



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:52 PM GMT

PDB ID : 4Q4Z  
Title : Thermus thermophilus RNA polymerase de novo transcription initiation complex  
Authors : Murakami, K.S.  
Deposited on : 2014-04-15  
Resolution : 2.90 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

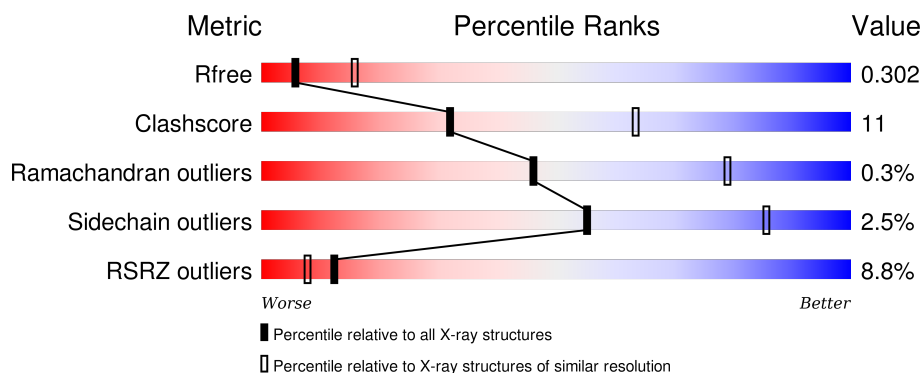
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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.





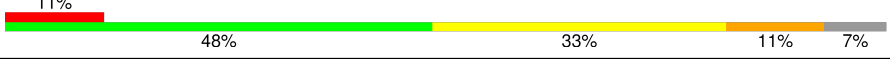
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>4%</div> <div>59%14%27%</div> </div>
1	B	315	<div> <div>4%</div> <div>60%12%28%</div> </div>
2	C	1119	<div> <div>7%</div> <div>79%19%..</div> </div>
3	D	1524	<div> <div>9%</div> <div>76%20%..</div> </div>
4	E	99	<div> <div>7%</div> <div>82%13%5%</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	423	
6	G	22	
7	H	27	

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28755 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	0	0
			1809	1155	315	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	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	0	0
			8774	5550	1565	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1494	Total	C	N	O	S	0	1	0
			11808	7484	2083	2205	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	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

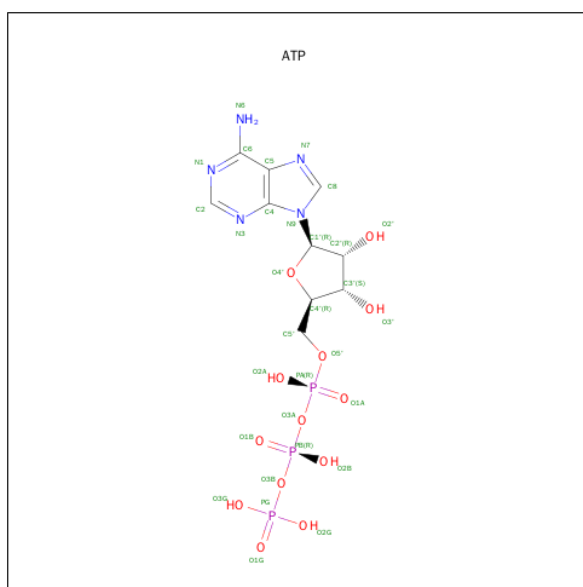
- Molecule 6 is a DNA chain called DNA (5'-D(\*CP\*CP\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*GP\*CP\*AP\*GP\*CP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	18	Total	C	N	O	P	0	0	0
			370	175	68	109	18			

- Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	25	Total 516	C 246	N 99	O 147	P 24	0	0	0

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

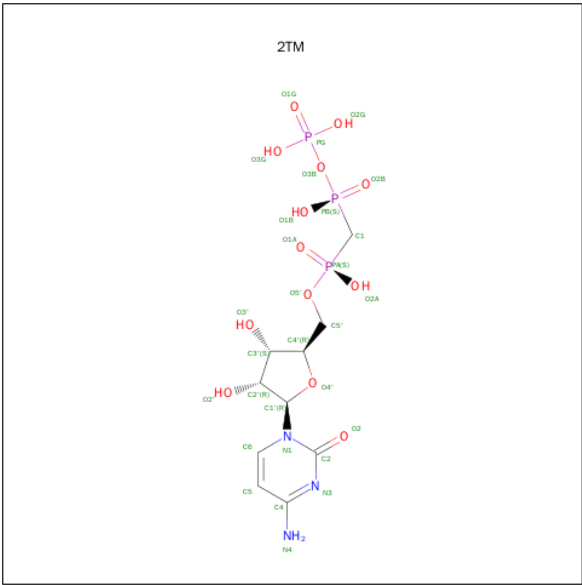
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	3	Total Mg 3 3	0	0

- Molecule 11 is 5'-O-[(S)-HYDROXY{[(S)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]METHYL}PHOSPHORYL]CYTIDINE (three-letter code: 2TM) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	D	1	29	10	3	13	3	0	0

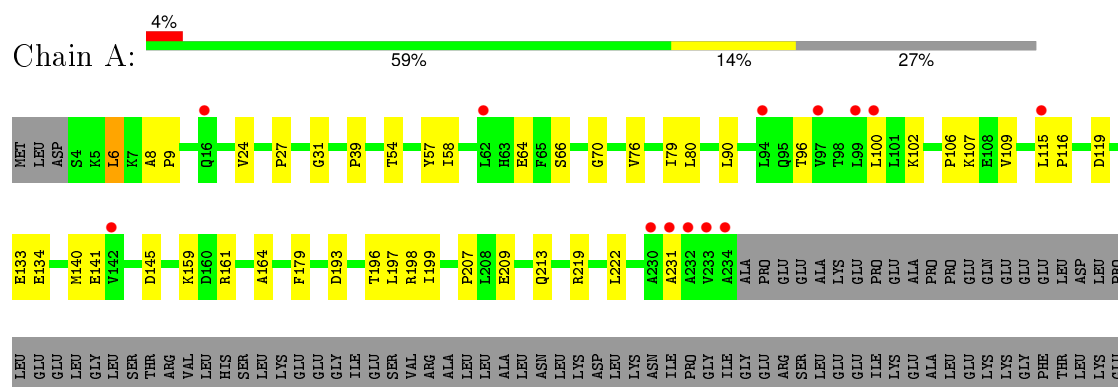
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	4	Total	O	0	0
			4	4		
12	B	1	Total	O	0	0
			1	1		
12	C	22	Total	O	0	0
			22	22		
12	D	26	Total	O	0	0
			26	26		
12	E	2	Total	O	0	0
			2	2		
12	G	1	Total	O	0	0
			1	1		

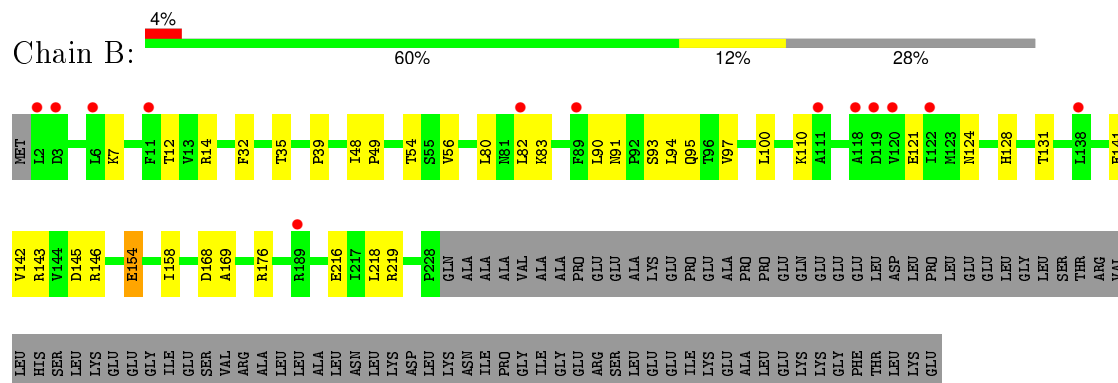
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

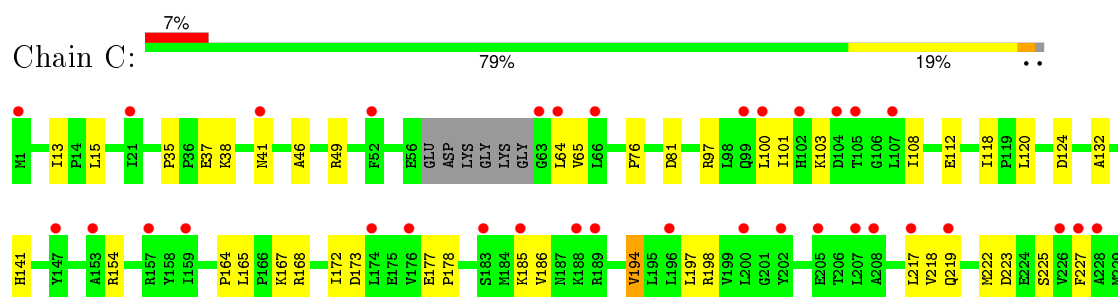
- Molecule 1: DNA-directed RNA polymerase subunit alpha

