



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:09 PM UTC

PDB ID : 5I2D / pdb_00005i2d
Title : Crystal structure of T. thermophilus TTHB099 class II transcription activation complex: TAP-RPo
Authors : Feng, Y.; Zhang, Y.; Ebright, R.H.
Deposited on : 2016-02-08
Resolution : 4.41 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

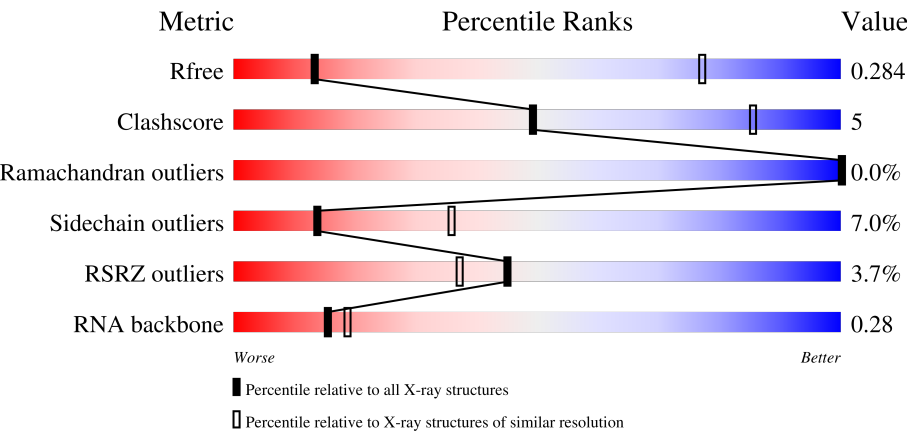
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.41 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)
RNA backbone	3983	1037 (5.60-3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	3% 73% 15% • 10%
1	B	315	4% 71% 15% • 11%
1	L	315	3% 76% 12% • 10%
1	M	315	3% 72% 14% • 11%

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	N	1119	
3	D	1524	
3	O	1524	
4	E	99	
4	P	99	
5	F	443	
5	Q	443	
6	G	215	
6	H	215	
6	R	215	
6	S	215	
7	I	72	
7	T	72	
8	J	72	
8	U	72	
9	K	4	
9	V	4	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 66882 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	284	Total	C	N	O	S	0	0	0
			2231	1421	387	421	2			
1	B	280	Total	C	N	O	S	0	0	0
			2199	1401	381	415	2			
1	L	284	Total	C	N	O	S	0	0	0
			2231	1421	387	421	2			
1	M	280	Total	C	N	O	S	0	0	0
			2199	1401	381	415	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	0	0
			8770	5548	1564	1634	24			
2	N	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1363	Total	C	N	O	S	0	0	0
			10754	6804	1906	2011	33			
3	O	1363	Total	C	N	O	S	0	0	0
			10754	6804	1906	2011	33			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			
4	P	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			
5	Q	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There are 40 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-5	VAL	-	expression tag	UNP Q5SKW1
Q	-4	PRO	-	expression tag	UNP Q5SKW1
Q	-3	ARG	-	expression tag	UNP Q5SKW1
Q	-2	GLY	-	expression tag	UNP Q5SKW1
Q	-1	SER	-	expression tag	UNP Q5SKW1
Q	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a protein called Transcriptional regulator, Crp family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	195	Total	C	N	O	S	0	0	0
			1559	974	293	288	4			
6	H	195	Total	C	N	O	S	0	0	0
			1559	974	293	288	4			
6	R	195	Total	C	N	O	S	0	0	0
			1559	974	293	288	4			
6	S	195	Total	C	N	O	S	0	0	0
			1559	974	293	288	4			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	MET	-	initiating methionine	UNP Q53W63
G	-18	GLY	-	expression tag	UNP Q53W63
G	-17	SER	-	expression tag	UNP Q53W63
G	-16	SER	-	expression tag	UNP Q53W63
G	-15	HIS	-	expression tag	UNP Q53W63
G	-14	HIS	-	expression tag	UNP Q53W63
G	-13	HIS	-	expression tag	UNP Q53W63
G	-12	HIS	-	expression tag	UNP Q53W63
G	-11	HIS	-	expression tag	UNP Q53W63
G	-10	HIS	-	expression tag	UNP Q53W63
G	-9	SER	-	expression tag	UNP Q53W63
G	-8	SER	-	expression tag	UNP Q53W63
G	-7	GLY	-	expression tag	UNP Q53W63
G	-6	LEU	-	expression tag	UNP Q53W63
G	-5	VAL	-	expression tag	UNP Q53W63
G	-4	PRO	-	expression tag	UNP Q53W63
G	-3	ARG	-	expression tag	UNP Q53W63
G	-2	GLY	-	expression tag	UNP Q53W63
G	-1	SER	-	expression tag	UNP Q53W63
G	0	HIS	-	expression tag	UNP Q53W63

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-19	MET	-	initiating methionine	UNP Q53W63
H	-18	GLY	-	expression tag	UNP Q53W63
H	-17	SER	-	expression tag	UNP Q53W63
H	-16	SER	-	expression tag	UNP Q53W63
H	-15	HIS	-	expression tag	UNP Q53W63
H	-14	HIS	-	expression tag	UNP Q53W63
H	-13	HIS	-	expression tag	UNP Q53W63
H	-12	HIS	-	expression tag	UNP Q53W63
H	-11	HIS	-	expression tag	UNP Q53W63
H	-10	HIS	-	expression tag	UNP Q53W63
H	-9	SER	-	expression tag	UNP Q53W63
H	-8	SER	-	expression tag	UNP Q53W63
H	-7	GLY	-	expression tag	UNP Q53W63
H	-6	LEU	-	expression tag	UNP Q53W63
H	-5	VAL	-	expression tag	UNP Q53W63
H	-4	PRO	-	expression tag	UNP Q53W63
H	-3	ARG	-	expression tag	UNP Q53W63
H	-2	GLY	-	expression tag	UNP Q53W63
H	-1	SER	-	expression tag	UNP Q53W63
H	0	HIS	-	expression tag	UNP Q53W63
R	-19	MET	-	initiating methionine	UNP Q53W63
R	-18	GLY	-	expression tag	UNP Q53W63
R	-17	SER	-	expression tag	UNP Q53W63
R	-16	SER	-	expression tag	UNP Q53W63
R	-15	HIS	-	expression tag	UNP Q53W63
R	-14	HIS	-	expression tag	UNP Q53W63
R	-13	HIS	-	expression tag	UNP Q53W63
R	-12	HIS	-	expression tag	UNP Q53W63
R	-11	HIS	-	expression tag	UNP Q53W63
R	-10	HIS	-	expression tag	UNP Q53W63
R	-9	SER	-	expression tag	UNP Q53W63
R	-8	SER	-	expression tag	UNP Q53W63
R	-7	GLY	-	expression tag	UNP Q53W63
R	-6	LEU	-	expression tag	UNP Q53W63
R	-5	VAL	-	expression tag	UNP Q53W63
R	-4	PRO	-	expression tag	UNP Q53W63
R	-3	ARG	-	expression tag	UNP Q53W63
R	-2	GLY	-	expression tag	UNP Q53W63
R	-1	SER	-	expression tag	UNP Q53W63
R	0	HIS	-	expression tag	UNP Q53W63
S	-19	MET	-	initiating methionine	UNP Q53W63
S	-18	GLY	-	expression tag	UNP Q53W63

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-17	SER	-	expression tag	UNP Q53W63
S	-16	SER	-	expression tag	UNP Q53W63
S	-15	HIS	-	expression tag	UNP Q53W63
S	-14	HIS	-	expression tag	UNP Q53W63
S	-13	HIS	-	expression tag	UNP Q53W63
S	-12	HIS	-	expression tag	UNP Q53W63
S	-11	HIS	-	expression tag	UNP Q53W63
S	-10	HIS	-	expression tag	UNP Q53W63
S	-9	SER	-	expression tag	UNP Q53W63
S	-8	SER	-	expression tag	UNP Q53W63
S	-7	GLY	-	expression tag	UNP Q53W63
S	-6	LEU	-	expression tag	UNP Q53W63
S	-5	VAL	-	expression tag	UNP Q53W63
S	-4	PRO	-	expression tag	UNP Q53W63
S	-3	ARG	-	expression tag	UNP Q53W63
S	-2	GLY	-	expression tag	UNP Q53W63
S	-1	SER	-	expression tag	UNP Q53W63
S	0	HIS	-	expression tag	UNP Q53W63

- Molecule 7 is a DNA chain called DNA (72-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	66	Total	C	N	O	P	0	0	0
			1349	639	246	398	66			
7	T	66	Total	C	N	O	P	0	0	0
			1349	639	246	398	66			

- Molecule 8 is a DNA chain called DNA (72-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	66	Total	C	N	O	P	0	0	0
			1367	645	267	390	65			
8	U	66	Total	C	N	O	P	0	0	0
			1367	645	267	390	65			

- Molecule 9 is a RNA chain called RNA (5'-R(*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	4	Total	C	N	O	P	0	0	0
			82	38	15	26	3			
9	V	4	Total	C	N	O	P	0	0	0
			82	38	15	26	3			

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total 2	Zn 2	0	0
10	O	2	Total 2	Zn 2	0	0

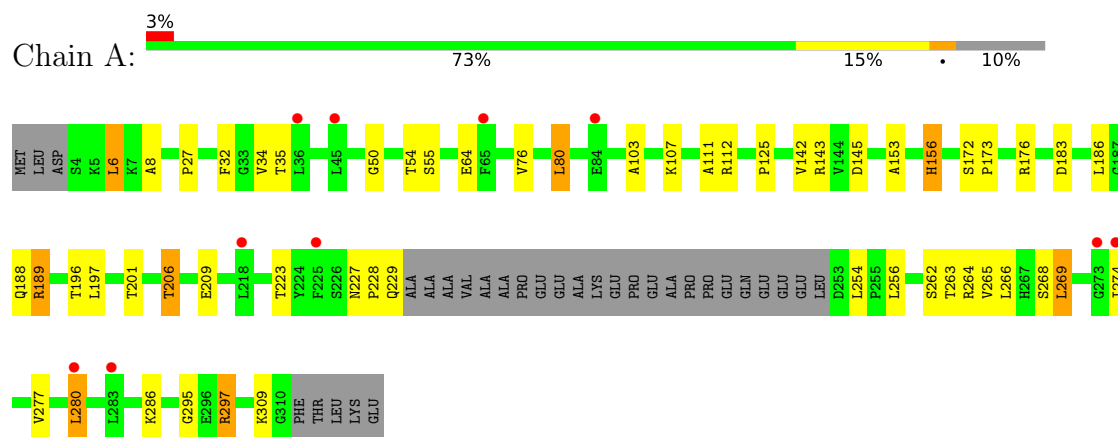
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total 1	Mg 1	0	0
11	O	1	Total 1	Mg 1	0	0

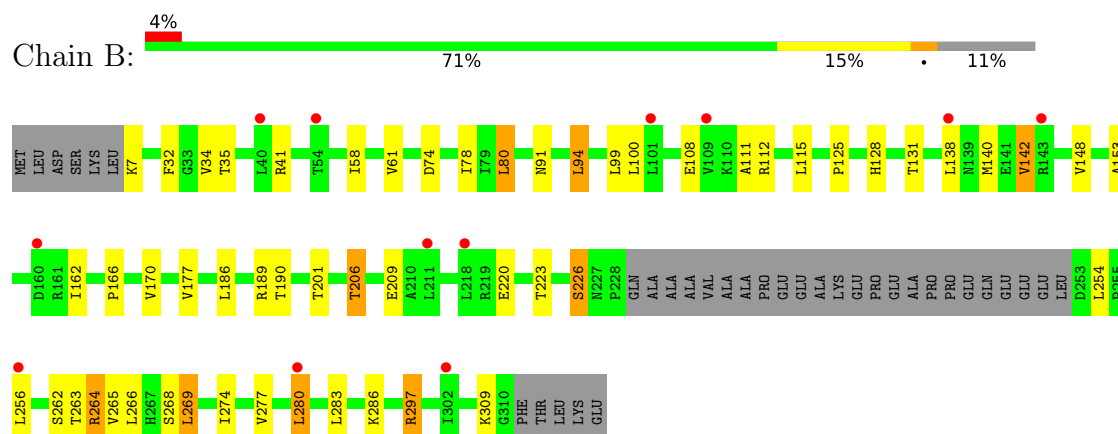
3 Residue-property plots [i](#)

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

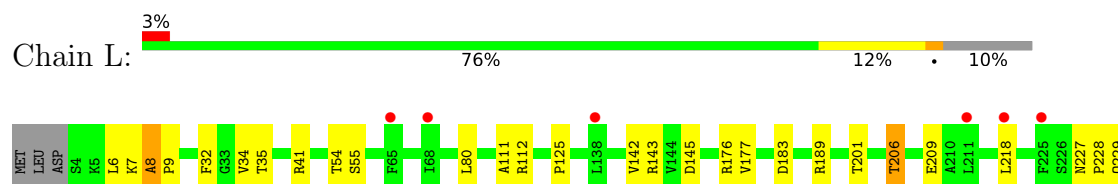
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

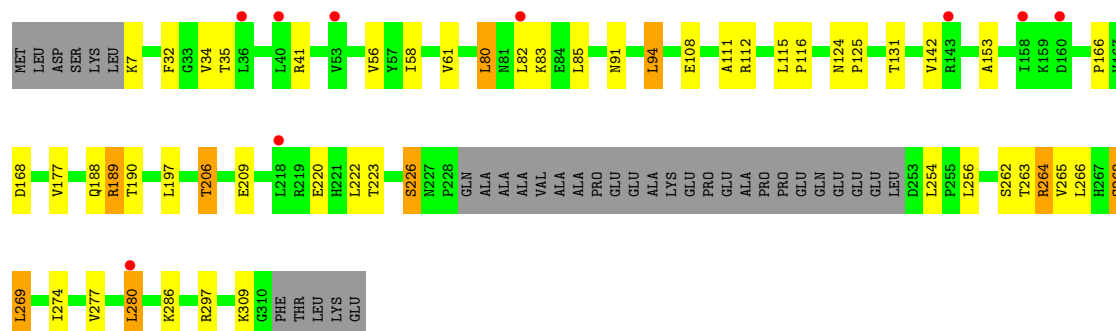
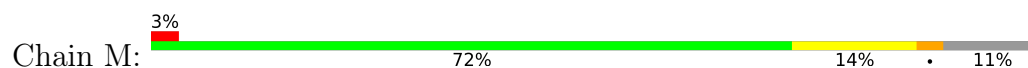


