



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:03 PM GMT

PDB ID : 3M3Y  
Title : RNA polymerase II elongation complex C  
Authors : Wang, D.; Zhu, G.; Huang, X.; Lippard, S.J.  
Deposited on : 2010-03-10  
Resolution : 3.18 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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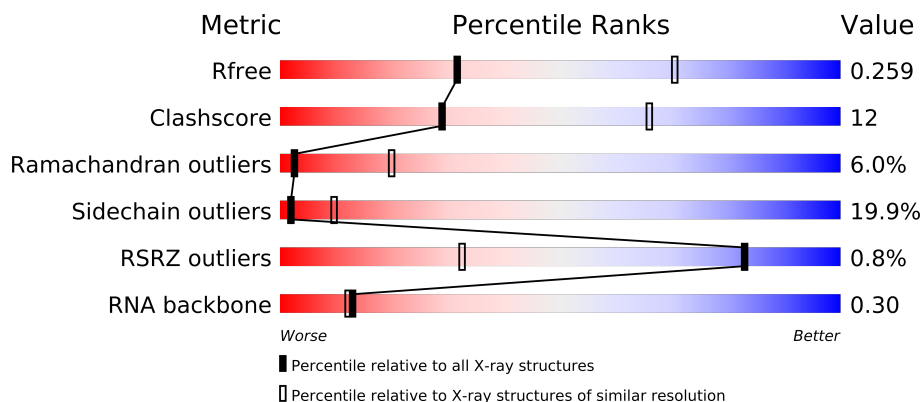
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance





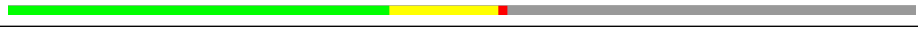




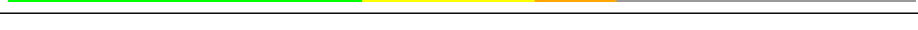

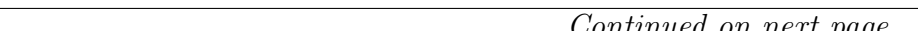
The reported resolution of this entry is 3.18 Å.

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))
$R_{free}$	66092	1472 (3.26-3.10)
Clashscore	79885	1024 (3.24-3.12)
Ramachandran outliers	78287	1002 (3.24-3.12)
Sidechain outliers	78261	1001 (3.24-3.12)
RSRZ outliers	66119	1473 (3.26-3.10)
RNA backbone	1838	1009 (3.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	E	215	
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	11	
12	T	28	

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Mol	Chain	Length	Quality of chain
13	N	14	 A horizontal bar chart representing the quality of chain 13. The bar is divided into three segments: a red segment (approximately 10% of the total length), a green segment (approximately 40% of the total length), and a yellow segment (approximately 50% of the total length).

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29241 atoms, of which 0 are hydrogen and 0 are deuterium.

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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(\*AP\*UP\*GP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	11	Total	C	N	O	P	0	0	0
			240	108	50	72	10			

- Molecule 12 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	28	Total	C	N	O	P	0	0	0
			550	265	92	166	27			

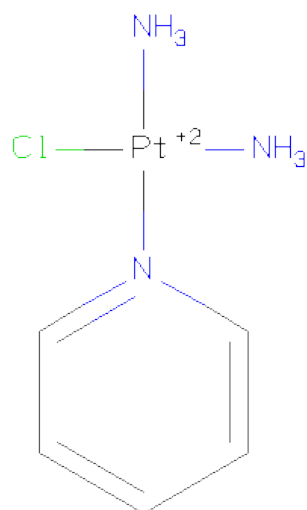
- Molecule 13 is a DNA chain called DNA (5'-D(\*GP\*TP\*GP\*GP\*TP\*TP\*AP\*TP\*GP\*GP\*GP\*TP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			293	140	55	85	13			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	Zn	0	0
			1	1		
14	B	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	C	1	Total	Zn	0	0
			1	1		
14	A	2	Total	Zn	0	0
			2	2		
14	L	1	Total	Zn	0	0
			1	1		

- Molecule 15 is CIS-DIAMMINE(PYRIDINE)CHLOROPLATINUM(II) (three-letter code: C7P) (formula: C<sub>5</sub>H<sub>11</sub>ClN<sub>3</sub>Pt).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	T	1	Total	C	N	Pt	0	0
			9	5	3	1		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

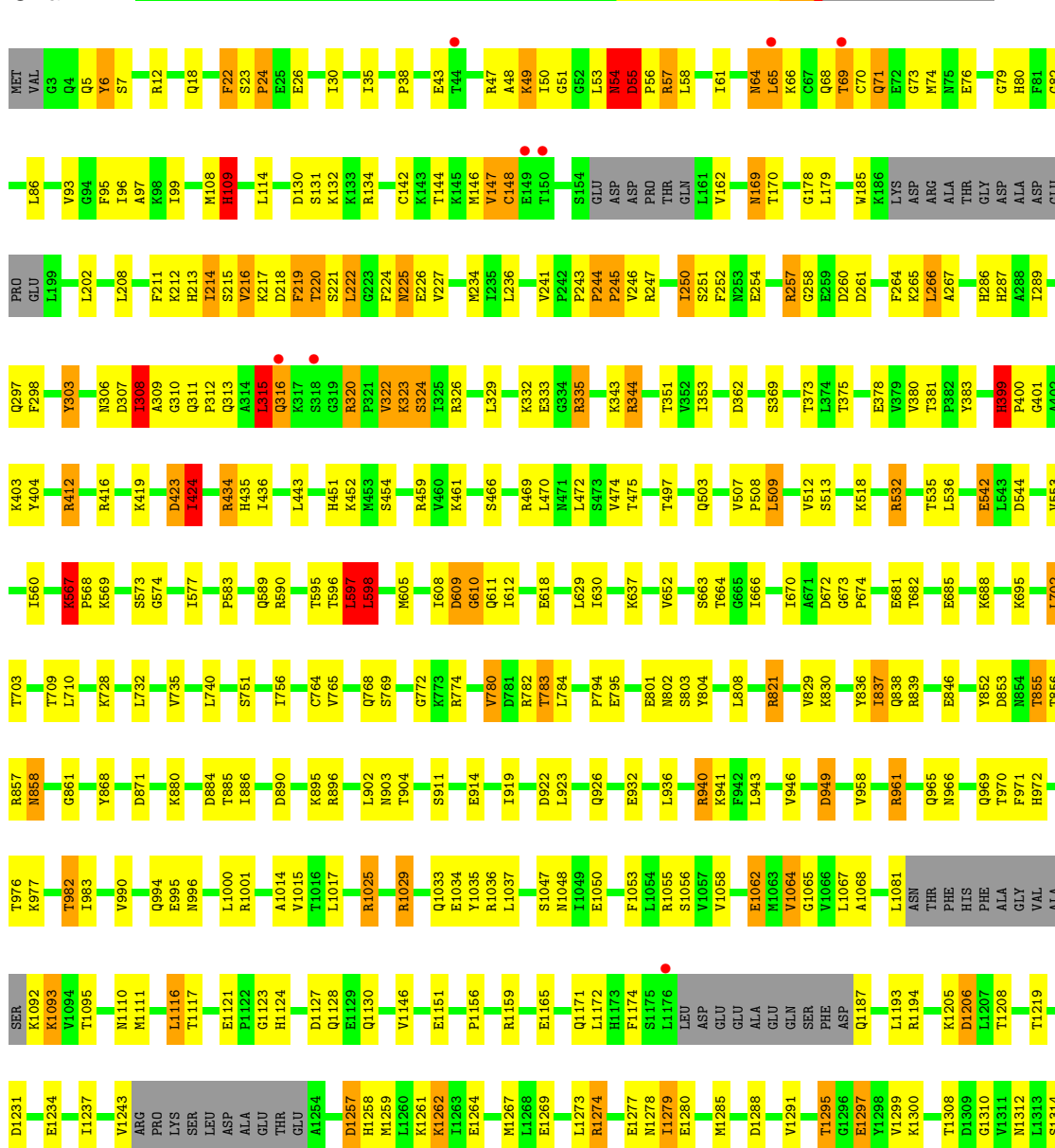
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

### 3 Residue-property plots

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

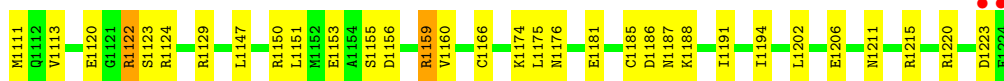
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A:



