



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:42 PM GMT

PDB ID : 4A3B  
Title : RNA POLYMERASE II INITIAL TRANSCRIBING COMPLEX WITH A  
4NT DNA-RNA HYBRID  
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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

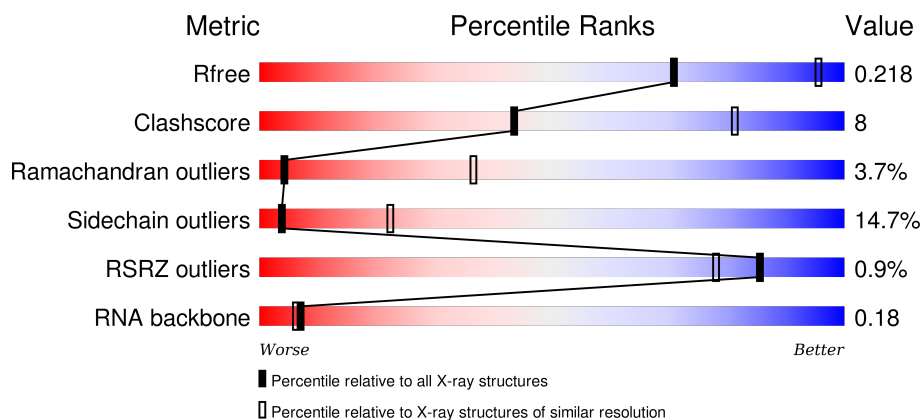
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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>58%</div> <div>20%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>26%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div>57%</div> <div>22%</div> <div>•</div> <div>16%</div> </div> </div>
4	D	221	<div> <div></div> <div> <div>54%</div> <div>22%</div> <div>• •</div> <div>19%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	215	<p>70% 27% 3% 2%</p>
6	F	155	<p>33% 19% 46% 2%</p>
7	G	171	<p>68% 26% 5% 1%</p>
8	H	146	<p>61% 23% 5% 9% 2%</p>
9	I	122	<p>75% 20% 5% 2%</p>
10	J	70	<p>61% 23% 7% 7%</p>
11	K	120	<p>68% 24% 8%</p>
12	L	70	<p>34% 19% 13% 34% 4%</p>
13	N	14	<p>14% 14% 71%</p>
14	P	4	<p>50% 50%</p>
15	T	26	<p>31% 12% 54% 3%</p>

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31612 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	1422	Total	C	N	O	S	0	0	0
			11174	7037	1954	2121	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	4	Total	C	N	O	P	0	0	0
			84	40	17	23	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	4	Total	C	N	O	P	0	0	0
			90	40	20	26	4			

- Molecule 15 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	12	Total	Br	C	N	O	P	0	0
			242	1	116	36	77	12		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

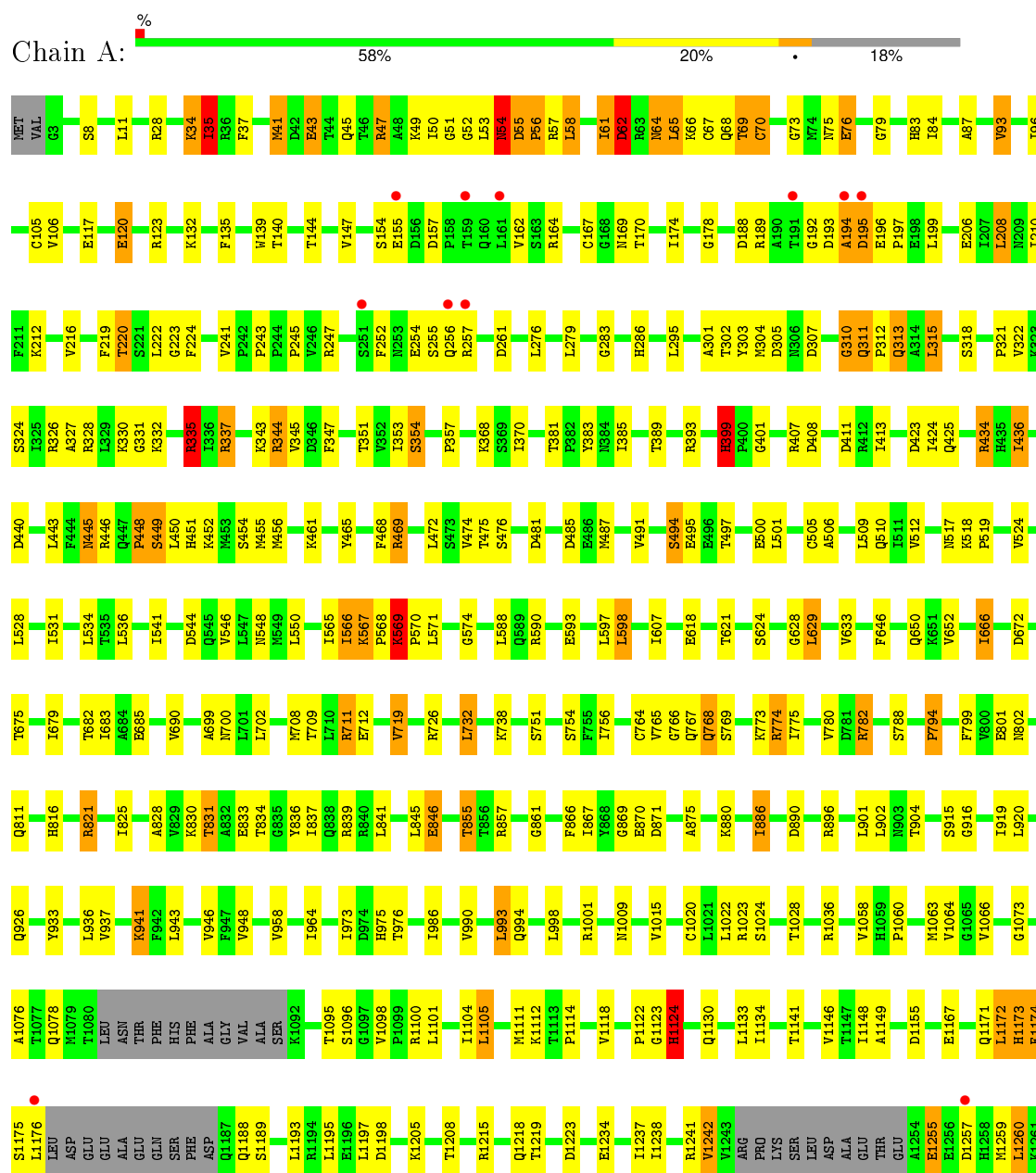
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

### 3 Residue-property plots

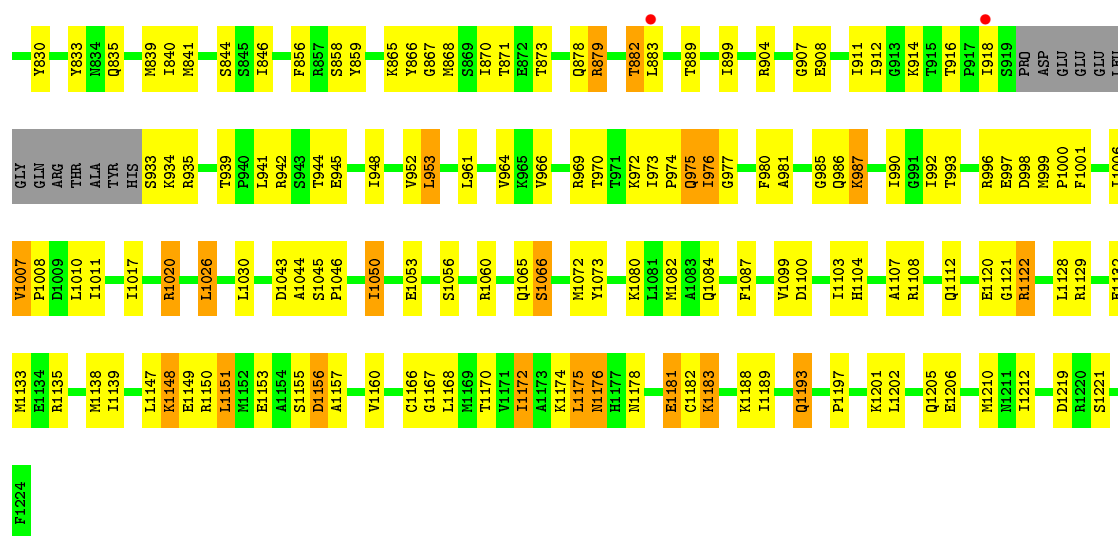
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

