



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2019 – 10:14 PM EST

PDB ID : 4A3F  
Title : RNA Polymerase II initial transcribing complex with a 6nt DNA-RNA hybrid and soaked with AMPCPP  
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.  
Deposited on : 2011-09-30  
Resolution : 3.50 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](mailto: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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

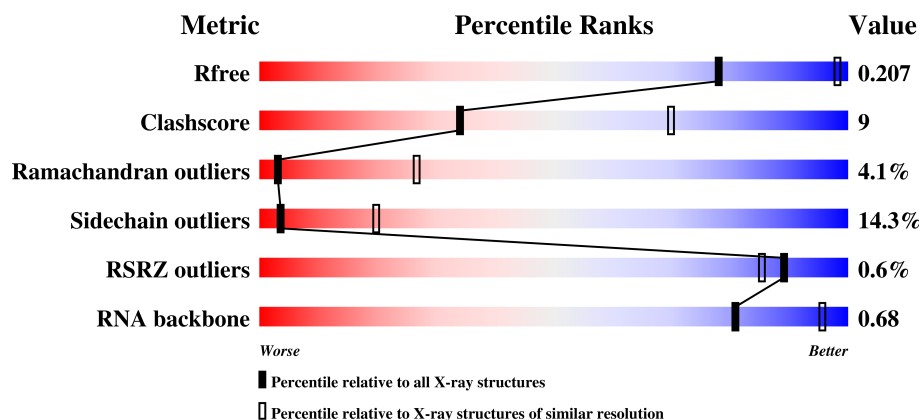
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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.




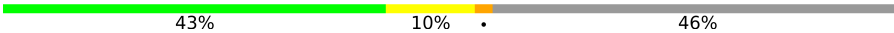









Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1391 (3.60-3.40)
Clashscore	122126	1485 (3.60-3.40)
Ramachandran outliers	120053	1446 (3.60-3.40)
Sidechain outliers	120020	1447 (3.60-3.40)
RSRZ outliers	108989	1303 (3.60-3.40)
RNA backbone	2636	1052 (4.10-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1732	<div> <div></div> <div> <div></div> <div>55%</div> <div>22%</div> <div>5%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div></div> <div> <div></div> <div>59%</div> <div>27%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div></div> <div>52%</div> <div>28%</div> <div>•</div> <div>16%</div> </div> </div>
4	D	221	<div> <div></div> <div> <div></div> <div>55%</div> <div>19%</div> <div>5%</div> <div>•</div> <div>19%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	6	
15	T	26	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32010 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 II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1425	Total	C	N	O	S	0	0	0
			11197	7051	1958	2126	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	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 POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

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

- Molecule 7 is a protein called RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	11	Total	C	N	O	P	0	0	0
			226	109	44	63	10			

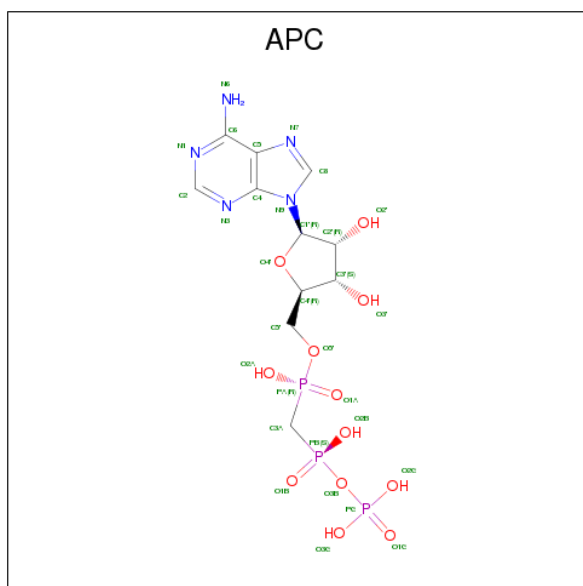
- Molecule 14 is a RNA chain called TRANSCRIPT RNA 5'-R(\*CP\*CP\*AP\*GP\*GP\*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	6	Total	C	N	O	P	0	0	0
			130	58	26	40	6			

- Molecule 15 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*DTP \*TP\*TP\*CP\*C BRU\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	20	Total	Br	C	N	O	P	0	0	0
			404	1	194	63	126	20			

- Molecule 16 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

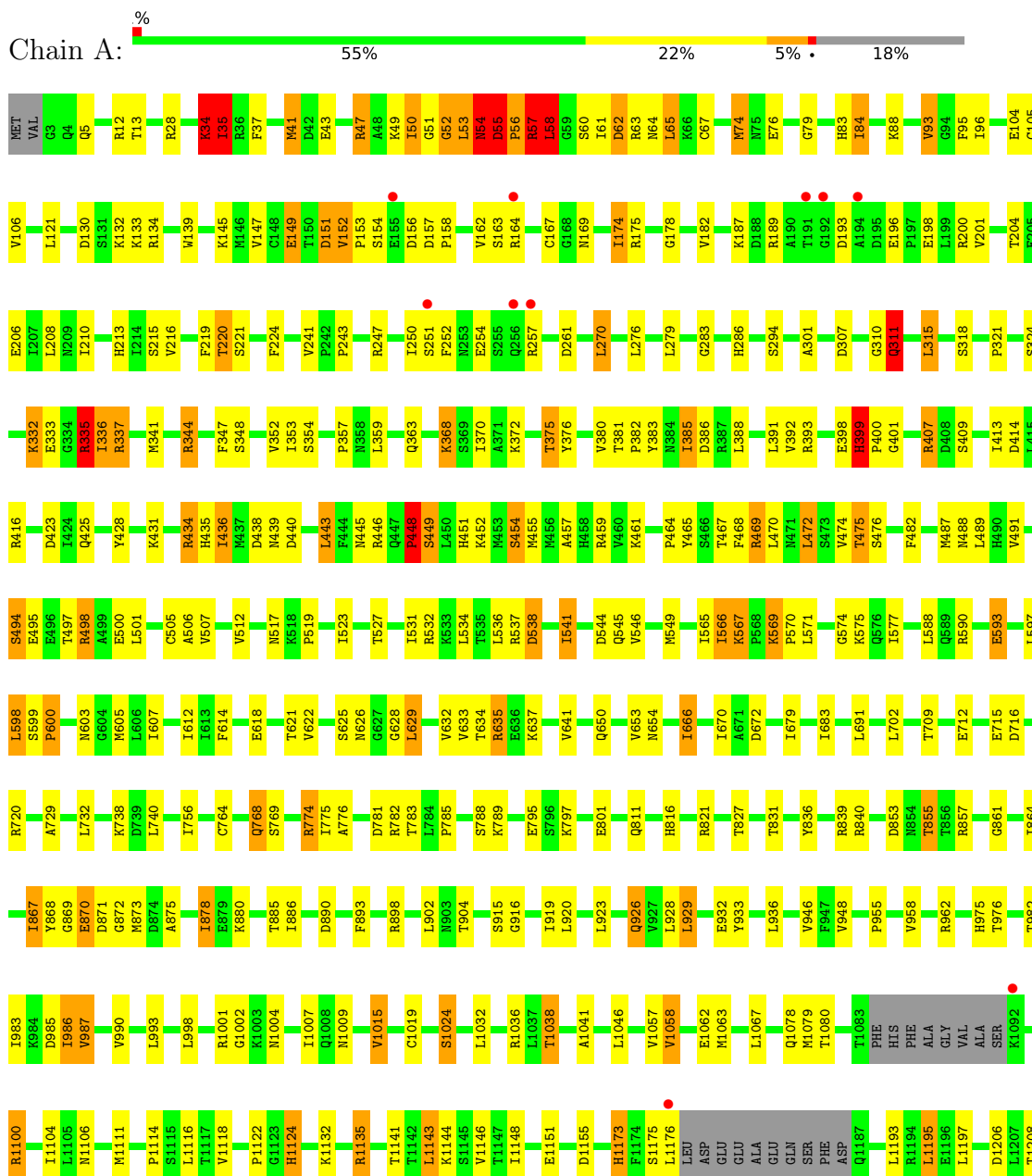
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

### 3 Residue-property plots

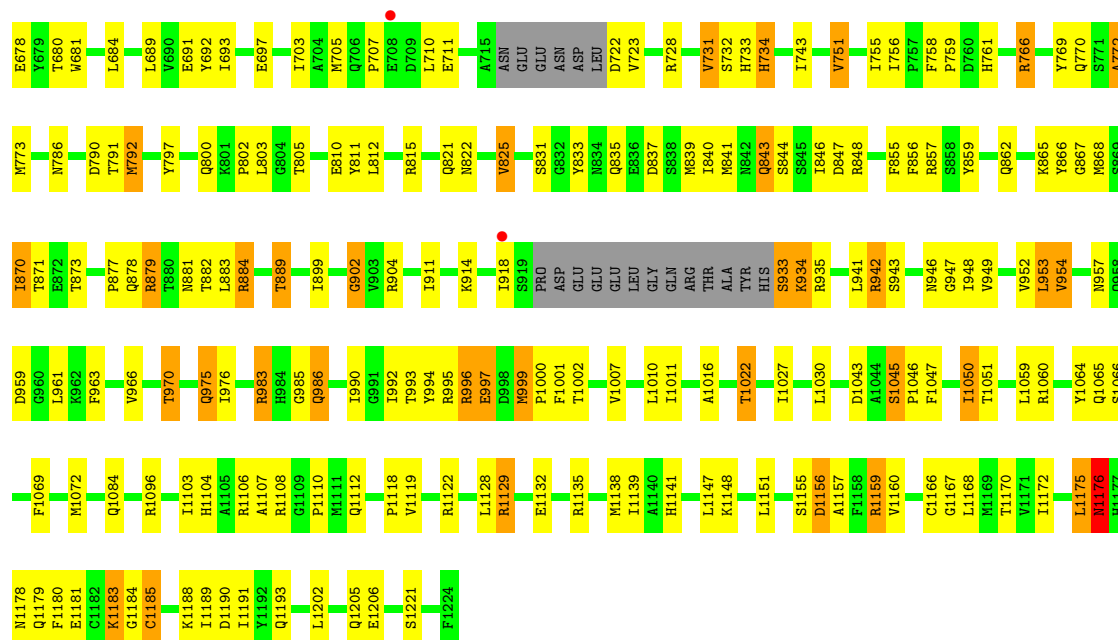
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 II SUBUNIT RPB1