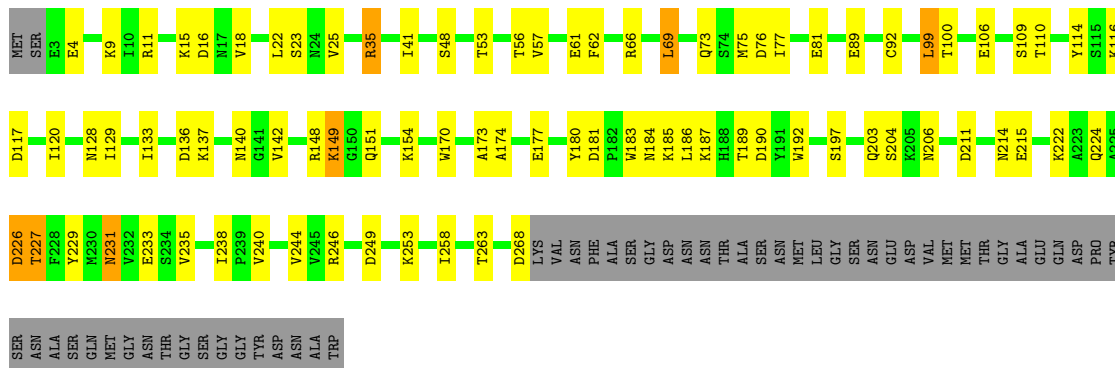






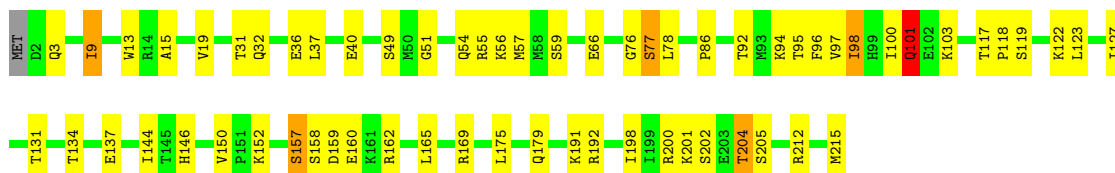
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



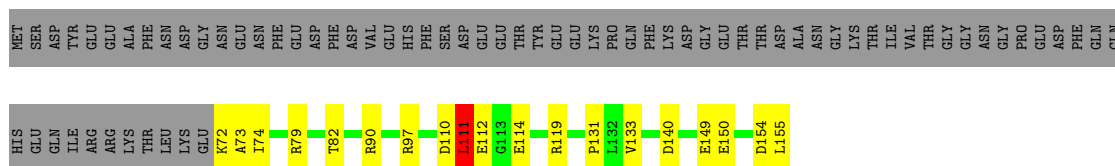
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



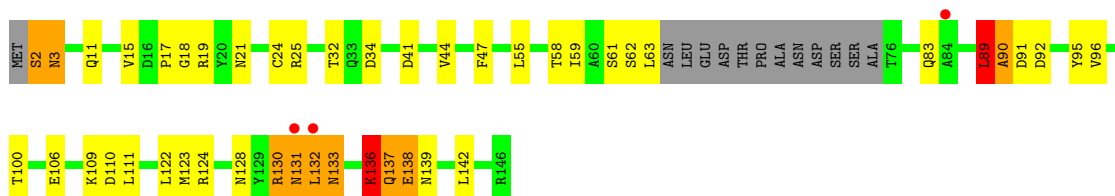
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



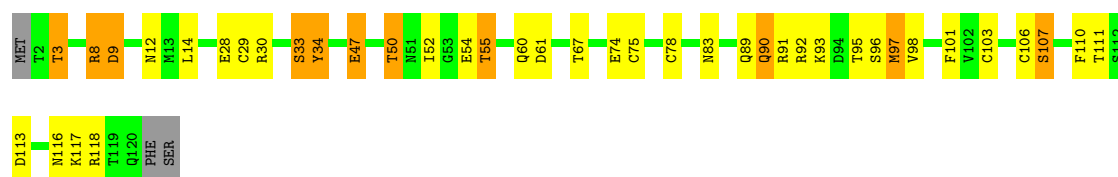
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



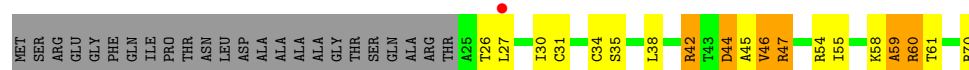
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



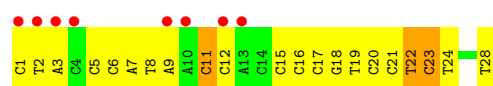
- Molecule 11: RNA (5'-R(\*AP\*UP\*GP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*C)-3')

Chain R:



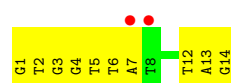
- Molecule 12: DNA (28-MER)

Chain T:



- Molecule 13: DNA (5'-D(\*GP\*TP\*GP\*GP\*TP\*TP\*AP\*TP\*GP\*GP\*GP\*TP\*AP\*G)-3')

Chain N:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.48Å 223.12Å 193.81Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	40.00 – 3.18 36.31 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.00-3.18) 98.6 (36.31-3.18)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.207 , 0.255 0.223 , 0.259	Depositor DCC
$R_{free}$ test set	5827 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.3	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 56.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 116095 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	29241	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: C7P, 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	0.73	1/11163 (0.0%)	0.87	8/15091 (0.1%)
2	B	0.84	2/8963 (0.0%)	0.94	11/12086 (0.1%)
3	C	0.84	1/2133 (0.0%)	0.93	0/2891
4	E	0.60	0/1788	0.75	1/2406 (0.0%)
5	F	0.71	0/691	0.79	0/933
6	H	0.69	0/1086	0.91	1/1470 (0.1%)
7	I	0.81	1/989 (0.1%)	0.94	1/1331 (0.1%)
8	J	0.85	0/541	1.01	2/727 (0.3%)
9	K	0.74	0/937	0.82	0/1265
10	L	0.88	0/365	1.10	0/485
11	R	1.25	0/270	2.01	15/421 (3.6%)
12	T	1.34	5/612 (0.8%)	2.03	35/937 (3.7%)
13	N	0.50	0/329	0.94	0/509
All	All	0.79	10/29867 (0.0%)	0.96	74/40552 (0.2%)

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
1	A	0	3
2	B	0	5
4	E	0	1
6	H	0	3
8	J	0	1
10	L	0	1
All	All	0	14

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	18	DG	C8-N7	9.27	1.36	1.30
12	T	21	DC	C3'-O3'	-6.85	1.35	1.44
12	T	18	DG	C6-N1	-6.38	1.35	1.39
12	T	18	DG	N9-C4	-5.70	1.33	1.38
1	A	795	GLU	CG-CD	5.61	1.60	1.51
12	T	19	DT	C3'-O3'	-5.54	1.36	1.44
3	C	92	CYS	CB-SG	-5.45	1.73	1.81
2	B	477	ALA	CA-CB	5.31	1.63	1.52
2	B	183	GLU	CG-CD	5.28	1.59	1.51
7	I	107	SER	CB-OG	5.04	1.48	1.42

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	18	DG	N3-C4-C5	-16.47	120.37	128.60
12	T	18	DG	C2-N3-C4	14.35	119.07	111.90
12	T	18	DG	C5-C6-N1	12.95	117.97	111.50
12	T	18	DG	N3-C4-N9	11.38	132.83	126.00
12	T	18	DG	O4'-C1'-N9	10.61	115.43	108.00
12	T	18	DG	O4'-C4'-C3'	-10.30	99.82	106.00
12	T	23	DC	O4'-C1'-N1	9.31	114.51	108.00
12	T	21	DC	O4'-C4'-C3'	-9.12	100.53	106.00
2	B	883	LEU	CA-CB-CG	9.10	136.23	115.30
11	R	8	G	C4'-C3'-C2'	-8.88	93.72	102.60
12	T	18	DG	C5-C6-O6	-8.82	123.31	128.60
12	T	20	DC	C4'-C3'-C2'	-8.45	95.49	103.10
1	A	702	LEU	CA-CB-CG	8.14	134.02	115.30
2	B	211	VAL	CB-CA-C	-8.07	96.07	111.40
2	B	167	ILE	CB-CA-C	-7.55	96.51	111.60
12	T	19	DT	C4-C5-C7	7.49	123.50	119.00
12	T	18	DG	C4'-C3'-C2'	-7.43	96.41	103.10
2	B	651	LEU	CA-CB-CG	7.42	132.35	115.30
11	R	11	C	C6-N1-C2	-7.41	117.33	120.30
11	R	11	C	O4'-C1'-N1	6.86	113.69	108.20
12	T	16	DC	C1'-O4'-C4'	-6.86	103.24	110.10
11	R	3	G	O4'-C1'-N9	6.84	113.67	108.20
8	J	3	VAL	CB-CA-C	-6.79	98.50	111.40
12	T	16	DC	O4'-C1'-N1	6.75	112.72	108.00
12	T	16	DC	O4'-C1'-C2'	-6.61	100.61	105.90
1	A	597	LEU	CB-CA-C	-6.61	97.65	110.20
1	A	936	LEU	CA-CB-CG	6.50	130.25	115.30
2	B	478	GLY	N-CA-C	-6.45	96.98	113.10
12	T	18	DG	C1'-O4'-C4'	-6.30	103.80	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	89	LEU	CA-CB-CG	6.16	129.47	115.30
12	T	22	DT	N3-C4-O4	6.14	123.58	119.90
11	R	1	A	O4'-C1'-N9	5.98	112.98	108.20
11	R	11	C	C3'-C2'-C1'	5.98	106.28	101.50
12	T	16	DC	P-O3'-C3'	5.95	126.84	119.70
12	T	17	DC	C4'-C3'-C2'	-5.91	97.78	103.10
12	T	19	DT	C6-C5-C7	-5.90	119.36	122.90
2	B	128	LEU	CA-CB-CG	5.89	128.84	115.30
11	R	8	G	C1'-O4'-C4'	-5.88	105.20	109.90
12	T	19	DT	O4'-C1'-N1	5.83	112.08	108.00
1	A	509	LEU	CA-CB-CG	5.81	128.66	115.30
12	T	18	DG	C6-N1-C2	-5.75	121.65	125.10
12	T	17	DC	C6-N1-C2	-5.73	118.01	120.30
11	R	10	A	C4'-C3'-C2'	-5.67	96.93	102.60
12	T	11	DC	O4'-C1'-N1	5.65	111.95	108.00
11	R	6	G	O4'-C1'-N9	5.63	112.70	108.20
4	E	175	LEU	CA-CB-CG	5.62	128.22	115.30
11	R	7	A	P-O3'-C3'	-5.57	113.02	119.70
2	B	390	LEU	CA-CB-CG	5.54	128.05	115.30
12	T	15	DC	O4'-C1'-N1	5.53	111.87	108.00
12	T	18	DG	N7-C8-N9	-5.48	110.36	113.10
1	A	821	ARG	NE-CZ-NH1	-5.47	117.56	120.30
12	T	22	DT	C4'-C3'-C2'	-5.46	98.18	103.10
11	R	7	A	OP1-P-O3'	5.45	117.20	105.20
12	T	28	DT	O4'-C4'-C3'	5.45	109.27	106.00
12	T	11	DC	C1'-O4'-C4'	-5.44	104.66	110.10
2	B	37	PHE	N-CA-C	-5.39	96.44	111.00
12	T	19	DT	C4'-C3'-C2'	-5.39	98.25	103.10
11	R	11	C	C4'-C3'-C2'	-5.39	97.21	102.60
7	I	78	CYS	CA-CB-SG	5.38	123.68	114.00
2	B	866	TYR	N-CA-C	5.36	125.47	111.00
12	T	17	DC	C2-N1-C1'	5.29	124.62	118.80
12	T	18	DG	N9-C1'-C2'	-5.29	102.54	112.60
2	B	1099	VAL	CB-CA-C	-5.27	101.39	111.40
11	R	7	A	C3'-C2'-C1'	5.25	105.70	101.50
11	R	2	U	O4'-C1'-N1	5.25	112.40	108.20
12	T	18	DG	C8-N9-C4	5.19	108.47	106.40
12	T	24	DT	C5-C4-O4	-5.16	121.29	124.90
1	A	598	LEU	N-CA-CB	5.13	120.65	110.40
2	B	766	ARG	NE-CZ-NH2	-5.11	117.75	120.30
11	R	3	G	N1-C6-O6	5.09	122.95	119.90
8	J	43	ARG	NE-CZ-NH1	-5.08	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1067	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	399	HIS	C-N-CD	5.02	138.95	128.40
12	T	17	DC	O4'-C1'-C2'	-5.01	101.89	105.90