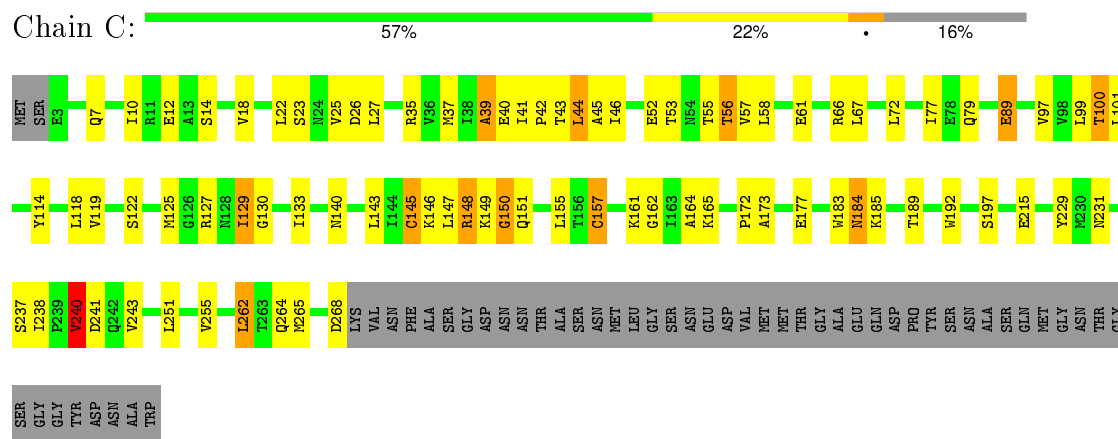




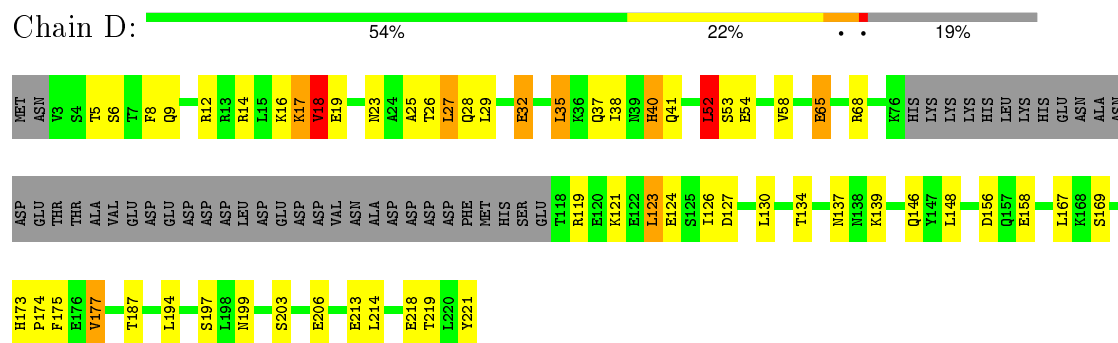




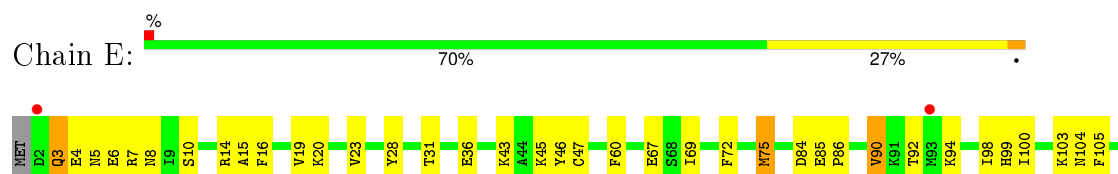
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

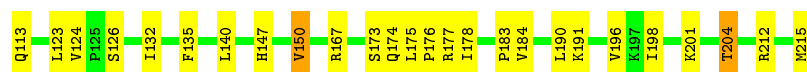


• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



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





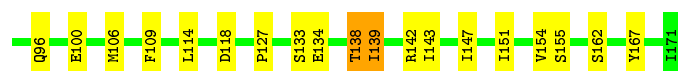
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 33% 19% • 46%



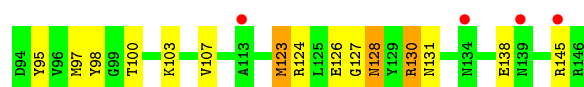
- Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 68% 26% 5%



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

Chain H: 3% 61% 23% 5% • 9%



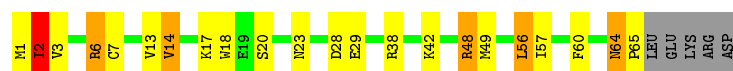
- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I: 2% 75% 20% • •



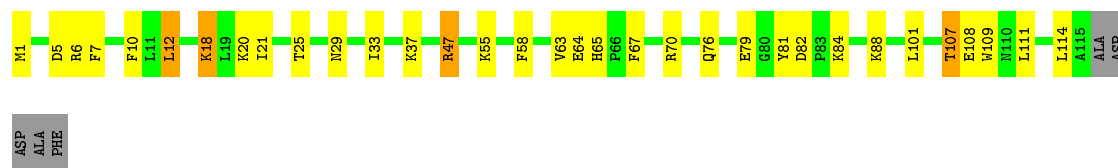
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J: 61% 23% 7% • 7%




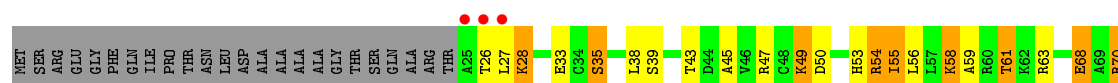
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:  68% 24% . .



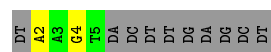
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:  4% 34% 19% 13% 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:  14% 14% 71%




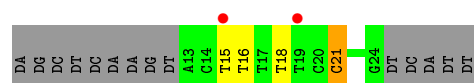
- Molecule 14: TRANSCRIPT RNA 5'-R(\*AP\*GP\*GP\*A)-3'

Chain P:  50% 50%



- Molecule 15: TEMPLATE DNA

Chain T:  8% 31% 12% 54%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.09 Å   392.97 Å   281.84 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.89 – 3.50 48.89 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.89-3.50) 98.9 (48.89-3.50)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 3.48 Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.166 , 0.197 0.191 , 0.218	Depositor DCC
$R_{free}$ test set	3021 reflections (2.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	112.6	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 100.2	EDS
Estimated twinning fraction	0.025 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 152634 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	31612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0/11374	0.84	12/15383 (0.1%)
2	B	0.52	0/9029	0.80	1/12171 (0.0%)
3	C	0.49	0/2133	0.79	1/2891 (0.0%)
4	D	0.52	0/1444	0.84	2/1935 (0.1%)
5	E	0.48	0/1788	0.74	0/2406
6	F	0.61	0/691	0.82	0/933
7	G	0.50	0/1368	0.78	0/1844
8	H	0.52	0/1086	0.80	0/1470
9	I	0.46	0/989	0.77	0/1331
10	J	0.54	0/541	0.83	0/727
11	K	0.50	0/938	0.72	0/1267
12	L	0.56	0/365	1.06	1/485 (0.2%)
13	N	1.22	0/94	0.97	0/143
14	P	1.08	0/101	0.78	0/156
15	T	1.42	2/245 (0.8%)	1.14	0/373
All	All	0.54	2/32186 (0.0%)	0.82	17/43515 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	15	DT	C1'-N1	5.44	1.56	1.49
15	T	21	DC	C1'-N1	5.12	1.55	1.49

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	LYS	C-N-CA	7.41	140.22	121.70
1	A	399	HIS	N-CA-CB	6.52	122.34	110.60
1	A	56	PRO	C-N-CA	5.87	136.38	121.70
1	A	194	ALA	C-N-CA	5.67	135.87	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	338	GLY	C-N-CA	5.54	135.56	121.70
1	A	34	LYS	N-CA-C	-5.50	96.16	111.00
1	A	54	ASN	C-N-CA	5.47	135.39	121.70
1	A	311	GLN	N-CA-C	5.47	125.77	111.00
1	A	310	GLY	C-N-CA	5.41	135.21	121.70
4	D	26	THR	N-CA-C	-5.32	96.64	111.00
1	A	55	ASP	N-CA-CB	5.18	119.92	110.60
12	L	49	LYS	C-N-CA	5.09	134.43	121.70
1	A	35	ILE	N-CA-CB	5.08	122.47	110.80
3	C	39	ALA	N-CA-C	5.04	124.61	111.00
1	A	68	GLN	C-N-CA	5.03	134.26	121.70
4	D	25	ALA	C-N-CA	5.02	134.25	121.70
1	A	69	THR	N-CA-CB	5.00	119.80	110.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	11233	186	0
2	B	8859	0	8901	171	0
3	C	2095	0	2051	45	0
4	D	1434	0	1460	22	0
5	E	1752	0	1776	27	0
6	F	679	0	701	23	0
7	G	1340	0	1357	29	0
8	H	1068	0	1040	19	0
9	I	971	0	927	13	0
10	J	532	0	542	14	0
11	K	920	0	929	14	0
12	L	363	0	386	9	0
13	N	84	0	46	3	0
14	P	90	0	45	1	0
15	T	242	0	136	3	0
16	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31612	0	31530	509	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 8.

