Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 01:52 AM EDT

PDB ID	:	4OIO
Title	:	Crystal structure of Thermus thermophilus pre-insertion substrate complex for de novo transcription initiation
Authors	:	Zhang, Y.; Ebright, R.H.; Arnold, E.
Deposited on	:	2014-01-20
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

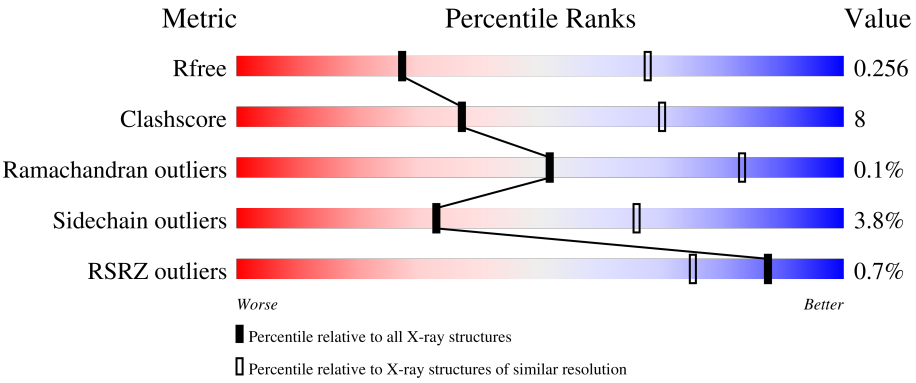
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	58% 14% 28%
1	B	315	57% 12% • 30%
2	C	1119	% 79% 19% ••
3	D	1524	% 74% 21% • •
4	E	99	71% 23% • 5%

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Mol	Chain	Length	Quality of chain
5	F	443	59% 18% 22%
6	G	21	57% 19% 24%
7	H	27	52% 33% 11%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 28649 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	1	0
			8779	5556	1564	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1479	Total	C	N	O	S	0	0	0
			11684	7408	2059	2181	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
			758	483	132	139	4			

- Molecule 5 is a protein called DNA directed RNA polymerase sigma factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	344	Total	C	N	O	S	0	0	0
			2791	1760	507	520	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			331	156	63	96	16			

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

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

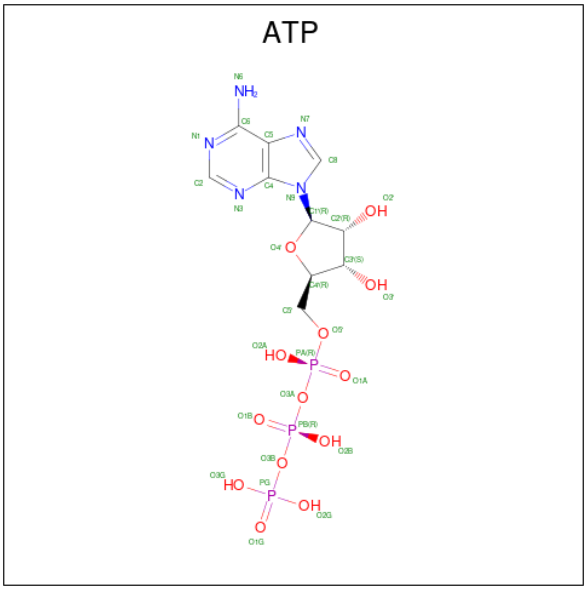
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

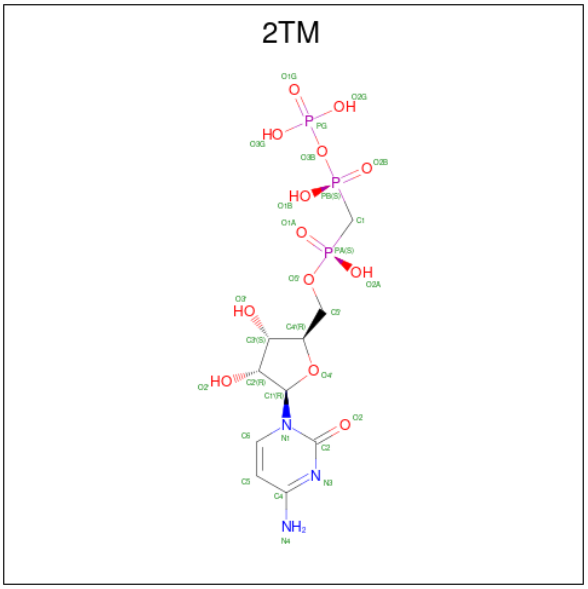
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	Total Mg 2 2	0	0

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 11 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (three-letter code: 2TM) (formula: $C_{10}H_{18}N_3O_{13}P_3$).



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.

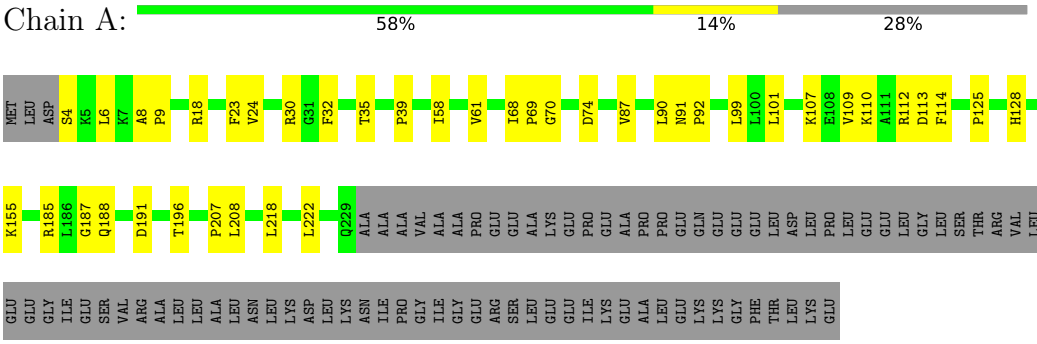
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	16	Total	O	0	0
			16	16		
12	B	7	Total	O	0	0
			7	7		
12	C	68	Total	O	0	0
			68	68		
12	D	89	Total	O	0	0
			89	89		
12	E	13	Total	O	0	0
			13	13		
12	F	15	Total	O	0	0
			15	15		
12	G	5	Total	O	0	0
			5	5		
12	H	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

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

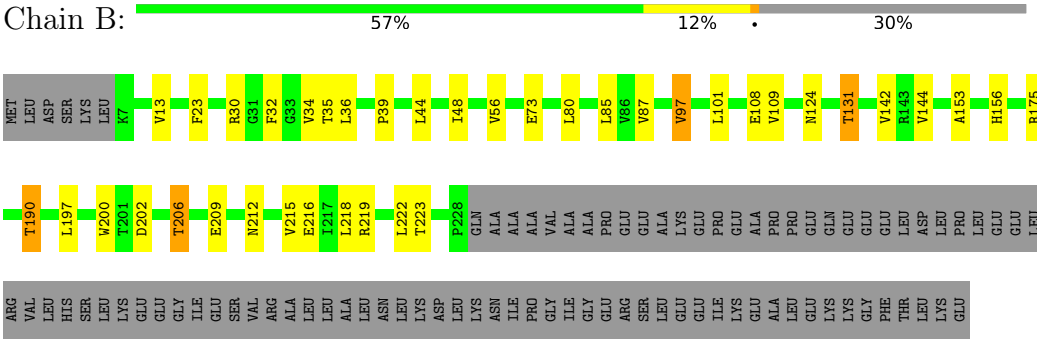
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



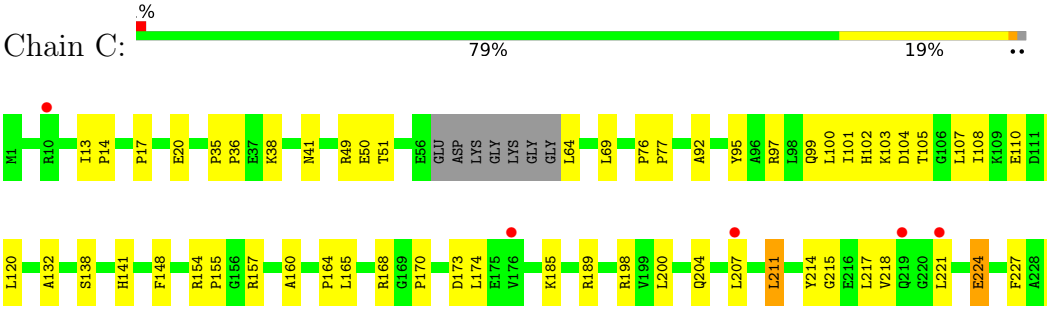
• Molecule 1: DNA-directed RNA polymerase subunit alpha