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1391	ARG	Peptide
1	A	252	PHE	Peptide
1	A	71	GLN	Peptide
2	B	1076	HIS	Peptide
2	B	245	GLU	Peptide
2	B	265	SER	Peptide
2	B	644	GLU	Peptide
2	B	882	THR	Peptide
4	E	157	SER	Peptide
6	H	136	LYS	Peptide
6	H	138	GLU	Peptide
6	H	61	SER	Peptide
8	J	64	ASN	Peptide
10	L	42	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10969	0	23	121	0
2	B	8792	0	0	110	0
3	C	2095	0	0	20	0
4	E	1752	0	0	13	0
5	F	679	0	0	2	0
6	H	1068	0	0	18	0
7	I	971	0	0	10	0
8	J	532	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	919	0	0	2	0
10	L	363	0	0	5	0
11	R	240	0	0	0	0
12	T	550	0	0	41	0
13	N	293	0	0	43	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	1	0
14	L	1	0	0	0	0
15	T	9	0	0	0	0
16	A	1	0	0	0	0
All	All	29241	0	23	355	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (355) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:T:7:DA:C2	12:T:8:DT:C4	2.41	1.07
12:T:2:DT:C2'	12:T:3:DA:C5'	2.38	1.02
13:N:4:DG:C2	13:N:5:DT:C2	2.51	0.98
13:N:4:DG:N2	13:N:5:DT:C2	2.33	0.95
13:N:1:DG:C2'	13:N:2:DT:C7	2.46	0.93
1:A:567:LYS:CG	1:A:568:PRO:CD	2.47	0.92
13:N:4:DG:C6	13:N:5:DT:C4	2.59	0.90
12:T:8:DT:C2'	12:T:9:DA:C8	2.54	0.90
12:T:6:DC:C2	12:T:7:DA:N7	2.40	0.89
12:T:7:DA:C2	12:T:8:DT:N3	2.42	0.88
13:N:6:DT:C2	13:N:7:DA:C5	2.63	0.86
1:A:567:LYS:CB	1:A:568:PRO:CD	2.55	0.84
12:T:6:DC:C2	12:T:7:DA:C8	2.66	0.84
13:N:13:DA:OP2	13:N:13:DA:C8	2.30	0.84
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.28	0.81
12:T:1:DC:C2'	12:T:2:DT:OP2	2.30	0.80
13:N:6:DT:O2	13:N:7:DA:C5	2.36	0.79
13:N:6:DT:C2	13:N:7:DA:C6	2.71	0.78
1:A:423:ASP:O	1:A:424:ILE:CB	2.32	0.78
13:N:4:DG:C2	13:N:5:DT:N1	2.54	0.76
1:A:55:ASP:O	1:A:56:PRO:C	2.22	0.75
1:A:1029:ARG:NH1	1:A:1029:ARG:CG	2.49	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:T:6:DC:N1	12:T:7:DA:N7	2.35	0.74
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.21	0.74
1:A:596:THR:O	1:A:598:LEU:N	2.22	0.73
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.23	0.72
2:B:175:ARG:CG	2:B:175:ARG:NH1	2.53	0.72
12:T:6:DC:C1'	12:T:7:DA:C8	2.72	0.72
12:T:8:DT:O4	13:N:7:DA:N1	2.23	0.71
12:T:9:DA:C2	13:N:7:DA:C2	2.78	0.71
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.23	0.71
12:T:7:DA:N1	12:T:8:DT:C4	2.59	0.71
13:N:6:DT:N3	13:N:7:DA:N6	2.38	0.71
1:A:567:LYS:NZ	6:H:95:TYR:CZ	2.59	0.70
13:N:4:DG:N1	13:N:5:DT:C4	2.60	0.70
1:A:532:ARG:CG	1:A:532:ARG:NH1	2.55	0.70
1:A:55:ASP:O	1:A:57:ARG:N	2.25	0.69
12:T:6:DC:N1	12:T:7:DA:C8	2.60	0.69
13:N:1:DG:C2'	13:N:2:DT:C5	2.76	0.69
3:C:66:ARG:NH2	8:J:3:VAL:O	2.26	0.68
1:A:260:ASP:OD1	1:A:261:ASP:N	2.25	0.68
1:A:64:ASN:O	1:A:66:LYS:N	2.27	0.68
2:B:476:ARG:O	2:B:478:GLY:N	2.26	0.68
1:A:399:HIS:O	1:A:401:GLY:N	2.27	0.68
1:A:412:ARG:CG	1:A:412:ARG:NH1	2.56	0.68
1:A:1437:GLY:O	1:A:1439:GLY:N	2.27	0.68
13:N:4:DG:N1	13:N:5:DT:N3	2.41	0.67
6:H:63:LEU:C	6:H:90:ALA:CB	2.62	0.67
1:A:378:GLU:OE1	1:A:434:ARG:NH1	2.27	0.67
1:A:343:LYS:NZ	2:B:1156:ASP:OD2	2.28	0.67
13:N:4:DG:C5	13:N:5:DT:C5	2.83	0.67
2:B:880:THR:CG2	2:B:880:THR:O	2.43	0.66
1:A:542:GLU:OE1	1:A:569:LYS:NZ	2.28	0.66
1:A:609:ASP:O	1:A:611:GLN:N	2.28	0.66
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.28	0.66
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.29	0.66
13:N:6:DT:N3	13:N:7:DA:C6	2.64	0.66
1:A:1206:ASP:N	1:A:1274:ARG:HH12	1.92	0.66
6:H:89:LEU:O	6:H:91:ASP:N	2.30	0.64
2:B:770:GLN:O	2:B:770:GLN:CG	2.45	0.64
2:B:363:HIS:O	2:B:364:ILE:CB	2.45	0.64
7:I:8:ARG:O	7:I:9:ASP:CB	2.45	0.64
13:N:4:DG:C4	13:N:5:DT:C6	2.85	0.64
2:B:167:ILE:O	2:B:168:GLY:O	2.15	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:T:6:DC:C2	12:T:7:DA:C5	2.86	0.64
2:B:822:ASN:O	8:J:48:ARG:NH1	2.31	0.63
2:B:482:VAL:O	2:B:483:LEU:O	2.16	0.63
3:C:185:LYS:NZ	3:C:211:ASP:O	2.31	0.63
8:J:46:CYS:SG	14:J:101:ZN:ZN	1.85	0.63
2:B:732:SER:CB	2:B:734:HIS:CD2	2.82	0.62
6:H:89:LEU:CD2	6:H:92:ASP:N	2.62	0.62
13:N:4:DG:N3	13:N:5:DT:C6	2.67	0.62
1:A:780:VAL:CG2	2:B:699:GLU:OE2	2.48	0.62
12:T:6:DC:C2'	12:T:7:DA:OP2	2.48	0.62
13:N:4:DG:N2	13:N:5:DT:O2	2.33	0.61
2:B:708:GLU:O	2:B:710:LEU:N	2.33	0.61
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.49	0.61
2:B:751:VAL:CG1	2:B:752:ALA:N	2.63	0.61
1:A:630:ILE:CD1	1:A:630:ILE:N	2.64	0.60
1:A:567:LYS:CB	6:H:96:VAL:N	2.64	0.60
2:B:482:VAL:C	2:B:483:LEU:O	2.36	0.60
13:N:5:DT:C2'	13:N:6:DT:C7	2.81	0.59
2:B:744:HIS:CD2	2:B:746:SER:N	2.70	0.59
13:N:4:DG:C2	13:N:5:DT:C6	2.91	0.59
3:C:73:GLN:NE2	3:C:75:MET:N	2.49	0.59
13:N:3:DG:C2'	13:N:4:DG:OP2	2.50	0.59
1:A:265:LYS:C	1:A:267:ALA:N	2.55	0.59
2:B:1153:GLU:OE2	2:B:1153:GLU:N	2.36	0.59
2:B:647:GLY:C	2:B:648:HIS:ND1	2.57	0.58
1:A:1053:PHE:O	1:A:1056:SER:N	2.36	0.58
1:A:215:SER:C	1:A:217:LYS:N	2.57	0.58
12:T:8:DT:C4	13:N:7:DA:N1	2.72	0.58
1:A:215:SER:O	1:A:217:LYS:N	2.37	0.58
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.37	0.57
1:A:567:LYS:CD	6:H:95:TYR:CD1	2.87	0.57
2:B:760:ASP:OD1	2:B:760:ASP:N	2.36	0.57
2:B:778:MET:CE	2:B:853:SER:CB	2.83	0.57
6:H:131:ASN:O	6:H:133:ASN:N	2.36	0.57
6:H:47:PHE:CB	6:H:95:TYR:CD1	2.87	0.57
10:L:47:ARG:NH1	10:L:54:ARG:NE	2.52	0.56
1:A:344:ARG:NH1	1:A:344:ARG:CG	2.68	0.56
1:A:1364:ASN:ND2	1:A:1366:ARG:CG	2.69	0.56
2:B:485:ARG:NH1	2:B:485:ARG:CG	2.68	0.56
2:B:708:GLU:O	2:B:709:ASP:C	2.44	0.56
2:B:1096:ARG:O	2:B:1097:HIS:CD2	2.59	0.56
12:T:3:DA:C2	13:N:12:DT:N3	2.73	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:T:11:DC:C5	12:T:12:DC:N4	2.74	0.56
1:A:1436:ILE:O	1:A:1437:GLY:C	2.43	0.56
6:H:44:VAL:CG1	6:H:44:VAL:O	2.53	0.56
6:H:17:PRO:O	6:H:19:ARG:N	2.38	0.56
4:E:117:THR:O	4:E:119:SER:N	2.39	0.56
2:B:547:VAL:N	2:B:612:GLU:OE2	2.39	0.56
2:B:636:PRO:O	2:B:691:GLU:O	2.24	0.56
12:T:6:DC:C6	12:T:7:DA:N7	2.74	0.55
1:A:399:HIS:O	1:A:400:PRO:C	2.41	0.55
13:N:4:DG:C4	13:N:5:DT:C5	2.94	0.55
6:H:41:ASP:OD2	6:H:122:LEU:N	2.39	0.55
2:B:801:LYS:O	8:J:52:THR:CG2	2.54	0.55
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.40	0.55
12:T:8:DT:N3	13:N:7:DA:C2	2.74	0.55
1:A:244:PRO:O	1:A:246:VAL:N	2.39	0.55
2:B:63:ILE:O	2:B:67:SER:CB	2.55	0.55
7:I:47:GLU:OE1	7:I:50:THR:CG2	2.54	0.55
13:N:4:DG:C6	13:N:5:DT:C5	2.95	0.55
1:A:214:ILE:CG2	1:A:215:SER:N	2.70	0.54
12:T:6:DC:C4	12:T:7:DA:N6	2.75	0.54
4:E:100:ILE:O	4:E:101:GLN:C	2.45	0.54
5:F:110:ASP:O	5:F:111:LEU:C	2.46	0.54
13:N:6:DT:O2	13:N:7:DA:C4	2.60	0.54
1:A:265:LYS:O	1:A:267:ALA:N	2.40	0.54
1:A:320:ARG:NH1	1:A:320:ARG:CG	2.70	0.54
12:T:2:DT:O2	13:N:13:DA:N1	2.40	0.54
1:A:424:ILE:O	1:A:424:ILE:CG2	2.54	0.54
12:T:7:DA:N1	12:T:8:DT:O4	2.40	0.54
1:A:56:PRO:O	1:A:58:LEU:N	2.41	0.54
2:B:473:MET:O	2:B:475:SER:N	2.41	0.54
1:A:608:ILE:O	1:A:609:ASP:O	2.26	0.53
2:B:1096:ARG:O	2:B:1097:HIS:CG	2.61	0.53
13:N:6:DT:C4	13:N:7:DA:N6	2.77	0.53
13:N:12:DT:C2'	13:N:13:DA:OP2	2.57	0.53
12:T:3:DA:N1	13:N:12:DT:C4	2.77	0.53
4:E:55:ARG:O	4:E:57:MET:N	2.42	0.53
2:B:986:GLN:NE2	2:B:1022:THR:CG2	2.72	0.52
2:B:881:ASN:ND2	2:B:933:SER:OG	2.42	0.52
1:A:307:ASP:O	1:A:308:ILE:C	2.48	0.52
2:B:635:ARG:O	2:B:636:PRO:O	2.26	0.52
2:B:747:MET:CA	2:B:747:MET:CE	2.88	0.52
2:B:1103:ILE:CG2	2:B:1103:ILE:O	2.58	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:H:131:ASN:OD1	6:H:132:LEU:N	2.42	0.52
2:B:325:GLN:NE2	7:I:12:ASN:OD1	2.43	0.52
8:J:32:GLU:N	8:J:32:GLU:OE1	2.43	0.52
2:B:230:ALA:N	2:B:231:PRO:CD	2.73	0.52
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.52
3:C:69:LEU:CB	8:J:5:VAL:CG1	2.88	0.52
1:A:853:ASP:OD1	1:A:855:THR:CB	2.59	0.51
1:A:1116:LEU:CD1	1:A:1329:THR:CG2	2.88	0.51
2:B:254:LEU:CD2	2:B:381:MET:CE	2.87	0.51
2:B:487:THR:CG2	2:B:488:TYR:N	2.73	0.51
10:L:44:ASP:O	10:L:46:VAL:N	2.43	0.51
1:A:23:SER:O	1:A:26:GLU:N	2.43	0.51
6:H:89:LEU:C	6:H:91:ASP:N	2.63	0.51
12:T:7:DA:C2	12:T:8:DT:C5	2.97	0.51
2:B:287:ARG:NH1	2:B:324:ILE:O	2.44	0.51
1:A:401:GLY:C	1:A:435:HIS:CD2	2.84	0.51
1:A:1437:GLY:O	1:A:1440:ALA:N	2.43	0.51
1:A:219:PHE:O	1:A:222:LEU:N	2.43	0.51
12:T:7:DA:N3	12:T:8:DT:C5	2.78	0.51
7:I:101:PHE:N	7:I:110:PHE:O	2.44	0.51
1:A:507:VAL:N	1:A:508:PRO:CD	2.73	0.51
1:A:1121:GLU:O	1:A:1124:HIS:O	2.29	0.51
7:I:96:SER:O	7:I:98:VAL:N	2.44	0.50
1:A:553:VAL:CG2	1:A:652:VAL:CG2	2.88	0.50
2:B:635:ARG:O	2:B:635:ARG:CG	2.59	0.50
12:T:7:DA:C2	12:T:8:DT:C2	3.00	0.50
1:A:244:PRO:O	1:A:247:ARG:N	2.43	0.50