- Molecule 1: DNA-directed RNA polymerase subunit alpha

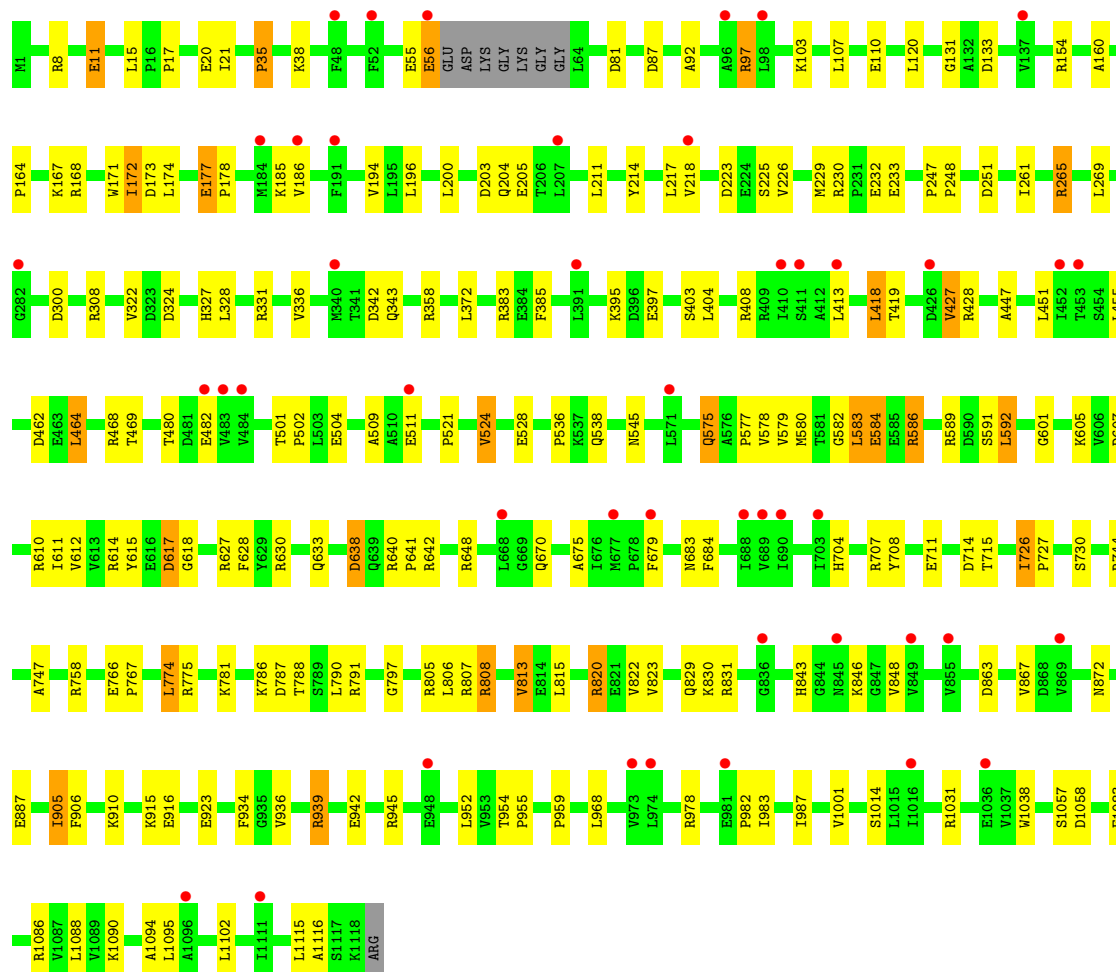
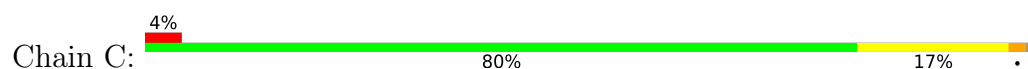




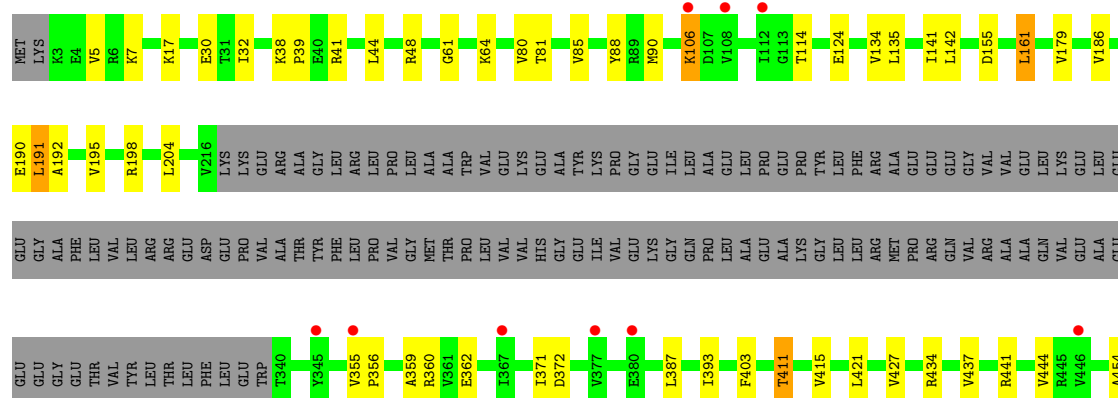
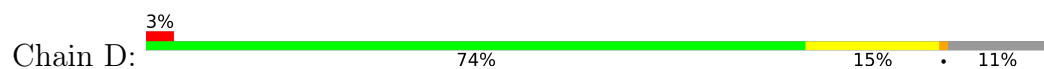
• Molecule 1: DNA-directed RNA polymerase subunit alpha

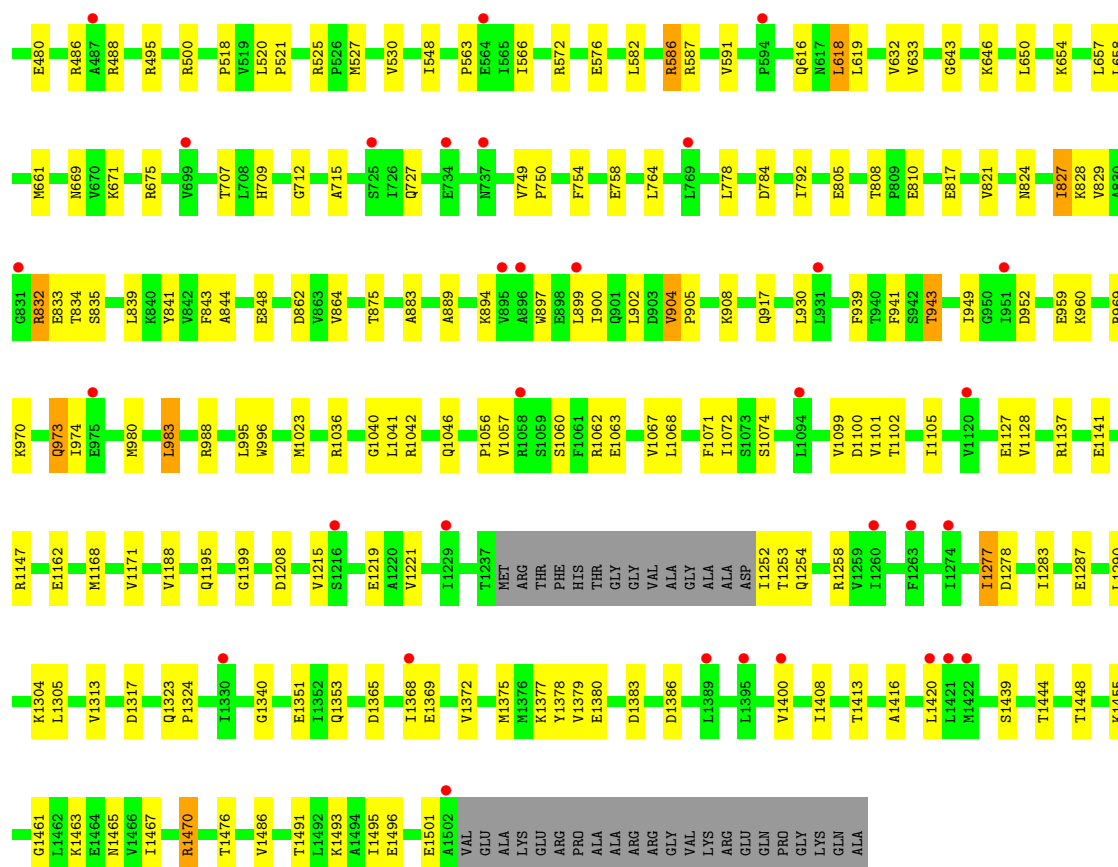


• Molecule 2: DNA-directed RNA polymerase subunit beta

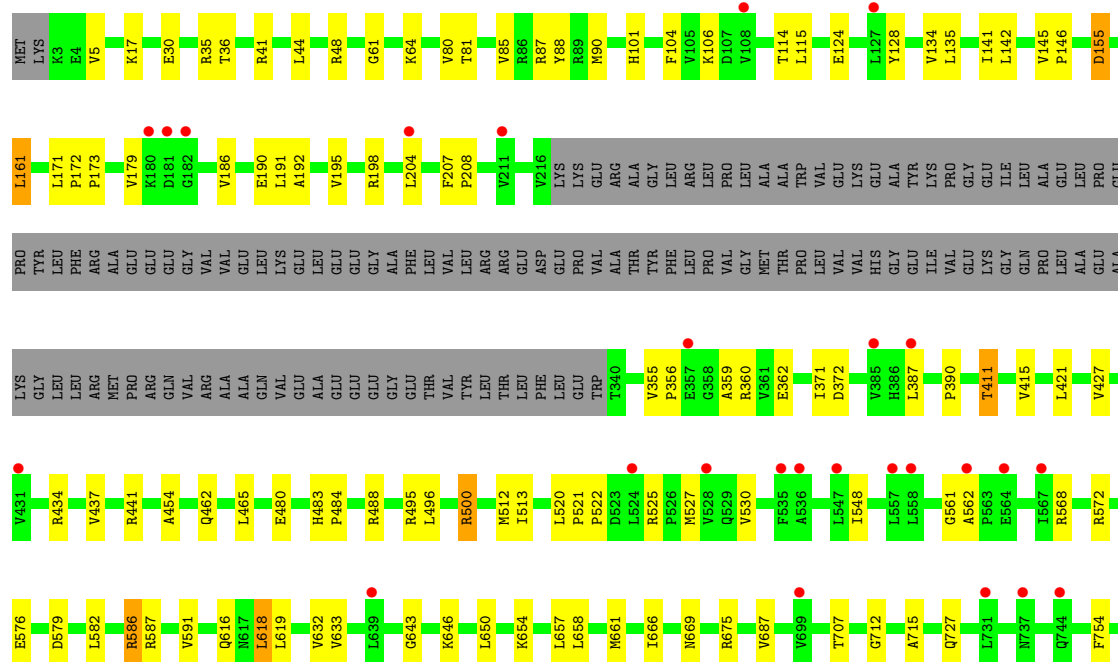
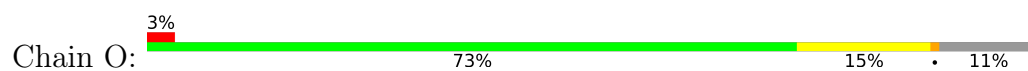


Chain N: 5% 81% 17% ..



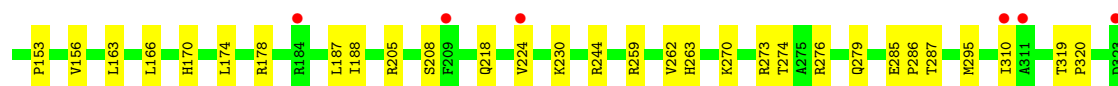
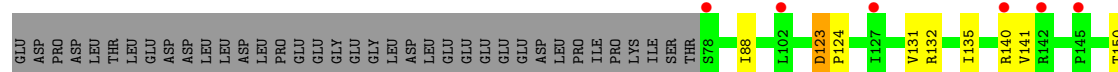
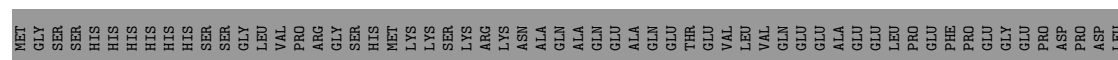


• Molecule 3: DNA-directed RNA polymerase subunit beta'

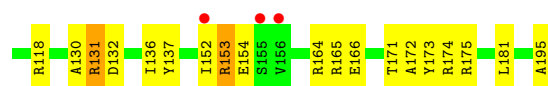
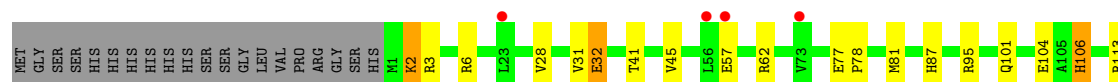




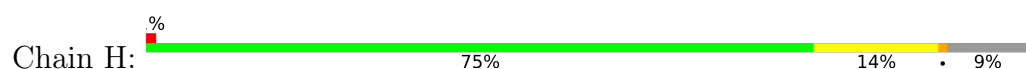
• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 6: Transcriptional regulator, Crp family

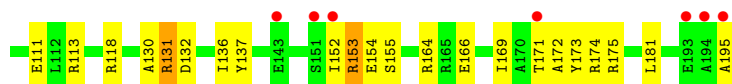


• Molecule 6: Transcriptional regulator, Crp family

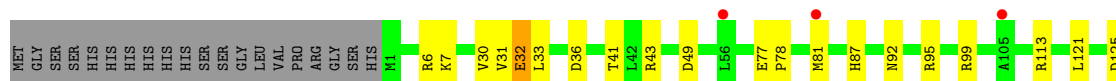
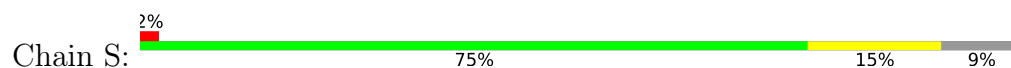


• Molecule 6: Transcriptional regulator, Crp family





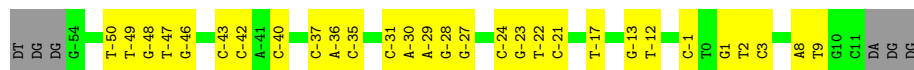
- Molecule 6: Transcriptional regulator, Crp family



- Molecule 7: DNA (72-MER)



- Molecule 7: DNA (72-MER)



- Molecule 8: DNA (72-MER)



- Molecule 8: DNA (72-MER)