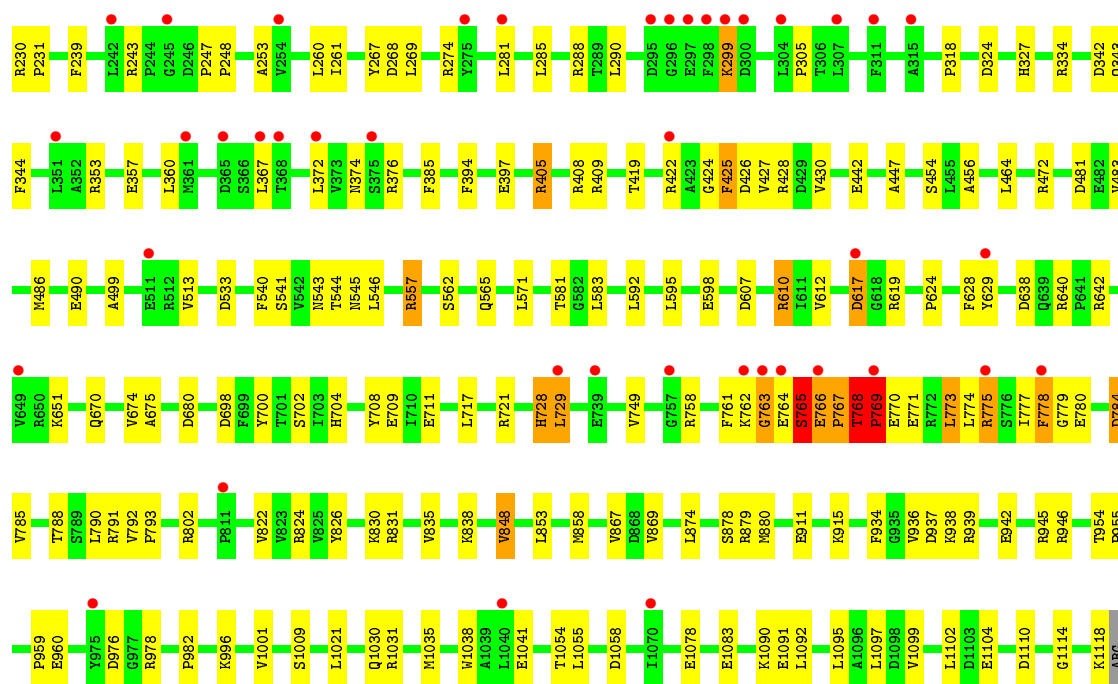


- Molecule 1: DNA-directed RNA polymerase subunit alpha

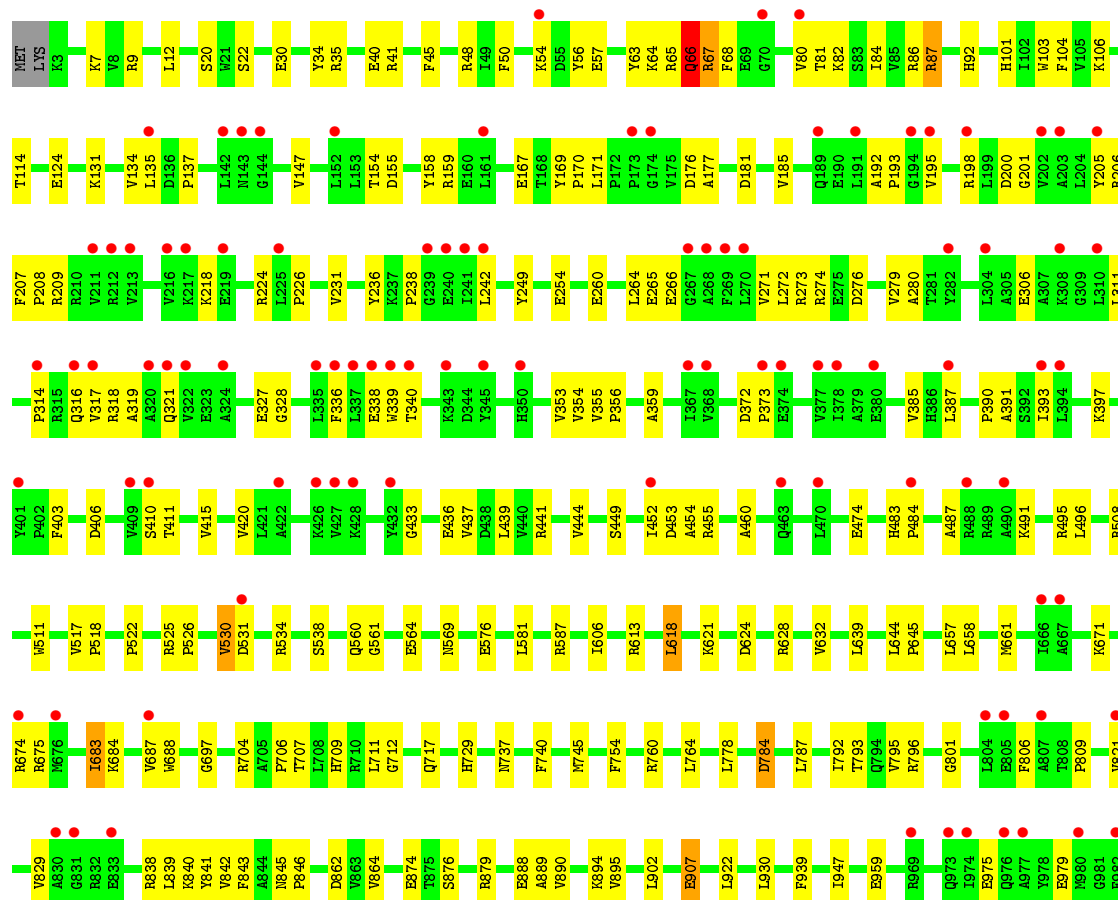
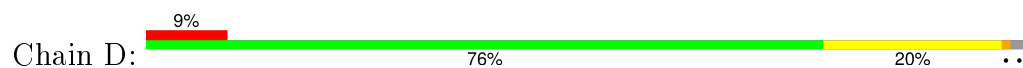


- Molecule 2: DNA-directed RNA polymerase subunit beta

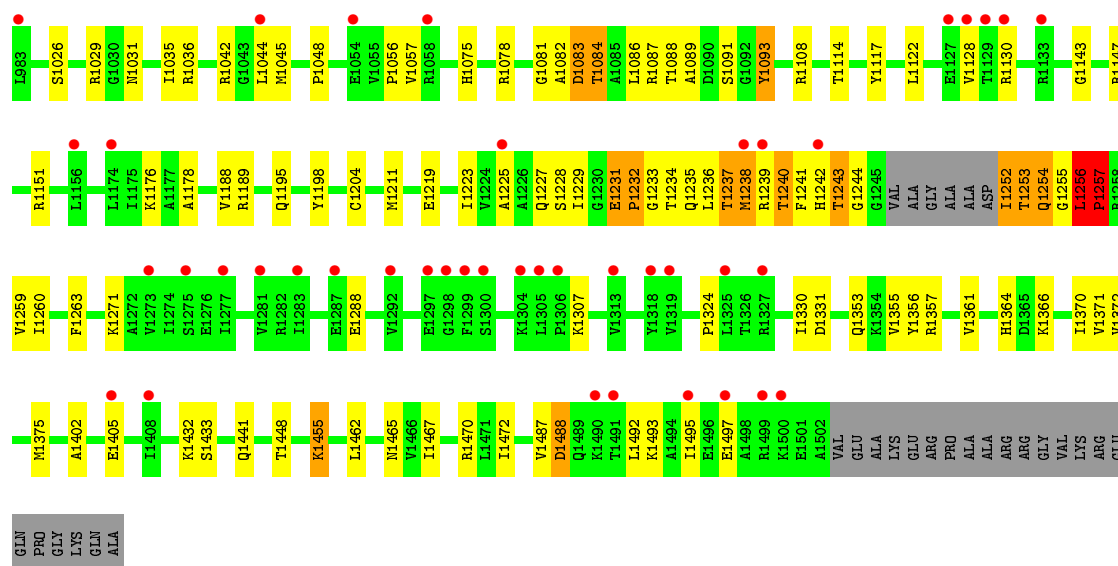




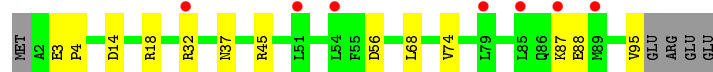
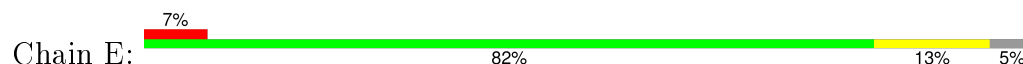
• Molecule 3: DNA-directed RNA polymerase subunit beta'



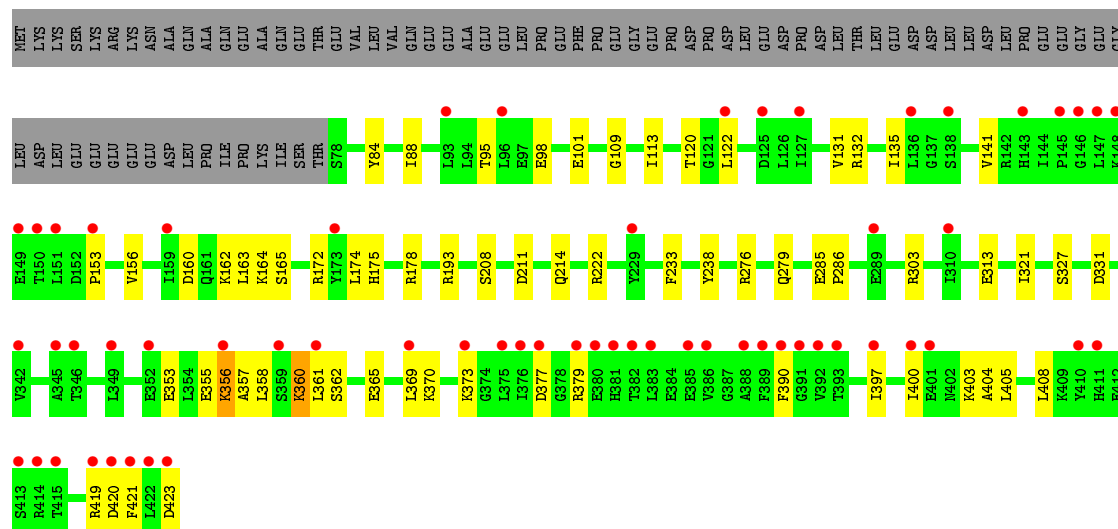




- Molecule 4: DNA-directed RNA polymerase subunit omega

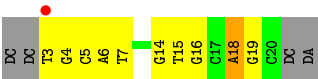


- Molecule 5: RNA polymerase sigma factor SigA

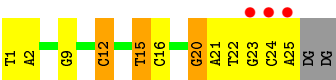


- Molecule 6: DNA (5'-D(\*CP\*CP\*TP\*GP\*CP\*AP\*TP\*CP\*CP\*GP\*TP\*GP\*AP\*GP\*TP\*GP\*CP\*AP\*GP\*CP\*CP\*A)-3')





● Molecule 7: DNA (25-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.49Å 102.16Å 294.72Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	29.78 – 2.90 43.54 – 2.85	Depositor EDS
% Data completeness (in resolution range)	89.5 (29.78-2.90) 84.3 (43.54-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.256 , 0.275 0.292 , 0.302	Depositor DCC
$R_{free}$ test set	1686 reflections (1.66%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 18.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	3 of 111819 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	28755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 2TM, MG, ZN, ATP