2:B:894:ASP:OD2	10:L:58:LYS:NZ	2.44	0.50
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.60	0.50
13:N:2:DT:C2'	13:N:3:DG:C8	2.95	0.50
12:T:5:DC:C4	12:T:6:DC:C4	2.99	0.50
2:B:797:TYR:CE2	3:C:62:PHE:CD2	3.00	0.50
12:T:6:DC:N3	12:T:7:DA:C5	2.79	0.49
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.59	0.49
1:A:303:TYR:O	1:A:303:TYR:CG	2.66	0.49
1:A:315:LEU:CB	1:A:316:GLN:CA	2.91	0.49
7:I:92:ARG:CG	7:I:93:LYS:N	2.75	0.49
2:B:487:THR:OG1	2:B:777:ALA:O	2.28	0.49
7:I:33:SER:O	7:I:34:TYR:O	2.30	0.49
3:C:76:ASP:OD2	3:C:128:ASN:N	2.46	0.49
3:C:99:LEU:CD2	3:C:99:LEU:N	2.76	0.49
1:A:1117:THR:N	1:A:1328:TYR:O	2.46	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:244:PRO:CB	1:A:245:PRO:CD	2.92	0.48
2:B:25:ILE:CG2	2:B:26:THR:N	2.76	0.48
1:A:1392:SER:O	1:A:1394:THR:N	2.46	0.48
12:T:7:DA:C4	12:T:8:DT:C5	3.01	0.48
6:H:91:ASP:O	6:H:92:ASP:OD2	2.31	0.48
1:A:218:ASP:O	1:A:222:LEU:CD1	2.61	0.48
3:C:206:ASN:ND2	3:C:229:TYR:CB	2.76	0.48
2:B:435:THR:O	2:B:437:GLU:N	2.46	0.48
12:T:2:DT:C2'	12:T:3:DA:C8	2.96	0.48
1:A:868:TYR:CZ	1:A:1064:VAL:CG2	2.97	0.48
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.46	0.48
2:B:591:ARG:O	2:B:592:ASN:CB	2.61	0.48
1:A:1258:HIS:O	1:A:1262:LYS:NZ	2.47	0.48
4:E:55:ARG:C	4:E:57:MET:N	2.67	0.48
1:A:961:ARG:NH1	1:A:961:ARG:CB	2.77	0.48
12:T:5:DC:C5	12:T:6:DC:C4	3.03	0.47
1:A:1206:ASP:N	1:A:1274:ARG:NH1	2.62	0.47
1:A:6:TYR:CD2	1:A:7:SER:N	2.82	0.47
4:E:15:ALA:O	4:E:19:VAL:CG2	2.62	0.47
2:B:732:SER:CB	2:B:734:HIS:NE2	2.78	0.47
1:A:1312:ASN:ND2	1:A:1314:SER:OG	2.47	0.47
2:B:423:LYS:O	2:B:427:ASP:CB	2.62	0.47
13:N:5:DT:C2'	13:N:6:DT:C6	2.97	0.47
12:T:6:DC:N4	12:T:7:DA:N6	2.62	0.47
1:A:43:GLU:N	1:A:43:GLU:OE1	2.48	0.47
2:B:64:CYS:O	2:B:65:GLU:CD	2.53	0.47
7:I:111:THR:CG2	7:I:113:ASP:CB	2.93	0.47
1:A:804:TYR:O	2:B:761:HIS:ND1	2.48	0.47
13:N:4:DG:N1	13:N:5:DT:C2	2.81	0.47
2:B:475:SER:O	2:B:476:ARG:C	2.52	0.47
1:A:108:MET:O	1:A:109:HIS:CB	2.62	0.47
1:A:134:ARG:CD	1:A:221:SER:O	2.63	0.47
2:B:612:GLU:O	2:B:632:ARG:NH2	2.49	0.46
2:B:1166:CYS:O	2:B:1215:ARG:NH1	2.48	0.46
2:B:1074:ASN:OD1	2:B:1076:HIS:N	2.48	0.46
1:A:596:THR:O	1:A:597:LEU:C	2.52	0.46
2:B:260:GLY:O	2:B:267:ARG:CD	2.64	0.46
1:A:1423:GLY:O	1:A:1424:VAL:C	2.53	0.46
6:H:131:ASN:C	6:H:133:ASN:N	2.69	0.46
2:B:36:ALA:C	2:B:37:PHE:O	2.42	0.46
1:A:225:ASN:ND2	1:A:225:ASN:C	2.69	0.46
1:A:596:THR:C	1:A:598:LEU:N	2.67	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.48	0.46
13:N:4:DG:C5	13:N:5:DT:C7	2.98	0.46
2:B:176:SER:OG	2:B:177:LYS:N	2.48	0.46
12:T:1:DC:N4	13:N:13:DA:N6	2.63	0.46
3:C:69:LEU:O	8:J:6:ARG:NH1	2.49	0.46
1:A:868:TYR:CE1	1:A:1064:VAL:CG2	2.98	0.46
1:A:1035:TYR:O	1:A:1037:LEU:N	2.49	0.46
2:B:878:GLN:O	2:B:879:ARG:C	2.55	0.45
2:B:512:ARG:NH2	2:B:531:GLN:O	2.50	0.45
1:A:53:LEU:CD1	1:A:266:LEU:O	2.65	0.45
1:A:362:ASP:OD2	1:A:362:ASP:N	2.48	0.45
1:A:858:ASN:C	1:A:858:ASN:ND2	2.70	0.45
2:B:680:THR:O	2:B:681:TRP:C	2.53	0.45
12:T:2:DT:O2	13:N:13:DA:C2	2.69	0.45
2:B:647:GLY:O	2:B:648:HIS:ND1	2.50	0.45
1:A:362:ASP:OD1	1:A:459:ARG:NH1	2.50	0.45
13:N:5:DT:C2'	13:N:6:DT:C5	2.99	0.45
2:B:855:PHE:N	2:B:970:THR:O	2.50	0.45
1:A:1322:ILE:CG1	1:A:1323:ASP:N	2.80	0.45
4:E:96:PHE:C	4:E:98:ILE:N	2.70	0.44
1:A:949:ASP:N	1:A:949:ASP:OD1	2.50	0.44
2:B:712:PRO:O	2:B:733:HIS:NE2	2.50	0.44
1:A:1206:ASP:N	1:A:1206:ASP:OD2	2.51	0.44
1:A:1194:ARG:NH2	1:A:1237:ILE:CD1	2.80	0.44
2:B:764:SER:O	2:B:765:PRO:C	2.55	0.44
1:A:783:THR:CG2	1:A:784:LEU:N	2.80	0.44
2:B:764:SER:O	2:B:766:ARG:N	2.51	0.44
3:C:114:TYR:O	3:C:117:ASP:N	2.51	0.44
12:T:5:DC:C4	12:T:6:DC:N3	2.85	0.44
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.50	0.44
3:C:148:ARG:CG	3:C:149:LYS:N	2.81	0.44
12:T:22:DT:C2'	12:T:23:DC:O5'	2.65	0.44
2:B:167:ILE:N	2:B:167:ILE:CD1	2.79	0.44
1:A:22:PHE:CB	2:B:1211:ASN:OD1	2.65	0.44
2:B:100:PRO:O	2:B:101:MET:CG	2.66	0.44
2:B:879:ARG:O	2:B:880:THR:C	2.56	0.44
2:B:635:ARG:C	2:B:636:PRO:O	2.56	0.44
1:A:836:TYR:O	1:A:837:ILE:C	2.56	0.44
13:N:13:DA:C2'	13:N:14:DG:C8	3.01	0.43
1:A:943:LEU:O	1:A:946:VAL:N	2.51	0.43
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.36	0.43
1:A:610:GLY:O	1:A:611:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:9:ILE:O	4:E:13:TRP:N	2.51	0.43
3:C:231:ASN:C	3:C:231:ASN:ND2	2.71	0.43
6:H:25:ARG:NH2	6:H:41:ASP:OD2	2.52	0.43
1:A:858:ASN:O	1:A:861:GLY:N	2.50	0.43
2:B:549:THR:O	2:B:628:THR:CG2	2.67	0.43
1:A:855:THR:CG2	1:A:857:ARG:NE	2.82	0.43
2:B:378:LEU:O	2:B:382:ILE:CG1	2.67	0.43
1:A:1015:VAL:CG1	1:A:1015:VAL:O	2.66	0.43
2:B:96:TYR:N	2:B:129:PHE:O	2.51	0.43
1:A:211:PHE:O	1:A:213:HIS:N	2.52	0.43
2:B:770:GLN:O	2:B:770:GLN:CD	2.57	0.43
1:A:53:LEU:CD2	1:A:54:ASN:N	2.82	0.43
2:B:957:ASN:CG	2:B:958:GLN:N	2.73	0.43
1:A:982:THR:O	1:A:983:ILE:C	2.57	0.43
13:N:6:DT:C2	13:N:7:DA:N7	2.87	0.42
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.37	0.42
1:A:969:GLN:O	1:A:971:PHE:N	2.52	0.42
1:A:96:ILE:O	1:A:97:ALA:C	2.58	0.42
4:E:157:SER:O	4:E:159:ASP:N	2.52	0.42
4:E:157:SER:N	4:E:160:GLU:OE1	2.52	0.42
3:C:233:GLU:OE2	8:J:43:ARG:NH2	2.52	0.42
4:E:76:GLY:O	4:E:77:SER:C	2.58	0.42
2:B:642:ASP:O	2:B:644:GLU:N	2.52	0.42
1:A:95:PHE:O	1:A:99:ILE:N	2.52	0.42
3:C:226:ASP:O	3:C:227:THR:O	2.37	0.42
1:A:535:THR:O	1:A:536:LEU:C	2.58	0.42
1:A:1336:MET:CE	1:A:1380:GLY:CA	2.97	0.42
1:A:323:LYS:O	1:A:324:SER:CB	2.66	0.42
2:B:473:MET:C	2:B:475:SER:N	2.72	0.42
9:K:40:HIS:ND1	9:K:61:TYR:OH	2.53	0.42
2:B:412:LEU:O	2:B:413:LEU:C	2.57	0.42
2:B:1035:ALA:O	2:B:1039:GLY:N	2.52	0.42
1:A:243:PRO:O	1:A:244:PRO:C	2.57	0.42
12:T:7:DA:C8	12:T:7:DA:OP2	2.73	0.42
6:H:2:SER:O	6:H:3:ASN:CB	2.67	0.42
1:A:86:LEU:CD1	1:A:236:LEU:O	2.67	0.42
2:B:221:ASN:N	2:B:241:ARG:O	2.53	0.42
2:B:35:SER:O	2:B:37:PHE:O	2.38	0.42
3:C:190:ASP:C	3:C:190:ASP:OD1	2.58	0.42
1:A:1065:GLY:O	1:A:1068:ALA:N	2.53	0.42
13:N:4:DG:C2	13:N:5:DT:N3	2.80	0.42
2:B:640:VAL:CG1	2:B:640:VAL:O	2.63	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:GLY:O	1:A:241:VAL:N	2.52	0.42
6:H:137:GLN:O	6:H:139:ASN:N	2.53	0.41
1:A:808:LEU:O	2:B:728:ARG:NH1	2.53	0.41
4:E:198:ILE:CD1	4:E:212:ARG:CG	2.99	0.41
1:A:1328:TYR:OH	1:A:1351:GLU:OE1	2.39	0.41
3:C:184:ASN:OD1	3:C:187:LYS:CA	2.69	0.41
2:B:708:GLU:O	2:B:711:GLU:N	2.54	0.41
10:L:59:ALA:O	10:L:60:ARG:CB	2.68	0.41
1:A:573:SER:O	1:A:574:GLY:C	2.59	0.41
1:A:401:GLY:CA	1:A:435:HIS:CD2	3.03	0.41
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.54	0.41
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.54	0.41
12:T:2:DT:OP2	12:T:2:DT:C7	2.68	0.41
2:B:635:ARG:O	2:B:636:PRO:C	2.59	0.41
2:B:28:GLU:C	2:B:30:SER:N	2.74	0.41
12:T:7:DA:C6	12:T:8:DT:O4	2.74	0.41
1:A:23:SER:O	1:A:24:PRO:C	2.59	0.41
2:B:644:GLU:CA	2:B:644:GLU:OE1	2.69	0.41
1:A:782:ARG:NH2	7:I:67:THR:CG2	2.84	0.41
1:A:802:ASN:OD1	2:B:729:ILE:N	2.54	0.41
7:I:55:THR:O	7:I:55:THR:CG2	2.68	0.41
2:B:817:LEU:N	2:B:818:PRO:CD	2.84	0.41
3:C:180:TYR:O	3:C:181:ASP:C	2.59	0.41
12:T:7:DA:N3	12:T:8:DT:C6	2.89	0.40
1:A:1062:GLU:O	1:A:1064:VAL:N	2.53	0.40
2:B:605:ARG:NE	2:B:691:GLU:OE2	2.54	0.40
8:J:23:ASN:CB	8:J:27:GLU:OE2	2.69	0.40
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.75	0.40
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.55	0.40
1:A:1279:ILE:N	1:A:1279:ILE:CD1	2.84	0.40
1:A:1025:ARG:O	1:A:1035:TYR:OH	2.39	0.40
2:B:879:ARG:CG	2:B:880:THR:N	2.84	0.40
2:B:706:GLN:O	2:B:707:PRO:C	2.58	0.40
4:E:204:THR:CG2	4:E:205:SER:N	2.85	0.40
2:B:199:MET:N	2:B:199:MET:SD	2.95	0.40
2:B:852:ARG:NH2	10:L:70:ARG:O	2.54	0.40
2:B:516:ASN:ND2	2:B:516:ASN:N	2.69	0.40
1:A:1365:TYR:CD2	1:A:1365:TYR:C	2.94	0.40
2:B:826:ALA:N	2:B:1010:LEU:O	2.54	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1383/1733 (80%)	1094 (79%)	201 (14%)	88 (6%)	2	17
2	B	1088/1224 (89%)	900 (83%)	126 (12%)	62 (6%)	3	22
3	C	264/318 (83%)	226 (86%)	30 (11%)	8 (3%)	7	43
4	E	212/215 (99%)	173 (82%)	28 (13%)	11 (5%)	3	25
5	F	82/155 (53%)	63 (77%)	13 (16%)	6 (7%)	2	12
6	H	129/146 (88%)	94 (73%)	23 (18%)	12 (9%)	1	7
7	I	117/122 (96%)	97 (83%)	13 (11%)	7 (6%)	2	20
8	J	63/70 (90%)	52 (82%)	6 (10%)	5 (8%)	1	10
9	K	112/120 (93%)	105 (94%)	7 (6%)	0	100	100
10	L	44/70 (63%)	25 (57%)	10 (23%)	9 (20%)	0	0
All	All	3494/4173 (84%)	2829 (81%)	457 (13%)	208 (6%)	2	20

