4%)	3 16
3	L	270/277~(98%)	241 (89%)	17~(6%)	12~(4%)	2 12
3	Ο	274/277~(99%)	242 (88%)	25~(9%)	7 (3%)	4 21
3	Р	270/277~(98%)	239~(88%)	20 (7%)	11 (4%)	2 13
All	All	2176/2216 (98%)	1932 (89%)	164 (8%)	80 (4%)	2 16

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	А	86	GLU
3	А	87	PHE
3	А	89	PRO
3	А	134	ILE
3	В	93	PRO
3	В	137	CYS
3	В	138	ASP
3	В	152	ASP
3	В	153	GLU
3	В	224	SER
3	G	86	GLU
3	G	89	PRO
3	G	134	ILE
3	G	157	PHE
3	Н	93	PRO
3	Н	137	CYS
3	Н	138	ASP
3	Н	152	ASP
3	Н	153	GLU
3	Н	224	SER
3	К	86	GLU
3	Κ	87	PHE
3	Κ	89	PRO
3	K	134	ILE
3	К	153	GLU
3	К	224	SER
3	L	93	PRO



Mol	Chain	Res	Type
3	L	137	CYS
3	L	138	ASP
3	L	152	ASP
3	L	153	GLU
3	L	224	SER
3	0	86	GLU
3	0	89	PRO
3	0	134	ILE
3	0	153	GLU
3	0	157	PHE
3	Р	93	PRO
3	Р	137	CYS
3	Р	138	ASP
3	Р	152	ASP
3	Р	153	GLU
3	Р	224	SER
3	А	153	GLU
3	А	224	SER
3	В	90	GLU
3	В	91	ARG
3	G	87	PHE
3	G	153	GLU
3	G	224	SER
3	Н	90	GLU
3	Н	91	ARG
3	K	85	ALA
3	L	24	ARG
3	L	90	GLU
3	L	91	ARG
3	L	134	ILE
3	0	87	PHE
3	Р	90	GLU
3	Р	91	ARG
3	Р	134	ILE
3	A	136	ASP
3	A	157	PHE
3	В	223	GLY
3	G	136	ASP
3	Η	134	ILE
3	Н	223	GLY
3	К	136	ASP
3	K	157	PHE



Mol	Chain	Res	Type
3	0	136	ASP
3	Р	66	HIS
3	G	85	ALA
3	Κ	223	GLY
3	А	160	ALA
3	Р	223	GLY
3	А	85	ALA
3	L	125	ASN
3	В	134	ILE
3	L	223	GLY
3	G	217	PRO

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	\mathbf{P}	erc	entiles
3	А	245/246~(100%)	223~(91%)	22 (9%)		8	29
3	В	244/246~(99%)	226~(93%)	18 (7%)		11	36
3	G	245/246~(100%)	222~(91%)	23~(9%)		7	27
3	Н	244/246~(99%)	224 (92%)	20 (8%)		9	33
3	Κ	245/246~(100%)	223~(91%)	22 (9%)		8	29
3	L	244/246~(99%)	221 (91%)	23~(9%)		7	27
3	Ο	245/246~(100%)	228~(93%)	17 (7%)		13	39
3	Р	244/246~(99%)	220 (90%)	24 (10%)		6	25
All	All	1956/1968~(99%)	1787 (91%)	169 (9%)		8	31

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	А	16	ARG
3	А	20	LYS
3	А	38	THR
3	А	47	ASN



Mol	Chain	Res	Type
3	А	54	THR
3	А	90	GLU
3	А	94	LEU
3	А	98	ASN
3	А	115	LEU
3	А	132	LEU
3	А	136	ASP
3	А	138	ASP
3	А	150	LEU
3	А	158	THR
3	А	184	ARG
3	А	187	ARG
3	А	208	GLU
3	А	220	GLU
3	А	222	ARG
3	A	226	SER
3	А	239	ARG
3	А	262	SER
3	В	7	ILE
3	В	8	GLU
3	В	9	GLN
3	В	33	ARG
3	В	79	ARG
3	В	86	GLU
3	В	91	ARG
3	В	105	LYS
3	В	115	LEU
3	В	116	ARG
3	В	132	LEU
3	В	134	ILE
3	B	150	LEU
3	В	187	ARG
3	B	208	GLU
3	B	252	VAL
3	В	273	GLN
3	В	277	ASP
3	G	15	MET
3	G	16	ARG
3	G	20	LYS
3	G	37	THR
3	G	38	THR
3	G	47	ASN



