Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 04:48 AM JST

PDB ID	:	6KQN
Title	:	Thermus thermophilus initial transcription complex comprising sigma A and 5'-triphosphate RNA of 6 nt
Authors	:	Zhang, Y.; Li, L.; Ebright, R.H.
Deposited on	:	2019-08-18
Resolution	:	3.49 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 ⓘ 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 ⓘ) were used in the production of this report:

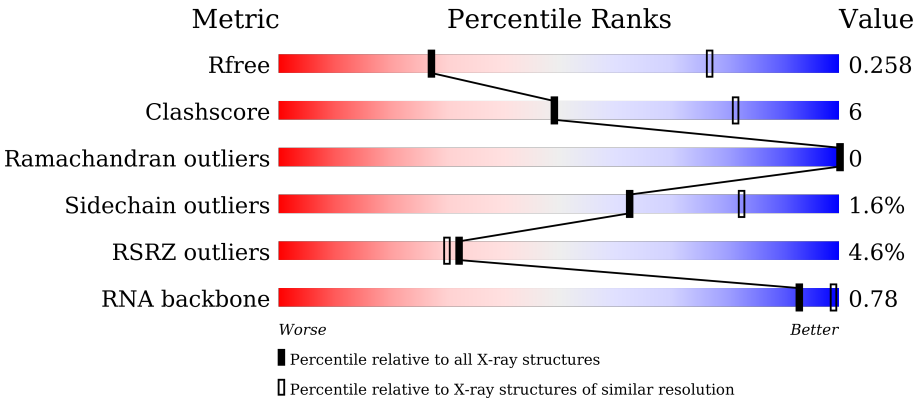
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)
RNA backbone	3102	1054 (4.00-2.96)

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	315	2% 62% 11% 27%
1	B	315	% 62% 9% 29%
2	C	1119	5% 82% 16% ••
3	D	1524	4% 82% 15% •

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Mol	Chain	Length	Quality of chain
4	E	99	2% 80% 15% 5%
5	F	443	7% 68% 7% 24%
6	G	21	38% 48% 14%
7	H	27	44% 44% 11%
8	I	6	67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MG	B	2001	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28637 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	1	0
			1814	1158	316	338	2			
1	B	223	Total	C	N	O	S	0	0	0
			1755	1123	304	326	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	3	0
			8785	5556	1570	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	3	0
			11753	7455	2067	2195	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	337	Total	C	N	O	S	0	0	0
			2737	1726	499	508	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	18	372	176	73	106	17	0	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G*)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	H	24	495	236	94	142	23	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	6	134	56	21	49	8	0	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	2	Total Mg 2 2	0	0
9	F	1	Total Mg 1 1	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is water.

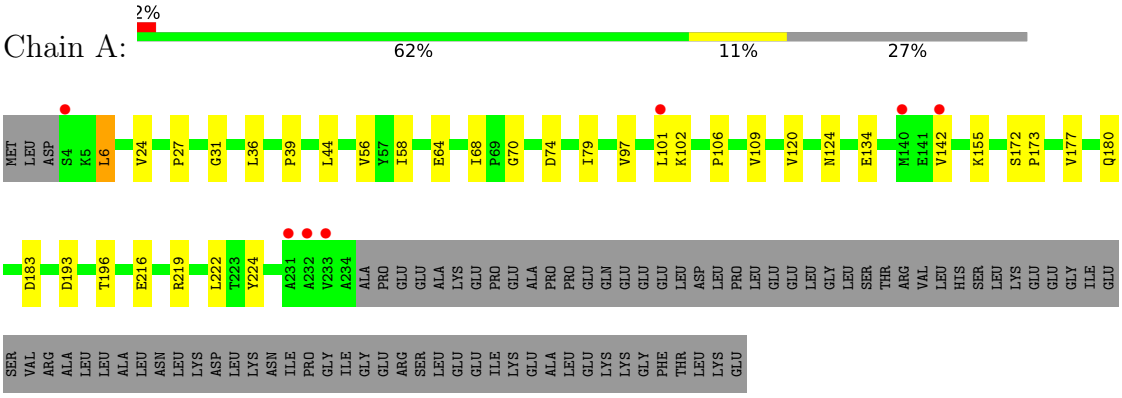
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	2	Total O 2 2	0	0
11	C	7	Total O 7 7	0	0
11	D	14	Total O 14 14	0	0
11	G	1	Total O 1 1	0	0
11	H	1	Total O 1 1	0	0

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.

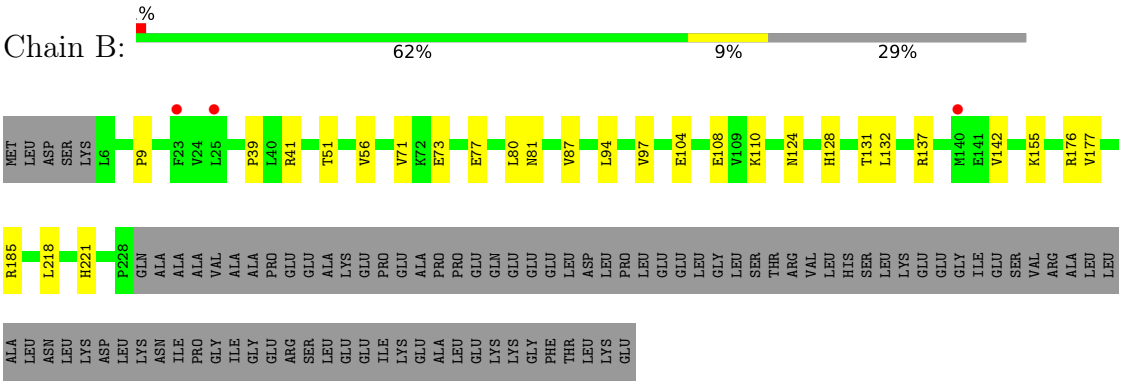
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