- Molecule 9: RNA (5'-R(*UP*CP*GP*A)-3')



- Molecule 9: RNA (5'-R(*UP*CP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	171.49Å 105.45Å 374.58Å 90.00° 102.39° 90.00°	Depositor
Resolution (Å)	49.31 – 4.41 49.31 – 4.41	Depositor EDS
% Data completeness (in resolution range)	85.8 (49.31-4.41) 84.8 (49.31-4.41)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.241 , 0.284 0.239 , 0.284	Depositor DCC
R_{free} test set	2033 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	156.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 84.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	66882	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6653e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.28	0/2265	0.78	4/3069 (0.1%)
1	B	0.28	0/2233	0.77	0/3027
1	L	0.28	0/2265	0.79	2/3069 (0.1%)
1	M	0.29	0/2233	0.76	0/3027
2	C	0.27	0/8937	0.74	6/12087 (0.0%)
2	N	0.27	0/8937	0.74	5/12087 (0.0%)
3	D	0.27	0/10937	0.74	2/14781 (0.0%)
3	O	0.27	0/10937	0.74	2/14781 (0.0%)
4	E	0.25	0/775	0.74	0/1045
4	P	0.25	0/775	0.73	0/1045
5	F	0.27	0/2852	0.76	0/3837
5	Q	0.27	0/2852	0.77	0/3837
6	G	0.28	0/1580	0.72	2/2129 (0.1%)
6	H	0.28	0/1580	0.72	2/2129 (0.1%)
6	R	0.28	0/1580	0.73	2/2129 (0.1%)
6	S	0.28	0/1580	0.72	2/2129 (0.1%)
7	I	0.11	0/1511	0.55	0/2329
7	T	0.11	0/1511	0.56	0/2329
8	J	0.12	0/1538	0.54	0/2376
8	U	0.12	0/1538	0.54	0/2376
9	K	0.08	0/91	0.23	0/140
9	V	0.09	0/91	0.26	0/140
All	All	0.26	0/68598	0.73	29/93898 (0.0%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1340	GLY	CA-C-N	6.67	125.90	118.97
3	O	1340	GLY	C-N-CA	6.67	125.90	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1340	GLY	CA-C-N	6.35	125.57	118.97
3	D	1340	GLY	C-N-CA	6.35	125.57	118.97
2	N	35	PRO	CA-C-N	6.07	126.23	119.32
2	N	35	PRO	C-N-CA	6.07	126.23	119.32
2	N	154	ARG	CA-C-N	5.96	125.17	118.97
2	N	154	ARG	C-N-CA	5.96	125.17	118.97
1	L	8	ALA	CA-C-N	5.93	125.90	120.03
1	L	8	ALA	C-N-CA	5.93	125.90	120.03
2	C	154	ARG	CA-C-N	5.81	125.01	118.97
2	C	154	ARG	C-N-CA	5.81	125.01	118.97
6	H	77	GLU	CA-C-N	5.77	125.25	119.24
6	H	77	GLU	C-N-CA	5.77	125.25	119.24
2	C	35	PRO	CA-C-N	5.70	125.81	119.32
2	C	35	PRO	C-N-CA	5.70	125.81	119.32
6	S	77	GLU	CA-C-N	5.37	125.44	119.32
6	S	77	GLU	C-N-CA	5.37	125.44	119.32
6	G	77	GLU	CA-C-N	5.25	124.70	119.24
6	G	77	GLU	C-N-CA	5.25	124.70	119.24
2	C	726	ILE	CA-C-N	5.18	125.48	119.93
2	C	726	ILE	C-N-CA	5.18	125.48	119.93
1	A	8	ALA	CA-C-N	5.15	125.13	120.03
1	A	8	ALA	C-N-CA	5.15	125.13	120.03
6	R	77	GLU	CA-C-N	5.13	124.58	119.24
6	R	77	GLU	C-N-CA	5.13	124.58	119.24
2	N	271	GLU	N-CA-C	-5.08	105.83	111.36
1	A	172	SER	CA-C-N	5.03	124.64	119.56
1	A	172	SER	C-N-CA	5.03	124.64	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2231	0	2313	21	0
1	B	2199	0	2276	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2231	0	2313	17	0
1	M	2199	0	2276	24	0
2	C	8770	0	8874	102	0
2	N	8770	0	8874	98	0
3	D	10754	0	10975	112	0
3	O	10754	0	10975	121	0
4	E	761	0	778	8	0
4	P	761	0	778	10	0
5	F	2807	0	2882	29	0
5	Q	2807	0	2882	32	0
6	G	1559	0	1587	25	0
6	H	1559	0	1587	20	0
6	R	1559	0	1587	29	0
6	S	1559	0	1587	19	0
7	I	1349	0	741	25	0
7	T	1349	0	741	27	0
8	J	1367	0	739	32	0
8	U	1367	0	739	28	0
9	K	82	0	44	2	0
9	V	82	0	44	2	0
10	D	2	0	0	0	0
10	O	2	0	0	0	0
11	D	1	0	0	0	0
11	O	1	0	0	0	0
All	All	66882	0	65592	713	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 5.

