



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:55 AM UTC

PDB ID : 4Q4Z / pdb_00004q4z
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

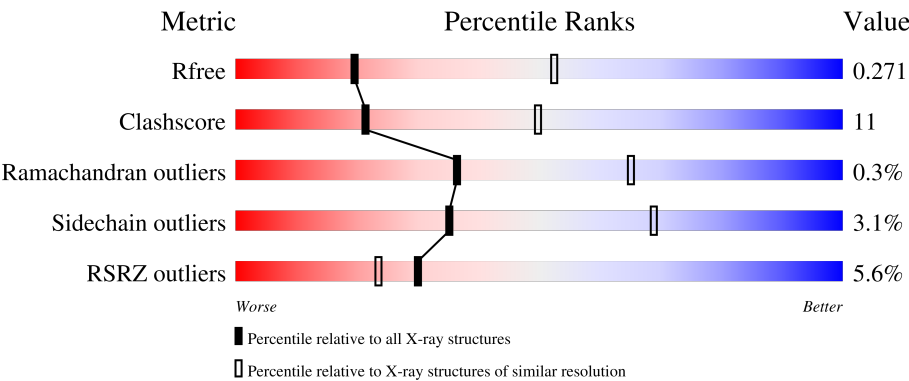
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 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.



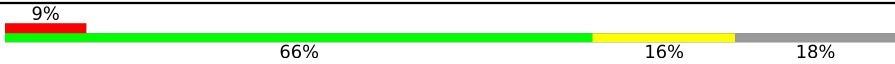
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	3% 58% 15% • 27%
1	B	315	3% 58% 14% 28%
2	C	1119	5% 78% 20% ••
3	D	1524	5% 75% 21% ••
4	E	99	4% 80% 14% • 5%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MG	D	2004	-	-	-	X

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			

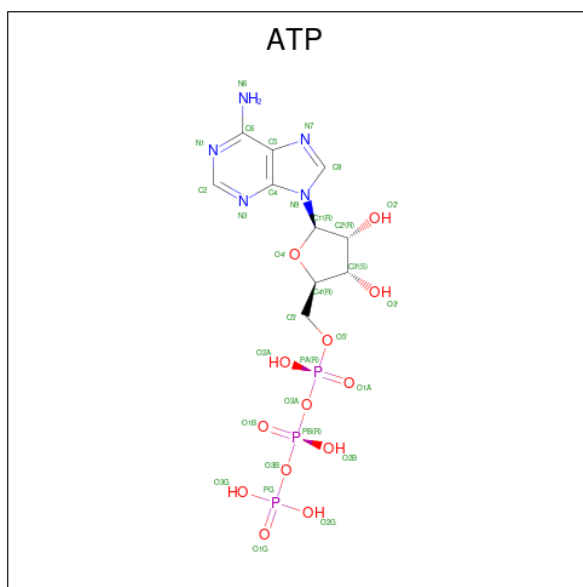
- Molecule 6 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*GP*CP*AP*GP*CP*CP*A)-3').

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	C	N	O	P	0	0	0
			516	246	99	147	24			

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

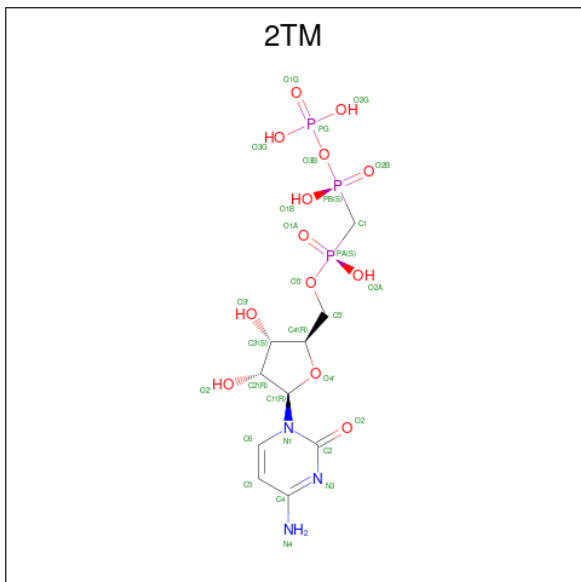
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 11 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (CCD ID: 2TM) (formula: C₁₀H₁₈N₃O₁₃P₃).



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

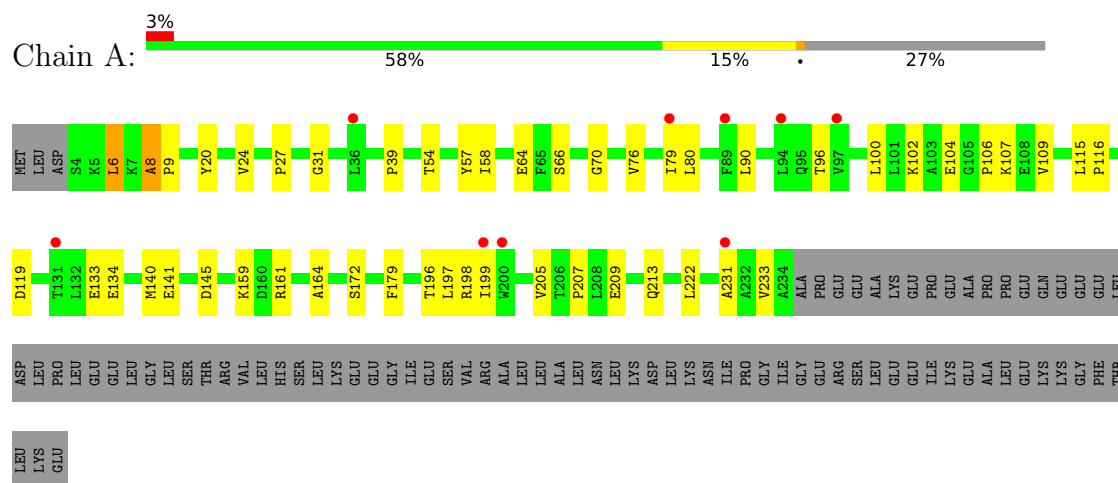
- Molecule 12 is water.

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

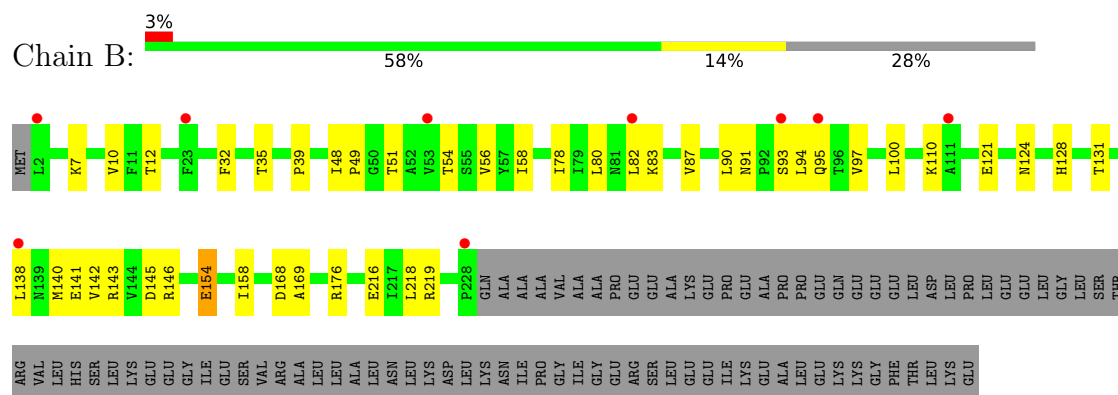
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

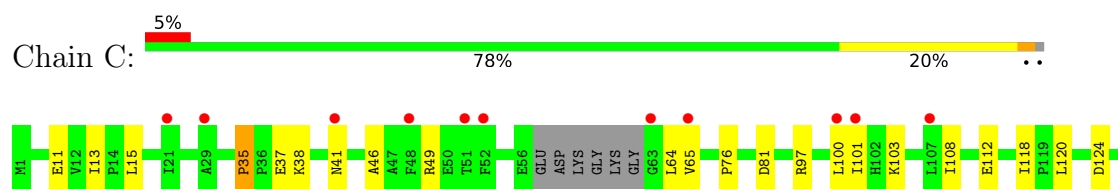
- Molecule 1: DNA-directed RNA polymerase subunit alpha