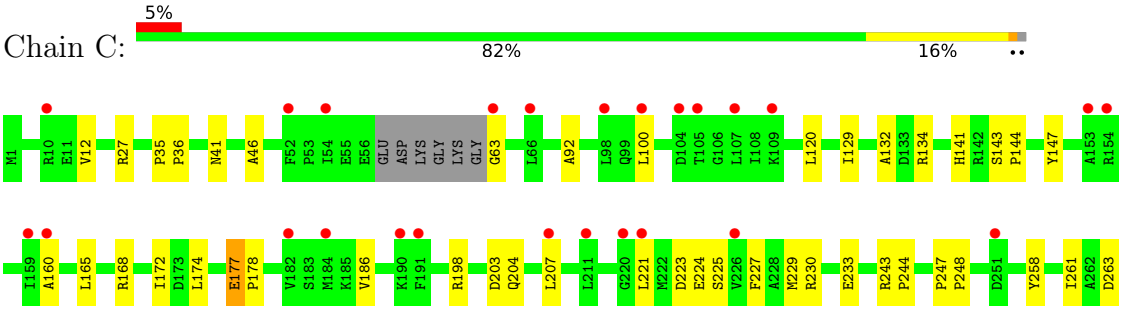
• Molecule 1: DNA-directed RNA polymerase subunit alpha

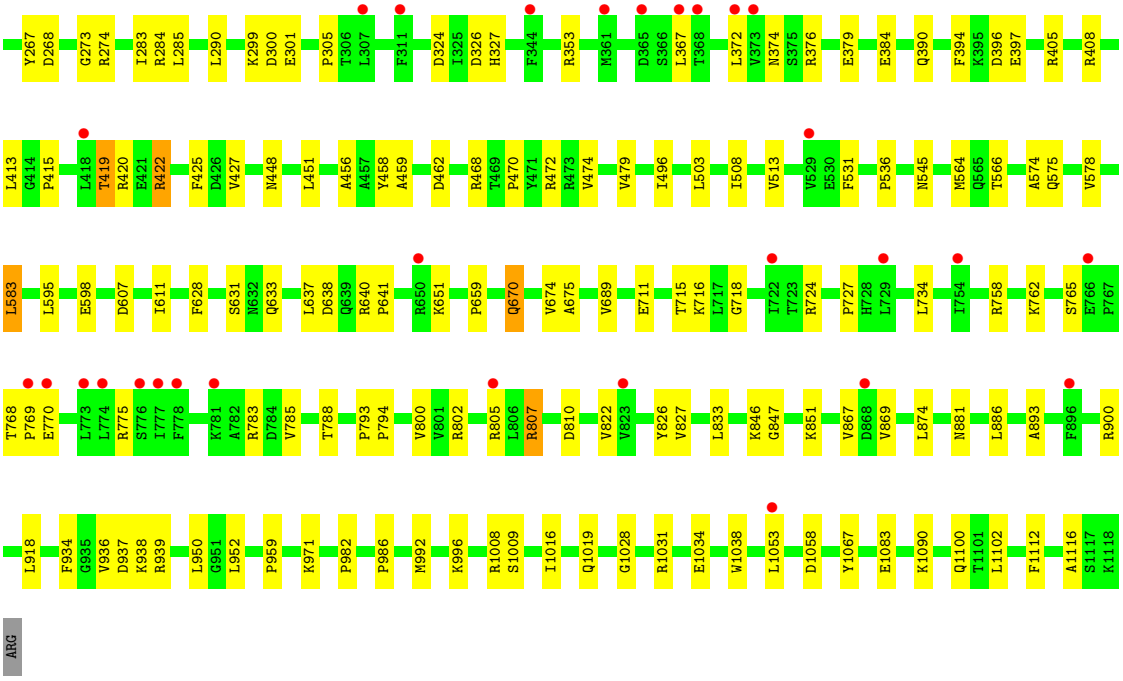
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

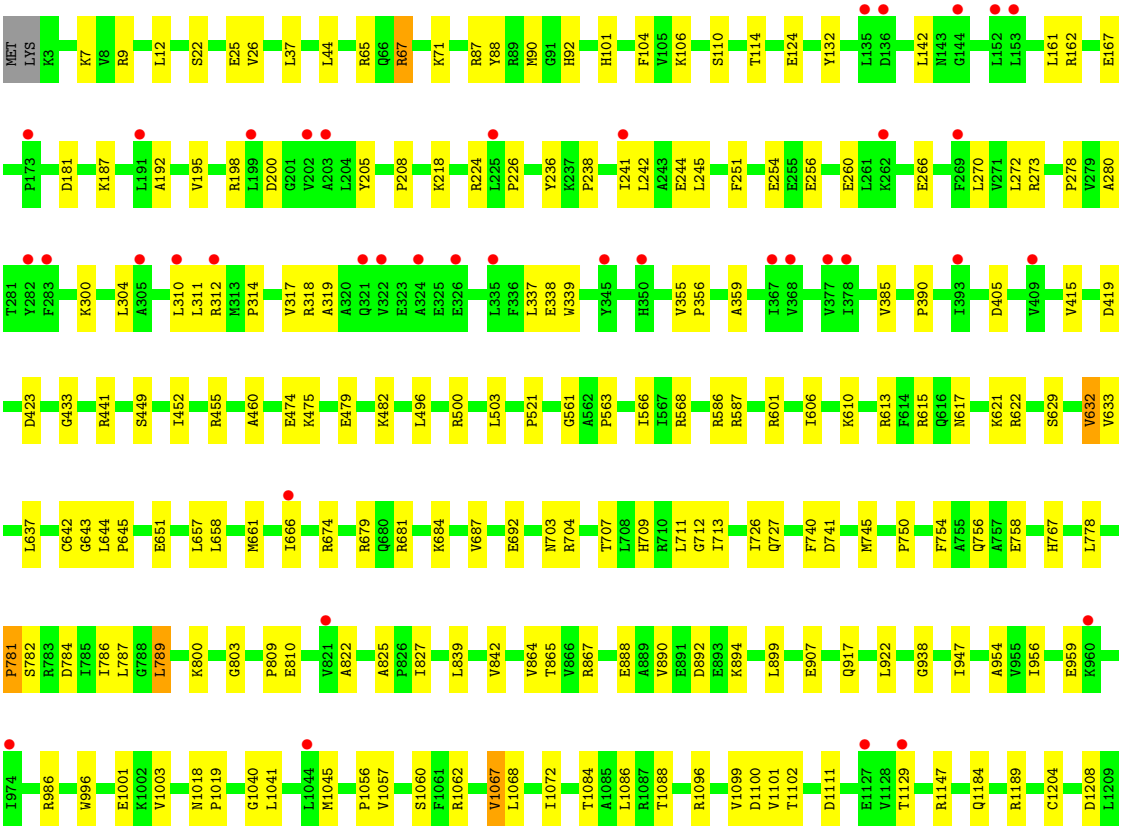
Chain C:

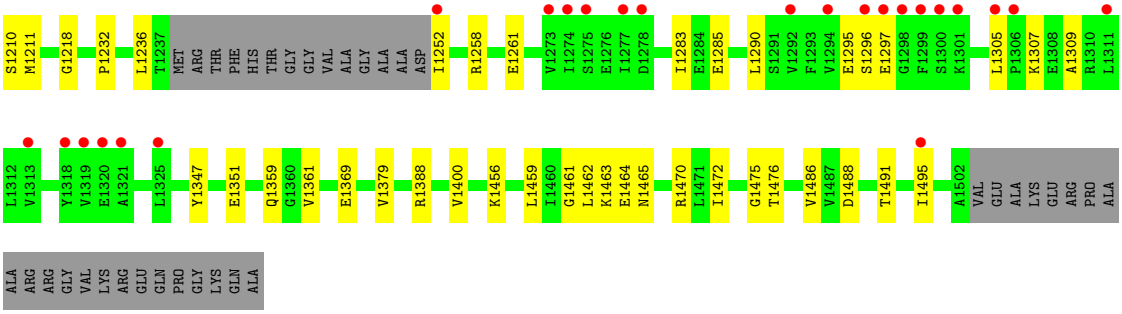




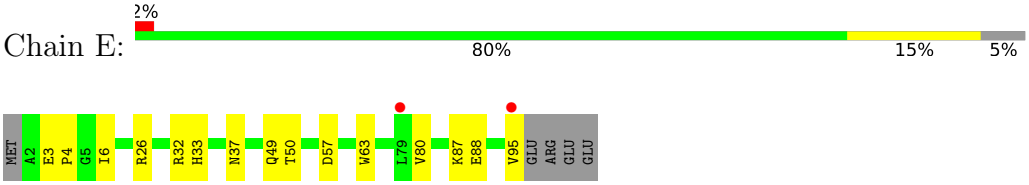
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:

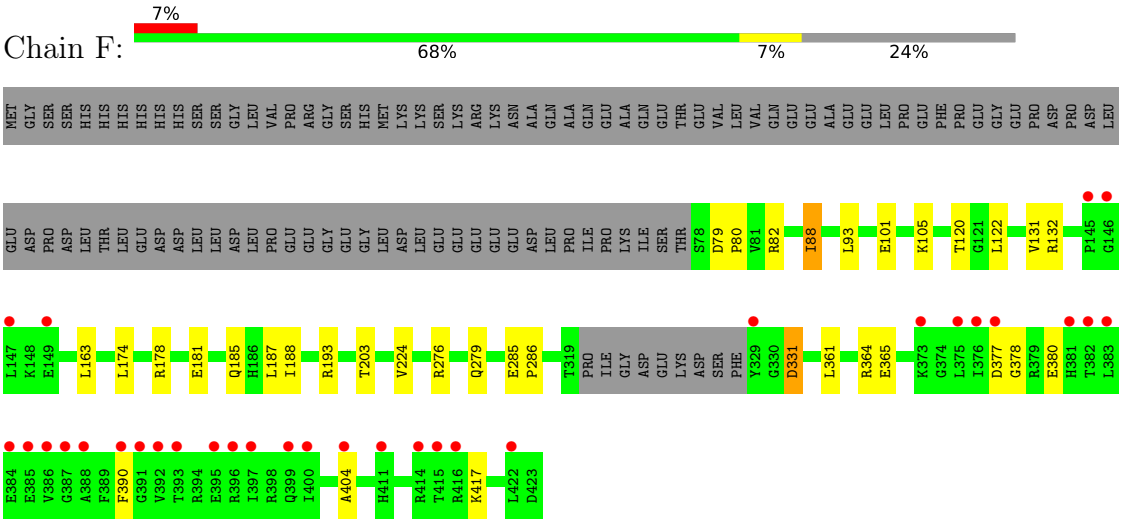




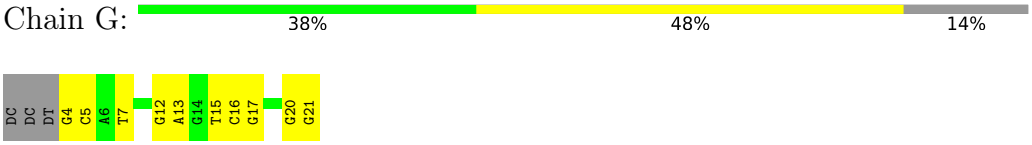
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor SigA



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



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

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

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.62Å 101.92Å 296.11Å 90.00° 98.83° 90.00°	Depositor
Resolution (Å)	48.79 – 3.49 48.79 – 3.49	Depositor EDS
% Data completeness (in resolution range)	93.2 (48.79-3.49) 93.5 (48.79-3.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.213 , 0.258 0.213 , 0.258	Depositor DCC
R_{free} test set	3249 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	99.9	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28637	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CTP, 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	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.22	0/1849	0.40	0/2515
1	B	0.21	0/1787	0.43	0/2431
2	C	0.21	0/8961	0.41	0/12118
3	D	0.22	0/11969	0.41	0/16182
4	E	0.21	0/775	0.38	0/1045
5	F	0.20	0/2779	0.36	0/3737
6	G	0.43	0/418	0.89	0/645
7	H	0.42	0/556	0.96	0/858
8	I	0.16	0/116	0.64	0/178
All	All	0.23	0/29210	0.44	0/39709

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

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	1814	0	1869	24	0
1	B	1755	0	1804	20	0
2	C	8785	0	8895	117	0
3	D	11753	0	11992	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	761	0	778	10	0
5	F	2737	0	2819	24	0
6	G	372	0	203	21	0
7	H	495	0	272	16	0
8	I	134	0	65	1	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	B	2	0	0	0	0
11	C	7	0	0	0	0
11	D	14	0	0	0	0
11	G	1	0	0	0	0
11	H	1	0	0	0	0
All	All	28637	0	28697	335	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.

