



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 12:55 PM BST

PDB ID : 6JCX
Title : Mycobacterium tuberculosis transcription initiation complex with ECF sigma factor sigma H and 6nt RNA
Authors : Li, L.; Zhang, Y.
Deposited on : 2019-01-30
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

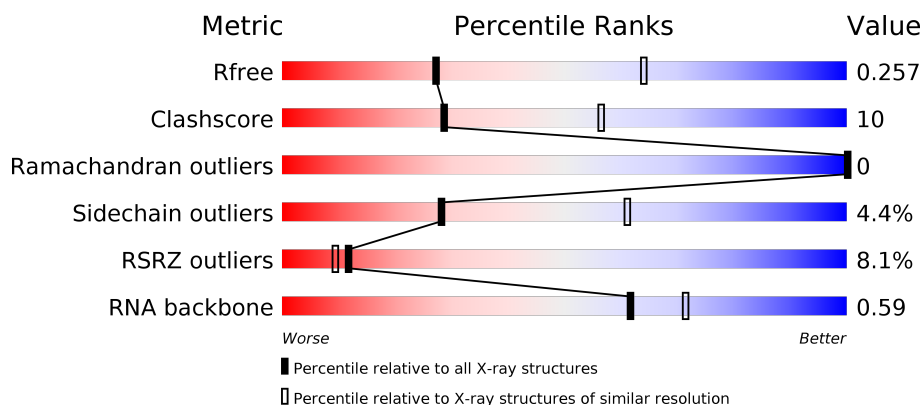
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	368	<div> <div>45%</div> <div>13%</div> <div>•</div> <div>40%</div> </div>
1	B	368	<div>11%</div> <div>46%</div> <div>17%</div> <div>37%</div>

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Mol	Chain	Length	Quality of chain
4	E	110	<div><div></div><div>4%</div><div>49%</div><div>15%</div><div>35%</div></div>
5	F	218	<div><div></div><div>12%</div><div>61%</div><div>24%</div><div>15%</div></div>
6	H	20	<div><div></div><div>20%</div><div>35%</div><div>65%</div></div>
7	G	23	<div><div></div><div>35%</div><div>39%</div><div>57%</div><div></div></div>
8	I	6	<div><div></div><div>67%</div><div>33%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 25143 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	219	Total	C	N	O	S	0	0	0
			1654	1044	282	326	2			
1	B	232	Total	C	N	O	S	0	0	0
			1696	1073	287	334	2			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P9WGZ1
A	-19	GLY	-	expression tag	UNP P9WGZ1
A	-18	HIS	-	expression tag	UNP P9WGZ1
A	-17	HIS	-	expression tag	UNP P9WGZ1
A	-16	HIS	-	expression tag	UNP P9WGZ1
A	-15	HIS	-	expression tag	UNP P9WGZ1
A	-14	HIS	-	expression tag	UNP P9WGZ1
A	-13	HIS	-	expression tag	UNP P9WGZ1
A	-12	HIS	-	expression tag	UNP P9WGZ1
A	-11	HIS	-	expression tag	UNP P9WGZ1
A	-10	HIS	-	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	SER	-	expression tag	UNP P9WGZ1
A	-7	SER	-	expression tag	UNP P9WGZ1
A	-6	GLY	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	ILE	-	expression tag	UNP P9WGZ1
A	-3	GLU	-	expression tag	UNP P9WGZ1
A	-2	GLY	-	expression tag	UNP P9WGZ1
A	-1	ARG	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
B	-20	MET	-	initiating methionine	UNP P9WGZ1
B	-19	GLY	-	expression tag	UNP P9WGZ1
B	-18	HIS	-	expression tag	UNP P9WGZ1
B	-17	HIS	-	expression tag	UNP P9WGZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP P9WGZ1
B	-15	HIS	-	expression tag	UNP P9WGZ1
B	-14	HIS	-	expression tag	UNP P9WGZ1
B	-13	HIS	-	expression tag	UNP P9WGZ1
B	-12	HIS	-	expression tag	UNP P9WGZ1
B	-11	HIS	-	expression tag	UNP P9WGZ1
B	-10	HIS	-	expression tag	UNP P9WGZ1
B	-9	HIS	-	expression tag	UNP P9WGZ1
B	-8	SER	-	expression tag	UNP P9WGZ1
B	-7	SER	-	expression tag	UNP P9WGZ1
B	-6	GLY	-	expression tag	UNP P9WGZ1
B	-5	HIS	-	expression tag	UNP P9WGZ1
B	-4	ILE	-	expression tag	UNP P9WGZ1
B	-3	GLU	-	expression tag	UNP P9WGZ1
B	-2	GLY	-	expression tag	UNP P9WGZ1
B	-1	ARG	-	expression tag	UNP P9WGZ1
B	0	HIS	-	expression tag	UNP P9WGZ1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1138	Total	C	N	O	S	0	0	0
			8731	5458	1528	1706	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	initiating methionine	UNP P9WGY9
C	6	VAL	-	expression tag	UNP P9WGY9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1258	Total	C	N	O	S	0	0	0
			9822	6153	1776	1852	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P9WGY7
D	1	VAL	-	expression tag	UNP P9WGY7

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	71	Total	C	N	O	0	0	0
			566	362	95	109			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	186	Total	C	N	O	S	0	0	0
			1477	926	260	286	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P9WGH9
F	0	ALA	-	expression tag	UNP P9WGH9

- Molecule 6 is a DNA chain called DNA (5'-D(*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	20	Total	C	N	O	P	0	0	0
			412	196	77	120	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	23	Total	C	N	O	P	0	0	0
			475	226	89	138	22			

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

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

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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


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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	Mg	0	0
			1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	9	Total	O	0	0
			9	9		
11	B	9	Total	O	0	0
			9	9		
11	C	66	Total	O	0	0
			66	66		
11	D	71	Total	O	0	0
			71	71		
11	E	3	Total	O	0	0
			3	3		
11	F	11	Total	O	0	0
			11	11		
11	H	7	Total	O	0	0
			7	7		
11	G	4	Total	O	0	0
			4	4		
11	I	5	Total	O	0	0
			5	5		

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.

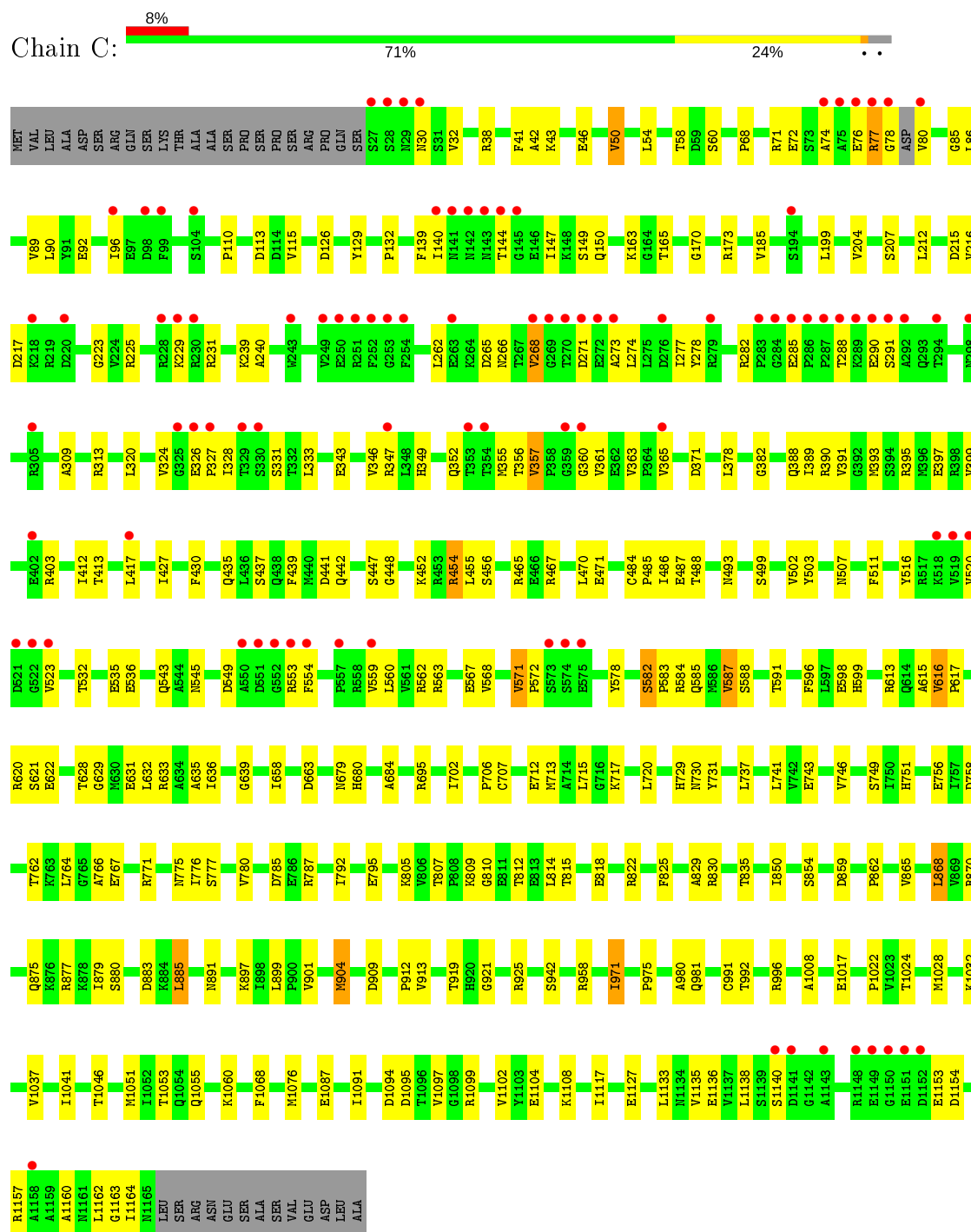
- Chain A: 

- Chain B:

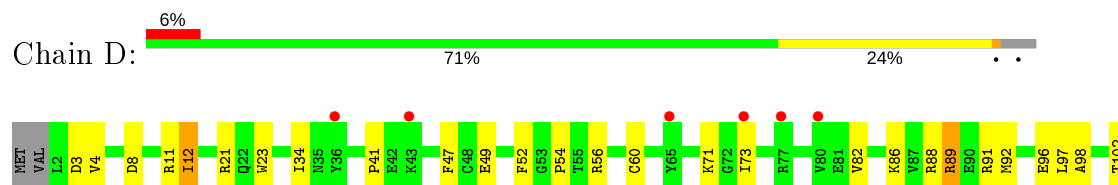
Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.30). The x-axis shows positions 1 to 200. The color scale at the top indicates conservation levels: 11% (red), 46% (green), 17% (yellow), and 37% (grey).

