



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:21 PM BST

PDB ID : 6KQG  
Title : Thermus thermophilus initial transcription complex comprising sigma A and 5'-OH RNA of 6 nt  
Authors : Zhang, Y.; Li, L.; Ebright, R.H.  
Deposited on : 2019-08-17  
Resolution : 2.78 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

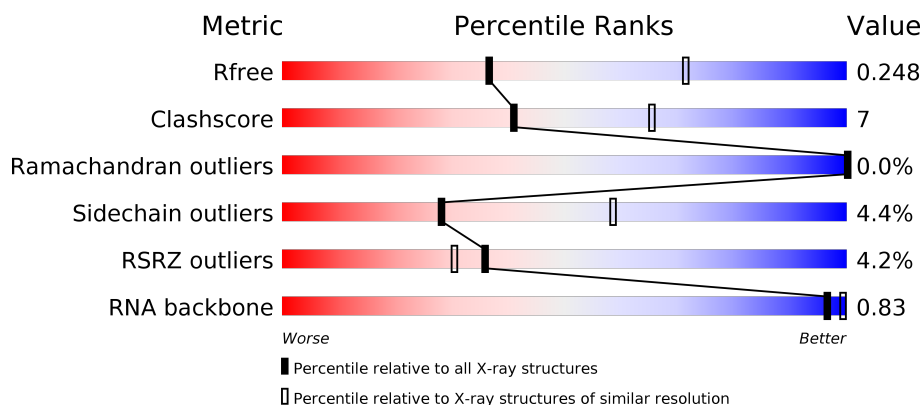
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)
RNA backbone	3102	1092 (3.06-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>17%</div> <div>•</div> <div>27%</div> </div> </div>
1	B	315	<div> <div>0%</div> <div> <div></div> <div>54%</div> <div>15%</div> <div>•</div> <div>29%</div> </div> </div>
2	C	1119	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>••</div> </div> </div>
3	D	1524	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>82%13%5%</div></div>
5	F	443	<div><div>2%</div><div></div><div>65%11%24%</div></div>
6	G	21	<div><div></div><div>24%62%14%</div></div>
7	H	27	<div><div></div><div>41%48%11%</div></div>
8	I	6	<div><div></div><div>83%17%</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28816 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
			1758	1124	305	327	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
			8788	5560	1570	1634	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
			11732	7442	2063	2191	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	338	Total	C	N	O	S	0	0	0
			2748	1735	500	509	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\*T\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*T  
P\*GP\*AP\*GP\*TP\*CP\*GP\*AP\*GP\*GP\*G)-3').

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

- 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\*G)-3').

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	6	Total	C	N	O	P	0	0	0
			122	56	21	40	5			

- 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

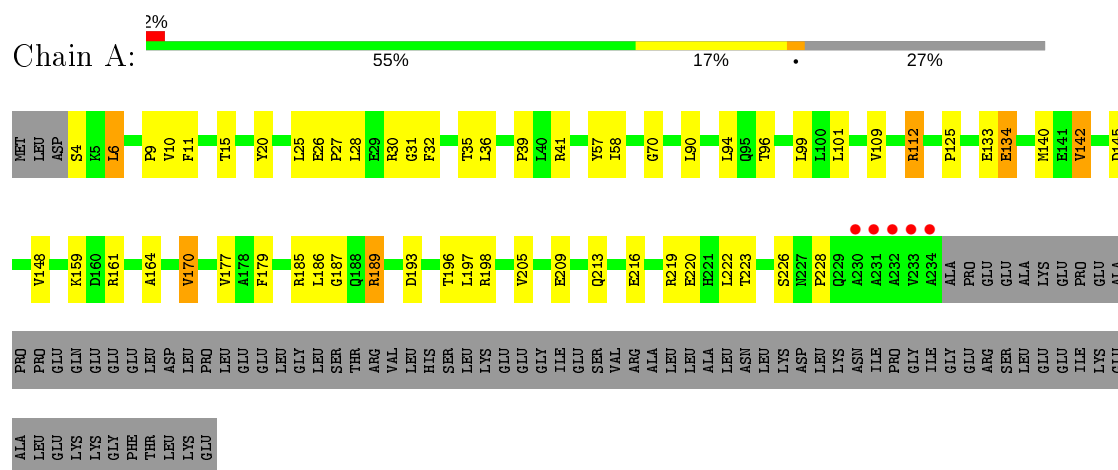
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	9	Total O 9 9	0	0
11	B	9	Total O 9 9	0	0
11	C	60	Total O 60 60	0	0
11	D	94	Total O 94 94	0	0
11	E	8	Total O 8 8	0	0
11	F	23	Total O 23 23	0	0
11	G	10	Total O 10 10	0	0
11	H	6	Total O 6 6	0	0
11	I	1	Total O 1 1	0	0

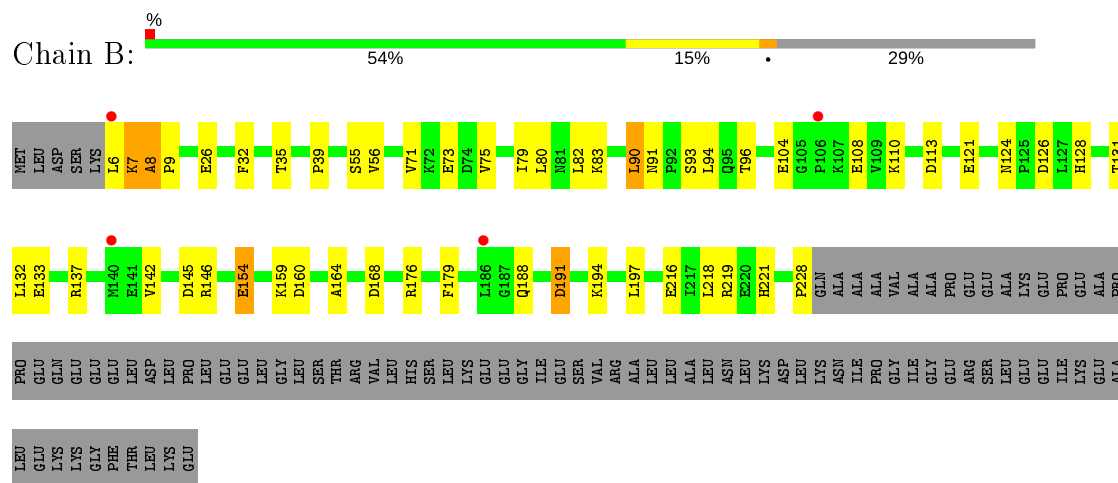
### 3 Residue-property plots

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.