All (208) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	55	ASP
1	A	57	ARG
1	A	65	LEU
1	A	73	GLY
1	A	109	HIS
1	A	148	CYS
1	A	169	ASN
1	A	216	VAL
1	A	226	GLU
1	A	245	PRO
1	A	250	ILE
1	A	258	GLY
1	A	286	HIS
1	A	308	ILE
1	A	315	LEU

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Mol	Chain	Res	Type
1	A	399	HIS
1	A	424	ILE
1	A	567	LYS
1	A	597	LEU
1	A	609	ASP
1	A	610	GLY
1	A	846	GLU
1	A	923	LEU
1	A	972	HIS
1	A	994	GLN
1	A	1014	ALA
1	A	1036	ARG
1	A	1393	ASN
1	A	1403	GLU
1	A	1438	THR
2	B	65	GLU
2	B	168	GLY
2	B	229	ALA
2	B	230	ALA
2	B	245	GLU
2	B	266	ALA
2	B	395	GLN
2	B	436	VAL
2	B	469	GLN
2	B	473	MET
2	B	474	SER
2	B	477	ALA
2	B	483	LEU
2	B	531	GLN
2	B	592	ASN
2	B	629	ASP
2	B	636	PRO
2	B	645	SER
2	B	708	GLU
2	B	709	ASP
2	B	713	ALA
2	B	733	HIS
2	B	734	HIS
2	B	751	VAL
2	B	866	TYR
2	B	879	ARG
2	B	881	ASN