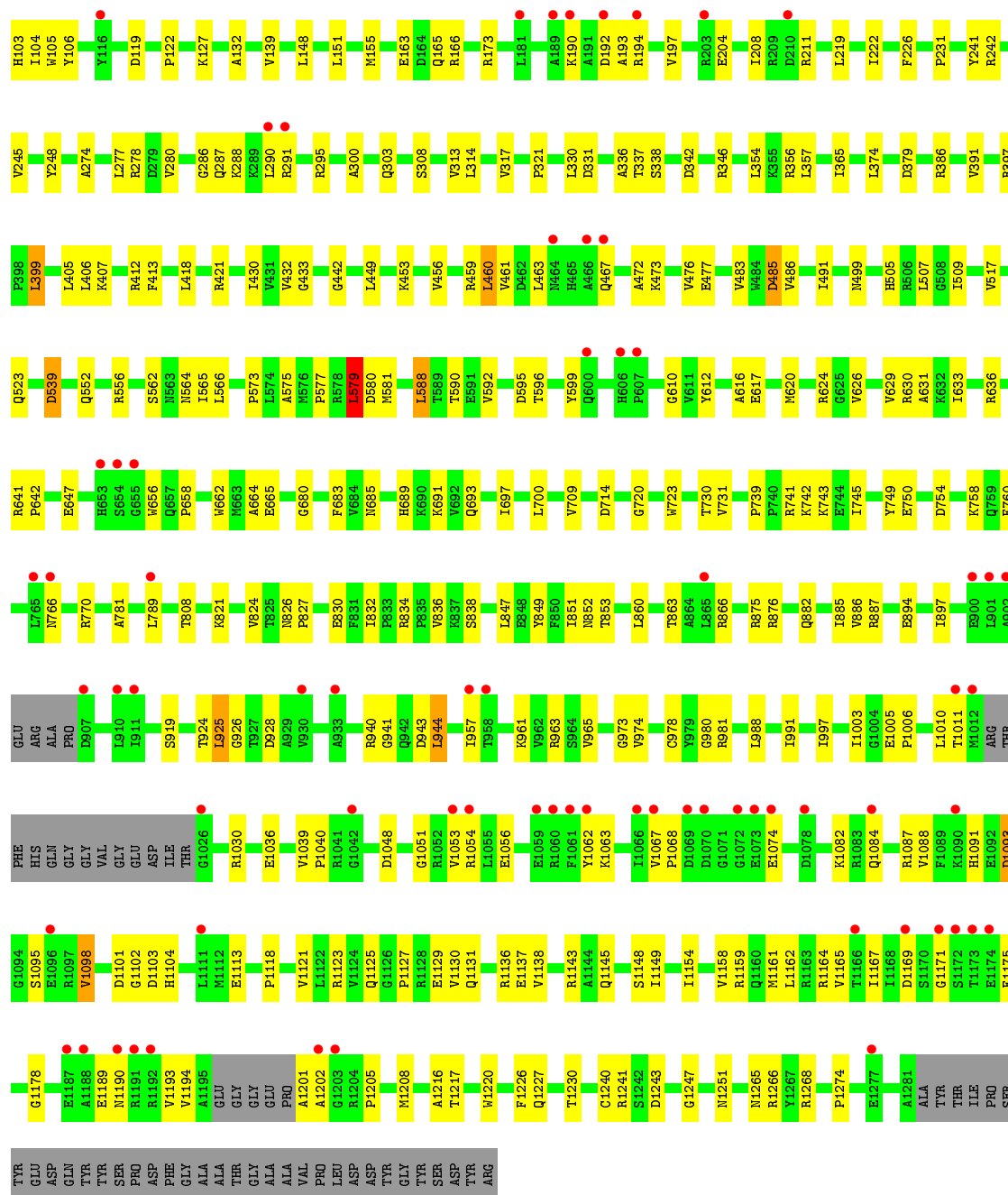
Position	Amino Acid	Information Content (bits)
1	GLU	0.05
2	GLU	0.05
3	VAL	0.05
4	ARG	0.05
5	ARG	0.05
6	R182	0.05
7	V69	0.05
8	K70	0.05
9	GLY	0.05
10	ALA	0.05
11	ASN	0.05
12	Tyr	0.05
13	E184	0.05
14	R185	0.05
15	ASN	0.05
16	R186	0.05
17	CYS	0.05
18	T187	0.05
19	VAL	0.05
20	D188	0.05
21	ARG	0.05
22	F189	0.05
23	ALA	0.05
24	D190	0.05
25	GLU	0.05
26	K191	0.05
27	GLY	0.05
28	VAL	0.05
29	TRP	0.05
30	L194	0.05
31	HIS	0.05
32	THR	0.05
33	SER	0.05
34	THR	0.05
35	VAL	0.05
36	K199	0.05
37	THR	0.05
38	R200	0.05
39	GLY	0.05
40	S201	0.05
41	GLU	0.05
42	I202	0.05
43	LEU	0.05
44	VAL	0.05
45	R205	0.05
46	ALA	0.05
47	ARG	0.05
48	THR	0.05
49	L208	0.05
50	GLU	0.05
51	THR	0.05
52	SER	0.05
53	L218	0.05
54	ASP	0.05
55	F219	0.05
56	LEU	0.05
57	G220	0.05
58	LEU	0.05
59	L221	0.05
60	ASP	0.05
61	A222	0.05
62	R223	0.05
63	ILE	0.05
64	ARG	0.05
65	E224	0.05
66	ASN	0.05
67	PHE	0.05
68	GLN	0.05
69	E229	0.05
70	GLN	0.05
71	E230	0.05
72	L231	0.05
73	LYS	0.05
74	SER	0.05
75	ILE	0.05
76	I234	0.05
77	ASP	0.05
78	G235	0.05
79	GLU	0.05
80	P236	0.05
81	VAL	0.05
82	SER	0.05
83	LYS	0.05
84	PRO	0.05
85	ALA	0.05
86	ILE	0.05
87	LYS	0.05
88	GLU	0.05
89	ALA	0.05
90	ASP	0.05
91	HIS	0.05
92	LEU	0.05
93	TYR	0.05
94	ILE	0.05
95	ALA	0.05
96	GLY	0.05
97	LEU	0.05
98	SER	0.05
99	PHE	0.05
100	LEU	0.05
101	ALA	0.05
102	LYS	0.05
103	LEU	0.05
104	ASP	0.05
105	PRO	0.05
106	ILE	0.05
107	SER	0.05
108	ASP	0.05
109	PRO	0.05
110	PRO	0.05
111	ASP	0.05
112	ASP	0.05
113	F63	0.05
114	V171	0.05
115	P170	0.05
116	H61	0.05
117	G58	0.05
118	ALA	0.05
119	ARG	0.05
120	ASN	0.05
121	Q151	0.05
122	L138	0.05
123	E137	0.05
124	L134	0.05
125	K133	0.05
126	G132	0.05
127	K131	0.05
128	D130	0.05
129	H129	0.05
130	L128	0.05
131	T127	0.05
132	D16	0.05
133	T15	0.05
134	L14	0.05
135	V13	0.05
136	D12	0.05
137	E11	

• Molecule 2: DNA-directed RNA polymerase subunit beta

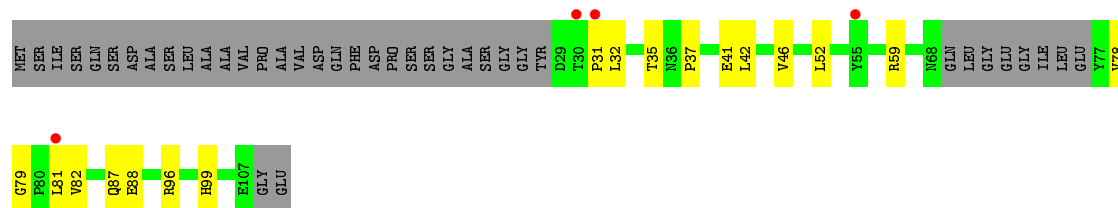


• Molecule 3: DNA-directed RNA polymerase subunit beta'