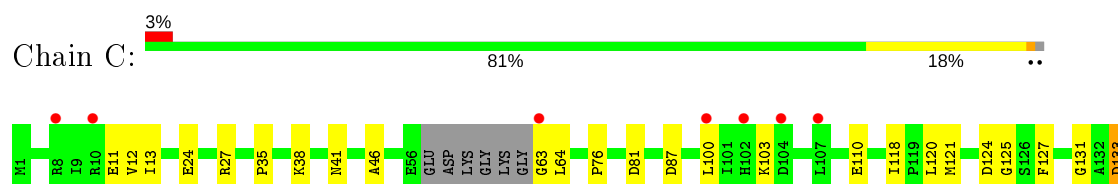
- Molecule 1: DNA-directed RNA polymerase subunit alpha

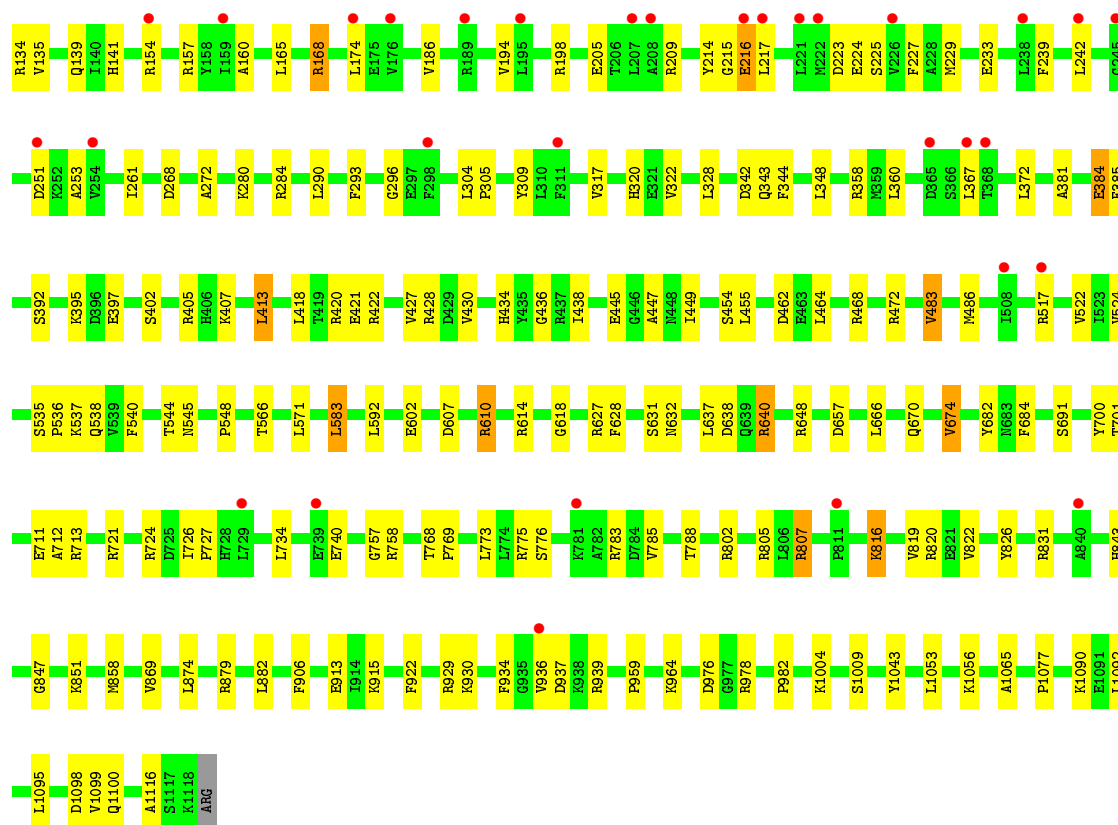


- Molecule 1: DNA-directed RNA polymerase subunit alpha

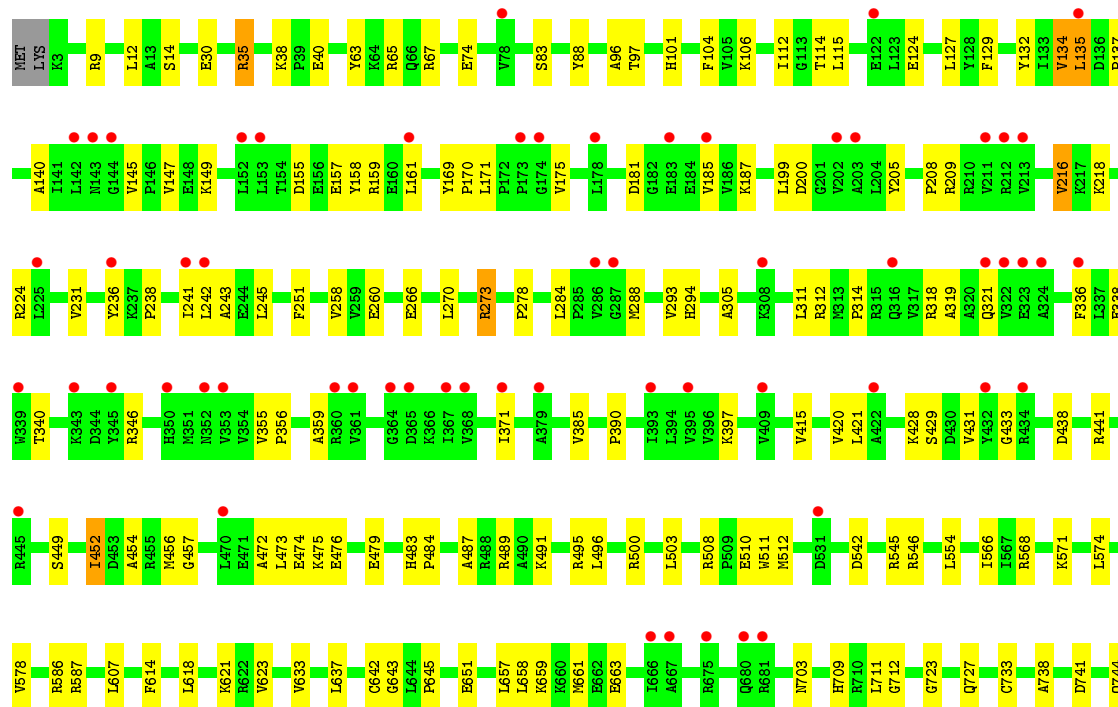
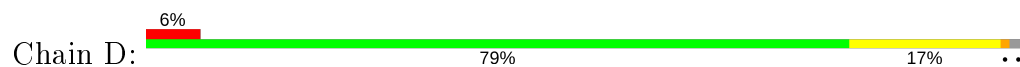