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Mol	Chain	Res	Type
2	B	1046	PRO
2	B	1097	HIS
2	B	1223	ASP
3	C	173	ALA
4	E	49	SER
4	E	59	SER
4	E	118	PRO
5	F	73	ALA
6	H	90	ALA
6	H	109	LYS
6	H	111	LEU
6	H	131	ASN
6	H	132	LEU
6	H	138	GLU
7	I	34	TYR
8	J	2	ILE
10	L	34	CYS
10	L	35	SER
10	L	45	ALA
10	L	59	ALA
10	L	60	ARG
1	A	130	ASP
1	A	224	PHE
1	A	257	ARG
1	A	266	LEU
1	A	298	PHE
1	A	309	ALA
1	A	322	VAL
1	A	324	SER
1	A	837	ILE
1	A	1123	GLY
1	A	1174	PHE
1	A	1234	GLU
1	A	1257	ASP
1	A	1388	GLY
1	A	1420	ASP
2	B	67	SER
2	B	249	ARG
2	B	288	ALA
2	B	466	TRP
2	B	643	ASP
2	B	737	THR

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Mol	Chain	Res	Type
2	B	880	THR
2	B	1021	MET
2	B	1103	ILE
2	B	1185	CYS
3	C	48	SER
3	C	142	VAL
3	C	174	ALA
3	C	227	THR
4	E	56	LYS
4	E	77	SER
5	F	111	LEU
6	H	3	ASN
6	H	62	SER
6	H	136	LYS
7	I	3	THR
7	I	9	ASP
7	I	54	GLU
7	I	97	MET
8	J	8	PHE
8	J	30	LEU
10	L	46	VAL
1	A	35	ILE
1	A	54	ASN
1	A	131	SER
1	A	142	CYS
1	A	214	ILE
1	A	251	SER
1	A	673	GLY
1	A	674	PRO
1	A	852	TYR
1	A	1127	ASP
1	A	1278	ASN
2	B	364	ILE
2	B	468	GLU
2	B	471	LYS
2	B	480	SER
2	B	555	ILE
2	B	732	SER
2	B	735	ALA
2	B	792	MET
2	B	864	LYS
4	E	101	GLN

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Mol	Chain	Res	Type
4	E	158	SER
5	F	114	GLU
6	H	128	ASN
7	I	90	GLN
8	J	9	SER
8	J	19	GLU
10	L	44	ASP
1	A	48	ALA
1	A	49	LYS
1	A	69	THR
1	A	147	VAL
1	A	178	GLY
1	A	219	PHE
1	A	220	THR
1	A	404	TYR
1	A	423	ASP
1	A	583	PRO
1	A	958	VAL
1	A	1093	LYS
2	B	367	LEU
2	B	479	VAL
2	B	561	TRP
2	B	644	GLU
2	B	711	GLU
2	B	1108	ARG
4	E	97	VAL
6	H	130	ARG
7	I	47	GLU
1	A	24	PRO
1	A	51	GLY
1	A	234	MET
1	A	254	GLU
1	A	903	ASN
1	A	970	THR
1	A	1151	GLU
2	B	333	PHE
2	B	413	LEU
2	B	476	ARG
2	B	707	PRO
3	C	214	ASN
3	C	215	GLU
4	E	36	GLU