All (713) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:164:ARG:NH1	6:G:171:THR:OG1	2.20	0.75
8:U:15:DG:H2"	8:U:16:DC:H5"	1.66	0.75
2:N:630:ARG:CZ	2:N:707:ARG:HD3	2.17	0.74
2:N:683:ASN:HB3	2:N:872:ASN:HB2	1.69	0.74
6:R:164:ARG:NH1	6:R:171:THR:OG1	2.21	0.73
3:O:1491:THR:HG21	4:P:89:MET:HG2	1.71	0.73
6:H:136:ILE:HD11	6:H:181:LEU:HD21	1.71	0.73
8:J:15:DG:H2"	8:J:16:DC:H5"	1.70	0.72
1:B:269:LEU:HD12	1:B:274:ILE:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:269:LEU:HD12	1:M:274:ILE:HD11	1.72	0.71
3:D:61:GLY:O	3:D:64:LYS:NZ	2.24	0.71
1:L:269:LEU:HD12	1:L:274:ILE:HD11	1.72	0.70
6:R:164:ARG:NH1	8:U:35:DG:OP1	2.24	0.70
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.72	0.70
6:R:154:GLU:OE1	7:T:-37:DC:N4	2.21	0.69
1:A:269:LEU:HD12	1:A:274:ILE:HD11	1.71	0.69
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.26	0.69
3:O:61:GLY:O	3:O:64:LYS:NZ	2.26	0.69
3:D:1491:THR:HG21	4:E:89:MET:HG2	1.73	0.68
2:N:17:PRO:HB2	2:N:20:GLU:HB3	1.74	0.68
7:I:-47:DT:H2''	7:I:-46:DG:H5'	1.75	0.68
6:G:136:ILE:HD11	6:G:181:LEU:HD21	1.74	0.68
6:R:31:VAL:HG12	6:R:41:THR:HA	1.74	0.68
1:M:206:THR:HG22	1:M:209:GLU:H	1.58	0.68
6:S:31:VAL:HG12	6:S:41:THR:HA	1.76	0.67
1:L:55:SER:HB3	1:L:143:ARG:HB3	1.76	0.67
6:S:136:ILE:HD11	6:S:181:LEU:HD21	1.76	0.67
3:O:1254:GLN:HB3	3:O:1258:ARG:HB2	1.76	0.66
6:R:136:ILE:HD11	6:R:181:LEU:HD21	1.77	0.66
1:B:206:THR:HG22	1:B:209:GLU:H	1.60	0.66
6:G:164:ARG:NH1	8:J:35:DG:OP1	2.28	0.65
1:L:111:ALA:HB3	1:L:125:PRO:HA	1.78	0.65
6:G:165:ARG:NH2	8:J:36:DT:OP2	2.29	0.65
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.29	0.65
8:U:44:DC:H2''	8:U:45:DT:H5'	1.77	0.65
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.30	0.65
6:H:78:PRO:HA	6:H:81:MET:HE2	1.79	0.65
1:A:6:LEU:HD23	1:A:189:ARG:HH11	1.59	0.64
1:A:176:ARG:NH1	2:C:863:ASP:O	2.30	0.64
6:H:31:VAL:HG12	6:H:41:THR:HA	1.78	0.64
1:L:297:ARG:HH21	6:S:121:LEU:HB3	1.62	0.64
2:N:630:ARG:NH1	2:N:707:ARG:HD3	2.12	0.64
2:N:97:ARG:NH1	2:N:110:GLU:OE1	2.31	0.64
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.78	0.64
7:T:-47:DT:H2''	7:T:-46:DG:H5'	1.79	0.64
2:N:905:ILE:HG23	2:N:906:PHE:HD2	1.62	0.63
6:G:31:VAL:HG12	6:G:41:THR:HA	1.80	0.63
6:H:6:ARG:HH11	6:H:174:ARG:HH21	1.47	0.63
2:C:55:GLU:O	2:C:56:GLU:HB3	1.98	0.63
8:J:44:DC:H2''	8:J:45:DT:H5'	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.81	0.63
1:A:111:ALA:HB3	1:A:125:PRO:HA	1.81	0.63
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.80	0.63
2:N:55:GLU:O	2:N:56:GLU:HB3	1.99	0.63
1:A:297:ARG:HH21	6:H:121:LEU:HB3	1.63	0.63
3:D:1353:GLN:NE2	3:D:1365:ASP:OD1	2.28	0.62
8:U:1:DC:H2'	8:U:2:DG:H8	1.64	0.62
2:C:905:ILE:HG23	2:C:906:PHE:HD2	1.63	0.62
1:A:265:VAL:HG13	1:A:269:LEU:HD23	1.82	0.62
1:L:176:ARG:NH1	2:N:863:ASP:O	2.32	0.62
6:S:78:PRO:HA	6:S:81:MET:HE2	1.82	0.62
1:L:265:VAL:HG13	1:L:269:LEU:HD23	1.82	0.62
2:N:983:ILE:HG21	2:N:987:ILE:HD11	1.80	0.62
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.82	0.62
8:U:24:DG:H2''	8:U:25:DG:H5''	1.82	0.62
3:O:1353:GLN:NE2	3:O:1365:ASP:OD1	2.32	0.61
1:B:265:VAL:HG13	1:B:269:LEU:HD23	1.82	0.61
3:O:128:TYR:OH	3:O:579:ASP:OD2	2.16	0.61
7:T:-22:DT:H1'	7:T:-21:DC:H5'	1.82	0.61
8:J:1:DC:H2'	8:J:2:DG:H8	1.65	0.61
2:N:797:GLY:O	2:N:829:GLN:NE2	2.34	0.61
5:Q:131:VAL:HG13	5:Q:178:ARG:HD3	1.83	0.61
6:R:78:PRO:HA	6:R:81:MET:HE2	1.82	0.61
1:L:295:GLY:HA3	6:S:125:ASP:HA	1.83	0.60
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.33	0.60
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.83	0.60
3:D:657:LEU:HG	3:D:661:MET:HE2	1.84	0.60
3:O:142:LEU:HB2	3:O:161:LEU:HD11	1.82	0.60
2:N:428:ARG:NH2	2:N:447:ALA:O	2.35	0.60
2:N:504:GLU:HG2	2:N:509:ALA:HB2	1.84	0.59
3:D:973:GLN:HB2	3:O:976:GLN:HB2	1.84	0.59
1:M:265:VAL:HG13	1:M:269:LEU:HD23	1.82	0.59
3:O:1495:ILE:HD13	4:P:80:VAL:HG21	1.83	0.59
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.85	0.59
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.85	0.59
3:D:980:MET:HG3	3:O:972:LEU:HD21	1.85	0.59
3:O:124:GLU:OE2	3:O:587:ARG:NH2	2.35	0.59
6:S:49:ASP:HA	6:S:92:ASN:HD21	1.68	0.59
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.85	0.59
7:I:-22:DT:H1'	7:I:-21:DC:H5'	1.85	0.59
3:O:1495:ILE:HG12	4:P:88:GLU:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:707:THR:HG23	3:O:712:GLY:HA3	1.85	0.59
2:N:168:ARG:NH2	2:N:265:ARG:O	2.36	0.58
5:Q:397:ILE:HD12	5:Q:400:ILE:HD11	1.85	0.58
2:C:797:GLY:O	2:C:829:GLN:NE2	2.37	0.58
2:N:160:ALA:HB3	2:N:174:LEU:HB2	1.86	0.58
2:N:343:GLN:HG3	2:N:385:PHE:HB2	1.85	0.58
6:R:6:ARG:HH11	6:R:174:ARG:HH21	1.52	0.58
8:J:24:DG:H2''	8:J:25:DG:H5''	1.86	0.58
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.84	0.58
6:G:2:LYS:HD3	6:G:3:ARG:N	2.19	0.58
1:A:295:GLY:HA3	6:H:125:ASP:HA	1.86	0.58
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.86	0.58
2:N:521:PRO:HB3	3:O:1068:LEU:HD21	1.86	0.58
2:N:92:ALA:HB2	2:N:120:LEU:HD11	1.86	0.57
2:C:469:THR:HG1	2:C:538:GLN:NE2	2.01	0.57
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.37	0.57
3:O:480:GLU:OE2	3:O:488:ARG:NH2	2.36	0.57
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.87	0.57
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.86	0.57
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.87	0.56
3:O:1432:LYS:O	3:O:1455:LYS:NZ	2.38	0.56
2:C:628:PHE:H	2:C:638:ASP:HB2	1.71	0.56
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.88	0.56
6:G:78:PRO:HA	6:G:81:MET:HE2	1.87	0.56
8:U:1:DC:H2'	8:U:2:DG:C8	2.41	0.56
3:O:1372:VAL:HA	3:O:1375:MET:HE3	1.88	0.56
2:C:172:ILE:HG13	2:C:186:VAL:HG22	1.88	0.56
1:A:206:THR:HG22	1:A:209:GLU:H	1.71	0.56
2:C:428:ARG:NH2	2:C:447:ALA:O	2.39	0.56
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.88	0.55
8:J:1:DC:H2'	8:J:2:DG:C8	2.41	0.55
2:N:787:ASP:OD2	2:N:791:ARG:NH2	2.36	0.55
1:B:153:ALA:HB1	1:B:166:PRO:HB2	1.89	0.55
3:O:1380:GLU:HB2	3:O:1420:LEU:HD22	1.87	0.55
3:D:671:LYS:NZ	5:F:423:ASP:OD1	2.36	0.55
3:O:356:PRO:HG2	3:O:359:ALA:HB2	1.89	0.55
6:S:154:GLU:OE2	8:U:46:DC:N4	2.39	0.55
7:T:-48:DG:H2''	7:T:-47:DT:H5''	1.88	0.55
2:N:628:PHE:H	2:N:638:ASP:HB2	1.71	0.55
3:O:520:LEU:O	3:O:525:ARG:NH1	2.39	0.55
6:R:153:ARG:NH2	8:U:35:DG:O6	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:-31:DC:H1'	7:T:-30:DA:H5'	1.89	0.55
2:C:939:ARG:HB2	2:C:982:PRO:HG3	1.89	0.55
3:D:520:LEU:O	3:D:525:ARG:NH1	2.40	0.55
6:R:173:TYR:CG	7:T:-30:DA:H5''	2.42	0.55
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.89	0.55
1:B:58:ILE:HB	1:B:61:VAL:HB	1.89	0.54
3:O:1108:ARG:NH2	3:O:1198:TYR:O	2.38	0.54
1:M:111:ALA:HB3	1:M:125:PRO:HA	1.90	0.54
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.88	0.54
1:B:223:THR:O	1:B:226:SER:OG	2.24	0.54
3:O:1042:ARG:HB3	3:O:1057:VAL:HB	1.90	0.54
3:O:949:ILE:HD11	3:O:1023:MET:HE1	1.89	0.54
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.42	0.54
2:N:469:THR:OG1	2:N:538:GLN:NE2	2.40	0.54
3:O:411:THR:HB	3:O:437:VAL:H	1.73	0.54
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.90	0.54
1:M:80:LEU:HG	3:O:844:ALA:HA	1.88	0.54
6:G:153:ARG:NH2	8:J:35:DG:O6	2.36	0.54
2:N:462:ASP:HB3	2:N:468:ARG:HD2	1.89	0.53
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.90	0.53
2:N:1083:GLU:OE1	2:N:1086:ARG:NH1	2.41	0.53
3:O:904:VAL:HG22	3:O:905:PRO:HD2	1.89	0.53
7:T:-50:DT:H2''	7:T:-49:DT:H5''	1.89	0.53
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.90	0.53
4:E:37:ASN:HD22	4:E:89:MET:HE1	1.74	0.53
7:I:-37:DC:H2''	7:I:-36:DA:H5'	1.90	0.53
2:N:1116:ALA:HB2	3:O:88:TYR:HB3	1.90	0.53
6:G:6:ARG:HH11	6:G:174:ARG:HH21	1.57	0.53
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.89	0.53
3:O:1045:MET:HE2	3:O:1073:SER:HA	1.90	0.53
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.91	0.53
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.90	0.53
7:I:-50:DT:H2''	7:I:-49:DT:H5''	1.90	0.53
6:R:6:ARG:NH2	6:R:68:MET:O	2.38	0.53
6:H:95:ARG:NH1	6:H:195:ALA:OXT	2.42	0.53
3:O:1046:GLN:OE1	3:O:1046:GLN:N	2.41	0.53
1:B:100:LEU:HB2	1:B:115:LEU:HD12	1.91	0.53
3:O:657:LEU:HG	3:O:661:MET:HE2	1.90	0.53
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.89	0.52
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.92	0.52
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:627:ARG:NH1	2:N:638:ASP:OD2	2.43	0.52
2:C:758:ARG:HH21	2:C:788:THR:HB	1.73	0.52
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.37	0.52
3:O:715:ALA:HB3	3:O:764:LEU:HA	1.90	0.52
6:G:154:GLU:OE1	7:I:-37:DC:N4	2.34	0.52
2:N:605:LYS:HB2	2:N:612:VAL:HB	1.90	0.52
2:N:915:LYS:NZ	3:O:952:ASP:OD2	2.42	0.52
6:R:113:ARG:NH2	6:R:166:GLU:OE1	2.37	0.52
2:N:177:GLU:HG3	2:N:178:PRO:HD2	1.92	0.52
2:N:774:LEU:HG	5:Q:350:LEU:HD11	1.92	0.52
3:O:371:ILE:HG23	5:Q:230:LYS:HD2	1.92	0.52
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.91	0.52
1:M:91:ASN:HB3	1:M:94:LEU:HB2	1.91	0.52
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.92	0.52
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.40	0.52
3:D:434:ARG:NH2	5:F:135:ILE:O	2.43	0.52
5:F:270:LYS:O	5:F:274:THR:OG1	2.22	0.52
2:N:418:LEU:HD21	2:N:427:VAL:HG11	1.92	0.52
2:N:711:GLU:HG2	2:N:822:VAL:HG22	1.92	0.52
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.92	0.52
2:C:843:HIS:NE2	2:C:887:GLU:OE2	2.42	0.52
3:D:1071:PHE:O	3:D:1074:SER:OG	2.27	0.52
6:G:57:GLU:OE2	6:H:98:ARG:NH2	2.36	0.52
8:U:13:DC:H2"	8:U:14:DG:C8	2.45	0.52
1:M:58:ILE:HB	1:M:61:VAL:HB	1.92	0.51
1:B:220:GLU:O	1:B:223:THR:OG1	2.21	0.51
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.92	0.51
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.91	0.51
6:H:92:ASN:OD1	6:H:96:GLN:NE2	2.43	0.51
3:O:5:VAL:O	3:O:1470:ARG:NH2	2.43	0.51
3:O:1383:ASP:HB3	3:O:1416:ALA:HB3	1.92	0.51
6:S:130:ALA:HB3	6:S:137:TYR:CE1	2.46	0.51
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.92	0.51
3:D:618:LEU:HG	3:D:1467:ILE:HG23	1.92	0.51
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.91	0.51
3:O:1147:ARG:NH2	3:O:1369:GLU:OE1	2.38	0.51
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.91	0.51
5:F:372:ARG:NH2	8:J:31:DG:OP2	2.43	0.51
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.92	0.51
2:N:843:HIS:NE2	2:N:887:GLU:OE2	2.35	0.51
7:T:-29:DA:H2"	7:T:-28:DG:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:HA	1:B:177:VAL:HG11	1.93	0.51
3:D:969:ARG:HD3	3:O:980:MET:HA	1.92	0.51
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.11	0.51
2:N:617:ASP:N	2:N:617:ASP:OD1	2.41	0.51
2:N:805:ARG:HG3	2:N:823:VAL:HG22	1.93	0.51
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.93	0.51
1:M:153:ALA:HB1	1:M:166:PRO:HB2	1.93	0.51
2:N:1038:TRP:CE2	3:O:1099:VAL:HG11	2.46	0.51
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.92	0.50
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.43	0.50
7:T:-37:DC:H2''	7:T:-36:DA:H5'	1.92	0.50
2:C:617:ASP:OD1	2:C:617:ASP:N	2.43	0.50
3:D:1046:GLN:OE1	3:D:1046:GLN:N	2.40	0.50
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.93	0.50
6:H:49:ASP:HA	6:H:92:ASN:HD21	1.76	0.50
2:N:1115:LEU:HG	3:O:85:VAL:HG12	1.92	0.50
2:C:214:TYR:HE2	2:C:308:ARG:HG3	1.76	0.50
2:N:172:ILE:HG13	2:N:186:VAL:HG22	1.93	0.50
3:D:1386:ASP:OD2	3:D:1413:THR:N	2.38	0.50
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.93	0.50
1:A:153:ALA:HA	1:A:156:HIS:CE1	2.47	0.50
2:N:143:SER:O	2:N:147:TYR:OH	2.26	0.50
2:N:164:PRO:HA	2:N:269:LEU:HD12	1.94	0.50
3:O:356:PRO:HB3	3:O:441:ARG:HA	1.94	0.50
6:S:95:ARG:NH1	6:S:195:ALA:OXT	2.44	0.50
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.92	0.50
3:O:899:LEU:HD22	3:O:917:GLN:HB3	1.93	0.50
7:T:-13:DG:H1'	7:T:-12:DT:H5'	1.93	0.50
1:A:27:PRO:HG3	1:A:186:LEU:HD13	1.93	0.50
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.94	0.50
6:R:92:ASN:OD1	6:R:96:GLN:NE2	2.44	0.50
3:O:1071:PHE:O	3:O:1074:SER:OG	2.28	0.50
2:C:226:VAL:HA	2:C:229:MET:HE2	1.93	0.49
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.94	0.49
2:C:1115:LEU:HG	3:D:85:VAL:HG12	1.94	0.49
7:I:-48:DG:H2''	7:I:-47:DT:H5''	1.92	0.49
6:R:95:ARG:NH1	6:R:195:ALA:OXT	2.45	0.49
1:B:91:ASN:HB3	1:B:94:LEU:HB2	1.94	0.49
2:C:21:ILE:HD12	2:C:455:LEU:HD22	1.93	0.49
3:D:1380:GLU:HB2	3:D:1420:LEU:HD22	1.94	0.49
2:C:167:LYS:HD3	7:I:-1:DC:H5	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.47	0.49
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.95	0.49
7:I:-29:DA:H2''	7:I:-28:DG:C8	2.47	0.49
3:O:643:GLY:HA3	3:O:727:GLN:HB2	1.95	0.49
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.94	0.49
1:M:220:GLU:O	1:M:223:THR:OG1	2.23	0.49
1:M:223:THR:O	1:M:226:SER:OG	2.30	0.49
1:B:32:PHE:HA	1:B:35:THR:HB	1.94	0.49
6:H:130:ALA:HB3	6:H:137:TYR:CE1	2.47	0.49
6:R:2:LYS:HD3	6:R:3:ARG:N	2.27	0.49
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.77	0.49
1:L:206:THR:HG22	1:L:209:GLU:H	1.77	0.49
1:M:32:PHE:HA	1:M:35:THR:HB	1.94	0.49
2:N:577:PRO:HG2	2:N:580:MET:HG2	1.95	0.49
7:I:-36:DA:H1'	7:I:-35:DC:H5''	1.95	0.49
6:G:130:ALA:HB3	6:G:137:TYR:CE1	2.48	0.49
6:G:172:ALA:O	6:G:175:ARG:HB2	2.13	0.49
1:L:32:PHE:HA	1:L:35:THR:HB	1.94	0.49
3:O:824:ASN:ND2	3:O:862:ASP:OD1	2.38	0.49
3:O:1208:ASP:HB2	3:O:1215:VAL:HA	1.94	0.49
1:B:256:LEU:HD11	1:B:280:LEU:HD23	1.95	0.49
2:C:630:ARG:CZ	2:C:707:ARG:HD3	2.43	0.49
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.48	0.49
3:O:192:ALA:HB3	3:O:195:VAL:HB	1.95	0.49
2:N:1095:LEU:HD23	3:O:582:LEU:HD22	1.94	0.48
1:B:80:LEU:HG	3:D:844:ALA:HA	1.95	0.48
6:G:164:ARG:HD2	6:G:171:THR:HG23	1.95	0.48
2:N:524:VAL:HG13	2:N:528:GLU:HB2	1.95	0.48
3:O:101:HIS:HB3	3:O:104:PHE:HD2	1.79	0.48
3:O:1101:VAL:HG13	3:O:1102:THR:HG23	1.95	0.48
5:Q:188:ILE:HG12	5:Q:224:VAL:HG21	1.95	0.48
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.94	0.48
1:M:256:LEU:HD11	1:M:280:LEU:HD23	1.95	0.48
5:Q:263:HIS:NE2	7:T:-17:DT:OP2	2.45	0.48
6:S:6:ARG:HH11	6:S:174:ARG:HH21	1.60	0.48
2:C:614:ARG:NH2	2:C:618:GLY:O	2.47	0.48
3:O:44:LEU:HB3	3:O:525:ARG:NH2	2.29	0.48
6:R:30:VAL:HB	6:R:43:ARG:HG2	1.94	0.48
6:R:172:ALA:O	6:R:175:ARG:HB2	2.13	0.48
8:U:33:DC:H2'	8:U:34:DT:H72	1.96	0.48
3:D:586:ARG:HH22	8:J:-5:DG:H5''	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:264:ARG:O	1:M:268:SER:OG	2.27	0.48
3:O:134:VAL:HG12	3:O:454:ALA:HB2	1.95	0.48
6:R:164:ARG:NH2	8:U:35:DG:OP2	2.42	0.48
2:C:524:VAL:HG13	2:C:528:GLU:HB2	1.96	0.48
8:J:25:DG:H2''	8:J:26:DG:C8	2.49	0.48
6:R:130:ALA:HB3	6:R:137:TYR:CE1	2.48	0.48
8:U:2:DG:H1	9:V:2:C:N4	2.12	0.48
1:A:54:THR:HG21	1:A:145:ASP:HB2	1.94	0.48
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.14	0.48
8:U:30:DT:H2''	8:U:31:DG:H5'	1.96	0.48
2:N:557:ARG:HG3	2:N:844:GLY:HA3	1.95	0.48
6:H:153:ARG:NH2	7:I:-48:DG:N7	2.62	0.47
2:N:331:ARG:NH2	7:T:1:DG:O6	2.43	0.47
2:N:744:ARG:HG3	2:N:747:ALA:HB2	1.95	0.47
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.97	0.47
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.95	0.47
4:E:83:ASP:OD1	4:E:83:ASP:N	2.47	0.47
8:J:13:DC:H2''	8:J:14:DG:C8	2.49	0.47
4:P:83:ASP:N	4:P:83:ASP:OD1	2.48	0.47
3:D:805:GLU:HG3	3:D:828:LYS:HB2	1.96	0.47
2:N:211:LEU:HB3	2:N:218:VAL:HB	1.96	0.47
3:O:832:ARG:HD2	3:O:833:GLU:H	1.79	0.47
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.96	0.47
3:O:821:VAL:HG11	3:O:827:ILE:HD12	1.96	0.47
1:A:32:PHE:HA	1:A:35:THR:HB	1.97	0.47
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.96	0.47
2:N:324:ASP:HB3	2:N:327:HIS:HB2	1.96	0.47
3:O:41:ARG:HG3	3:O:48:ARG:HE	1.79	0.47
3:D:5:VAL:O	3:D:1470:ARG:NH2	2.45	0.47
3:D:829:VAL:HG21	3:D:839:LEU:HD11	1.96	0.47
1:M:41:ARG:HA	1:M:177:VAL:HG11	1.97	0.47
2:N:942:GLU:HG2	2:N:945:ARG:HH21	1.80	0.47
8:U:0:DT:H2'	8:U:1:DC:C6	2.50	0.47
8:U:2:DG:H1	9:V:2:C:H42	1.61	0.47
3:O:155:ASP:OD2	3:O:568:ARG:NH1	2.38	0.46
3:O:561:GLY:HA3	5:Q:132:ARG:HD3	1.97	0.46
5:Q:187:LEU:HD23	5:Q:224:VAL:HG13	1.97	0.46
2:C:536:PRO:HB2	2:C:905:ILE:HG22	1.97	0.46
3:O:586:ARG:HH22	8:U:-5:DG:H5''	1.80	0.46
3:O:1258:ARG:HH21	3:O:1351:GLU:HG2	1.80	0.46
5:Q:153:PRO:HA	5:Q:156:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:-23:DG:H1'	7:T:-22:DT:H5'	1.96	0.46
7:T:2:DT:H2''	7:T:3:DC:H5'	1.96	0.46
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.96	0.46
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.96	0.46
2:C:714:ASP:OD1	2:C:820:ARG:NE	2.46	0.46
3:D:784:ASP:HB2	3:D:939:PHE:HE1	1.80	0.46
3:O:1040:GLY:O	3:O:1060:SER:HB3	2.15	0.46
5:Q:263:HIS:HE1	7:T:-17:DT:H2'	1.80	0.46
8:U:24:DG:C2'	8:U:25:DG:H5''	2.45	0.46
2:C:1031:ARG:HH12	3:D:616:GLN:HA	1.80	0.46
3:D:832:ARG:HD2	3:D:833:GLU:H	1.80	0.46
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.47	0.46
3:O:114:THR:HG23	3:O:495:ARG:HG2	1.98	0.46
3:D:824:ASN:ND2	3:D:862:ASP:OD1	2.38	0.46
3:D:983:LEU:HD13	3:D:988:ARG:HB2	1.98	0.46
6:S:49:ASP:HA	6:S:92:ASN:ND2	2.28	0.46
6:G:28:VAL:HB	6:G:45:VAL:HB	1.98	0.46
2:N:571:LEU:HB2	2:N:574:ALA:HB2	1.98	0.46
2:N:1057:SER:HB3	2:N:1058:ASP:H	1.58	0.46
3:O:371:ILE:HD12	5:Q:230:LYS:HA	1.98	0.46
6:R:131:ARG:HG2	6:R:132:ASP:N	2.30	0.46