All (335) 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)
3:D:782:SER:HA	3:D:786:ILE:HD12	1.49	0.95
2:C:874:LEU:HD22	3:D:784:ASP:OD1	1.75	0.87
3:D:782:SER:HA	3:D:786:ILE:CD1	2.05	0.85
2:C:768:THR:CG2	2:C:769:PRO:HD2	2.06	0.85
2:C:768:THR:HG23	2:C:769:PRO:HD2	1.59	0.85
6:G:12:DG:N2	7:H:16:DC:N3	2.27	0.80
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.64	0.78
2:C:628:PHE:H	2:C:638:ASP:HB3	1.48	0.77
7:H:17:DA:C2	7:H:18:DC:C2	2.74	0.76
6:G:16:DC:H2'	6:G:17:DG:H8	1.50	0.74
6:G:20:DG:H1	8:I:2:CTP:HN41	1.35	0.74
6:G:12:DG:N2	7:H:16:DC:C2	2.56	0.72
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.70	0.71
7:H:17:DA:N3	7:H:18:DC:C2	2.61	0.69
4:E:32:ARG:O	4:E:95:VAL:HG13	1.93	0.69
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.76	0.67
2:C:758:ARG:HH21	2:C:788:THR:HB	1.59	0.67
3:D:405:ASP:HB3	3:D:423:ASP:HA	1.77	0.67
2:C:63:GLY:HA3	2:C:100:LEU:HD21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.28	0.65
6:G:12:DG:H1	7:H:16:DC:H42	1.44	0.65
3:D:65:ARG:NH1	5:F:378:GLY:O	2.29	0.65
6:G:16:DC:H2'	6:G:17:DG:C8	2.32	0.65
2:C:768:THR:HG22	2:C:770:GLU:OE1	1.98	0.64
2:C:1019:GLN:HG2	2:C:1058:ASP:HB3	1.80	0.63
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.79	0.63
2:C:800:VAL:HG22	2:C:827:VAL:HG22	1.79	0.63
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.32	0.62
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.80	0.62
2:C:420:ARG:NH2	2:C:448:ASN:OD1	2.30	0.62
3:D:711:LEU:HD22	3:D:778:LEU:HD23	1.82	0.62
6:G:21:DG:OP2	6:G:21:DG:H8	1.82	0.62
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.82	0.61
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.83	0.61
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.34	0.61
2:C:575:GLN:HG3	2:C:670:GLN:HE21	1.66	0.61
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.34	0.60
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.83	0.60
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.82	0.60
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.84	0.59
3:D:803:GLY:HA2	3:D:827:ILE:HA	1.83	0.59
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.83	0.59
2:C:874:LEU:HD11	3:D:787:LEU:HD22	1.84	0.59
6:G:20:DG:C2'	6:G:21:DG:O4'	2.50	0.59
6:G:20:DG:H2"	6:G:21:DG:O4'	2.03	0.59
3:D:1258:ARG:NH1	3:D:1261:GLU:OE2	2.36	0.58
7:H:17:DA:C2	7:H:18:DC:O2	2.56	0.58
2:C:768:THR:HG22	2:C:769:PRO:HD2	1.84	0.58
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.83	0.58
5:F:331:ASP:OD2	5:F:331:ASP:N	2.36	0.58
2:C:1034:GLU:OE2	3:D:1096:ARG:NH2	2.37	0.58
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.85	0.58
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.86	0.58
3:D:106:LYS:O	3:D:586:ARG:NH1	2.37	0.57
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.85	0.57
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.86	0.57
7:H:15:DT:H1'	7:H:16:DC:H5'	1.86	0.57
2:C:768:THR:CG2	2:C:769:PRO:CD	2.80	0.57
6:G:15:DT:H2'	6:G:16:DC:C6	2.39	0.57
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.34	0.57
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.38	0.57
2:C:326:ASP:OD1	7:H:14:DG:N2	2.32	0.56
5:F:193:ARG:NH1	7:H:7:DG:N7	2.54	0.56
2:C:223:ASP:OD1	2:C:225:SER:OG	2.21	0.56
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.88	0.56
1:A:196:THR:HG21	2:C:934:PHE:HE2	1.70	0.55
2:C:715:THR:OG1	2:C:718:GLY:O	2.24	0.55
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.87	0.55
4:E:33:HIS:HA	4:E:95:VAL:HG22	1.88	0.55
3:D:241:ILE:HA	3:D:312:ARG:HG2	1.89	0.55
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.88	0.55
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.89	0.55
2:C:637:LEU:HG	2:C:659:PRO:HG3	1.89	0.55
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.89	0.55
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.39	0.55
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.88	0.55
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.88	0.54
2:C:244:PRO:O	5:F:82:ARG:NH1	2.40	0.54
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	1.89	0.54
2:C:1031:ARG:HA	3:D:622:ARG:HA	1.89	0.54
2:C:207:LEU:HD13	2:C:221:LEU:HD21	1.89	0.54
2:C:611:ILE:HD11	2:C:641:PRO:HB3	1.89	0.54
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.90	0.54
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.41	0.54
3:D:789:LEU:HD23	3:D:938:GLY:HA2	1.89	0.54
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.90	0.54