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Mol	Chain	Res	Type
6	H	18	GLY
10	L	26	THR
1	A	38	PRO
1	A	1062	GLU
2	B	233	PRO
2	B	1175	LEU
3	C	136	ASP
4	E	51	GLY
5	F	74	ILE
5	F	154	ASP
1	A	79	GLY
1	A	244	PRO
1	A	1156	PRO
1	A	1424	VAL
1	A	1437	GLY
2	B	467	GLY
1	A	794	PRO
5	F	131	PRO
1	A	312	PRO
1	A	990	VAL
10	L	30	ILE
1	A	310	GLY
1	A	772	GLY
4	E	86	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1218/1520 (80%)	974 (80%)	244 (20%)	2	9
2	B	960/1061 (90%)	772 (80%)	188 (20%)	2	10
3	C	234/274 (85%)	180 (77%)	54 (23%)	1	6
4	E	196/197 (100%)	160 (82%)	36 (18%)	2	12
5	F	74/137 (54%)	62 (84%)	12 (16%)	3	16
6	H	117/128 (91%)	95 (81%)	22 (19%)	2	11
7	I	113/116 (97%)	87 (77%)	26 (23%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	60/65 (92%)	42 (70%)	18 (30%)	0	1
9	K	99/102 (97%)	87 (88%)	12 (12%)	7	31
10	L	40/57 (70%)	33 (82%)	7 (18%)	3	13
All	All	3111/3657 (85%)	2492 (80%)	619 (20%)	2	9

All (619) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	12	ARG
1	A	18	GLN
1	A	22	PHE
1	A	30	ILE
1	A	47	ARG
1	A	49	LYS
1	A	54	ASN
1	A	55	ASP
1	A	61	ILE
1	A	64	ASN
1	A	65	LEU
1	A	68	GLN
1	A	69	THR
1	A	70	CYS
1	A	71	GLN
1	A	74	MET
1	A	80	HIS
1	A	93	VAL
1	A	109	HIS
1	A	114	LEU
1	A	132	LYS
1	A	144	THR
1	A	146	MET
1	A	147	VAL
1	A	148	CYS
1	A	162	VAL
1	A	169	ASN
1	A	170	THR
1	A	179	LEU
1	A	185	TRP
1	A	202	LEU
1	A	208	LEU

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Mol	Chain	Res	Type
1	A	212	LYS
1	A	216	VAL
1	A	220	THR
1	A	222	LEU
1	A	225	ASN
1	A	227	VAL
1	A	250	ILE
1	A	257	ARG
1	A	264	PHE
1	A	287	HIS
1	A	289	ILE
1	A	297	GLN
1	A	303	TYR
1	A	306	ASN
1	A	308	ILE
1	A	311	GLN
1	A	313	GLN
1	A	315	LEU
1	A	316	GLN
1	A	320	ARG
1	A	322	VAL
1	A	323	LYS
1	A	326	ARG
1	A	329	LEU
1	A	332	LYS
1	A	333	GLU
1	A	335	ARG
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	369	SER
1	A	373	THR
1	A	375	THR
1	A	380	VAL
1	A	381	THR
1	A	383	TYR
1	A	403	LYS
1	A	412	ARG
1	A	416	ARG
1	A	419	LYS
1	A	424	ILE
1	A	434	ARG

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Mol	Chain	Res	Type
1	A	436	ILE
1	A	443	LEU
1	A	451	HIS
1	A	452	LYS
1	A	454	SER
1	A	461	LYS
1	A	466	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	497	THR
1	A	509	LEU
1	A	512	VAL
1	A	513	SER
1	A	518	LYS
1	A	532	ARG
1	A	542	GLU
1	A	544	ASP
1	A	560	ILE
1	A	567	LYS
1	A	577	ILE
1	A	589	GLN
1	A	590	ARG
1	A	595	THR
1	A	598	LEU
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	629	LEU
1	A	637	LYS
1	A	663	SER
1	A	664	THR
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	681	GLU
1	A	682	THR
1	A	685	GLU
1	A	688	LYS
1	A	695	LYS

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Mol	Chain	Res	Type
1	A	702	LEU
1	A	703	THR
1	A	709	THR
1	A	710	LEU
1	A	728	LYS
1	A	732	LEU
1	A	735	VAL
1	A	740	LEU
1	A	756	ILE
1	A	764	CYS
1	A	765	VAL
1	A	768	GLN
1	A	769	SER
1	A	774	ARG
1	A	780	VAL
1	A	783	THR
1	A	801	GLU
1	A	803	SER
1	A	821	ARG
1	A	829	VAL
1	A	830	LYS
1	A	838	GLN
1	A	839	ARG
1	A	855	THR
1	A	856	THR
1	A	858	ASN
1	A	880	LYS
1	A	884	ASP
1	A	885	THR
1	A	886	ILE
1	A	895	LYS
1	A	896	ARG
1	A	902	LEU
1	A	904	THR
1	A	911	SER
1	A	914	GLU
1	A	919	ILE
1	A	922	ASP
1	A	926	GLN
1	A	932	GLU
1	A	940	ARG
1	A	941	LYS

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Mol	Chain	Res	Type
1	A	949	ASP
1	A	961	ARG
1	A	965	GLN
1	A	966	ASN
1	A	976	THR
1	A	977	LYS
1	A	982	THR
1	A	995	GLU
1	A	996	ASN
1	A	1000	LEU
1	A	1001	ARG
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1034	GLU
1	A	1047	SER
1	A	1048	ASN
1	A	1050	GLU
1	A	1055	ARG
1	A	1058	VAL
1	A	1064	VAL
1	A	1081	LEU
1	A	1092	LYS
1	A	1093	LYS
1	A	1095	THR
1	A	1110	ASN
1	A	1111	MET
1	A	1116	LEU
1	A	1128	GLN
1	A	1130	GLN
1	A	1146	VAL
1	A	1159	ARG
1	A	1165	GLU
1	A	1171	GLN
1	A	1172	LEU
1	A	1187	GLN
1	A	1193	LEU
1	A	1205	LYS
1	A	1206	ASP
1	A	1208	THR
1	A	1219	THR

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Mol	Chain	Res	Type
1	A	1231	ASP
1	A	1243	VAL
1	A	1257	ASP
1	A	1259	MET
1	A	1261	LYS
1	A	1262	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1269	GLU
1	A	1273	LEU
1	A	1274	ARG
1	A	1277	GLU
1	A	1279	ILE
1	A	1280	GLU
1	A	1285	MET
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1300	LYS
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1336	MET
1	A	1345	ARG
1	A	1354	ASN
1	A	1359	ASP
1	A	1366	ARG
1	A	1374	VAL
1	A	1376	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1406	VAL
1	A	1407	GLU
1	A	1422	ARG
1	A	1426	GLU

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Mol	Chain	Res	Type
1	A	1445	ILE
2	B	20	ASP
2	B	28	GLU
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	65	GLU
2	B	66	ASP
2	B	67	SER
2	B	70	ILE
2	B	94	LYS
2	B	97	VAL
2	B	98	THR
2	B	102	VAL
2	B	108	VAL
2	B	120	ARG
2	B	133	LYS
2	B	134	LYS
2	B	167	ILE
2	B	175	ARG
2	B	179	CYS
2	B	181	LEU
2	B	194	GLU
2	B	199	MET
2	B	217	ARG
2	B	225	VAL
2	B	234	ILE
2	B	239	GLU
2	B	242	SER
2	B	245	GLU
2	B	246	LYS
2	B	249	ARG
2	B	252	SER
2	B	268	THR
2	B	272	THR
2	B	275	TYR
2	B	276	ILE
2	B	284	ILE
2	B	310	MET
2	B	313	MET
2	B	315	LYS
2	B	323	VAL

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Mol	Chain	Res	Type
2	B	324	ILE
2	B	328	GLU
2	B	331	LEU
2	B	345	LYS
2	B	346	GLU
2	B	350	GLN
2	B	354	ASP
2	B	361	LEU
2	B	365	THR
2	B	366	GLN
2	B	367	LEU
2	B	368	GLU
2	B	376	PHE
2	B	382	ILE
2	B	384	ARG
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	395	GLN
2	B	398	ARG
2	B	415	GLN
2	B	425	THR
2	B	426	LYS
2	B	428	ILE
2	B	429	PHE
2	B	436	VAL
2	B	437	GLU
2	B	448	ILE
2	B	455	SER
2	B	461	LEU
2	B	468	GLU
2	B	471	LYS
2	B	474	SER
2	B	479	VAL
2	B	483	LEU
2	B	485	ARG
2	B	487	THR
2	B	498	THR
2	B	512	ARG
2	B	513	GLN
2	B	516	ASN
2	B	527	THR

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Mol	Chain	Res	Type
2	B	531	GLN
2	B	544	CYS
2	B	549	THR
2	B	552	MET
2	B	554	ILE
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	591	ARG
2	B	598	GLU
2	B	606	LYS
2	B	617	ARG
2	B	619	ILE
2	B	624	LEU
2	B	629	ASP
2	B	633	VAL
2	B	635	ARG
2	B	637	LEU
2	B	643	ASP
2	B	644	GLU
2	B	651	LEU
2	B	653	VAL
2	B	666	TYR
2	B	690	VAL
2	B	706	GLN
2	B	708	GLU
2	B	710	LEU
2	B	731	VAL
2	B	732	SER
2	B	742	GLU
2	B	747	MET
2	B	751	VAL
2	B	764	SER
2	B	786	ASN
2	B	787	VAL
2	B	790	ASP
2	B	791	THR
2	B	792	MET
2	B	815	ARG
2	B	827	ILE
2	B	844	SER
2	B	864	LYS