1:A:256:LEU:HD11	1:A:280:LEU:HD23	1.97	0.46
2:C:168:ARG:NH2	2:C:265:ARG:O	2.48	0.46
2:C:383:ARG:NH2	8:J:9:DA:H5''	2.31	0.46
6:G:113:ARG:NH2	6:G:166:GLU:OE1	2.41	0.46
3:O:619:LEU:HD11	3:O:1439:SER:HB2	1.98	0.46
3:O:787:LEU:HD21	3:O:947:ILE:HG21	1.98	0.46
8:J:35:DG:H1'	8:J:36:DT:H5''	1.98	0.46
2:N:1072:LYS:NZ	5:Q:352:GLU:OE2	2.39	0.46
3:O:562:ALA:O	5:Q:140:ARG:NH1	2.38	0.46
2:C:164:PRO:HD2	2:C:171:TRP:CD1	2.50	0.45
1:L:256:LEU:HD11	1:L:280:LEU:HD23	1.98	0.45
1:M:83:LYS:HE2	1:M:168:ASP:HB2	1.98	0.45
6:R:49:ASP:HA	6:R:92:ASN:HD21	1.80	0.45
2:C:582:GLY:N	2:C:584:GLU:OE2	2.49	0.45
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.98	0.45
7:I:2:DT:H2''	7:I:3:DC:H5'	1.98	0.45
7:T:-36:DA:H1'	7:T:-35:DC:H5''	1.98	0.45
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.98	0.45
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.31	0.45
5:F:368:VAL:O	5:F:372:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:-31:DC:H1'	7:I:-30:DA:H5'	1.99	0.45
8:J:30:DT:H2''	8:J:31:DG:H5'	1.99	0.45
2:N:853:LEU:HB2	2:N:858:MET:HE1	1.99	0.45
3:O:1258:ARG:NH1	3:O:1261:GLU:OE2	2.43	0.45
7:I:-23:DG:H1'	7:I:-22:DT:H5'	1.99	0.45
1:M:56:VAL:HG21	1:M:82:LEU:HD13	1.98	0.45
2:C:203:ASP:OD1	2:C:204:GLN:N	2.50	0.45
2:C:586:ARG:HD2	2:C:586:ARG:HA	1.67	0.45
7:I:8:DA:H1'	7:I:9:DT:H5'	1.99	0.45
1:M:108:GLU:HG2	1:M:131:THR:HG22	1.98	0.45
2:N:203:ASP:OD1	2:N:204:GLN:N	2.49	0.45
2:N:686:ASP:OD2	2:N:879:ARG:NH2	2.42	0.45
3:O:618:LEU:HG	3:O:1467:ILE:HG23	1.98	0.45
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.98	0.45
6:H:49:ASP:HA	6:H:92:ASN:ND2	2.31	0.45
2:N:578:VAL:HG23	2:N:579:VAL:HG23	1.97	0.45
2:N:586:ARG:HA	2:N:586:ARG:HD2	1.69	0.45
6:G:174:ARG:NH2	8:J:33:DC:OP1	2.47	0.45
8:J:2:DG:H1	9:K:2:C:H42	1.65	0.45
3:O:784:ASP:HB2	3:O:939:PHE:HE1	1.82	0.45
3:O:1168:MET:HE2	3:O:1172:HIS:CE1	2.52	0.45
2:C:395:LYS:HD3	2:C:397:GLU:HB3	1.98	0.45
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.50	0.45
1:L:218:LEU:HD23	1:M:222:LEU:HD21	1.99	0.45
2:N:758:ARG:HH21	2:N:788:THR:HB	1.82	0.45
2:N:1101:THR:OG1	2:N:1109:VAL:O	2.35	0.45
4:P:52:GLU:OE1	4:P:52:GLU:N	2.47	0.45
5:Q:338:LEU:HA	5:Q:339:PRO:HD3	1.85	0.45
6:S:172:ALA:O	6:S:175:ARG:HB2	2.17	0.45
3:D:17:LYS:HB2	3:D:17:LYS:HE3	1.77	0.45
3:D:90:MET:SD	3:D:521:PRO:HD3	2.57	0.45
3:D:191:LEU:HB3	3:D:393:ILE:HD12	1.98	0.45
3:D:758:GLU:OE1	3:D:1476:THR:OG1	2.32	0.45
6:G:131:ARG:HG2	6:G:132:ASP:N	2.31	0.45
3:O:434:ARG:NH2	5:Q:135:ILE:O	2.50	0.45
2:N:395:LYS:HD3	2:N:397:GLU:HB3	2.00	0.44
2:N:561:GLY:O	2:N:565:GLN:HG3	2.18	0.44
2:N:704:HIS:CD2	2:N:831:ARG:HD2	2.52	0.44
2:N:766:GLU:HG3	3:O:64:LYS:HD2	1.99	0.44
2:N:939:ARG:HB2	2:N:982:PRO:HG3	1.99	0.44
3:O:1252:ILE:HG23	3:O:1253:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1324:PRO:HG3	3:O:1330:ILE:HD11	1.97	0.44
5:Q:166:LEU:HD13	5:Q:170:HIS:HB3	2.00	0.44
2:C:578:VAL:HG23	2:C:579:VAL:HG23	1.98	0.44
3:D:1252:ILE:HG23	3:D:1253:THR:HG23	2.00	0.44
8:J:41:DT:H1'	8:J:42:DG:C8	2.52	0.44
2:N:383:ARG:NH2	8:U:9:DA:H5''	2.32	0.44
5:Q:333:ILE:HA	5:Q:334:PRO:HD3	1.84	0.44
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.18	0.44
8:J:0:DT:H2'	8:J:1:DC:C6	2.52	0.44
2:N:679:PHE:HA	3:O:943:THR:HB	1.99	0.44
2:N:719:PRO:HB3	2:N:820:ARG:NE	2.32	0.44
5:Q:372:ARG:HB3	5:Q:372:ARG:NH1	2.32	0.44
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.99	0.44
7:I:-13:DG:H1'	7:I:-12:DT:H5'	1.99	0.44
2:N:936:VAL:HG11	2:N:959:PRO:HB2	1.98	0.44
2:C:1083:GLU:OE1	2:C:1086:ARG:NH1	2.51	0.44
2:C:1088:LEU:HD22	3:D:618:LEU:HD21	1.99	0.44
3:D:1168:MET:HE3	3:D:1171:VAL:HB	1.98	0.44
6:G:2:LYS:HD3	6:G:3:ARG:H	1.83	0.44
2:N:164:PRO:HD2	2:N:171:TRP:CD1	2.52	0.44
2:N:1016:ILE:O	3:O:87:ARG:NH1	2.45	0.44
1:B:170:VAL:HG21	3:D:848:GLU:HG3	2.00	0.44
3:D:843:PHE:CE2	3:D:864:VAL:HG11	2.53	0.44
1:B:74:ASP:OD1	1:B:74:ASP:N	2.46	0.44
1:B:99:LEU:HB2	1:B:142:VAL:HG22	1.99	0.44
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.99	0.44
2:N:87:ASP:HA	2:N:131:GLY:HA3	1.99	0.44
3:O:834:THR:OG1	3:O:835:SER:N	2.51	0.44
8:U:41:DT:H1'	8:U:42:DG:C8	2.53	0.44
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.88	0.44
6:G:106:HIS:ND1	6:G:118:ARG:HD2	2.32	0.44
6:H:6:ARG:NH2	6:H:68:MET:O	2.45	0.44
1:L:264:ARG:NH1	1:L:297:ARG:HD2	2.33	0.44
5:Q:273:ARG:HH22	8:U:13:DC:P	2.41	0.44
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.99	0.44
7:I:-24:DC:H2''	7:I:-23:DG:C8	2.53	0.44
3:O:1068:LEU:O	3:O:1072:ILE:HG12	2.18	0.44
1:B:78:ILE:HG21	1:B:140:MET:HE1	2.00	0.43
2:C:707:ARG:O	2:C:707:ARG:HG2	2.18	0.43
3:D:106:LYS:HE3	3:D:587:ARG:HG3	2.00	0.43
3:D:974:ILE:HG22	3:D:988:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:964:LEU:HB3	3:O:1058:ARG:HH21	1.83	0.43
6:S:173:TYR:CZ	8:U:53:DG:H5''	2.53	0.43
3:D:821:VAL:HG11	3:D:827:ILE:HD12	2.00	0.43
3:O:829:VAL:HG21	3:O:839:LEU:HD11	2.00	0.43
3:O:983:LEU:HD13	3:O:988:ARG:HB2	2.00	0.43
6:R:111:GLU:HB3	7:T:-40:DC:OP1	2.18	0.43
7:T:-28:DG:H2''	7:T:-27:DG:H5'	2.00	0.43
2:C:684:PHE:HB3	3:D:633:VAL:HG21	2.00	0.43
6:H:28:VAL:HB	6:H:45:VAL:HB	2.00	0.43
7:I:-50:DT:H2''	7:I:-49:DT:C5'	2.48	0.43
1:L:8:ALA:HA	1:L:9:PRO:HD3	1.74	0.43
1:A:188:GLN:NE2	1:A:189:ARG:HG2	2.33	0.43
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	2.00	0.43
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.79	0.43
8:J:24:DG:C2'	8:J:25:DG:H5''	2.47	0.43
2:N:167:LYS:HD3	7:T:-1:DC:H5	1.83	0.43
4:P:14:ASP:OD1	4:P:14:ASP:N	2.50	0.43
6:R:152:ILE:HD12	6:R:155:SER:H	1.82	0.43
6:R:173:TYR:CE1	7:T:-30:DA:H4'	2.53	0.43
1:A:103:ALA:HB1	1:A:107:LYS:HD3	2.00	0.43
2:C:404:LEU:O	2:C:408:ARG:HG3	2.18	0.43
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.50	0.43
4:E:52:GLU:OE1	4:E:52:GLU:N	2.48	0.43
8:J:29:DT:H2''	8:J:30:DT:O5'	2.18	0.43
2:N:21:ILE:HD12	2:N:455:LEU:HD22	2.01	0.43
2:N:591:SER:O	2:N:592:LEU:HB2	2.18	0.43
2:N:946:ARG:O	2:N:950:LEU:HG	2.19	0.43
3:O:1371:VAL:HG12	3:O:1375:MET:HE2	2.01	0.43
5:Q:394:ARG:O	5:Q:397:ILE:HG22	2.19	0.43
2:C:846:LYS:NZ	9:K:4:A:OP1	2.42	0.43
6:H:131:ARG:HG2	6:H:132:ASP:N	2.34	0.43
3:O:1094:LEU:HD22	3:O:1260:ILE:HG12	2.01	0.43
6:R:6:ARG:HH11	6:R:174:ARG:NH2	2.16	0.43
6:S:49:ASP:OD2	6:S:99:ARG:NH2	2.40	0.43
7:T:-50:DT:H4'	7:T:-49:DT:OP1	2.18	0.43
2:C:35:PRO:HG2	2:C:38:LYS:HB2	2.00	0.43
2:C:774:LEU:HD23	5:F:354:LEU:HD21	2.00	0.43
2:C:1094:ALA:HA	3:D:518:PRO:HB2	2.01	0.43
2:N:83:CYS:HA	2:N:88:LEU:HB2	2.00	0.43
3:O:654:LYS:O	3:O:658:LEU:HG	2.19	0.43
3:O:1137:ARG:O	3:O:1141:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:-50:DT:H2''	7:T:-49:DT:C5'	2.49	0.43
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.89	0.43
6:G:6:ARG:HH11	6:G:174:ARG:NH2	2.16	0.43
6:H:164:ARG:HG2	6:H:170:ALA:HA	2.01	0.43
6:H:172:ALA:O	6:H:175:ARG:HB2	2.19	0.43
3:O:939:PHE:O	3:O:943:THR:HG22	2.19	0.43
6:R:28:VAL:HB	6:R:45:VAL:HB	2.00	0.43
2:C:328:LEU:HD23	2:C:328:LEU:HA	1.89	0.43
2:N:545:ASN:HB3	2:N:583:LEU:HD22	2.00	0.43
3:O:1018:ASN:HA	3:O:1019:PRO:HD3	1.89	0.43
2:C:575:GLN:HG3	2:C:670:GLN:HA	2.00	0.43
3:D:784:ASP:HB2	3:D:939:PHE:CE1	2.53	0.43
3:D:970:LYS:HD3	3:D:995:LEU:HD13	2.00	0.43
3:D:1105:ILE:HG23	3:D:1199:GLY:HA2	2.00	0.43
7:I:-43:DC:H2''	7:I:-42:DC:H5'	2.01	0.43
6:R:164:ARG:HD3	6:R:169:ILE:HG13	2.01	0.43
2:C:211:LEU:HB3	2:C:218:VAL:HB	2.01	0.42
2:C:591:SER:O	2:C:592:LEU:HB2	2.19	0.42
3:D:486:ARG:H	3:D:486:ARG:HG3	1.59	0.42
2:N:229:MET:HB2	2:N:233:GLU:HB2	2.01	0.42
2:N:582:GLY:N	2:N:584:GLU:OE2	2.52	0.42
5:Q:372:ARG:HG2	5:Q:386:VAL:HG21	2.01	0.42
2:C:324:ASP:HB3	2:C:327:HIS:HB2	2.01	0.42
2:C:418:LEU:HD21	2:C:427:VAL:HG11	2.01	0.42
2:C:744:ARG:HG3	2:C:747:ALA:HB2	2.00	0.42
3:D:843:PHE:HE2	3:D:864:VAL:HG11	1.85	0.42
6:G:173:TYR:CG	7:I:-30:DA:H5''	2.54	0.42
1:L:54:THR:HG21	1:L:145:ASP:HB2	2.00	0.42
3:O:172:PRO:HA	3:O:173:PRO:HD3	1.90	0.42
3:O:527:MET:HE2	3:O:527:MET:HB2	1.91	0.42
4:P:45:ARG:HA	4:P:46:PRO:HD3	1.91	0.42
6:S:173:TYR:O	6:S:174:ARG:HG2	2.19	0.42
8:U:14:DG:H2''	8:U:15:DG:O5'	2.18	0.42
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.54	0.42
1:B:274:ILE:HD13	1:B:283:LEU:HD11	2.01	0.42
5:F:372:ARG:NH1	5:F:372:ARG:HB3	2.34	0.42
7:I:-50:DT:H4'	7:I:-49:DT:OP1	2.19	0.42
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.35	0.42
3:D:654:LYS:O	3:D:658:LEU:HG	2.19	0.42
2:C:942:GLU:HG2	2:C:945:ARG:HH21	1.85	0.42
3:D:32:ILE:HG22	3:D:39:PRO:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:373:LYS:HD3	5:F:373:LYS:HA	1.76	0.42
1:L:227:ASN:HA	1:L:228:PRO:HD3	1.86	0.42
3:O:1147:ARG:HD3	3:O:1188:VAL:HG11	2.01	0.42
2:C:501:THR:HA	2:C:502:PRO:HD3	1.92	0.42
2:C:679:PHE:HA	3:D:943:THR:HB	2.00	0.42
5:F:166:LEU:HD13	5:F:170:HIS:HB3	2.00	0.42
5:F:193:ARG:HB2	7:I:-7:DT:H1'	2.01	0.42
7:I:-47:DT:C2'	7:I:-46:DG:H5'	2.48	0.42
3:O:792:ILE:HD13	3:O:941:PHE:CD2	2.54	0.42
5:Q:420:ASP:OD1	5:Q:420:ASP:N	2.52	0.42
3:D:41:ARG:HG3	3:D:48:ARG:HE	1.84	0.42
2:N:247:PRO:HA	2:N:248:PRO:HD3	1.70	0.42
6:R:106:HIS:ND1	6:R:118:ARG:HD2	2.35	0.42
7:T:-43:DC:H2''	7:T:-42:DC:H5'	2.01	0.42
7:I:-28:DG:H2''	7:I:-27:DG:H5'	2.01	0.42
3:O:1493:LYS:HD2	3:O:1493:LYS:HA	1.72	0.42
5:Q:163:LEU:HD13	5:Q:174:LEU:HD13	2.01	0.42
8:U:15:DG:C2'	8:U:16:DC:H5''	2.43	0.42
6:G:95:ARG:NH1	6:G:195:ALA:OXT	2.53	0.42
1:M:80:LEU:HD11	3:O:842:VAL:HG12	2.01	0.42
3:O:17:LYS:HB2	3:O:17:LYS:HE3	1.83	0.42
3:O:1047:LYS:HG2	3:O:1053:PHE:CZ	2.54	0.42
6:R:49:ASP:HA	6:R:92:ASN:ND2	2.35	0.42
6:H:173:TYR:O	6:H:174:ARG:HG2	2.19	0.42
1:L:41:ARG:HA	1:L:177:VAL:HG11	2.02	0.42
2:N:1031:ARG:HH12	3:O:616:GLN:HA	1.85	0.42
2:N:1043:TYR:CG	3:O:763:MET:HG2	2.55	0.42
4:P:68:LEU:HD12	4:P:68:LEU:HA	1.85	0.42
5:Q:285:GLU:HA	5:Q:286:PRO:HD3	1.79	0.42
7:T:-49:DT:H2''	7:T:-48:DG:C8	2.55	0.42
2:C:611:ILE:HD11	2:C:641:PRO:HB3	2.02	0.41
2:C:726:ILE:HA	2:C:727:PRO:HD3	1.91	0.41
2:C:1058:ASP:OD1	2:C:1058:ASP:N	2.52	0.41
5:F:93:LEU:HD21	5:F:193:ARG:HD2	2.02	0.41
6:G:101:GLN:O	6:G:104:GLU:HB2	2.20	0.41
1:M:188:GLN:HG2	1:M:189:ARG:HG2	2.02	0.41
2:N:243:ARG:HD2	2:N:256:TYR:CE1	2.55	0.41
3:O:1122:LEU:HD13	3:O:1178:ALA:HB2	2.01	0.41
4:P:13:VAL:HG21	4:P:19:LEU:HB2	2.00	0.41
5:Q:360:LYS:HA	5:Q:360:LYS:HD3	1.93	0.41
2:C:11:GLU:H	2:C:11:GLU:HG2	1.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.68	0.41
3:D:411:THR:HB	3:D:437:VAL:H	1.84	0.41
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.54	0.41
6:G:32:GLU:OE1	6:G:62:ARG:NH2	2.50	0.41
2:N:553:ASP:OD2	2:N:843:HIS:ND1	2.53	0.41
1:A:50:GLY:HA3	1:A:173:PRO:HD3	2.02	0.41
1:A:227:ASN:HA	1:A:228:PRO:HD3	1.83	0.41
5:F:212:LEU:HD22	5:F:247:ILE:HG23	2.03	0.41
2:N:246:ASP:HA	2:N:247:PRO:HD2	1.90	0.41
3:O:35:ARG:HH11	3:O:36:THR:HG22	1.85	0.41
5:Q:270:LYS:O	5:Q:274:THR:OG1	2.24	0.41
8:U:25:DG:H2''	8:U:26:DG:C8	2.54	0.41
8:U:49:DA:H2''	8:U:50:DA:O5'	2.20	0.41
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	2.01	0.41
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.91	0.41
2:N:464:LEU:HD12	2:N:464:LEU:HA	1.85	0.41
5:Q:123:ASP:HA	5:Q:124:PRO:HD3	1.91	0.41
5:Q:354:LEU:HD23	5:Q:354:LEU:HA	1.91	0.41
6:S:6:ARG:HG2	6:S:7:LYS:HG2	2.02	0.41
3:D:749:VAL:HA	3:D:750:PRO:HD2	1.93	0.41
3:D:959:GLU:OE1	3:D:959:GLU:N	2.47	0.41
3:D:1463:LYS:HB3	3:D:1463:LYS:HE2	1.92	0.41
5:F:123:ASP:HA	5:F:124:PRO:HD3	1.93	0.41
5:F:162:LYS:HB2	5:F:162:LYS:HE3	1.79	0.41
8:J:49:DA:H2''	8:J:50:DA:O5'	2.20	0.41
3:O:521:PRO:HA	3:O:522:PRO:HD3	1.85	0.41
3:O:666:ILE:HG21	3:O:687:VAL:HG12	2.01	0.41
7:T:-24:DC:H2''	7:T:-23:DG:C8	2.55	0.41
2:C:223:ASP:OD1	2:C:225:SER:OG	2.33	0.41
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.55	0.41
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.55	0.41
3:O:145:VAL:HA	3:O:146:PRO:HD3	1.91	0.41
3:O:208:PRO:HA	3:O:390:PRO:HA	2.03	0.41
3:O:758:GLU:OE1	3:O:1476:THR:OG1	2.33	0.41
3:O:1490:LYS:HE3	3:O:1490:LYS:HB2	1.92	0.41
5:Q:319:THR:HA	5:Q:320:PRO:HD3	1.85	0.41
7:T:8:DA:H5'	7:T:8:DA:C8	2.56	0.41
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.91	0.41
3:D:841:TYR:HB2	3:D:864:VAL:HG13	2.02	0.41
8:J:45:DT:H2''	8:J:46:DC:H5'	2.02	0.41
2:N:684:PHE:HB3	3:O:633:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1032:PHE:CZ	2:N:1036:GLU:HB3	2.56	0.41
3:O:171:LEU:HD22	3:O:390:PRO:HG2	2.02	0.41
3:O:1383:ASP:HA	3:O:1384:PRO:HD3	1.82	0.41
7:T:8:DA:H1'	7:T:9:DT:H5'	2.02	0.41
3:D:38:LYS:HA	3:D:38:LYS:HD3	1.90	0.41
3:D:1147:ARG:HH22	3:D:1369:GLU:CD	2.29	0.41
5:F:135:ILE:HD11	5:F:178:ARG:HB3	2.03	0.41
6:H:173:TYR:CZ	8:J:53:DG:H5''	2.55	0.41
1:M:265:VAL:O	1:M:269:LEU:HB2	2.20	0.41
2:N:214:TYR:HE2	2:N:308:ARG:HG3	1.86	0.41
2:N:774:LEU:HD23	5:Q:354:LEU:HD21	2.01	0.41
2:N:802:ARG:HB2	2:N:826:TYR:HB2	2.03	0.41
3:O:115:LEU:HD12	3:O:512:MET:HE1	2.03	0.41
6:S:30:VAL:HB	6:S:43:ARG:HG2	2.02	0.41
1:B:264:ARG:NH1	1:B:297:ARG:HD2	2.36	0.41
2:C:230:ARG:HG3	2:C:233:GLU:HG3	2.03	0.41
2:C:601:GLY:HA3	2:C:615:TYR:HA	2.02	0.41
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.02	0.41
3:D:403:PHE:CD1	3:D:444:VAL:HG23	2.55	0.41
3:D:527:MET:HE2	3:D:527:MET:HB2	1.92	0.41
3:D:834:THR:OG1	3:D:835:SER:N	2.53	0.41
3:D:939:PHE:O	3:D:943:THR:HG22	2.20	0.41
4:E:66:LYS:O	4:E:70:THR:HG23	2.21	0.41
5:F:354:LEU:HD23	5:F:354:LEU:HA	1.92	0.41
5:F:382:THR:CB	8:J:30:DT:H5'	2.51	0.41
8:J:14:DG:H2''	8:J:15:DG:O5'	2.20	0.41
1:L:264:ARG:O	1:L:268:SER:OG	2.25	0.41
2:N:168:ARG:O	2:N:267:TYR:HA	2.21	0.41
2:N:348:LEU:HD12	2:N:348:LEU:HA	1.92	0.41
2:N:577:PRO:HA	2:N:671:ASN:OD1	2.21	0.41
2:N:740:GLU:HB3	2:N:805:ARG:NH1	2.36	0.41
3:O:462:GLN:HB2	3:O:513:ILE:HG21	2.01	0.41
3:O:465:LEU:HD12	3:O:513:ILE:HD13	2.03	0.41
3:O:1057:VAL:HG13	3:O:1069:GLU:CD	2.45	0.41
3:O:1147:ARG:HH22	3:O:1369:GLU:CD	2.26	0.41
3:O:1331:ASP:HA	3:O:1332:PRO:HD3	1.91	0.41
5:Q:408:LEU:HD23	5:Q:408:LEU:HA	1.91	0.41
8:U:35:DG:H1'	8:U:36:DT:H5''	2.03	0.41
1:B:265:VAL:O	1:B:269:LEU:HB2	2.20	0.41
3:D:883:ALA:HA	3:D:900:ILE:HD13	2.02	0.41
8:J:15:DG:C2'	8:J:16:DC:H5''	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:80:LEU:HD12	1:M:80:LEU:HA	1.85	0.41
3:O:1232:PRO:HG2	3:O:1356:TYR:HE1	1.86	0.41
3:O:1444:THR:O	3:O:1448:THR:HG23	2.20	0.41
2:C:766:GLU:HA	2:C:767:PRO:HD2	1.92	0.40
3:D:114:THR:HG23	3:D:495:ARG:HG2	2.03	0.40
2:N:16:PRO:O	2:N:586:ARG:NH2	2.55	0.40
2:N:607:ASP:HB2	2:N:610:ARG:NH1	2.36	0.40
3:O:90:MET:HE3	3:O:90:MET:HB3	1.97	0.40
3:O:483:HIS:HA	3:O:484:PRO:HD3	1.91	0.40
3:O:1044:LEU:H	3:O:1044:LEU:HD12	1.86	0.40
5:Q:368:VAL:O	5:Q:372:ARG:HG3	2.21	0.40
6:S:32:GLU:HG3	6:S:33:LEU:N	2.33	0.40
3:D:1323:GLN:HA	3:D:1324:PRO:HD3	1.87	0.40
5:F:420:ASP:OD1	5:F:420:ASP:N	2.53	0.40
8:J:41:DT:H1'	8:J:42:DG:N7	2.35	0.40
2:C:464:LEU:HD12	2:C:464:LEU:HA	1.85	0.40
2:C:642:ARG:HD3	2:C:642:ARG:HA	1.93	0.40
8:J:28:DC:H2''	8:J:29:DT:C6	2.56	0.40
2:N:11:GLU:H	2:N:11:GLU:HG2	1.59	0.40
3:O:207:PHE:HA	3:O:208:PRO:HD2	1.95	0.40
4:P:66:LYS:O	4:P:70:THR:HG23	2.22	0.40
1:B:269:LEU:HD13	1:B:269:LEU:HA	1.92	0.40
2:C:627:ARG:NH1	2:C:638:ASP:OD2	2.54	0.40
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.86	0.40
3:D:1444:THR:O	3:D:1448:THR:HG23	2.21	0.40
5:F:263:HIS:NE2	7:I:17:DT:OP2	2.54	0.40
5:F:372:ARG:HH22	8:J:31:DG:P	2.44	0.40
8:J:33:DC:H2'	8:J:34:DT:H72	2.02	0.40
1:M:85:LEU:HA	1:M:124:ASN:HD21	1.86	0.40
1:M:115:LEU:HA	1:M:116:PRO:HD3	1.90	0.40
2:N:617:ASP:HB2	2:N:619:ARG:HG2	2.03	0.40
2:N:774:LEU:HD22	2:N:774:LEU:HA	1.86	0.40
3:O:496:LEU:O	3:O:500:ARG:HB2	2.22	0.40
3:O:843:PHE:CE2	3:O:864:VAL:HG11	2.56	0.40
3:O:897:TRP:CH2	3:O:902:LEU:HD22	2.56	0.40
1:B:162:ILE:HD12	1:B:162:ILE:HA	1.92	0.40
2:C:427:VAL:HG13	7:I:1:DG:N1	2.36	0.40
2:C:806:LEU:HB3	2:C:813:VAL:HG21	2.04	0.40
2:C:954:THR:HA	2:C:955:PRO:HD3	1.85	0.40
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.37	0.40
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1353:GLN:HG2	3:D:1368:ILE:HD12	2.03	0.40
8:J:43:DG:H1'	8:J:44:DC:C6	2.57	0.40
3:O:1377:LYS:HE3	3:O:1378:TYR:CZ	2.56	0.40
6:R:173:TYR:O	6:R:174:ARG:HG2	2.22	0.40
6:S:113:ARG:NH2	6:S:166:GLU:OE1	2.49	0.40
8:U:28:DC:H2''	8:U:29:DT:C6	2.55	0.40
8:U:29:DT:H2''	8:U:30:DT:O5'	2.20	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	280/315 (89%)	269 (96%)	11 (4%)	0	100	100
1	B	276/315 (88%)	264 (96%)	12 (4%)	0	100	100
1	L	280/315 (89%)	269 (96%)	11 (4%)	0	100	100
1	M	276/315 (88%)	264 (96%)	12 (4%)	0	100	100
2	C	1107/1119 (99%)	1090 (98%)	17 (2%)	0	100	100
2	N	1107/1119 (99%)	1088 (98%)	19 (2%)	0	100	100
3	D	1357/1524 (89%)	1337 (98%)	19 (1%)	1 (0%)	48	83
3	O	1357/1524 (89%)	1339 (99%)	17 (1%)	1 (0%)	48	83
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
4	P	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/443 (78%)	337 (98%)	7 (2%)	0	100	100
5	Q	344/443 (78%)	337 (98%)	7 (2%)	0	100	100
6	G	193/215 (90%)	190 (98%)	3 (2%)	0	100	100
6	H	193/215 (90%)	190 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	R	193/215 (90%)	190 (98%)	3 (2%)	0	100	100
6	S	193/215 (90%)	190 (98%)	3 (2%)	0	100	100
All	All	7684/8490 (90%)	7532 (98%)	150 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	530	VAL
3	O	530	VAL