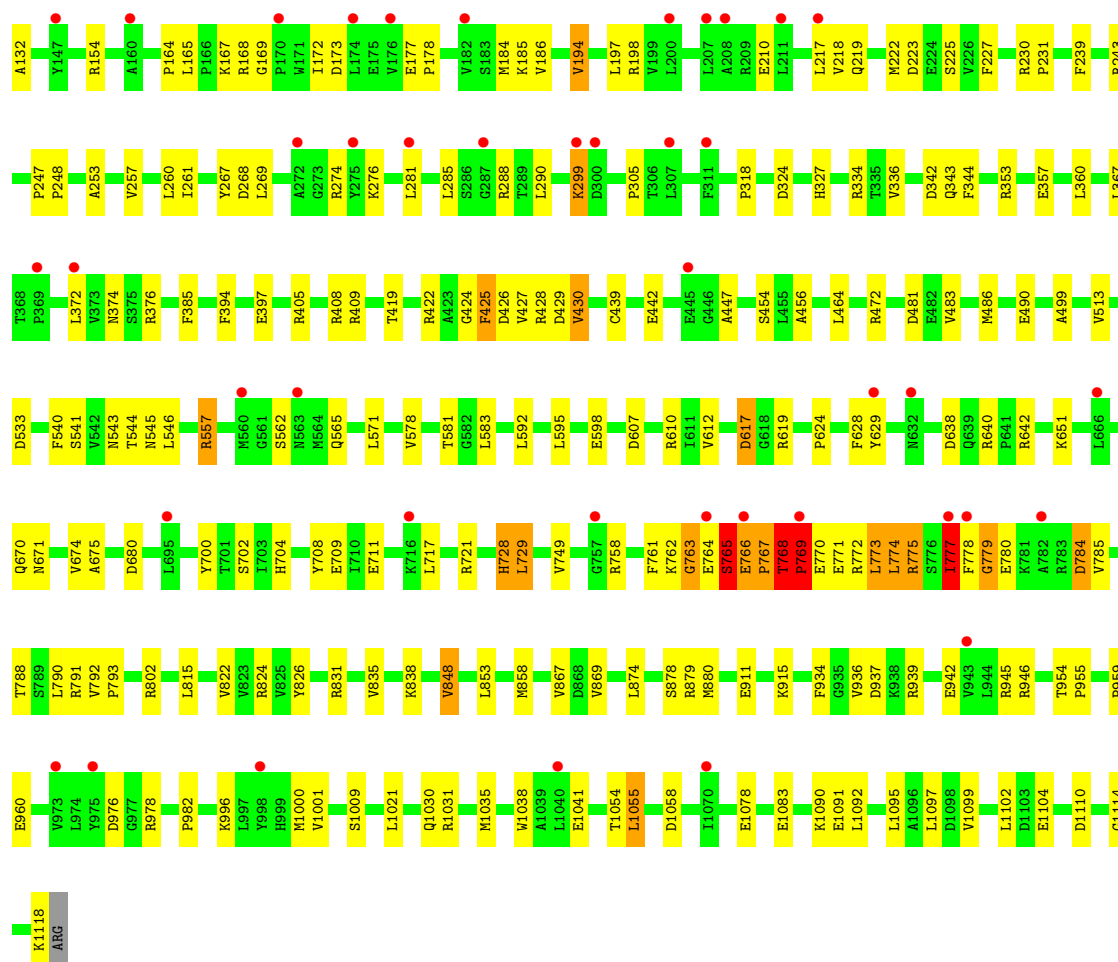


- Molecule 1: DNA-directed RNA polymerase subunit alpha

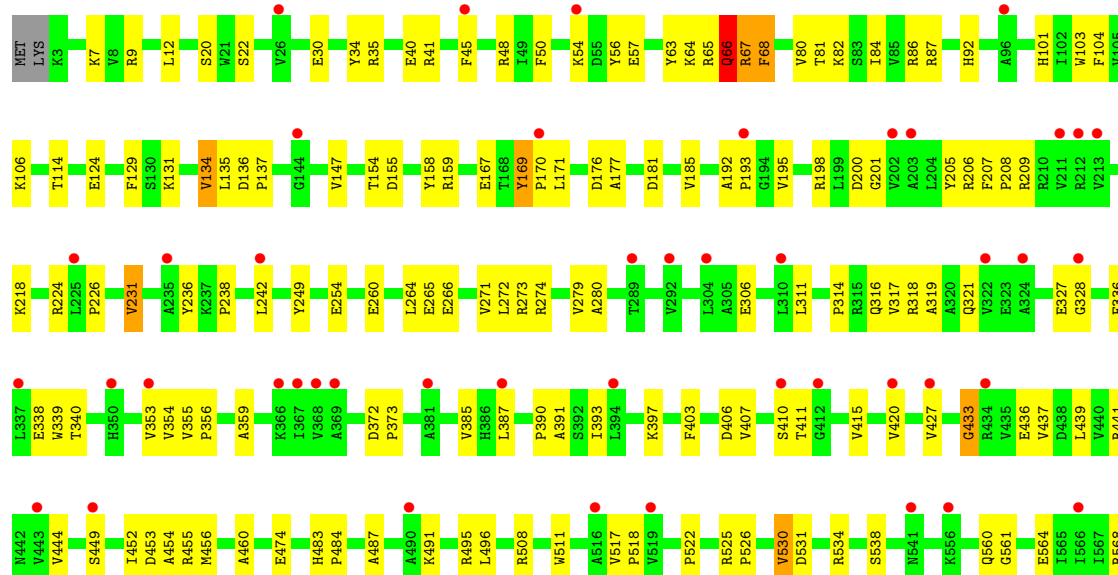
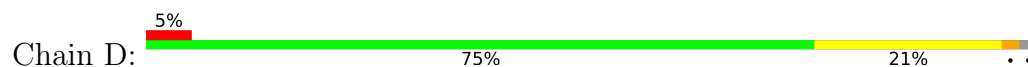


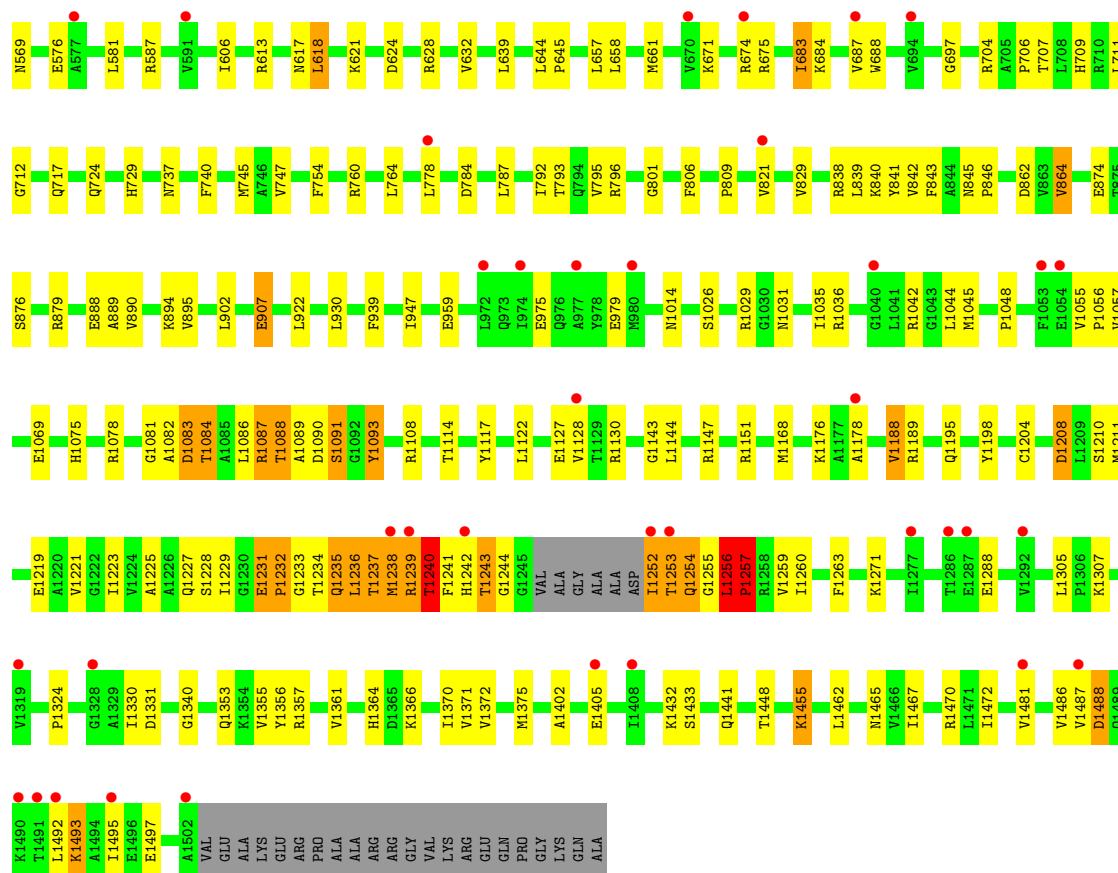
- Molecule 2: DNA-directed RNA polymerase subunit beta



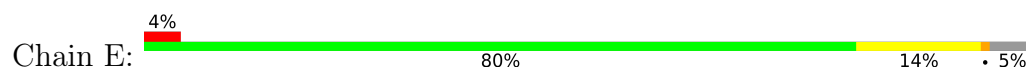


• Molecule 3: DNA-directed RNA polymerase subunit beta'

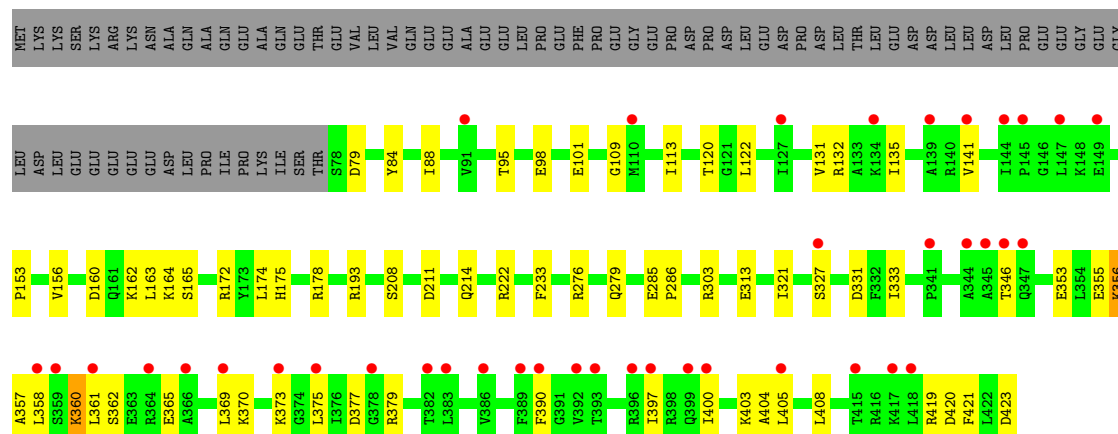




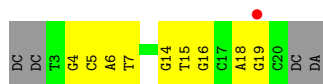
• Molecule 4: DNA-directed RNA polymerase subunit omega