All (509) 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	1.75	1.56
1:A:53:LEU:HD23	1:A:54:ASN:H	1.27	0.98
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.46	0.97
6:F:90:ARG:HG3	6:F:90:ARG:HH11	1.31	0.94
1:A:855:THR:HG21	1:A:857:ARG:HE	1.32	0.94
10:J:48:ARG:HE	10:J:49:MET:HE2	1.33	0.92
1:A:35:ILE:HG21	1:A:241:VAL:HG21	1.46	0.92
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.55	0.88
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.40	0.85
12:L:28:LYS:HB2	12:L:39:SER:HA	1.58	0.83
3:C:56:THR:HG21	3:C:145:CYS:SG	2.19	0.82
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.61	0.82
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.61	0.82
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.61	0.81
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.65	0.79
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.48	0.79
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.63	0.79
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.63	0.79
8:H:47:PHE:HB3	8:H:95:TYR:HD2	1.49	0.78
3:C:46:ILE:H	3:C:46:ILE:HD12	1.47	0.78
2:B:1172:ILE:HD11	2:B:1183:LYS:HE2	1.65	0.77
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.67	0.76
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.22	0.75
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.67	0.75
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.68	0.75
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.70	0.74
1:A:53:LEU:HD23	1:A:54:ASN:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.72	0.71
1:A:855:THR:CG2	1:A:857:ARG:HE	2.04	0.71
3:C:46:ILE:HD13	3:C:67:LEU:O	1.91	0.71
1:A:216:VAL:O	1:A:220:THR:HB	1.91	0.70
2:B:705:MET:H	2:B:710:LEU:HD12	1.56	0.70
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.73	0.70
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.74	0.70
2:B:168:GLY:H	2:B:450:ALA:HB1	1.57	0.70
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.32	0.69
3:C:66:ARG:NH2	10:J:3:VAL:O	2.25	0.68
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.76	0.68
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.74	0.67
3:C:43:THR:HG22	3:C:44:LEU:H	1.60	0.67
1:A:64:ASN:O	1:A:65:LEU:HB3	1.93	0.67
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.75	0.66
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.75	0.66
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.78	0.66
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.78	0.65
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.77	0.65
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.78	0.65
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.97	0.65
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.80	0.64
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.79	0.64
4:D:40:HIS:HA	7:G:73:LYS:HE3	1.80	0.64
3:C:56:THR:HG23	3:C:147:LEU:HD23	1.78	0.64
2:B:126:SER:CB	2:B:172:ILE:HD11	2.28	0.64
1:A:646:PHE:O	1:A:650:GLN:HG2	1.97	0.64
1:A:49:LYS:HD3	1:A:61:ILE:HG13	1.80	0.64
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.79	0.63
9:I:50:THR:HG22	9:I:52:ILE:H	1.63	0.63
8:H:82:PRO:C	8:H:84:ALA:H	2.02	0.63
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.29	0.63
1:A:857:ARG:HD3	1:A:861:GLY:O	1.99	0.62
2:B:70:ILE:HD13	2:B:429:PHE:HZ	1.64	0.62
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.80	0.62
1:A:1387:HIS:CE1	13:N:4:DG:H4'	2.34	0.62
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.33	0.62
7:G:1:MET:SD	7:G:2:PHE:N	2.68	0.62
1:A:53:LEU:CD2	1:A:54:ASN:H	2.09	0.61
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.64	0.61
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:918:ILE:HD13	2:B:935:ARG:HH12	1.65	0.61
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.82	0.61
2:B:247:GLY:H	2:B:418:LYS:NZ	1.99	0.60
1:A:869:GLY:O	5:E:204:THR:HG21	2.02	0.60
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.83	0.60
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.83	0.60
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.82	0.60
2:B:826:ALA:HB2	2:B:1087:PHE:CD1	2.37	0.60
6:F:94:LEU:HD21	6:F:125:LEU:HD22	1.84	0.60
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.84	0.59
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.83	0.59
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.84	0.59
4:D:32:GLU:HG3	7:G:5:LYS:NZ	2.18	0.59
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.68	0.59
2:B:882:THR:HG1	2:B:935:ARG:N	1.99	0.59
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.67	0.59
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.36	0.59
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.84	0.59
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.84	0.59
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.83	0.59
7:G:1:MET:CE	7:G:80:LYS:O	2.51	0.58
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.67	0.58
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.02	0.58
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.86	0.58
11:K:82:ASP:OD2	11:K:84:LYS:HB2	2.04	0.58
1:A:565:ILE:O	1:A:570:PRO:HA	2.04	0.58
2:B:1168:LEU:HB2	2:B:1170:THR:OG1	2.04	0.58
8:H:127:GLY:N	8:H:130:ARG:HH21	2.01	0.58
1:A:310:GLY:O	1:A:312:PRO:HD2	2.04	0.57
1:A:446:ARG:HB2	1:A:487:MET:SD	2.44	0.57
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.51	0.57
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.87	0.57
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.85	0.57
1:A:75:ASN:O	1:A:76:GLU:HB2	2.05	0.57
6:F:90:ARG:CG	6:F:90:ARG:HH11	2.07	0.57
7:G:1:MET:HE1	7:G:80:LYS:O	2.05	0.57
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.87	0.57
1:A:567:LYS:HA	1:A:569:LYS:N	2.20	0.57
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.05	0.57
1:A:709:THR:HB	1:A:712:GLU:H	1.70	0.56
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:VAL:HG22	8:H:26:ILE:HD11	1.88	0.56
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.88	0.56
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.87	0.56
1:A:933:TYR:HA	1:A:936:LEU:HD12	1.88	0.56
4:D:32:GLU:HG3	7:G:5:LYS:HZ1	1.70	0.56
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.88	0.56
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.88	0.55
1:A:120:GLU:HA	1:A:123:ARG:HG2	1.88	0.55
9:I:4:PHE:HE2	9:I:13:MET:HB2	1.71	0.55
1:A:61:ILE:HG22	1:A:62:ASP:H	1.70	0.55
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.87	0.55
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.88	0.55
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.88	0.55
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.89	0.55
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.72	0.55
2:B:425:THR:HA	2:B:428:ILE:HD12	1.88	0.55
2:B:247:GLY:H	2:B:418:LYS:HZ1	1.53	0.55
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.88	0.55
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.72	0.54
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.88	0.54
2:B:662:MET:HA	2:B:665:GLU:HB2	1.89	0.54
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.89	0.54
3:C:149:LYS:HG3	3:C:150:GLY:H	1.72	0.54
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.89	0.54
6:F:90:ARG:NH1	6:F:90:ARG:HG3	2.09	0.54
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.37	0.54
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.05	0.54
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.89	0.54
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.90	0.54
2:B:1166:CYS:O	2:B:1168:LEU:N	2.41	0.54
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.90	0.54
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.89	0.54
14:P:8:G:H1	15:T:21:DC:H42	1.56	0.54
6:F:90:ARG:NH1	6:F:90:ARG:CG	2.69	0.53
1:A:34:LYS:HB2	1:A:83:HIS:CE1	2.43	0.53
3:C:100:THR:HG22	3:C:119:VAL:HG13	1.89	0.53
1:A:494:SER:HB3	1:A:497:THR:H	1.74	0.53
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.74	0.53
3:C:66:ARG:NH2	10:J:2:ILE:HG23	2.23	0.53
1:A:933:TYR:O	1:A:937:VAL:HG23	2.09	0.53
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:GLU:HG3	6:F:98:ALA:HB1	1.89	0.53
2:B:846:ILE:HG23	2:B:974:PRO:HD2	1.90	0.53
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.89	0.53
7:G:34:VAL:O	7:G:37:SER:HB3	2.08	0.53
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.91	0.53
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.44	0.53
1:A:1451:VAL:HG23	7:G:20:PRO:HB3	1.92	0.52
5:E:176:PRO:O	5:E:212:ARG:HA	2.09	0.52
2:B:34:ILE:HG12	2:B:542:MET:CE	2.40	0.52
1:A:55:ASP:N	1:A:56:PRO:HD3	2.23	0.52
1:A:1445:ILE:HG23	6:F:132:LEU:HD23	1.91	0.52
10:J:65:PRO:HB3	12:L:35:SER:OG	2.10	0.52
1:A:568:PRO:HG2	8:H:46:LEU:HD12	1.91	0.52
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.92	0.52
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.91	0.52