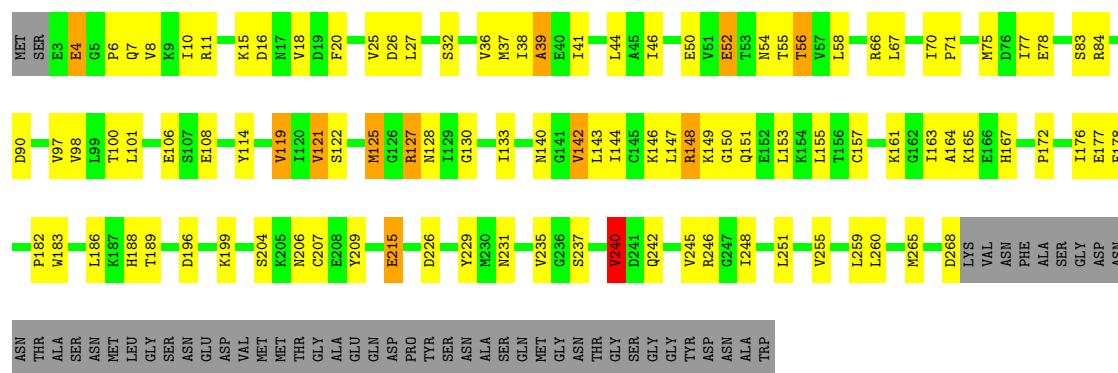






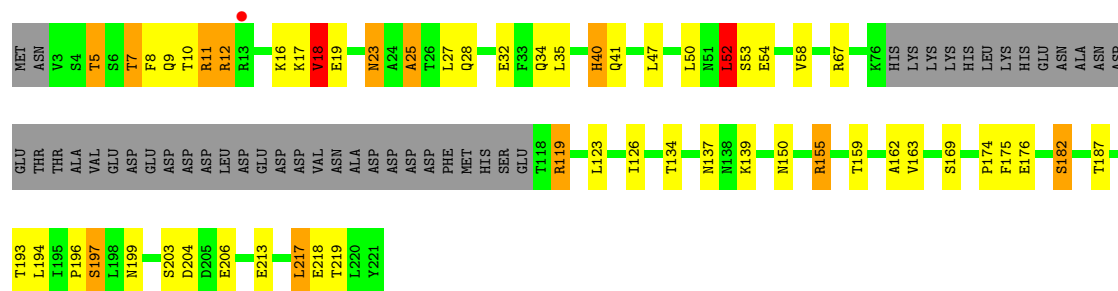
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 52% 28% 16%



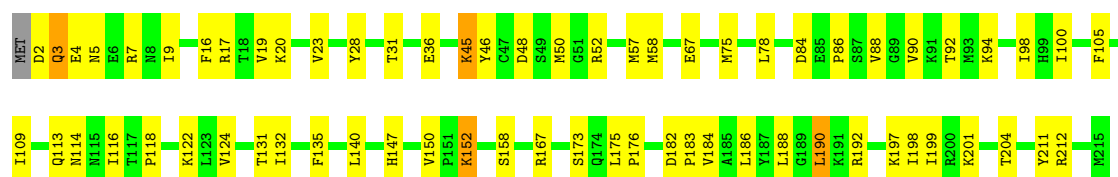
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D: 55% 19% 5% 19%

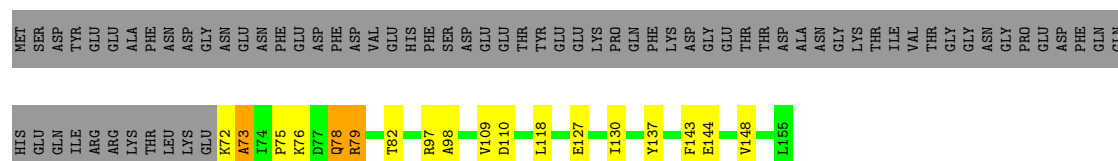


• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

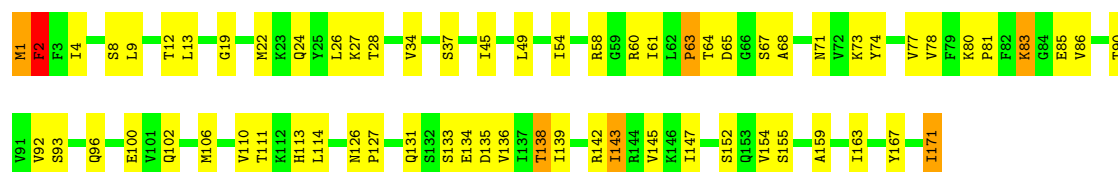
Chain E: 69% 29%



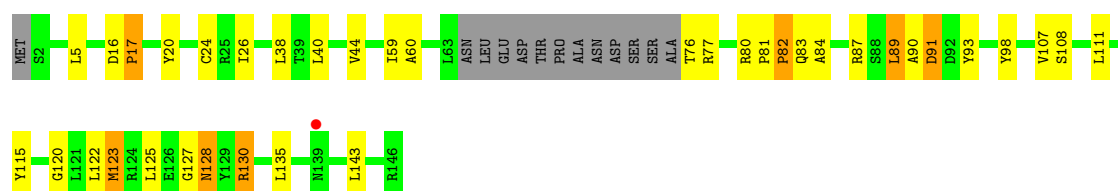
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



- Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

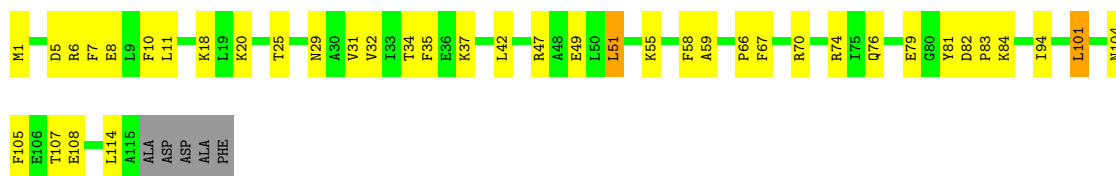


- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5




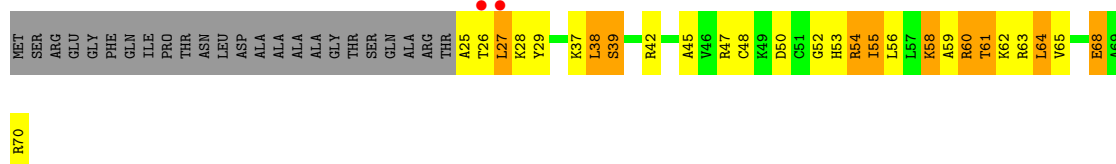
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:  63% 32%




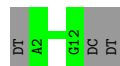
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:  3% 26% 26% 14% 34%



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

Chain N:  79% 21%



- Molecule 14: TRANSCRIPT RNA 5'-R(\*CP\*CP\*AP\*GP\*GP\*AP)-3'

Chain P:  67% 33%



- Molecule 15: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*DTP\*TP\*TP\*CP\*CBRU\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'

Chain T:  42% 27% 8% 23%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.60Å 391.30Å 283.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.89 – 3.50 52.78 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.89-3.50) 98.2 (52.78-3.40)	Depositor EDS
$R_{merge}$	0.68	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.156 , 0.185 0.180 , 0.207	Depositor DCC
$R_{free}$ test set	3255 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	110.5	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 101.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.036 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32010	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: MG, APC, ZN, BRU

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	0.54	0/11397	0.86	13/15415 (0.1%)
2	B	0.52	0/9029	0.81	3/12171 (0.0%)
3	C	0.49	0/2133	0.78	1/2891 (0.0%)
4	D	0.53	0/1444	0.84	1/1935 (0.1%)
5	E	0.46	0/1788	0.71	0/2406
6	F	0.57	0/691	0.80	0/933
7	G	0.53	0/1368	0.83	0/1844
8	H	0.51	0/1086	0.80	0/1470
9	I	0.46	0/989	0.76	0/1331
10	J	0.55	0/541	0.83	0/727
11	K	0.50	0/938	0.75	0/1267
12	L	0.52	0/365	0.95	0/485
13	N	1.11	0/254	1.01	0/391
14	P	1.13	0/145	0.78	0/224
15	T	1.36	4/426 (0.9%)	1.12	1/652 (0.2%)
All	All	0.55	4/32594 (0.0%)	0.83	19/44142 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	25	DT	N1-C2	7.74	1.44	1.38
15	T	25	DT	C1'-N1	7.62	1.59	1.49
15	T	13	DA	C3'-O3'	5.37	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	25	DT	N1-C6	5.08	1.41	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	HIS	N-CA-CB	7.22	123.60	110.60
1	A	34	LYS	C-N-CA	6.76	138.61	121.70
1	A	57	ARG	C-N-CA	5.96	136.60	121.70
1	A	54	ASN	C-N-CA	5.95	136.58	121.70
1	A	34	LYS	N-CA-C	-5.92	95.02	111.00
15	T	21	DC	O4'-C4'-C3'	-5.79	102.19	104.50
1	A	54	ASN	CB-CA-C	5.76	121.92	110.40
1	A	56	PRO	C-N-CA	5.71	135.97	121.70
4	D	25	ALA	C-N-CA	5.64	135.81	121.70
2	B	628	THR	C-N-CA	5.62	135.75	121.70
1	A	310	GLY	C-N-CA	5.62	135.74	121.70
1	A	35	ILE	N-CA-CB	5.30	123.00	110.80
2	B	338	GLY	C-N-CA	5.29	134.93	121.70
3	C	39	ALA	N-CA-C	5.26	125.20	111.00
2	B	1184	GLY	C-N-CA	5.21	134.73	121.70
1	A	1404	GLU	N-CA-C	5.14	124.89	111.00
1	A	55	ASP	N-CA-CB	5.11	119.80	110.60
1	A	53	LEU	N-CA-CB	5.02	120.45	110.40
1	A	311	GLN	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide

## 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	11197	0	11257	222	0
2	B	8859	0	8901	185	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2095	0	2051	56	0
4	D	1434	0	1460	25	0
5	E	1752	0	1776	33	0
6	F	679	0	701	10	0
7	G	1340	0	1357	37	0
8	H	1068	0	1040	21	0
9	I	971	0	927	10	0
10	J	532	0	542	14	0
11	K	920	0	929	22	0
12	L	363	0	386	15	0
13	N	226	0	126	0	0
14	P	130	0	66	1	0
15	T	404	0	227	6	0
16	A	31	0	14	2	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	32010	0	31760	583	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 9.

All (583) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.79	1.60
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.43	0.98
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.48	0.95
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.54	0.90
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.55	0.87
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.57	0.87
3:C:66:ARG:NH2	10:J:3:VAL:O	2.08	0.86
16:A:2455:APC:H8	16:A:2455:APC:H5'2	1.58	0.86
1:A:855:THR:HG21	1:A:857:ARG:HE	1.37	0.86
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.58	0.84
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.42	0.83
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG22	3:C:58:LEU:H	1.44	0.81
1:A:53:LEU:HD23	1:A:54:ASN:HB3	1.63	0.80
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.46	0.80
12:L:28:LYS:HB2	12:L:39:SER:HA	1.64	0.80
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.67	0.77
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.67	0.77
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.67	0.76
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.69	0.75
1:A:348:SER:HB2	2:B:1128:LEU:HD12	1.68	0.74
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.69	0.74
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.68	0.74
4:D:176:GLU:OE2	4:D:197:SER:HB2	1.86	0.74
1:A:472:LEU:O	1:A:475:THR:HB	1.87	0.74
1:A:61:ILE:HG22	1:A:62:ASP:H	1.51	0.74
2:B:882:THR:HG21	2:B:935:ARG:HA	1.70	0.74
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.53	0.73
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.70	0.73
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.17	0.73
2:B:1172:ILE:HD11	2:B:1183:LYS:HE2	1.69	0.72
7:G:111:THR:HG22	7:G:113:HIS:H	1.55	0.72
2:B:642:ASP:HA	2:B:649:LYS:HA	1.71	0.72
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.73	0.71
1:A:1445:ILE:HD11	7:G:68:ALA:CB	2.19	0.71
1:A:650:GLN:O	1:A:654:ASN:HB2	1.91	0.70
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.72	0.70
1:A:63:ARG:HA	1:A:74:MET:HG3	1.74	0.70
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.74	0.69
2:B:101:MET:HG2	2:B:111:ALA:HA	1.74	0.69
3:C:182:PRO:HB3	3:C:204:SER:HB3	1.73	0.69
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.56	0.69
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.57	0.69
7:G:138:THR:HG22	7:G:139:ILE:H	1.57	0.68
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.75	0.68
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.74	0.68
3:C:55:THR:HB	3:C:151:GLN:HA	1.76	0.68
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.28	0.68
3:C:100:THR:HG22	3:C:119:VAL:HG22	1.76	0.67
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.23	0.67
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.76	0.67
7:G:1:MET:SD	7:G:2:PHE:N	2.64	0.67
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.94	0.66
6:F:76:LYS:HA	6:F:79:ARG:CD	2.25	0.66
2:B:1175:LEU:O	2:B:1176:ASN:HB3	1.95	0.66
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.76	0.66
3:C:54:ASN:OD1	3:C:56:THR:HB	1.96	0.65
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.79	0.65
2:B:273:LEU:HD12	2:B:280:ILE:HD13	1.77	0.65
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.78	0.65
2:B:510:LYS:N	2:B:511:PRO:HD3	2.12	0.65
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.36	0.65
1:A:982:THR:HB	1:A:985:ASP:H	1.61	0.65
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.78	0.65
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.79	0.65
2:B:705:MET:H	2:B:710:LEU:HD12	1.61	0.64
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.36	0.64
2:B:484:ASN:HB3	2:B:486:TYR:CE2	2.33	0.64
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.28	0.64
1:A:982:THR:H	1:A:985:ASP:HB2	1.63	0.64
1:A:629:LEU:O	1:A:633:VAL:HG23	1.96	0.64
2:B:563:MET:CE	2:B:580:VAL:HB	2.28	0.64
3:C:52:GLU:HA	12:L:64:LEU:HD21	1.78	0.64
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.81	0.63
1:A:315:LEU:HA	1:A:321:PRO:HA	1.80	0.63
5:E:176:PRO:O	5:E:212:ARG:HA	1.97	0.63
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.79	0.63
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.81	0.62
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.80	0.62
1:A:35:ILE:HG21	1:A:241:VAL:HG21	1.82	0.62
1:A:388:LEU:O	1:A:392:VAL:HG23	2.00	0.62
1:A:56:PRO:O	1:A:57:ARG:HG3	2.00	0.62
2:B:882:THR:HG1	2:B:935:ARG:N	1.98	0.61
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.82	0.61
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.81	0.61
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.81	0.61
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.83	0.61
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.36	0.61
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.82	0.61
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.82	0.61
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.33	0.61
2:B:296:GLU:O	2:B:300:HIS:HD2	1.83	0.61
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LYS:H	1:A:337:ARG:HB3	1.67	0.60
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.84	0.60
1:A:1288:ASP:HA	1:A:1302:PRO:HB3	1.82	0.60
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.84	0.60
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.02	0.60
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.83	0.59
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.37	0.59
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.66	0.59
1:A:446:ARG:HB2	1:A:487:MET:SD	2.42	0.59
2:B:825:VAL:HG13	2:B:1010:LEU:HB3	1.85	0.59
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.02	0.58
1:A:869:GLY:O	5:E:204:THR:HG21	2.02	0.58
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.84	0.58
12:L:27:LEU:HD22	12:L:37:LYS:HE3	1.84	0.58
1:A:105:CYS:SG	1:A:139:TRP:HA	2.44	0.58
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.85	0.58
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.18	0.58
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.69	0.58
8:H:82:PRO:C	8:H:84:ALA:H	2.07	0.58
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.83	0.58
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.85	0.58
1:A:449:SER:HA	1:A:454:SER:HB3	1.85	0.57
1:A:448:PRO:O	1:A:449:SER:HB2	2.04	0.57
1:A:41:MET:HB3	1:A:49:LYS:HA	1.86	0.57
2:B:563:MET:HE2	2:B:580:VAL:HB	1.85	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.86	0.57
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.87	0.57
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.87	0.57
1:A:855:THR:CG2	1:A:857:ARG:HE	2.13	0.57
1:A:885:THR:HG23	1:A:893:PHE:HE2	1.69	0.57
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.87	0.57
2:B:882:THR:CG2	2:B:935:ARG:HA	2.34	0.57
3:C:11:ARG:HH21	3:C:229:TYR:HD1	1.53	0.56
1:A:534:LEU:O	1:A:574:GLY:HA3	2.05	0.56
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.88	0.56
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.86	0.56
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.88	0.56
11:K:7:PHE:O	11:K:11:LEU:HB2	2.05	0.56
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.71	0.56
2:B:815:ARG:HH11	2:B:815:ARG:HG3	1.71	0.56
7:G:34:VAL:O	7:G:37:SER:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.88	0.56
2:B:957:ASN:HB3	2:B:961:LEU:H	1.71	0.56
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.86	0.56
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.39	0.55
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.87	0.55
5:E:188:LEU:HB2	5:E:190:LEU:HD23	1.88	0.55
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.53	0.55
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.88	0.55
1:A:216:VAL:O	1:A:220:THR:HB	2.05	0.55
2:B:1172:ILE:HD11	2:B:1183:LYS:CE	2.36	0.55
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.89	0.55
1:A:494:SER:HB3	1:A:497:THR:H	1.72	0.55
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.72	0.55
2:B:590:HIS:HD2	2:B:592:ASN:H	1.53	0.55
2:B:597:MET:HG3	2:B:601:ARG:HH12	1.71	0.55
2:B:475:SER:O	2:B:476:ARG:HB3	2.07	0.54
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.89	0.54
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.88	0.54
2:B:1022:THR:HG23	2:B:1022:THR:O	2.08	0.54
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.89	0.54
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.89	0.54
2:B:902:GLY:O	12:L:65:VAL:HG11	2.08	0.54
1:A:134:ARG:HD2	1:A:221:SER:O	2.07	0.54
2:B:166:PHE:HZ	2:B:169:ARG:HG2	1.72	0.54
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.89	0.54
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.90	0.54
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.43	0.54
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.08	0.53
1:A:55:ASP:H	1:A:56:PRO:HD3	1.73	0.53
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.89	0.53
2:B:877:PRO:HA	2:B:934:LYS:HZ3	1.74	0.53
4:D:23:ASN:HA	4:D:28:GLN:O	2.08	0.53
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.90	0.53
1:A:709:THR:HB	1:A:712:GLU:H	1.73	0.53
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.90	0.53
1:A:1442:ASP:HB2	6:F:137:TYR:CE1	2.41	0.53
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.91	0.53
4:D:155:ARG:HB3	4:D:219:THR:HG21	1.90	0.53
1:A:54:ASN:HB2	1:A:247:ARG:HH12	1.74	0.53
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.91	0.53
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.90	0.53
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.09	0.53
2:B:899:ILE:HD12	2:B:911:ILE:HA	1.90	0.53
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.90	0.53
3:C:148:ARG:HG3	3:C:151:GLN:HG3	1.91	0.52
3:C:251:LEU:O	3:C:255:VAL:HG23	2.08	0.52
4:D:10:THR:HB	4:D:12:ARG:HH22	1.74	0.52
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.90	0.52