• 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, α , β , γ	184.49Å 102.16Å 294.72Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	29.78 – 2.90 29.78 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.5 (29.78-2.90) 85.7 (29.78-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.256 , 0.275 0.256 , 0.271	Depositor DCC
R_{free} test set	1753 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	28755	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ZN, 2TM

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	0.31	0/1841	0.81	4/2504 (0.2%)
1	B	0.29	0/1821	0.79	0/2476
2	C	0.40	3/8941 (0.0%)	0.81	15/12092 (0.1%)
3	D	0.48	6/12019 (0.0%)	0.83	24/16248 (0.1%)
4	E	0.29	0/775	0.70	0/1045
5	F	0.30	0/2852	0.74	3/3837 (0.1%)
6	G	0.46	0/414	0.82	0/637
7	H	0.29	0/580	0.74	0/895
All	All	0.41	9/29243 (0.0%)	0.81	46/39734 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1093	TYR	C-O	-7.60	1.15	1.24
3	D	1091	SER	CA-C	-6.45	1.44	1.52
3	D	1231	GLU	CA-C	-6.31	1.45	1.52
3	D	1231	GLU	N-CA	-5.84	1.42	1.46
3	D	1090	ASP	C-O	-5.59	1.17	1.24
2	C	769	PRO	N-CD	5.50	1.55	1.47
2	C	430	VAL	C-O	-5.16	1.18	1.24
2	C	429	ASP	C-O	-5.10	1.17	1.24
3	D	1088	THR	CA-C	-5.08	1.46	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	761	PHE	O-C-N	-13.71	106.01	122.87
2	C	761	PHE	CA-C-N	12.57	139.47	121.50
2	C	761	PHE	C-N-CA	12.57	139.47	121.50
3	D	1257	PRO	CA-N-CD	-8.77	99.72	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1232	PRO	CA-N-CD	-7.94	100.88	112.00
2	C	777	ILE	CB-CA-C	-7.92	101.84	111.97
2	C	765	SER	N-CA-C	-6.92	96.06	110.80
3	D	1231	GLU	CA-C-N	-6.67	111.50	119.84
3	D	1231	GLU	C-N-CA	-6.67	111.50	119.84
3	D	1231	GLU	O-C-N	6.45	125.47	120.38
3	D	68	PHE	N-CA-C	-6.41	97.76	109.56
3	D	1208	ASP	N-CA-C	-6.27	99.66	109.25
1	A	8	ALA	CA-C-N	6.14	126.65	120.14
1	A	8	ALA	C-N-CA	6.14	126.65	120.14
3	D	433	GLY	N-CA-C	6.14	119.46	110.80
2	C	169	GLY	CA-C-N	6.06	125.97	119.85
2	C	169	GLY	C-N-CA	6.06	125.97	119.85
3	D	1240	THR	N-CA-C	5.87	123.29	110.80
2	C	772	ARG	N-CA-C	-5.77	104.90	111.07
1	A	172	SER	CA-C-N	5.76	125.38	119.56
1	A	172	SER	C-N-CA	5.76	125.38	119.56
3	D	1236	LEU	N-CA-C	-5.70	104.98	111.07
3	D	1256	LEU	CA-C-N	-5.69	112.73	119.84
3	D	1256	LEU	C-N-CA	-5.69	112.73	119.84
2	C	769	PRO	CA-N-CD	-5.60	104.16	112.00
3	D	1144	LEU	N-CA-C	5.60	120.26	113.38
3	D	1235	GLN	CB-CA-C	-5.57	101.91	110.81
2	C	35	PRO	CA-C-N	5.54	125.64	119.32
2	C	35	PRO	C-N-CA	5.54	125.64	119.32
3	D	1340	GLY	CA-C-N	5.54	124.73	118.97
3	D	1340	GLY	C-N-CA	5.54	124.73	118.97
5	F	333	ILE	N-CA-C	5.43	112.92	107.55
3	D	169	TYR	CA-C-N	5.29	125.71	119.99
3	D	169	TYR	C-N-CA	5.29	125.71	119.99
3	D	1087	ARG	CB-CA-C	5.27	119.84	109.72
3	D	1481	VAL	N-CA-C	5.22	119.64	113.22
3	D	617	ASN	N-CA-C	5.16	119.67	113.17
2	C	766	GLU	CA-C-N	-5.11	113.45	119.84
2	C	766	GLU	C-N-CA	-5.11	113.45	119.84
3	D	1014	ASN	N-CA-C	5.06	117.91	111.69
3	D	136	ASP	CA-C-N	5.05	124.71	119.56
3	D	136	ASP	C-N-CA	5.05	124.71	119.56
5	F	79	ASP	CA-C-N	5.02	125.04	119.32
5	F	79	ASP	C-N-CA	5.02	125.04	119.32
2	C	439	CYS	CA-C-N	5.00	124.61	119.56
2	C	439	CYS	C-N-CA	5.00	124.61	119.56