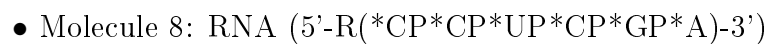
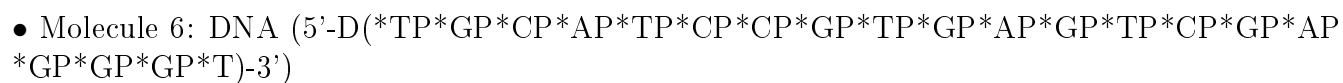




- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: ECF RNA polymerase sigma factor SigH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.14Å 161.00Å 128.85Å 90.00° 117.06° 90.00°	Depositor
Resolution (Å)	36.09 – 2.90 36.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.5 (36.09-2.90) 97.7 (36.72-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.210 , 0.256 0.210 , 0.257	Depositor DCC
R_{free} test set	2446 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25143	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/1679	0.52	0/2285
1	B	0.27	0/1722	0.49	0/2351
2	C	0.31	0/8889	0.50	0/12067
3	D	0.30	0/9984	0.50	1/13500 (0.0%)
4	E	0.27	0/577	0.50	0/786
5	F	0.28	0/1506	0.46	0/2041
6	H	0.70	0/462	0.95	0/713
7	G	0.66	0/533	1.11	3/823 (0.4%)
8	I	0.41	0/135	1.04	0/208
All	All	0.32	0/25487	0.54	4/34774 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	8	DG	OP1-P-O3'	-10.49	82.12	105.20
7	G	8	DG	OP2-P-O3'	-10.08	83.03	105.20
7	G	9	DG	OP1-P-OP2	7.77	131.26	119.60
3	D	579	LEU	CA-CB-CG	6.98	131.35	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	579	LEU	Mainchain