Mol	Chain	Res	Type
3	G	54	THR
3	G	90	GLU
3	G	94	LEU
3	G	98	ASN
3	G	115	LEU
3	G	132	LEU
3	G	136	ASP
3	G	138	ASP
3	G	150	LEU
3	G	158	THR
3	G	161	LEU
3	G	187	ARG
3	G	208	GLU
3	G	222	ARG
3	G	226	SER
3	G	239	ARG
3	G	252	VAL
3	Н	3	TYR
3	Н	7	ILE
3	Н	8	GLU
3	Н	9	GLN
3	Н	33	ARG
3	Н	38	THR
3	Н	54	THR
3	Н	64	PRO
3	Н	79	ARG
3	Н	115	LEU
3	Н	116	ARG
3	Н	131	LEU
3	Н	132	LEU
3	Н	134	ILE
3	H	150	LEU
3	H	187	ARG
3	H	208	GLU
3	Н	271	GLU
3	Н	273	GLN
3	H	277	ASP
3	K	15	MET
3	K	16	ARG
3	K	47	ASN
3	K	54	THR
3	Κ	90	GLU



Mol	Chain	Res	Type
3	K	94	LEU
3	K	98	ASN
3	K	106	LYS
3	Κ	115	LEU
3	K	132	LEU
3	Κ	136	ASP
3	K	138	ASP
3	Κ	150	LEU
3	K	158	THR
3	Κ	161	LEU
3	Κ	184	ARG
3	K	187	ARG
3	Κ	207	LYS
3	K	208	GLU
3	Κ	220	GLU
3	K	226	SER
3	Κ	239	ARG
3	L	3	TYR
3	L	7	ILE
3	L	8	GLU
3	L	9	GLN
3	L	33	ARG
3	L	54	THR
3	L	66	HIS
3	L	79	ARG
3	L	86	GLU
3	L	91	ARG
3	L	105	LYS
3	L	115	LEU
3	L	116	ARG
3	L	131	LEU
3	L	132	LEU
3	L	134	ILE
3	L	150	LEU
3	L	187	ARG
3	L	198	ILE
3	L	208	GLU
3	L	262	SER
3	L	273	GLN
3	L	277	ASP
3	Ō	16	ARG
3	0	38	THR



Mol	Chain	Res	Type	
3	0	47	ASN	
3	0	54	THR	
3	0	90	GLU	
3	0	94	LEU	
3	0	98	ASN	
3	0	132	LEU	
3	0	136	ASP	
3	0	138	ASP	
3	0	150	LEU	
3	0	161	LEU	
3	0	164	ILE	
3	0	187	ARG	
3	0	208	GLU	
3	0	239	ARG	
3	0	262	SER	
3	Р	7	ILE	
3	Р	8	GLU	
3	Р	9	GLN	
3	Р	33	ARG	
3	Р	38	THR	
3	Р	54	THR	
3	Р	79	ARG	
3	Р	86	GLU	
3	Р	91	ARG	
3	Р	101	ILE	
3	Р	105	LYS	
3	Р	114	ILE	
3	Р	115	LEU	
3	Р	116	ARG	
3	Р	131	LEU	
3	Р	132	LEU	
3	Р	134	ILE	
3	Р	150	LEU	
3	Р	158	THR	
3	Р	187	ARG	
3	Р	208	GLU	
3	Р	262	SER	
3	Р	273	GLN	
3	Р	277	ASP	

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:



Mol	Chain	Res	Type
3	Κ	273	GLN
3	L	273	GLN
3	Р	69	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	$\langle RSRZ \rangle$	#RSRZ>2		Z>2	$OWAB(Å^2)$	Q < 0.9
1	С	20/20~(100%)	-1.69	0	100	100	58, 73, 101, 109	0
1	Е	20/20~(100%)	-1.37	0	100	100	47, 100, 151, 152	0
1	Ι	20/20~(100%)	-1.87	0	100	100	49, 68, 93, 96	0
1	М	20/20~(100%)	-1.83	0	100	100	46, 76, 118, 123	0
2	D	20/20~(100%)	-1.71	0	100	100	43, 97, 119, 119	0
2	F	20/20~(100%)	-1.75	0	100	100	55, 82, 118, 121	0
2	J	20/20~(100%)	-1.60	0	100	100	39, 63, 130, 143	0
2	N	20/20~(100%)	-1.76	0	100	100	51, 71, 89, 99	0
3	А	276/277~(99%)	-1.39	0	100	100	60, 82, 133, 168	0
3	В	274/277~(98%)	-1.30	0	100	100	56, 83, 141, 166	0
3	G	276/277~(99%)	-1.36	0	100	100	49, 79, 135, 157	0
3	Н	274/277~(98%)	-1.33	0	100	100	48, 79, 141, 164	0
3	Κ	276/277~(99%)	-1.36	0	100	100	56, 84, 128, 166	0
3	L	274/277~(98%)	-1.45	0	100	100	45, 77, 118, 170	0
3	Ο	276/277~(99%)	-1.45	0	100	100	48, 83, 125, 155	0
3	Р	274/277~(98%)	-1.42	0	100	100	51, 77, 117, 173	0
All	All	2360/2376~(99%)	-1.41	0	100	100	39, 80, 131, 173	0

There are no RSRZ outliers to report.

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