- Molecule 2: DNA-directed RNA polymerase subunit beta

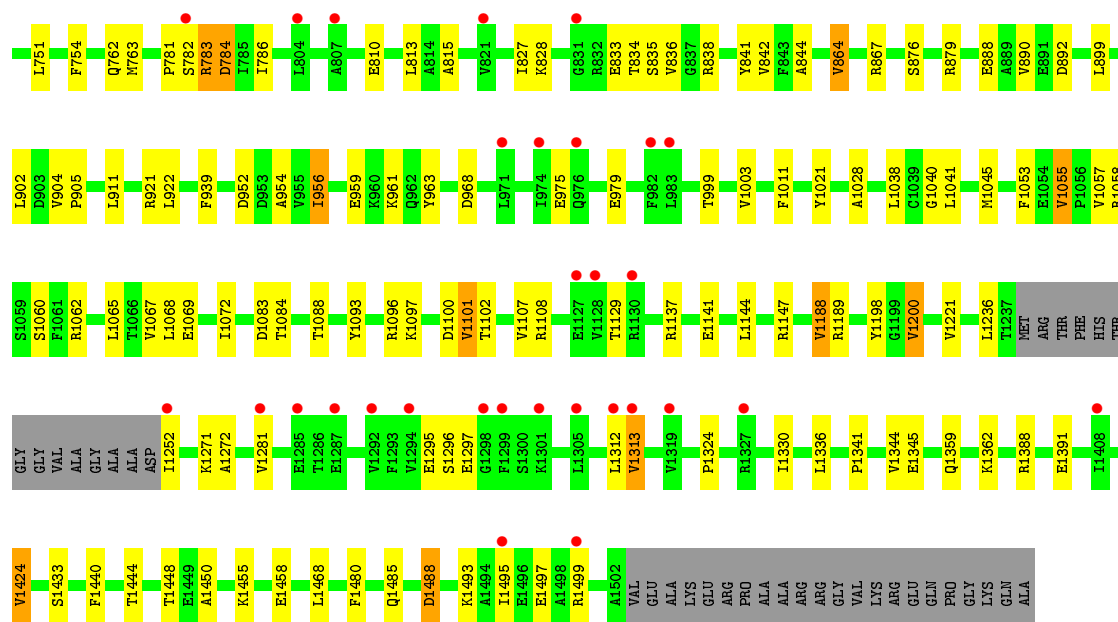




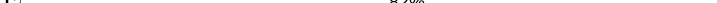
• Molecule 3: DNA-directed RNA polymerase subunit beta'







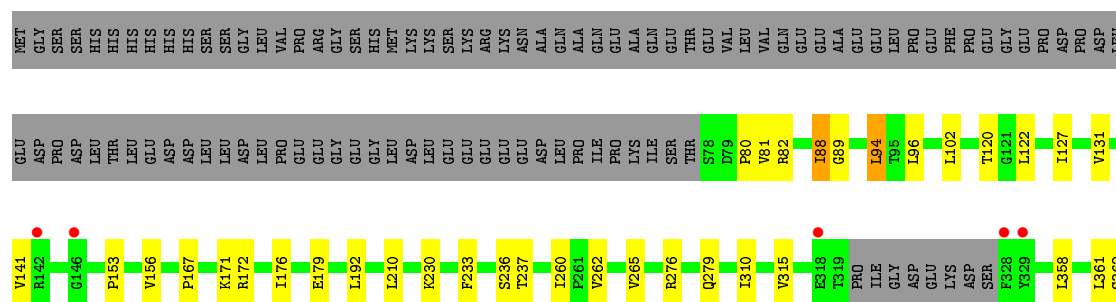
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:  82% 13% 5%

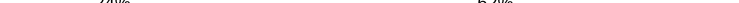


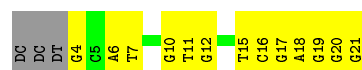
- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 



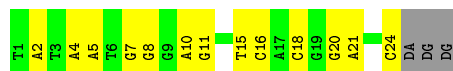
- Molecule 6: DNA (5'-D(\*CP\*CP\*T\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*CP\*GP\*AP\*GP\*GP\*G)-3')

Chain G:  24% 62% 14%




- 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')

Chain H:  41% 48% 11%



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

Chain I:  83% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.24Å 104.04Å 296.85Å 90.00° 98.65° 90.00°	Depositor
Resolution (Å)	49.03 – 2.78 49.03 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.03-2.78) 98.3 (49.03-2.78)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.205 , 0.248 0.205 , 0.248	Depositor DCC
$R_{free}$ test set	6829 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.1	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28816	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.30	0/1849	0.52	0/2515
1	B	0.31	0/1790	0.50	0/2435
2	C	0.30	0/8965	0.49	0/12124
3	D	0.30	0/11948	0.49	0/16157
4	E	0.35	0/775	0.50	1/1045 (0.1%)
5	F	0.29	0/2791	0.44	0/3753
6	G	0.69	0/418	0.86	0/645
7	H	0.62	0/556	0.89	0/858
8	I	0.52	0/135	1.05	0/208
All	All	0.32	0/29227	0.51	1/39740 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	E	93	TYR	C-N-CD	5.00	138.91	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1814	0	1869	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1758	0	1808	45	0
2	C	8788	0	8898	128	0
3	D	11732	0	11952	178	0
4	E	761	0	778	8	0
5	F	2748	0	2828	28	0
6	G	372	0	203	18	0
7	H	495	0	272	11	0
8	I	122	0	66	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	A	9	0	0	0	0
11	B	9	0	0	0	0
11	C	60	0	0	4	0
11	D	94	0	0	5	0
11	E	8	0	0	1	0
11	F	23	0	0	0	0
11	G	10	0	0	1	0
11	H	6	0	0	0	0
11	I	1	0	0	0	0
All	All	28816	0	28674	404	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 7.