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	37	0
1	B	1789	0	1841	28	0
2	C	8774	0	8877	232	3
3	D	11808	0	12041	265	4
4	E	761	0	778	11	1
5	F	2807	0	2882	100	2
6	G	370	0	202	19	0
7	H	516	0	283	30	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	622	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 (622) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:C:768:THR:C	2:C:770:GLU:H	1.75	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:538:SER:CB	12:D:2119:HOH:O	2.16	0.93
5:F:358:LEU:HD13	5:F:370:LYS:HZ1	0.85	0.93
2:C:880:MET:HE1	3:D:1242:HIS:CD2	2.05	0.92
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:764:GLU:CD	3:D:54:LYS:HE2	1.96	0.89
2:C:768:THR:C	2:C:770:GLU:N	2.27	0.89
2:C:481:ASP:HA	12:C:1322:HOH:O	1.72	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:O	2:C:765:SER:C	2.20	0.84
3:D:581:LEU:HD21	12:D:2108:HOH:O	1.77	0.84
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
5:F:357:ALA:O	5:F:360:LYS:HB2	1.78	0.82
5:F:358:LEU:CD1	5:F:370:LYS:HZ3	1.88	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
5:F:355:GLU:CD	5:F:358:LEU:HD12	2.07	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
5:F:358:LEU:CD1	5:F:370:LYS:HZ1	1.72	0.78
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
2:C:762:LYS:HG2	2:C:784:ASP:O	1.85	0.77
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:773:LEU:HD23	5:F:373:LYS:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:1082:ALA:O	3:D:1086:LEU:HD13	1.87	0.74
5:F:358:LEU:CD2	5:F:370:LYS:HE3	2.17	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
2:C:768:THR:O	2:C:770:GLU:C	2.35	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:657:LEU:HG	3:D:661:MET:HE2	1.75	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
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.77	0.67
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.75	0.67
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.75	0.67
3:D:576:GLU:HB3	12:D:2102:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:21:DA:H2''	7:H:22:DT:C5'	2.18	0.67
2:C:773:LEU:HD12	2:C:777:ILE:CD1	2.17	0.66
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.28	0.66
3:D:1228:SER:O	3:D:1232:PRO:HD2	1.95	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:230:ARG:HD3	2:C:231:PRO:HD2	1.78	0.66
3:D:526:PRO:HD2	12:D:2119:HOH:O	1.95	0.66
2:C:670:GLN:HE21	2:C:700:TYR:H	1.42	0.65
2:C:784:ASP:OD2	2:C:784:ASP:N	2.29	0.65
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.77	0.65
3:D:1044:LEU:O	3:D:1244:GLY:HA2	1.95	0.65
2:C:763:GLY:C	2:C:765:SER:H	2.04	0.65
3:D:1240:THR:O	3:D:1241:PHE:HB2	1.94	0.65
2:C:880:MET:HE2	3:D:1242:HIS:CD2	2.30	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
2:C:717:LEU:HD21	2:C:763:GLY:CA	2.24	0.64
5:F:355:GLU:O	5:F:358:LEU:HB2	1.97	0.64
6:G:7:DT:N3	7:H:21:DA:N6	2.28	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.80	0.64
3:D:63:TYR:CD1	3:D:68:PHE:CE1	2.85	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
3:D:316:GLN:NE2	3:D:340:THR:O	2.31	0.63
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.81	0.63
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.80	0.63
3:D:711:LEU:HD13	3:D:778:LEU:HD23	1.80	0.63
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.31	0.63
5:F:357:ALA:HA	5:F:360:LYS:HG2	1.81	0.63
2:C:562:SER:HA	12:C:1316:HOH:O	1.99	0.62
3:D:1083:ASP:OD2	3:D:1253:THR:HG22	2.00	0.62
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.82	0.62
3:D:569:ASN:ND2	5:F:214:GLN:OE1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.82	0.61
5:F:358:LEU:HD13	5:F:370:LYS:HE3	1.73	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:376:ARG:HE	5:F:276:ARG:HG3	1.66	0.60
2:C:598:GLU:O	2:C:651:LYS:NZ	2.35	0.60
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.83	0.60
2:C:274:ARG:HD2	2:C:288:ARG:HG2	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
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.66	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
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
5:F:357:ALA:C	5:F:360:LYS:HB2	2.28	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
1:B:94:LEU:O	1:B:146:ARG:NH2	2.36	0.57
3:D:1371:VAL:HG12	3:D:1375:MET:HE2	1.85	0.57
7:H:20:DG:C2'	7:H:21:DA:H5''	2.33	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
2:C:376:ARG:NE	5:F:276:ARG:HG3	2.19	0.57
2:C:778:PHE:CE2	5:F:419:ARG:NH1	2.71	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:45:PHE:O	3:D:86:ARG:NH2	2.37	0.57
3:D:65:ARG:NE	3:D:68:PHE:CE2	2.71	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
2:C:164:PRO:HA	2:C:269:LEU:HD23	1.87	0.56
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.41	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
3:D:1168:MET:HE3	3:D:1168:MET:HA	1.88	0.56
1:A:106:PRO:HD3	1:A:134:GLU:HG2	1.88	0.56
2:C:628:PHE:H	2:C:638:ASP:CB	2.19	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: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:198:ARG:HE	2:C:227:PHE:HA	1.72	0.55
2:C:728:HIS:CB	5:F:423:ASP:O	2.45	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
2:C:409:ARG:HD2	12:C:1311:HOH:O	2.06	0.55
2:C:419:THR:HG22	2:C:422:ARG:HE	1.71	0.55
1:B:93:SER:O	1:B:95:GLN:NE2	2.39	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
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
6:G:6:DA:H2''	6:G:7:DT:H5'	1.87	0.55
3:D:63:TYR:CD1	3:D:68:PHE:HE1	2.25	0.55
1:A:31:GLY:HA2	12:A:403:HOH:O	2.06	0.55
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.88	0.55
2:C:353:ARG:NH1	2:C:357:GLU:OE2	2.40	0.54
3:D:65:ARG:C	3:D:66:GLN:O	2.46	0.54
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.87	0.54
2:C:629:TYR:HB3	12:C:1319:HOH:O	2.08	0.54
3:D:56:TYR:CE2	3:D:66:GLN:HG3	2.42	0.54
3:D:658:LEU:HA	3:D:661:MET:HE3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:773:LEU:CD1	2:C:777:ILE:CG1	2.85	0.54
6:G:7:DT:O2	7:H:21:DA:C2	2.59	0.54
2:C:167:LYS:HD3	7:H:12:DC:C5	2.41	0.54
2:C:778:PHE:CZ	5:F:419:ARG:NE	2.75	0.54
3:D:846:PRO:CD	12:D:2115:HOH:O	2.55	0.54
3:D:1045:MET:HE1	3:D:1243:THR:O	2.08	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
2:C:64:LEU:HB3	2:C:100:LEU:HD11	1.90	0.53
3:D:697:GLY:HA3	12:E:101:HOH:O	2.09	0.53
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.90	0.53
3:D:1235:GLN:O	3:D:1239:ARG:HB2	2.09	0.53
5:F:358:LEU:HD22	5:F:370:LYS:HE3	1.89	0.53
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.89	0.53
2:C:778:PHE:HZ	5:F:419:ARG:NE	2.07	0.53
2:C:835:VAL:HG23	12:C:1308:HOH:O	2.09	0.53
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.90	0.53
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.90	0.53
3:D:894:LYS:H	3:D:894:LYS:HD2	1.74	0.53
1:A:199:ILE:HB	1:A:207:PRO:HB3	1.91	0.52
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
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.92	0.52
2:C:260:LEU:HB3	2:C:261:ILE:HD12	1.92	0.52
2:C:763:GLY:C	2:C:765:SER:N	2.68	0.52
3:D:439:LEU:CD1	5:F:172:ARG:HG3	2.40	0.52
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.91	0.52
3:D:684:LYS:O	3:D:687:VAL:HG12	2.09	0.52
2:C:223:ASP:OD1	2:C:225:SER:OG	2.24	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
3:D:1086:LEU:CD1	3:D:1086:LEU:N	2.72	0.52
2:C:217:LEU:HD12	2:C:217:LEU:H	1.73	0.52
2:C:427:VAL:O	2:C:427:VAL:HG22	2.08	0.52
2:C:541:SER:O	2:C:545:ASN:ND2	2.43	0.52
3:D:65:ARG:O	3:D:68:PHE:HB2	2.08	0.52
3:D:1253:THR:O	3:D:1257:PRO:HD2	2.10	0.52
5:F:355:GLU:HA	5:F:358:LEU:HG	1.91	0.52
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:439:LEU:HD13	5:F:172:ARG:HG3	1.91	0.52
3:D:1253:THR:O	3:D:1257:PRO:HG2	2.10	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:564:GLU:HG3	12:D:2110:HOH:O	2.09	0.52
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.10	0.52
2:C:729:LEU:HD11	2:C:791:ARG:HH22	1.75	0.52
2:C:880:MET:HE1	3:D:1242:HIS:CG	2.45	0.52
3:D:321:GLN:HB2	3:D:336:PHE:HB2	1.92	0.52
12:C:1315:HOH:O	3:D:1462:LEU:HD13	2.10	0.51
3:D:1042:ARG:HG3	3:D:1045:MET:HE3	1.91	0.51
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.92	0.51
3:D:231:VAL:O	3:D:236:TYR:OH	2.28	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
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.93	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
2:C:774:LEU:C	2:C:777:ILE:HD12	2.36	0.50
1:B:54:THR:OG1	1:B:145:ASP:OD1	2.27	0.50
3:D:209:ARG:HE	3:D:391:ALA:HB2	1.74	0.50
3:D:671:LYS:HZ3	5:F:421:PHE:HA	1.74	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:1271:LYS:HE2	3:D:1331:ASP:HB2	1.93	0.50
2:C:15:LEU:HD11	2:C:583:LEU:HD11	1.93	0.50
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.92	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
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.46	0.50
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.31	0.50
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
2:C:168:ARG:O	2:C:267:TYR:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:O	1:A:213:GLN:HG2	2.12	0.49
3:D:274:ARG:NH2	3:D:279:VAL:HG21	2.27	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
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
3:D:1087:ARG:HB2	3:D:1237:THR:CG2	2.42	0.49
5:F:353:GLU:O	5:F:356:LYS:HB2	2.12	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
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
2:C:218:VAL:HG22	2:C:222:MET:HE2	1.95	0.48
2:C:774:LEU:O	2:C:777:ILE:HD12	2.12	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
3:D:1114:THR:OG1	3:D:1195:GLN:NE2	2.45	0.48
7:H:24:DC:N3	7:H:25:DA:C6	2.81	0.48
2:C:1031:ARG:NE	6:G:16:DG:OP1	2.36	0.48
1:B:154:GLU:HG3	3:D:840:LYS:HZ1	1.78	0.48
2:C:543:ASN:C	12:C:1316:HOH:O	2.49	0.48
2:C:777:ILE:HA	5:F:405:LEU:CD1	2.33	0.48
2:C:1035:MET:SD	6:G:15:DT:H4'	2.53	0.48
3:D:846:PRO:N	12:D:2115:HOH:O	2.47	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
3:D:1229:ILE:HG23	3:D:1356:TYR:OH	2.14	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
2:C:1102:LEU:HD11	3:D:9:ARG:HH11	1.78	0.48
5:F:361:LEU:HD11	5:F:408:LEU:CG	2.42	0.48
1:B:58:ILE:HG12	1:B:140:MET:HE2	1.95	0.48
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.95	0.48
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.96	0.48
2:C:767:PRO:O	2:C:769:PRO:HD3	2.14	0.47
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.47	0.47
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.95	0.47
2:C:540:PHE:HB3	2:C:544:THR:HB	1.95	0.47
3:D:264:LEU:HB3	12:D:2116:HOH:O	2.13	0.47
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.36	0.47