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	1654	0	1687	32	0
1	B	1696	0	1683	39	0
2	C	8731	0	8564	191	0
3	D	9822	0	9862	197	0
4	E	566	0	567	10	0
5	F	1477	0	1422	38	0
6	H	412	0	227	11	0
7	G	475	0	261	18	0
8	I	122	0	66	3	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	A	9	0	0	0	0
11	B	9	0	0	1	0
11	C	66	0	0	4	0
11	D	71	0	0	2	0
11	E	3	0	0	0	0
11	F	11	0	0	0	0
11	G	4	0	0	0	0
11	H	7	0	0	0	0
11	I	5	0	0	0	0
All	All	25143	0	24339	478	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (478) 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:485:PRO:HB2	3:D:853:THR:HG21	1.52	0.89
2:C:1051:MET:O	3:D:89:ARG:NH2	2.08	0.87
2:C:1053:THR:HG23	2:C:1055:GLN:H	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1024:THR:H	3:D:730:THR:HG21	1.43	0.84
3:D:505:HIS:HD2	3:D:1005:GLU:HG3	1.49	0.77
3:D:925:LEU:HG	3:D:944:LEU:HD21	1.67	0.77
4:E:59:ARG:HH22	4:E:79:GLY:HA3	1.49	0.77
3:D:1056:GLU:HB3	3:D:1063:LYS:HB3	1.66	0.76
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.69	0.74
4:E:37:PRO:HG2	4:E:42:LEU:HD11	1.70	0.74
3:D:629:VAL:HG12	3:D:630:ARG:HG3	1.71	0.73
3:D:346:ARG:NH2	5:F:53:ASP:OD1	2.21	0.73
6:H:11:DT:H2'	6:H:12:DG:C8	2.24	0.72
2:C:78:GLY:O	2:C:80:VAL:N	2.23	0.72
2:C:50:VAL:O	2:C:633:ARG:NH2	2.22	0.71
3:D:190:LYS:HE2	3:D:192:ASP:HB3	1.73	0.71
6:H:17:DG:N2	8:I:5:C:O2	2.18	0.71
3:D:875:ARG:NH2	3:D:1226:PHE:O	2.24	0.70
2:C:92:GLU:OE1	2:C:390:ARG:NH2	2.25	0.70
2:C:1046:THR:HG21	5:F:129:GLU:H	1.56	0.70
2:C:758:ASP:HB3	2:C:868:LEU:HD23	1.74	0.70
4:E:31:PRO:HB2	4:E:35:THR:HG23	1.75	0.68
3:D:981:ARG:HA	3:D:988:LEU:HA	1.76	0.68
6:H:16:DC:H2'	6:H:17:DG:H5''	1.76	0.68
4:E:46:VAL:HG21	4:E:52:LEU:HB2	1.76	0.68
2:C:395:ARG:NH1	7:G:10:DA:OP1	2.26	0.67
3:D:1118:PRO:HA	3:D:1121:VAL:HG12	1.77	0.67
1:B:102:PRO:HA	1:B:128:LEU:O	1.95	0.67
1:A:144:ARG:NH2	1:B:27:GLU:OE1	2.25	0.67
2:C:1046:THR:HG22	5:F:127:SER:HB2	1.77	0.66
2:C:74:ALA:HA	2:C:77:ARG:HD2	1.76	0.66
3:D:1062:TYR:HE1	3:D:1082:LYS:HA	1.61	0.66
2:C:357:VAL:HG13	2:C:360:GLY:HA3	1.78	0.66
2:C:751:HIS:CD2	2:C:877:ARG:HG3	2.31	0.66
2:C:815:THR:HG23	2:C:818:GLU:H	1.61	0.66
3:D:1167:ILE:HD13	3:D:1175:PHE:HB3	1.78	0.65
3:D:876:ARG:NH1	3:D:1036:GLU:OE1	2.28	0.65
3:D:885:ILE:HG13	3:D:887:ARG:HD3	1.79	0.65
3:D:173:ARG:NE	3:D:204:GLU:OE1	2.27	0.65
2:C:631:GLU:OE1	2:C:631:GLU:N	2.26	0.65
5:F:44:ALA:HB2	5:F:86:LEU:HD11	1.80	0.64
2:C:507:ASN:HD21	2:C:511:PHE:HB2	1.62	0.64
2:C:921:GLY:O	2:C:925:ARG:HG3	1.98	0.64
2:C:684:ALA:HA	2:C:706:PRO:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:97:LEU:HD22	3:D:374:LEU:HD21	1.79	0.64
3:D:973:GLY:O	3:D:1159:ARG:NH2	2.31	0.63
3:D:642:PRO:HG2	3:D:647:GLU:HB2	1.79	0.63
2:C:467:ARG:NH1	7:G:13:DT:O4'	2.32	0.63
2:C:582:SER:OG	2:C:583:PRO:O	2.16	0.63
3:D:163:GLU:HG2	3:D:166:ARG:HH21	1.62	0.63
3:D:1158:VAL:HG22	3:D:1161:MET:HE3	1.82	0.62
5:F:141:ILE:HD13	5:F:195:LEU:HD11	1.82	0.62
2:C:1136:GLU:OE1	3:D:11:ARG:NH2	2.34	0.61
3:D:47:PHE:O	3:D:88:ARG:NH2	2.33	0.61
2:C:571:VAL:HG22	2:C:572:PRO:HD2	1.82	0.60
1:A:87:SER:HB2	1:A:116:VAL:HG22	1.84	0.60
2:C:173:ARG:NH2	11:C:1202:HOH:O	2.34	0.60
3:D:562:SER:HA	3:D:565:ILE:HD11	1.83	0.60
2:C:822:ARG:NH2	2:C:829:ALA:O	2.34	0.60
7:G:13:DT:H1'	7:G:14:DG:H5''	1.83	0.60
3:D:824:VAL:HG11	3:D:852:ASN:HA	1.82	0.60
1:B:220:GLY:HA2	1:B:223:ARG:HG2	1.82	0.60
2:C:901:VAL:HG22	2:C:912:PRO:HG2	1.83	0.60
1:B:110:ILE:HD11	1:B:118:VAL:HG21	1.84	0.60
3:D:1274:PRO:HG3	4:E:78:VAL:HG11	1.84	0.59
3:D:866:ARG:HD3	3:D:1010:LEU:O	2.02	0.59
2:C:388:GLN:HG2	2:C:430:PHE:HB2	1.84	0.59
1:B:97:LEU:HB2	1:B:110:ILE:HG22	1.85	0.59
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.68	0.59
2:C:313:ARG:HD3	2:C:331:SER:HA	1.85	0.59
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.85	0.59
2:C:536:GLU:OE2	2:C:562:ARG:NH2	2.35	0.59
2:C:741:LEU:HD22	2:C:746:VAL:HG21	1.85	0.58
2:C:805:LYS:NZ	2:C:835:THR:OG1	2.36	0.58
2:C:1140:SER:HA	3:D:8:ASP:HB2	1.85	0.58
2:C:814:LEU:HD11	2:C:822:ARG:HH11	1.68	0.58
2:C:391:VAL:O	2:C:395:ARG:HG2	2.03	0.58
6:H:18:DA:H2'	6:H:19:DG:C8	2.38	0.58
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.38	0.58
2:C:919:THR:HG23	3:D:731:VAL:HG23	1.86	0.58
3:D:1088:VAL:HA	3:D:1098:VAL:HA	1.84	0.58
2:C:756:GLU:OE1	2:C:870:ARG:NH1	2.37	0.58
2:C:96:ILE:HD13	2:C:397:GLU:HG3	1.86	0.58
2:C:1091:ILE:HD12	2:C:1102:VAL:HG21	1.84	0.58
3:D:539:ASP:OD1	8:I:7:A:O3'	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.68	0.57
3:D:300:ALA:HA	3:D:303:GLN:HG2	1.86	0.57
5:F:160:ASP:OD1	5:F:188:ARG:NH1	2.33	0.57
3:D:505:HIS:CD2	3:D:1005:GLU:HG3	2.37	0.57
1:A:197:GLU:OE1	2:C:996:ARG:NH2	2.30	0.57
2:C:282:ARG:HD3	2:C:285:GLU:HG2	1.86	0.57
2:C:560:LEU:HD11	2:C:568:VAL:HB	1.87	0.57
2:C:663:ASP:OD2	2:C:695:ARG:NH2	2.37	0.56
2:C:809:LYS:HA	5:F:122:SER:HB2	1.87	0.56
6:H:7:DT:H1'	6:H:8:DC:H5'	1.86	0.56
3:D:499:ASN:HB2	3:D:509:ILE:HG12	1.88	0.56
2:C:628:THR:HG23	2:C:975:PRO:HA	1.87	0.56
2:C:658:ILE:HD13	2:C:702:ILE:HG22	1.87	0.56
3:D:386:ARG:HH12	3:D:1230:THR:HG21	1.71	0.56
3:D:12:ILE:HD11	3:D:1220:TRP:CE3	2.41	0.56
3:D:34:ILE:HG22	3:D:41:PRO:HA	1.87	0.56
3:D:92:MET:HG3	3:D:321:PRO:HD3	1.88	0.56
2:C:239:LYS:NZ	2:C:262:LEU:HD11	2.21	0.56
2:C:815:THR:HG22	2:C:818:GLU:HB2	1.87	0.56
2:C:126:ASP:HA	2:C:170:GLY:HA3	1.87	0.56
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.87	0.56
3:D:139:VAL:HG12	3:D:231:PRO:HD3	1.87	0.56
1:B:9:LEU:HD13	1:B:23:ILE:HG12	1.87	0.55
2:C:587:VAL:HG13	2:C:591:THR:HB	1.87	0.55
2:C:140:ILE:HG12	2:C:147:ILE:HG12	1.88	0.55
2:C:792:ILE:HG13	2:C:850:ILE:HD12	1.88	0.55
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.89	0.55
3:D:1265:ASN:HA	3:D:1268:ARG:HG2	1.89	0.55
3:D:832:ILE:HG22	3:D:834:ARG:H	1.72	0.55
2:C:239:LYS:HZ2	2:C:262:LEU:HD11	1.71	0.55
3:D:1136:ARG:HH21	3:D:1143:ARG:HH22	1.52	0.55
2:C:68:PRO:HA	2:C:71:ARG:HB3	1.89	0.55
3:D:739:PRO:HG2	3:D:742:LYS:HB2	1.89	0.55
4:E:41:GLU:OE1	4:E:99:HIS:NE2	2.30	0.55
6:H:3:DT:H2''	6:H:4:DG:C8	2.42	0.54
3:D:21:ARG:NE	3:D:96:GLU:OE2	2.32	0.54
3:D:1054:ARG:NH1	3:D:1056:GLU:OE1	2.40	0.54
5:F:39:GLN:OE1	5:F:79:LYS:NZ	2.34	0.54
2:C:1041:ILE:O	2:C:1060:LYS:NZ	2.34	0.54
2:C:454:ARG:HH11	2:C:499:SER:HB3	1.72	0.54
2:C:516:TYR:HB3	2:C:578:TYR:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:194:ARG:HA	3:D:197:VAL:HG22	1.90	0.54
1:A:213:LYS:HB2	1:B:223:ARG:HE	1.74	0.53
2:C:622:GLU:HB3	2:C:717:LYS:HD3	1.89	0.53
3:D:421:ARG:NH1	6:H:17:DG:OP1	2.40	0.53
6:H:5:DC:H2"	6:H:6:DA:C8	2.43	0.53
1:A:222:ALA:HB1	1:B:208:LEU:HG	1.91	0.53
2:C:899:LEU:HB2	2:C:904:MET:CE	2.38	0.53
3:D:1087:ARG:NH1	3:D:1113:GLU:OE2	2.39	0.53
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.90	0.53
2:C:615:ALA:HB3	2:C:715:LEU:HD22	1.91	0.53
3:D:453:LYS:NZ	5:F:129:GLU:OE2	2.42	0.53
2:C:729:HIS:CD2	2:C:897:LYS:HD2	2.43	0.53
2:C:741:LEU:HA	2:C:746:VAL:HG13	1.90	0.53
5:F:148:LEU:HD13	5:F:191:LEU:HD13	1.91	0.53
2:C:635:ALA:HB2	2:C:713:MET:HG2	1.90	0.53
2:C:767:GLU:OE2	2:C:807:THR:OG1	2.25	0.53
3:D:963:ARG:NH1	3:D:978:CYS:SG	2.82	0.53
2:C:487:GLU:OE2	2:C:613:ARG:NH2	2.42	0.52
3:D:1091:HIS:HB3	3:D:1095:SER:O	2.10	0.52
1:A:146:TYR:CD2	2:C:743:GLU:HG2	2.44	0.52
2:C:880:SER:N	2:C:883:ASP:OD2	2.41	0.52
3:D:739:PRO:HD3	3:D:789:LEU:HD13	1.90	0.52
2:C:1117:ILE:HD13	3:D:3:ASP:HB2	1.90	0.52
3:D:1164:ARG:HD2	3:D:1208:MET:SD	2.50	0.52
3:D:539:ASP:CG	8:I:7:A:O3'	2.48	0.52
1:B:75:GLU:HG2	3:D:636:ARG:NH2	2.25	0.52
3:D:683:PHE:HE1	3:D:685:ASN:HB2	1.75	0.52
1:A:72:ASP:N	1:A:72:ASP:OD1	2.42	0.52
3:D:928:ASP:OD1	3:D:940:ARG:N	2.36	0.52