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.90	0.54
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.89	0.53
3:D:1045[B]:MET:HE1	3:D:1057:VAL:HG23	1.90	0.53
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.89	0.53
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.90	0.53
2:C:456:ALA:HB3	2:C:459:ALA:HB2	1.91	0.53
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.91	0.53
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.90	0.53
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.90	0.53
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.91	0.53
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.90	0.53
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.90	0.53
3:D:142:LEU:HB2	3:D:161:LEU:HD21	1.91	0.52
3:D:781:PRO:O	3:D:786:ILE:HD11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.34	0.52
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.42	0.52
2:C:408:ARG:NH1	2:C:456:ALA:O	2.42	0.52
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.92	0.52
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.43	0.52
3:D:1111:ASP:OD1	3:D:1189:ARG:NH2	2.42	0.52
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.74	0.51
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.90	0.51
3:D:226:PRO:HG2	3:D:245:LEU:HD11	1.92	0.51
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.93	0.51
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.91	0.51
6:G:12:DG:H2'	6:G:13:DA:C8	2.45	0.51
6:G:12:DG:H1	7:H:16:DC:N4	2.09	0.51
5:F:279:GLN:HB3	5:F:286:PRO:HD3	1.91	0.51
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.92	0.51
6:G:20:DG:H2'	6:G:21:DG:C1'	2.41	0.51
4:E:32:ARG:O	4:E:95:VAL:CG1	2.58	0.51
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.93	0.50
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.93	0.50
2:C:41:ASN:O	2:C:46:ALA:HB2	2.11	0.50
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.93	0.50
2:C:807[A]:ARG:NH1	2:C:810:ASP:OD2	2.44	0.50
3:D:110:SER:O	3:D:114:THR:OG1	2.21	0.50
3:D:1100:ASP:OD2	3:D:1463:LYS:NZ	2.36	0.50
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.92	0.50
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.92	0.50
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.92	0.50
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.93	0.50
6:G:4:DG:H2"	6:G:5:DC:C6	2.46	0.50
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.92	0.50
4:E:57:ASP:HB3	4:E:63:TRP:HE1	1.77	0.50
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.94	0.50
6:G:20:DG:C2'	6:G:21:DG:C1'	2.89	0.50
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.93	0.50
4:E:37:ASN:OD1	4:E:37:ASN:N	2.42	0.50
2:C:243:ARG:NH1	7:H:9:DG:O6	2.45	0.49
2:C:129:ILE:HB	2:C:134:ARG:HD2	1.94	0.49
2:C:419:THR:HG23	2:C:422:ARG:HB2	1.94	0.49
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.94	0.49
3:D:208:PRO:HA	3:D:390:PRO:HA	1.94	0.49
3:D:657:LEU:HG	3:D:661:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.95	0.49
2:C:390:GLN:HB3	2:C:415:PRO:HD3	1.94	0.49
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.93	0.49
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.12	0.49
1:A:31:GLY:N	1:A:193:ASP:OD1	2.43	0.49
3:D:758:GLU:HG2	3:D:1476:THR:HG21	1.95	0.49
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.45	0.49
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.93	0.49
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.95	0.49
6:G:20:DG:H2'	6:G:21:DG:C8	2.48	0.49
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.95	0.49
1:B:81:ASN:OD1	3:D:867:ARG:NH2	2.41	0.49
2:C:168:ARG:HE	2:C:168:ARG:HA	1.78	0.49
3:D:842:VAL:HG22	3:D:865:THR:HB	1.95	0.48
3:D:433:GLY:HA2	3:D:449:SER:H	1.78	0.48
2:C:598:GLU:O	2:C:651:LYS:NZ	2.43	0.48
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.95	0.48
3:D:959:GLU:N	3:D:959:GLU:OE1	2.44	0.48
2:C:937:ASP:OD1	2:C:938:LYS:N	2.46	0.48
3:D:658:LEU:HA	3:D:661:MET:HE3	1.95	0.48
3:D:1486:VAL:HG11	4:E:26:ARG:HB2	1.95	0.48
3:D:789:LEU:HD23	3:D:789:LEU:N	2.29	0.48
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.96	0.48
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.49	0.48
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.79	0.47
3:D:187:LYS:N	3:D:200:ASP:OD1	2.39	0.47
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.96	0.47
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.78	0.47
3:D:162:ARG:HH11	3:D:452:ILE:H	1.61	0.47