All (404) 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)
6:G:20:DG:H2'	6:G:21:DG:C4'	1.81	1.11
3:D:783:ARG:HB3	3:D:1028:ALA:O	1.54	1.06
6:G:20:DG:H2'	6:G:21:DG:O4'	1.60	1.02
1:B:6:LEU:HD12	1:B:7:LYS:H	1.26	0.99
2:C:684:PHE:HE1	3:D:782:SER:OG	1.45	0.97
1:B:7:LYS:NZ	1:B:8:ALA:HB2	1.83	0.94
1:B:7:LYS:HZ1	1:B:8:ALA:HB2	1.36	0.89
3:D:783:ARG:CB	3:D:1028:ALA:O	2.24	0.85
6:G:20:DG:H2'	6:G:21:DG:H4'	1.58	0.85
6:G:19:DG:H2''	6:G:20:DG:H5'	1.59	0.85
6:G:20:DG:C2'	6:G:21:DG:H4'	2.07	0.85
3:D:827:ILE:HG12	3:D:834:THR:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:O	1:B:9:PRO:HD3	1.79	0.81
2:C:684:PHE:CE1	3:D:782:SER:OG	2.27	0.80
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.64	0.79
1:B:7:LYS:HD2	1:B:8:ALA:N	2.00	0.77
2:C:628:PHE:H	2:C:638:ASP:HB3	1.49	0.76
1:B:7:LYS:HD2	1:B:8:ALA:H	1.50	0.74
3:D:782:SER:O	3:D:786:ILE:HG13	1.84	0.74
6:G:20:DG:C2'	6:G:21:DG:C4'	2.61	0.73
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.71	0.73
6:G:20:DG:H1	8:I:2:C:H42	1.36	0.73
1:B:6:LEU:CD1	1:B:7:LYS:H	1.98	0.73
3:D:273:ARG:HG3	3:D:278:PRO:HA	1.70	0.73
5:F:374:GLY:HA2	5:F:379:ARG:O	1.88	0.72
3:D:241:ILE:HA	3:D:312:ARG:HG2	1.71	0.72
6:G:19:DG:H2'	6:G:20:DG:C8	2.24	0.72
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.72	0.71
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.73	0.71
3:D:1045[B]:MET:HE1	3:D:1057:VAL:HG23	1.72	0.70
3:D:835:SER:OG	3:D:838:ARG:HG3	1.92	0.70
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.74	0.69
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.73	0.69
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.25	0.69
2:C:428:ARG:NH2	2:C:447:ALA:O	2.24	0.69
2:C:198:ARG:HE	2:C:227:PHE:HA	1.58	0.69
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.74	0.69
3:D:65:ARG:NH1	5:F:378:GLY:O	2.25	0.69
6:G:15:DT:H2'	6:G:16:DC:C6	2.29	0.68
3:D:260:GLU:HG2	3:D:294:HIS:HE1	1.58	0.68
6:G:18:DA:H2'	6:G:19:DG:C8	2.30	0.67
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.28	0.67
2:C:63:GLY:HA3	2:C:100:LEU:HD21	1.77	0.67
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.28	0.66
1:B:6:LEU:HD12	1:B:7:LYS:N	2.08	0.66
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.26	0.66
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.78	0.65
1:A:112:ARG:HG3	1:A:125:PRO:HB2	1.78	0.65
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.29	0.65
3:D:1450:ALA:HA	3:D:1455:LYS:HE3	1.78	0.65
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.79	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.79	0.64
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:4:DG:H1	7:H:24:DC:H42	1.47	0.63
3:D:959:GLU:OE1	3:D:959:GLU:N	2.31	0.63
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.81	0.63
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.32	0.63
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.29	0.63
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.81	0.63
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.82	0.62
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.80	0.62
3:D:657:LEU:HG	3:D:661:MET:HE2	1.80	0.62
1:A:6:LEU:HD21	1:A:27:PRO:HG2	1.82	0.62
3:D:1053[B]:PHE:CZ	3:D:1055:VAL:HG13	2.36	0.61
1:A:31:GLY:N	1:A:193:ASP:OD2	2.34	0.60
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.84	0.60
1:A:209:GLU:O	1:A:213:GLN:HG2	2.02	0.60
1:A:185:ARG:NH2	1:A:187:GLY:O	2.34	0.60
7:H:10:DA:H2"	7:H:11:DG:H5"	1.84	0.60
2:C:773:LEU:HB2	5:F:373:LYS:HG3	1.83	0.60
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.84	0.59
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.84	0.59
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.67	0.59
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.85	0.59
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.01	0.59
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.84	0.58
5:F:395:GLU:OE2	5:F:398:ARG:NH2	2.30	0.58
3:D:835:SER:OG	3:D:838:ARG:CG	2.50	0.58
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.85	0.58
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.86	0.58
2:C:713:ARG:HA	2:C:819:VAL:HA	1.85	0.58
3:D:208:PRO:HA	3:D:390:PRO:HA	1.86	0.58
3:D:783:ARG:HA	3:D:1028:ALA:HA	1.86	0.57
3:D:155:ASP:OD2	3:D:159:ARG:NH1	2.37	0.57
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.87	0.57
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.23	0.57
1:B:191:ASP:N	1:B:191:ASP:OD1	2.30	0.57
3:D:231:VAL:O	3:D:236:TYR:OH	2.22	0.57
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.37	0.57
6:G:11:DT:H2"	6:G:12:DG:C8	2.39	0.57
3:D:273:ARG:HG3	3:D:278:PRO:CA	2.33	0.56
7:H:15:DT:H2"	7:H:16:DC:C6	2.40	0.56
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.38	0.56
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:536:PRO:HB3	3:D:1067:VAL:HG11	1.87	0.56
2:C:874:LEU:HD12	3:D:784:ASP:OD1	2.04	0.56
1:B:7:LYS:O	1:B:8:ALA:HB3	2.05	0.56
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.88	0.56
3:D:1444:THR:O	3:D:1448:THR:HG23	2.05	0.56
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.88	0.56
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.88	0.56
2:C:614:ARG:NH2	2:C:618:GLY:O	2.39	0.56
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.87	0.56
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.88	0.56
2:C:816:LYS:HG3	2:C:819:VAL:HG11	1.89	0.55
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.88	0.55
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.89	0.55
2:C:317:VAL:HG22	2:C:320:HIS:HD1	1.72	0.55
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.88	0.55
3:D:1488:ASP:N	3:D:1488:ASP:OD1	2.35	0.55
5:F:172:ARG:O	5:F:176:ILE:HG12	2.06	0.55
3:D:815:ALA:HB3	11:D:2137:HOH:O	2.06	0.55
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.42	0.55
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.88	0.55
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.07	0.55
4:E:95:VAL:O	4:E:95:VAL:HG12	2.06	0.55
3:D:658:LEU:HA	3:D:661:MET:HE3	1.88	0.55
2:C:684:PHE:HE1	3:D:782:SER:HG	0.66	0.54
3:D:783:ARG:HD3	3:D:1028:ALA:O	2.07	0.54
3:D:975:GLU:O	3:D:979:GLU:HG2	2.07	0.54
2:C:906:PHE:CG	3:D:1067:VAL:HG12	2.43	0.54
2:C:139:GLN:NE2	2:C:413:LEU:O	2.41	0.54
2:C:776:SER:OG	5:F:373:LYS:NZ	2.41	0.54
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.90	0.54
3:D:438:ASP:OD2	3:D:441:ARG:NH2	2.41	0.54
3:D:1499:ARG:HH21	4:E:81:PRO:HD3	1.73	0.54
3:D:1084:THR:O	3:D:1088:THR:HG23	2.07	0.53
2:C:224:GLU:CD	2:C:224:GLU:H	2.10	0.53
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.43	0.53
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.43	0.53
3:D:288:MET:HG2	3:D:305:ALA:HB1	1.91	0.53
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.90	0.53
2:C:405:ARG:HD3	2:C:566:THR:HG21	1.90	0.53
2:C:13:ILE:HD13	2:C:483:VAL:HG21	1.91	0.53