2:C:862:PRO:HG2	2:C:865:VAL:HG21	1.92	0.51
1:B:231:GLY:HA3	11:B:408:HOH:O	2.11	0.51
2:C:352:GLN:O	2:C:365:VAL:HB	2.10	0.51
2:C:395:ARG:HH22	7:G:10:DA:H5"	1.75	0.51
5:F:79:LYS:HE3	7:G:7:DG:C8	2.46	0.51
3:D:943:ASP:OD1	3:D:981:ARG:HD2	2.11	0.51
1:B:124:HIS:CE1	1:B:127:THR:HG23	2.46	0.51
3:D:1167:ILE:O	3:D:1178:GLY:N	2.41	0.51
2:C:442:GLN:H	2:C:680:HIS:HD2	1.59	0.51
1:B:98:ARG:HA	1:B:134:LEU:O	2.10	0.51
3:D:1006:PRO:HG3	3:D:1149:ILE:HD11	1.93	0.51
3:D:23:TRP:HB3	3:D:92:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TYR:O	3:D:624:ARG:NE	2.44	0.50
2:C:46:GLU:OE1	2:C:503:TYR:OH	2.28	0.50
3:D:356:ARG:NH2	5:F:60:GLU:OE1	2.43	0.50
2:C:326:GLU:N	2:C:327:PRO:HD3	2.27	0.50
3:D:1190:ASN:HD21	3:D:1201:ALA:HB1	1.77	0.50
1:B:218:LEU:O	1:B:221:LEU:HB2	2.12	0.50
3:D:599:TYR:HB2	3:D:610:GLY:HA3	1.94	0.50
2:C:484:CYS:HB2	2:C:588:SER:HB3	1.93	0.50
4:E:32:LEU:O	4:E:35:THR:HG22	2.12	0.50
2:C:737:LEU:HD22	2:C:741:LEU:HD12	1.94	0.50
3:D:1053:VAL:HG12	3:D:1103:ASP:O	2.12	0.50
3:D:190:LYS:HD3	3:D:193:ALA:HB2	1.94	0.50
1:A:175:THR:HG22	1:A:195:ASP:HB3	1.93	0.49
2:C:632:LEU:HB2	2:C:712:GLU:HG2	1.93	0.49
2:C:854:SER:O	2:C:859:ASP:HB2	2.12	0.49
3:D:242:ARG:HA	3:D:245:VAL:HG22	1.93	0.49
2:C:470:LEU:HD12	2:C:470:LEU:H	1.77	0.49
2:C:758:ASP:OD1	5:F:120:HIS:NE2	2.45	0.49
3:D:365:ILE:HD12	5:F:34:ILE:HD13	1.93	0.49
2:C:1104:GLU:HG2	2:C:1108:LYS:HE2	1.93	0.49
2:C:41:PHE:CG	2:C:980:ALA:HB2	2.48	0.49
3:D:1011:THR:O	3:D:1145:GLN:NE2	2.46	0.49
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.94	0.49
3:D:689:HIS:CE1	3:D:691:LYS:HE2	2.47	0.49
3:D:1030:ARG:NH2	3:D:1137:GLU:OE1	2.40	0.49
3:D:847:LEU:O	3:D:851:ILE:HG12	2.12	0.49
3:D:86:LYS:O	3:D:89:ARG:HG2	2.13	0.49
3:D:926:GLY:O	3:D:940:ARG:NH2	2.40	0.49
2:C:113:ASP:HB3	2:C:132:PRO:HD2	1.94	0.49
7:G:9:DG:H2"	7:G:10:DA:C8	2.48	0.49
2:C:38:ARG:HA	2:C:971:ILE:HG22	1.93	0.49
1:A:99:LYS:HG2	1:A:105:VAL:HG22	1.93	0.49
2:C:412:ILE:HD12	2:C:417:LEU:HD21	1.95	0.49
2:C:583:PRO:O	2:C:584:ARG:HG2	2.12	0.49
2:C:810:GLY:H	3:D:56:ARG:NH2	2.10	0.49
3:D:219:LEU:HA	3:D:222:ILE:HD12	1.95	0.49
2:C:207:SER:OG	2:C:309:ALA:N	2.46	0.49
3:D:1003:ILE:O	11:D:2101:HOH:O	2.20	0.49
3:D:552:GLN:O	3:D:556:ARG:HG3	2.13	0.49
3:D:73:ILE:O	3:D:82:VAL:HG12	2.13	0.49
2:C:532:THR:HG22	2:C:535:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:DG:H2"	7:G:12:DC:H5"	1.94	0.48
2:C:762:THR:HG22	2:C:764:LEU:H	1.79	0.48
3:D:357:LEU:HD21	5:F:63:VAL:HG22	1.96	0.48
2:C:265:ASP:OD1	2:C:266:ASN:N	2.46	0.48
3:D:1226:PHE:CD2	3:D:1227:GLN:HG2	2.48	0.48
3:D:579:LEU:HD23	3:D:808:THR:HB	1.95	0.48
3:D:1274:PRO:HB3	4:E:81:LEU:HD11	1.94	0.48
2:C:139:PHE:CZ	2:C:412:ILE:HD11	2.49	0.48
3:D:754:ASP:O	3:D:758:LYS:HG2	2.12	0.48
2:C:1135:VAL:HG13	3:D:12:ILE:HG23	1.95	0.48
3:D:208:ILE:HG23	3:D:211:ARG:HH22	1.78	0.48
1:A:3:ILE:HG13	1:A:4:SER:H	1.78	0.48
3:D:750:GLU:OE1	3:D:834:ARG:NH2	2.47	0.48
5:F:22:ASP:O	5:F:26:THR:HG23	2.14	0.48
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.96	0.48
3:D:459:ARG:NH2	4:E:87:GLN:OE1	2.47	0.48
2:C:441:ASP:HA	2:C:680:HIS:NE2	2.29	0.48
3:D:876:ARG:HG2	3:D:1226:PHE:HZ	1.78	0.48
3:D:882:GLN:HG3	3:D:997:ILE:HD11	1.96	0.48
2:C:1068:PHE:HZ	2:C:1076:MET:HE2	1.79	0.47
3:D:449:LEU:HD11	3:D:476:VAL:HG13	1.96	0.47
2:C:467:ARG:HA	7:G:15:DT:H5'	1.95	0.47
1:A:149:ALA:HB1	1:A:163:PRO:HB2	1.95	0.47
2:C:199:LEU:HG	2:C:216:VAL:HG23	1.96	0.47
2:C:815:THR:CG2	2:C:818:GLU:HB2	2.44	0.47
2:C:173:ARG:NH1	2:C:437:SER:O	2.47	0.47
7:G:13:DT:H2"	7:G:14:DG:OP2	2.15	0.47
3:D:566:LEU:HA	3:D:573:PRO:HA	1.95	0.47
1:A:86:SER:HG	1:A:119:HIS:HE2	1.60	0.47
2:C:616:VAL:HG13	2:C:1032:LYS:O	2.14	0.47
2:C:549:ASP:OD1	2:C:553:ARG:N	2.27	0.47
3:D:683:PHE:CE1	3:D:685:ASN:HB2	2.50	0.47
1:A:7:PRO:HA	1:A:25:PRO:HD2	1.96	0.47
3:D:1062:TYR:CE1	3:D:1082:LYS:HA	2.45	0.47
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.47	0.47
3:D:612:TYR:HD2	3:D:617:GLU:HG2	1.79	0.47
3:D:1068:PRO:HD3	3:D:1074:GLU:HA	1.96	0.47
3:D:847:LEU:H	3:D:847:LEU:HD12	1.80	0.47
3:D:287:GLN:HA	3:D:290:LEU:HD12	1.96	0.47
2:C:448:GLY:O	2:C:452:LYS:HG3	2.14	0.46
2:C:598:GLU:OE1	2:C:598:GLU:N	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:633:ILE:O	3:D:665:GLU:HA	2.15	0.46
2:C:165:THR:HB	2:C:173:ARG:O	2.15	0.46
2:C:273:ALA:O	2:C:277:ILE:HG12	2.16	0.46
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.96	0.46
3:D:127:LYS:HA	3:D:132:ALA:HB3	1.96	0.46
3:D:596:THR:HG22	3:D:626:VAL:O	2.15	0.46
3:D:760:PHE:CG	3:D:770:ARG:HD3	2.50	0.46
2:C:1154:ASP:OD2	2:C:1157:ARG:NH2	2.48	0.46
2:C:216:VAL:HG21	2:C:349:HIS:NE2	2.30	0.46
3:D:280:VAL:HG13	3:D:288:LYS:HE3	1.98	0.46
2:C:1160:ALA:HA	2:C:1164:ILE:HB	1.97	0.46
2:C:1087:GLU:HG3	2:C:1091:ILE:HD11	1.98	0.46
3:D:1101:ASP:OD1	3:D:1102:GLY:N	2.48	0.46
3:D:1136:ARG:HD2	3:D:1136:ARG:HA	1.71	0.46
3:D:460:LEU:HD12	3:D:486:VAL:HG21	1.98	0.46
6:H:15:DT:H2'	6:H:16:DC:C6	2.51	0.46
2:C:628:THR:HG22	2:C:629:GLY:H	1.81	0.46
2:C:632:LEU:HA	2:C:712:GLU:HA	1.97	0.46
2:C:981:GLN:NE2	11:C:1201:HOH:O	2.30	0.46
3:D:689:HIS:O	3:D:693:GLN:HG3	2.16	0.46
1:B:128:LEU:HD21	1:B:134:LEU:HB2	1.98	0.46
2:C:239:LYS:HZ3	2:C:268:VAL:HA	1.79	0.46
2:C:60:SER:OG	2:C:382:GLY:N	2.36	0.46
2:C:879:ILE:HD12	2:C:1032:LYS:HE3	1.98	0.46
3:D:461:VAL:HG23	3:D:472:ALA:HB2	1.97	0.46
2:C:1076:MET:HE2	2:C:1076:MET:HB2	1.86	0.45
2:C:229:LYS:HD3	2:C:229:LYS:HA	1.75	0.45
2:C:766:ALA:O	2:C:830:ARG:NH1	2.49	0.45
3:D:98:ALA:HB3	3:D:354:LEU:HD23	1.98	0.45
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.97	0.45
3:D:581:MET:HA	3:D:720:GLY:HA3	1.97	0.45
5:F:41:TYR:HB2	5:F:58:LEU:HD22	1.97	0.45
6:H:4:DG:H2''	6:H:5:DC:O5'	2.15	0.45
3:D:1136:ARG:NH2	3:D:1143:ARG:HH22	2.14	0.45
2:C:225:ARG:HG3	2:C:229:LYS:O	2.17	0.45
2:C:731:TYR:HB3	3:D:432:VAL:HG21	1.98	0.45
3:D:924:THR:HG22	3:D:941:GLY:HA2	1.98	0.45
1:B:170:PRO:HB2	1:B:202:ILE:HD11	1.97	0.45
2:C:1127:GLU:OE1	3:D:412:ARG:HG3	2.16	0.45
2:C:343:GLU:HA	2:C:346:VAL:HG22	1.98	0.45
2:C:347:ARG:HD2	2:C:355:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:520:VAL:O	2:C:523:VAL:HG12	2.17	0.45
3:D:1131:GLN:HG3	3:D:1162:LEU:HD12	1.99	0.45
3:D:662:TRP:CZ3	3:D:664:ALA:HB2	2.52	0.45
2:C:1104:GLU:HG3	5:F:136:LEU:HD21	1.99	0.45
3:D:741:ARG:O	3:D:745:ILE:HG13	2.16	0.45
3:D:1093:ASP:OD2	3:D:1104:HIS:ND1	2.44	0.45
3:D:826:ASN:OD1	3:D:827:PRO:HD2	2.17	0.45
5:F:154:MET:HG3	5:F:158:TYR:CE2	2.51	0.45
5:F:166:TYR:HA	5:F:169:ILE:HG22	1.99	0.45
2:C:771:ARG:HG2	2:C:771:ARG:O	2.17	0.45
2:C:288:THR:HB	2:C:291:SER:OG	2.17	0.45
2:C:751:HIS:HD2	2:C:877:ARG:HG3	1.81	0.45
2:C:1133:LEU:HD11	3:D:105:TRP:CZ3	2.52	0.45
3:D:342:ASP:O	3:D:346:ARG:HG3	2.16	0.45
3:D:980:GLY:O	3:D:988:LEU:HD12	2.17	0.45
2:C:775:ASN:HA	5:F:202:ARG:HB3	1.99	0.45
7:G:20:DG:H2"	7:G:21:DA:C8	2.52	0.45
2:C:389:ILE:HG12	2:C:427:ILE:HD11	1.97	0.44
2:C:596:PHE:HB3	2:C:599:HIS:CD2	2.52	0.44
3:D:226:PHE:CE1	3:D:248:TYR:HB3	2.52	0.44
3:D:616:ALA:O	3:D:620:MET:HG3	2.17	0.44
3:D:641:ARG:HD3	3:D:680:GLY:O	2.17	0.44
5:F:29:PHE:HB2	5:F:69:PHE:CE2	2.51	0.44
1:B:100:GLN:HA	1:B:133:LYS:HA	1.99	0.44
1:B:107:ALA:HB3	1:B:121:PRO:HA	2.00	0.44
3:D:1171:GLY:H	3:D:1201:ALA:N	2.15	0.44
3:D:287:GLN:OE1	3:D:287:GLN:N	2.51	0.44
3:D:592:VAL:HB	3:D:595:ASP:HB2	1.99	0.44
3:D:894:GLU:O	3:D:961:LYS:NZ	2.45	0.44
2:C:435:GLN:NE2	11:C:1205:HOH:O	2.48	0.44
2:C:54:LEU:O	2:C:58:THR:HG23	2.18	0.44
2:C:792:ILE:H	2:C:792:ILE:HD12	1.82	0.44
3:D:507:LEU:HD11	3:D:564:ASN:HB3	2.00	0.44
3:D:826:ASN:HB2	3:D:830:GLU:O	2.17	0.44
7:G:14:DG:H4'	7:G:15:DT:OP1	2.16	0.44