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	249/273 (91%)	224 (90%)	25 (10%)	7	24
1	B	245/273 (90%)	220 (90%)	25 (10%)	7	23
1	L	249/273 (91%)	226 (91%)	23 (9%)	8	27
1	M	245/273 (90%)	222 (91%)	23 (9%)	8	26
2	C	936/941 (100%)	867 (93%)	69 (7%)	13	33
2	N	936/941 (100%)	868 (93%)	68 (7%)	13	34
3	D	1152/1279 (90%)	1077 (94%)	75 (6%)	15	37
3	O	1152/1279 (90%)	1079 (94%)	73 (6%)	16	38
4	E	83/88 (94%)	82 (99%)	1 (1%)	63	73
4	P	83/88 (94%)	82 (99%)	1 (1%)	63	73
5	F	301/388 (78%)	276 (92%)	25 (8%)	10	30
5	Q	301/388 (78%)	276 (92%)	25 (8%)	10	30
6	G	155/172 (90%)	148 (96%)	7 (4%)	24	46
6	H	155/172 (90%)	150 (97%)	5 (3%)	34	55
6	R	155/172 (90%)	149 (96%)	6 (4%)	28	49
6	S	155/172 (90%)	150 (97%)	5 (3%)	34	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6552/7172 (91%)	6096 (93%)	456 (7%)	14	36