5:F:360:LYS:HA	5:F:360:LYS:HD3	1.63	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:405:ARG:NE	2:C:442:GLU:OE2	2.37	0.47
2:C:976:ASP:OD1	2:C:978:ARG:HG3	2.15	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
3:D:1253:THR:OG1	3:D:1254:GLN:N	2.31	0.47
2:C:1021:LEU:HD22	5:F:331:ASP:O	2.15	0.47
2:C:1058:ASP:OD1	3:D:621:LYS:HE2	2.14	0.47
3:D:207:PHE:HE2	5:F:98:GLU:HG2	1.79	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
5:F:355:GLU:O	5:F:356:LYS:C	2.58	0.47
6:G:6:DA:N1	7:H:22:DT:C4	2.80	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
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.47	0.47
3:D:683:ILE:HD11	3:D:688:TRP:CZ2	2.50	0.47
2:C:773:LEU:O	2:C:773:LEU:HD13	2.15	0.47
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.39	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
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
3:D:65:ARG:NE	5:F:379:ARG:HB3	2.30	0.46
7:H:21:DA:C2'	7:H:22:DT:C5'	2.86	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
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.48	0.46
3:D:1239:ARG:O	3:D:1241:PHE:CD1	2.68	0.46
3:D:737:ASN:ND2	3:D:1235:GLN:HE22	2.13	0.46
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.68	0.46
2:C:543:ASN:CB	12:C:1316:HOH:O	1.70	0.46
2:C:773:LEU:HD13	2:C:777:ILE:HG13	1.98	0.46
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.51	0.46
3:D:879:ARG:HD3	3:D:902:LEU:O	2.16	0.46
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:LYS:HE2	2:C:299:LYS:HA	1.96	0.45
2:C:773:LEU:CD1	2:C:773:LEU:C	2.89	0.45
11:D:2006:2TM:H2	12:D:2123:HOH:O	2.16	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
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	1.99	0.45
1:A:102:LYS:HB2	1:A:102:LYS:HE3	1.75	0.45
2:C:334:ARG:NH2	2:C:342:ASP:OD2	2.46	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:218:LYS:HG2	3:D:338:GLU:HG2	1.98	0.45
5:F:357:ALA:HA	5:F:360:LYS:HB2	1.99	0.45
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.98	0.45
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.51	0.45
3:D:525:ARG:C	12:D:2119:HOH:O	2.59	0.45
3:D:1091:SER:OG	3:D:1234:THR:CA	2.64	0.45
3:D:1211:MET:HE1	4:E:16:LYS:HD2	1.98	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.45
3:D:456:MET:HE1	3:D:568:ARG:NE	2.31	0.45
2:C:76:PRO:HG3	2:C:120:LEU:HD12	1.99	0.45
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.82	0.45
2:C:172:ILE:HD13	2:C:184:MET:HE3	1.97	0.45
2:C:1118:LYS:HE2	3:D:20:SER:O	2.17	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.45
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.99	0.45
1:A:198:ARG:HD3	2:C:934:PHE:CE1	2.52	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:424:GLY:O	2:C:426:ASP:N	2.49	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
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.87	0.44
3:D:264:LEU:CB	12:D:2116:HOH:O	2.65	0.44
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.16	0.44
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.50	0.44
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.00	0.44
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.82	0.44
4:E:95:VAL:O	4:E:95:VAL:HG12	2.16	0.44
2:C:367:LEU:HD13	2:C:372:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:422:ARG:HG2	7:H:15:DT:C6	2.52	0.44
2:C:763:GLY:O	2:C:765:SER:N	2.51	0.44
3:D:66:GLN:C	3:D:68:PHE:N	2.73	0.44
3:D:717:GLN:NE2	12:D:2118:HOH:O	2.50	0.44
3:D:1232:PRO:HB3	3:D:1361:VAL:HG11	1.99	0.44
5:F:109:GLY:O	5:F:113:ILE:HG13	2.17	0.44
5:F:362:SER:OG	5:F:365:GLU:HG2	2.18	0.44
2:C:778:PHE:C	2:C:780:GLU:H	2.26	0.44
2:C:1001:VAL:HG12	12:C:1317:HOH:O	2.17	0.44
3:D:260:GLU:HB3	3:D:271:VAL:HB	2.00	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
1:A:6:LEU:HD11	1:A:27:PRO:HG2	1.99	0.44
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.99	0.44
2:C:425:PHE:C	2:C:427:VAL:H	2.26	0.44
3:D:84:ILE:O	3:D:87:ARG:HG2	2.18	0.44
3:D:265:GLU:N	12:D:2116:HOH:O	2.51	0.44
3:D:1176:LYS:HB3	3:D:1176:LYS:HE2	1.79	0.44
3:D:1219:GLU:OE1	4:E:17:TYR:OH	2.32	0.44
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.17	0.44
7:H:15:DT:H2''	7:H:16:DC:H5'	1.99	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
8:C:1201:ATP:H5'1	12:D:2123:HOH:O	2.16	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
2:C:194:VAL:HA	2:C:197:LEU:HD12	2.00	0.43
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.00	0.43
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.43
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:768:THR:HB	2:C:770:GLU:HB2	2.01	0.43
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.53	0.43
1:A:159:LYS:HE3	1:A:164:ALA:O	2.17	0.43
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.73	0.43
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.00	0.43
2:C:101:ILE:HG12	2:C:108:ILE:HG12	2.01	0.43
2:C:425:PHE:C	2:C:427:VAL:N	2.75	0.43
2:C:154:ARG:H	2:C:154:ARG:HG2	1.68	0.43
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:97:ARG:HG2	2:C:112:GLU:HB2	2.00	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
1:A:20:TYR:C	1:A:207:PRO:HG2	2.44	0.43
2:C:1009:SER:O	3:D:624:ASP:HB3	2.19	0.43
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.00	0.43
2:C:996:LYS:CG	12:C:1321:HOH:O	2.29	0.43
1:B:94:LEU:HD11	1:B:97:VAL:HG22	2.01	0.43
2:C:642:ARG:HD3	2:C:642:ARG:HA	1.87	0.43
3:D:526:PRO:N	12:D:2119:HOH:O	2.51	0.43
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.53	0.43
5:F:355:GLU:HA	5:F:358:LEU:CG	2.49	0.43
2:C:768:THR:OG1	2:C:771:GLU:CD	2.62	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
1:B:51:THR:OG1	1:B:87:VAL:O	2.32	0.42
3:D:81:THR:OG1	3:D:82:LYS:N	2.52	0.42
3:D:103:TRP:HB3	3:D:1448:THR:HG21	2.01	0.42
3:D:1086:LEU:N	3:D:1086:LEU:HD12	2.33	0.42
4:E:37:ASN:OD1	4:E:37:ASN:N	2.44	0.42
2:C:562:SER:CA	12:C:1316:HOH:O	2.63	0.42
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.85	0.42
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.54	0.42
3:D:129:PHE:HD1	3:D:456:MET:HE3	1.83	0.42
3:D:1255:GLY:HA2	3:D:1355:VAL:HG13	2.01	0.42
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.19	0.42
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.77	0.42
3:D:66:GLN:C	3:D:68:PHE:H	2.26	0.42
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.19	0.42
3:D:1208:ASP:OD1	3:D:1210:SER:OG	2.34	0.42
3:D:1254:GLN:O	3:D:1257:PRO:HB2	2.19	0.42
3:D:560:GLN:HE22	5:F:222:ARG:HH12	1.68	0.42
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.50	0.42
2:C:546:LEU:HB2	2:C:565:GLN:HE22	1.84	0.42
2:C:1091:GLU:OE2	3:D:606:ILE:HG21	2.19	0.42
3:D:795:VAL:HG12	3:D:876:SER:HB3	2.00	0.42
2:C:218:VAL:O	2:C:222:MET:HG2	2.19	0.42
2:C:878:SER:N	12:C:1301:HOH:O	2.44	0.42
3:D:131:LYS:NZ	3:D:154:THR:HG22	2.34	0.42
2:C:777:ILE:C	2:C:779:GLY:H	2.27	0.42
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.88	0.42
3:D:706:PRO:HG3	6:G:14:DG:H21	1.84	0.42
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.52	0.42
2:C:624:PRO:CA	12:C:1313:HOH:O	2.68	0.42
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.80	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
3:D:1057:VAL:HG13	3:D:1069:GLU:CD	2.44	0.42
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.55	0.42
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.42
2:C:954:THR:HA	2:C:955:PRO:HD3	1.91	0.42
1:A:133:GLU:HG2	1:A:134:GLU:N	2.35	0.42
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.54	0.42
5:F:355:GLU:HA	5:F:358:LEU:HB2	2.02	0.42
2:C:545:ASN:HB3	2:C:583:LEU:HD22	2.02	0.41
3:D:801:GLY:HA3	3:D:821:VAL:HG13	2.01	0.41
3:D:1117:TYR:HB2	3:D:1188:VAL:O	2.20	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
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.95	0.41
1:B:83:LYS:HE2	1:B:168:ASP:HB2	2.02	0.41
3:D:1253:THR:O	3:D:1257:PRO:CD	2.68	0.41
2:C:486:MET:HB3	2:C:490:GLU:HB3	2.01	0.41
3:D:176:ASP:OD1	3:D:177:ALA:N	2.44	0.41
3:D:185:VAL:N	3:D:201:GLY:O	2.45	0.41
3:D:455:ARG:HB2	3:D:460:ALA:HB2	2.02	0.41
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.20	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
3:D:889:ALA:HB1	3:D:930:LEU:HA	2.02	0.41
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.84	0.41
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.46	0.41
2:C:771:GLU:HB3	2:C:775:ARG:HH21	1.83	0.41
5:F:321:ILE:O	5:F:327:SER:HB3	2.20	0.41
5:F:358:LEU:HD11	5:F:370:LYS:NZ	1.97	0.41
1:B:56:VAL:HG21	1:B:82:LEU:HD13	2.02	0.41
2:C:765:SER:O	2:C:767:PRO:HD3	2.21	0.41
3:D:68:PHE:O	3:D:80:VAL:HG21	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.96	0.41
5:F:88:ILE:CG2	5:F:193:ARG:HG2	2.50	0.41
6:G:5:DC:H1'	6:G:6:DA:H8	1.85	0.41
2:C:408:ARG:NH1	2:C:456:ALA:O	2.53	0.41
2:C:571:LEU:HD23	2:C:702:SER:HB3	2.03	0.41
2:C:1102:LEU:HD11	3:D:9:ARG:HB2	2.03	0.41
3:D:538:SER:HB3	12:D:2119:HOH:O	2.03	0.41
3:D:707:THR:HG23	3:D:712:GLY:HA3	2.01	0.41
1:B:124:ASN:OD1	1:B:124:ASN:N	2.53	0.41
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.03	0.41
2:C:749:VAL:HB	2:C:792:VAL:HG21	2.03	0.41
2:C:946:ARG:HG3	12:C:1320:HOH:O	2.20	0.41
3:D:171:LEU:HD11	3:D:393:ILE:HD11	2.03	0.41
3:D:192:ALA:HB1	3:D:193:PRO:HD2	2.02	0.41
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.56	0.41
3:D:675:ARG:HH22	5:F:420:ASP:HB3	1.85	0.41
3:D:843:PHE:HE1	3:D:864:VAL:HG21	1.86	0.41
1:A:109:VAL:CG2	12:A:404:HOH:O	2.69	0.41
2:C:773:LEU:HD13	2:C:777:ILE:CG1	2.51	0.41
2:C:942:GLU:HG3	2:C:945:ARG:HH21	1.85	0.41
3:D:613:ARG:HG3	3:D:618:LEU:HD22	2.03	0.41
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
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
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
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.55	0.40
3:D:517:VAL:HA	3:D:518:PRO:HD3	1.95	0.40
5:F:162:LYS:O	5:F:165:SER:OG	2.34	0.40
2:C:773:LEU:HD22	5:F:373:LYS:CD	2.42	0.40
2:C:1054:THR:OG1	2:C:1055:LEU:N	2.53	0.40
3:D:134:VAL:C	3:D:135:LEU:HD12	2.46	0.40
3:D:403:PHE:CD2	3:D:444:VAL:HG23	2.57	0.40
3:D:784:ASP:HB2	3:D:939:PHE:CE2	2.56	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
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:704:HIS:CD2	2:C:831:ARG:HD2	2.57	0.40
2:C:858:MET:HG2	2:C:867:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.57	0.40
3:D:907:GLU:HB2	3:D:1026:SER:HA	2.03	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
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	24	54
3	D	1491/1524 (98%)	1454 (98%)	33 (2%)	4 (0%)	36	65
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/423 (81%)	336 (98%)	7 (2%)	1 (0%)	36	65
All	All	3489/3795 (92%)	3403 (98%)	75 (2%)	11 (0%)	36	65