1:A:93:VAL:HG11	1:A:116:VAL:HG21	2.00	0.44
1:A:81:LYS:NZ	1:A:165:ASP:HB2	2.32	0.44
1:B:182:ARG:CB	1:B:189:PHE:HB2	2.47	0.44
3:D:1048:ASP:OD2	3:D:1123:ARG:NH2	2.40	0.44
3:D:1051:GLY:HA3	3:D:1067:VAL:O	2.18	0.44
2:C:583:PRO:C	2:C:585:GLN:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:85:GLY:O	2:C:89:VAL:HG23	2.18	0.44
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.47	0.44
1:A:78:LEU:HD23	2:C:620:ARG:NH1	2.32	0.44
2:C:737:LEU:HD11	2:C:885:LEU:HD21	2.00	0.44
3:D:274:ALA:O	3:D:278:ARG:HG3	2.17	0.44
3:D:97:LEU:HD11	3:D:317:VAL:HG23	2.00	0.44
3:D:656:TRP:CH2	3:D:658:PRO:HA	2.53	0.44
7:G:6:DT:H2''	7:G:7:DG:O5'	2.17	0.44
2:C:215:ASP:N	2:C:215:ASP:OD1	2.50	0.44
1:B:146:TYR:CE2	3:D:617:GLU:HG3	2.52	0.43
2:C:1163:GLY:O	5:F:153:ARG:HD2	2.18	0.43
2:C:313:ARG:HB2	2:C:331:SER:HB2	1.99	0.43
3:D:391:VAL:HG12	3:D:399:LEU:HD22	2.00	0.43
3:D:204:GLU:O	3:D:208:ILE:HG13	2.17	0.43
3:D:886:VAL:HB	3:D:991:ILE:O	2.18	0.43
3:D:122:PRO:HG2	7:G:22:DT:H3'	2.01	0.43
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.84	0.43
3:D:1217:THR:O	3:D:1241:ARG:NH2	2.52	0.43
3:D:965:VAL:HG13	3:D:974:VAL:HG11	2.00	0.43
2:C:899:LEU:HB2	2:C:904:MET:HE1	2.00	0.43
3:D:155:MET:CE	3:D:219:LEU:HB3	2.48	0.43
3:D:473:LYS:O	3:D:477:GLU:HG3	2.18	0.43
4:E:88:GLU:OE2	4:E:96:ARG:NH1	2.51	0.43
1:A:213:LYS:HZ3	1:B:223:ARG:HH21	1.66	0.43
3:D:432:VAL:HG13	3:D:433:GLY:H	1.83	0.43
3:D:430:ILE:HD11	3:D:539:ASP:HB2	2.00	0.43
3:D:588:LEU:HG	3:D:723:TRP:CD1	2.53	0.43
2:C:320:LEU:C	2:C:363:VAL:HG11	2.39	0.43
3:D:397:ARG:HH21	5:F:107:GLU:HG2	1.82	0.43
5:F:81:TRP:O	5:F:85:ILE:HG13	2.19	0.43
3:D:693:GLN:O	3:D:697:ILE:HG13	2.18	0.43
1:A:66:VAL:O	1:A:69:VAL:HG22	2.18	0.43
2:C:240:ALA:HA	2:C:274:LEU:HG	2.01	0.43
2:C:399:VAL:O	2:C:403:ARG:HG2	2.19	0.43
2:C:730:ASN:N	2:C:730:ASN:OD1	2.48	0.43
1:B:176:TYR:HB3	1:B:194:LEU:HD23	2.01	0.43
3:D:330:LEU:HD11	3:D:336:ALA:HB2	2.00	0.43
5:F:59:GLN:O	5:F:63:VAL:HG23	2.19	0.43
1:A:152:ASN:HA	1:A:157:ALA:HB3	2.01	0.43
1:A:46:ILE:HD12	1:A:210:SER:OG	2.19	0.43
2:C:891:ASN:HD21	2:C:1028:MET:CE	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:GLN:HG3	2:C:679:ASN:HB2	2.00	0.42
2:C:1138:LEU:HD11	3:D:11:ARG:NH1	2.33	0.42
7:G:10:DA:H2"	7:G:11:DG:H5"	2.01	0.42
2:C:371:ASP:OD1	7:G:14:DG:N2	2.51	0.42
1:B:69:VAL:HG22	1:B:128:LEU:HD23	2.01	0.42
1:B:7:PRO:HB3	1:B:25:PRO:O	2.19	0.42
2:C:389:ILE:O	2:C:393:MET:HG2	2.18	0.42
2:C:163:LYS:HD2	2:C:639:GLY:HA3	2.02	0.42
3:D:1162:LEU:HD23	3:D:1162:LEU:HA	1.92	0.42
3:D:1189:GLU:O	3:D:1193:VAL:HG23	2.19	0.42
11:C:1238:HOH:O	3:D:418:LEU:HD13	2.20	0.42
1:A:146:TYR:CG	2:C:743:GLU:HG2	2.54	0.42
5:F:104:TYR:HA	5:F:105:PRO:HD3	1.87	0.42
1:A:173:LYS:HD3	2:C:909:ASP:O	2.20	0.42
3:D:577:PRO:HB3	3:D:581:MET:HB2	2.02	0.42
1:A:61:HIS:HE1	1:A:63:PHE:O	2.02	0.42
1:B:28:PRO:HB3	1:B:188:ASP:O	2.20	0.42
2:C:1095:ASP:O	2:C:1099:ARG:HG3	2.19	0.42
2:C:439:PHE:CE2	2:C:679:ASN:HB3	2.55	0.42
3:D:1125:GLN:NE2	3:D:1129:GLU:HG2	2.35	0.42
1:B:101:GLY:N	1:B:132:GLY:O	2.53	0.42
1:A:205:ARG:HG2	1:B:225:LEU:HD22	2.02	0.42
2:C:324:VAL:HG11	2:C:361:VAL:HG21	2.02	0.42
3:D:151:LEU:HD22	3:D:248:TYR:HE1	1.85	0.42
3:D:749:TYR:CG	3:D:781:ALA:HB2	2.55	0.42
5:F:44:ALA:HB1	5:F:57:LEU:HD23	2.02	0.42
5:F:79:LYS:HE3	7:G:7:DG:H8	1.84	0.42
1:B:94:THR:O	1:B:113:PRO:HG3	2.20	0.42
3:D:1039:VAL:HA	3:D:1040:PRO:HD3	1.89	0.42
3:D:241:TYR:O	3:D:245:VAL:HG13	2.20	0.42
3:D:119:ASP:HB2	3:D:295:ARG:NH2	2.35	0.42
5:F:82:LEU:HD23	5:F:85:ILE:HD12	2.01	0.42
3:D:460:LEU:HD21	3:D:483:VAL:HG12	2.02	0.42
5:F:25:LEU:HD12	5:F:70:ARG:NH1	2.35	0.42
5:F:40:LEU:HD11	5:F:82:LEU:HB3	2.02	0.42
2:C:825:PHE:CE2	5:F:192:ARG:HG3	2.55	0.42
1:A:95:MET:HE2	1:A:95:MET:HB3	1.91	0.41
2:C:617:PRO:HA	2:C:707:CYS:SG	2.60	0.41
3:D:71:LYS:HB3	3:D:71:LYS:HE3	1.80	0.41
5:F:26:THR:O	5:F:30:GLU:HG3	2.20	0.41
1:B:186:ARG:O	1:B:187:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:405:LEU:HA	3:D:405:LEU:HD23	1.94	0.41
2:C:1017:GLU:H	2:C:1017:GLU:HG2	1.66	0.41
3:D:641:ARG:HG3	3:D:642:PRO:HD2	2.02	0.41
2:C:32:VAL:HG11	2:C:632:LEU:HD11	2.01	0.41
2:C:502:VAL:HG23	2:C:587:VAL:O	2.20	0.41
2:C:72:GLU:O	2:C:76:GLU:N	2.50	0.41
2:C:86:LEU:HD21	2:C:389:ILE:HD13	2.02	0.41
1:A:213:LYS:NZ	1:B:223:ARG:HH21	2.19	0.41
7:G:25:DA:OP2	7:G:25:DA:H3'	2.20	0.41
1:A:11:GLU:OE1	1:A:205:ARG:HD3	2.19	0.41
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.87	0.41
2:C:223:GLY:HA3	2:C:231:ARG:HE	1.86	0.41
1:A:57:ASP:HB2	1:A:135:GLU:HB3	2.03	0.41
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.84	0.41
2:C:212:LEU:HD22	2:C:333:LEU:HD21	2.02	0.41
3:D:12:ILE:HD11	3:D:1220:TRP:CZ3	2.55	0.41
1:B:184:GLU:HG2	3:D:485:ASP:OD2	2.21	0.41
3:D:700:LEU:HB3	3:D:709:VAL:HG22	2.02	0.41
5:F:34:ILE:HA	5:F:37:LEU:HD23	2.03	0.41
6:H:17:DG:H8	6:H:17:DG:H5''	1.86	0.41
1:B:172:LEU:HD13	1:B:199:LYS:HG3	2.02	0.41
2:C:185:VAL:HG22	2:C:204:VAL:HG22	2.01	0.41
3:D:413:PHE:HB2	11:D:2104:HOH:O	2.20	0.41
3:D:887:ARG:HA	3:D:887:ARG:HD2	1.95	0.41
3:D:52:PHE:O	3:D:91:ARG:HD2	2.21	0.41
1:B:24:GLU:HB2	1:B:191:LYS:HG3	2.03	0.41
2:C:776:ILE:HG23	2:C:780:VAL:HB	2.02	0.41
2:C:771:ARG:NH1	2:C:785:ASP:O	2.49	0.41
3:D:287:GLN:O	3:D:291:ARG:HG2	2.20	0.41
1:B:112:PRO:HA	1:B:113:PRO:HD2	1.92	0.41
2:C:507:ASN:ND2	2:C:511:PHE:HB2	2.32	0.41
3:D:49:GLU:HG2	3:D:54:PRO:HA	2.01	0.41
5:F:33:ALA:O	5:F:36:LEU:HB2	2.21	0.41
5:F:80:ALA:HA	7:G:7:DG:O6	2.20	0.41
1:A:199:LYS:O	1:A:200:ASN:HB2	2.21	0.41
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.88	0.41
1:A:46:ILE:HD11	1:A:211:ALA:HB2	2.03	0.41
2:C:223:GLY:HA3	2:C:231:ARG:HH21	1.85	0.41
2:C:90:LEU:HD12	2:C:110:PRO:HG3	2.03	0.41
3:D:12:ILE:HD11	3:D:1220:TRP:CD2	2.56	0.41
3:D:277:LEU:HD21	3:D:295:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLN:HB3	2:C:795:GLU:OE2	2.22	0.40
2:C:454:ARG:O	2:C:455:LEU:HD23	2.20	0.40
2:C:149:SER:OG	2:C:150:GLN:N	2.54	0.40
2:C:465:ARG:NH2	2:C:493:ASN:OD1	2.54	0.40
2:C:563:ARG:N	2:C:567:GLU:O	2.53	0.40
2:C:942:SER:OG	2:C:992:THR:HG23	2.20	0.40
3:D:1127:PRO:HA	3:D:1130:VAL:HG23	2.03	0.40
3:D:925:LEU:HD23	3:D:925:LEU:HA	1.92	0.40
1:B:10:SER:HB3	1:B:22:VAL:HG23	2.03	0.40
2:C:217:ASP:OD2	2:C:231:ARG:NH1	2.54	0.40
2:C:278:TYR:CZ	2:C:282:ARG:HD2	2.55	0.40
2:C:484:CYS:CB	2:C:588:SER:HB3	2.51	0.40
3:D:1138:VAL:HG12	3:D:1154:ILE:HD13	2.02	0.40
3:D:286:GLY:O	3:D:290:LEU:HG	2.21	0.40
1:B:30:PHE:HA	1:B:33:THR:HB	2.03	0.40
2:C:1008:ALA:O	2:C:1022:PRO:HA	2.21	0.40
2:C:262:LEU:HA	2:C:265:ASP:HB2	2.02	0.40
2:C:271:ASP:N	2:C:271:ASP:OD1	2.52	0.40
2:C:825:PHE:CZ	5:F:199:ALA:HB2	2.56	0.40
3:D:1220:TRP:NE1	3:D:1243:ASP:HB2	2.37	0.40
3:D:821:LYS:HB3	3:D:836:VAL:HB	2.03	0.40
2:C:150:GLN:NE2	2:C:413:THR:OG1	2.49	0.40
2:C:749:SER:OG	2:C:751:HIS:NE2	2.46	0.40
3:D:766:ASN:O	3:D:770:ARG:N	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	215/368 (58%)	210 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	228/368 (62%)	213 (93%)	15 (7%)	0	100	100
2	C	1134/1174 (97%)	1084 (96%)	50 (4%)	0	100	100
3	D	1250/1317 (95%)	1205 (96%)	45 (4%)	0	100	100
4	E	67/110 (61%)	62 (92%)	5 (8%)	0	100	100
5	F	184/218 (84%)	180 (98%)	4 (2%)	0	100	100
All	All	3078/3555 (87%)	2954 (96%)	124 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/315 (59%)	174 (94%)	12 (6%)	17	45
1	B	181/315 (58%)	171 (94%)	10 (6%)	21	53
2	C	940/995 (94%)	899 (96%)	41 (4%)	28	61
3	D	1040/1096 (95%)	997 (96%)	43 (4%)	30	64
4	E	62/90 (69%)	61 (98%)	1 (2%)	62	86
5	F	149/175 (85%)	144 (97%)	5 (3%)	37	71
All	All	2558/2986 (86%)	2446 (96%)	112 (4%)	28	61