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	0.24	0/1841	0.46	0/2504
1	B	0.22	0/1821	0.44	0/2476
2	C	0.31	1/8941 (0.0%)	0.50	6/12092 (0.0%)
3	D	0.35	1/12019 (0.0%)	0.50	4/16248 (0.0%)
4	E	0.24	0/775	0.41	0/1045
5	F	0.23	0/2852	0.40	0/3837
6	G	0.72	2/414 (0.5%)	1.16	3/637 (0.5%)
7	H	0.57	0/580	1.13	3/895 (0.3%)
All	All	0.33	4/29243 (0.0%)	0.52	16/39734 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1093	TYR	CE2-CZ	-6.38	1.30	1.38
6	G	18	DA	O3'-P	-5.67	1.54	1.61
6	G	3	DT	O3'-P	-5.63	1.54	1.61
2	C	769	PRO	N-CD	5.43	1.55	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	761	PHE	O-C-N	-10.43	106.01	122.70
6	G	18	DA	O4'-C1'-N9	9.34	114.54	108.00
3	D	1257	PRO	CA-N-CD	-8.41	99.72	111.50
3	D	1232	PRO	CA-N-CD	-7.58	100.88	111.50
2	C	761	PHE	C-N-CA	7.11	139.47	121.70
2	C	761	PHE	CA-C-N	7.08	132.78	117.20
6	G	18	DA	C4'-C3'-C2'	6.18	108.67	103.10
3	D	1256	LEU	C-N-CD	6.01	141.01	128.40
2	C	766	GLU	C-N-CD	5.84	140.67	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	765	SER	N-CA-C	-5.53	96.06	111.00
3	D	1231	GLU	C-N-CD	5.36	139.65	128.40
6	G	18	DA	O5'-P-OP1	5.31	117.08	110.70
7	H	15	DT	O4'-C1'-N1	5.30	111.71	108.00
2	C	769	PRO	CA-N-CD	-5.24	104.16	111.50
7	H	20	DG	C1'-O4'-C4'	-5.24	104.86	110.10
7	H	12	DC	O4'-C1'-N1	5.20	111.64	108.00

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	1809	0	1863	38	0
1	B	1789	0	1841	24	0
2	C	8774	0	8877	226	3
3	D	11808	0	12041	258	4
4	E	761	0	778	9	1
5	F	2807	0	2882	101	2
6	G	370	0	202	19	0
7	H	516	0	283	31	1
8	C	31	0	11	2	0
9	D	2	0	0	0	0
10	D	3	0	0	0	0
11	D	29	0	14	2	0
12	A	4	0	0	9	0
12	B	1	0	0	0	0
12	C	22	0	0	29	0
12	D	26	0	0	26	0
12	E	2	0	0	1	0
12	G	1	0	0	0	0
All	All	28755	0	28792	605	6

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 11.