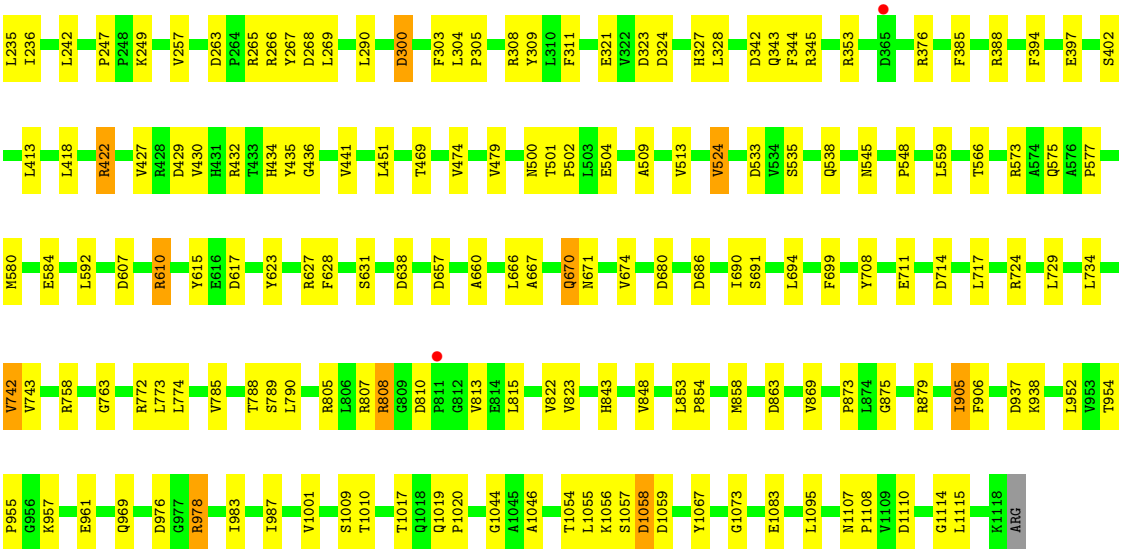
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

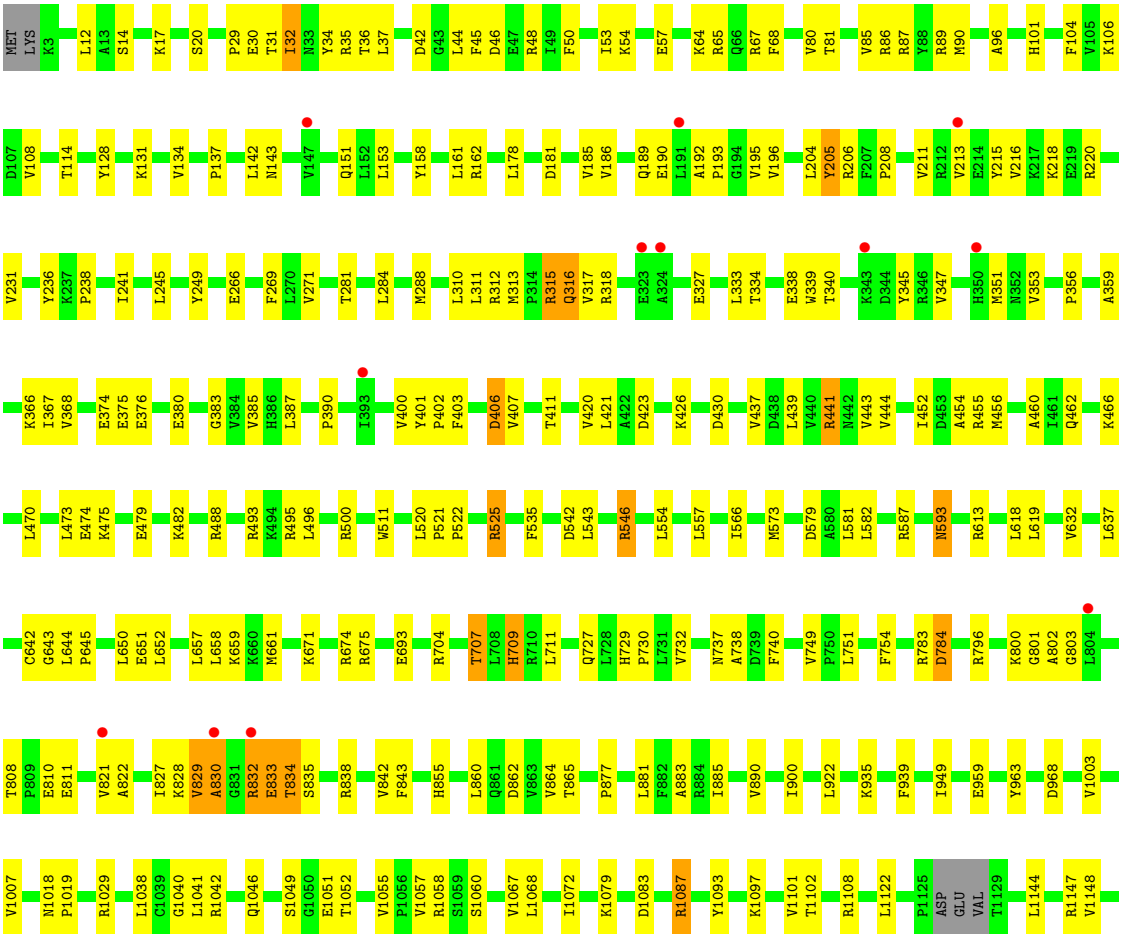
Chain C:

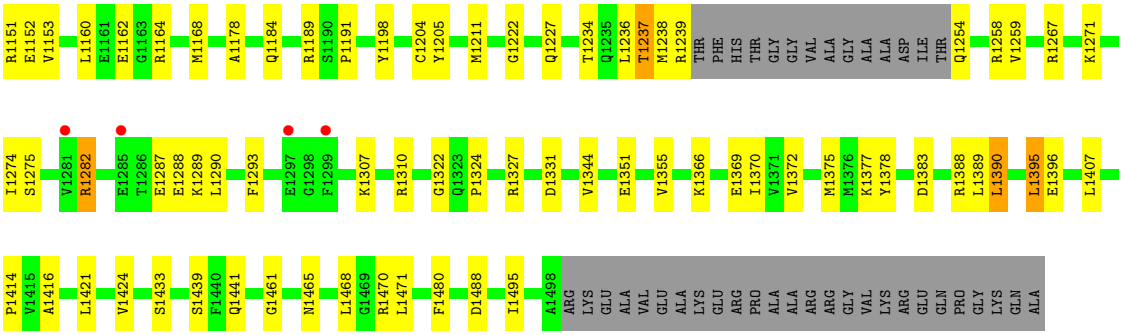




• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



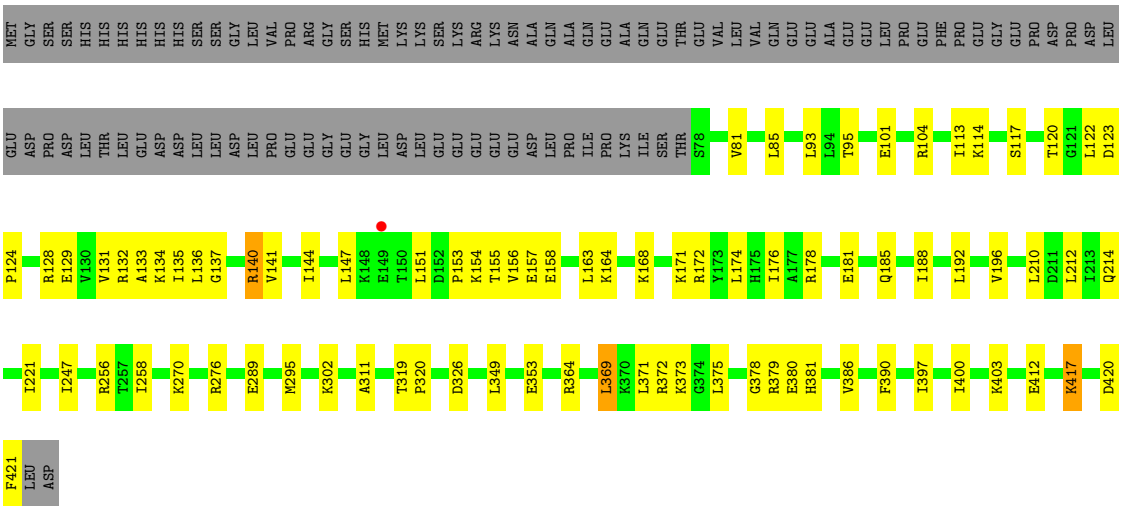


• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

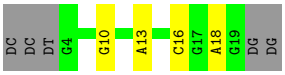
• Molecule 5: DNA directed RNA polymerase sigma factor A

Chain F:



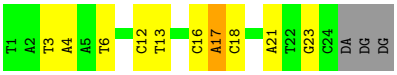
• Molecule 6: 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'

Chain G:



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

Chain H:


T1
A2
T3
A4
A5
T6
C12
T13
C16
A17
C18
A21
T22
G23
C24
DA
DG
DG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.11Å 103.78Å 296.09Å 90.00° 98.86° 90.00°	Depositor
Resolution (Å)	48.92 – 3.10 48.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (48.92-3.10) 94.8 (48.92-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.205 , 0.256 0.207 , 0.256	Depositor DCC
R_{free} test set	2110 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 21.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.022 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.019 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	28649	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.23	0/1814	0.43	0/2466
1	B	0.24	0/1782	0.44	0/2424
2	C	0.25	0/8950	0.46	0/12105
3	D	0.24	0/11889	0.45	0/16072
4	E	0.24	0/772	0.42	0/1040
5	F	0.24	0/2836	0.42	0/3815
6	G	0.45	0/371	1.05	1/571 (0.2%)
7	H	0.48	0/556	1.13	4/858 (0.5%)
All	All	0.25	0/28970	0.49	5/39351 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	17	DA	O4'-C4'-C3'	-7.00	101.70	104.50
6	G	16	DC	O4'-C4'-C3'	-6.27	101.99	104.50
7	H	17	DA	O4'-C1'-N9	6.11	112.28	108.00
7	H	17	DA	C1'-O4'-C4'	-6.05	104.05	110.10
7	H	23	DG	O4'-C1'-N9	5.17	111.62	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	1782	0	1834	23	0
1	B	1750	0	1797	27	0
2	C	8779	0	8883	143	0
3	D	11684	0	11918	212	1
4	E	758	0	770	18	0
5	F	2791	0	2867	56	0
6	G	331	0	180	3	0
7	H	495	0	272	6	0
8	D	2	0	0	0	0
9	D	2	0	0	0	0
10	D	31	0	11	0	0
11	D	29	0	14	1	0
12	A	16	0	0	0	0
12	B	7	0	0	0	0
12	C	68	0	0	4	0
12	D	89	0	0	2	0
12	E	13	0	0	0	0
12	F	15	0	0	0	0
12	G	5	0	0	0	0
12	H	2	0	0	0	0
All	All	28649	0	28546	440	1

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 8.