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	10	SER
1	A	51	VAL
1	A	85	VAL
1	A	88	GLU
1	A	93	VAL
1	A	100	GLN
1	A	111	VAL

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Mol	Chain	Res	Type
1	A	133	LYS
1	A	146	TYR
1	A	208	LEU
1	A	213	LYS
1	B	11	GLU
1	B	16	ASP
1	B	34	LEU
1	B	45	SER
1	B	64	THR
1	B	65	THR
1	B	74	THR
1	B	171	VAL
1	B	172	LEU
1	B	175	THR
2	C	30	ASN
2	C	43	LYS
2	C	50	VAL
2	C	77	ARG
2	C	144	THR
2	C	268	VAL
2	C	290	GLU
2	C	328	ILE
2	C	356	THR
2	C	357	VAL
2	C	378	LEU
2	C	447	SER
2	C	454	ARG
2	C	456	SER
2	C	471	GLU
2	C	488	THR
2	C	543	GLN
2	C	545	ASN
2	C	554	PHE
2	C	559	VAL
2	C	571	VAL
2	C	582	SER
2	C	587	VAL
2	C	616	VAL
2	C	621	SER
2	C	636	ILE
2	C	777	SER
2	C	787	ARG

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Mol	Chain	Res	Type
2	C	812	THR
2	C	868	LEU
2	C	875	GLN
2	C	885	LEU
2	C	904	MET
2	C	958	ARG
2	C	971	ILE
2	C	991	CYS
2	C	1037	VAL
2	C	1094	ASP
2	C	1097	VAL
2	C	1153	GLU
2	C	1162	LEU
3	D	4	VAL
3	D	12	ILE
3	D	60	CYS
3	D	89	ARG
3	D	148	LEU
3	D	165	GLN
3	D	308	SER
3	D	314	LEU
3	D	331	ASP
3	D	337	THR
3	D	338	SER
3	D	399	LEU
3	D	406	LEU
3	D	407	LYS
3	D	456	VAL
3	D	460	LEU
3	D	463	LEU
3	D	467	GLN
3	D	485	ASP
3	D	491	ILE
3	D	517	VAL
3	D	539	ASP
3	D	579	LEU
3	D	580	ASP
3	D	588	LEU
3	D	590	THR
3	D	714	ASP
3	D	743	LYS
3	D	838	SER

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Mol	Chain	Res	Type
3	D	860	LEU
3	D	863	THR
3	D	897	ILE
3	D	919	SER
3	D	925	LEU
3	D	944	LEU
3	D	957	ILE
3	D	1084	GLN
3	D	1093	ASP
3	D	1098	VAL
3	D	1148	SER
3	D	1194	VAL
3	D	1240	CYS
3	D	1266	ARG
4	E	82	VAL
5	F	37	LEU
5	F	45	LEU
5	F	83	TYR
5	F	194	LEU
5	F	206	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	262	GLN
3	D	505	HIS

5.3.3 RNA ⓘ

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

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	219/368 (59%)	0.05	5 (2%) 60 58	46, 62, 95, 132	0
1	B	232/368 (63%)	0.83	41 (17%) 1 1	64, 100, 128, 144	0
2	C	1138/1174 (96%)	0.40	93 (8%) 11 9	36, 64, 143, 173	0
3	D	1258/1317 (95%)	0.26	75 (5%) 21 18	39, 67, 111, 144	0
4	E	71/110 (64%)	0.38	4 (5%) 24 20	65, 84, 112, 120	0
5	F	186/218 (85%)	0.86	26 (13%) 2 2	38, 92, 131, 141	12 (6%)
6	H	20/20 (100%)	0.69	4 (20%) 1 0	47, 70, 137, 142	0
7	G	23/23 (100%)	1.76	8 (34%) 0 0	80, 117, 162, 169	3 (13%)
8	I	6/6 (100%)	0.02	0 100 100	47, 52, 65, 69	0
All	All	3153/3604 (87%)	0.39	256 (8%) 12 9	36, 70, 130, 173	15 (0%)