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	425	PHE

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Mol	Chain	Res	Type
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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/273 (73%)	194 (97%)	6 (3%)	36	70
1	B	200/273 (73%)	196 (98%)	4 (2%)	48	78
2	C	936/941 (100%)	903 (96%)	33 (4%)	32	66
3	D	1260/1279 (98%)	1218 (97%)	42 (3%)	33	67
4	E	83/88 (94%)	82 (99%)	1 (1%)	63	86
5	F	301/371 (81%)	294 (98%)	7 (2%)	44	76
All	All	2980/3225 (92%)	2887 (97%)	93 (3%)	35	69

All (93) 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	104	GLU
1	A	205	VAL
1	A	233	VAL
1	B	7	LYS
1	B	10	VAL

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Mol	Chain	Res	Type
1	B	91	ASN
1	B	154	GLU
2	C	11	GLU
2	C	81	ASP
2	C	194	VAL
2	C	210	GLU
2	C	219	GLN
2	C	257	VAL
2	C	276	LYS
2	C	285	LEU
2	C	299	LYS
2	C	336	VAL
2	C	360	LEU
2	C	397	GLU
2	C	464	LEU
2	C	513	VAL
2	C	557	ARG
2	C	595	LEU
2	C	617	ASP
2	C	640	ARG
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	774	LEU
2	C	775	ARG
2	C	777	ILE
2	C	784	ASP
2	C	815	LEU
2	C	848	VAL
2	C	1055	LEU
2	C	1078	GLU
3	D	66	GLN
3	D	67	ARG
3	D	134	VAL
3	D	231	VAL
3	D	354	VAL
3	D	406	ASP
3	D	407	VAL

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Mol	Chain	Res	Type
3	D	415	VAL
3	D	420	VAL
3	D	427	VAL
3	D	530	VAL
3	D	618	LEU
3	D	632	VAL
3	D	683	ILE
3	D	709	HIS
3	D	724	GLN
3	D	747	VAL
3	D	754	PHE
3	D	864	VAL
3	D	907	GLU
3	D	1055	VAL
3	D	1083	ASP
3	D	1084	THR
3	D	1127	GLU
3	D	1188	VAL
3	D	1221	VAL
3	D	1236	LEU
3	D	1237	THR
3	D	1238	MET
3	D	1239	ARG
3	D	1243	THR
3	D	1252	ILE
3	D	1254	GLN
3	D	1256	LEU
3	D	1288	GLU
3	D	1305	LEU
3	D	1307	LYS
3	D	1433	SER
3	D	1455	LYS
3	D	1486	VAL
3	D	1488	ASP
3	D	1493	LYS
4	E	37	ASN
5	F	95	THR
5	F	141	VAL
5	F	279	GLN
5	F	346	THR
5	F	356	LYS
5	F	369	LEU

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Mol	Chain	Res	Type
5	F	375	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	HIS
1	B	95	GLN
2	C	390	GLN
2	C	565	GLN
2	C	670	GLN
2	C	728	HIS
2	C	860	HIS
2	C	1047	HIS
3	D	66	GLN
3	D	560	GLN
3	D	669	ASN
3	D	717	GLN
3	D	724	GLN
3	D	737	ASN
3	D	768	ASN
3	D	994	GLN
3	D	1046	GLN
3	D	1124	GLN
3	D	1195	GLN
3	D	1242	HIS
3	D	1254	GLN
3	D	1441	GLN
3	D	1442	ASN
5	F	83	GLN
5	F	312	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
11	2TM	D	2006	-	26,30,30	2.18	8 (30%)	39,47,47	1.78	10 (25%)
8	ATP	C	1201	10	32,33,33	1.84	6 (18%)	48,52,52	1.85	9 (18%)

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
11	2TM	D	2006	-	-	5/19/38/38	0/2/2/2
8	ATP	C	1201	10	-	8/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1201	ATP	PB-O3A	5.30	1.65	1.59
11	D	2006	2TM	C5-C4	-4.41	1.32	1.42
8	C	1201	ATP	C5-C4	4.38	1.46	1.39
11	D	2006	2TM	PB-O3B	4.37	1.63	1.58
8	C	1201	ATP	PA-O3A	4.24	1.64	1.59
11	D	2006	2TM	PB-O1B	-3.94	1.46	1.56
8	C	1201	ATP	PB-O3B	3.53	1.63	1.59
11	D	2006	2TM	C6-N1	-3.47	1.29	1.38
11	D	2006	2TM	PA-O2A	-3.40	1.48	1.56
8	C	1201	ATP	C5-N7	-2.69	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2006	2TM	O4'-C4'	-2.41	1.39	1.45
11	D	2006	2TM	C4-N3	-2.39	1.30	1.34
8	C	1201	ATP	C4-N9	-2.14	1.33	1.37
11	D	2006	2TM	C2-N3	-2.00	1.32	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1201	ATP	C2'-C1'-N9	-6.24	97.79	113.30
8	C	1201	ATP	C5-C4-N3	-5.35	119.35	126.72
8	C	1201	ATP	N3-C4-N9	4.78	135.30	127.17
11	D	2006	2TM	O4'-C1'-N1	3.96	117.33	108.36
11	D	2006	2TM	C2'-C1'-N1	-3.89	102.43	113.25
11	D	2006	2TM	O3G-PG-O1G	3.78	125.58	110.83
11	D	2006	2TM	O1B-PB-O2B	3.76	122.18	109.95
11	D	2006	2TM	O2-C2-N3	-3.37	117.03	122.33
8	C	1201	ATP	C2-N3-C4	3.08	119.35	111.83
8	C	1201	ATP	N3-C2-N1	-3.03	123.99	128.58
11	D	2006	2TM	C6-N1-C2	-2.57	116.11	120.46
11	D	2006	2TM	O2A-PA-C1	2.52	117.16	106.73
8	C	1201	ATP	N6-C6-N1	2.40	123.73	118.38
8	C	1201	ATP	C4-N9-C8	2.37	108.23	105.74
11	D	2006	2TM	O2B-PB-C1	2.17	114.76	109.05
11	D	2006	2TM	C1'-N1-C2	2.14	123.16	118.44
8	C	1201	ATP	C2-N1-C6	2.11	122.19	118.73
8	C	1201	ATP	O4'-C1'-N9	2.06	112.05	108.09
11	D	2006	2TM	N4-C4-N3	2.04	121.55	117.91

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1201	ATP	PB-O3B-PG-O3G
8	C	1201	ATP	C5'-O5'-PA-O3A
11	D	2006	2TM	PB-O3B-PG-O2G
11	D	2006	2TM	PA-C1-PB-O2B
11	D	2006	2TM	O4'-C4'-C5'-O5'
8	C	1201	ATP	C5'-O5'-PA-O1A
8	C	1201	ATP	PA-O3A-PB-O2B
8	C	1201	ATP	PB-O3A-PA-O1A
11	D	2006	2TM	C3'-C4'-C5'-O5'
8	C	1201	ATP	PB-O3A-PA-O2A