All (605) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:773:LEU:CD2	5:F:373:LYS:HG3	1.14	1.60
5:F:358:LEU:HD13	5:F:370:LYS:NZ	1.33	1.41
2:C:773:LEU:CD2	5:F:373:LYS:CG	2.03	1.36
2:C:778:PHE:HE2	5:F:419:ARG:NH2	1.25	1.35
2:C:764:GLU:O	2:C:766:GLU:N	1.62	1.32
5:F:358:LEU:CD1	5:F:370:LYS:CE	2.09	1.30
5:F:358:LEU:CD1	5:F:370:LYS:NZ	1.92	1.30
2:C:768:THR:O	2:C:771:GLU:N	1.65	1.28
5:F:355:GLU:OE1	5:F:358:LEU:HD12	1.21	1.27
5:F:358:LEU:HD11	5:F:370:LYS:CE	1.64	1.26
1:A:107:LYS:HG3	12:A:404:HOH:O	1.23	1.25
2:C:778:PHE:CE2	5:F:419:ARG:NH2	2.08	1.21
2:C:764:GLU:OE1	3:D:54:LYS:HE2	1.37	1.20
2:C:778:PHE:HE2	5:F:419:ARG:CZ	1.55	1.19
3:D:1091:SER:OG	3:D:1234:THR:OG1	1.61	1.17
2:C:778:PHE:CE2	5:F:419:ARG:CZ	2.26	1.17
2:C:996:LYS:HG2	12:C:1321:HOH:O	1.44	1.17
2:C:878:SER:HB3	12:C:1301:HOH:O	1.44	1.16
2:C:773:LEU:HD23	5:F:373:LYS:HG3	1.25	1.15
5:F:358:LEU:CD1	5:F:370:LYS:HZ1	1.50	1.14
12:C:1314:HOH:O	5:F:331:ASP:HA	1.45	1.14
2:C:773:LEU:HD22	5:F:373:LYS:CG	1.69	1.11
5:F:358:LEU:HD11	5:F:370:LYS:HE2	1.21	1.11
2:C:773:LEU:HD23	5:F:373:LYS:CB	1.80	1.10
2:C:773:LEU:HD12	2:C:777:ILE:HD11	1.29	1.10
7:H:21:DA:H2"	7:H:22:DT:H5'	1.30	1.09
6:G:6:DA:N1	7:H:22:DT:N3	2.01	1.08
2:C:717:LEU:CD2	2:C:763:GLY:HA2	1.86	1.06
2:C:773:LEU:HD23	5:F:373:LYS:CG	1.73	1.06
3:D:1056:PRO:HA	12:D:2114:HOH:O	1.54	1.04
1:A:107:LYS:CG	12:A:404:HOH:O	1.83	1.04
1:A:107:LYS:CD	12:A:404:HOH:O	2.01	1.04
3:D:1044:LEU:HA	12:D:2114:HOH:O	1.57	1.04
1:A:107:LYS:HE2	12:A:404:HOH:O	1.54	1.03
2:C:774:LEU:HA	2:C:777:ILE:HD12	1.39	1.01
3:D:538:SER:HB2	12:D:2119:HOH:O	1.60	1.01
3:D:1223:ILE:O	3:D:1227:GLN:HG3	1.60	1.01
2:C:717:LEU:HD21	2:C:763:GLY:HA2	1.44	1.00
2:C:768:THR:O	2:C:770:GLU:N	1.95	0.99
2:C:728:HIS:HB3	5:F:423:ASP:O	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:65:ARG:CZ	3:D:68:PHE:CE2	2.47	0.97
1:A:107:LYS:CE	12:A:404:HOH:O	2.08	0.97
2:C:543:ASN:HB3	12:C:1316:HOH:O	0.79	0.96
5:F:358:LEU:HD13	5:F:370:LYS:CE	1.82	0.96
6:G:7:DT:H3	7:H:21:DA:N6	1.65	0.95
2:C:777:ILE:HA	5:F:405:LEU:HD11	1.48	0.94
3:D:538:SER:CB	12:D:2119:HOH:O	2.16	0.93
3:D:1235:GLN:HG3	3:D:1239:ARG:HD3	1.50	0.92
3:D:1081:GLY:O	3:D:1084:THR:OG1	1.85	0.92
2:C:764:GLU:OE1	3:D:54:LYS:CE	2.19	0.91
2:C:1041:GLU:HG2	12:C:1315:HOH:O	1.69	0.91
2:C:268:ASP:HA	12:C:1307:HOH:O	1.71	0.90
2:C:768:THR:C	2:C:770:GLU:H	1.75	0.89
2:C:481:ASP:HA	12:C:1322:HOH:O	1.72	0.88
5:F:358:LEU:HD13	5:F:370:LYS:HZ1	0.71	0.88
2:C:880:MET:CE	3:D:1242:HIS:CD2	2.55	0.88
2:C:774:LEU:HA	2:C:777:ILE:CD1	2.02	0.88
3:D:206:ARG:NH2	5:F:101:GLU:OE2	2.06	0.88
3:D:65:ARG:NH2	3:D:68:PHE:CE2	2.41	0.88
5:F:358:LEU:CD1	5:F:370:LYS:HE3	2.04	0.87
3:D:65:ARG:CZ	3:D:68:PHE:HE2	1.87	0.87
3:D:947:ILE:HA	12:D:2120:HOH:O	1.73	0.86
3:D:1225:ALA:O	3:D:1229:ILE:HD12	1.76	0.85
5:F:355:GLU:OE1	5:F:358:LEU:CD1	2.18	0.85
2:C:764:GLU:CD	3:D:54:LYS:HE2	1.96	0.85
3:D:581:LEU:HD21	12:D:2108:HOH:O	1.77	0.84
2:C:768:THR:C	2:C:770:GLU:N	2.27	0.83
2:C:778:PHE:CZ	5:F:419:ARG:CZ	2.61	0.83
11:D:2006:2TM:H1	11:D:2006:2TM:H10	1.60	0.83
2:C:880:MET:HE1	3:D:1242:HIS:CD2	2.14	0.83
5:F:357:ALA:O	5:F:360:LYS:HB2	1.78	0.82
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.62	0.81
2:C:717:LEU:HD23	2:C:763:GLY:HA2	1.61	0.81
7:H:21:DA:C2'	7:H:22:DT:H5'	2.09	0.81
2:C:764:GLU:O	2:C:765:SER:C	2.20	0.80
2:C:472:ARG:HD2	12:C:1322:HOH:O	1.83	0.79
2:C:774:LEU:CA	2:C:777:ILE:HD12	2.11	0.79
3:D:1086:LEU:O	3:D:1089:ALA:HB3	1.82	0.78
7:H:20:DG:H2''	7:H:21:DA:C5'	2.14	0.78
2:C:773:LEU:CD1	2:C:777:ILE:HD11	2.13	0.77
3:D:675:ARG:NH2	5:F:420:ASP:O	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:773:LEU:HD22	5:F:373:LYS:HG3	0.77	0.77
3:D:68:PHE:O	3:D:80:VAL:HG23	1.84	0.77
2:C:762:LYS:HG2	2:C:784:ASP:O	1.85	0.77
2:C:773:LEU:HD23	5:F:373:LYS:HB2	1.67	0.77
2:C:880:MET:HE2	3:D:1242:HIS:CD2	2.19	0.77
3:D:65:ARG:NH2	3:D:68:PHE:HE2	1.78	0.77
6:G:7:DT:C2	7:H:21:DA:N1	2.53	0.77
2:C:422:ARG:HD2	7:H:15:DT:OP2	1.84	0.76
5:F:355:GLU:CD	5:F:358:LEU:HD12	2.07	0.76
5:F:358:LEU:CD2	5:F:370:LYS:HE3	2.17	0.74
3:D:1082:ALA:O	3:D:1086:LEU:HD13	1.87	0.74
3:D:1432:LYS:HD3	12:D:2122:HOH:O	1.86	0.74
2:C:409:ARG:HH11	2:C:454:SER:HB2	1.53	0.74
2:C:758:ARG:HH21	2:C:788:THR:HB	1.53	0.73
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.68	0.73
2:C:1030:GLN:OE1	3:D:628:ARG:NH1	2.20	0.73
6:G:7:DT:O2	7:H:21:DA:N1	2.21	0.73
5:F:361:LEU:HD11	5:F:408:LEU:HG	1.72	0.72
7:H:20:DG:H2"	7:H:21:DA:H5"	1.72	0.72
3:D:1084:THR:O	3:D:1088:THR:OG1	2.07	0.72
2:C:764:GLU:O	2:C:766:GLU:HG3	1.90	0.71
2:C:541:SER:HB2	12:C:1302:HOH:O	1.90	0.71
2:C:167:LYS:HD3	7:H:12:DC:H5	1.55	0.71
2:C:728:HIS:HD2	5:F:423:ASP:HB2	1.54	0.71
3:D:65:ARG:CD	5:F:379:ARG:HB3	2.21	0.71
3:D:63:TYR:HD1	3:D:68:PHE:CE1	2.09	0.70
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.73	0.70
6:G:4:DG:H2"	6:G:5:DC:OP2	1.91	0.70
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.25	0.70
3:D:68:PHE:O	3:D:80:VAL:CG2	2.39	0.70
2:C:628:PHE:H	2:C:638:ASP:HB3	1.57	0.69
2:C:717:LEU:CD2	2:C:763:GLY:CA	2.69	0.69
3:D:65:ARG:NH2	3:D:68:PHE:CZ	2.60	0.69
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.73	0.69
3:D:1255:GLY:O	3:D:1259:VAL:HG23	1.93	0.69
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.75	0.68
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.74	0.68
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.75	0.68
2:C:428:ARG:NH2	2:C:447:ALA:O	2.27	0.68
2:C:771:GLU:HB3	2:C:775:ARG:NH2	2.09	0.67
3:D:208:PRO:HA	3:D:390:PRO:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.77	0.67
7:H:21:DA:H2"	7:H:22:DT:C5'	2.18	0.67
3:D:576:GLU:HB3	12:D:2102:HOH:O	1.95	0.67
2:C:773:LEU:HD12	2:C:777:ILE:CD1	2.17	0.66
3:D:1240:THR:O	3:D:1241:PHE:HB2	1.94	0.66
3:D:1228:SER:O	3:D:1232:PRO:HD2	1.95	0.66
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.28	0.66
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.29	0.66
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.61	0.66
2:C:768:THR:O	2:C:770:GLU:C	2.35	0.66
3:D:526:PRO:HD2	12:D:2119:HOH:O	1.95	0.66
2:C:230:ARG:HD3	2:C:231:PRO:HD2	1.78	0.66
2:C:784:ASP:N	2:C:784:ASP:OD2	2.29	0.65
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.77	0.65
2:C:670:GLN:HE21	2:C:700:TYR:H	1.42	0.65
3:D:1044:LEU:O	3:D:1244:GLY:HA2	1.95	0.65
3:D:433:GLY:HA2	3:D:449:SER:H	1.62	0.65
5:F:357:ALA:HA	5:F:360:LYS:CG	2.27	0.65
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.79	0.65
3:D:411:THR:O	5:F:178:ARG:NH1	2.26	0.65
2:C:778:PHE:HE2	5:F:419:ARG:HH22	1.37	0.65
3:D:947:ILE:HD13	12:D:2120:HOH:O	1.97	0.65
3:D:1231:GLU:OE1	3:D:1232:PRO:HD3	1.97	0.65
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.30	0.64
5:F:355:GLU:O	5:F:358:LEU:HB2	1.97	0.64
2:C:717:LEU:HD21	2:C:763:GLY:CA	2.24	0.64
6:G:7:DT:N3	7:H:21:DA:N6	2.28	0.64
3:D:1253:THR:OG1	3:D:1254:GLN:N	2.31	0.64
3:D:63:TYR:CD1	3:D:68:PHE:CE1	2.85	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.80	0.64
2:C:764:GLU:C	2:C:766:GLU:N	2.49	0.64
3:D:1233:GLY:O	3:D:1237:THR:OG1	2.16	0.63
3:D:1252:ILE:HG13	3:D:1252:ILE:O	1.98	0.63
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.79	0.63
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.81	0.63
3:D:316:GLN:NE2	3:D:340:THR:O	2.31	0.63
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.80	0.63
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.80	0.63
5:F:357:ALA:HA	5:F:360:LYS:HG2	1.81	0.63
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.31	0.63
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:562:SER:HA	12:C:1316:HOH:O	1.99	0.62
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.82	0.62
3:D:1083:ASP:OD2	3:D:1253:THR:HG22	2.00	0.62
3:D:569:ASN:ND2	5:F:214:GLN:OE1	2.28	0.62
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.81	0.62
3:D:65:ARG:HD3	5:F:379:ARG:HB3	1.81	0.61
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.82	0.61
3:D:534:ARG:NH2	5:F:313:GLU:O	2.33	0.61
5:F:358:LEU:HD13	5:F:370:LYS:HE3	1.73	0.61
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.82	0.61
3:D:671:LYS:NZ	5:F:421:PHE:HA	2.14	0.61
2:C:773:LEU:O	2:C:777:ILE:HG13	2.01	0.61
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.32	0.61
6:G:6:DA:H2''	6:G:7:DT:C5'	2.30	0.61
2:C:763:GLY:C	2:C:765:SER:H	2.04	0.60
2:C:376:ARG:HE	5:F:276:ARG:HG3	1.66	0.60
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.83	0.60
12:C:1315:HOH:O	3:D:1462:LEU:HB3	2.01	0.60
3:D:1432:LYS:O	3:D:1455:LYS:NZ	2.34	0.60
2:C:274:ARG:HD2	2:C:288:ARG:HG2	1.83	0.60
2:C:764:GLU:O	2:C:766:GLU:CA	2.48	0.60
3:D:959:GLU:OE1	3:D:959:GLU:N	2.30	0.60
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.66	0.60
3:D:846:PRO:HD2	12:D:2115:HOH:O	2.02	0.60
4:E:32:ARG:O	4:E:95:VAL:HG21	2.01	0.60
3:D:1091:SER:OG	3:D:1234:THR:CB	2.48	0.60
3:D:1231:GLU:HB3	3:D:1232:PRO:CD	2.32	0.59
2:C:960:GLU:CB	12:C:1303:HOH:O	2.51	0.59
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.32	0.59
1:A:196:THR:HG21	2:C:934:PHE:HE2	1.68	0.59
2:C:768:THR:O	2:C:770:GLU:CA	2.51	0.59
6:G:7:DT:C4	7:H:21:DA:N6	2.57	0.59
7:H:20:DG:H2''	7:H:21:DA:H5'	1.83	0.59
3:D:65:ARG:NE	3:D:68:PHE:HE2	1.99	0.59
3:D:845:ASN:HB2	12:D:2115:HOH:O	2.01	0.58
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.86	0.58
3:D:1231:GLU:HB3	3:D:1232:PRO:HD2	1.85	0.58
7:H:20:DG:C2'	7:H:21:DA:H5''	2.33	0.57
1:B:94:LEU:O	1:B:146:ARG:NH2	2.36	0.57
2:C:422:ARG:CD	7:H:15:DT:OP2	2.51	0.57
2:C:581:THR:HB	12:C:1312:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:358:LEU:CD1	5:F:370:LYS:HZ3	2.12	0.57
2:C:778:PHE:CE2	5:F:419:ARG:NH1	2.71	0.57
2:C:376:ARG:NE	5:F:276:ARG:HG3	2.19	0.57
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.87	0.57
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.38	0.57
3:D:65:ARG:NE	3:D:68:PHE:CE2	2.71	0.57
3:D:45:PHE:O	3:D:86:ARG:NH2	2.37	0.57
5:F:233:PHE:CD2	7:H:2:DA:H1'	2.40	0.57