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.45	0.52
2:B:843:GLN:HE21	11:K:6:ARG:HH21	1.57	0.52
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.39	0.52
1:A:376:TYR:CE1	1:A:498:ARG:HD2	2.44	0.52
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.91	0.52
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.92	0.52
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.92	0.52
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.91	0.52
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.91	0.52
1:A:565:ILE:O	1:A:570:PRO:HA	2.08	0.52
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.91	0.52
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.92	0.52
3:C:32:SER:O	3:C:36:VAL:HG23	2.10	0.52
1:A:449:SER:HA	1:A:454:SER:CB	2.40	0.52
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.58	0.52
2:B:918:ILE:HD13	2:B:935:ARG:HH12	1.74	0.52
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.75	0.52
1:A:332:LYS:H	1:A:337:ARG:CB	2.23	0.52
1:A:729:ALA:HA	1:A:732:LEU:HD12	1.91	0.52
7:G:143:ILE:HG22	7:G:145:VAL:HG23	1.91	0.52
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.43	0.52
5:E:19:VAL:O	5:E:23:VAL:HG23	2.09	0.52
4:D:40:HIS:CB	7:G:73:LYS:HE3	2.30	0.52
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.73	0.51
4:D:159:THR:O	4:D:163:VAL:HG23	2.10	0.51
1:A:149:GLU:HG2	1:A:152:VAL:HG23	1.92	0.51
2:B:1185:CYS:HA	4:D:17:LYS:HD3	1.91	0.51
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.91	0.51
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.93	0.51
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.93	0.51
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.93	0.51
5:E:197:LYS:HD3	5:E:199:ILE:HD11	1.91	0.51
2:B:247:GLY:H	2:B:418:LYS:HZ3	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.92	0.51
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.92	0.51
1:A:855:THR:HG21	1:A:857:ARG:NE	2.16	0.51
2:B:882:THR:C	2:B:884:ARG:H	2.14	0.51
1:A:827:THR:O	1:A:831:THR:HB	2.11	0.51
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.93	0.51
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.93	0.51
7:G:8:SER:HB2	7:G:71:ASN:HD21	1.75	0.51
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.93	0.50
2:B:1129:ARG:HG2	15:T:20:DC:H5"	1.92	0.50
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.45	0.50
3:C:206:ASN:HA	3:C:209:TYR:HD1	1.75	0.50
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.47	0.50
1:A:1132:LYS:HG2	1:A:1135:ARG:HH12	1.77	0.50
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.47	0.50
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.93	0.50
3:C:242:GLN:O	3:C:246:ARG:HB2	2.12	0.50
4:D:193:THR:HG21	7:G:167:TYR:HD2	1.76	0.50
10:J:6:ARG:H	10:J:14:VAL:H	1.57	0.50
2:B:35:SER:HA	2:B:811:TYR:HE1	1.77	0.50
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.94	0.50
1:A:62:ASP:HB3	1:A:64:ASN:O	2.11	0.50
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.94	0.50
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.77	0.50
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.93	0.50
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.45	0.50
2:B:254:LEU:HD11	2:B:273:LEU:HD23	1.93	0.50
1:A:53:LEU:HD23	1:A:54:ASN:N	2.26	0.49
4:D:5:THR:HG21	7:G:74:TYR:OH	2.12	0.49
1:A:1264:GLU:HA	1:A:1267:MET:HE2	1.93	0.49
1:A:1143:LEU:HD22	1:A:1267:MET:HB3	1.93	0.49
1:A:52:GLY:N	1:A:56:PRO:HB3	2.27	0.49
2:B:291:ILE:HD12	2:B:291:ILE:H	1.77	0.49
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.93	0.49
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.93	0.49
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.41	0.49
1:A:354:SER:O	1:A:469:ARG:HA	2.11	0.49
2:B:276:ILE:HA	2:B:338:GLY:O	2.12	0.49
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.13	0.49
3:C:148:ARG:H	3:C:151:GLN:HG3	1.77	0.49
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:LEU:HB3	1:A:987:VAL:HG11	1.94	0.49
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.78	0.49
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.77	0.49
2:B:486:TYR:HB3	2:B:1096:ARG:HD2	1.94	0.49
2:B:933:SER:O	2:B:935:ARG:N	2.46	0.49
1:A:716:ASP:O	1:A:720:ARG:HB2	2.13	0.49
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.78	0.49
2:B:953:LEU:HD11	12:L:55:ILE:HG22	1.95	0.49
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.94	0.48
1:A:88:LYS:HB2	1:A:276:LEU:HD21	1.95	0.48
1:A:35:ILE:HG22	1:A:84:ILE:HG23	1.94	0.48
1:A:370:ILE:HD11	2:B:1103:ILE:HG13	1.95	0.48
2:B:841:MET:O	2:B:993:THR:HA	2.13	0.48
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.78	0.48
4:D:23:ASN:O	7:G:83:LYS:HG2	2.12	0.48
16:A:2455:APC:C8	16:A:2455:APC:H5'2	2.38	0.48
2:B:577:ALA:HB1	2:B:589:VAL:HB	1.95	0.48
1:A:632:VAL:HG13	1:A:962:ARG:HD3	1.95	0.48
4:D:162:ALA:HB3	4:D:217:LEU:HD21	1.95	0.48
8:H:5:LEU:HB2	8:H:59:ILE:HG22	1.96	0.48
9:I:73:ARG:HH12	9:I:112:SER:HA	1.78	0.48
11:K:8:GLU:O	11:K:37:LYS:HD2	2.14	0.48
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.96	0.48
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.95	0.48
12:L:61:THR:HG22	12:L:63:ARG:H	1.79	0.48
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.94	0.48
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.96	0.48
1:A:414:ASP:OD1	1:A:416:ARG:HB2	2.13	0.47
2:B:769:TYR:O	2:B:772:ALA:HB3	2.14	0.47
1:A:781:ASP:HB2	1:A:789:LYS:HG2	1.95	0.47
2:B:206:ASN:HD21	2:B:458:LYS:HD3	1.79	0.47
8:H:127:GLY:N	8:H:130:ARG:HH21	2.11	0.47
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.35	0.47
1:A:531:ILE:HD12	1:A:653:VAL:HG21	1.96	0.47
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.50	0.47
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.95	0.47
7:G:1:MET:CG	7:G:2:PHE:N	2.77	0.47
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.97	0.47
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.45	0.47
1:A:399:HIS:O	1:A:401:GLY:N	2.47	0.47
2:B:123:THR:HG23	2:B:205:ILE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.96	0.47
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.95	0.47
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.97	0.47
3:C:98:VAL:H	3:C:122:SER:HB3	1.80	0.47
2:B:873:THR:O	2:B:914:LYS:HA	2.15	0.47
8:H:89:LEU:C	8:H:91:ASP:H	2.18	0.47
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.97	0.47
1:A:1215:ARG:HG3	1:A:1273:LEU:HA	1.97	0.47
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.96	0.47
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.15	0.47
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.96	0.47
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.80	0.47
2:B:986:GLN:OE1	2:B:1016:ALA:HB1	2.15	0.47
2:B:732:SER:HB2	2:B:734:HIS:ND1	2.30	0.47
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.97	0.47
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.56	0.46
2:B:1221:SER:HB3	4:D:12:ARG:HD2	1.97	0.46
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.96	0.46
1:A:457:ALA:O	1:A:507:VAL:HG23	2.15	0.46
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.97	0.46
1:A:873:MET:C	1:A:1058:VAL:HG22	2.36	0.46
1:A:495:GLU:HG3	6:F:98:ALA:HB1	1.97	0.46
1:A:567:LYS:HD3	1:A:569:LYS:H	1.80	0.46
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.97	0.46
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.98	0.46
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	1.98	0.46
8:H:80:ARG:HH11	8:H:87:ARG:HH22	1.62	0.46
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.96	0.46
10:J:32:GLU:CD	10:J:32:GLU:H	2.18	0.46
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.51	0.46
1:A:448:PRO:O	1:A:449:SER:CB	2.64	0.46
11:K:35:PHE:O	11:K:70:ARG:HA	2.15	0.46
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.98	0.46
7:G:93:SER:OG	7:G:100:GLU:HB2	2.16	0.46
1:A:575:LYS:HD2	8:H:120:GLY:HA3	1.98	0.46
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.81	0.46
4:D:52:LEU:HG	4:D:182:SER:HB3	1.97	0.46
4:D:54:GLU:O	4:D:58:VAL:HG23	2.16	0.46
1:A:541:ILE:HG21	1:A:549:MET:HE2	1.96	0.46
2:B:383:ASN:O	2:B:387:LEU:HB2	2.16	0.46
2:B:551:PRO:HA	2:B:554:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.98	0.46
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.46	0.46
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.97	0.46
1:A:605:MET:CE	1:A:612:ILE:HG23	2.46	0.46
3:C:149:LYS:C	3:C:151:GLN:H	2.19	0.46
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.98	0.46
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.98	0.45
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.46	0.45
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.98	0.45
2:B:242:SER:OG	2:B:362:PRO:HD2	2.16	0.45
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.97	0.45
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.97	0.45
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.97	0.45
1:A:537:ARG:HB2	8:H:20:TYR:CE1	2.52	0.45
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.99	0.45
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.98	0.45
2:B:803:LEU:HG	10:J:52:THR:HG21	1.98	0.45
2:B:446:LEU:HD12	2:B:448:ILE:HD11	1.98	0.45
4:D:150:ASN:HB3	7:G:142:ARG:NH2	2.31	0.45
15:T:25:DT:H6	15:T:25:DT:H5"	1.80	0.45
1:A:1323:ASP:CG	1:A:1326:ARG:HG3	2.37	0.45
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.51	0.45
12:L:25:ALA:HB1	12:L:62:LYS:HZ1	1.81	0.45
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.98	0.45
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.98	0.45
2:B:343:ILE:O	2:B:344:LYS:HB2	2.16	0.45
5:E:182:ASP:O	5:E:186:LEU:HG	2.16	0.45
11:K:82:ASP:OD2	11:K:84:LYS:HB2	2.17	0.45
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.16	0.45
2:B:865:LYS:HB2	2:B:961:LEU:HD21	1.98	0.45
2:B:947:GLY:HA2	2:B:970:THR:HG23	1.98	0.45
2:B:831:SER:HG	2:B:994:TYR:HE2	1.65	0.45
5:E:78:LEU:HD11	5:E:109:ILE:HG13	1.99	0.45
1:A:567:LYS:HA	1:A:569:LYS:N	2.31	0.45
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.99	0.45
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.98	0.45
7:G:81:PRO:HG3	7:G:106:MET:SD	2.57	0.45
2:B:296:GLU:O	2:B:300:HIS:CD2	2.66	0.45
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.82	0.45
1:A:880:LYS:HA	1:A:955:PRO:HA	1.99	0.44
2:B:249:ARG:HE	2:B:418:LYS:HZ2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:GLY:HA2	2:B:327:ARG:HD2	1.98	0.44