1:B:91:ASN:OD1	1:B:93:SER:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:ASN:O	2:C:46:ALA:HB2	2.09	0.53
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.44	0.53
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.31	0.52
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.08	0.52
3:D:827:ILE:O	3:D:834:THR:N	2.24	0.52
1:A:32:PHE:HA	1:A:35:THR:HB	1.92	0.52
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.92	0.52
2:C:682:TYR:CE1	2:C:851:LYS:HD3	2.44	0.52
3:D:1296:SER:OG	3:D:1297:GLU:N	2.42	0.52
5:F:236:SER:OG	7:H:5:DA:OP2	2.21	0.52
1:B:6:LEU:CG	1:B:7:LYS:N	2.73	0.52
3:D:487:ALA:O	3:D:491:LYS:HG2	2.10	0.52
5:F:94:LEU:HD21	5:F:102:LEU:HD12	1.91	0.52
3:D:137:PRO:HA	3:D:452:ILE:HG23	1.92	0.52
3:D:783:ARG:HB3	3:D:1028:ALA:C	2.28	0.52
2:C:205:GLU:O	2:C:209:ARG:HG2	2.10	0.52
2:C:134:ARG:NH1	2:C:392:SER:O	2.39	0.52
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.75	0.52
2:C:127:PHE:O	2:C:133:ASP:HA	2.10	0.52
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.74	0.52
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.92	0.51
1:B:32:PHE:HA	1:B:35:THR:HB	1.93	0.51
2:C:805:ARG:O	2:C:807[A]:ARG:NH2	2.43	0.51
2:C:328:LEU:HD11	2:C:438:ILE:HD12	1.91	0.51
3:D:472:ALA:O	3:D:476:GLU:HG2	2.09	0.51
3:D:828:LYS:HA	3:D:833:GLU:HA	1.92	0.51
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.92	0.51
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.91	0.51
2:C:631:SER:HB3	2:C:637:LEU:HG	1.93	0.51
2:C:381:ALA:O	2:C:384:GLU:HG3	2.10	0.51
3:D:1093:TYR:O	3:D:1097:LYS:HG3	2.11	0.51
1:A:133:GLU:HG2	1:A:134:GLU:H	1.75	0.51
2:C:740:GLU:OE1	2:C:807[B]:ARG:NH2	2.44	0.51
3:D:956:ILE:HD11	3:D:1062:ARG:HG2	1.92	0.51
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.11	0.50
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.45	0.50
3:D:835:SER:O	3:D:836:VAL:C	2.48	0.50
3:D:959:GLU:HB3	3:D:963:TYR:HE2	1.74	0.50
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.93	0.50
2:C:64:LEU:HD12	2:C:103:LYS:HB2	1.92	0.50
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:10:DG:N2	7:H:18:DC:O2	2.45	0.50
2:C:517:ARG:HD2	2:C:522:VAL:HG11	1.93	0.50
3:D:106:LYS:O	3:D:586:ARG:NH1	2.45	0.50
3:D:781:PRO:HG2	3:D:911:LEU:HB3	1.93	0.50
5:F:167:PRO:O	5:F:171:LYS:N	2.45	0.49
7:H:10:DA:H2''	7:H:11:DG:C8	2.47	0.49
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.94	0.49
1:B:6:LEU:HG	1:B:7:LYS:N	2.27	0.49
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.12	0.49
5:F:89:GLY:HA3	7:H:7:DG:C6	2.47	0.49
3:D:546:ARG:NH2	11:D:2104:HOH:O	2.45	0.49
3:D:1057:VAL:HG22	3:D:1069:GLU:HG2	1.94	0.49
6:G:17:DG:H2'	6:G:17:DG:N3	2.28	0.49
1:B:73:GLU:OE1	1:B:73:GLU:N	2.44	0.49
2:C:628:PHE:H	2:C:638:ASP:CB	2.22	0.49
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.95	0.49
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.48	0.49
3:D:187:LYS:N	3:D:200:ASP:OD1	2.37	0.48
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.94	0.48
2:C:724:ARG:NH2	2:C:734:LEU:O	2.45	0.48
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.45	0.48
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.48	0.48
1:A:9:PRO:HB3	1:A:27:PRO:O	2.14	0.48
6:G:6:DA:C8	6:G:7:DT:H72	2.49	0.48
2:C:602:GLU:HB2	2:C:648:ARG:HH21	1.78	0.48
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.44	0.48
1:A:226:SER:O	1:A:228:PRO:HD3	2.14	0.48
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.94	0.48
3:D:134:VAL:HG22	3:D:149:LYS:HA	1.94	0.48
1:A:186:LEU:O	1:A:189:ARG:HG3	2.13	0.48
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.14	0.48
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.96	0.48
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.96	0.48
2:C:816:LYS:O	2:C:819:VAL:HG13	2.13	0.48
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.47	0.48
5:F:276:ARG:O	5:F:279:GLN:HG3	2.14	0.48
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.47	0.48
2:C:436:GLY:HA2	2:C:538:GLN:O	2.13	0.47
3:D:224:ARG:H	3:D:251:PHE:HE1	1.61	0.47
5:F:127:ILE:O	5:F:131:VAL:HG23	2.14	0.47
2:C:1009:SER:HB3	3:D:651:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.96	0.47
5:F:237:THR:OG1	7:H:4:DA:H8	1.96	0.47
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.79	0.47
1:A:4:SER:O	1:A:189:ARG:NH2	2.48	0.47
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.79	0.47
2:C:758:ARG:HH21	2:C:788:THR:HB	1.79	0.47
1:A:25:LEU:HB3	1:A:28:LEU:HD11	1.96	0.47
3:D:260:GLU:HG2	3:D:294:HIS:CE1	2.44	0.47
3:D:784:ASP:HB3	3:D:939:PHE:HE1	1.79	0.47
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.50	0.47
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.96	0.47
1:B:6:LEU:CD1	1:B:7:LYS:N	2.73	0.47
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.47	0.47
2:C:674:VAL:HG22	2:C:869:VAL:HG22	1.97	0.47
3:D:1341:PRO:O	3:D:1345:GLU:HG3	2.15	0.47
4:E:39:VAL:O	4:E:72:ARG:NH1	2.41	0.47
1:B:7:LYS:CD	1:B:8:ALA:N	2.73	0.47
2:C:214:TYR:HB3	2:C:217:LEU:HD12	1.97	0.47
3:D:200:ASP:O	3:D:397:LYS:HG2	2.15	0.47
3:D:542:ASP:OD1	3:D:545:ARG:NH2	2.41	0.46
2:C:317:VAL:HG22	2:C:320:HIS:ND1	2.30	0.46
2:C:607:ASP:HB3	2:C:610:ARG:H	1.79	0.46
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.97	0.46
5:F:88:ILE:HD11	5:F:192:LEU:HD13	1.96	0.46
1:B:8:ALA:N	1:B:9:PRO:CD	2.78	0.46
3:D:1485:GLN:O	4:E:75:PHE:HA	2.16	0.46
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.96	0.46
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.97	0.46
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.97	0.46
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.98	0.46
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.74	0.46
6:G:19:DG:N7	11:G:101:HOH:O	2.36	0.46
2:C:1098:ASP:OD2	2:C:1100:GLN:NE2	2.49	0.46
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.44	0.46
3:D:999:THR:O	3:D:1003:VAL:HG13	2.16	0.46
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.98	0.46
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.31	0.46
3:D:733:CYS:HB3	3:D:738:ALA:O	2.16	0.46
3:D:921:ARG:NH1	11:D:2106:HOH:O	2.49	0.46
1:B:75:VAL:O	1:B:79:ILE:HG13	2.16	0.46
2:C:712:ALA:O	2:C:820:ARG:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1065:ALA:HB1	2:C:1077:PRO:HG3	1.98	0.45
1:A:70:GLY:N	2:C:607:ASP:OD1	2.48	0.45
2:C:879:ARG:NE	11:C:1202:HOH:O	2.39	0.45
3:D:35:ARG:HB3	3:D:35:ARG:HH21	1.81	0.45
5:F:374:GLY:CA	5:F:379:ARG:O	2.62	0.45
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.97	0.45
5:F:370:LYS:HD3	5:F:376:ILE:HD11	1.98	0.45
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.51	0.45
3:D:659:LYS:HE3	3:D:663:GLU:OE2	2.17	0.45
5:F:82:ARG:HB2	7:H:8:DG:O6	2.16	0.45
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.82	0.45
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.16	0.45
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.43	0.45