All (440) 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)
1:A:58:ILE:HB	1:A:61:VAL:HB	1.69	0.74
3:D:245:LEU:HD21	3:D:249:TYR:HB3	1.68	0.73
1:B:206:THR:HG22	1:B:209:GLU:H	1.53	0.72
3:D:829:VAL:HG12	3:D:830:ALA:H	1.57	0.69
3:D:208:PRO:HA	3:D:390:PRO:HA	1.73	0.69
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.75	0.69
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.74	0.68
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.74	0.68
2:C:1019:GLN:HG3	2:C:1058:ASP:HB3	1.75	0.68
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.59	0.68
3:D:366:LYS:NZ	3:D:376:GLU:OE1	2.25	0.68
3:D:213:VAL:HG21	3:D:367:ILE:HD13	1.76	0.67
3:D:493:ARG:HG3	3:D:1390:LEU:HD12	1.75	0.67
3:D:828:LYS:HA	3:D:833:GLU:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.76	0.67
3:D:835:SER:HB3	3:D:838:ARG:HE	1.59	0.67
3:D:106:LYS:HE2	3:D:587:ARG:HG3	1.76	0.67
3:D:67:ARG:HD2	5:F:379:ARG:H	1.58	0.67
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.78	0.66
1:B:44:LEU:HA	1:B:48:ILE:HD13	1.78	0.65
3:D:266:GLU:OE1	3:D:315:ARG:NH2	2.28	0.65
5:F:353:GLU:OE1	5:F:417:LYS:NZ	2.24	0.64
1:A:30:ARG:HH22	3:D:855:HIS:HD2	1.43	0.64
2:C:501:THR:HG21	2:C:513:VAL:HG23	1.78	0.64
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.30	0.63
4:E:44:GLU:OE2	4:E:72:ARG:NH1	2.30	0.63
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.79	0.63
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.80	0.63
3:D:31:THR:HG22	3:D:44:LEU:HB2	1.80	0.62
2:C:978:ARG:HH21	2:C:978:ARG:HG3	1.63	0.61
4:E:33:HIS:CE1	4:E:89:MET:HB3	2.34	0.61
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.83	0.61
4:E:33:HIS:HE1	4:E:89:MET:HB3	1.66	0.61
2:C:49:ARG:NH1	12:C:1207:HOH:O	2.34	0.60
2:C:101:ILE:HG12	2:C:108:ILE:HG22	1.83	0.60
2:C:628:PHE:H	2:C:638:ASP:HB3	1.66	0.60
3:D:671:LYS:HD3	5:F:420:ASP:HB2	1.83	0.60
1:B:34:VAL:HG21	2:C:978:ARG:HB3	1.83	0.60
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.83	0.60
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.83	0.60
5:F:256:ARG:NH2	5:F:311:ALA:O	2.35	0.60
2:C:714:ASP:OD2	2:C:808:ARG:NH2	2.34	0.60
3:D:520:LEU:O	3:D:525:ARG:NH1	2.35	0.59
2:C:772:ARG:NH2	5:F:380:GLU:OE1	2.35	0.59
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.84	0.59
5:F:134:LYS:NZ	5:F:157:GLU:OE2	2.31	0.59
3:D:206:ARG:NH2	5:F:101:GLU:OE2	2.36	0.59
2:C:168:ARG:HB3	2:C:268:ASP:HB3	1.84	0.58
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.84	0.58
5:F:326:ASP:OD2	6:G:18:DA:N6	2.36	0.58
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.86	0.58
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.86	0.58
3:D:1122:LEU:HD23	3:D:1178:ALA:HB2	1.85	0.58
3:D:400:VAL:HG12	3:D:402:PRO:HD3	1.86	0.58
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:198:ARG:HE	2:C:227:PHE:HA	1.69	0.57
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.86	0.57
1:B:216:GLU:OE2	1:B:219:ARG:NH2	2.34	0.57
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.86	0.57
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.86	0.57
3:D:400:VAL:HG13	3:D:443:VAL:HG21	1.85	0.57
1:B:185:ARG:HB2	1:B:190:THR:HG23	1.86	0.57
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.37	0.56
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.86	0.56
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.38	0.56
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.05	0.56
5:F:133:ALA:O	5:F:137:GLY:N	2.37	0.56
2:C:808:ARG:HG2	2:C:808:ARG:HH11	1.70	0.56
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.87	0.56
2:C:474:VAL:HG22	2:C:479:VAL:HG22	1.86	0.56
3:D:42:ASP:N	3:D:46:ASP:OD2	2.33	0.55
3:D:190:GLU:HG2	3:D:196:VAL:HG22	1.88	0.55
3:D:186:VAL:HB	3:D:189:GLN:HB2	1.89	0.55
3:D:1152:GLU:HG2	3:D:1162:GLU:H	1.70	0.55
2:C:64:LEU:HD23	2:C:102:HIS:HA	1.87	0.55
3:D:1237:THR:HG23	3:D:1238:MET:HG3	1.88	0.55
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.89	0.55
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.88	0.55
3:D:367:ILE:HG22	3:D:368:VAL:HG23	1.88	0.55
2:C:397:GLU:HB3	2:C:631:SER:HB2	1.88	0.55
3:D:1254:GLN:HB2	3:D:1258:ARG:HB2	1.88	0.55
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.88	0.55
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.88	0.55
3:D:411:THR:HB	3:D:437:VAL:H	1.72	0.55
2:C:50:GLU:OE1	2:C:345:ARG:NE	2.39	0.54
2:C:402:SER:HA	2:C:566:THR:HG23	1.87	0.54
2:C:905:ILE:HG22	2:C:906:PHE:CD2	2.43	0.54
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.90	0.54
2:C:198:ARG:NH1	2:C:229:MET:O	2.41	0.54
3:D:317:VAL:HB	3:D:339:TRP:HB3	1.88	0.54
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.89	0.54
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.36	0.54
3:D:543:LEU:O	3:D:546:ARG:HG2	2.07	0.54
3:D:796:ARG:NH1	3:D:862:ASP:OD2	2.41	0.54
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.23	0.54
2:C:774:LEU:HD13	5:F:421:PHE:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:406:ASP:HB2	5:F:168:LYS:HB3	1.89	0.53
2:C:189:ARG:HD2	2:C:242:LEU:HD13	1.90	0.53
3:D:181:ASP:N	3:D:205:TYR:OH	2.42	0.53
1:B:175:ARG:HD3	1:B:202:ASP:HB3	1.89	0.53
3:D:1275:SER:O	3:D:1322:GLY:N	2.41	0.53
1:A:112:ARG:HB3	1:A:125:PRO:HB3	1.91	0.53
1:B:97:VAL:HG12	1:B:144:VAL:HB	1.91	0.53
2:C:978:ARG:HH21	2:C:978:ARG:CG	2.20	0.53
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.73	0.53
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.90	0.53
1:B:73:GLU:OE1	1:B:131:THR:OG1	2.27	0.52
3:D:181:ASP:OD1	3:D:441:ARG:NH1	2.43	0.52
3:D:1287:GLU:O	3:D:1307:LYS:NZ	2.38	0.52
1:A:185:ARG:NH2	1:A:187:GLY:HA2	2.23	0.52
2:C:905:ILE:HG22	2:C:906:PHE:HD2	1.75	0.52
2:C:230:ARG:HG3	2:C:231:PRO:HD2	1.90	0.52
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.91	0.52
3:D:220:ARG:HH21	3:D:334:THR:HG21	1.72	0.52
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.92	0.52
2:C:200:LEU:HG	2:C:300:ASP:HB3	1.92	0.52
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.92	0.52
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.74	0.51
3:D:1259:VAL:HG23	3:D:1355:VAL:HG11	1.92	0.51
2:C:1009:SER:HB3	3:D:651:GLU:O	2.10	0.51
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.10	0.51
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.93	0.51
3:D:808:THR:HG22	3:D:810:GLU:H	1.75	0.51
2:C:773:LEU:HD13	5:F:373:LYS:HG3	1.92	0.51
2:C:976:ASP:OD1	2:C:978:ARG:NH2	2.43	0.51
3:D:53:ILE:HG23	3:D:54:LYS:HG3	1.93	0.51
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.76	0.51
2:C:810:ASP:HB2	2:C:813:VAL:HB	1.92	0.51
2:C:873:PRO:HB2	3:D:949:ILE:HD13	1.92	0.51
4:E:47:LYS:NZ	4:E:56:ASP:OD1	2.41	0.51
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.92	0.50
2:C:758:ARG:HH21	2:C:788:THR:HB	1.76	0.50
2:C:772:ARG:HH22	5:F:380:GLU:HB3	1.76	0.50
3:D:883:ALA:HA	3:D:900:ILE:HD13	1.94	0.50
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.92	0.50
2:C:1083:GLU:OE2	3:D:87:ARG:NH1	2.44	0.50
3:D:241:ILE:HD13	3:D:310:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:32:ILE:HG22	5:F:258:ILE:HG23	1.93	0.50
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.27	0.50
5:F:131:VAL:O	5:F:135:ILE:HG22	2.10	0.50
2:C:170:PRO:HD2	2:C:267:TYR:HD1	1.76	0.50
3:D:835:SER:HB3	3:D:838:ARG:HG3	1.93	0.50
3:D:808:THR:HB	3:D:811:GLU:HG3	1.94	0.49
3:D:1282:ARG:HD2	3:D:1293:PHE:HB2	1.93	0.49
2:C:805:ARG:NH1	2:C:807:ARG:HE	2.10	0.49
1:B:32:PHE:HA	1:B:35:THR:HB	1.95	0.49
3:D:45:PHE:O	3:D:86:ARG:NH2	2.45	0.49
3:D:573:MET:SD	5:F:210:LEU:HB3	2.52	0.49
3:D:968:ASP:OD1	3:D:1058:ARG:NH2	2.45	0.49
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.42	0.49
1:B:30:ARG:HH21	2:C:854:PRO:HB3	1.77	0.49
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.77	0.49
3:D:204:LEU:HD23	3:D:441:ARG:NH2	2.28	0.49
3:D:613:ARG:HG3	3:D:618:LEU:HD23	1.93	0.49
3:D:1389:LEU:HD21	3:D:1395:LEU:HD21	1.95	0.49
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.95	0.48
3:D:657:LEU:HG	3:D:661:MET:HE2	1.95	0.48
3:D:211:VAL:HG13	3:D:345:TYR:HB2	1.94	0.48
3:D:241:ILE:HA	3:D:312:ARG:HB3	1.96	0.48
5:F:141:VAL:HG13	5:F:151:LEU:HD23	1.95	0.48
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.65	0.48
3:D:347:VAL:HG13	3:D:351:MET:HG3	1.95	0.48
7:H:3:DT:H2'	7:H:4:DA:C8	2.48	0.48
2:C:848:VAL:HG22	3:D:740:PHE:O	2.13	0.48
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.96	0.48
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.94	0.48
3:D:315:ARG:H	3:D:315:ARG:HD2	1.79	0.48
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.47	0.48
2:C:1046:ALA:HB1	3:D:1471:LEU:HG	1.96	0.48
3:D:90:MET:HG2	3:D:521:PRO:HD3	1.96	0.47
3:D:215:TYR:HA	3:D:383:GLY:HA3	1.96	0.47
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.96	0.47
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.48	0.47
2:C:978:ARG:HG3	2:C:978:ARG:NH2	2.28	0.47
3:D:737:ASN:ND2	11:D:2006:2TM:O3'	2.47	0.47
2:C:758:ARG:H	2:C:789:SER:HB3	1.80	0.47
3:D:29:PRO:O	3:D:31:THR:HG23	2.14	0.47
3:D:709:HIS:HA	3:D:1227:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:801:GLY:HA3	3:D:821:VAL:HG13	1.96	0.47
3:D:316:GLN:HE21	3:D:316:GLN:HB2	1.53	0.47
3:D:707:THR:O	3:D:707:THR:OG1	2.33	0.47
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.97	0.47
2:C:1073:GLY:HA3	3:D:659:LYS:HE2	1.97	0.47
3:D:496:LEU:HD23	3:D:1390:LEU:HD13	1.96	0.47
2:C:211:LEU:HD23	2:C:218:VAL:HG23	1.96	0.47
3:D:1079:LYS:O	3:D:1083:ASP:HB2	2.14	0.47
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.46	0.47
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.80	0.47
2:C:628:PHE:H	2:C:638:ASP:CB	2.28	0.47
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.15	0.47
3:D:142:LEU:HG	3:D:143:ASN:H	1.80	0.47
2:C:41:ASN:O	2:C:41:ASN:ND2	2.48	0.46
2:C:690:ILE:HD12	2:C:694:LEU:HD12	1.96	0.46
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.97	0.46
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.80	0.46
3:D:1468:LEU:HD12	3:D:1470:ARG:HD2	1.97	0.46
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.47	0.46
2:C:853:LEU:HB2	2:C:858:MET:CE	2.44	0.46
3:D:421:LEU:HD23	3:D:444:VAL:HG11	1.97	0.46
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.24	0.46
2:C:513:VAL:HG13	2:C:524:VAL:HG12	1.96	0.46
3:D:37:LEU:HD13	3:D:535:PHE:HZ	1.80	0.46
3:D:42:ASP:OD1	3:D:48:ARG:NH2	2.49	0.46
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.97	0.46
2:C:211:LEU:HD21	2:C:311:PHE:CE2	2.50	0.46
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.97	0.46
2:C:573:ARG:O	2:C:670:GLN:NE2	2.43	0.46
3:D:162:ARG:HH11	3:D:452:ILE:H	1.63	0.46
3:D:542:ASP:OD2	3:D:593:ASN:ND2	2.42	0.46
1:A:4:SER:O	1:A:188:GLN:NE2	2.48	0.46
3:D:65:ARG:HH21	5:F:379:ARG:HD2	1.81	0.46
5:F:369:LEU:HD12	5:F:369:LEU:HA	1.77	0.46
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.51	0.46