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.95	0.47
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.97	0.47
2:C:768:THR:CG2	2:C:770:GLU:OE1	2.62	0.47
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.96	0.47
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.96	0.47
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.96	0.47
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.44	0.47
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.96	0.47
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.96	0.47
3:D:1459:LEU:HD22	3:D:1464:GLU:HB3	1.97	0.47
1:A:97:VAL:HG11	1:A:120:VAL:HG21	1.96	0.46
2:C:168:ARG:O	2:C:267:TYR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:458:TYR:HB3	2:C:470:PRO:HG3	1.97	0.46
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.96	0.46
3:D:890:VAL:HG23	3:D:892:ASP:H	1.80	0.46
2:C:768:THR:HG22	2:C:769:PRO:CD	2.46	0.46
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.98	0.46
2:C:574:ALA:HA	2:C:670:GLN:HE22	1.81	0.46
2:C:578:VAL:HA	2:C:900:ARG:HG2	1.98	0.46
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.16	0.46
2:C:689:VAL:HG13	2:C:851:LYS:HB3	1.96	0.46
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.97	0.46
1:A:180:GLN:HB3	1:A:196:THR:HB	1.97	0.46
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.97	0.46
3:D:629:SER:HB3	3:D:726:ILE:HG13	1.97	0.46
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.97	0.45
2:C:1009:SER:HB3	3:D:651:GLU:O	2.15	0.45
2:C:300:ASP:OD1	2:C:301:GLU:N	2.49	0.45
3:D:789:LEU:CD2	3:D:938:GLY:HA2	2.46	0.45
1:A:124:ASN:OD1	1:A:124:ASN:N	2.49	0.45
2:C:283:ILE:HD13	2:C:305:PRO:HG2	1.96	0.45
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.98	0.45
3:D:319:ALA:HA	3:D:337:LEU:HD23	1.98	0.45
3:D:679:ARG:HH22	3:D:681:ARG:HD2	1.81	0.45
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.75	0.45
2:C:203:ASP:OD2	2:C:204:GLN:N	2.50	0.45
2:C:847:GLY:HA2	3:D:741:ASP:HA	1.98	0.45
2:C:893:ALA:HB2	2:C:918:LEU:HD23	1.97	0.45
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.99	0.45
3:D:479:GLU:HA	3:D:482:LYS:HE2	1.99	0.45
2:C:833:LEU:HD13	2:C:996:LYS:HE2	1.98	0.45
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.97	0.45
1:B:41:ARG:HA	1:B:177:VAL:HG11	1.98	0.44
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.98	0.44
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.99	0.44
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.98	0.44
2:C:950:LEU:HB3	2:C:952:LEU:HD13	1.98	0.44
3:D:633:VAL:HB	3:D:740:PHE:CZ	2.52	0.44
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.98	0.44
3:D:1296:SER:OG	3:D:1297:GLU:N	2.50	0.44
1:B:185:ARG:HH21	3:D:692:GLU:HG3	1.83	0.44
3:D:65:ARG:HD3	3:D:65:ARG:HA	1.81	0.44
1:B:155:LYS:HD3	1:B:155:LYS:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:12:DG:H5"	6:G:12:DG:H8	1.83	0.44
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.33	0.44
7:H:10:DA:H2"	7:H:11:DG:C8	2.52	0.44
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.99	0.44
2:C:564:MET:SD	2:C:846:LYS:HD3	2.57	0.44
2:C:536:PRO:HB3	3:D:1067:VAL:HG11	1.99	0.44
3:D:632:VAL:O	3:D:727:GLN:HA	2.18	0.44
3:D:661:MET:HG2	3:D:666:ILE:HD12	2.00	0.44
7:H:10:DA:H2"	7:H:11:DG:H5"	1.99	0.44
1:A:172:SER:HA	1:A:173:PRO:HD2	1.85	0.43
2:C:881:ASN:OD1	2:C:881:ASN:N	2.51	0.43
3:D:864:VAL:HG22	3:D:865:THR:H	1.83	0.43
3:D:1290:LEU:HD22	3:D:1305:LEU:HD11	2.00	0.43
5:F:101:GLU:HG2	5:F:105:LYS:HE2	2.00	0.43
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.81	0.43
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.82	0.43
2:C:224:GLU:CD	2:C:224:GLU:H	2.21	0.43
3:D:601:ARG:NH1	3:D:606:ILE:HG12	2.33	0.43
6:G:20:DG:H2"	6:G:21:DG:C1'	2.48	0.43
2:C:724:ARG:NH2	2:C:734:LEU:O	2.51	0.43
3:D:606:ILE:O	3:D:613:ARG:N	2.47	0.43
3:D:1283:ILE:H	3:D:1283:ILE:HG13	1.71	0.43
5:F:93:LEU:HD21	5:F:193:ARG:HD2	2.00	0.43
2:C:496:ILE:HG12	2:C:531:PHE:HB2	2.00	0.43
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	1.99	0.43
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.48	0.43
6:G:7:DT:H3	7:H:21:DA:H61	1.66	0.43
2:C:425:PHE:CE1	3:D:1086:LEU:HD12	2.53	0.43
3:D:90:MET:SD	3:D:521:PRO:HD3	2.58	0.43
7:H:18:DC:H2'	7:H:19:DG:C8	2.54	0.43
2:C:397:GLU:HB2	2:C:631:SER:HB2	2.00	0.43
3:D:25:GLU:HB2	3:D:92:HIS:CE1	2.54	0.43
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.01	0.43
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.48	0.43