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.85	0.44
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.99	0.44
2:B:758:PHE:CE2	2:B:1027:ILE:HG22	2.52	0.44
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.99	0.44
3:C:100:THR:HB	3:C:121:VAL:HG21	2.00	0.44
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.98	0.44
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.17	0.44
2:B:629:ASP:HB3	2:B:632:ARG:NE	2.31	0.44
2:B:70:ILE:H	2:B:70:ILE:HD12	1.81	0.44
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.99	0.44
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.99	0.44
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.52	0.44
1:A:452:LYS:HG2	2:B:1141:HIS:CE1	2.52	0.44
5:E:197:LYS:HG3	5:E:211:TYR:CE2	2.52	0.44
5:E:50:MET:HB3	5:E:52:ARG:HG3	2.00	0.44
1:A:867:ILE:CD1	1:A:867:ILE:CB	2.85	0.44
3:C:71:PRO:HG3	10:J:13:VAL:HG11	2.00	0.44
8:H:82:PRO:O	8:H:84:ALA:N	2.47	0.44
1:A:439:ASN:HD21	1:A:459:ARG:HE	1.65	0.44
2:B:510:LYS:N	2:B:511:PRO:CD	2.81	0.44
2:B:810:GLU:HA	2:B:815:ARG:NH1	2.33	0.44
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.91	0.44
7:G:147:ILE:HG23	7:G:159:ALA:HB1	2.00	0.44
7:G:142:ARG:HB3	7:G:171:ILE:HD12	2.00	0.44
1:A:1148:ILE:HG23	9:I:49:ILE:HB	2.00	0.44
2:B:1050:ILE:H	2:B:1050:ILE:HG13	1.63	0.44
1:A:151:ASP:HA	1:A:163:SER:HA	2.00	0.44
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.99	0.44
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.00	0.44
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.77	0.44
5:E:5:ASN:HD21	5:E:52:ARG:HE	1.66	0.44
10:J:7:CYS:HA	10:J:49:MET:HG2	2.00	0.44
4:D:5:THR:HG23	7:G:9:LEU:HB2	2.00	0.44
11:K:5:ASP:HB2	11:K:8:GLU:HG3	1.98	0.44
1:A:182:VAL:HB	1:A:201:VAL:HG23	2.00	0.43
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.86	0.43
3:C:142:VAL:HG22	10:J:15:GLY:HA3	2.00	0.43
1:A:104:GLU:HG2	1:A:174:ILE:HD12	2.00	0.43
1:A:55:ASP:CG	1:A:55:ASP:O	2.55	0.43
2:B:1106:ARG:NH1	2:B:1110:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.83	0.43
1:A:49:LYS:HE2	1:A:61:ILE:H	1.82	0.43
1:A:857:ARG:HD3	1:A:861:GLY:O	2.18	0.43
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.53	0.43
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.53	0.43
3:C:6:PRO:HB2	11:K:101:LEU:HD23	2.00	0.43
4:D:50:LEU:HD11	7:G:4:ILE:HG13	2.01	0.43
1:A:443:LEU:HD23	1:A:501:LEU:HD22	2.00	0.43
1:A:932:GLU:O	1:A:936:LEU:HG	2.19	0.43
2:B:128:LEU:HD21	2:B:170:LEU:CB	2.48	0.43
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.53	0.43
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.83	0.43
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.47	0.43
1:A:55:ASP:N	1:A:56:PRO:HD3	2.33	0.43
1:A:929:LEU:HD21	1:A:983:ILE:HG12	2.00	0.43
2:B:291:ILE:HD12	2:B:291:ILE:N	2.32	0.43
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.43
1:A:598:LEU:HB2	8:H:115:TYR:HE2	1.84	0.43
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.00	0.43
2:B:954:VAL:HG21	12:L:29:TYR:CE1	2.53	0.43
2:B:693:ILE:HG23	2:B:697:GLU:HB3	2.01	0.43
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.31	0.43
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.01	0.43
2:B:39:ARG:NE	2:B:665:GLU:HG2	2.33	0.43
5:E:46:TYR:CE1	5:E:58:MET:HA	2.54	0.43
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.19	0.43
1:A:546:VAL:HG13	1:A:577:ILE:HG21	2.00	0.43
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.65	0.43
2:B:344:LYS:O	2:B:348:ARG:HD2	2.18	0.43
2:B:485:ARG:NH1	2:B:491:THR:HG21	2.34	0.43
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.84	0.43
1:A:1443:VAL:HG12	7:G:61:ILE:HD13	2.01	0.42
1:A:49:LYS:NZ	1:A:60:SER:HA	2.34	0.42
1:A:628:GLY:O	1:A:632:VAL:HG23	2.19	0.42
8:H:107:VAL:O	8:H:111:LEU:HB2	2.19	0.42
14:P:5:C:H2'	14:P:6:C:C6	2.54	0.42
2:B:770:GLN:CD	2:B:983:ARG:HA	2.39	0.42
2:B:773:MET:HE1	2:B:985:GLY:HA2	2.01	0.42
15:T:15:DT:H2'	15:T:16:DT:C6	2.54	0.42
1:A:354:SER:HA	1:A:482:PHE:CD1	2.54	0.42
1:A:53:LEU:HD12	1:A:270:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:ALA:O	1:A:783:THR:HG22	2.18	0.42
2:B:548:GLY:HA3	2:B:630:ALA:HB2	2.00	0.42
2:B:792:MET:HG2	2:B:855:PHE:CZ	2.53	0.42
7:G:126:ASN:HA	7:G:127:PRO:HA	1.88	0.42
15:T:13:DA:H2''	15:T:14:DC:O4'	2.20	0.42
1:A:885:THR:OG1	1:A:1024:SER:HB2	2.19	0.42
2:B:281:PRO:HD2	2:B:284:ILE:HD13	2.01	0.42
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.02	0.42
2:B:882:THR:O	2:B:884:ARG:N	2.52	0.42
2:B:35:SER:HA	2:B:811:TYR:CE1	2.53	0.42
3:C:37:MET:HA	3:C:41:ILE:HD12	2.01	0.42
1:A:152:VAL:HG22	1:A:153:PRO:HD2	2.01	0.42
1:A:774:ARG:CZ	1:A:797:LYS:HB2	2.49	0.42
2:B:512:ARG:CZ	2:B:535:LEU:HD11	2.50	0.42
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.20	0.42
1:A:1285:MET:HG3	1:A:1307:GLU:HG3	2.00	0.42
1:A:35:ILE:HA	1:A:52:GLY:O	2.20	0.42
1:A:538:ASP:H	8:H:20:TYR:HE1	1.68	0.42
2:B:634:TYR:CD2	2:B:692:TYR:HB3	2.55	0.42
2:B:792:MET:HA	2:B:856:PHE:O	2.20	0.42
1:A:1143:LEU:HD21	1:A:1195:LEU:HD13	2.01	0.42
1:A:336:ILE:HG21	1:A:1401:SER:HA	2.02	0.42
1:A:64:ASN:O	1:A:65:LEU:HB3	2.19	0.42
1:A:347:PHE:H	2:B:1107:ALA:HA	1.85	0.42
2:B:126:SER:HB2	2:B:172:ILE:HD11	2.02	0.42
2:B:542:MET:HB3	2:B:636:PRO:HD2	2.02	0.42
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.55	0.42
2:B:459:TYR:CE2	2:B:470:LYS:HG3	2.54	0.42
1:A:840:ARG:NH2	1:A:1106:ASN:ND2	2.67	0.42
10:J:8:PHE:H	10:J:49:MET:CE	2.33	0.42
15:T:8:DC:H2'	15:T:9:DA:C8	2.55	0.42
1:A:382:PRO:HG3	1:A:428:TYR:CZ	2.55	0.41
3:C:125:MET:HB2	3:C:127:ARG:NE	2.35	0.41
3:C:114:TYR:HB3	3:C:140:ASN:O	2.20	0.41
5:E:3:GLN:HE22	5:E:5:ASN:HD22	1.68	0.41
1:A:359:LEU:HD22	1:A:363:GLN:HG3	2.02	0.41
4:D:7:THR:HB	4:D:8:PHE:H	1.45	0.41
15:T:13:DA:H4'	15:T:14:DC:OP1	2.20	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.19	0.41
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.01	0.41
1:A:1173:HIS:HB3	1:A:1227:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:VAL:HA	1:A:519:PRO:HA	2.03	0.41
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.01	0.41
2:B:1043:ASP:OD2	2:B:1045:SER:HB2	2.20	0.41
2:B:1110:PRO:HG2	2:B:1119:VAL:HG21	2.03	0.41
2:B:345:LYS:HA	2:B:348:ARG:CD	2.50	0.41
2:B:351:TYR:HB3	2:B:352:ALA:N	2.35	0.41
2:B:486:TYR:HD2	2:B:490:SER:HG	1.67	0.41
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.85	0.41
5:E:23:VAL:HG12	5:E:28:TYR:HB2	2.03	0.41
7:G:110:VAL:HG11	7:G:163:ILE:HG12	2.02	0.41
9:I:118:ARG:HB3	9:I:119:THR:H	1.69	0.41
1:A:1400:CYS:HA	1:A:1408:ILE:HD12	2.02	0.41
1:A:599:SER:HA	1:A:600:PRO:HD3	1.83	0.41
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.54	0.41
1:A:1335:ILE:HG21	1:A:1347:ALA:HB2	2.02	0.41
1:A:872:GLY:O	1:A:1057:VAL:HG13	2.20	0.41
1:A:488:ASN:HD22	2:B:1128:LEU:HD13	1.85	0.41
2:B:168:GLY:H	2:B:450:ALA:HB1	1.86	0.41
2:B:464:GLY:HA2	2:B:480:SER:HB3	2.02	0.41
2:B:847:ASP:HB3	3:C:167:HIS:CE1	2.55	0.41
5:E:118:PRO:O	5:E:122:LYS:HG2	2.21	0.41
9:I:7:CYS:SG	9:I:10:CYS:HB2	2.59	0.41
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.21	0.41
2:B:365:THR:HG21	2:B:370:PHE:HB2	2.02	0.41
2:B:530:GLY:H	2:B:533:CYS:HB2	1.85	0.41
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.56	0.41
1:A:1450:LEU:HD22	7:G:19:GLY:O	2.21	0.41
1:A:840:ARG:NH2	1:A:1106:ASN:HD21	2.18	0.41
1:A:336:ILE:CG2	1:A:1401:SER:HA	2.50	0.41
2:B:33:VAL:HG23	2:B:658:ILE:HD11	2.03	0.41
3:C:84:ARG:CZ	11:K:11:LEU:HD11	2.50	0.41
5:E:152:LYS:H	5:E:152:LYS:HG3	1.67	0.41
5:E:94:LYS:HE2	5:E:98:ILE:HD11	2.02	0.41
3:C:4:GLU:OE1	11:K:104:ASN:ND2	2.53	0.41
11:K:82:ASP:OD1	11:K:83:PRO:HD2	2.21	0.41
1:A:41:MET:HA	1:A:50:ILE:HB	2.02	0.41
1:A:157:ASP:HA	1:A:158:PRO:HD3	1.96	0.41
1:A:352:VAL:HG12	1:A:467:THR:HG22	2.02	0.41
1:A:79:GLY:HA3	1:A:243:PRO:HG3	2.03	0.41
2:B:564:GLU:O	2:B:588:GLY:HA3	2.21	0.41
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:47:ARG:HG3	12:L:54:ARG:HG3	2.03	0.41
1:A:1038:THR:HG23	1:A:1041:ALA:HB2	2.03	0.40
1:A:1215:ARG:O	1:A:1218:GLN:HG2	2.21	0.40
1:A:206:GLU:O	1:A:210:ILE:HG12	2.21	0.40
1:A:200:ARG:NH2	1:A:206:GLU:OE1	2.50	0.40
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.57	0.40
3:C:100:THR:HG22	3:C:119:VAL:CG2	2.48	0.40
1:A:709:THR:HG23	9:I:94:ASP:HA	2.02	0.40
1:A:1444:MET:HG3	7:G:58:ARG:HB3	2.02	0.40
2:B:102:VAL:HG13	2:B:112:LEU:HD22	2.04	0.40
2:B:1059:LEU:HG	2:B:1064:TYR:HB2	2.04	0.40
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.36	0.40
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.80	0.40
2:B:756:ILE:O	2:B:759:PRO:HD3	2.20	0.40
2:B:766:ARG:NH1	2:B:769:TYR:HD2	2.19	0.40
4:D:25:ALA:HB1	4:D:196:PRO:HD2	2.04	0.40
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.56	0.40
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.03	0.40
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.03	0.40
2:B:481:GLN:HE21	2:B:481:GLN:HB3	1.74	0.40
2:B:54:PHE:HA	2:B:58:THR:HB	2.03	0.40
2:B:69:LEU:HD11	2:B:425:THR:HG23	2.02	0.40
2:B:710:LEU:HA	2:B:733:HIS:HB3	2.03	0.40
10:J:8:PHE:H	10:J:49:MET:HE3	1.86	0.40
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.20	0.40
1:A:368:LYS:HE2	1:A:399:HIS:HB2	2.03	0.40
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.55	0.40
1:A:986:ILE:O	1:A:990:VAL:HG23	2.22	0.40
2:B:728:ARG:HH12	2:B:1047:PHE:HA	1.87	0.40
2:B:975:GLN:O	2:B:990:ILE:HD12	2.21	0.40
2:B:773:MET:CE	2:B:985:GLY:HA2	2.51	0.40
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.03	0.40
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.21	0.40
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.52	0.40
3:C:153:LEU:HD11	3:C:155:LEU:HD23	2.04	0.40
3:C:15:LYS:O	3:C:240:VAL:HG22	2.20	0.40
1:A:946:VAL:HG22	5:E:201:LYS:HD2	2.03	0.40
11:K:10:PHE:CD2	11:K:11:LEU:HD13	2.56	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	1417/1732 (82%)	1225 (86%)	135 (10%)	57 (4%)	3	27
2	B	1095/1224 (90%)	951 (87%)	92 (8%)	52 (5%)	2	23
3	C	264/318 (83%)	237 (90%)	20 (8%)	7 (3%)	5	36
4	D	174/221 (79%)	153 (88%)	11 (6%)	10 (6%)	2	19
5	E	212/215 (99%)	196 (92%)	12 (6%)	4 (2%)	9	43
6	F	82/155 (53%)	77 (94%)	4 (5%)	1 (1%)	14	53
7	G	169/171 (99%)	156 (92%)	9 (5%)	4 (2%)	6	38
8	H	129/146 (88%)	104 (81%)	17 (13%)	8 (6%)	1	17
9	I	117/122 (96%)	93 (80%)	19 (16%)	5 (4%)	3	25
10	J	63/70 (90%)	53 (84%)	7 (11%)	3 (5%)	2	22
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	24 (54%)	12 (27%)	8 (18%)	0	1
All	All	3879/4564 (85%)	3377 (87%)	343 (9%)	159 (4%)	3	27