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.87	0.57
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.41	0.56
2:C:164:PRO:HA	2:C:269:LEU:HD23	1.87	0.56
2:C:878:SER:CB	12:C:1301:HOH:O	2.24	0.56
3:D:1492:LEU:HD22	4:E:74:VAL:HG21	1.87	0.56
2:C:628:PHE:H	2:C:638:ASP:CB	2.19	0.56
1:A:106:PRO:HD3	1:A:134:GLU:HG2	1.88	0.56
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.88	0.56
1:A:70:GLY:N	2:C:607:ASP:OD1	2.38	0.56
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.87	0.55
3:D:1045:MET:HE1	3:D:1243:THR:O	2.07	0.55
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.88	0.55
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.87	0.55
2:C:728:HIS:CB	5:F:423:ASP:O	2.45	0.55
2:C:198:ARG:HE	2:C:227:PHE:HA	1.72	0.55
2:C:419:THR:HG22	2:C:422:ARG:HE	1.71	0.55
2:C:409:ARG:HD2	12:C:1311:HOH:O	2.06	0.55
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.41	0.55
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.88	0.55
3:D:526:PRO:CD	12:D:2119:HOH:O	2.54	0.55
3:D:1229:ILE:CG2	3:D:1356:TYR:OH	2.55	0.55
1:B:93:SER:O	1:B:95:GLN:NE2	2.39	0.55
6:G:6:DA:H2''	6:G:7:DT:H5'	1.87	0.55
3:D:411:THR:HG23	3:D:436:GLU:HA	1.89	0.55
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.06	0.55
3:D:63:TYR:CD1	3:D:68:PHE:HE1	2.25	0.55
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.88	0.55
1:A:31:GLY:HA2	12:A:403:HOH:O	2.06	0.55
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.87	0.54
2:C:353:ARG:NH1	2:C:357:GLU:OE2	2.40	0.54
3:D:56:TYR:CE2	3:D:66:GLN:HG3	2.42	0.54
2:C:629:TYR:HB3	12:C:1319:HOH:O	2.08	0.54
2:C:773:LEU:CD1	2:C:777:ILE:CG1	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:7:DT:O2	7:H:21:DA:C2	2.59	0.54
1:A:231:ALA:HB2	1:B:12:THR:HG22	1.89	0.54
2:C:243:ARG:NH1	7:H:9:DG:O6	2.39	0.54
3:D:657:LEU:HG	3:D:661:MET:HE2	1.89	0.54
2:C:778:PHE:CZ	5:F:419:ARG:NE	2.75	0.54
2:C:167:LYS:HD3	7:H:12:DC:C5	2.41	0.54
3:D:846:PRO:CD	12:D:2115:HOH:O	2.55	0.54
6:G:5:DC:H1'	6:G:6:DA:C8	2.43	0.54
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.08	0.54
2:C:838:LYS:NZ	8:C:1201:ATP:O1A	2.41	0.53
5:F:357:ALA:C	5:F:360:LYS:HB2	2.28	0.53
3:D:697:GLY:HA3	12:E:101:HOH:O	2.09	0.53
2:C:64:LEU:HB3	2:C:100:LEU:HD11	1.90	0.53
5:F:358:LEU:HD22	5:F:370:LYS:HE3	1.89	0.53
3:D:1235:GLN:O	3:D:1239:ARG:HB2	2.09	0.53
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.90	0.53
2:C:778:PHE:HZ	5:F:419:ARG:NE	2.07	0.53
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.90	0.53
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.89	0.53
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.90	0.53
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.90	0.53
2:C:835:VAL:HG23	12:C:1308:HOH:O	2.09	0.53
2:C:598:GLU:O	2:C:651:LYS:NZ	2.35	0.53
3:D:894:LYS:HD2	3:D:894:LYS:H	1.74	0.53
2:C:422:ARG:CG	7:H:15:DT:OP2	2.57	0.52
2:C:425:PHE:O	2:C:427:VAL:N	2.42	0.52
2:C:557:ARG:HD3	2:C:879:ARG:HB3	1.90	0.52
1:A:199:ILE:HB	1:A:207:PRO:HB3	1.91	0.52
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.92	0.52
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.91	0.52
3:D:658:LEU:HA	3:D:661:MET:HE3	1.92	0.52
2:C:260:LEU:HB3	2:C:261:ILE:HD12	1.92	0.52
3:D:439:LEU:CD1	5:F:172:ARG:HG3	2.40	0.52
3:D:65:ARG:C	3:D:66:GLN:O	2.46	0.52
3:D:684:LYS:O	3:D:687:VAL:HG12	2.09	0.52
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.90	0.52
6:G:15:DT:H2'	6:G:16:DG:C8	2.44	0.52
2:C:223:ASP:OD1	2:C:225:SER:OG	2.24	0.52
3:D:1086:LEU:N	3:D:1086:LEU:CD1	2.72	0.52
5:F:355:GLU:HA	5:F:358:LEU:HG	1.91	0.52
3:D:65:ARG:O	3:D:68:PHE:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:541:SER:O	2:C:545:ASN:ND2	2.43	0.52
3:D:1253:THR:O	3:D:1257:PRO:HD2	2.10	0.52
2:C:427:VAL:O	2:C:427:VAL:HG22	2.08	0.52
2:C:217:LEU:H	2:C:217:LEU:HD12	1.73	0.52
3:D:1253:THR:O	3:D:1257:PRO:HG2	2.10	0.52
3:D:439:LEU:HD13	5:F:172:ARG:HG3	1.91	0.52
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.91	0.52
2:C:717:LEU:HD23	2:C:763:GLY:CA	2.37	0.52
3:D:200:ASP:O	3:D:397:LYS:HG2	2.10	0.52
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.10	0.52
3:D:564:GLU:HG3	12:D:2110:HOH:O	2.09	0.52
3:D:321:GLN:HB2	3:D:336:PHE:HB2	1.92	0.52
2:C:729:LEU:HD11	2:C:791:ARG:HH22	1.75	0.52
12:C:1315:HOH:O	3:D:1462:LEU:HD13	2.10	0.51
3:D:231:VAL:O	3:D:236:TYR:OH	2.28	0.51
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.92	0.51
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.93	0.51
3:D:1048:PRO:HG3	3:D:1075:HIS:ND1	2.25	0.51
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.51
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.75	0.51
7:H:24:DC:C2	7:H:25:DA:C5	2.99	0.51
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.93	0.51
3:D:1219:GLU:HA	12:D:2117:HOH:O	2.09	0.51
2:C:778:PHE:O	2:C:780:GLU:N	2.44	0.51
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.46	0.51
2:C:624:PRO:CB	12:C:1313:HOH:O	2.58	0.50
3:D:671:LYS:HZ3	5:F:421:PHE:HA	1.74	0.50
3:D:209:ARG:HE	3:D:391:ALA:HB2	1.74	0.50
1:B:54:THR:OG1	1:B:145:ASP:OD1	2.27	0.50
3:D:1271:LYS:HE2	3:D:1331:ASP:HB2	1.93	0.50
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.93	0.50
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.93	0.50
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.92	0.50
2:C:15:LEU:HD11	2:C:583:LEU:HD11	1.93	0.50
3:D:975:GLU:O	3:D:979:GLU:HG2	2.12	0.50
2:C:610:ARG:HD3	2:C:612:VAL:HG23	1.92	0.50
3:D:1488:ASP:N	3:D:1488:ASP:OD1	2.31	0.50
2:C:543:ASN:C	12:C:1316:HOH:O	2.49	0.49
2:C:374:ASN:OD1	5:F:276:ARG:HD2	2.13	0.49
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.94	0.49
5:F:160:ASP:O	5:F:164:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:ARG:O	2:C:267:TYR:HA	2.13	0.49
1:B:154:GLU:HG3	3:D:840:LYS:HZ1	1.76	0.49
3:D:274:ARG:NH2	3:D:279:VAL:HG21	2.27	0.49
1:A:209:GLU:O	1:A:213:GLN:HG2	2.12	0.49
2:C:430:VAL:HG23	3:D:1078:ARG:HG2	1.95	0.49
2:C:773:LEU:CD1	2:C:777:ILE:CD1	2.86	0.49
5:F:353:GLU:O	5:F:356:LYS:HB2	2.12	0.49
3:D:1087:ARG:HB2	3:D:1237:THR:CG2	2.42	0.49
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.47	0.49
3:D:508:ARG:HB2	3:D:511:TRP:CE2	2.48	0.49
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.95	0.49
2:C:874:LEU:O	3:D:1029:ARG:HG3	2.12	0.49
3:D:155:ASP:OD1	3:D:159:ARG:NH1	2.46	0.49
5:F:238:TYR:HH	7:H:1:DT:H6	1.59	0.48
2:C:774:LEU:O	2:C:777:ILE:HD12	2.12	0.48
1:B:54:THR:HG22	1:B:169:ALA:HB2	1.95	0.48
2:C:65:VAL:HG21	2:C:103:LYS:HE3	1.95	0.48
7:H:24:DC:N3	7:H:25:DA:C6	2.81	0.48
3:D:1114:THR:OG1	3:D:1195:GLN:NE2	2.45	0.48
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.94	0.48
3:D:530:VAL:HG12	3:D:531:ASP:H	1.77	0.48
2:C:1031:ARG:NE	6:G:16:DG:OP1	2.36	0.48
2:C:777:ILE:HA	5:F:405:LEU:CD1	2.33	0.48
3:D:846:PRO:N	12:D:2115:HOH:O	2.47	0.48
2:C:1035:MET:SD	6:G:15:DT:H4'	2.53	0.48
3:D:1229:ILE:HG23	3:D:1356:TYR:OH	2.14	0.48
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.95	0.48
3:D:1128:VAL:HG23	3:D:1130:ARG:H	1.79	0.48
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.95	0.48
2:C:376:ARG:HD3	5:F:276:ARG:HD2	1.94	0.48
2:C:960:GLU:HB2	12:C:1303:HOH:O	2.11	0.48
5:F:361:LEU:HD11	5:F:408:LEU:CG	2.42	0.48
2:C:1102:LEU:HD11	3:D:9:ARG:HH11	1.78	0.48
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.96	0.48
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.95	0.48
2:C:767:PRO:O	2:C:769:PRO:HD3	2.14	0.47
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.95	0.47
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.47	0.47
3:D:1042:ARG:HG3	3:D:1045:MET:HE3	1.96	0.47
3:D:264:LEU:HB3	12:D:2116:HOH:O	2.13	0.47
2:C:540:PHE:HB3	2:C:544:THR:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:360:LYS:HD3	5:F:360:LYS:HA	1.63	0.47
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.96	0.47
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.36	0.47
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.97	0.47
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.96	0.47
1:A:109:VAL:HG22	12:A:404:HOH:O	2.13	0.47
2:C:976:ASP:OD1	2:C:978:ARG:HG3	2.15	0.47
2:C:405:ARG:NE	2:C:442:GLU:OE2	2.37	0.47
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.97	0.47
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.97	0.47
2:C:763:GLY:C	2:C:765:SER:N	2.68	0.47
2:C:1021:LEU:HD22	5:F:331:ASP:O	2.15	0.47
6:G:6:DA:N1	7:H:22:DT:C4	2.80	0.47
3:D:272:LEU:O	3:D:279:VAL:N	2.47	0.47
3:D:658:LEU:HD11	3:D:674[A]:ARG:HH11	1.80	0.47
3:D:207:PHE:HE2	5:F:98:GLU:HG2	1.79	0.47
2:C:1058:ASP:OD1	3:D:621:LYS:HE2	2.14	0.47
6:G:18:DA:H2"	6:G:19:DG:O5'	2.14	0.47
1:A:196:THR:HG21	2:C:934:PHE:CE2	2.47	0.47
3:D:683:ILE:HD11	3:D:688:TRP:CZ2	2.50	0.47
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.47	0.47
2:C:773:LEU:HD13	2:C:773:LEU:O	2.15	0.47
12:C:1315:HOH:O	3:D:1472:ILE:HG21	2.15	0.47
5:F:84:TYR:O	5:F:88:ILE:HG12	2.15	0.47
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.39	0.47
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.97	0.46
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.96	0.46
7:H:21:DA:C2'	7:H:22:DT:C5'	2.86	0.46
3:D:65:ARG:NE	5:F:379:ARG:HB3	2.30	0.46
2:C:880:MET:HE1	3:D:1242:HIS:CG	2.49	0.46
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.97	0.46
3:D:1088:THR:HG23	3:D:1238:MET:SD	2.56	0.46
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.96	0.46
3:D:1239:ARG:O	3:D:1241:PHE:CD1	2.68	0.46
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.48	0.46
3:D:737:ASN:ND2	3:D:1235:GLN:HE22	2.13	0.46
2:C:543:ASN:CB	12:C:1316:HOH:O	1.70	0.46
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.68	0.46
1:A:193:ASP:OD2	2:C:938:LYS:NZ	2.40	0.46
2:C:773:LEU:HD13	2:C:777:ILE:HG13	1.98	0.46
2:C:774:LEU:C	2:C:777:ILE:HD12	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:879:ARG:HD3	3:D:902:LEU:O	2.16	0.46
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.51	0.46
11:D:2006:2TM:H2	12:D:2123:HOH:O	2.16	0.45