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.92	0.52
2:B:599:THR:O	2:B:603:LEU:HD12	2.10	0.52
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.92	0.52
8:H:63:LEU:C	8:H:90:ALA:HB3	2.30	0.52
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.90	0.51
1:A:315:LEU:HA	1:A:321:PRO:HA	1.93	0.51
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.92	0.51
3:C:173:ALA:HB2	3:C:243:VAL:HG11	1.91	0.51
1:A:528:LEU:HD23	1:A:751:SER:HA	1.91	0.51
8:H:89:LEU:C	8:H:91:ASP:H	2.13	0.51
2:B:68:THR:HG23	2:B:91:SER:HB3	1.91	0.51
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.92	0.51
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.91	0.51
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.45	0.51
2:B:246:LYS:HG2	2:B:249:ARG:HH21	1.76	0.51
1:A:629:LEU:O	1:A:633:VAL:HG23	2.10	0.51
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.93	0.51
2:B:841:MET:O	2:B:993:THR:HA	2.10	0.51
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.76	0.51
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	1.91	0.51
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.93	0.51
1:A:208:LEU:HD22	1:A:212:LYS:HE3	1.93	0.51
1:A:135:PHE:HD2	1:A:223:GLY:H	1.58	0.51
3:C:46:ILE:H	3:C:46:ILE:CD1	2.16	0.51
1:A:867:ILE:CD1	1:A:867:ILE:CB	2.80	0.50
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:MET:HA	3:C:41:ILE:HD12	1.94	0.50
2:B:313:MET:HG2	2:B:386:LEU:HD22	1.92	0.50
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.46	0.50
4:D:123:LEU:HD21	4:D:146:GLN:HG2	1.92	0.50
3:C:14:SER:O	3:C:240:VAL:HG21	2.11	0.50
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.94	0.50
2:B:976:ILE:HG13	2:B:990:ILE:HG22	1.93	0.50
1:A:353:ILE:HG12	1:A:487:MET:HG3	1.92	0.50
1:A:370:ILE:HD11	2:B:1103:ILE:HG13	1.94	0.50
2:B:792:MET:HA	2:B:856:PHE:O	2.12	0.50
5:E:72:PHE:HB2	5:E:75:MET:HB2	1.93	0.50
1:A:506:ALA:H	1:A:509:LEU:HD12	1.77	0.50
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	1.94	0.49
2:B:839:MET:HE2	2:B:980:PHE:HB2	1.94	0.49
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.47	0.49
2:B:911:ILE:HG23	2:B:966:VAL:HG11	1.93	0.49
8:H:36:CYS:HA	8:H:126:GLU:O	2.12	0.49
2:B:210:LYS:NZ	2:B:462:ALA:O	2.46	0.49
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.94	0.49
2:B:1043:ASP:O	2:B:1050:ILE:HD13	2.12	0.49
1:A:846:GLU:HA	1:A:1066:VAL:HG22	1.95	0.49
2:B:487:THR:HG23	2:B:490:SER:H	1.78	0.49
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	1.95	0.49
1:A:327:ALA:HA	1:A:330:LYS:HE3	1.95	0.49
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.94	0.49
2:B:128:LEU:HB2	2:B:167:ILE:O	2.12	0.49
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.95	0.49
5:E:10:SER:O	5:E:14:ARG:HG3	2.13	0.49
3:C:99:LEU:HB3	3:C:118:LEU:HD22	1.94	0.49
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.94	0.49
2:B:824:ILE:HG22	2:B:1008:PRO:HA	1.94	0.49
5:E:15:ALA:O	5:E:19:VAL:HG23	2.12	0.49
8:H:100:THR:HG23	8:H:138:GLU:HA	1.94	0.49
1:A:765:VAL:HG23	1:A:802:ASN:O	2.13	0.49
1:A:448:PRO:O	1:A:449:SER:HB2	2.13	0.49
2:B:416:LEU:HD11	2:B:460:ALA:HB1	1.93	0.49
1:A:1325:THR:HA	5:E:147:HIS:HA	1.94	0.48
3:C:165:LYS:O	11:K:6:ARG:NH1	2.46	0.48
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.94	0.48
1:A:1444:MET:HE1	6:F:135:ARG:HE	1.78	0.48
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:NE	2.15	0.48
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.94	0.48
2:B:311:LEU:HA	2:B:314:LEU:HD12	1.96	0.48
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.95	0.48
7:G:90:THR:HG22	7:G:142:ARG:HG2	1.94	0.48
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.48	0.48
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.95	0.48
1:A:56:PRO:CD	1:A:58:LEU:HG	2.44	0.48
1:A:518:LYS:HE2	1:A:624:SER:O	2.13	0.48
1:A:337:ARG:HD2	2:B:1132:GLU:OE1	2.14	0.48
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.47	0.48
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.60	0.48
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.49	0.48
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.44	0.48
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.96	0.48
6:F:72:LYS:HE3	6:F:142:SER:OG	2.14	0.48
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.95	0.48
1:A:866:PHE:O	1:A:867:ILE:HD12	2.14	0.47
5:E:43:LYS:O	5:E:47:CYS:HB2	2.14	0.47
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.96	0.47
2:B:839:MET:CE	2:B:980:PHE:HB2	2.44	0.47
6:F:93:ILE:HG12	6:F:148:VAL:HG11	1.95	0.47
2:B:446:LEU:HD12	2:B:448:ILE:HD11	1.96	0.47
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.95	0.47
7:G:138:THR:HG22	7:G:139:ILE:H	1.78	0.47
4:D:65:GLU:HA	4:D:68:ARG:HG3	1.96	0.47
2:B:563:MET:HG3	2:B:580:VAL:HG21	1.96	0.47
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.96	0.47
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.96	0.47
1:A:1189:SER:HB3	1:A:1242:VAL:H	1.79	0.47
2:B:953:LEU:HD11	12:L:55:ILE:HG22	1.97	0.47
4:D:27:LEU:HD23	4:D:197:SER:CB	2.45	0.47
2:B:310:MET:O	2:B:313:MET:HB3	2.15	0.47
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.62	0.47
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.95	0.47
1:A:567:LYS:HA	1:A:568:PRO:C	2.35	0.47
1:A:679:ILE:HG13	1:A:732:LEU:HD13	1.95	0.47
2:B:766:ARG:HH21	2:B:1020:ARG:HG2	1.78	0.47
1:A:70:CYS:SG	1:A:70:CYS:O	2.72	0.47
1:A:206:GLU:O	1:A:210:ILE:HG12	2.14	0.47
1:A:41:MET:CB	1:A:49:LYS:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:HA	1:A:50:ILE:H	1.80	0.46
2:B:283:VAL:HG13	2:B:297:ILE:HD13	1.96	0.46
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.97	0.46
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.96	0.46
1:A:719:VAL:HG23	1:A:774:ARG:HD2	1.97	0.46
2:B:778:MET:O	2:B:819:ALA:HA	2.15	0.46
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.97	0.46
1:A:886:ILE:HG12	1:A:943:LEU:HB3	1.97	0.46
3:C:66:ARG:HH21	10:J:2:ILE:HG23	1.80	0.46
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.51	0.46
1:A:709:THR:HG22	1:A:711:ARG:H	1.80	0.46
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.98	0.46
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.49	0.46
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.15	0.46
2:B:64:CYS:HA	2:B:67:SER:HB3	1.96	0.46
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	2.45	0.46
1:A:534:LEU:O	1:A:574:GLY:HA3	2.15	0.46
2:B:70:ILE:HD13	2:B:429:PHE:CZ	2.47	0.46
2:B:916:THR:O	2:B:935:ARG:N	2.48	0.46
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.97	0.46
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.98	0.46
1:A:1387:HIS:HE1	13:N:4:DG:H4'	1.78	0.46
1:A:313:GLN:O	1:A:315:LEU:HG	2.16	0.46
1:A:1172:LEU:C	1:A:1174:PHE:H	2.18	0.46
2:B:485:ARG:NH1	2:B:491:THR:HG21	2.30	0.46
4:D:8:PHE:HB2	4:D:38:ILE:HB	1.98	0.46
11:K:65:HIS:HE1	11:K:67:PHE:CD1	2.34	0.46
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.97	0.46
2:B:102:VAL:HG13	2:B:112:LEU:HD22	1.98	0.45
11:K:107:THR:O	11:K:111:LEU:HG	2.16	0.45
1:A:833:GLU:O	1:A:837:ILE:HD13	2.15	0.45
2:B:622:LYS:HE3	9:I:59:VAL:HG22	1.97	0.45
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.49	0.45
6:F:101:ILE:HG12	6:F:107:VAL:HG22	1.99	0.45
3:C:251:LEU:O	3:C:255:VAL:HG23	2.16	0.45
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.52	0.45
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.51	0.45
4:D:35:LEU:HD11	4:D:174:PRO:HD2	1.98	0.45
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.97	0.45
2:B:343:ILE:HD13	2:B:344:LYS:H	1.81	0.45
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ILE:HG23	2:B:418:LYS:HG3	1.99	0.45
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.52	0.45
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.65	0.45
2:B:1221:SER:HB3	4:D:12:ARG:HD2	1.98	0.45
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.99	0.45
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.98	0.45
3:C:148:ARG:HG3	3:C:149:LYS:H	1.82	0.44
2:B:338:GLY:HA3	2:B:340:ALA:H	1.82	0.44
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.99	0.44
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.48	0.44
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.99	0.44
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.98	0.44
3:C:184:ASN:HD21	3:C:189:THR:H	1.64	0.44
7:G:27:LYS:HD3	7:G:51:TYR:CE1	2.52	0.44
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.00	0.44
1:A:836:TYR:HB2	15:T:18:DT:H4'	2.00	0.44
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.81	0.44
3:C:89:GLU:HG2	3:C:89:GLU:O	2.18	0.44
1:A:1400:CYS:HB2	1:A:1405:THR:HA	1.99	0.44
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.57	0.44
3:C:148:ARG:HH11	3:C:149:LYS:HE2	1.82	0.44
1:A:588:LEU:HD23	1:A:607:ILE:HD12	2.00	0.44
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.00	0.44