All (159) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	58	LEU
1	A	169	ASN
1	A	189	ARG
1	A	251	SER
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	448	PRO
1	A	449	SER
1	A	1122	PRO
1	A	1175	SER

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Mol	Chain	Res	Type
1	A	1206	ASP
2	B	229	ALA
2	B	340	ALA
2	B	344	LYS
2	B	367	LEU
2	B	731	VAL
2	B	751	VAL
2	B	879	ARG
2	B	943	SER
2	B	1046	PRO
2	B	1066	SER
2	B	1157	ALA
2	B	1181	GLU
3	C	215	GLU
3	C	237	SER
4	D	18	VAL
4	D	119	ARG
4	D	199	ASN
5	E	48	ASP
8	H	90	ALA
9	I	95	THR
10	J	6	ARG
12	L	56	LEU
12	L	60	ARG
1	A	52	GLY
1	A	55	ASP
1	A	57	ARG
1	A	76	GLU
1	A	167	CYS
1	A	178	GLY
1	A	257	ARG
1	A	332	LYS
1	A	335	ARG
1	A	465	TYR
1	A	775	ILE
1	A	1403	GLU
1	A	1405	THR
2	B	67	SER
2	B	262	GLU
2	B	307	ASP
2	B	343	ILE
2	B	369	GLY

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Mol	Chain	Res	Type
2	B	473	MET
2	B	629	ASP
2	B	643	ASP
2	B	667	GLN
2	B	707	PRO
2	B	711	GLU
2	B	772	ALA
2	B	792	MET
2	B	867	GLY
2	B	883	LEU
2	B	1069	PHE
2	B	1155	SER
2	B	1156	ASP
2	B	1176	ASN
2	B	1185	CYS
2	B	1190	ASP
4	D	11	ARG
4	D	16	LYS
4	D	53	SER
5	E	45	LYS
8	H	83	GLN
8	H	128	ASN
9	I	88	SER
12	L	39	SER
1	A	43	GLU
1	A	74	MET
1	A	156	ASP
1	A	164	ARG
1	A	975	HIS
1	A	1079	MET
2	B	338	GLY
2	B	341	LEU
2	B	449	ASN
2	B	889	THR
2	B	902	GLY
2	B	942	ARG
2	B	1167	GLY
4	D	52	LEU
4	D	169	SER
4	D	174	PRO
4	D	218	GLU
5	E	36	GLU