3:D:178:LEU:HD13	3:D:193:PRO:HD3	1.98	0.46
2:C:99:GLN:HB3	2:C:110:GLU:HG2	1.98	0.46
2:C:1019:GLN:HG3	2:C:1058:ASP:CB	2.44	0.46
2:C:1115:LEU:HD23	3:D:85:VAL:HG12	1.97	0.46
5:F:181:GLU:O	5:F:185:GLN:HG2	2.16	0.46
2:C:742:VAL:HG12	2:C:743:VAL:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.97	0.46
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.97	0.46
5:F:93:LEU:HD11	7:H:6:DT:H2"	1.96	0.46
2:C:69:LEU:HD12	2:C:97:ARG:HG2	1.97	0.46
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.97	0.46
2:C:247:PRO:HG2	2:C:249:LYS:HE3	1.97	0.46
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.96	0.45
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.45	0.45
3:D:1148:VAL:HA	3:D:1164:ARG:O	2.17	0.45
3:D:1310:ARG:HB2	3:D:1327:ARG:HB2	1.98	0.45
12:D:2106:HOH:O	4:E:37:ASN:HB2	2.15	0.45
5:F:101:GLU:HG3	5:F:104:ARG:NH2	2.31	0.45
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.97	0.45
3:D:784:ASP:HB2	3:D:939:PHE:HE2	1.81	0.45
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.97	0.45
2:C:660:ALA:HB1	2:C:667:ALA:O	2.16	0.45
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.51	0.45
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.51	0.45
3:D:403:PHE:HE2	3:D:443:VAL:N	2.13	0.45
3:D:1168:MET:HE3	3:D:1168:MET:HA	1.98	0.45
3:D:1290:LEU:HD13	3:D:1307:LYS:HA	1.99	0.45
3:D:231:VAL:O	3:D:236:TYR:OH	2.32	0.45
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.98	0.45
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.99	0.45
3:D:462:GLN:HG2	3:D:466:LYS:HE3	1.97	0.45
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.98	0.45
3:D:1254:GLN:NE2	12:D:2150:HOH:O	2.41	0.45
5:F:302:LYS:HE2	5:F:302:LYS:HB3	1.86	0.45
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.98	0.45
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.99	0.45
2:C:154:ARG:HE	2:C:157:ARG:HG3	1.82	0.45
5:F:85:LEU:HD11	5:F:196:VAL:HG11	1.99	0.45
5:F:114:LYS:O	5:F:117:SER:OG	2.27	0.45
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.82	0.44
2:C:1054:THR:O	2:C:1059:ASP:HB3	2.16	0.44
3:D:67:ARG:HD2	5:F:378:GLY:HA3	1.98	0.44
2:C:535:SER:O	2:C:538:GLN:HG2	2.17	0.44
2:C:680:ASP:OD2	2:C:978:ARG:NH1	2.32	0.44
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.52	0.44
1:B:87:VAL:HG21	1:B:144:VAL:HG11	2.00	0.44
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:875:GLY:O	2:C:879:ARG:HD3	2.18	0.44
3:D:31:THR:HB	3:D:45:PHE:CD2	2.53	0.44
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.99	0.44
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.52	0.44
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.50	0.44
1:A:32:PHE:HA	1:A:35:THR:HB	1.98	0.44
1:B:124:ASN:OD1	1:B:124:ASN:N	2.50	0.44
2:C:376:ARG:HE	5:F:276:ARG:HG2	1.81	0.44
2:C:670:GLN:HG2	2:C:699:PHE:CD2	2.53	0.44
2:C:1067:TYR:OH	3:D:674:ARG:NH1	2.51	0.44
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.26	0.44
3:D:17:LYS:O	3:D:20:SER:HB3	2.17	0.44
3:D:238:PRO:HD3	3:D:318:ARG:HG2	2.00	0.44
3:D:832:ARG:HH21	3:D:832:ARG:CG	2.31	0.44
5:F:417:LYS:HZ2	5:F:417:LYS:HB2	1.83	0.44
1:A:101:LEU:HB2	1:A:114:PHE:CE2	2.53	0.44
2:C:224:GLU:CD	2:C:224:GLU:H	2.21	0.44
2:C:267:TYR:CE2	2:C:290:LEU:HD13	2.53	0.44
2:C:615:TYR:OH	2:C:623:TYR:OH	2.22	0.44
3:D:284:LEU:HD22	3:D:288:MET:HE1	2.00	0.44
3:D:401:TYR:OH	3:D:430:ASP:HB2	2.18	0.44
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.18	0.44
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.98	0.44
2:C:432:ARG:NH2	12:C:1261:HOH:O	2.38	0.44
2:C:1019:GLN:HA	2:C:1020:PRO:HD3	1.92	0.44
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.52	0.44
3:D:374:GLU:HG3	3:D:375:GLU:HG3	2.00	0.44
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.98	0.44
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.83	0.44
3:D:482:LYS:HE2	3:D:482:LYS:HB2	1.85	0.43
3:D:1093:TYR:OH	3:D:1441:GLN:OE1	2.23	0.43
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.99	0.43
2:C:937:ASP:OD1	2:C:938:LYS:N	2.51	0.43
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.52	0.43
5:F:144:ILE:HB	5:F:147:LEU:HG	1.99	0.43
2:C:436:GLY:HA2	2:C:538:GLN:O	2.19	0.43
2:C:501:THR:HA	2:C:502:PRO:HD3	1.83	0.43
2:C:545:ASN:O	2:C:905:ILE:HD11	2.18	0.43
2:C:952:LEU:O	2:C:969:GLN:NE2	2.48	0.43
3:D:671:LYS:NZ	3:D:675:ARG:HH21	2.15	0.43
1:A:99:LEU:HD23	1:A:114:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:76:PRO:HA	2:C:77:PRO:HD3	1.90	0.43
5:F:129:GLU:HG3	5:F:147:LEU:HD11	1.99	0.43
2:C:165:LEU:HB2	2:C:168:ARG:HB2	1.99	0.43
2:C:211:LEU:HD22	2:C:221:LEU:HD22	2.01	0.43
2:C:328:LEU:HD23	2:C:328:LEU:HA	1.82	0.43
3:D:236:TYR:HB3	3:D:313:MET:HG3	2.00	0.43
2:C:102:HIS:CE1	2:C:105:THR:HG1	2.36	0.43
2:C:154:ARG:HA	2:C:155:PRO:HD3	1.89	0.43
3:D:68:PHE:HB2	3:D:80:VAL:HG21	2.00	0.43
3:D:423:ASP:HB2	3:D:426:LYS:HB2	2.01	0.43
3:D:1153:VAL:HG22	3:D:1160:LEU:HB2	2.00	0.43
3:D:1211:MET:SD	4:E:16:LYS:HE3	2.58	0.43
5:F:319:THR:HA	5:F:320:PRO:HD3	1.90	0.43
2:C:724:ARG:NH2	2:C:734:LEU:O	2.51	0.43
3:D:131:LYS:O	3:D:456:MET:HG2	2.18	0.43
3:D:693:GLU:HG2	4:E:48:MET:HE1	1.99	0.43
1:A:18:ARG:O	1:A:207:PRO:HD3	2.19	0.43
2:C:758:ARG:HE	2:C:788:THR:HB	1.83	0.43
1:A:58:ILE:HD13	1:A:140:MET:HB3	2.00	0.43
1:A:107:LYS:NZ	1:A:113:ASP:OD2	2.50	0.43
2:C:148:PHE:CZ	2:C:309:TYR:HB3	2.54	0.43
2:C:204:GLN:HG3	2:C:227:PHE:CG	2.54	0.43
2:C:215:GLY:HA2	2:C:218:VAL:HG12	2.01	0.43
2:C:717:LEU:HD13	2:C:763:GLY:HA2	2.01	0.43
2:C:500:ASN:ND2	12:C:1223:HOH:O	2.51	0.43
3:D:353:VAL:HG11	3:D:387:LEU:HD11	2.01	0.42
3:D:864:VAL:HG12	3:D:865:THR:N	2.34	0.42
5:F:140:ARG:HH21	5:F:140:ARG:HB3	1.84	0.42
5:F:172:ARG:O	5:F:176:ILE:HG12	2.19	0.42
1:A:23:PHE:HE1	1:A:208:LEU:HD13	1.85	0.42
2:C:575:GLN:NE2	2:C:671:ASN:HB2	2.35	0.42
2:C:954:THR:HA	2:C:955:PRO:HD3	1.87	0.42
3:D:185:VAL:HG13	3:D:189:GLN:HE21	1.83	0.42
3:D:557:LEU:HD23	3:D:557:LEU:HA	1.87	0.42
3:D:1038:LEU:O	3:D:1060:SER:HB2	2.19	0.42
1:B:212:ASN:HA	1:B:215:VAL:HG22	2.01	0.42
3:D:658:LEU:HA	3:D:661:MET:HE3	2.02	0.42
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	2.01	0.42
5:F:386:VAL:HB	5:F:397:ILE:HG21	2.00	0.42
2:C:729:LEU:HD23	2:C:729:LEU:HA	1.90	0.42
3:D:142:LEU:HD12	3:D:161:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:123:ASP:HA	5:F:124:PRO:HD3	1.92	0.42
1:A:74:ASP:OD2	2:C:627:ARG:NH1	2.52	0.42
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.86	0.42
2:C:422:ARG:NH2	6:G:13:DA:H61	2.18	0.42
2:C:429:ASP:OD2	3:D:1079:LYS:NZ	2.49	0.42
3:D:1236:LEU:HD23	3:D:1236:LEU:HA	1.87	0.42
5:F:155:THR:HA	5:F:158:GLU:HG2	2.02	0.42
7:H:16:DC:H2"	7:H:17:DA:C8	2.54	0.42
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.90	0.42
2:C:51:THR:O	2:C:265:ARG:NH2	2.53	0.42
3:D:1344:VAL:HG11	3:D:1421:LEU:HD22	2.00	0.42
4:E:50:THR:HG22	4:E:51:LEU:H	1.84	0.42
5:F:372:ARG:HA	5:F:381:HIS:H	1.85	0.42
4:E:8:LYS:HE3	4:E:8:LYS:HB2	1.80	0.42
2:C:290:LEU:HB3	2:C:303:PHE:CE1	2.55	0.42
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.84	0.42
5:F:397:ILE:HD13	5:F:397:ILE:HA	1.85	0.42
2:C:1107:ASN:HA	2:C:1108:PRO:HD3	1.92	0.42
3:D:833:GLU:O	3:D:834:THR:HB	2.19	0.42
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	2.02	0.42
3:D:1378:TYR:CE2	3:D:1396:GLU:HG2	2.55	0.42
5:F:188:ILE:HD13	5:F:221:ILE:HG12	2.01	0.42
7:H:12:DC:H1'	7:H:13:DT:C4	2.55	0.42
1:B:175:ARG:N	1:B:200:TRP:O	2.46	0.42
2:C:211:LEU:HD21	2:C:311:PHE:HE2	1.85	0.42
3:D:134:VAL:CG2	3:D:151:GLN:H	2.33	0.42
3:D:271:VAL:HG22	3:D:281:THR:HG23	2.01	0.42
3:D:566:ILE:HG23	5:F:214:GLN:HE22	1.85	0.42
3:D:729:HIS:O	3:D:732:VAL:HG22	2.20	0.42
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.20	0.42
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	2.01	0.42
5:F:163:LEU:HD13	5:F:174:LEU:HD11	2.01	0.42
3:D:475:LYS:O	3:D:479:GLU:HG2	2.20	0.41
3:D:652:LEU:HB3	3:D:749:VAL:HG21	2.02	0.41
5:F:349:LEU:O	5:F:353:GLU:HG2	2.20	0.41
6:G:10:DG:H1	7:H:18:DC:H42	1.68	0.41
2:C:957:LYS:HD3	2:C:961:GLU:HB3	2.01	0.41
3:D:134:VAL:HG22	3:D:151:GLN:H	1.85	0.41
3:D:637:LEU:O	3:D:935:LYS:NZ	2.53	0.41
3:D:900:ILE:H	3:D:900:ILE:HG13	1.71	0.41
5:F:164:LYS:HA	5:F:171:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:VAL:HG22	1:B:23:PHE:HD1	1.85	0.41
2:C:580:MET:HB3	2:C:584:GLU:CD	2.40	0.41
2:C:584:GLU:OE1	2:C:584:GLU:N	2.52	0.41
3:D:50:PHE:O	3:D:89:ARG:HD2	2.19	0.41
3:D:802:ALA:HA	3:D:803:GLY:HA2	1.80	0.41
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.02	0.41
1:A:39:PRO:HG3	1:B:39:PRO:HG3	2.02	0.41
3:D:108:VAL:HG12	7:H:21:DA:H4'	2.01	0.41
5:F:93:LEU:HD23	5:F:93:LEU:HA	1.96	0.41
1:B:153:ALA:HA	1:B:156:HIS:CE1	2.55	0.41
2:C:13:ILE:HD12	2:C:14:PRO:HD2	2.01	0.41
5:F:132:ARG:O	5:F:136:LEU:HB3	2.20	0.41
5:F:212:LEU:HD22	5:F:247:ILE:HG23	2.02	0.41
2:C:207:LEU:HD13	2:C:221:LEU:HD21	2.03	0.41
3:D:881:LEU:O	3:D:885:ILE:HG13	2.20	0.41
3:D:1144:LEU:HD23	3:D:1144:LEU:HA	1.90	0.41
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.93	0.41
2:C:686:ASP:CG	2:C:879:ARG:HH22	2.23	0.41
3:D:30:GLU:H	3:D:30:GLU:HG2	1.64	0.41
1:A:70:GLY:N	2:C:607:ASP:OD1	2.53	0.41
3:D:216:VAL:HG22	3:D:340:THR:HG22	2.03	0.41
5:F:364:ARG:HG3	5:F:390:PHE:CE2	2.56	0.41
1:A:110:LYS:HD3	1:A:128:HIS:HA	2.03	0.41
2:C:263:ASP:HB3	2:C:266:ARG:HB2	2.03	0.41
2:C:548:PRO:O	2:C:843:HIS:HE1	2.04	0.41
2:C:1056:LYS:NZ	3:D:749:VAL:O	2.39	0.41
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.84	0.41
3:D:643:GLY:HA3	3:D:727:GLN:HB2	2.02	0.41
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.86	0.41
3:D:1288:GLU:HG2	3:D:1289:LYS:HG3	2.01	0.41
4:E:14:ASP:OD1	4:E:14:ASP:N	2.54	0.41
3:D:1191:PRO:HB3	3:D:1370:ILE:HD13	2.03	0.41
1:A:68:ILE:HA	1:A:69:PRO:HD3	1.94	0.40
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.03	0.40
3:D:1267:ARG:HG2	3:D:1331:ASP:OD1	2.22	0.40
1:B:153:ALA:HA	1:B:156:HIS:HE1	1.86	0.40
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.94	0.40
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.21	0.40
3:D:1271:LYS:HD3	3:D:1331:ASP:HB2	2.03	0.40
3:D:1407:LEU:HD11	3:D:1414:PRO:HA	2.04	0.40
4:E:40:LEU:HG	4:E:67:GLU:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.36	0.40
2:C:905:ILE:HG12	12:C:1244:HOH:O	2.20	0.40
3:D:101:HIS:CE1	3:D:582:LEU:HD13	2.56	0.40
3:D:439:LEU:HD21	5:F:172:ARG:HG3	2.03	0.40
3:D:704:ARG:HD2	3:D:738:ALA:HB2	2.04	0.40
4:E:47:LYS:HD3	4:E:47:LYS:HA	1.93	0.40
2:C:1009:SER:OG	2:C:1010:THR:N	2.55	0.40
3:D:1102:THR:O	3:D:1222:GLY:HA3	2.20	0.40
3:D:1205:TYR:CZ	3:D:1366:LYS:HE2	2.57	0.40
5:F:113:ILE:HD13	5:F:128:ARG:HG3	2.03	0.40
2:C:95:TYR:HB3	2:C:112:GLU:HG2	2.03	0.40
2:C:168:ARG:O	2:C:267:TYR:HA	2.22	0.40
2:C:418:LEU:HD11	2:C:427:VAL:HG21	2.02	0.40
3:D:213:VAL:HG22	3:D:385:VAL:HG22	2.03	0.40
3:D:835:SER:HB3	3:D:838:ARG:NE	2.32	0.40
3:D:1282:ARG:HB3	3:D:1293:PHE:HB2	2.04	0.40