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.99	0.45
2:C:293:PHE:CZ	2:C:296:GLY:HA2	2.51	0.45
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.51	0.45
2:C:769:PRO:HG3	3:D:65:ARG:HH12	1.81	0.45
3:D:371:ILE:HD12	5:F:230:LYS:HA	1.98	0.45
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.98	0.45
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.98	0.45
1:B:154:GLU:CD	1:B:154:GLU:H	2.20	0.45
2:C:239:PHE:CD1	2:C:253:ALA:HA	2.52	0.45
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.98	0.45
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.52	0.44
2:C:121:MET:SD	2:C:125:GLY:HA2	2.58	0.44
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.98	0.44
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	2.00	0.44
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.81	0.44
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.52	0.44
3:D:137:PRO:HB3	3:D:147:VAL:HG12	2.00	0.44
3:D:475:LYS:O	3:D:479:GLU:HG2	2.18	0.44
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.99	0.44
1:B:7:LYS:CE	1:B:8:ALA:HB2	2.47	0.44
3:D:1271:LYS:HG3	3:D:1272:ALA:O	2.18	0.44
3:D:645:PRO:HB3	3:D:723:GLY:O	2.17	0.44
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.52	0.43
2:C:691:SER:HB2	2:C:858:MET:HG3	1.99	0.43
2:C:674:VAL:CG2	2:C:869:VAL:HG22	2.48	0.43
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.17	0.43
2:C:135:VAL:HG23	2:C:395:LYS:HG3	2.00	0.43
3:D:1144:LEU:O	3:D:1147:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:20:DG:H1'	7:H:21:DA:C8	2.53	0.43
2:C:215:GLY:O	2:C:216:GLU:HG3	2.18	0.43
3:D:1011:PHE:HB3	3:D:1021:TYR:CD1	2.54	0.43
3:D:1362:LYS:HB2	3:D:1362:LYS:HE3	1.84	0.43
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.77	0.43
3:D:420:VAL:HA	11:D:2182:HOH:O	2.19	0.43
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.99	0.43
3:D:1458:GLU:HG3	11:D:2143:HOH:O	2.19	0.43
3:D:112:ILE:HD11	3:D:512:MET:HB3	2.01	0.43
3:D:879:ARG:HD3	3:D:902:LEU:O	2.18	0.43
1:A:101:LEU:HD21	1:A:109:VAL:HG11	2.01	0.43
1:B:159:LYS:HE3	1:B:164:ALA:O	2.19	0.43
2:C:261:ILE:HG13	2:C:290:LEU:HD12	2.01	0.43
2:C:272:ALA:HB2	2:C:464:LEU:HB3	2.00	0.43
2:C:882:LEU:HD11	3:D:1038:LEU:HD22	2.00	0.43
2:C:1004:LYS:HD3	3:D:744:GLN:OE1	2.18	0.43
1:B:113:ASP:OD1	1:B:113:ASP:N	2.52	0.43
1:A:11:PHE:O	1:B:228:PRO:HA	2.18	0.43
2:C:540:PHE:HB3	2:C:544:THR:HB	2.01	0.43
2:C:627:ARG:NH2	2:C:640:ARG:HG3	2.34	0.43
2:C:816:LYS:HG3	2:C:819:VAL:CG1	2.48	0.43
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.54	0.43
3:D:129:PHE:CD1	3:D:456:MET:HB3	2.54	0.43
3:D:508:ARG:HD3	3:D:510:GLU:OE1	2.19	0.43
1:B:124:ASN:OD1	1:B:124:ASN:N	2.52	0.42
2:C:11:GLU:OE2	2:C:537:LYS:HE2	2.19	0.42
3:D:321:GLN:HB2	3:D:336:PHE:HD2	1.83	0.42
3:D:1101:VAL:HG23	3:D:1102:THR:HG23	2.01	0.42
3:D:574:LEU:O	3:D:578:VAL:HG23	2.19	0.42
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.01	0.42
2:C:468:ARG:HA	2:C:486:MET:O	2.18	0.42
3:D:1281:VAL:HG21	3:D:1313:VAL:CG2	2.49	0.42
2:C:420:ARG:C	2:C:422:ARG:H	2.23	0.42
3:D:614:PHE:HA	3:D:618:LEU:HD12	2.01	0.42
5:F:362:SER:OG	5:F:365:GLU:HG2	2.19	0.42
3:D:158:TYR:HE1	3:D:454:ALA:HB3	1.83	0.42
1:B:56:VAL:HG21	1:B:82:LEU:HD13	2.01	0.42
2:C:1053:LEU:HA	3:D:621:LYS:HD2	2.01	0.42
2:C:571:LEU:HD22	2:C:700:TYR:HA	2.02	0.42
2:C:936:VAL:HG11	2:C:959:PRO:HB2	2.01	0.42
3:D:115:LEU:HD23	3:D:115:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:876:SER:OG	3:D:879:ARG:HG3	2.20	0.42
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.64	0.42
5:F:233:PHE:CD2	7:H:2:DA:H1'	2.53	0.42
1:B:110:LYS:HD2	1:B:126:ASP:O	2.20	0.42
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.91	0.42
3:D:231:VAL:HG23	3:D:243:ALA:HA	2.02	0.42
2:C:110:GLU:HB2	11:C:1235:HOH:O	2.19	0.42
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.01	0.42
3:D:127:LEU:HA	3:D:457:GLY:HA2	2.02	0.42
2:C:63:GLY:N	2:C:367:LEU:HD12	2.35	0.42
2:C:372:LEU:HD12	2:C:372:LEU:HA	1.89	0.42
1:A:196:THR:HG21	2:C:934:PHE:CE1	2.55	0.42
2:C:930:LYS:HA	2:C:930:LYS:HD2	1.81	0.42
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.20	0.42
3:D:428:LYS:HB3	3:D:428:LYS:HE2	1.85	0.42
3:D:956:ILE:H	3:D:956:ILE:HG12	1.66	0.42
3:D:157:GLU:O	3:D:161:LEU:HG	2.19	0.41
2:C:194:VAL:HG23	11:C:1201:HOH:O	2.21	0.41
2:C:462:ASP:HB3	2:C:468:ARG:HD2	2.02	0.41
3:D:258:VAL:HG12	3:D:273:ARG:O	2.20	0.41
3:D:433:GLY:HA2	3:D:449:SER:H	1.85	0.41
6:G:16:DC:H2'	6:G:17:DG:H8	1.85	0.41
1:A:41:ARG:HA	1:A:177:VAL:HG11	2.03	0.41
2:C:548:PRO:O	2:C:843:HIS:HE1	2.03	0.41
3:D:1096:ARG:NH1	3:D:1440:PHE:O	2.53	0.41
3:D:961:LYS:HB2	3:D:961:LYS:HE3	1.80	0.41
1:A:10:VAL:HG12	1:A:26:GLU:O	2.20	0.41
3:D:135:LEU:HD23	3:D:135:LEU:N	2.36	0.41
3:D:703:ASN:HA	3:D:712:GLY:O	2.20	0.41
1:A:220:GLU:O	1:A:223:THR:HB	2.21	0.41
2:C:701:THR:HA	2:C:831:ARG:O	2.21	0.41
2:C:847:GLY:HA2	3:D:741:ASP:HA	2.01	0.41
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.56	0.41
3:D:1045[B]:MET:HE3	3:D:1045[B]:MET:HB2	1.74	0.41
1:B:96:THR:HB	1:B:145:ASP:OD1	2.21	0.41
3:D:762:GLN:HA	11:E:104:HOH:O	2.20	0.41
1:B:90:LEU:HD11	1:B:121:GLU:HB2	2.02	0.41
3:D:784:ASP:HB3	3:D:939:PHE:CE1	2.56	0.41
1:A:133:GLU:HG2	1:A:134:GLU:N	2.36	0.41
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.03	0.41
3:D:844:ALA:O	3:D:867:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:154:ARG:HH21	2:C:157:ARG:HG3	1.86	0.41
3:D:140:ALA:HB2	3:D:452:ILE:HG12	2.02	0.41
3:D:209:ARG:O	3:D:346:ARG:HD3	2.21	0.41
1:A:159:LYS:HE3	1:A:164:ALA:O	2.21	0.41
1:A:170:VAL:HG22	1:A:170:VAL:O	2.21	0.41
2:C:223:ASP:OD2	2:C:225:SER:OG	2.35	0.41
2:C:229:MET:HB2	2:C:233:GLU:HB2	2.02	0.41
5:F:260:ILE:HG22	5:F:265:VAL:HG23	2.03	0.41
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.86	0.40
3:D:270:LEU:HD12	3:D:284:LEU:HD11	2.03	0.40
3:D:783:ARG:HG2	3:D:783:ARG:H	1.55	0.40
2:C:168:ARG:HD3	2:C:268:ASP:HB3	2.04	0.40
2:C:434:HIS:HE1	11:C:1203:HOH:O	2.03	0.40
6:G:17:DG:H3'	6:G:18:DA:H8	1.85	0.40
3:D:114:THR:HG23	3:D:495:ARG:HG2	2.02	0.40
2:C:397:GLU:HG2	2:C:632:ASN:HB2	2.02	0.40
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.02	0.40
3:D:216:VAL:HA	3:D:340:THR:HG22	2.02	0.40
3:D:355:VAL:HG11	3:D:385:VAL:HG21	2.02	0.40
3:D:38:LYS:HD3	3:D:38:LYS:HA	1.83	0.40
3:D:74:GLU:H	3:D:74:GLU:CD	2.24	0.40
1:A:133:GLU:OE1	2:C:610:ARG:NH1	2.55	0.40
3:D:904:VAL:CG2	3:D:905:PRO:HD2	2.50	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%)	229 (100%)	1 (0%)	0	100	100
1	B	221/315 (70%)	218 (99%)	2 (1%)	1 (0%)	29	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1111/1119 (99%)	1091 (98%)	20 (2%)	0	100	100
3	D	1485/1524 (97%)	1461 (98%)	24 (2%)	0	100	100
4	E	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
5	F	334/443 (75%)	333 (100%)	1 (0%)	0	100	100
All	All	3473/3815 (91%)	3423 (99%)	49 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ALA