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.97	0.45
2:C:299:LYS:HE2	2:C:299:LYS:HA	1.96	0.45
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	1.99	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.65	0.45
1:A:90:LEU:HB2	1:A:119:ASP:HB3	1.98	0.45
2:C:334:ARG:NH2	2:C:342:ASP:OD2	2.46	0.45
1:A:102:LYS:HB2	1:A:102:LYS:HE3	1.75	0.45
5:F:357:ALA:HA	5:F:360:LYS:HB2	1.99	0.45
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.98	0.45
1:A:100:LEU:HD22	1:A:141:GLU:HG2	1.98	0.45
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.17	0.45
3:D:41:ARG:HE	3:D:48:ARG:CZ	2.30	0.45
3:D:1091:SER:OG	3:D:1234:THR:CA	2.64	0.45
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.51	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.45
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.82	0.45
2:C:1118:LYS:HE2	3:D:20:SER:O	2.17	0.45
2:C:76:PRO:HG3	2:C:120:LEU:HD12	1.99	0.45
1:A:198:ARG:HD3	2:C:934:PHE:CE1	2.52	0.45
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.99	0.45
1:B:32:PHE:HA	1:B:35:THR:HB	1.98	0.45
2:C:41:ASN:O	2:C:46:ALA:HB2	2.17	0.45
3:D:353:VAL:HG11	3:D:387:LEU:HD11	1.98	0.45
2:C:764:GLU:O	2:C:766:GLU:CG	2.61	0.45
3:D:238:PRO:HG3	3:D:318:ARG:HB2	1.99	0.45
2:C:424:GLY:O	2:C:426:ASP:N	2.49	0.45
3:D:264:LEU:CB	12:D:2116:HOH:O	2.65	0.44
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.50	0.44
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.16	0.44
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.87	0.44
4:E:95:VAL:O	4:E:95:VAL:HG12	2.16	0.44
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.82	0.44
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.00	0.44
2:C:763:GLY:O	2:C:765:SER:N	2.51	0.44
2:C:422:ARG:HG2	7:H:15:DT:C6	2.52	0.44
5:F:362:SER:OG	5:F:365:GLU:HG2	2.18	0.44
3:D:1232:PRO:HB3	3:D:1361:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:LEU:HD13	2:C:372:LEU:HD21	2.00	0.44
5:F:109:GLY:O	5:F:113:ILE:HG13	2.17	0.44
3:D:717:GLN:NE2	12:D:2118:HOH:O	2.50	0.44
3:D:260:GLU:HB3	3:D:271:VAL:HB	2.00	0.44
2:C:1001:VAL:HG12	12:C:1317:HOH:O	2.17	0.44
2:C:422:ARG:HG2	7:H:15:DT:OP2	2.18	0.44
3:D:67:ARG:HG3	5:F:377:ASP:O	2.18	0.44
7:H:15:DT:H2''	7:H:16:DC:H5'	1.99	0.44
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.99	0.44
3:D:265:GLU:N	12:D:2116:HOH:O	2.51	0.44
3:D:84:ILE:O	3:D:87:ARG:HG2	2.18	0.44
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.99	0.44
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.17	0.44
3:D:1176:LYS:HE2	3:D:1176:LYS:HB3	1.79	0.44
3:D:1211:MET:HE3	3:D:1211:MET:HB2	1.89	0.44
8:C:1201:ATP:H5'1	12:D:2123:HOH:O	2.16	0.44
1:A:31:GLY:CA	12:A:403:HOH:O	2.64	0.44
2:C:1095:LEU:O	3:D:101:HIS:NE2	2.39	0.44
3:D:135:LEU:O	3:D:453:ASP:HB3	2.18	0.44
2:C:324:ASP:HB3	2:C:327:HIS:HB2	2.00	0.44
4:E:14:ASP:OD2	4:E:18:ARG:NH1	2.50	0.44
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.53	0.43
3:D:1487:VAL:HG11	3:D:1492:LEU:HD13	2.00	0.43
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.43
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.00	0.43
2:C:194:VAL:HA	2:C:197:LEU:HD12	2.00	0.43
2:C:768:THR:HB	2:C:770:GLU:HB2	2.01	0.43
1:A:159:LYS:HE3	1:A:164:ALA:O	2.17	0.43
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.00	0.43
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.53	0.43
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.73	0.43
2:C:101:ILE:HG12	2:C:108:ILE:HG12	2.01	0.43
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.00	0.43
2:C:154:ARG:H	2:C:154:ARG:HG2	1.68	0.43
3:D:410:SER:H	5:F:164:LYS:NZ	2.16	0.43
3:D:796:ARG:NH1	3:D:862:ASP:OD2	2.47	0.43
2:C:97:ARG:HG2	2:C:112:GLU:HB2	2.00	0.43
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.00	0.43
2:C:1009:SER:O	3:D:624:ASP:HB3	2.19	0.43
2:C:996:LYS:CG	12:C:1321:HOH:O	2.29	0.43
5:F:355:GLU:HA	5:F:358:LEU:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:526:PRO:N	12:D:2119:HOH:O	2.51	0.43
3:D:1263:PHE:CD2	3:D:1375:MET:HE2	2.48	0.43
1:B:94:LEU:HD11	1:B:97:VAL:HG22	2.01	0.43
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.53	0.43
2:C:642:ARG:HA	2:C:642:ARG:HD3	1.87	0.43
2:C:773:LEU:HD23	5:F:373:LYS:HB3	1.91	0.43
7:H:23:DG:H2"	7:H:24:DC:C6	2.53	0.43
3:D:1086:LEU:HD12	3:D:1086:LEU:N	2.33	0.42
3:D:103:TRP:HB3	3:D:1448:THR:HG21	2.01	0.42
3:D:81:THR:OG1	3:D:82:LYS:N	2.52	0.42
4:E:37:ASN:N	4:E:37:ASN:OD1	2.44	0.42
2:C:562:SER:CA	12:C:1316:HOH:O	2.63	0.42
3:D:1255:GLY:HA2	3:D:1355:VAL:HG13	2.01	0.42
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.54	0.42
3:D:12:LEU:HA	3:D:12:LEU:HD23	1.85	0.42
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.19	0.42
4:E:68:LEU:HA	4:E:68:LEU:HD12	1.77	0.42
3:D:1254:GLN:O	3:D:1257:PRO:HB2	2.19	0.42
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.19	0.42
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.50	0.42
3:D:560:GLN:HE22	5:F:222:ARG:HH12	1.68	0.42
3:D:795:VAL:HG12	3:D:876:SER:HB3	2.00	0.42
2:C:1091:GLU:OE2	3:D:606:ILE:HG21	2.19	0.42
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.84	0.42
5:F:355:GLU:O	5:F:356:LYS:C	2.58	0.42
2:C:878:SER:N	12:C:1301:HOH:O	2.44	0.42
2:C:218:VAL:O	2:C:222:MET:HG2	2.19	0.42
3:D:131:LYS:NZ	3:D:154:THR:HG22	2.34	0.42
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.52	0.42
3:D:706:PRO:HG3	6:G:14:DG:H21	1.84	0.42
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.92	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.88	0.42
2:C:624:PRO:CA	12:C:1313:HOH:O	2.68	0.42
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.54	0.42
3:D:838:ARG:HD3	3:D:874:GLU:OE1	2.20	0.42
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.80	0.42
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.55	0.42
2:C:954:THR:HA	2:C:955:PRO:HD3	1.91	0.42
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.42
5:F:355:GLU:HA	5:F:358:LEU:HB2	2.02	0.42
1:A:133:GLU:HG2	1:A:134:GLU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.54	0.42
2:C:545:ASN:HB3	2:C:583:LEU:HD22	2.02	0.41
3:D:1117:TYR:HB2	3:D:1188:VAL:O	2.20	0.41
3:D:801:GLY:HA3	3:D:821:VAL:HG13	2.01	0.41
2:C:768:THR:OG1	2:C:771:GLU:HG3	2.20	0.41
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.41
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.01	0.41
3:D:1253:THR:O	3:D:1257:PRO:CD	2.68	0.41
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.95	0.41
1:B:83:LYS:HE2	1:B:168:ASP:HB2	2.02	0.41
3:D:185:VAL:N	3:D:201:GLY:O	2.45	0.41
3:D:176:ASP:OD1	3:D:177:ALA:N	2.44	0.41
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.20	0.41
3:D:455:ARG:HB2	3:D:460:ALA:HB2	2.02	0.41
2:C:486:MET:HB3	2:C:490:GLU:HB3	2.01	0.41
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	0.41
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.02	0.41
3:D:760:ARG:O	3:D:764:LEU:HB2	2.21	0.41
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.84	0.41
5:F:358:LEU:HD11	5:F:370:LYS:NZ	1.97	0.41
2:C:771:GLU:HB3	2:C:775:ARG:HH21	1.83	0.41
3:D:66:GLN:C	3:D:68:PHE:N	2.73	0.41
5:F:321:ILE:O	5:F:327:SER:HB3	2.20	0.41
2:C:765:SER:O	2:C:767:PRO:HD3	2.21	0.41
6:G:5:DC:H1'	6:G:6:DA:H8	1.85	0.41
3:D:68:PHE:O	3:D:80:VAL:HG21	2.19	0.41
1:B:56:VAL:HG21	1:B:82:LEU:HD13	2.02	0.41
5:F:88:ILE:CG2	5:F:193:ARG:HG2	2.50	0.41
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.96	0.41
3:D:106:LYS:HD2	3:D:106:LYS:HA	1.75	0.41
3:D:704:ARG:HB2	3:D:745:MET:HG2	2.03	0.41
3:D:538:SER:HB3	12:D:2119:HOH:O	2.03	0.41
2:C:1102:LEU:HD11	3:D:9:ARG:HB2	2.03	0.41
2:C:408:ARG:NH1	2:C:456:ALA:O	2.53	0.41
3:D:707:THR:HG23	3:D:712:GLY:HA3	2.01	0.41
2:C:571:LEU:HD23	2:C:702:SER:HB3	2.03	0.41
2:C:773:LEU:C	2:C:773:LEU:CD1	2.89	0.41
3:D:525:ARG:C	12:D:2119:HOH:O	2.59	0.41
3:D:675:ARG:HH22	5:F:420:ASP:HB3	1.85	0.41
3:D:192:ALA:HB1	3:D:193:PRO:HD2	2.02	0.41
2:C:749:VAL:HB	2:C:792:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:171:LEU:HD11	3:D:393:ILE:HD11	2.03	0.41
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.03	0.41
1:B:124:ASN:N	1:B:124:ASN:OD1	2.53	0.41
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.56	0.41
3:D:843:PHE:HE1	3:D:864:VAL:HG21	1.86	0.41
2:C:946:ARG:HG3	12:C:1320:HOH:O	2.20	0.41
2:C:773:LEU:HD13	2:C:777:ILE:CG1	2.51	0.41
1:A:109:VAL:CG2	12:A:404:HOH:O	2.69	0.41
3:D:613:ARG:HG3	3:D:618:LEU:HD22	2.03	0.41
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.85	0.41
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.93	0.40
7:H:21:DA:H1'	7:H:22:DT:C5'	2.51	0.40
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.35	0.40
3:D:226:PRO:HD3	3:D:249:TYR:CE2	2.56	0.40
3:D:517:VAL:HA	3:D:518:PRO:HD3	1.95	0.40
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.55	0.40
5:F:162:LYS:O	5:F:165:SER:OG	2.34	0.40
2:C:848:VAL:HB	3:D:740:PHE:O	2.21	0.40
2:C:1104:GLU:HA	3:D:7:LYS:HE3	2.03	0.40
2:C:773:LEU:HD22	5:F:373:LYS:CD	2.42	0.40
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.21	0.40
6:G:15:DT:H2'	6:G:16:DG:H8	1.87	0.40
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.51	0.40
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.53	0.40
3:D:784:ASP:HB2	3:D:939:PHE:CE2	2.56	0.40
3:D:403:PHE:CD2	3:D:444:VAL:HG23	2.57	0.40
2:C:1097:LEU:HD11	3:D:103:TRP:HZ3	1.86	0.40
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.57	0.40
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.57	0.40
2:C:858:MET:HG2	2:C:867:VAL:O	2.22	0.40
3:D:907:GLU:HB2	3:D:1026:SER:HA	2.03	0.40
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.57	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:306:GLU:OE1	7:H:1:DT:O5'[4_745]	1.70	0.50
2:C:318:PRO:CB	4:E:87:LYS:CG[1_545]	1.77	0.43
3:D:34:TYR:OH	3:D:327:GLU:OE1[4_755]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:328:GLY:O	5:F:303:ARG:NH2[4_745]	2.11	0.09
2:C:37:GLU:OE1	3:D:1151:ARG:NH1[3_545]	2.12	0.08
2:C:49:ARG:NH2	5:F:390:PHE:O[1_545]	2.18	0.02