12:L:33:GLU:OE1	12:L:55:ILE:HD11	2.18	0.44
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.98	0.44
2:B:1174:LYS:O	2:B:1176:ASN:N	2.50	0.44
1:A:828:ALA:O	1:A:831:THR:HG22	2.18	0.44
6:F:118:LEU:O	6:F:122:MET:HG3	2.18	0.44
1:A:343:LYS:HD3	2:B:1156:ASP:HB2	2.00	0.44
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.53	0.44
6:F:111:LEU:H	6:F:111:LEU:HD12	1.81	0.44
1:A:399:HIS:O	1:A:401:GLY:N	2.50	0.44
7:G:31:LEU:HD11	7:G:51:TYR:CE2	2.53	0.44
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.52	0.44
2:B:564:GLU:HB2	2:B:589:VAL:HG23	2.00	0.44
2:B:865:LYS:HB2	2:B:961:LEU:HD21	1.98	0.44
1:A:51:GLY:C	1:A:56:PRO:HB3	2.38	0.44
5:E:90:VAL:HG23	5:E:123:LEU:HD11	2.00	0.44
10:J:6:ARG:H	10:J:14:VAL:H	1.64	0.44
1:A:443:LEU:HD23	1:A:501:LEU:HD22	1.99	0.44
1:A:50:ILE:HG22	1:A:52:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:ILE:O	1:A:990:VAL:HG23	2.17	0.44
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.99	0.44
2:B:405:ARG:HB3	2:B:631:GLY:HA3	1.99	0.44
2:B:343:ILE:O	2:B:344:LYS:HB2	2.18	0.44
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.53	0.44
1:A:354:SER:O	1:A:469:ARG:HA	2.17	0.44
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.53	0.44
4:D:52:LEU:HB2	4:D:148:LEU:HD23	1.99	0.44
13:N:2:DA:H61	15:T:16:DT:H3	1.65	0.43
2:B:351:TYR:O	2:B:352:ALA:HA	2.18	0.43
2:B:952:VAL:HB	12:L:58:LYS:HB2	2.00	0.43
3:C:147:LEU:HB3	3:C:151:GLN:HB2	2.00	0.43
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.00	0.43
2:B:981:ALA:HB2	2:B:987:LYS:HA	2.00	0.43
1:A:310:GLY:C	1:A:312:PRO:HD2	2.38	0.43
1:A:528:LEU:O	1:A:531:ILE:HG22	2.18	0.43
11:K:7:PHE:HA	11:K:10:PHE:CZ	2.54	0.43
2:B:234:ILE:HG12	2:B:257:LYS:HB3	2.00	0.43
2:B:364:ILE:HA	2:B:585:VAL:HG13	2.00	0.43
5:E:86:PRO:HA	5:E:113:GLN:HB2	2.00	0.43
1:A:780:VAL:O	1:A:782:ARG:HD3	2.18	0.43
2:B:822:ASN:O	10:J:48:ARG:NH1	2.52	0.43
4:D:121:LYS:HA	4:D:124:GLU:HG2	2.00	0.43
2:B:449:ASN:HD22	2:B:452:THR:HG23	1.84	0.43
9:I:102:VAL:HG22	9:I:109:ILE:HG13	2.00	0.43
2:B:70:ILE:H	2:B:70:ILE:HD12	1.84	0.43
2:B:114:PRO:HG3	2:B:181:LEU:HD11	2.00	0.43
7:G:26:LEU:HD13	7:G:56:ILE:HD11	2.00	0.43
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	2.18	0.43
1:A:194:ALA:HA	1:A:195:ASP:C	2.39	0.43
3:C:183:TRP:O	3:C:185:LYS:N	2.49	0.43
1:A:62:ASP:HB3	1:A:64:ASN:O	2.18	0.43
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.66	0.43
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.82	0.43
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.18	0.43
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.34	0.43
7:G:19:GLY:O	7:G:22:MET:HB2	2.19	0.43
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.00	0.43
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.50	0.43
1:A:50:ILE:HG22	1:A:52:GLY:H	1.84	0.43
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:HB3	1:A:162:VAL:HG23	2.01	0.42
2:B:773:MET:CE	2:B:985:GLY:HA2	2.49	0.42
2:B:1181:GLU:HG2	2:B:1182:CYS:N	2.34	0.42
1:A:841:LEU:O	1:A:845:LEU:HG	2.19	0.42
2:B:780:VAL:HG21	10:J:56:LEU:HD22	2.01	0.42
4:D:167:LEU:HB3	4:D:177:VAL:HG22	2.01	0.42
2:B:745:PRO:O	2:B:748:ILE:HG12	2.18	0.42
2:B:46:GLN:HG3	2:B:46:GLN:H	1.50	0.42
1:A:708:MET:HG2	1:A:712:GLU:HB3	2.02	0.42
2:B:69:LEU:HD11	2:B:425:THR:HG23	2.00	0.42
2:B:766:ARG:NH2	2:B:1020:ARG:HG2	2.33	0.42
2:B:710:LEU:HA	2:B:733:HIS:HB3	2.02	0.42
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.19	0.42
11:K:12:LEU:HD11	11:K:18:LYS:HG2	2.00	0.42
7:G:127:PRO:HB2	7:G:139:ILE:HD13	2.02	0.42
5:E:3:GLN:HE21	5:E:5:ASN:HB2	1.84	0.42
2:B:20:ASP:C	2:B:22:SER:H	2.23	0.42
3:C:56:THR:HG22	3:C:57:VAL:HG22	2.01	0.42
7:G:62:LEU:HA	7:G:63:PRO:HD2	1.81	0.42
2:B:806:THR:HG22	2:B:808:ALA:H	1.84	0.42
2:B:638:PHE:CD1	2:B:653:VAL:HG21	2.55	0.42
4:D:17:LYS:H	4:D:17:LYS:HG3	1.68	0.42
1:A:304:MET:HG2	2:B:1210:MET:HG2	2.02	0.42
6:F:79:ARG:HB2	6:F:79:ARG:HH11	1.83	0.42
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.50	0.42
1:A:700:ASN:HB3	9:I:115:LYS:HB2	2.02	0.42
2:B:284:ILE:HG12	2:B:324:ILE:HD13	2.01	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.02	0.42
3:C:262:LEU:HD22	11:K:88:LYS:HE3	2.01	0.42
2:B:365:THR:HG21	2:B:370:PHE:CD2	2.55	0.42
2:B:1219:ASP:OD1	4:D:14:ARG:NH2	2.53	0.42
1:A:56:PRO:HD3	1:A:58:LEU:HG	2.01	0.42
2:B:542:MET:HG2	2:B:747:MET:HE3	2.02	0.42
4:D:54:GLU:O	4:D:58:VAL:HG23	2.19	0.42
1:A:546:VAL:O	1:A:550:LEU:HG	2.20	0.42
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.54	0.42
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.02	0.42
2:B:558:LEU:HD23	2:B:596:LEU:HD11	2.01	0.42
1:A:64:ASN:O	1:A:65:LEU:CB	2.64	0.41
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.20	0.41
1:A:512:VAL:HA	1:A:519:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:GLN:CG	1:A:816:HIS:HA	2.42	0.41
2:B:705:MET:N	2:B:710:LEU:HD12	2.30	0.41
8:H:82:PRO:O	8:H:84:ALA:N	2.49	0.41
2:B:424:LEU:O	2:B:428:ILE:HG13	2.20	0.41
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.53	0.41
1:A:456:MET:HG2	1:A:510:GLN:HG3	2.02	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.55	0.41
7:G:100:GLU:HG3	7:G:109:PHE:HB2	2.02	0.41
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.02	0.41
7:G:9:LEU:HD22	7:G:34:VAL:HG23	2.02	0.41
2:B:90:ILE:HA	2:B:133:LYS:O	2.20	0.41
1:A:946:VAL:HG22	5:E:201:LYS:HD2	2.01	0.41
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.56	0.41
1:A:1426:GLU:HG2	1:A:1426:GLU:H	1.62	0.41
1:A:675:THR:HG23	1:A:732:LEU:HD22	2.02	0.41
1:A:598:LEU:HG	8:H:124:ARG:HB2	2.03	0.41
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.53	0.41
1:A:767:GLN:HA	1:A:799:PHE:HA	2.01	0.41
7:G:8:SER:HB2	7:G:71:ASN:HD21	1.86	0.41
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.79	0.41
2:B:406:LEU:HD12	2:B:545:ILE:HD11	2.01	0.41
2:B:112:LEU:HD21	2:B:117:ALA:HB2	2.03	0.41
5:E:3:GLN:NE2	5:E:5:ASN:HB2	2.35	0.41
4:D:127:ASP:HA	4:D:130:LEU:HD12	2.03	0.41
1:A:1105:LEU:HB3	1:A:1384:VAL:HB	2.02	0.41
2:B:115:GLN:O	2:B:119:LEU:HD12	2.20	0.41
4:D:23:ASN:HA	4:D:28:GLN:O	2.19	0.41
1:A:56:PRO:HD2	1:A:58:LEU:HG	2.02	0.41
7:G:34:VAL:HG13	7:G:45:ILE:HG21	2.02	0.41
2:B:295:GLY:H	2:B:298:LEU:CD1	2.34	0.41
1:A:105:CYS:SG	1:A:139:TRP:HA	2.61	0.41
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.35	0.41
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	2.02	0.41
2:B:873:THR:O	2:B:914:LYS:HA	2.21	0.41
1:A:699:ALA:HB1	9:I:114:GLN:HG3	2.03	0.41
1:A:37:PHE:HD2	1:A:52:GLY:CA	2.34	0.41
7:G:1:MET:HE3	7:G:81:PRO:HA	2.03	0.41
1:A:937:VAL:O	1:A:941:LYS:HG2	2.20	0.41
2:B:34:ILE:HG12	2:B:542:MET:HE2	2.03	0.41
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.21	0.41
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1148:LYS:HE2	2:B:1153:GLU:OE1	2.20	0.41
2:B:1056:SER:HB3	2:B:1066:SER:HB2	2.03	0.41
2:B:703:ILE:HA	2:B:740:HIS:O	2.21	0.41
2:B:295:GLY:O	2:B:299:GLU:HB2	2.21	0.41
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.56	0.41
4:D:194:LEU:HD21	7:G:167:TYR:HB2	2.03	0.41
1:A:830:LYS:HE3	1:A:1098:VAL:HB	2.03	0.41
2:B:286:PHE:HD1	2:B:291:ILE:HD13	1.86	0.41
1:A:347:PHE:H	2:B:1107:ALA:HA	1.86	0.41
4:D:27:LEU:HD11	4:D:173:HIS:HB2	2.03	0.40
1:A:1149:ALA:HB2	9:I:47:GLU:HA	2.03	0.40
1:A:302:THR:HA	1:A:305:ASP:O	2.21	0.40
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.61	0.40
5:E:124:VAL:HG13	5:E:132:ILE:HB	2.03	0.40
1:A:1436:ILE:O	1:A:1437:GLY:C	2.60	0.40
2:B:128:LEU:HD21	2:B:170:LEU:CB	2.51	0.40
2:B:766:ARG:HH21	2:B:1020:ARG:HH11	1.68	0.40
2:B:299:GLU:HG3	2:B:572:HIS:NE2	2.37	0.40
3:C:149:LYS:C	3:C:151:GLN:H	2.25	0.40
7:G:60:ARG:HG3	7:G:60:ARG:O	2.20	0.40
1:A:383:TYR:HB3	6:F:115:THR:HG22	2.04	0.40
6:F:109:VAL:HG12	6:F:124:GLU:HG2	2.02	0.40
8:H:5:LEU:HD11	8:H:61:SER:HB3	2.04	0.40
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.88	0.40
2:B:412:LEU:HA	2:B:412:LEU:HD13	1.96	0.40
2:B:123:THR:HG23	2:B:205:ILE:HA	2.02	0.40
2:B:249:ARG:HH12	2:B:415:GLN:HA	1.87	0.40
2:B:1156:ASP:HB3	2:B:1197:PRO:HB3	2.04	0.40
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.03	0.40
2:B:35:SER:HA	2:B:811:TYR:CE1	2.57	0.40
1:A:219:PHE:HA	1:A:222:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1414/1732 (82%)	1211 (86%)	145 (10%)	58 (4%)	3	33
2	B	1095/1224 (90%)	951 (87%)	114 (10%)	30 (3%)	6	44
3	C	264/318 (83%)	231 (88%)	26 (10%)	7 (3%)	6	44
4	D	174/221 (79%)	147 (84%)	19 (11%)	8 (5%)	3	29
5	E	212/215 (99%)	194 (92%)	11 (5%)	7 (3%)	5	39
6	F	82/155 (53%)	75 (92%)	6 (7%)	1 (1%)	16	61
7	G	169/171 (99%)	158 (94%)	7 (4%)	4 (2%)	7	47
8	H	129/146 (88%)	100 (78%)	15 (12%)	14 (11%)	0	8
9	I	117/122 (96%)	99 (85%)	16 (14%)	2 (2%)	11	54
10	J	63/70 (90%)	54 (86%)	5 (8%)	4 (6%)	2	21
11	K	113/120 (94%)	104 (92%)	8 (7%)	1 (1%)	21	68
12	L	44/70 (63%)	30 (68%)	6 (14%)	8 (18%)	0	2
All	All	3876/4564 (85%)	3354 (86%)	378 (10%)	144 (4%)	4	36