All (456) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	80	LEU
1	A	112	ARG
1	A	142	VAL
1	A	156	HIS
1	A	183	ASP
1	A	189	ARG
1	A	197	LEU
1	A	201	THR
1	A	206	THR
1	A	223	THR
1	A	229	GLN
1	A	254	LEU
1	A	262	SER
1	A	263	THR
1	A	264	ARG
1	A	266	LEU
1	A	268	SER
1	A	269	LEU
1	A	277	VAL
1	A	280	LEU
1	A	286	LYS
1	A	297	ARG
1	A	309	LYS
1	B	7	LYS
1	B	34	VAL
1	B	80	LEU
1	B	94	LEU
1	B	112	ARG
1	B	142	VAL
1	B	148	VAL
1	B	186	LEU
1	B	189	ARG
1	B	190	THR
1	B	201	THR
1	B	206	THR

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Mol	Chain	Res	Type
1	B	226	SER
1	B	254	LEU
1	B	262	SER
1	B	263	THR
1	B	264	ARG
1	B	266	LEU
1	B	268	SER
1	B	269	LEU
1	B	277	VAL
1	B	280	LEU
1	B	286	LYS
1	B	297	ARG
1	B	309	LYS
2	C	8	ARG
2	C	11	GLU
2	C	15	LEU
2	C	56	GLU
2	C	81	ASP
2	C	97	ARG
2	C	103	LYS
2	C	107	LEU
2	C	133	ASP
2	C	172	ILE
2	C	177	GLU
2	C	194	VAL
2	C	196	LEU
2	C	205	GLU
2	C	217	LEU
2	C	232	GLU
2	C	251	ASP
2	C	261	ILE
2	C	265	ARG
2	C	322	VAL
2	C	331	ARG
2	C	336	VAL
2	C	342	ASP
2	C	358	ARG
2	C	372	LEU
2	C	403	SER
2	C	418	LEU
2	C	419	THR
2	C	427	VAL

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Mol	Chain	Res	Type
2	C	464	LEU
2	C	480	THR
2	C	482	GLU
2	C	511	GLU
2	C	524	VAL
2	C	575	GLN
2	C	583	LEU
2	C	584	GLU
2	C	586	ARG
2	C	589	ARG
2	C	592	LEU
2	C	617	ASP
2	C	633	GLN
2	C	638	ASP
2	C	640	ARG
2	C	648	ARG
2	C	715	THR
2	C	730	SER
2	C	774	LEU
2	C	775	ARG
2	C	781	LYS
2	C	786	LYS
2	C	807	ARG
2	C	808	ARG
2	C	813	VAL
2	C	815	LEU
2	C	820	ARG
2	C	830	LYS
2	C	848	VAL
2	C	905	ILE
2	C	910	LYS
2	C	916	GLU
2	C	923	GLU
2	C	939	ARG
2	C	952	LEU
2	C	968	LEU
2	C	978	ARG
2	C	1001	VAL
2	C	1014	SER
2	C	1057	SER
3	D	30	GLU
3	D	80	VAL

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Mol	Chain	Res	Type
3	D	81	THR
3	D	106	LYS
3	D	135	LEU
3	D	141	ILE
3	D	155	ASP
3	D	161	LEU
3	D	179	VAL
3	D	186	VAL
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	204	LEU
3	D	355	VAL
3	D	360	ARG
3	D	362	GLU
3	D	372	ASP
3	D	387	LEU
3	D	411	THR
3	D	415	VAL
3	D	421	LEU
3	D	427	VAL
3	D	500	ARG
3	D	548	ILE
3	D	572	ARG
3	D	576	GLU
3	D	586	ARG
3	D	591	VAL
3	D	618	LEU
3	D	632	VAL
3	D	646	LYS
3	D	650	LEU
3	D	669	ASN
3	D	675	ARG
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	810	GLU
3	D	817	GLU
3	D	827	ILE
3	D	832	ARG
3	D	875	THR

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Mol	Chain	Res	Type
3	D	894	LYS
3	D	904	VAL
3	D	908	LYS
3	D	943	THR
3	D	973	GLN
3	D	983	LEU
3	D	1041	LEU
3	D	1062	ARG
3	D	1067	VAL
3	D	1127	GLU
3	D	1128	VAL
3	D	1162	GLU
3	D	1188	VAL
3	D	1195	GLN
3	D	1219	GLU
3	D	1221	VAL
3	D	1277	ILE
3	D	1283	ILE
3	D	1287	GLU
3	D	1290	LEU
3	D	1304	LYS
3	D	1305	LEU
3	D	1313	VAL
3	D	1317	ASP
3	D	1408	ILE
3	D	1455	LYS
3	D	1470	ARG
3	D	1486	VAL
3	D	1493	LYS
3	D	1496	GLU
3	D	1501	GLU
4	E	50	THR
5	F	88	ILE
5	F	123	ASP
5	F	141	VAL
5	F	150	THR
5	F	205	ARG
5	F	208	SER
5	F	218	GLN
5	F	244	ARG
5	F	259	ARG
5	F	262	VAL

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Mol	Chain	Res	Type
5	F	276	ARG
5	F	279	GLN
5	F	287	THR
5	F	295	MET
5	F	310	ILE
5	F	364	ARG
5	F	377	ASP
5	F	382	THR
5	F	398	ARG
5	F	402	ASN
5	F	403	LYS
5	F	406	ARG
5	F	419	ARG
5	F	420	ASP
5	F	422	LEU
6	G	2	LYS
6	G	32	GLU
6	G	87	HIS
6	G	106	HIS
6	G	131	ARG
6	G	152	ILE
6	G	153	ARG
6	H	32	GLU
6	H	87	HIS
6	H	131	ARG
6	H	152	ILE
6	H	153	ARG
1	L	6	LEU
1	L	7	LYS
1	L	34	VAL
1	L	80	LEU
1	L	112	ARG
1	L	142	VAL
1	L	183	ASP
1	L	189	ARG
1	L	201	THR
1	L	206	THR
1	L	229	GLN
1	L	254	LEU
1	L	262	SER
1	L	263	THR
1	L	264	ARG

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Mol	Chain	Res	Type
1	L	266	LEU
1	L	268	SER
1	L	269	LEU
1	L	277	VAL
1	L	280	LEU
1	L	286	LYS
1	L	297	ARG
1	L	309	LYS
1	M	7	LYS
1	M	34	VAL
1	M	80	LEU
1	M	94	LEU
1	M	112	ARG
1	M	142	VAL
1	M	189	ARG
1	M	190	THR
1	M	197	LEU
1	M	206	THR
1	M	226	SER
1	M	254	LEU
1	M	262	SER
1	M	263	THR
1	M	264	ARG
1	M	266	LEU
1	M	268	SER
1	M	269	LEU
1	M	277	VAL
1	M	280	LEU
1	M	286	LYS
1	M	297	ARG
1	M	309	LYS
2	N	8	ARG
2	N	11	GLU
2	N	15	LEU
2	N	56	GLU
2	N	81	ASP
2	N	97	ARG
2	N	103	LYS
2	N	107	LEU
2	N	133	ASP
2	N	172	ILE
2	N	177	GLU

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Mol	Chain	Res	Type
2	N	194	VAL
2	N	196	LEU
2	N	205	GLU
2	N	217	LEU
2	N	232	GLU
2	N	251	ASP
2	N	261	ILE
2	N	265	ARG
2	N	322	VAL
2	N	331	ARG
2	N	336	VAL
2	N	342	ASP
2	N	358	ARG
2	N	372	LEU
2	N	403	SER
2	N	418	LEU
2	N	419	THR
2	N	427	VAL
2	N	464	LEU
2	N	480	THR
2	N	482	GLU
2	N	524	VAL
2	N	575	GLN
2	N	583	LEU
2	N	584	GLU
2	N	586	ARG
2	N	589	ARG
2	N	592	LEU
2	N	617	ASP
2	N	633	GLN
2	N	638	ASP
2	N	640	ARG
2	N	648	ARG
2	N	715	THR
2	N	730	SER
2	N	774	LEU
2	N	775	ARG
2	N	781	LYS
2	N	786	LYS
2	N	807	ARG
2	N	808	ARG
2	N	813	VAL

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Mol	Chain	Res	Type
2	N	815	LEU
2	N	820	ARG
2	N	830	LYS
2	N	848	VAL
2	N	905	ILE
2	N	910	LYS
2	N	916	GLU
2	N	923	GLU
2	N	939	ARG
2	N	952	LEU
2	N	968	LEU
2	N	978	ARG
2	N	1001	VAL
2	N	1014	SER
2	N	1057	SER
3	O	30	GLU
3	O	80	VAL
3	O	81	THR
3	O	106	LYS
3	O	135	LEU
3	O	141	ILE
3	O	155	ASP
3	O	161	LEU
3	O	179	VAL
3	O	186	VAL
3	O	190	GLU
3	O	191	LEU
3	O	198	ARG
3	O	204	LEU
3	O	355	VAL
3	O	360	ARG
3	O	362	GLU
3	O	372	ASP
3	O	387	LEU
3	O	411	THR
3	O	415	VAL
3	O	421	LEU
3	O	427	VAL
3	O	500	ARG
3	O	548	ILE
3	O	572	ARG
3	O	576	GLU

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Mol	Chain	Res	Type
3	O	586	ARG
3	O	591	VAL
3	O	618	LEU
3	O	632	VAL
3	O	646	LYS
3	O	650	LEU
3	O	669	ASN
3	O	675	ARG
3	O	754	PHE
3	O	778	LEU
3	O	808	THR
3	O	810	GLU
3	O	817	GLU
3	O	827	ILE
3	O	832	ARG
3	O	875	THR
3	O	894	LYS
3	O	904	VAL
3	O	908	LYS
3	O	943	THR
3	O	970	LYS
3	O	983	LEU
3	O	1041	LEU
3	O	1062	ARG
3	O	1067	VAL
3	O	1127	GLU
3	O	1128	VAL
3	O	1162	GLU
3	O	1188	VAL
3	O	1195	GLN
3	O	1219	GLU
3	O	1221	VAL
3	O	1277	ILE
3	O	1283	ILE
3	O	1287	GLU
3	O	1290	LEU
3	O	1304	LYS
3	O	1305	LEU
3	O	1313	VAL
3	O	1317	ASP
3	O	1455	LYS
3	O	1470	ARG