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Mol	Chain	Res	Type
7	G	63	PRO
7	G	154	VAL
8	H	60	ALA
8	H	81	PRO
8	H	82	PRO
9	I	89	GLN
10	J	17	LYS
12	L	53	HIS
12	L	59	ALA
1	A	224	PHE
1	A	399	HIS
1	A	409	SER
1	A	569	LYS
1	A	593	GLU
1	A	870	GLU
1	A	1255	GLU
1	A	1281	ARG
1	A	1377	THR
2	B	68	THR
2	B	282	ILE
2	B	466	TRP
2	B	476	ARG
3	C	78	GLU
7	G	2	PHE
7	G	67	SER
8	H	17	PRO
9	I	23	ASN
10	J	2	ILE
12	L	26	THR
1	A	196	GLU
1	A	250	ILE
1	A	336	ILE
1	A	600	PRO
1	A	635	ARG
1	A	958	VAL
1	A	986	ILE
1	A	1124	HIS
1	A	1242	VAL
2	B	353	LYS
2	B	1108	ARG
3	C	56	THR
3	C	90	ASP

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Mol	Chain	Res	Type
6	F	73	ALA
8	H	108	SER
9	I	105	SER
12	L	45	ALA
1	A	54	ASN
1	A	283	GLY
1	A	916	GLY
2	B	648	HIS
5	E	90	VAL
1	A	35	ILE
2	B	108	VAL
2	B	251	ILE
2	B	870	ILE
3	C	150	GLY
3	C	240	VAL
12	L	52	GLY
2	B	510	LYS
1	A	987	VAL
2	B	364	ILE
1	A	400	PRO
1	A	567	LYS

### 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	1243/1519 (82%)	1046 (84%)	197 (16%)	3	16
2	B	966/1061 (91%)	833 (86%)	133 (14%)	4	21
3	C	234/274 (85%)	206 (88%)	28 (12%)	5	26
4	D	160/200 (80%)	131 (82%)	29 (18%)	2	10
5	E	196/197 (100%)	176 (90%)	20 (10%)	8	34
6	F	74/137 (54%)	66 (89%)	8 (11%)	7	31
7	G	152/152 (100%)	128 (84%)	24 (16%)	3	16
8	H	117/128 (91%)	108 (92%)	9 (8%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	113/116 (97%)	102 (90%)	11 (10%)	9	35
10	J	60/65 (92%)	50 (83%)	10 (17%)	2	13
11	K	99/102 (97%)	85 (86%)	14 (14%)	4	20
12	L	40/57 (70%)	29 (72%)	11 (28%)	0	3
All	All	3454/4008 (86%)	2960 (86%)	494 (14%)	3	20

All (494) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	THR
1	A	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	47	ARG
1	A	50	ILE
1	A	54	ASN
1	A	58	LEU
1	A	62	ASP
1	A	65	LEU
1	A	67	CYS
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	106	VAL
1	A	121	LEU
1	A	132	LYS
1	A	145	LYS
1	A	147	VAL
1	A	149	GLU
1	A	151	ASP
1	A	152	VAL
1	A	174	ILE
1	A	175	ARG
1	A	193	ASP
1	A	204	THR
1	A	208	LEU
1	A	213	HIS
1	A	215	SER
1	A	219	PHE
1	A	220	THR

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Mol	Chain	Res	Type
1	A	252	PHE
1	A	261	ASP
1	A	270	LEU
1	A	279	LEU
1	A	294	SER
1	A	307	ASP
1	A	311	GLN
1	A	315	LEU
1	A	324	SER
1	A	333	GLU
1	A	335	ARG
1	A	337	ARG
1	A	341	MET
1	A	344	ARG
1	A	368	LYS
1	A	375	THR
1	A	381	THR
1	A	383	TYR
1	A	385	ILE
1	A	386	ASP
1	A	393	ARG
1	A	398	GLU
1	A	407	ARG
1	A	423	ASP
1	A	425	GLN
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	438	ASP
1	A	443	LEU
1	A	448	PRO
1	A	451	HIS
1	A	454	SER
1	A	461	LYS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	494	SER

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Mol	Chain	Res	Type
1	A	498	ARG
1	A	500	GLU
1	A	505	CYS
1	A	517	ASN
1	A	523	ILE
1	A	527	THR
1	A	532	ARG
1	A	536	LEU
1	A	538	ASP
1	A	541	ILE
1	A	544	ASP
1	A	545	GLN
1	A	566	ILE
1	A	571	LEU
1	A	593	GLU
1	A	597	LEU
1	A	598	LEU
1	A	603	ASN
1	A	618	GLU
1	A	622	VAL
1	A	625	SER
1	A	626	ASN
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	691	LEU
1	A	702	LEU
1	A	738	LYS
1	A	740	LEU
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	774	ARG
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	811	GLN
1	A	821	ARG

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Mol	Chain	Res	Type
1	A	839	ARG
1	A	855	THR
1	A	864	ILE
1	A	867	ILE
1	A	878	ILE
1	A	886	ILE
1	A	890	ASP
1	A	904	THR
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	926	GLN
1	A	929	LEU
1	A	948	VAL
1	A	976	THR
1	A	998	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1015	VAL
1	A	1024	SER
1	A	1038	THR
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1080	THR
1	A	1100	ARG
1	A	1116	LEU
1	A	1124	HIS
1	A	1135	ARG
1	A	1141	THR
1	A	1143	LEU
1	A	1146	VAL
1	A	1173	HIS
1	A	1176	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1222	ASN
1	A	1223	ASP
1	A	1232	ASN

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Mol	Chain	Res	Type
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1270	ASN
1	A	1274	ARG
1	A	1277	GLU
1	A	1289	ARG
1	A	1291	VAL
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1301	GLU
1	A	1303	GLU
1	A	1309	ASP
1	A	1325	THR
1	A	1327	ILE
1	A	1329	THR
1	A	1336	MET
1	A	1341	ILE
1	A	1366	ARG
1	A	1376	THR
1	A	1383	SER
1	A	1392	SER
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET
1	A	1400	CYS
1	A	1405	THR
1	A	1418	LEU
1	A	1426	GLU
1	A	1432	GLN
1	A	1442	ASP
1	A	1445	ILE
1	A	1449	SER
1	A	1451	VAL
1	A	1454	MET
2	B	25	ILE
2	B	35	SER
2	B	40	GLU

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Mol	Chain	Res	Type
2	B	46	GLN
2	B	63	ILE
2	B	134	LYS
2	B	185	THR
2	B	187	SER
2	B	218	SER
2	B	240	ILE
2	B	251	ILE
2	B	252	SER
2	B	261	ARG
2	B	262	GLU
2	B	264	SER
2	B	267	ARG
2	B	272	THR
2	B	279	ASP
2	B	313	MET
2	B	324	ILE
2	B	337	ARG
2	B	339	THR
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	348	ARG
2	B	356	LEU
2	B	364	ILE
2	B	365	THR
2	B	384	ARG
2	B	393	LYS
2	B	398	ARG
2	B	401	PHE
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	429	PHE
2	B	446	LEU
2	B	453	ILE
2	B	470	LYS
2	B	475	SER
2	B	481	GLN
2	B	485	ARG
2	B	486	TYR

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Mol	Chain	Res	Type
2	B	490	SER
2	B	500	THR
2	B	531	GLN
2	B	537	LYS
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	554	ILE
2	B	570	VAL
2	B	574	SER
2	B	595	ARG
2	B	603	LEU
2	B	616	ILE
2	B	617	ARG
2	B	620	ARG
2	B	628	THR
2	B	637	LEU
2	B	644	GLU
2	B	658	ILE
2	B	678	GLU
2	B	680	THR
2	B	722	ASP
2	B	723	VAL
2	B	731	VAL
2	B	734	HIS
2	B	743	ILE
2	B	755	ILE
2	B	766	ARG
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	797	TYR
2	B	825	VAL
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	843	GLN
2	B	844	SER
2	B	857	ARG
2	B	868	MET
2	B	871	THR
2	B	878	GLN

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Mol	Chain	Res	Type
2	B	879	ARG
2	B	881	ASN
2	B	884	ARG
2	B	889	THR
2	B	933	SER
2	B	934	LYS
2	B	942	ARG
2	B	946	ASN
2	B	953	LEU
2	B	954	VAL
2	B	959	ASP
2	B	970	THR
2	B	975	GLN
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1022	THR
2	B	1045	SER
2	B	1050	ILE
2	B	1051	THR
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1112	GLN
2	B	1129	ARG
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1168	LEU
2	B	1170	THR
2	B	1175	LEU
2	B	1176	ASN
2	B	1178	ASN
2	B	1179	GLN

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Mol	Chain	Res	Type
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1202	LEU
3	C	4	GLU
3	C	7	GLN
3	C	16	ASP
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	50	GLU
3	C	52	GLU
3	C	83	SER
3	C	101	LEU
3	C	106	GLU
3	C	108	GLU
3	C	119	VAL
3	C	121	VAL
3	C	125	MET
3	C	127	ARG
3	C	133	ILE
3	C	142	VAL
3	C	148	ARG
3	C	189	THR
3	C	215	GLU
3	C	226	ASP
3	C	235	VAL
3	C	240	VAL
3	C	259	LEU
3	C	260	LEU
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	9	GLN
4	D	11	ARG
4	D	12	ARG
4	D	18	VAL
4	D	23	ASN
4	D	27	LEU
4	D	32	GLU
4	D	34	GLN