### 5.3.2 Protein sidechains ⓘ

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%)	187 (93%)	14 (7%)	15	37
1	B	196/273 (72%)	186 (95%)	10 (5%)	24	53
2	C	938/941 (100%)	896 (96%)	42 (4%)	27	58
3	D	1250/1279 (98%)	1203 (96%)	47 (4%)	33	64
4	E	83/88 (94%)	80 (96%)	3 (4%)	35	66
5	F	294/388 (76%)	278 (95%)	16 (5%)	22	50
All	All	2962/3242 (91%)	2830 (96%)	132 (4%)	28	58

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	15	THR
1	A	30	ARG
1	A	90	LEU
1	A	94	LEU
1	A	96	THR

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Mol	Chain	Res	Type
1	A	112	ARG
1	A	134	GLU
1	A	142	VAL
1	A	145	ASP
1	A	148	VAL
1	A	170	VAL
1	A	189	ARG
1	A	205	VAL
1	B	7	LYS
1	B	55	SER
1	B	90	LEU
1	B	94	LEU
1	B	133	GLU
1	B	146	ARG
1	B	154	GLU
1	B	160	ASP
1	B	188	GLN
1	B	191	ASP
2	C	81	ASP
2	C	133	ASP
2	C	141	HIS
2	C	168	ARG
2	C	186	VAL
2	C	216	GLU
2	C	242	LEU
2	C	251	ASP
2	C	284	ARG
2	C	322	VAL
2	C	342	ASP
2	C	348	LEU
2	C	358	ARG
2	C	360	LEU
2	C	384	GLU
2	C	402	SER
2	C	413	LEU
2	C	418	LEU
2	C	421	GLU
2	C	427	VAL
2	C	430	VAL
2	C	445	GLU
2	C	449	ILE
2	C	454	SER

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Mol	Chain	Res	Type
2	C	455	LEU
2	C	483	VAL
2	C	524	VAL
2	C	583	LEU
2	C	610	ARG
2	C	640	ARG
2	C	657	ASP
2	C	666	LEU
2	C	670	GLN
2	C	674	VAL
2	C	768	THR
2	C	775	ARG
2	C	807[A]	ARG
2	C	807[B]	ARG
2	C	816	LYS
2	C	913	GLU
2	C	929	ARG
2	C	1095	LEU
3	D	35	ARG
3	D	67	ARG
3	D	83	SER
3	D	134	VAL
3	D	135	LEU
3	D	145	VAL
3	D	175	VAL
3	D	185	VAL
3	D	199	LEU
3	D	216	VAL
3	D	245	LEU
3	D	273	ARG
3	D	293	VAL
3	D	415	VAL
3	D	431	VAL
3	D	452	ILE
3	D	503	LEU
3	D	607	LEU
3	D	623	VAL
3	D	709	HIS
3	D	711	LEU
3	D	754	PHE
3	D	783	ARG
3	D	784	ASP

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Mol	Chain	Res	Type
3	D	810	GLU
3	D	813	LEU
3	D	864	VAL
3	D	892	ASP
3	D	899	LEU
3	D	956	ILE
3	D	1055	VAL
3	D	1083	ASP
3	D	1100	ASP
3	D	1101	VAL
3	D	1129	THR
3	D	1188	VAL
3	D	1189	ARG
3	D	1200	VAL
3	D	1221	VAL
3	D	1252	ILE
3	D	1295	GLU
3	D	1312	LEU
3	D	1313	VAL
3	D	1424	VAL
3	D	1433	SER
3	D	1468	LEU
3	D	1488	ASP
4	E	15	SER
4	E	50	THR
4	E	84	ARG
5	F	81	VAL
5	F	88	ILE
5	F	94	LEU
5	F	96	LEU
5	F	141	VAL
5	F	179	GLU
5	F	262	VAL
5	F	310	ILE
5	F	315	VAL
5	F	358	LEU
5	F	369	LEU
5	F	373	LYS
5	F	380	GLU
5	F	392	VAL
5	F	399	GLN
5	F	417	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