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	57	ARG
1	A	58	LEU
1	A	69	THR
1	A	193	ASP
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	332	LYS
1	A	335	ARG
1	A	399	HIS
1	A	449	SER
1	A	775	ILE
1	A	1124	HIS
1	A	1405	THR
2	B	229	ALA
2	B	731	VAL
2	B	879	ARG

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Mol	Chain	Res	Type
2	B	1167	GLY
2	B	1175	LEU
3	C	161	LYS
4	D	18	VAL
4	D	199	ASN
7	G	63	PRO
9	I	95	THR
10	J	6	ARG
12	L	43	THR
12	L	53	HIS
12	L	56	LEU
12	L	59	ALA
1	A	35	ILE
1	A	54	ASN
1	A	61	ILE
1	A	76	GLU
1	A	178	GLY
1	A	189	ARG
1	A	195	ASP
1	A	331	GLY
1	A	385	ILE
1	A	628	GLY
1	A	1175	SER
1	A	1403	GLU
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	367	LEU
2	B	449	ASN
2	B	473	MET
2	B	476	ARG
2	B	772	ALA
2	B	867	GLY
2	B	1046	PRO
2	B	1066	SER
2	B	1157	ALA
2	B	1176	ASN
3	C	150	GLY
3	C	162	GLY
3	C	184	ASN
3	C	229	TYR
3	C	240	VAL