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Mol	Chain	Res	Type
2	B	865	LYS
2	B	868	MET
2	B	871	THR
2	B	879	ARG
2	B	880	THR
2	B	886	LYS
2	B	894	ASP
2	B	901	PRO
2	B	904	ARG
2	B	943	SER
2	B	944	THR
2	B	955	THR
2	B	957	ASN
2	B	963	PHE
2	B	969	ARG
2	B	970	THR
2	B	976	ILE
2	B	983	ARG
2	B	987	LYS
2	B	992	ILE
2	B	996	ARG
2	B	997	GLU
2	B	1002	THR
2	B	1004	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1021	MET
2	B	1028	GLU
2	B	1032	SER
2	B	1046	PRO
2	B	1051	THR
2	B	1055	ILE
2	B	1065	GLN
2	B	1077	THR
2	B	1082	MET
2	B	1093	GLN
2	B	1094	ARG
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE
2	B	1111	MET
2	B	1113	VAL

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Mol	Chain	Res	Type
2	B	1120	GLU
2	B	1122	ARG
2	B	1123	SER
2	B	1124	ARG
2	B	1129	ARG
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1155	SER
2	B	1159	ARG
2	B	1160	VAL
2	B	1174	LYS
2	B	1176	ASN
2	B	1181	GLU
2	B	1186	ASP
2	B	1187	ASN
2	B	1188	LYS
2	B	1191	ILE
2	B	1194	ILE
2	B	1202	LEU
2	B	1220	ARG
3	C	4	GLU
3	C	9	LYS
3	C	11	ARG
3	C	15	LYS
3	C	16	ASP
3	C	18	VAL
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	35	ARG
3	C	41	ILE
3	C	53	THR
3	C	56	THR
3	C	57	VAL
3	C	69	LEU
3	C	77	ILE
3	C	81	GLU
3	C	89	GLU
3	C	99	LEU
3	C	100	THR
3	C	106	GLU

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Mol	Chain	Res	Type
3	C	109	SER
3	C	110	THR
3	C	116	LYS
3	C	120	ILE
3	C	129	ILE
3	C	133	ILE
3	C	137	LYS
3	C	140	ASN
3	C	149	LYS
3	C	151	GLN
3	C	154	LYS
3	C	170	TRP
3	C	177	GLU
3	C	183	TRP
3	C	186	LEU
3	C	189	THR
3	C	197	SER
3	C	203	GLN
3	C	204	SER
3	C	222	LYS
3	C	224	GLN
3	C	226	ASP
3	C	231	ASN
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	244	VAL
3	C	246	ARG
3	C	249	ASP
3	C	253	LYS
3	C	258	ILE
3	C	263	THR
3	C	268	ASP
4	E	3	GLN
4	E	9	ILE
4	E	31	THR
4	E	32	GLN
4	E	37	LEU
4	E	40	GLU
4	E	54	GLN
4	E	66	GLU
4	E	78	LEU

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Mol	Chain	Res	Type
4	E	92	THR
4	E	94	LYS
4	E	95	THR
4	E	98	ILE
4	E	101	GLN
4	E	103	LYS
4	E	122	LYS
4	E	123	LEU
4	E	127	ILE
4	E	131	THR
4	E	134	THR
4	E	137	GLU
4	E	144	ILE
4	E	146	HIS
4	E	150	VAL
4	E	152	LYS
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
4	E	179	GLN
4	E	191	LYS
4	E	192	ARG
4	E	200	ARG
4	E	201	LYS
4	E	202	SER
4	E	204	THR
4	E	215	MET
5	F	72	LYS
5	F	79	ARG
5	F	82	THR
5	F	97	ARG
5	F	111	LEU
5	F	112	GLU
5	F	119	ARG
5	F	133	VAL
5	F	140	ASP
5	F	149	GLU
5	F	150	GLU
5	F	155	LEU
6	H	2	SER
6	H	11	GLN
6	H	15	VAL

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Mol	Chain	Res	Type
6	H	21	ASN
6	H	24	CYS
6	H	32	THR
6	H	34	ASP
6	H	55	LEU
6	H	58	THR
6	H	59	ILE
6	H	83	GLN
6	H	89	LEU
6	H	100	THR
6	H	106	GLU
6	H	110	ASP
6	H	123	MET
6	H	124	ARG
6	H	130	ARG
6	H	133	ASN
6	H	136	LYS
6	H	137	GLN
6	H	142	LEU
7	I	3	THR
7	I	8	ARG
7	I	14	LEU
7	I	28	GLU
7	I	29	CYS
7	I	30	ARG
7	I	33	SER
7	I	50	THR
7	I	52	ILE
7	I	55	THR
7	I	60	GLN
7	I	61	ASP
7	I	74	GLU
7	I	75	CYS
7	I	83	ASN
7	I	89	GLN
7	I	90	GLN
7	I	91	ARG
7	I	95	THR
7	I	97	MET
7	I	103	CYS
7	I	106	CYS
7	I	107	SER

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Mol	Chain	Res	Type
7	I	116	ASN
7	I	117	LYS
7	I	118	ARG
8	J	1	MET
8	J	3	VAL
8	J	6	ARG
8	J	7	CYS
8	J	9	SER
8	J	10	CYS
8	J	13	VAL
8	J	22	LEU
8	J	26	GLN
8	J	27	GLU
8	J	28	ASP
8	J	29	GLU
8	J	31	ASP
8	J	42	LYS
8	J	43	ARG
8	J	48	ARG
8	J	59	LYS
8	J	64	ASN
9	K	1	MET
9	K	14	GLU
9	K	17	SER
9	K	20	LYS
9	K	26	LYS
9	K	31	VAL
9	K	51	LEU
9	K	77	THR
9	K	82	ASP
9	K	103	THR
9	K	106	GLU
9	K	107	THR
10	L	27	LEU
10	L	31	CYS
10	L	38	LEU
10	L	42	ARG
10	L	47	ARG
10	L	55	ILE
10	L	61	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	10/11 (90%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	3	G
11	R	11	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	C7P	T	29	12	5,9,10	1.05	0	5,11,14	1.21	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	C7P	T	29	12	-	0/0/12/14	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	29	C7P	C2-C3-C4	-2.34	118.22	120.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1395/1733 (80%)	-0.20	8 (0%) 86 40	47, 104, 216, 308	0
2	B	1106/1224 (90%)	-0.27	6 (0%) 88 43	43, 86, 154, 209	0
3	C	266/318 (83%)	-0.32	0 100 100	62, 91, 135, 158	0
4	E	214/215 (99%)	-0.12	0 100 100	81, 159, 225, 242	0
5	F	84/155 (54%)	-0.21	0 100 100	77, 110, 142, 150	0
6	H	133/146 (91%)	-0.02	3 (2%) 57 11	101, 153, 199, 211	0
7	I	119/122 (97%)	-0.16	0 100 100	75, 118, 158, 172	0
8	J	65/70 (92%)	-0.43	0 100 100	56, 73, 100, 116	0
9	K	114/120 (95%)	-0.30	0 100 100	59, 103, 131, 141	0
10	L	46/70 (65%)	0.15	1 (2%) 59 12	72, 144, 173, 182	0
11	R	11/11 (100%)	0.70	0 100 100	141, 156, 211, 217	0
12	T	28/28 (100%)	1.57	8 (28%) 1 0	146, 286, 394, 400	0
13	N	14/14 (100%)	1.39	2 (14%) 3 1	309, 352, 380, 391	0
All	All	3595/4226 (85%)	-0.20	28 (0%) 83 32	43, 103, 203, 400	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	6.3
2	B	866	TYR	5.1
12	T	3	DA	3.9
12	T	4	DC	3.5
1	A	44	THR	3.4
12	T	2	DT	3.3
2	B	1224	PHE	3.3
2	B	477	ALA	3.1
2	B	1223	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
6	H	84	ALA	2.9
12	T	13	DA	2.9
10	L	27	LEU	2.7
2	B	476	ARG	2.7
1	A	69	THR	2.6
1	A	149	GLU	2.6
12	T	12	DC	2.6
2	B	865	LYS	2.5
12	T	1	DC	2.5
1	A	150	THR	2.3
1	A	65	LEU	2.3
12	T	9	DA	2.3
1	A	316	GLN	2.3
6	H	131	ASN	2.2
6	H	132	LEU	2.2
13	N	8	DT	2.2
13	N	7	DA	2.1
1	A	318	SER	2.1
12	T	10	DA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	C7P	T	29	9/10	0.29	0.14	205,229,260,269	1
16	MG	A	2001	1/1	0.10	-1.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
14	ZN	I	204	1/1	0.07	-1.89	59,59,59,59	0
14	ZN	C	319	1/1	0.03	-2.59	63,63,63,63	0
14	ZN	I	203	1/1	0.02	-2.65	74,74,74,74	0
14	ZN	B	1307	1/1	0.04	-2.70	92,92,92,92	0
14	ZN	A	1734	1/1	0.10	-3.03	113,113,113,113	0
14	ZN	A	1735	1/1	0.04	-3.14	83,83,83,83	0
14	ZN	L	105	1/1	0.05	-3.67	101,101,101,101	1
14	ZN	J	101	1/1	0.06	-4.72	61,61,61,61	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.