## 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	229/315 (73%)	226 (99%)	3 (1%)	0	100	100
1	B	225/315 (71%)	222 (99%)	3 (1%)	0	100	100
2	C	1108/1119 (99%)	1076 (97%)	26 (2%)	6 (0%)	34	71
3	D	1491/1524 (98%)	1454 (98%)	33 (2%)	4 (0%)	46	79
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/423 (81%)	336 (98%)	7 (2%)	1 (0%)	46	79
All	All	3489/3795 (92%)	3403 (98%)	75 (2%)	11 (0%)	46	79

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	425	PHE
2	C	765	SER
2	C	769	PRO
3	D	1240	THR
2	C	779	GLY
3	D	66	GLN
5	F	360	LYS
2	C	763	GLY
3	D	1253	THR
2	C	768	THR
3	D	1257	PRO

### 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	200/273 (73%)	196 (98%)	4 (2%)	63	88
1	B	200/273 (73%)	196 (98%)	4 (2%)	63	88
2	C	936/941 (100%)	907 (97%)	29 (3%)	47	82
3	D	1260/1279 (98%)	1229 (98%)	31 (2%)	55	85
4	E	83/88 (94%)	83 (100%)	0	100	100
5	F	301/371 (81%)	296 (98%)	5 (2%)	68	91
All	All	2980/3225 (92%)	2907 (98%)	73 (2%)	55	86

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	66	SER
1	A	96	THR
1	A	219	ARG
1	B	7	LYS
1	B	14	ARG
1	B	91	ASN
1	B	154	GLU
2	C	81	ASP
2	C	141	HIS
2	C	194	VAL
2	C	219	GLN
2	C	285	LEU
2	C	299	LYS
2	C	360	LEU
2	C	397	GLU
2	C	405	ARG
2	C	464	LEU
2	C	513	VAL
2	C	557	ARG
2	C	595	LEU
2	C	610	ARG

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Mol	Chain	Res	Type
2	C	617	ASP
2	C	640	ARG
2	C	698	ASP
2	C	728	HIS
2	C	729	LEU
2	C	765	SER
2	C	767	PRO
2	C	768	THR
2	C	769	PRO
2	C	773	LEU
2	C	775	ARG
2	C	778	PHE
2	C	784	ASP
2	C	848	VAL
2	C	1078	GLU
3	D	66	GLN
3	D	67	ARG
3	D	87	ARG
3	D	134	VAL
3	D	276	ASP
3	D	354	VAL
3	D	406	ASP
3	D	415	VAL
3	D	420	VAL
3	D	530	VAL
3	D	618	LEU
3	D	632	VAL
3	D	683	ILE
3	D	709	HIS
3	D	754	PHE
3	D	784	ASP
3	D	907	GLU
3	D	1083	ASP
3	D	1084	THR
3	D	1236	LEU
3	D	1237	THR
3	D	1238	MET
3	D	1243	THR
3	D	1252	ILE
3	D	1254	GLN
3	D	1256	LEU
3	D	1288	GLU

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Mol	Chain	Res	Type
3	D	1307	LYS
3	D	1433	SER
3	D	1455	LYS
3	D	1488	ASP
5	F	95	THR
5	F	141	VAL
5	F	279	GLN
5	F	356	LYS
5	F	369	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
2	C	390	GLN
2	C	434	HIS
2	C	506	ASN
2	C	565	GLN
2	C	670	GLN
2	C	728	HIS
2	C	860	HIS
3	D	316	GLN
3	D	560	GLN
3	D	669	ASN
3	D	717	GLN
3	D	737	ASN
3	D	768	ASN
3	D	855	HIS
3	D	976	GLN
3	D	1124	GLN
3	D	1195	GLN
3	D	1242	HIS
3	D	1254	GLN
3	D	1441	GLN
5	F	83	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	ATP	C	1201	10	24,33,33	0.99	2 (8%)	31,52,52	2.49	4 (12%)
11	2TM	D	2006	-	22,30,30	2.31	8 (36%)	30,47,47	2.24	11 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ATP	C	1201	10	-	0/18/38/38	0/3/3/3
11	2TM	D	2006	-	-	0/15/38/38	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2006	2TM	C6-N1	-4.25	1.29	1.35
11	D	2006	2TM	PB-O1B	-3.94	1.46	1.56
11	D	2006	2TM	C5-C4	-3.60	1.32	1.40
11	D	2006	2TM	PA-O2A	-3.39	1.48	1.56
11	D	2006	2TM	C4-N3	-2.87	1.30	1.35
11	D	2006	2TM	O4'-C4'	-2.34	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2006	2TM	O4'-C1'	-2.14	1.38	1.41
8	C	1201	ATP	O4'-C1'	2.01	1.43	1.41
8	C	1201	ATP	C5-C4	2.84	1.46	1.40
11	D	2006	2TM	PB-O3B	4.30	1.63	1.58