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Mol	Chain	Res	Type
4	D	52	LEU
4	D	53	SER
4	D	119	ARG
5	E	104	ASN
5	E	126	SER
5	E	174	GLN
7	G	154	VAL
8	H	81	PRO
12	L	45	ALA
12	L	50	ASP
1	A	43	GLU
1	A	62	ASP
1	A	224	PHE
1	A	465	TYR
1	A	1064	VAL
1	A	1167	GLU
2	B	108	VAL
2	B	707	PRO
2	B	883	LEU
2	B	1181	GLU
5	E	36	GLU
7	G	2	PHE
8	H	46	LEU
8	H	82	PRO
8	H	83	GLN
8	H	90	ALA
8	H	128	ASN
9	I	3	THR
10	J	2	ILE
10	J	17	LYS
11	K	64	GLU
12	L	26	THR
1	A	169	ASN
1	A	569	LYS
1	A	1242	VAL
1	A	1366	ARG
2	B	575	PRO
2	B	711	GLU
2	B	751	VAL
4	D	16	LYS
4	D	169	SER
5	E	45	LYS

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Mol	Chain	Res	Type
8	H	89	LEU
1	A	155	GLU
1	A	167	CYS
1	A	196	GLU
1	A	846	GLU
1	A	958	VAL
1	A	975	HIS
1	A	1173	HIS
1	A	1255	GLU
1	A	1437	GLY
2	B	792	MET
3	C	237	SER
4	D	218	GLU
5	E	103	LYS
6	F	73	ALA
8	H	18	GLY
8	H	32	THR
8	H	52	GLN
8	H	60	ALA
8	H	131	ASN
1	A	65	LEU
1	A	1060	PRO
2	B	251	ILE
2	B	364	ILE
2	B	1108	ARG
7	G	139	ILE
8	H	78	SER
12	L	28	LYS
1	A	73	GLY
1	A	192	GLY
1	A	567	LYS
1	A	283	GLY
1	A	1122	PRO
1	A	1123	GLY
5	E	90	VAL
8	H	107	VAL
1	A	197	PRO
1	A	916	GLY
2	B	907	GLY
10	J	64	ASN
1	A	448	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	1240/1519 (82%)	1055 (85%)	185 (15%)	4	22
2	B	966/1061 (91%)	818 (85%)	148 (15%)	3	21
3	C	234/274 (85%)	199 (85%)	35 (15%)	3	21
4	D	160/200 (80%)	133 (83%)	27 (17%)	2	15
5	E	196/197 (100%)	172 (88%)	24 (12%)	6	29
6	F	74/137 (54%)	66 (89%)	8 (11%)	8	37
7	G	152/152 (100%)	130 (86%)	22 (14%)	4	23
8	H	117/128 (91%)	103 (88%)	14 (12%)	6	30
9	I	113/116 (97%)	105 (93%)	8 (7%)	18	58
10	J	60/65 (92%)	48 (80%)	12 (20%)	1	9
11	K	99/102 (97%)	85 (86%)	14 (14%)	4	24
12	L	40/57 (70%)	30 (75%)	10 (25%)	1	4
All	All	3451/4008 (86%)	2944 (85%)	507 (15%)	4	22

All (507) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	28	ARG
1	A	41	MET
1	A	43	GLU
1	A	45	GLN
1	A	47	ARG
1	A	62	ASP
1	A	64	ASN
1	A	66	LYS
1	A	67	CYS
1	A	70	CYS
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE

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Mol	Chain	Res	Type
1	A	106	VAL
1	A	117	GLU
1	A	120	GLU
1	A	132	LYS
1	A	140	THR
1	A	144	THR
1	A	147	VAL
1	A	157	ASP
1	A	164	ARG
1	A	170	THR
1	A	174	ILE
1	A	188	ASP
1	A	199	LEU
1	A	208	LEU
1	A	220	THR
1	A	252	PHE
1	A	255	SER
1	A	256	GLN
1	A	261	ASP
1	A	279	LEU
1	A	295	LEU
1	A	303	TYR
1	A	307	ASP
1	A	313	GLN
1	A	315	LEU
1	A	322	VAL
1	A	324	SER
1	A	328	ARG
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	354	SER
1	A	381	THR
1	A	389	THR
1	A	393	ARG
1	A	408	ASP
1	A	411	ASP
1	A	423	ASP
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE

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Mol	Chain	Res	Type
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	454	SER
1	A	461	LYS
1	A	469	ARG
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	485	ASP
1	A	494	SER
1	A	500	GLU
1	A	505	CYS
1	A	517	ASN
1	A	524	VAL
1	A	536	LEU
1	A	541	ILE
1	A	544	ASP
1	A	566	ILE
1	A	569	LYS
1	A	571	LEU
1	A	593	GLU
1	A	597	LEU
1	A	598	LEU
1	A	618	GLU
1	A	629	LEU
1	A	652	VAL
1	A	666	ILE
1	A	672	ASP
1	A	682	THR
1	A	685	GLU
1	A	702	LEU
1	A	711	ARG
1	A	719	VAL
1	A	732	LEU
1	A	738	LYS
1	A	754	SER
1	A	756	ILE
1	A	764	CYS

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Mol	Chain	Res	Type
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	774	ARG
1	A	782	ARG
1	A	788	SER
1	A	794	PRO
1	A	811	GLN
1	A	821	ARG
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	855	THR
1	A	880	LYS
1	A	886	ILE
1	A	890	ASP
1	A	896	ARG
1	A	904	THR
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	941	LYS
1	A	948	VAL
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	993	LEU
1	A	998	LEU
1	A	1001	ARG
1	A	1009	ASN
1	A	1015	VAL
1	A	1020	CYS
1	A	1024	SER
1	A	1028	THR
1	A	1036	ARG
1	A	1058	VAL
1	A	1078	GLN
1	A	1096	SER
1	A	1105	LEU
1	A	1118	VAL
1	A	1124	HIS
1	A	1134	ILE

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Mol	Chain	Res	Type
1	A	1146	VAL
1	A	1171	GLN
1	A	1172	LEU
1	A	1173	HIS
1	A	1174	PHE
1	A	1176	LEU
1	A	1188	GLN
1	A	1195	LEU
1	A	1208	THR
1	A	1215	ARG
1	A	1218	GLN
1	A	1223	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1280	GLU
1	A	1288	ASP
1	A	1290	LYS
1	A	1295	THR
1	A	1297	GLU
1	A	1301	GLU
1	A	1325	THR
1	A	1333	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1370	LEU
1	A	1376	THR
1	A	1386	ARG
1	A	1387	HIS
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1406	VAL
1	A	1418	LEU
1	A	1420	ASP
1	A	1426	GLU
1	A	1442	ASP
1	A	1444	MET

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Mol	Chain	Res	Type
1	A	1445	ILE
1	A	1451	VAL
1	A	1454	MET
2	B	25	ILE
2	B	28	GLU
2	B	35	SER
2	B	40	GLU
2	B	46	GLN
2	B	64	CYS
2	B	102	VAL
2	B	110	HIS
2	B	118	ARG
2	B	126	SER
2	B	185	THR
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	251	ILE
2	B	254	LEU
2	B	261	ARG
2	B	272	THR
2	B	273	LEU
2	B	278	GLN
2	B	279	ASP
2	B	289	LEU
2	B	312	GLU
2	B	313	MET
2	B	324	ILE
2	B	337	ARG
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	348	ARG
2	B	365	THR
2	B	372	SER
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	398	ARG
2	B	408	LEU
2	B	412	LEU

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Mol	Chain	Res	Type
2	B	416	LEU
2	B	423	LYS
2	B	429	PHE
2	B	436	VAL
2	B	446	LEU
2	B	448	ILE
2	B	453	ILE
2	B	458	LYS
2	B	461	LEU
2	B	466	TRP
2	B	468	GLU
2	B	470	LYS
2	B	474	SER
2	B	476	ARG
2	B	480	SER
2	B	485	ARG
2	B	545	ILE
2	B	547	VAL
2	B	570	VAL
2	B	572	HIS
2	B	573	GLN
2	B	574	SER
2	B	580	VAL
2	B	589	VAL
2	B	598	GLU
2	B	603	LEU
2	B	604	ARG
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	628	THR
2	B	629	ASP
2	B	642	ASP
2	B	646	LEU
2	B	651	LEU
2	B	652	LYS
2	B	653	VAL
2	B	658	ILE
2	B	668	ASP
2	B	678	GLU
2	B	680	THR
2	B	689	LEU

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Mol	Chain	Res	Type
2	B	696	GLU
2	B	723	VAL
2	B	729	ILE
2	B	734	HIS
2	B	766	ARG
2	B	786	ASN
2	B	790	ASP
2	B	830	TYR
2	B	835	GLN
2	B	844	SER
2	B	858	SER
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	889	THR
2	B	908	GLU
2	B	933	SER
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	945	GLU
2	B	953	LEU
2	B	964	VAL
2	B	970	THR
2	B	972	LYS
2	B	973	ILE
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	987	LYS
2	B	997	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1017	ILE
2	B	1020	ARG
2	B	1026	LEU
2	B	1050	ILE
2	B	1053	GLU
2	B	1060	ARG