All (1) 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:34:TYR:OH	3:D:327:GLU:OE2[4_555]	2.15	0.05

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	224/315 (71%)	219 (98%)	5 (2%)	0	100	100
1	B	220/315 (70%)	216 (98%)	4 (2%)	0	100	100
2	C	1108/1119 (99%)	1083 (98%)	24 (2%)	1 (0%)	51	83
3	D	1473/1524 (97%)	1445 (98%)	25 (2%)	3 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100 100
5	F	342/443 (77%)	335 (98%)	7 (2%)	0	100 100
All	All	3459/3815 (91%)	3388 (98%)	67 (2%)	4 (0%)	51 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	834	THR
3	D	830	ALA
2	C	905	ILE
3	D	829	VAL

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	199/273 (73%)	193 (97%)	6 (3%)	41 71
1	B	195/273 (71%)	189 (97%)	6 (3%)	40 70
2	C	937/941 (100%)	893 (95%)	44 (5%)	26 59
3	D	1247/1279 (98%)	1202 (96%)	45 (4%)	35 67
4	E	82/88 (93%)	80 (98%)	2 (2%)	49 76
5	F	299/388 (77%)	289 (97%)	10 (3%)	38 69
All	All	2959/3242 (91%)	2846 (96%)	113 (4%)	33 66

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	87	VAL
1	A	90	LEU
1	A	142	VAL
1	A	155	LYS
1	A	191	ASP

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Mol	Chain	Res	Type
1	B	36	LEU
1	B	97	VAL
1	B	131	THR
1	B	190	THR
1	B	206	THR
1	B	223	THR
2	C	103	LYS
2	C	104	ASP
2	C	107	LEU
2	C	138	SER
2	C	141	HIS
2	C	211	LEU
2	C	214	TYR
2	C	217	LEU
2	C	224	GLU
2	C	230	ARG
2	C	235	LEU
2	C	236	ILE
2	C	257	VAL
2	C	300	ASP
2	C	308	ARG
2	C	321	GLU
2	C	323	ASP
2	C	342	ASP
2	C	353	ARG
2	C	388	ARG
2	C	422	ARG
2	C	430	VAL
2	C	434	HIS
2	C	441	VAL
2	C	524	VAL
2	C	559	LEU
2	C	592	LEU
2	C	610	ARG
2	C	617	ASP
2	C	657	ASP
2	C	666	LEU
2	C	670	GLN
2	C	691	SER
2	C	742	VAL
2	C	785	VAL
2	C	808	ARG

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Mol	Chain	Res	Type
2	C	815	LEU
2	C	863	ASP
2	C	978	ARG
2	C	1001	VAL
2	C	1017	THR
2	C	1055	LEU
2	C	1057	SER
2	C	1058	ASP
3	D	32	ILE
3	D	35	ARG
3	D	36	THR
3	D	81	THR
3	D	153	LEU
3	D	205	TYR
3	D	269	PHE
3	D	311	LEU
3	D	315	ARG
3	D	316	GLN
3	D	333	LEU
3	D	380	GLU
3	D	406	ASP
3	D	407	VAL
3	D	420	VAL
3	D	441	ARG
3	D	470	LEU
3	D	488	ARG
3	D	525	ARG
3	D	546	ARG
3	D	593	ASN
3	D	632	VAL
3	D	650	LEU
3	D	707	THR
3	D	709	HIS
3	D	711	LEU
3	D	754	PHE
3	D	783	ARG
3	D	784	ASP
3	D	827	ILE
3	D	832	ARG
3	D	833	GLU
3	D	1029	ARG
3	D	1041	LEU