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1201	ATP	C2'-C1'-N9	-10.80	97.79	114.29
8	C	1201	ATP	N3-C2-N1	-6.41	123.99	128.89
11	D	2006	2TM	O5'-PA-O1A	-4.89	100.97	113.98
11	D	2006	2TM	C6-N1-C2	-3.19	116.11	121.28
11	D	2006	2TM	O5'-PA-C1	-2.58	97.21	104.42
8	C	1201	ATP	PB-O3B-PG	-2.17	125.38	132.67
11	D	2006	2TM	C5-C4-N4	-2.10	118.09	121.31
8	C	1201	ATP	N6-C6-N1	2.11	123.73	119.20
11	D	2006	2TM	O2B-PB-C1	2.28	114.76	109.02
11	D	2006	2TM	O2A-PA-C1	2.36	117.16	106.88
11	D	2006	2TM	N4-C4-N3	2.77	121.55	116.50
11	D	2006	2TM	C2-N3-C4	3.41	120.43	115.61
11	D	2006	2TM	O1B-PB-O2B	3.84	122.18	110.12
11	D	2006	2TM	O4'-C1'-N1	4.38	117.33	108.08
11	D	2006	2TM	O3G-PG-O1G	4.66	125.58	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1201	ATP	2	0
11	D	2006	2TM	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	0.45	13 (5%) 28 21	36, 68, 92, 101	0
1	B	227/315 (72%)	0.45	13 (5%) 27 21	41, 69, 100, 122	0
2	C	1112/1119 (99%)	0.50	75 (6%) 21 15	25, 58, 115, 135	0
3	D	1494/1524 (98%)	0.61	140 (9%) 11 6	19, 58, 122, 214	0
4	E	94/99 (94%)	0.55	7 (7%) 17 11	34, 73, 111, 114	0
5	F	346/423 (81%)	0.95	60 (17%) 2 1	43, 79, 152, 176	0
6	G	18/22 (81%)	0.24	1 (5%) 28 21	55, 81, 139, 140	0
7	H	25/27 (92%)	0.46	3 (12%) 6 3	70, 100, 149, 169	0
All	All	3547/3844 (92%)	0.58	312 (8%) 12 8	19, 64, 124, 214	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	173	PRO	9.0
2	C	311	PHE	7.7
2	C	300	ASP	7.6
2	C	207	LEU	7.1
3	D	211	VAL	7.0
5	F	149	GLU	7.0
3	D	427	VAL	6.9
5	F	373	LYS	6.5
5	F	150	THR	6.4
3	D	1499	ARG	6.3
5	F	381	HIS	6.2
2	C	107	LEU	6.1
3	D	241	ILE	6.1
5	F	386	VAL	6.0
3	D	1297	GLU	5.9
5	F	375	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
3	D	322	VAL	5.7
3	D	324	ALA	5.4
1	B	2	LEU	5.4
5	F	382	THR	5.3
1	A	231	ALA	5.3
3	D	1127	GLU	5.3
3	D	1298	GLY	5.2
2	C	365	ASP	5.2
3	D	1500	LYS	5.1
3	D	267	GLY	5.1
5	F	146	GLY	5.1
3	D	1305	LEU	5.1
3	D	976	GLN	5.0
5	F	369	LEU	4.9
2	C	219	GLN	4.9
3	D	977	ALA	4.8
3	D	203	ALA	4.8
2	C	64	LEU	4.7
5	F	423	ASP	4.6
4	E	85	LEU	4.6
3	D	268	ALA	4.6
5	F	145	PRO	4.6
5	F	356	LYS	4.6
3	D	1495	ILE	4.6
5	F	414	ARG	4.5
3	D	821	VAL	4.5
3	D	1497	GLU	4.5
2	C	769	PRO	4.4
5	F	376	ILE	4.4
5	F	151	LEU	4.4
5	F	359	SER	4.4
3	D	422	ALA	4.4
2	C	811	PRO	4.4
5	F	147	LEU	4.4
2	C	629	TYR	4.4
2	C	104	ASP	4.3
3	D	1299	PHE	4.3
5	F	388	ALA	4.3
3	D	339	TRP	4.3
3	D	368	VAL	4.3
3	D	195	VAL	4.2
1	A	94	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
3	D	202	VAL	4.2
3	D	393	ILE	4.1
5	F	143	HIS	4.1
3	D	310	LEU	4.1
2	C	208	ALA	4.0
2	C	766	GLU	4.0
2	C	296	GLY	4.0
1	A	230	ALA	4.0
3	D	1319	VAL	4.0
2	C	217	LEU	4.0
5	F	385	GLU	4.0
5	F	349	LEU	3.9
3	D	830	ALA	3.9
3	D	983	LEU	3.9
3	D	982	PHE	3.9
5	F	415	THR	3.9
3	D	191	LEU	3.9
5	F	392	VAL	3.8
2	C	299	LYS	3.8
2	C	729	LEU	3.8
1	A	97	VAL	3.8
3	D	974	ILE	3.7
2	C	307	LEU	3.7
5	F	127	ILE	3.7
7	H	24	DC	3.7
5	F	390	PHE	3.7
3	D	428	LYS	3.7
3	D	1490	LYS	3.7
2	C	763	GLY	3.6
3	D	335	LEU	3.5
3	D	488	ARG	3.5
3	D	666	ILE	3.5
3	D	174	GLY	3.5
3	D	973	GLN	3.5
3	D	345	TYR	3.5
3	D	1313	VAL	3.5
3	D	387	LEU	3.5
3	D	1300	SER	3.5
3	D	367	ILE	3.5
3	D	378	ILE	3.4
5	F	377	ASP	3.4
3	D	212	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	281	LEU	3.4
2	C	226	VAL	3.4
5	F	383	LEU	3.4
2	C	174	LEU	3.3
2	C	242	LEU	3.3
3	D	213	VAL	3.3
3	D	1058	ARG	3.3
5	F	361	LEU	3.3
2	C	52	PHE	3.3
2	C	778	PHE	3.3
3	D	1306	PRO	3.3
3	D	667	ALA	3.3
5	F	410	TYR	3.3
3	D	1242	HIS	3.3
3	D	674[A]	ARG	3.2
5	F	173	TYR	3.2
1	B	122	ILE	3.2
2	C	102	HIS	3.2
2	C	159	ILE	3.1
1	B	3	ASP	3.1
3	D	831	GLY	3.1
2	C	315	ALA	3.1
3	D	410	SER	3.1
5	F	421	PHE	3.1
3	D	1283	ILE	3.1
3	D	1405	GLU	3.1
2	C	189	ARG	3.1
2	C	200	LEU	3.1
2	C	228	ALA	3.1
3	D	1287	GLU	3.1
5	F	397	ILE	3.1
3	D	374	GLU	3.0
1	B	118	ALA	3.0
3	D	409	VAL	3.0
2	C	304	LEU	3.0
2	C	511	GLU	3.0
3	D	1491	THR	3.0
7	H	23	DG	3.0
1	B	120	VAL	3.0
5	F	345	ALA	3.0
2	C	275	TYR	3.0
3	D	377	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	298	PHE	3.0
4	E	89	MET	3.0
3	D	373	PRO	2.9
5	F	153	PRO	2.9
7	H	25	DA	2.9
1	B	82	LEU	2.9
3	D	320	ALA	2.9
5	F	413	SER	2.9
5	F	391	GLY	2.9
1	A	100	LEU	2.9
3	D	807	ALA	2.9
4	E	32	ARG	2.9
3	D	205	TYR	2.9
1	B	6	LEU	2.9
1	A	99	LEU	2.8
3	D	142	LEU	2.8
3	D	1130	ARG	2.8
3	D	336	PHE	2.8
3	D	316	GLN	2.8
5	F	310	ILE	2.8
5	F	393	THR	2.8
3	D	269	PHE	2.7
3	D	340	THR	2.7
2	C	775	ARG	2.7
3	D	144	GLY	2.7
1	A	233	VAL	2.7
3	D	969	ARG	2.7
3	D	1327	ARG	2.7
3	D	217	LYS	2.7
3	D	531	ASP	2.7
1	A	142	VAL	2.7
2	C	762	LYS	2.7
2	C	617	ASP	2.7
3	D	833	GLU	2.6
3	D	1054	GLU	2.6
3	D	687	VAL	2.6
2	C	196	LEU	2.6
3	D	135	LEU	2.6
3	D	337	LEU	2.6
3	D	805	GLU	2.6
2	C	100	LEU	2.6
3	D	1128	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	138	LEU	2.5
3	D	240	GLU	2.5
5	F	342	VAL	2.5
2	C	297	GLU	2.5
2	C	1070	ILE	2.5
3	D	1239	ARG	2.5
3	D	338	GLU	2.5
3	D	1277	ILE	2.5
5	F	419	ARG	2.5
2	C	41	ASN	2.5
3	D	270	LEU	2.5
2	C	227	PHE	2.5
3	D	143	ASN	2.5
3	D	216	VAL	2.5
3	D	1408	ILE	2.5
2	C	105	THR	2.5
3	D	1292	VAL	2.5
5	F	136	LEU	2.5
5	F	346	THR	2.5
3	D	54	LYS	2.5
1	A	62	LEU	2.5
3	D	70	GLY	2.5
5	F	93	LEU	2.5
3	D	198	ARG	2.5
3	D	350	HIS	2.5
5	F	379	ARG	2.4
1	A	115	LEU	2.4
4	E	51	LEU	2.4
3	D	189	GLN	2.4
2	C	185	LYS	2.4
1	A	234	ALA	2.4
3	D	239	GLY	2.4
3	D	1325	LEU	2.4
2	C	764	GLU	2.4
5	F	411	HIS	2.4
3	D	161	LEU	2.4
3	D	470	LEU	2.4
3	D	1238	MET	2.4
1	B	111	ALA	2.4
5	F	159	ILE	2.4
1	B	119	ASP	2.4
5	F	422	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	463	GLN	2.3
3	D	452	ILE	2.3
3	D	484	PRO	2.3
2	C	1040	LEU	2.3
3	D	225	LEU	2.3
3	D	980	MET	2.3
5	F	420	ASP	2.3
4	E	79	LEU	2.3
3	D	1174	LEU	2.3
5	F	125	ASP	2.3
3	D	1133	ARG	2.3
3	D	1304	LYS	2.3
3	D	219	GLU	2.3
3	D	321	GLN	2.3
4	E	54	LEU	2.3
3	D	1275	SER	2.3
5	F	401	GLU	2.3
2	C	422	ARG	2.3
1	A	232	ALA	2.3
3	D	401	TYR	2.3
5	F	138	SER	2.3
2	C	1	MET	2.3
3	D	343	LYS	2.3
5	F	148	LYS	2.2
3	D	304	LEU	2.2
3	D	1129	THR	2.2
1	B	89	PHE	2.2
6	G	3	DT	2.2
2	C	757	GLY	2.2
3	D	394	LEU	2.2
5	F	96	LEU	2.2
5	F	352	GLU	2.2
3	D	426	LYS	2.2
2	C	147	TYR	2.2
3	D	80	VAL	2.2
2	C	351	LEU	2.2
3	D	380	GLU	2.2
2	C	975	TYR	2.2
3	D	676	MET	2.2
2	C	739	GLU	2.2
3	D	242	LEU	2.2
3	D	804	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	490	ALA	2.2
3	D	1225	ALA	2.2
3	D	152	LEU	2.2
2	C	21	ILE	2.2
2	C	66	LEU	2.2
4	E	87	LYS	2.1
2	C	176	VAL	2.1
5	F	400	ILE	2.1
2	C	202	TYR	2.1
2	C	63	GLY	2.1
2	C	183	SER	2.1
3	D	314	PRO	2.1
2	C	99	GLN	2.1
2	C	153	ALA	2.1
2	C	157	ARG	2.1
2	C	367	LEU	2.1
5	F	229	TYR	2.1
2	C	254	VAL	2.1
2	C	188	LYS	2.1
2	C	361	MET	2.1
3	D	1281	VAL	2.1
2	C	245	GLY	2.1
2	C	295	ASP	2.1
2	C	375	SER	2.1
3	D	1273	VAL	2.1
1	B	189	ARG	2.1
3	D	194	GLY	2.0
3	D	1318	TYR	2.0
2	C	372	LEU	2.0
5	F	389	PHE	2.0
3	D	308	LYS	2.0
1	A	16	GLN	2.0
3	D	282	TYR	2.0
3	D	432	TYR	2.0
2	C	649	VAL	2.0
3	D	1044	LEU	2.0
2	C	205	GLU	2.0
5	F	380	GLU	2.0
3	D	1156	LEU	2.0
5	F	122	LEU	2.0
1	B	11	PHE	2.0
5	F	289	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	368	THR	2.0
3	D	317	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
10	MG	D	2005	1/1	0.96	0.32	1.65	45,45,45,45	0
8	ATP	C	1201	31/31	0.88	0.19	-0.78	38,47,75,83	0
11	2TM	D	2006	29/29	0.84	0.19	-0.85	38,51,69,94	0
9	ZN	D	2001	1/1	0.97	0.17	-1.80	38,38,38,38	0
9	ZN	D	2002	1/1	0.97	0.02	-2.17	59,59,59,59	0
10	MG	D	2003	1/1	0.95	0.26	-	38,38,38,38	0
10	MG	D	2004	1/1	0.40	0.66	-	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.