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	HIS	9.8
2	C	75	ALA	8.8
5	F	68	GLY	8.0
2	C	284	GLY	7.5
2	C	143	ASN	7.4
2	C	220	ASP	7.1
2	C	28	SER	6.9
2	C	575	GLU	6.9
2	C	271	ASP	6.6
2	C	1150	GLY	6.6
7	G	6	DT	6.6
2	C	253	GLY	6.5
2	C	294	THR	6.5
2	C	1151	GLU	6.3
1	B	96	TYR	6.2

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Mol	Chain	Res	Type	RSRZ
2	C	287	PRO	6.0
3	D	654	SER	5.7
7	G	5	DG	5.7
2	C	329	THR	5.6
2	C	252	PHE	5.5
2	C	573	SER	5.5
5	F	76	THR	5.5
1	B	62	GLU	5.4
2	C	353	THR	5.4
4	E	30	THR	5.4
7	G	25	DA	5.3
2	C	552	GLY	5.3
1	B	187	THR	5.2
1	B	128	LEU	5.2
2	C	521	ASP	5.1
1	A	4	SER	5.1
2	C	291	SER	5.0
2	C	74	ALA	4.9
2	C	273	ALA	4.8
1	A	2	LEU	4.7
1	A	3	ILE	4.6
2	C	574	SER	4.6
2	C	268	VAL	4.5
1	B	236	PRO	4.5
3	D	766	ASN	4.5
3	D	653	HIS	4.5
1	B	58	GLY	4.4
3	D	1026	GLY	4.4
2	C	140	ILE	4.4
1	B	188	ASP	4.4
1	B	184	GLU	4.4
5	F	67	ALA	4.3
3	D	1053	VAL	4.3
3	D	1059	GLU	4.3
2	C	325	GLY	4.3
2	C	520	VAL	4.3
1	B	16	ASP	4.2
4	E	31	PRO	4.2
2	C	1149	GLU	4.2
2	C	254	PHE	4.2
2	C	522	GLY	4.2
2	C	519	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
5	F	73	ARG	4.1
3	D	1054	ARG	4.1
2	C	327	PRO	4.0
5	F	71	SER	4.0
3	D	655	GLY	4.0
2	C	553	ARG	3.9
5	F	45	LEU	3.9
2	C	30	ASN	3.9
2	C	142	ASN	3.9
6	H	3	DT	3.8
5	F	69	PHE	3.8
5	F	74	HIS	3.7
2	C	290	GLU	3.7
2	C	283	PRO	3.7
2	C	141	ASN	3.7
1	A	187	THR	3.7
7	G	11	DG	3.7
3	D	291	ARG	3.7
2	C	263	GLU	3.7
2	C	523	VAL	3.6
3	D	1084	GLN	3.6
2	C	218	LYS	3.6
1	B	129	ASN	3.6
3	D	1203	GLY	3.6
2	C	330	SER	3.6
1	B	100	GLN	3.5
3	D	192	ASP	3.5
2	C	1148	ARG	3.5
5	F	31	ARG	3.5
2	C	551	ASP	3.4
2	C	1152	ASP	3.4
3	D	910	LEU	3.4
3	D	464	ASN	3.4
1	B	137	GLU	3.3
2	C	194	SER	3.3
2	C	354	THR	3.3
5	F	81	TRP	3.3
1	B	118	VAL	3.3
3	D	1060	ARG	3.3
5	F	72	PHE	3.3
3	D	36	TYR	3.3
1	B	133	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	1191	ARG	3.3
5	F	25	LEU	3.2
2	C	360	GLY	3.2
1	B	102	PRO	3.2
2	C	76	GLU	3.2
1	B	130	ASP	3.2
1	B	138	LEU	3.2
2	C	288	THR	3.2
2	C	145	GLY	3.2
3	D	1072	GLY	3.2
3	D	1061	PHE	3.2
2	C	1140	SER	3.1
1	B	111	VAL	3.1
1	B	67	PRO	3.1
2	C	557	PRO	3.1
2	C	269	GLY	3.1
6	H	4	DG	3.1
7	G	7	DG	3.1
1	B	234	ILE	3.1
3	D	1192	ARG	3.1
5	F	173	MET	3.1
2	C	78	GLY	3.1
5	F	177	ILE	3.0
6	H	5	DC	3.0
3	D	1090	LYS	3.0
3	D	210	ASP	3.0
2	C	550	ALA	3.0
5	F	88	ASN	3.0
2	C	228	ARG	2.9
2	C	250	GLU	2.9
3	D	902	ALA	2.9
2	C	272	GLU	2.9
3	D	1042	GLY	2.9
2	C	270	THR	2.9
3	D	1074	GLU	2.9
2	C	289	LYS	2.8
3	D	1073	GLU	2.8
3	D	65	TYR	2.8
2	C	1143	ALA	2.8
3	D	607	PRO	2.8
3	D	1190	ASN	2.8
7	G	4	DT	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	63	PHE	2.8
2	C	251	ARG	2.8
3	D	80	VAL	2.8
3	D	865	LEU	2.8
3	D	600	GLN	2.8
3	D	77	ARG	2.8
2	C	279	ARG	2.8
2	C	230	ARG	2.7
2	C	104	SER	2.6
1	B	69	VAL	2.6
5	F	95	ARG	2.6
2	C	292	ALA	2.6
2	C	554	PHE	2.6
1	B	11	GLU	2.6
3	D	765	LEU	2.6
2	C	98	ASP	2.6
3	D	1187	GLU	2.6
2	C	518	LYS	2.6
3	D	190	LYS	2.6
3	D	1171	GLY	2.6
3	D	1067	VAL	2.6
5	F	29	PHE	2.6
2	C	347	ARG	2.6
3	D	1066	ILE	2.6
3	D	181	LEU	2.6
3	D	189	ALA	2.6
1	B	185	GLN	2.5
1	B	12	ASP	2.5
3	D	1169	ASP	2.5
3	D	290	LEU	2.5
3	D	1174	GLU	2.5
7	G	8	DG	2.5
2	C	99	PHE	2.5
3	D	1078	ASP	2.5
1	B	14	LEU	2.5
6	H	6	DA	2.5
2	C	326	GLU	2.5
3	D	789	LEU	2.5
3	D	194	ARG	2.5
5	F	70	ARG	2.5
3	D	911	ILE	2.5
3	D	1070	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
5	F	21	THR	2.4
3	D	907	ASP	2.4
1	B	151	GLN	2.4
1	B	98	ARG	2.4
3	D	933	ALA	2.4
3	D	930	VAL	2.4
1	B	205	ARG	2.4
5	F	77	ASN	2.4
5	F	28	ARG	2.4
7	G	3	DT	2.4
1	A	221	LEU	2.4
2	C	249	VAL	2.3
1	B	70	LYS	2.3
3	D	466	ALA	2.3
1	B	103	GLY	2.3
2	C	285	GLU	2.3
3	D	900	GLU	2.3
2	C	1158	ALA	2.3
3	D	1172	SER	2.3
3	D	43	LYS	2.3
2	C	243	TRP	2.3
3	D	203	ARG	2.3
1	B	13	VAL	2.3
2	C	29	ASN	2.3
3	D	1011	THR	2.3
5	F	114	LEU	2.3
5	F	90	TYR	2.3
5	F	163	GLY	2.2
2	C	417	LEU	2.2
3	D	467	GLN	2.2
1	B	105	VAL	2.2
2	C	559	VAL	2.2
2	C	298	ASN	2.2
3	D	1173	THR	2.2
4	E	81	LEU	2.2
2	C	276	ASP	2.2
3	D	1012	MET	2.2
3	D	116	TYR	2.2
2	C	1141	ASP	2.2
3	D	901	LEU	2.2
3	D	606	HIS	2.2
3	D	1062	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	182	ARG	2.2
1	B	175	THR	2.2
2	C	77	ARG	2.2
1	B	200	ASN	2.1
3	D	73	ILE	2.1
2	C	305	ARG	2.1
5	F	180	VAL	2.1
3	D	1277	GLU	2.1
2	C	27	SER	2.1
1	B	229	ALA	2.1
3	D	1166	THR	2.1
3	D	1096	GLU	2.1
2	C	80	VAL	2.1
2	C	359	GLY	2.1
2	C	286	PRO	2.1
3	D	1111	LEU	2.1
3	D	957	ILE	2.1
3	D	1202	ALA	2.1
1	B	127	THR	2.1
2	C	144	THR	2.1
3	D	1188	ALA	2.1
2	C	229	LYS	2.1
1	B	110	ILE	2.0
5	F	169	ILE	2.0
3	D	958	THR	2.0
2	C	365	VAL	2.0
2	C	96	ILE	2.0
1	B	66	VAL	2.0
2	C	402	GLU	2.0
3	D	1069	ASP	2.0
4	E	55	TYR	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, 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(\AA^2)	Q<0.9
9	ZN	D	2001	1/1	0.97	0.11	71,71,71,71	0
9	ZN	D	2002	1/1	0.98	0.06	91,91,91,91	0
10	MG	D	2003	1/1	0.99	0.35	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.