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Mol	Chain	Res	Type
3	O	1486	VAL
3	O	1493	LYS
3	O	1496	GLU
3	O	1501	GLU
4	P	50	THR
5	Q	88	ILE
5	Q	123	ASP
5	Q	141	VAL
5	Q	150	THR
5	Q	205	ARG
5	Q	208	SER
5	Q	218	GLN
5	Q	244	ARG
5	Q	259	ARG
5	Q	262	VAL
5	Q	276	ARG
5	Q	279	GLN
5	Q	287	THR
5	Q	295	MET
5	Q	310	ILE
5	Q	364	ARG
5	Q	377	ASP
5	Q	382	THR
5	Q	398	ARG
5	Q	402	ASN
5	Q	403	LYS
5	Q	406	ARG
5	Q	419	ARG
5	Q	420	ASP
5	Q	422	LEU
6	R	2	LYS
6	R	32	GLU
6	R	87	HIS
6	R	106	HIS
6	R	131	ARG
6	R	153	ARG
6	S	32	GLU
6	S	36	ASP
6	S	87	HIS
6	S	131	ARG
6	S	153	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	188	GLN
1	A	284	ASN
1	B	81	ASN
1	B	284	ASN
2	C	117	HIS
2	C	187	ASN
2	C	219	GLN
2	C	538	GLN
2	C	565	GLN
2	C	567	GLN
2	C	704	HIS
2	C	991	GLN
3	D	611	GLN
3	D	680	GLN
3	D	737	ASN
3	D	973	GLN
3	D	1116	ASN
3	D	1172	HIS
3	D	1202	GLN
3	D	1359	GLN
3	D	1441	GLN
3	D	1442	ASN
4	E	33	HIS
6	G	108	GLN
6	H	108	GLN
1	L	188	GLN
1	L	284	ASN
1	M	38	ASN
1	M	284	ASN
2	N	139	GLN
2	N	219	GLN
2	N	320	HIS
2	N	538	GLN
2	N	575	GLN
2	N	991	GLN
2	N	1018	GLN
3	O	724	GLN
3	O	994	GLN
3	O	1014	ASN
3	O	1037	GLN
3	O	1116	ASN

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Mol	Chain	Res	Type
3	O	1172	HIS
3	O	1359	GLN
5	Q	399	GLN
5	Q	411	HIS
6	R	108	GLN
6	S	108	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	K	3/4 (75%)	1 (33%)	0
9	V	3/4 (75%)	1 (33%)	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	K	2	C
9	V	2	C

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	284/315 (90%)	-0.04	10 (3%) 47 38	40, 111, 176, 252	0
1	B	280/315 (88%)	0.22	12 (4%) 40 35	25, 117, 187, 259	0
1	L	284/315 (90%)	0.03	8 (2%) 55 43	24, 117, 191, 242	0
1	M	280/315 (88%)	0.02	9 (3%) 50 40	39, 117, 182, 232	0
2	C	1111/1119 (99%)	0.13	45 (4%) 41 36	10, 94, 167, 243	0
2	N	1111/1119 (99%)	0.22	60 (5%) 31 29	3, 99, 174, 254	0
3	D	1363/1524 (89%)	0.07	41 (3%) 52 41	6, 80, 179, 266	1 (0%)
3	O	1363/1524 (89%)	0.07	47 (3%) 48 38	6, 79, 187, 278	1 (0%)
4	E	94/99 (94%)	0.00	4 (4%) 40 35	8, 68, 147, 194	0
4	P	94/99 (94%)	-0.07	4 (4%) 40 35	19, 74, 143, 182	0
5	F	346/443 (78%)	0.19	16 (4%) 37 33	27, 107, 192, 270	0
5	Q	346/443 (78%)	0.12	14 (4%) 42 36	17, 104, 188, 271	0
6	G	195/215 (90%)	0.18	7 (3%) 46 38	8, 64, 155, 220	0
6	H	195/215 (90%)	0.01	3 (1%) 72 56	14, 86, 160, 231	0
6	R	195/215 (90%)	0.27	11 (5%) 30 29	7, 63, 151, 234	0
6	S	195/215 (90%)	-0.03	5 (2%) 57 44	17, 82, 163, 268	0
7	I	66/72 (91%)	0.18	0 100 100	60, 135, 247, 283	0
7	T	66/72 (91%)	0.23	0 100 100	60, 134, 217, 302	0
8	J	66/72 (91%)	0.30	1 (1%) 72 56	40, 145, 238, 270	0
8	U	66/72 (91%)	0.26	0 100 100	52, 137, 230, 280	0
9	K	4/4 (100%)	-0.03	0 100 100	71, 79, 107, 113	0
9	V	4/4 (100%)	0.10	0 100 100	62, 74, 97, 217	0
All	All	8008/8786 (91%)	0.11	297 (3%) 45 37	3, 94, 182, 302	2 (0%)

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	ARG	6.3
1	A	280	LEU	6.2
2	C	689	VAL	6.2
2	C	410	ILE	5.6
2	N	343	GLN	5.5
3	O	1094	LEU	5.3
2	N	96	ALA	5.2
3	O	934	LEU	5.1
2	N	391	LEU	4.9
1	B	211	LEU	4.9
2	N	690	ILE	4.9
2	N	137	VAL	4.8
2	C	690	ILE	4.7
2	C	137	VAL	4.7
2	N	51	THR	4.6
3	D	1368	ILE	4.5
4	P	10	PHE	4.4
2	C	391	LEU	4.3
5	F	140	ARG	4.3
3	O	924	MET	4.2
2	N	1081	VAL	4.1
1	B	160	ASP	4.1
3	O	769	LEU	4.0
5	Q	326	ASP	3.9
1	A	36	LEU	3.9
2	N	700	TYR	3.9
3	D	1400	VAL	3.8
1	L	225	PHE	3.8
1	B	40	LEU	3.8
2	C	482	GLU	3.8
2	C	96	ALA	3.7
4	E	10	PHE	3.7
5	F	113	ILE	3.7
1	L	280	LEU	3.6
2	N	98	LEU	3.6
2	C	688	ILE	3.6
1	A	84	GLU	3.6
3	O	930	LEU	3.5
1	M	160	ASP	3.5
2	C	679	PHE	3.5
1	B	280	LEU	3.5
1	A	225	PHE	3.5
5	F	138	SER	3.5

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Mol	Chain	Res	Type	RSRZ
5	Q	140	ARG	3.4
3	O	181	ASP	3.4
3	D	896	ALA	3.4
1	A	283	LEU	3.4
2	N	172	ILE	3.4
2	N	1111	ILE	3.4
2	C	677	MET	3.3
6	H	56	LEU	3.3
1	L	138	LEU	3.3
2	N	571	LEU	3.3
6	S	56	LEU	3.3
2	C	484	VAL	3.2
3	D	1229	ILE	3.2
1	M	40	LEU	3.2
2	N	413	LEU	3.2
1	M	36	LEU	3.2
3	D	1389	LEU	3.2
3	O	557	LEU	3.2
6	G	155	SER	3.2
3	D	487	ALA	3.2
5	Q	142	ARG	3.2
3	D	1330	ILE	3.2
5	F	129	GLU	3.2
2	N	643	VAL	3.2
2	N	390	GLN	3.1
2	N	161	SER	3.1
3	D	737	ASN	3.1
2	C	974	LEU	3.1
5	F	333	ILE	3.1
2	N	260	LEU	3.1
5	Q	310	ILE	3.1
1	B	138	LEU	3.1
1	B	218	LEU	3.1
2	C	483	VAL	3.1
6	G	152	ILE	3.1
2	C	191	PHE	3.0
4	E	9	LEU	3.0
5	F	233	PHE	3.0
1	B	302	ILE	3.0
2	N	340	MET	3.0
2	N	890	LEU	3.0
6	G	56	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	453	THR	3.0
2	N	1010	THR	3.0
2	N	207	LEU	2.9
2	N	152	PRO	2.9
6	R	35	PRO	2.9
2	C	340	MET	2.9
2	N	853	LEU	2.9
1	B	54	THR	2.9
3	O	767	HIS	2.9
1	L	218	LEU	2.9
2	N	833	LEU	2.9
2	N	895	TYR	2.9
5	Q	184	ARG	2.8
6	R	36	ASP	2.8
1	B	256	LEU	2.8
3	D	1094	LEU	2.8
2	N	119	PRO	2.8
2	C	413	LEU	2.8
2	C	1016	ILE	2.8
5	F	187	LEU	2.8
2	C	186	VAL	2.8
2	N	138	SER	2.8
2	C	668	LEU	2.8
6	R	171	THR	2.8
1	A	65	PHE	2.8
2	C	869	VAL	2.8
6	R	81	MET	2.8
3	D	106	LYS	2.8
6	R	194	ALA	2.8
3	D	112	ILE	2.7
2	N	668	LEU	2.7
3	D	345	TYR	2.7
3	O	1356	TYR	2.7
1	L	65	PHE	2.7
2	C	207	LEU	2.7
4	E	6	ILE	2.7
1	M	143	ARG	2.7
2	N	555	ALA	2.7
2	N	694	LEU	2.7
2	N	859	PRO	2.6
3	D	725	SER	2.6
3	D	1263	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	1096	ALA	2.6
3	O	1256	LEU	2.6
3	O	535	PHE	2.6
3	D	377	VAL	2.6
3	O	1263	PHE	2.6
5	F	332	PHE	2.6
1	L	288	LEU	2.6
2	N	569	VAL	2.6
3	O	524	LEU	2.6
2	C	1111	ILE	2.6
2	N	914	ILE	2.6
2	N	823	VAL	2.6
3	D	1120	VAL	2.6
6	S	191	ALA	2.6
3	O	1421	LEU	2.6
3	D	951	ILE	2.6
3	D	895	VAL	2.6
3	D	1421	LEU	2.6
2	N	174	LEU	2.5
5	F	99	GLU	2.5
6	S	81	MET	2.5
3	O	1397	LYS	2.5
1	A	274	ILE	2.5
1	M	82	LEU	2.5
2	N	22	GLN	2.5
5	F	326	ASP	2.5
3	O	1259	VAL	2.5
2	C	184	MET	2.5
3	O	744	GLN	2.5
2	C	426	ASP	2.5
3	O	731	LEU	2.5
2	N	386	PHE	2.5
3	O	547	LEU	2.5
3	D	1274	ILE	2.5
3	O	1233	GLY	2.5
2	N	94	LEU	2.5
1	L	68	ILE	2.5
3	O	699	VAL	2.5
3	D	1502	ALA	2.5
5	Q	407	LYS	2.5
2	N	52	PHE	2.4
3	D	446	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	N	1000	MET	2.4
2	C	571	LEU	2.4
2	N	994	ILE	2.4
2	C	1036	GLU	2.4
3	O	182	GLY	2.4
1	M	158	ILE	2.4
2	N	282	GLY	2.4
2	C	98	LEU	2.4
2	N	656	ALA	2.4
1	B	109	VAL	2.4
2	C	411	SER	2.4
2	C	836	GLY	2.4
3	D	734	GLU	2.4
3	D	899	LEU	2.4
6	G	23	LEU	2.4
6	H	178	LEU	2.4
2	C	849	VAL	2.4
6	G	57	GLU	2.4
5	Q	127	ILE	2.4
2	N	257	VAL	2.4
3	D	1422	MET	2.3
3	D	1420	LEU	2.3
3	O	564	GLU	2.3
3	D	769	LEU	2.3
2	C	282	GLY	2.3
3	D	367	ILE	2.3
3	O	1453	ALA	2.3
3	O	385	VAL	2.3
2	N	549	PHE	2.3
5	Q	209	PHE	2.3
3	O	1330	ILE	2.3
3	O	536	ALA	2.3
3	O	1450	ALA	2.3
2	C	981	GLU	2.3
1	M	53	VAL	2.3
3	O	528	VAL	2.3
2	N	30	LEU	2.3
3	O	127	LEU	2.3
4	E	85	LEU	2.3
2	C	452	ILE	2.3
1	M	280	LEU	2.3
2	C	948	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	973	VAL	2.3
3	O	558	LEU	2.3
5	Q	78	SER	2.3
3	O	919	PHE	2.3
2	N	125	GLY	2.3
2	N	686	ASP	2.3
2	N	1076	VAL	2.3
6	G	156	VAL	2.3
5	F	147	LEU	2.3
5	F	199	ALA	2.3
1	B	101	LEU	2.2
3	D	931	LEU	2.2
5	Q	311	ALA	2.2
3	O	180	LYS	2.2
1	L	211	LEU	2.2
5	Q	102	LEU	2.2
6	R	73	VAL	2.2
6	R	193	GLU	2.2
2	N	998	TYR	2.2
4	P	9	LEU	2.2
6	S	184	LEU	2.2
2	N	336	VAL	2.2
3	D	355	VAL	2.2
2	C	855	VAL	2.2
5	Q	224	VAL	2.2
3	O	387	LEU	2.2
2	N	162	ILE	2.2
1	M	218	LEU	2.2
2	N	463	GLU	2.2
2	N	1113	GLU	2.2
5	F	249	ARG	2.2
2	N	173	ASP	2.1
6	S	105	ALA	2.1
5	F	329	TYR	2.1
6	H	38	ARG	2.1
3	D	380	GLU	2.1
3	D	831	GLY	2.1
2	C	511	GLU	2.1
2	C	703	ILE	2.1
2	N	118	ILE	2.1
5	Q	323	ASP	2.1
2	C	845	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	56	GLU	2.1
1	A	218	LEU	2.1
2	C	52	PHE	2.1
3	D	1260	ILE	2.1
3	O	204	LEU	2.1
4	P	75	PHE	2.1
8	J	16	DC	2.1
3	D	1058	ARG	2.1
3	O	357	GLU	2.1
5	F	126	LEU	2.1
6	R	143	GLU	2.1
6	R	152	ILE	2.1
3	D	699	VAL	2.1
3	O	108	VAL	2.1
3	O	1213	ARG	2.1
3	O	1442	ASN	2.1
1	A	273	GLY	2.1
2	C	48	PHE	2.1
2	N	467	ILE	2.1
3	O	431	VAL	2.1
1	A	45	LEU	2.1
4	P	19	LEU	2.1
3	O	562	ALA	2.1
3	O	567	ILE	2.1
3	O	639	LEU	2.0
3	O	1468	LEU	2.0
3	D	564	GLU	2.0
6	R	195	ALA	2.0
3	D	975	GLU	2.0
3	O	211	VAL	2.0
3	O	737	ASN	2.0
3	O	890	VAL	2.0
5	F	128	ARG	2.0
2	N	411	SER	2.0
2	N	1085	PHE	2.0
2	C	218	VAL	2.0
2	N	641	PRO	2.0
3	D	108	VAL	2.0
3	D	594	PRO	2.0
5	Q	145	PRO	2.0
6	G	73	VAL	2.0
3	D	1395	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	1216	SER	2.0
6	R	151	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	MG	O	2003	1/1	0.93	0.17	13,13,13,13	0
11	MG	D	2003	1/1	0.99	0.09	18,18,18,18	0
10	ZN	O	2002	1/1	0.99	0.04	65,65,65,65	0
10	ZN	D	2001	1/1	1.00	0.07	52,52,52,52	0
10	ZN	D	2002	1/1	1.00	0.02	49,49,49,49	0
10	ZN	O	2001	1/1	1.00	0.08	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.