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Mol	Chain	Res	Type
3	D	1055	VAL
3	D	1067	VAL
3	D	1087	ARG
3	D	1151	ARG
3	D	1184	GLN
3	D	1237	THR
3	D	1239	ARG
3	D	1282	ARG
3	D	1390	LEU
3	D	1395	LEU
3	D	1433	SER
4	E	36	LYS
4	E	50	THR
5	F	81	VAL
5	F	95	THR
5	F	140	ARG
5	F	154	LYS
5	F	289	GLU
5	F	369	LEU
5	F	371	LEU
5	F	375	LEU
5	F	412	GLU
5	F	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	180	GLN
2	C	117	HIS
2	C	139	GLN
2	C	538	GLN
2	C	575	GLN
2	C	999	HIS
3	D	66	GLN
3	D	189	GLN
3	D	316	GLN
3	D	348	GLN
3	D	350	HIS
3	D	737	ASN
3	D	1172	HIS
3	D	1184	GLN
3	D	1195	GLN

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Mol	Chain	Res	Type
3	D	1202	GLN
3	D	1235	GLN
3	D	1489	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
10	ATP	D	2005	9	26,33,33	1.66	4 (15%)	31,52,52	1.59	5 (16%)
11	2TM	D	2006	9	27,30,30	1.70	6 (22%)	39,47,47	1.20	3 (7%)

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
10	ATP	D	2005	9	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	2TM	D	2006	9	-	6/19/38/38	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	2005	ATP	C2-N3	4.59	1.39	1.32
11	D	2006	2TM	C4-N4	4.17	1.43	1.33
10	D	2005	ATP	C2'-C1'	-3.59	1.48	1.53
11	D	2006	2TM	PA-O1A	2.95	1.58	1.51
10	D	2005	ATP	C6-N6	2.66	1.43	1.34
11	D	2006	2TM	PA-O2A	-2.56	1.50	1.56
11	D	2006	2TM	C2'-C3'	-2.56	1.46	1.53
11	D	2006	2TM	C3'-C4'	-2.49	1.46	1.53
10	D	2005	ATP	C2-N1	2.37	1.38	1.33
11	D	2006	2TM	C6-C5	2.12	1.39	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	2005	ATP	N3-C2-N1	-4.90	121.01	128.68
10	D	2005	ATP	PB-O3B-PG	-3.64	120.33	132.83
10	D	2005	ATP	PA-O3A-PB	-3.57	120.58	132.83
11	D	2006	2TM	PB-O3B-PG	-2.96	122.20	132.62
10	D	2005	ATP	C4-C5-N7	2.93	112.45	109.40
11	D	2006	2TM	O4'-C4'-C3'	2.87	110.79	105.11
11	D	2006	2TM	O2-C2-N3	-2.83	117.72	122.33
10	D	2005	ATP	C2-N1-C6	2.12	122.38	118.75

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	2005	ATP	PB-O3A-PA-O5'
10	D	2005	ATP	C5'-O5'-PA-O1A
10	D	2005	ATP	C5'-O5'-PA-O3A
10	D	2005	ATP	O4'-C4'-C5'-O5'
11	D	2006	2TM	PB-O3B-PG-O3G
11	D	2006	2TM	PA-C1-PB-O1B
10	D	2005	ATP	C3'-C4'-C5'-O5'
11	D	2006	2TM	O4'-C4'-C5'-O5'
11	D	2006	2TM	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
11	D	2006	2TM	PA-C1-PB-O2B
11	D	2006	2TM	PB-O3B-PG-O1G

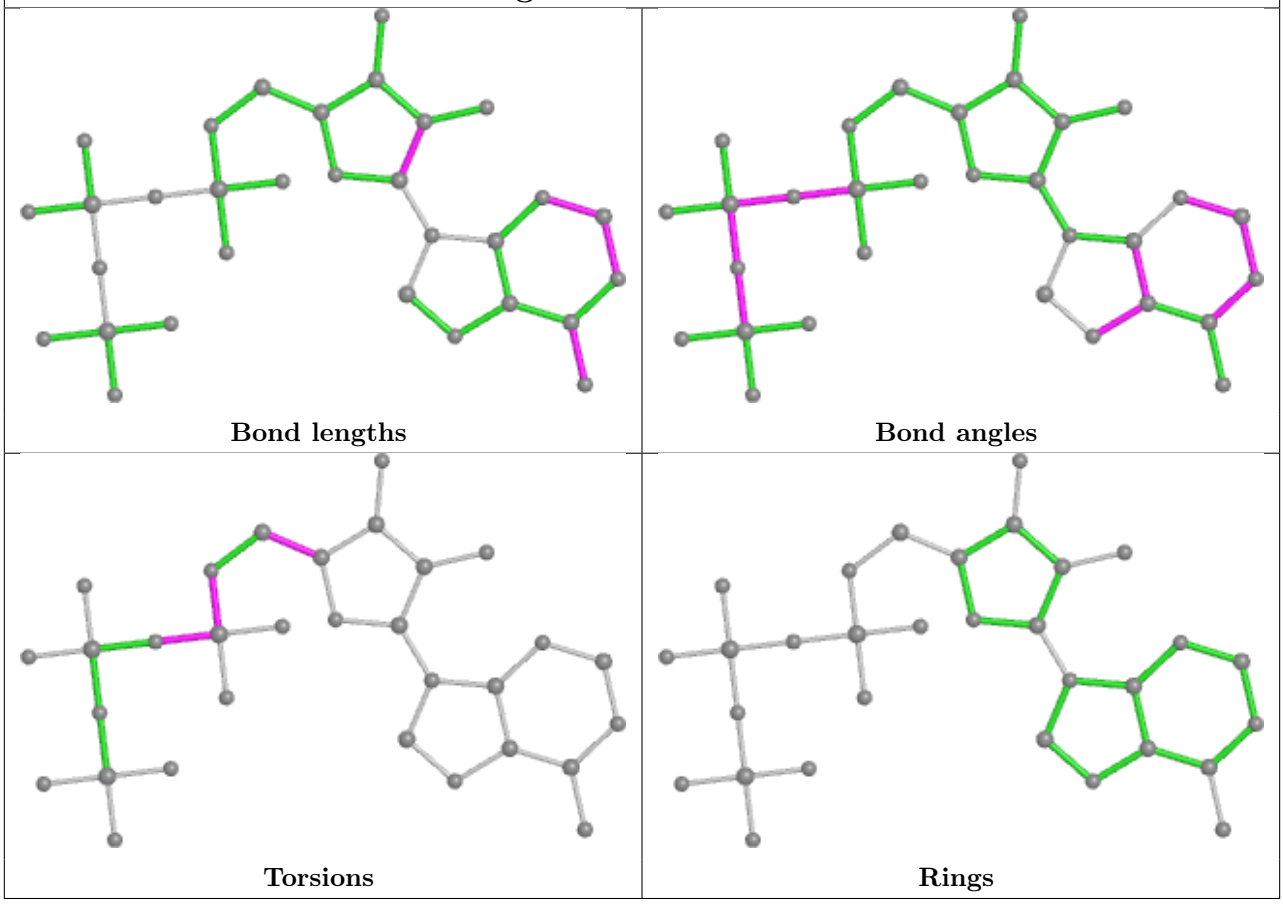
There are no ring outliers.

1 monomer is involved in 1 short contact:

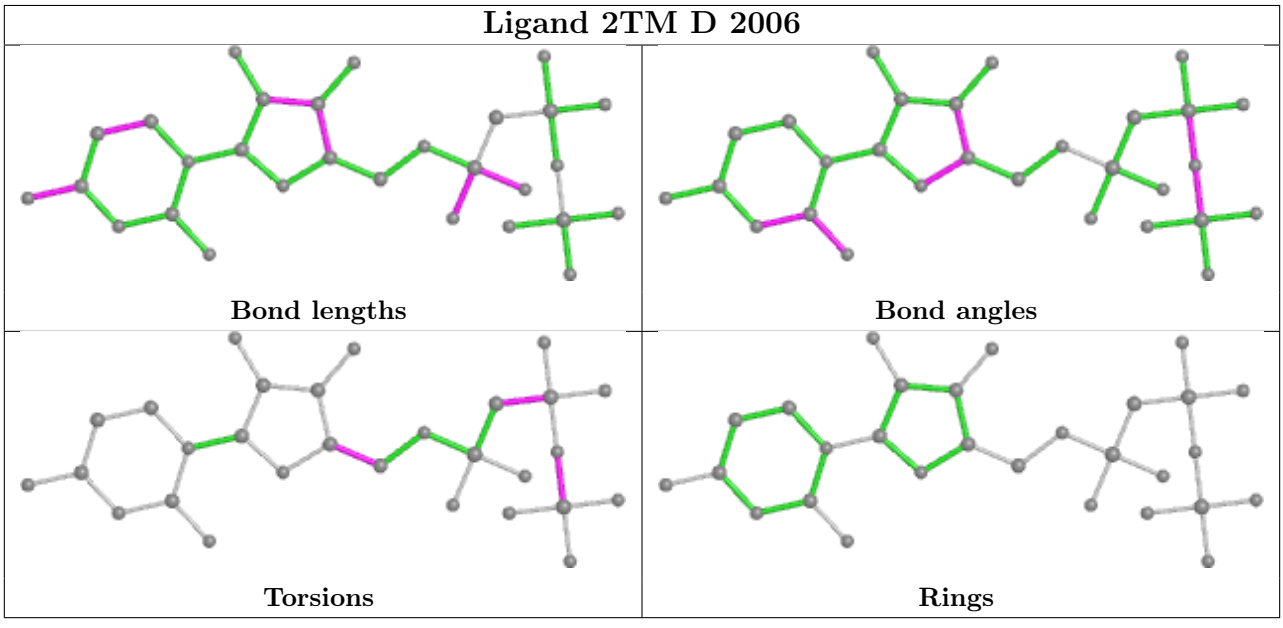
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2006	2TM	1	0

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 then 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.