5:F:364:ARG:HG3	5:F:390:PHE:CE2	2.53	0.43
2:C:143:SER:O	2:C:147:TYR:OH	2.27	0.42
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.54	0.42
3:D:684:LYS:O	3:D:687:VAL:HG22	2.19	0.42
6:G:20:DG:H2'	6:G:21:DG:N9	2.33	0.42
1:A:70:GLY:N	2:C:607:ASP:OD1	2.51	0.42
1:B:124:ASN:OD1	1:B:124:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.74	0.42
3:D:244:GLU:HG3	3:D:310:LEU:HG	2.02	0.42
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.55	0.42
1:A:183:ASP:HA	2:C:938:LYS:HE3	2.01	0.42
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.83	0.42
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.55	0.42
3:D:1211:MET:HE2	3:D:1211:MET:HB2	1.89	0.42
2:C:716:LYS:HE3	3:D:37:LEU:HG	2.00	0.42
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.54	0.42
2:C:1067:TYR:OH	3:D:674[B]:ARG:NH1	2.53	0.42
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.55	0.42
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.54	0.42
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	2.00	0.42
5:F:181:GLU:O	5:F:185:GLN:HG2	2.19	0.42
2:C:198:ARG:HE	2:C:227:PHE:HA	1.84	0.42
2:C:474:VAL:HG22	2:C:479:VAL:HG22	2.02	0.42
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	2.01	0.42
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.83	0.42
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.53	0.42
1:A:58:ILE:HG21	1:A:68:ILE:HD11	2.01	0.42
5:F:79:ASP:HA	5:F:80:PRO:HD3	1.93	0.42
2:C:805:ARG:HG2	2:C:807[A]:ARG:HE	1.84	0.42
2:C:376:ARG:NH1	2:C:379:GLU:OE1	2.53	0.41
3:D:67:ARG:HB3	5:F:377:ASP:O	2.19	0.41
3:D:610:LYS:HA	3:D:615:ARG:HD3	2.02	0.41
3:D:106:LYS:NZ	3:D:587:ARG:HG3	2.34	0.41
2:C:1031:ARG:HB2	3:D:622:ARG:HG2	2.02	0.41
3:D:500:ARG:HA	3:D:503:LEU:HB2	2.02	0.41
3:D:767:HIS:CE1	4:E:6:ILE:HG12	2.56	0.41
1:B:51:THR:OG1	1:B:87:VAL:O	2.23	0.41
2:C:374:ASN:OD1	5:F:276:ARG:HD2	2.20	0.41
1:A:196:THR:HG21	2:C:934:PHE:CE2	2.53	0.41
2:C:258:TYR:O	2:C:263:ASP:N	2.53	0.41
2:C:971:LYS:HB3	2:C:986:PRO:HB2	2.02	0.41
3:D:613:ARG:NH1	3:D:617:ASN:OD1	2.53	0.41
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.21	0.41
6:G:15:DT:C4	6:G:16:DC:N4	2.88	0.41
1:A:155:LYS:HA	1:A:155:LYS:HD2	1.86	0.41
3:D:1218:GLY:O	3:D:1475:GLY:N	2.43	0.41
3:D:475:LYS:O	3:D:479:GLU:HG2	2.20	0.41
3:D:1084:THR:O	3:D:1088:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:HB3	1:B:77:GLU:HB3	2.02	0.41
1:B:185:ARG:NH2	3:D:692:GLU:HG3	2.35	0.41
5:F:88:ILE:HG23	5:F:193:ARG:HG2	2.03	0.41
1:A:44:LEU:HB3	1:A:177:VAL:HG21	2.03	0.41
1:A:224:TYR:HB3	1:B:9:PRO:HG2	2.03	0.41
1:B:94:LEU:HD11	1:B:97:VAL:HG22	2.02	0.41
1:B:110:LYS:HD3	1:B:128:HIS:HA	2.03	0.41
2:C:230:ARG:HG3	2:C:233:GLU:HG3	2.03	0.41
2:C:762:LYS:HE3	2:C:785:VAL:O	2.20	0.41
2:C:793:PRO:HA	2:C:794:PRO:HD3	1.96	0.41
2:C:1008:ARG:NH1	2:C:1028:GLY:HA2	2.36	0.41
3:D:1208:ASP:OD1	3:D:1210:SER:OG	2.34	0.41
3:D:1285:GLU:HG3	3:D:1290:LEU:HG	2.03	0.41
5:F:163:LEU:HD13	5:F:174:LEU:HD13	2.02	0.41
1:A:102:LYS:HE3	1:A:102:LYS:HB2	1.91	0.40
1:A:39:PRO:HG3	1:B:39:PRO:HG3	2.03	0.40
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.86	0.40
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.36	0.40
2:C:413:LEU:HD21	2:C:451:LEU:HD13	2.02	0.40
3:D:809:PRO:HB3	3:D:839:LEU:HD13	2.02	0.40
3:D:1232:PRO:HG3	3:D:1361:VAL:HG11	2.03	0.40
5:F:188:ILE:HG12	5:F:224:VAL:HG21	2.04	0.40
2:C:353:ARG:NH2	5:F:203:THR:OG1	2.55	0.40
2:C:674:VAL:HG21	2:C:992:MET:HE3	2.03	0.40
2:C:936:VAL:HG11	2:C:959:PRO:HB2	2.02	0.40
3:D:251:PHE:HE2	3:D:304:LEU:HD12	1.86	0.40
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.97	0.40
2:C:886:LEU:HD23	2:C:886:LEU:HA	1.92	0.40
2:C:274:ARG:NH2	2:C:285:LEU:O	2.54	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	
1	A	230/315 (73%)	225 (98%)	5 (2%)	0	100	100
1	B	221/315 (70%)	215 (97%)	6 (3%)	0	100	100
2	C	1111/1119 (99%)	1082 (97%)	29 (3%)	0	100	100
3	D	1485/1524 (97%)	1449 (98%)	36 (2%)	0	100	100
4	E	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
5	F	333/443 (75%)	330 (99%)	3 (1%)	0	100	100
All	All	3472/3815 (91%)	3392 (98%)	80 (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	Percentiles	
1	A	201/273 (74%)	199 (99%)	2 (1%)	76	89
1	B	195/273 (71%)	195 (100%)	0	100	100
2	C	938/941 (100%)	919 (98%)	19 (2%)	55	79
3	D	1255/1279 (98%)	1236 (98%)	19 (2%)	65	84
4	E	83/88 (94%)	80 (96%)	3 (4%)	35	65
5	F	293/388 (76%)	289 (99%)	4 (1%)	67	85
All	All	2965/3242 (92%)	2918 (98%)	47 (2%)	62	82