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Mol	Chain	Res	Type
4	D	35	LEU
4	D	40	HIS
4	D	41	GLN
4	D	47	LEU
4	D	52	LEU
4	D	67	ARG
4	D	119	ARG
4	D	123	LEU
4	D	126	ILE
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	155	ARG
4	D	182	SER
4	D	187	THR
4	D	197	SER
4	D	204	ASP
4	D	213	GLU
4	D	217	LEU
5	E	2	ASP
5	E	3	GLN
5	E	9	ILE
5	E	17	ARG
5	E	31	THR
5	E	45	LYS
5	E	57	MET
5	E	67	GLU
5	E	75	MET
5	E	84	ASP
5	E	92	THR
5	E	114	ASN
5	E	131	THR
5	E	152	LYS
5	E	158	SER
5	E	173	SER
5	E	175	LEU
5	E	184	VAL
5	E	190	LEU
5	E	192	ARG
6	F	72	LYS
6	F	78	GLN
6	F	79	ARG

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Mol	Chain	Res	Type
6	F	82	THR
6	F	109	VAL
6	F	110	ASP
6	F	118	LEU
6	F	127	GLU
7	G	1	MET
7	G	2	PHE
7	G	12	THR
7	G	13	LEU
7	G	22	MET
7	G	24	GLN
7	G	26	LEU
7	G	28	THR
7	G	60	ARG
7	G	64	THR
7	G	65	ASP
7	G	80	LYS
7	G	83	LYS
7	G	90	THR
7	G	96	GLN
7	G	114	LEU
7	G	133	SER
7	G	134	GLU
7	G	135	ASP
7	G	138	THR
7	G	143	ILE
7	G	152	SER
7	G	155	SER
7	G	171	ILE
8	H	26	ILE
8	H	76	THR
8	H	77	ARG
8	H	89	LEU
8	H	91	ASP
8	H	123	MET
8	H	128	ASN
8	H	130	ARG
8	H	135	LEU
9	I	8	ARG
9	I	31	THR
9	I	42	LEU
9	I	50	THR

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Mol	Chain	Res	Type
9	I	55	THR
9	I	61	ASP
9	I	74	GLU
9	I	81	ARG
9	I	83	ASN
9	I	94	ASP
9	I	120	GLN
10	J	2	ILE
10	J	3	VAL
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	19	GLU
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
10	J	56	LEU
11	K	1	MET
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	34	THR
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	79	GLU
11	K	101	LEU
11	K	107	THR
11	K	114	LEU
12	L	27	LEU
12	L	38	LEU
12	L	42	ARG
12	L	50	ASP
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	60	ARG
12	L	61	THR
12	L	64	LEU
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	118	HIS
1	A	339	ASN
1	A	390	GLN
1	A	394	ASN
1	A	425	GLN
1	A	439	ASN
1	A	445	ASN
1	A	488	ASN
1	A	603	ASN
1	A	851	HIS
1	A	1106	ASN
1	A	1270	ASN
1	A	1312	ASN
1	A	1390	ASN
1	A	1393	ASN
2	B	46	GLN
2	B	47	GLN
2	B	206	ASN
2	B	300	HIS
2	B	465	ASN
2	B	572	HIS
2	B	573	GLN
2	B	590	HIS
2	B	842	ASN
2	B	843	GLN
2	B	975	GLN
2	B	1025	HIS
2	B	1040	ASN
2	B	1084	GLN
2	B	1117	GLN
2	B	1205	GLN
3	C	242	GLN
3	C	264	GLN
4	D	37	GLN
5	E	5	ASN
5	E	8	ASN
7	G	71	ASN
7	G	102	GLN
8	H	11	GLN
9	I	46	HIS

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Mol	Chain	Res	Type
9	I	51	ASN
9	I	83	ASN
9	I	89	GLN
9	I	108	HIS
9	I	114	GLN
11	K	76	GLN
11	K	89	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	BRU	T	22	15,14	14,21,22	1.70	3 (21%)	17,30,33	3.01	4 (23%)

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	BRU	T	22	15,14	-	0/3/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	O5'-C5'	-3.32	1.40	1.44
15	T	22	BRU	C2-N3	-2.53	1.33	1.38
15	T	22	BRU	C4-C5	4.16	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	-4.19	118.62	123.64
15	T	22	BRU	C2'-C1'-N1	-2.45	108.57	114.27
15	T	22	BRU	O4'-C1'-N1	5.21	116.57	107.78
15	T	22	BRU	C4-N3-C2	9.88	123.56	115.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
16	APC	A	2455	-	28,33,33	3.39	13 (46%)	27,52,52	2.44	7 (25%)

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
16	APC	A	2455	-	-	0/15/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	2455	APC	C8-N9	-3.10	1.33	1.36
16	A	2455	APC	C8-N7	-2.72	1.29	1.34
16	A	2455	APC	C5-N7	-2.43	1.31	1.39
16	A	2455	APC	C6-N1	-2.18	1.27	1.37
16	A	2455	APC	C4-N3	-2.06	1.32	1.35
16	A	2455	APC	O3'-C3'	2.11	1.48	1.43
16	A	2455	APC	PG-O2G	4.02	1.71	1.54
16	A	2455	APC	PA-O5'	4.03	1.63	1.57
16	A	2455	APC	PG-O1G	5.10	1.67	1.50
16	A	2455	APC	PA-O1A	5.46	1.65	1.51
16	A	2455	APC	PB-O2B	5.76	1.70	1.56
16	A	2455	APC	PG-O3B	7.23	1.71	1.60
16	A	2455	APC	PB-O3B	9.87	1.69	1.58

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	2455	APC	N3-C2-N1	-8.86	121.28	128.86
16	A	2455	APC	C4-C5-N7	-4.56	105.00	109.41
16	A	2455	APC	PG-O3B-PB	-3.15	121.35	132.40
16	A	2455	APC	C5'-C4'-C3'	-2.24	106.86	115.29
16	A	2455	APC	C5-C6-N6	2.07	124.69	120.47
16	A	2455	APC	O2'-C2'-C3'	2.23	118.96	111.83
16	A	2455	APC	O3'-C3'-C2'	3.26	122.26	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2455	APC	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.45
1	B	351:TYR	C	352:ALA	N	3.24

## 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	1425/1732 (82%)	-0.26	11 (0%) 86 80	58, 110, 173, 226	0
2	B	1115/1224 (91%)	-0.19	6 (0%) 90 87	69, 123, 181, 210	0
3	C	266/318 (83%)	-0.34	0 100 100	81, 110, 148, 178	0
4	D	178/221 (80%)	-0.20	1 (0%) 89 85	85, 121, 175, 193	0
5	E	214/215 (99%)	-0.21	0 100 100	91, 148, 190, 200	0
6	F	84/155 (54%)	-0.51	0 100 100	68, 92, 125, 138	0
7	G	171/171 (100%)	-0.20	0 100 100	82, 109, 145, 167	0
8	H	133/146 (91%)	0.17	1 (0%) 86 80	121, 153, 184, 218	0
9	I	119/122 (97%)	-0.13	3 (2%) 57 50	120, 158, 195, 213	0
10	J	65/70 (92%)	-0.31	0 100 100	90, 106, 145, 161	0
11	K	115/120 (95%)	-0.42	0 100 100	79, 110, 141, 156	0
12	L	46/70 (65%)	-0.02	2 (4%) 35 30	100, 180, 195, 199	0
13	N	11/14 (78%)	-0.39	0 100 100	181, 210, 266, 271	0
14	P	6/6 (100%)	-0.20	0 100 100	91, 95, 119, 147	0
15	T	19/26 (73%)	-0.34	0 100 100	84, 141, 264, 267	0
All	All	3967/4610 (86%)	-0.23	24 (0%) 89 85	58, 117, 182, 271	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	ARG	3.8
1	A	1176	LEU	3.7
2	B	340	ALA	3.6
8	H	139	ASN	3.6
2	B	509	ALA	3.2
9	I	119	THR	3.0
1	A	155	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	256	GLN	2.9
1	A	1092	LYS	2.8
12	L	27	LEU	2.7
9	I	118	ARG	2.7
2	B	918	ILE	2.5
2	B	708	GLU	2.4
2	B	250	PHE	2.4
1	A	164	ARG	2.4
1	A	251	SER	2.4
1	A	192	GLY	2.4
4	D	13	ARG	2.3
1	A	1455	PRO	2.3
9	I	117	LYS	2.2
1	A	194	ALA	2.2
12	L	26	THR	2.1
2	B	339	THR	2.0
1	A	191	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	BRU	T	22	20/21	0.95	0.16	86,97,107,113	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	APC	A	2455	31/31	0.88	0.24	112,115,143,144	0
17	ZN	L	1071	1/1	0.95	0.06	211,211,211,211	0
17	ZN	I	1122	1/1	0.97	0.05	201,201,201,201	0
18	MG	A	2458	1/1	0.98	0.16	86,86,86,86	0
17	ZN	A	2456	1/1	0.99	0.07	138,138,138,138	0
17	ZN	C	1269	1/1	0.99	0.12	93,93,93,93	0
17	ZN	I	1121	1/1	0.99	0.13	134,134,134,134	0
17	ZN	B	2225	1/1	0.99	0.21	81,81,81,81	0
17	ZN	J	1066	1/1	1.00	0.23	95,95,95,95	0
17	ZN	A	2457	1/1	1.00	0.15	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.