Ligand ATP D 2005



Ligand 2TM D 2006



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	226/315 (71%)	-0.53	0 100 100	24, 42, 69, 91	0
1	B	222/315 (70%)	-0.32	0 100 100	25, 56, 90, 106	0
2	C	1111/1119 (99%)	-0.36	7 (0%) 89 78	4, 35, 107, 145	0
3	D	1479/1524 (97%)	-0.25	16 (1%) 80 64	5, 40, 110, 149	1 (0%)
4	E	94/99 (94%)	-0.60	0 100 100	13, 35, 80, 89	0
5	F	344/443 (77%)	-0.38	1 (0%) 94 88	18, 57, 97, 125	0
6	G	16/21 (76%)	-0.73	0 100 100	34, 56, 146, 151	0
7	H	24/27 (88%)	-0.54	0 100 100	56, 90, 138, 164	0
All	All	3516/3863 (91%)	-0.33	24 (0%) 87 75	4, 42, 106, 164	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	191	LEU	3.3
3	D	1299	PHE	3.1
3	D	324	ALA	2.9
2	C	221	LEU	2.9
3	D	323	GLU	2.7
3	D	393	ILE	2.6
3	D	1285	GLU	2.5
3	D	1281	VAL	2.5
3	D	350	HIS	2.5
3	D	343	LYS	2.4
2	C	207	LEU	2.4
2	C	10	ARG	2.4
2	C	811	PRO	2.4
2	C	365	ASP	2.4
3	D	830	ALA	2.4
3	D	213	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	147	VAL	2.3
3	D	821	VAL	2.2
3	D	804	LEU	2.2
3	D	1297	GLU	2.2
2	C	219	GLN	2.2
3	D	832	ARG	2.2
2	C	176	VAL	2.1
5	F	149	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

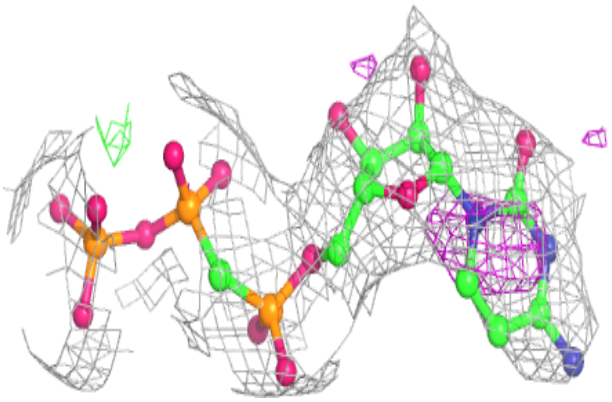
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

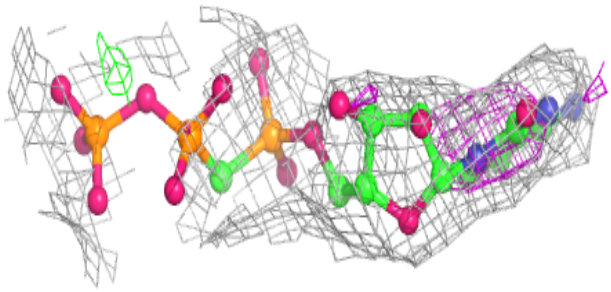
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	2TM	D	2006	29/29	0.89	0.18	31,48,75,85	0
10	ATP	D	2005	31/31	0.93	0.17	26,37,52,60	31
9	MG	D	2004	1/1	0.94	0.19	31,31,31,31	0
8	ZN	D	2001	1/1	0.99	0.16	20,20,20,20	0
8	ZN	D	2002	1/1	0.99	0.08	57,57,57,57	0
9	MG	D	2003	1/1	0.99	0.27	12,12,12,12	0

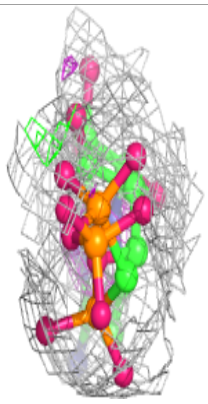
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

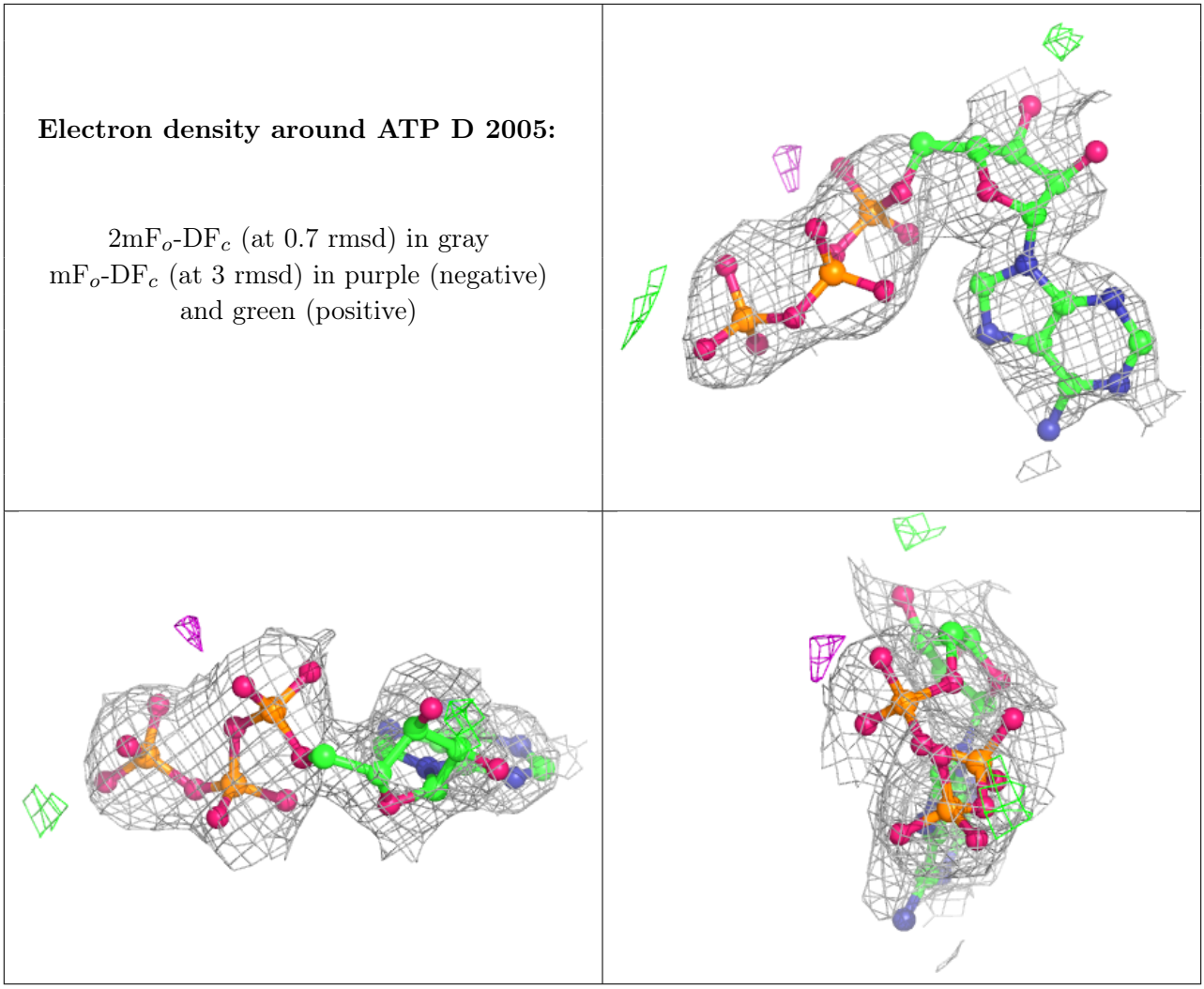






Electron density around ATP D 2005:

$2mF_o$-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.