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	74	ASP
2	C	27	ARG
2	C	141	HIS
2	C	177	GLU
2	C	261	ILE
2	C	284	ARG

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Mol	Chain	Res	Type
2	C	299	LYS
2	C	384	GLU
2	C	419	THR
2	C	422	ARG
2	C	427	VAL
2	C	513	VAL
2	C	583	LEU
2	C	595	LEU
2	C	640	ARG
2	C	670	GLN
2	C	765	SER
2	C	775	ARG
2	C	807[A]	ARG
2	C	807[B]	ARG
3	D	67	ARG
3	D	71	LYS
3	D	270	LEU
3	D	632	VAL
3	D	709	HIS
3	D	754	PHE
3	D	781	PRO
3	D	789	LEU
3	D	810	GLU
3	D	894	LYS
3	D	907	GLU
3	D	986	ARG
3	D	1001	GLU
3	D	1067	VAL
3	D	1129	THR
3	D	1184	GLN
3	D	1252	ILE
3	D	1295	GLU
3	D	1307	LYS
4	E	49	GLN
4	E	50	THR
4	E	87	LYS
5	F	88	ILE
5	F	331	ASP
5	F	380	GLU
5	F	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	99	GLN
2	C	390	GLN
2	C	834	GLN
2	C	860	HIS
3	D	709	HIS
3	D	724	GLN
3	D	976	GLN
3	D	1124	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	4/6 (66%)	1 (25%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	7	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	231/315 (73%)	0.20	7 (3%) 50 47	96, 129, 153, 181	0
1	B	223/315 (70%)	-0.05	3 (1%) 77 73	89, 124, 155, 169	0
2	C	1112/1119 (99%)	0.25	54 (4%) 29 28	70, 122, 175, 217	0
3	D	1486/1524 (97%)	0.24	63 (4%) 36 34	72, 118, 178, 205	1 (0%)
4	E	94/99 (94%)	-0.15	2 (2%) 63 60	89, 128, 169, 184	0
5	F	337/443 (76%)	0.42	32 (9%) 8 10	95, 140, 219, 231	0
6	G	18/21 (85%)	-0.30	0 100 100	87, 119, 213, 213	0
7	H	24/27 (88%)	-0.68	0 100 100	117, 137, 195, 221	0
8	I	5/6 (83%)	-0.04	0 100 100	92, 92, 94, 110	0
All	All	3530/3869 (91%)	0.22	161 (4%) 32 30	70, 124, 182, 231	1 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	63	GLY	7.8
5	F	381	HIS	7.2
5	F	386	VAL	6.9
5	F	390	PHE	6.5
5	F	422	LEU	6.3
2	C	777	ILE	6.0
5	F	375	LEU	6.0
5	F	392	VAL	5.5
5	F	415	THR	5.2
2	C	159	ILE	4.9
3	D	1313	VAL	4.9
5	F	414	ARG	4.9
3	D	173	PRO	4.9
2	C	207	LEU	4.8
3	D	1299	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
5	F	393	THR	4.7
3	D	322	VAL	4.7
5	F	399	GLN	4.6
5	F	373	LYS	4.6
3	D	1277	ILE	4.3
3	D	1292	VAL	4.2
1	A	233	VAL	4.2
3	D	1297	GLU	4.2
5	F	383	LEU	4.2
3	D	135	LEU	4.1
5	F	376	ILE	4.0
1	A	140	MET	3.9
2	C	66	LEU	3.8
1	A	101	LEU	3.8
5	F	382	THR	3.8
3	D	974	ILE	3.7
1	A	232	ALA	3.7
3	D	1278	ASP	3.7
2	C	191	PHE	3.6
3	D	409	VAL	3.6
1	A	4	SER	3.5
2	C	766	GLU	3.5
3	D	1294	VAL	3.5
3	D	203	ALA	3.5
5	F	149	GLU	3.4
2	C	773	LEU	3.4
2	C	344	PHE	3.4
5	F	400	ILE	3.3
5	F	396	ARG	3.2
5	F	388	ALA	3.2
2	C	221	LEU	3.1
2	C	107	LEU	3.0
5	F	146	GLY	3.0
5	F	404	ALA	3.0
2	C	769	PRO	3.0
3	D	1311	LEU	3.0
2	C	52	PHE	3.0
5	F	397	ILE	3.0
5	F	377	ASP	3.0
3	D	310	LEU	2.9
2	C	372	LEU	2.9
4	E	95	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	153	LEU	2.9
1	B	25	LEU	2.9
2	C	251	ASP	2.9
2	C	778	PHE	2.9
5	F	416	ARG	2.9
2	C	311	PHE	2.8
2	C	307	LEU	2.8
3	D	367	ILE	2.8
2	C	105	THR	2.8
3	D	305	ALA	2.8
5	F	147	LEU	2.8
2	C	361	MET	2.8
5	F	411	HIS	2.8
3	D	345	TYR	2.8
3	D	283	PHE	2.7
3	D	241	ILE	2.7
3	D	1305	LEU	2.7
2	C	154	ARG	2.6
2	C	823	VAL	2.6
5	F	391	GLY	2.6
2	C	896	PHE	2.6
2	C	184	MET	2.6
3	D	1273	VAL	2.6
3	D	378	ILE	2.6
3	D	269	PHE	2.6
3	D	1127	GLU	2.6
3	D	1319	VAL	2.6
2	C	367	LEU	2.5
2	C	373	VAL	2.5
3	D	393	ILE	2.5
5	F	385	GLU	2.5
2	C	365	ASP	2.5
3	D	666	ILE	2.5
5	F	384	GLU	2.5
3	D	1318	TYR	2.4
5	F	145	PRO	2.4
3	D	1301	LYS	2.4
5	F	395	GLU	2.4
3	D	1296	SER	2.4
3	D	326	GLU	2.4
2	C	770	GLU	2.4
3	D	1321	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	98	LEU	2.4
5	F	329	TYR	2.4
3	D	1044	LEU	2.4
2	C	220	GLY	2.4
3	D	350	HIS	2.4
2	C	10	ARG	2.3
1	B	140	MET	2.3
3	D	136	ASP	2.3
2	C	211	LEU	2.3
2	C	100	LEU	2.3
2	C	160	ALA	2.3
2	C	54	ILE	2.3
3	D	202	VAL	2.3
3	D	1298	GLY	2.3
2	C	805	ARG	2.3
3	D	1320	GLU	2.3
2	C	776	SER	2.3
3	D	1495	ILE	2.3
2	C	104	ASP	2.3
3	D	225	LEU	2.3
2	C	182	VAL	2.3
2	C	226	VAL	2.3
4	E	79	LEU	2.2
3	D	1129	THR	2.2
3	D	335	LEU	2.2
2	C	109	LYS	2.2
3	D	821	VAL	2.2
1	A	231	ALA	2.2
3	D	368	VAL	2.2
3	D	324	ALA	2.2
3	D	1300	SER	2.2
2	C	368	THR	2.2
2	C	754	ILE	2.2
3	D	1252	ILE	2.2
2	C	729	LEU	2.1
2	C	650	ARG	2.1
3	D	262	LYS	2.1
2	C	418	LEU	2.1
3	D	960	LYS	2.1
3	D	1275	SER	2.1
3	D	312	ARG	2.1
5	F	387	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	153	ALA	2.1
3	D	282	TYR	2.1
2	C	722	ILE	2.1
2	C	868	ASP	2.1
2	C	774	LEU	2.1
3	D	152	LEU	2.1
1	A	142	VAL	2.1
3	D	191	LEU	2.1
3	D	1274	ILE	2.0
2	C	529	VAL	2.0
3	D	199	LEU	2.0
2	C	190	LYS	2.0
3	D	1306	PRO	2.0
1	B	23	PHE	2.0
3	D	321	GLN	2.0
3	D	144	GLY	2.0
3	D	1325	LEU	2.0
2	C	781	LYS	2.0
2	C	1053	LEU	2.0
3	D	377	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MG	B	2001	1/1	0.72	1.42	132,132,132,132	0
9	MG	D	2003	1/1	0.92	0.22	84,84,84,84	0
10	ZN	D	2002	1/1	0.93	0.03	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MG	D	2004	1/1	0.94	0.47	67,67,67,67	0
9	MG	F	2001	1/1	0.98	0.12	137,137,137,137	0
10	ZN	D	2001	1/1	0.99	0.26	105,105,105,105	0

6.5 Other polymers (i)

There are no such residues in this entry.