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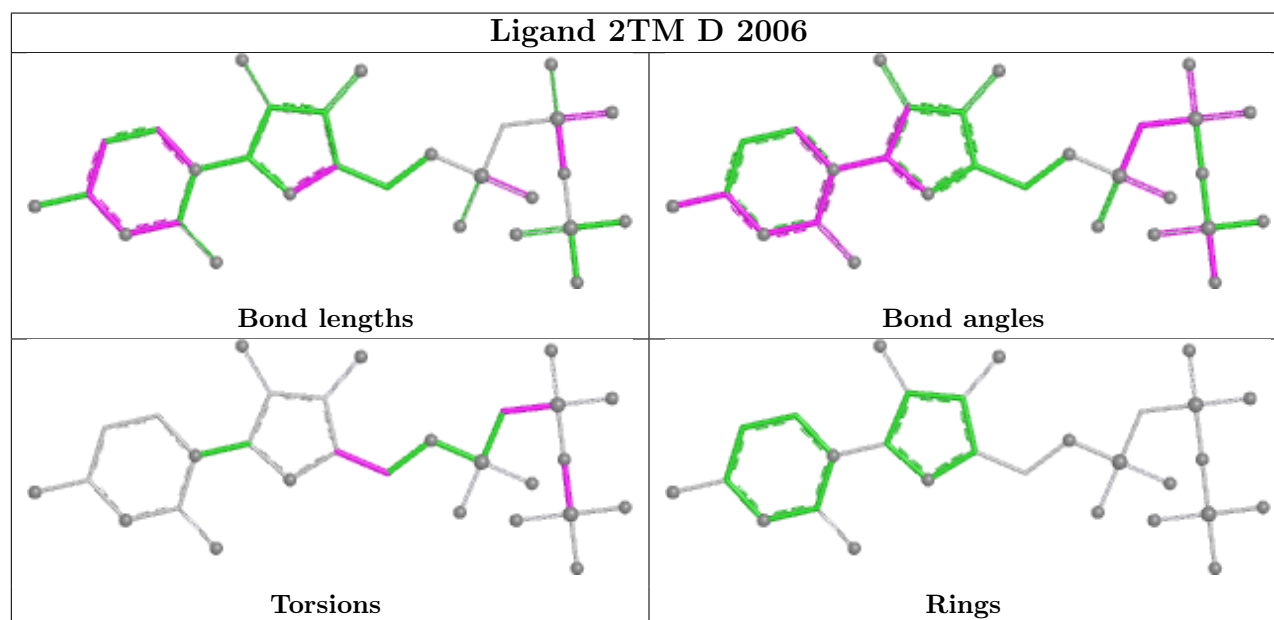
Mol	Chain	Res	Type	Atoms
11	D	2006	2TM	PB-O3B-PG-O1G
8	C	1201	ATP	PA-O3A-PB-O1B
8	C	1201	ATP	PB-O3B-PG-O1G

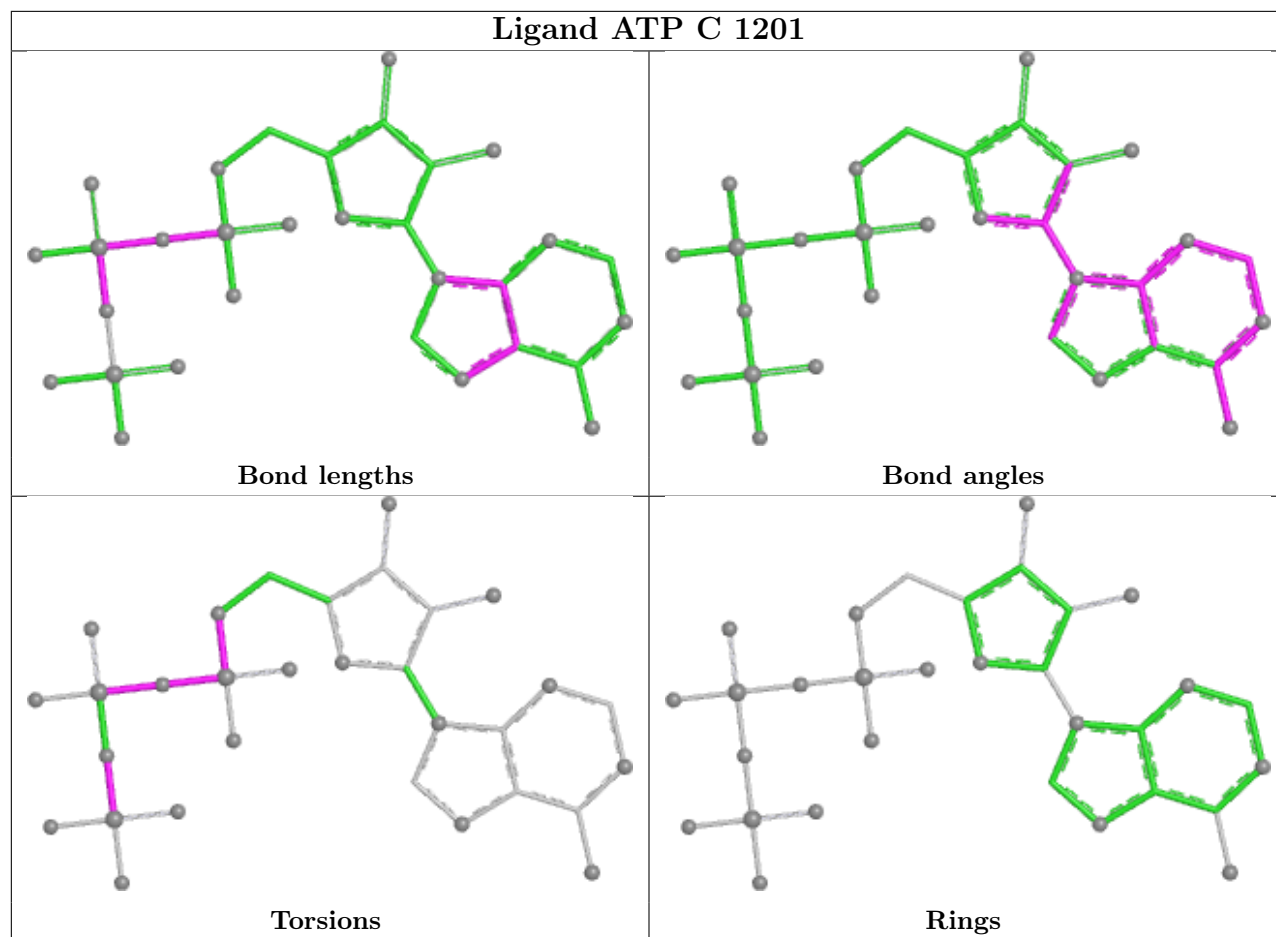
There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/315 (73%)	0.47	9 (3%) 43 35	36, 68, 92, 101	0
1	B	227/315 (72%)	0.44	9 (3%) 42 34	41, 69, 100, 122	0
2	C	1112/1119 (99%)	0.55	53 (4%) 35 28	25, 58, 115, 135	0
3	D	1494/1524 (98%)	0.57	82 (5%) 30 24	19, 58, 122, 199	1 (0%)
4	E	94/99 (94%)	0.65	4 (4%) 40 31	34, 73, 111, 114	0
5	F	346/423 (81%)	0.89	40 (11%) 9 8	43, 79, 152, 176	0
6	G	18/22 (81%)	0.63	1 (5%) 30 23	55, 81, 139, 140	0
7	H	25/27 (92%)	0.57	0 100 100	70, 100, 149, 169	0
All	All	3547/3844 (92%)	0.58	198 (5%) 30 23	19, 64, 124, 199	1 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	311	PHE	6.7
2	C	300	ASP	6.3
3	D	211	VAL	5.3
5	F	369	LEU	4.7
2	C	207	LEU	4.5
3	D	674[A]	ARG	4.4
3	D	412	GLY	4.0
2	C	41	ASN	4.0
3	D	1495	ILE	3.9
3	D	1242	HIS	3.9
5	F	386	VAL	3.9
5	F	373	LYS	3.7
5	F	378	GLY	3.7
3	D	203	ALA	3.6
5	F	382	THR	3.6
1	A	97	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	272	ALA	3.5
2	C	299	LYS	3.5
2	C	200	LEU	3.4
5	F	375	LEU	3.4
3	D	1487	VAL	3.4
5	F	393	THR	3.4
2	C	52	PHE	3.4
3	D	324	ALA	3.3
3	D	519	VAL	3.3
2	C	777	ILE	3.3
3	D	490	ALA	3.3
3	D	1252	ILE	3.3
2	C	174	LEU	3.3
3	D	1490	LYS	3.2
4	E	89	MET	3.2
3	D	977	ALA	3.2
3	D	577	ALA	3.1
2	C	101	ILE	3.1
2	C	63	GLY	3.1
5	F	400	ILE	3.1
3	D	96	ALA	3.1
2	C	65	VAL	3.1
5	F	127	ILE	3.1
2	C	769	PRO	3.1
5	F	392	VAL	3.0
1	B	138	LEU	3.0
3	D	322	VAL	3.0
3	D	420	VAL	3.0
3	D	974	ILE	3.0
5	F	145	PRO	3.0
5	F	344	ALA	3.0
1	B	82	LEU	3.0
3	D	1040	GLY	3.0
5	F	405	LEU	3.0
4	E	85	LEU	2.9
2	C	107	LEU	2.9
2	C	281	LEU	2.9
3	D	304	LEU	2.9
2	C	766	GLU	2.8
2	C	29	ALA	2.8
5	F	383	LEU	2.8
2	C	176	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	434	ARG	2.8
3	D	591	VAL	2.7
2	C	48	PHE	2.7
2	C	778	PHE	2.7
5	F	345	ALA	2.7
2	C	275	TYR	2.7
3	D	821	VAL	2.7
2	C	629	TYR	2.7
2	C	998	TYR	2.7
3	D	387	LEU	2.7
1	B	111	ALA	2.6
3	D	368	VAL	2.6
3	D	427	VAL	2.6
3	D	687	VAL	2.6
5	F	399	GLN	2.6
3	D	1178	ALA	2.6
2	C	147	TYR	2.6
2	C	287	GLY	2.6
2	C	632	ASN	2.6
5	F	358	LEU	2.6
3	D	369	ALA	2.6
2	C	764	GLU	2.6
5	F	347	GLN	2.6
1	A	89	PHE	2.6
2	C	369	PRO	2.5
2	C	307	LEU	2.5
3	D	1328	GLY	2.5
3	D	1491	THR	2.5
5	F	346	THR	2.5
1	B	93	SER	2.5
3	D	972	LEU	2.5
2	C	560	MET	2.5
3	D	541	ASN	2.5
5	F	327	SER	2.5
1	A	94	LEU	2.5
3	D	337	LEU	2.5
2	C	757	GLY	2.5
3	D	1054	GLU	2.5
2	C	51	THR	2.5
3	D	778	LEU	2.5
5	F	91	VAL	2.4
3	D	556	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
5	F	134	LYS	2.4
2	C	666	LEU	2.4
5	F	418	LEU	2.4
4	E	95	VAL	2.4
3	D	45	PHE	2.4
5	F	390	PHE	2.4
2	C	160	ALA	2.4
3	D	1502	ALA	2.4
2	C	563	ASN	2.4
3	D	566	ILE	2.4
3	D	353	VAL	2.4
3	D	694	VAL	2.4
3	D	1286	THR	2.4
3	D	443	VAL	2.4
1	B	23	PHE	2.4
6	G	19	DG	2.4
3	D	310	LEU	2.4
3	D	366	LYS	2.3
5	F	396	ARG	2.3
5	F	149	GLU	2.3
3	D	980	MET	2.3
3	D	350	HIS	2.3
5	F	397	ILE	2.3
5	F	141	VAL	2.3
3	D	144	GLY	2.3
3	D	394	LEU	2.3
3	D	367	ILE	2.3
3	D	54	LYS	2.3
5	F	389	PHE	2.3
1	A	131	THR	2.3
4	E	32	ARG	2.3
3	D	202	VAL	2.3
2	C	445	GLU	2.3
2	C	217	LEU	2.3
2	C	716	LYS	2.3
3	D	1239	ARG	2.3
5	F	415	THR	2.3
2	C	975	TYR	2.3
2	C	211	LEU	2.2
2	C	372	LEU	2.2
3	D	225	LEU	2.2
5	F	364	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	170	PRO	2.2
5	F	359	SER	2.2
3	D	1238	MET	2.2
3	D	1287	GLU	2.2
3	D	1128	VAL	2.2
5	F	341	PRO	2.2
3	D	328	GLY	2.2
1	A	79	ILE	2.2
2	C	21	ILE	2.2
5	F	144	ILE	2.2
1	B	228	PRO	2.2
3	D	1053	PHE	2.2
5	F	417	LYS	2.2
2	C	100	LEU	2.2
3	D	212	ARG	2.2
1	B	53	VAL	2.2
2	C	182	VAL	2.2
3	D	242	LEU	2.2
3	D	1277	ILE	2.1
3	D	1408	ILE	2.1
3	D	1492	LEU	2.1
5	F	361	LEU	2.1
2	C	170	PRO	2.1
2	C	943	VAL	2.1
2	C	973	VAL	2.1
5	F	110	MET	2.1
1	B	2	LEU	2.1
1	A	231	ALA	2.1
2	C	1070	ILE	2.1
5	F	147	LEU	2.1
1	A	200	TRP	2.1
2	C	208	ALA	2.1
3	D	410	SER	2.1
3	D	26	VAL	2.1
3	D	670	VAL	2.1
1	A	36	LEU	2.1
3	D	235	ALA	2.1
3	D	381	ALA	2.1
5	F	139	ALA	2.1
5	F	366	ALA	2.1
3	D	1405	GLU	2.1
3	D	292	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	1292	VAL	2.0
3	D	1481	VAL	2.0
3	D	193	PRO	2.0
2	C	695	LEU	2.0
1	A	199	ILE	2.0
3	D	1253	THR	2.0
1	B	95	GLN	2.0
3	D	213	VAL	2.0
3	D	449	SER	2.0
2	C	1040	LEU	2.0
2	C	782	ALA	2.0
3	D	289	THR	2.0
3	D	516	ALA	2.0
3	D	1319	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 oligosaccharides 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, 95th 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.