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

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	231/315 (73%)	0.01	5 (2%) 62 57	65, 85, 111, 148	0
1	B	223/315 (70%)	0.13	4 (1%) 68 65	68, 94, 122, 133	0
2	C	1112/1119 (99%)	0.21	38 (3%) 45 39	46, 78, 132, 155	0
3	D	1486/1524 (97%)	0.32	90 (6%) 21 16	46, 80, 135, 160	1 (0%)
4	E	94/99 (94%)	-0.20	0 100 100	61, 83, 115, 136	0
5	F	338/443 (76%)	0.16	10 (2%) 50 45	64, 93, 130, 147	0
6	G	18/21 (85%)	-0.35	0 100 100	67, 100, 176, 181	0
7	H	24/27 (88%)	-0.81	0 100 100	84, 105, 167, 193	0
8	I	6/6 (100%)	-0.31	0 100 100	66, 70, 84, 103	0
All	All	3532/3869 (91%)	0.21	147 (4%) 36 30	46, 83, 133, 193	1 (0%)

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ALA	7.6
1	B	6	LEU	6.3
3	D	409	VAL	6.1
2	C	63	GLY	6.0
1	A	233	VAL	5.3
2	C	365	ASP	5.0
2	C	811	PRO	4.6
3	D	203	ALA	4.4
3	D	974	ILE	4.3
2	C	159	ILE	4.2
3	D	371	ILE	4.2
2	C	207	LEU	4.1
3	D	286	VAL	4.0
3	D	173	PRO	4.0
3	D	531	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	C	189	ARG	3.9
3	D	368	VAL	3.9
2	C	100	LEU	3.8
3	D	360	ARG	3.8
3	D	241	ILE	3.8
3	D	1305	LEU	3.8
3	D	1313	VAL	3.7
3	D	1252	ILE	3.7
3	D	1408	ILE	3.6
3	D	470	LEU	3.6
5	F	146	GLY	3.6
3	D	144	GLY	3.5
1	A	231	ALA	3.5
3	D	213	VAL	3.5
2	C	254	VAL	3.4
3	D	321	GLN	3.4
3	D	1130	ARG	3.3
3	D	324	ALA	3.2
3	D	1319	VAL	3.2
3	D	804	LEU	3.2
3	D	143	ASN	3.1
3	D	343	LYS	3.1
2	C	739	GLU	3.1
3	D	393	ILE	3.1
3	D	152	LEU	3.1
3	D	971	LEU	3.1
3	D	821	VAL	3.1
2	C	176	VAL	3.0
3	D	1301	LYS	2.9
3	D	1299	PHE	2.9
5	F	328	PHE	2.9
2	C	367	LEU	2.9
3	D	831	GLY	2.9
3	D	782	SER	2.9
3	D	1292	VAL	2.9
3	D	316	GLN	2.9
3	D	142	LEU	2.9
2	C	217	LEU	2.9
3	D	1499	ARG	2.9
2	C	311	PHE	2.9
2	C	729	LEU	2.8
1	A	230	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	242	LEU	2.8
3	D	1127	GLU	2.8
3	D	352	ASN	2.8
2	C	107	LEU	2.8
3	D	983	LEU	2.7
3	D	1495	ILE	2.7
2	C	251	ASP	2.7
3	D	211	VAL	2.7
3	D	308	LYS	2.7
3	D	1294	VAL	2.7
3	D	1128	VAL	2.6
3	D	161	LEU	2.6
3	D	225	LEU	2.6
3	D	1312	LEU	2.6
1	B	106	PRO	2.6
2	C	154	ARG	2.6
1	B	140	MET	2.6
3	D	322	VAL	2.5
3	D	361	VAL	2.5
5	F	374	GLY	2.5
3	D	345	TYR	2.5
3	D	1281	VAL	2.5
3	D	379	ALA	2.5
2	C	221	LEU	2.5
3	D	336	PHE	2.5
5	F	318	GLU	2.5
2	C	238	LEU	2.5
3	D	185	VAL	2.5
3	D	422	ALA	2.4
3	D	236	TYR	2.4
3	D	807	ALA	2.4
3	D	445	ARG	2.4
3	D	982	PHE	2.4
5	F	414	ARG	2.4
2	C	508	ILE	2.4
2	C	195	LEU	2.4
3	D	666	ILE	2.4
2	C	781	LYS	2.3
3	D	350	HIS	2.3
1	A	234	ALA	2.3
3	D	135	LEU	2.3
2	C	245	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	122	GLU	2.3
5	F	373	LYS	2.3
3	D	675	ARG	2.3
5	F	329	TYR	2.3
3	D	364	GLY	2.3
2	C	208	ALA	2.3
2	C	936	VAL	2.3
3	D	365	ASP	2.3
3	D	242	LEU	2.3
2	C	216	GLU	2.3
3	D	367	ILE	2.3
3	D	153	LEU	2.2
2	C	840	ALA	2.2
3	D	339	TRP	2.2
3	D	667	ALA	2.2
3	D	1298	GLY	2.2
3	D	78	VAL	2.2
5	F	376	ILE	2.2
3	D	1327	ARG	2.2
2	C	368	THR	2.2
5	F	422	LEU	2.2
3	D	323	GLU	2.1
2	C	298	PHE	2.1
2	C	226	VAL	2.1
1	B	186	LEU	2.1
2	C	8	ARG	2.1
2	C	222	MET	2.1
3	D	1285	GLU	2.1
3	D	432	TYR	2.1
2	C	10	ARG	2.1
3	D	681	ARG	2.1
3	D	976	GLN	2.1
3	D	434	ARG	2.1
2	C	102[A]	HIS	2.1
3	D	202	VAL	2.1
2	C	104	ASP	2.1
3	D	287	GLY	2.1
2	C	174	LEU	2.0
3	D	212	ARG	2.0
5	F	142	ARG	2.0
3	D	174	GLY	2.0
3	D	178	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	1287	GLU	2.0
3	D	353	VAL	2.0
3	D	680	GLN	2.0
2	C	517	ARG	2.0
3	D	183	GLU	2.0
3	D	395	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
9	MG	B	2001	1/1	0.75	0.29	97,97,97,97	0
9	MG	F	2001	1/1	0.82	0.08	83,83,83,83	0
9	MG	D	2004	1/1	0.90	0.33	83,83,83,83	0
9	MG	D	2003	1/1	0.96	0.23	49,49,49,49	0
10	ZN	D	2002	1/1	0.98	0.12	107,107,107,107	0
10	ZN	D	2001	1/1	1.00	0.19	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.