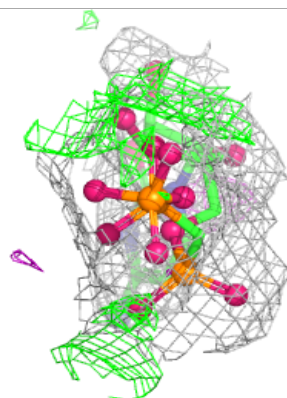
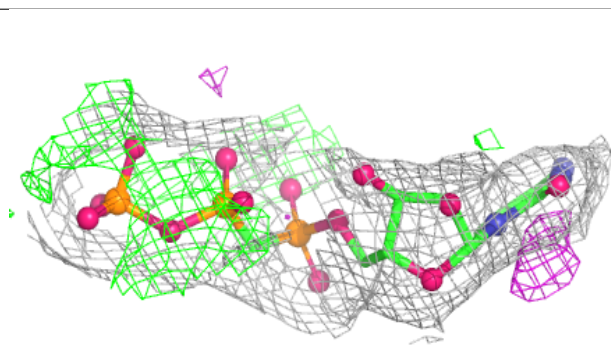
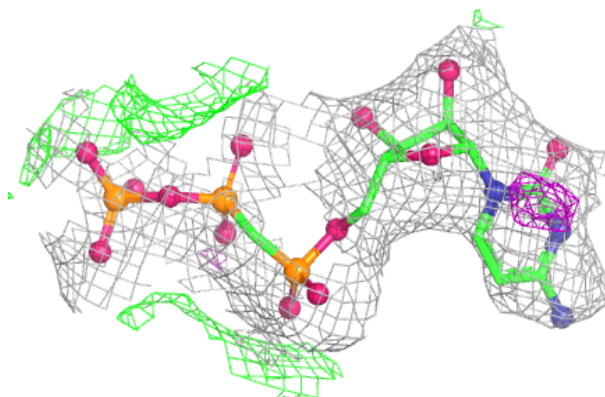
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MG	D	2004	1/1	0.41	0.41	54,54,54,54	0
11	2TM	D	2006	29/29	0.76	0.11	38,51,69,94	0
8	ATP	C	1201	31/31	0.86	0.10	38,47,75,83	0
10	MG	D	2005	1/1	0.89	0.16	45,45,45,45	0
9	ZN	D	2002	1/1	0.95	0.08	59,59,59,59	0
10	MG	D	2003	1/1	0.97	0.10	38,38,38,38	0
9	ZN	D	2001	1/1	0.99	0.03	38,38,38,38	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

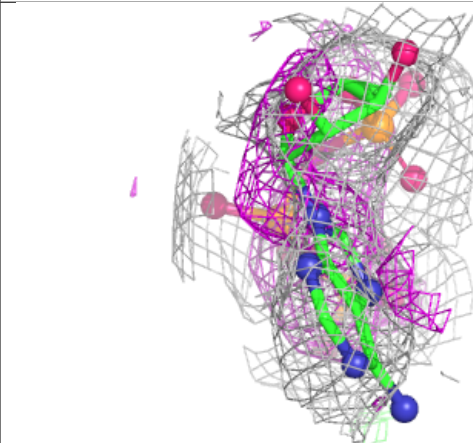
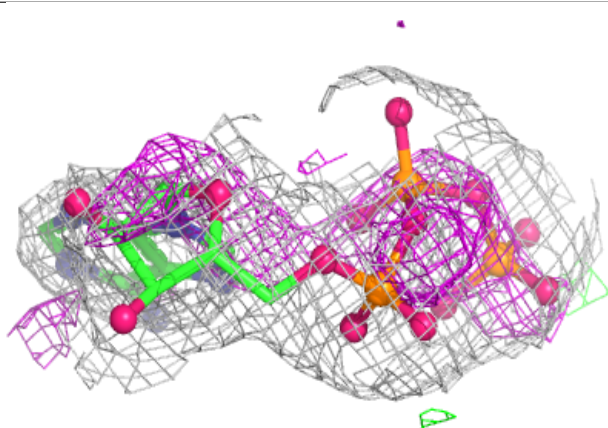
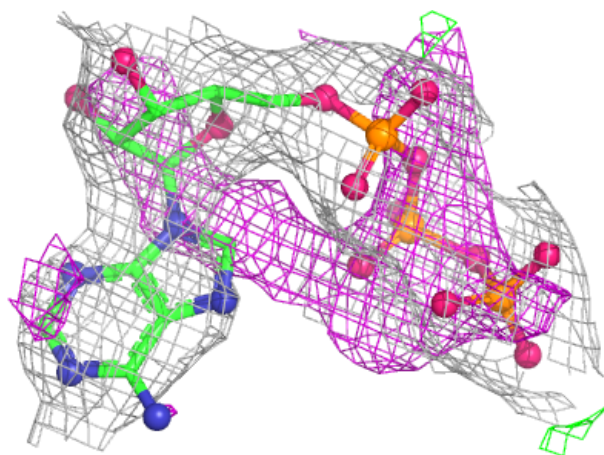
Electron density around 2TM D 2006:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP C 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.