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Mol	Chain	Res	Type
2	B	1065	GLN
2	B	1072	MET
2	B	1082	MET
2	B	1112	GLN
2	B	1122	ARG
2	B	1128	LEU
2	B	1129	ARG
2	B	1133	MET
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1149	GLU
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1160	VAL
2	B	1172	ILE
2	B	1175	LEU
2	B	1178	ASN
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1193	GLN
2	B	1202	LEU
2	B	1212	ILE
3	C	7	GLN
3	C	12	GLU
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	40	GLU
3	C	42	PRO
3	C	44	LEU
3	C	52	GLU
3	C	53	THR
3	C	55	THR
3	C	56	THR
3	C	79	GLN
3	C	89	GLU
3	C	100	THR

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Mol	Chain	Res	Type
3	C	101	LEU
3	C	122	SER
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	145	CYS
3	C	148	ARG
3	C	155	LEU
3	C	157	CYS
3	C	197	SER
3	C	215	GLU
3	C	238	ILE
3	C	240	VAL
3	C	262	LEU
3	C	264	GLN
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	6	SER
4	D	9	GLN
4	D	17	LYS
4	D	18	VAL
4	D	27	LEU
4	D	29	LEU
4	D	32	GLU
4	D	35	LEU
4	D	37	GLN
4	D	40	HIS
4	D	41	GLN
4	D	52	LEU
4	D	65	GLU
4	D	123	LEU
4	D	126	ILE
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	156	ASP
4	D	158	GLU
4	D	177	VAL
4	D	187	THR
4	D	213	GLU

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Mol	Chain	Res	Type
4	D	214	LEU
4	D	219	THR
4	D	221	TYR
5	E	3	GLN
5	E	6	GLU
5	E	8	ASN
5	E	31	THR
5	E	46	TYR
5	E	60	PHE
5	E	67	GLU
5	E	69	ILE
5	E	75	MET
5	E	84	ASP
5	E	85	GLU
5	E	92	THR
5	E	99	HIS
5	E	150	VAL
5	E	173	SER
5	E	175	LEU
5	E	177	ARG
5	E	178	ILE
5	E	184	VAL
5	E	190	LEU
5	E	191	LYS
5	E	196	VAL
5	E	204	THR
5	E	215	MET
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	90	ARG
6	F	93	ILE
6	F	110	ASP
6	F	111	LEU
6	F	123	LYS
7	G	8	SER
7	G	13	LEU
7	G	22	MET
7	G	24	GLN
7	G	26	LEU
7	G	39	THR
7	G	60	ARG

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Mol	Chain	Res	Type
7	G	64	THR
7	G	65	ASP
7	G	71	ASN
7	G	83	LYS
7	G	96	GLN
7	G	106	MET
7	G	114	LEU
7	G	118	ASP
7	G	133	SER
7	G	134	GLU
7	G	138	THR
7	G	143	ILE
7	G	151	ILE
7	G	155	SER
7	G	162	SER
8	H	13	SER
8	H	26	ILE
8	H	31	THR
8	H	46	LEU
8	H	63	LEU
8	H	76	THR
8	H	77	ARG
8	H	86	ASP
8	H	89	LEU
8	H	91	ASP
8	H	103	LYS
8	H	123	MET
8	H	128	ASN
8	H	130	ARG
9	I	4	PHE
9	I	8	ARG
9	I	31	THR
9	I	35	VAL
9	I	43	VAL
9	I	83	ASN
9	I	94	ASP
9	I	108	HIS
10	J	2	ILE
10	J	7	CYS
10	J	13	VAL
10	J	14	VAL
10	J	20	SER

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Mol	Chain	Res	Type
10	J	23	ASN
10	J	28	ASP
10	J	29	GLU
10	J	38	ARG
10	J	42	LYS
10	J	48	ARG
10	J	56	LEU
11	K	1	MET
11	K	12	LEU
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	37	LYS
11	K	47	ARG
11	K	63	VAL
11	K	70	ARG
11	K	79	GLU
11	K	101	LEU
11	K	107	THR
11	K	114	LEU
12	L	27	LEU
12	L	35	SER
12	L	38	LEU
12	L	49	LYS
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	253	ASN
1	A	425	GLN
1	A	439	ASN
1	A	548	ASN
1	A	968	GLN
1	A	994	GLN

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Mol	Chain	Res	Type
1	A	1106	ASN
1	A	1387	HIS
1	A	1390	ASN
1	A	1393	ASN
2	B	47	GLN
2	B	103	ASN
2	B	363	HIS
2	B	449	ASN
2	B	590	HIS
2	B	957	ASN
2	B	975	GLN
2	B	986	GLN
2	B	1065	GLN
2	B	1084	GLN
2	B	1117	GLN
2	B	1195	HIS
4	D	137	ASN
5	E	3	GLN
5	E	8	ASN
5	E	113	GLN
7	G	71	ASN
9	I	46	HIS
9	I	51	ASN
9	I	60	GLN
9	I	89	GLN
10	J	64	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	3/4 (75%)	1 (33%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	9	G

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	13,21,22	1.97	3 (23%)	16,30,33	2.57	4 (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
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	C4-N3	3.09	1.38	1.33
15	T	22	BRU	C6-N1	3.93	1.40	1.35
15	T	22	BRU	C4-C5	4.92	1.44	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C2'-C1'-N1	-5.22	101.46	114.16
15	T	22	BRU	C5-C4-N3	-3.90	119.83	124.00
15	T	22	BRU	O4'-C1'-N1	4.80	116.03	107.72
15	T	22	BRU	C4-N3-C2	6.14	120.56	115.25

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1422/1732 (82%)	-0.18	12 (0%) 87 80	64, 115, 172, 239	0
2	B	1115/1224 (91%)	-0.12	11 (0%) 84 76	71, 127, 187, 209	0
3	C	266/318 (83%)	-0.24	0 100 100	86, 115, 158, 185	0
4	D	178/221 (80%)	-0.17	0 100 100	96, 131, 179, 198	0
5	E	214/215 (99%)	-0.14	2 (0%) 85 78	89, 146, 193, 206	0
6	F	84/155 (54%)	-0.40	0 100 100	73, 97, 124, 137	0
7	G	171/171 (100%)	-0.18	0 100 100	85, 113, 154, 172	0
8	H	133/146 (91%)	0.32	5 (3%) 44 36	125, 157, 194, 214	0
9	I	119/122 (97%)	-0.05	2 (1%) 73 64	120, 151, 192, 199	0
10	J	65/70 (92%)	-0.27	0 100 100	95, 115, 151, 161	0
11	K	115/120 (95%)	-0.29	0 100 100	85, 114, 155, 174	0
12	L	46/70 (65%)	0.46	3 (6%) 22 17	103, 182, 199, 210	0
13	N	4/14 (28%)	0.36	0 100 100	230, 230, 234, 239	0
14	P	4/4 (100%)	0.24	0 100 100	211, 220, 228, 240	0
15	T	11/26 (42%)	0.85	2 (18%) 2 2	188, 216, 258, 264	0
All	All	3947/4608 (85%)	-0.14	37 (0%) 85 78	64, 122, 185, 264	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	5.0
12	L	26	THR	4.6
1	A	194	ALA	4.0
1	A	1455	PRO	3.8
2	B	883	LEU	3.3
2	B	709	ASP	3.3
2	B	340	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	469	GLN	3.1
1	A	257	ARG	3.0
15	T	15	DT	3.0
1	A	1176	LEU	3.0
8	H	134	ASN	2.8
5	E	2	ASP	2.7
12	L	25	ALA	2.6
8	H	86	ASP	2.6
2	B	470	LYS	2.6
1	A	195	ASP	2.5
2	B	708	GLU	2.5
1	A	191	THR	2.5
2	B	250	PHE	2.4
1	A	251	SER	2.4
1	A	256	GLN	2.3
2	B	468	GLU	2.3
8	H	145	ARG	2.3
1	A	155	GLU	2.2
9	I	119	THR	2.1
15	T	19	DT	2.1
8	H	139	ASN	2.1
5	E	93	MET	2.1
2	B	918	ILE	2.1
1	A	1257	ASP	2.0
1	A	159	THR	2.0
2	B	271	ALA	2.0
8	H	113	ALA	2.0
9	I	84	VAL	2.0
1	A	161	LEU	2.0
2	B	339	THR	2.0

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

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	BRU	T	22	20/21	0.84	0.21	-	221,231,240,243	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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	ZN	B	2225	1/1	0.99	0.21	-0.10	91,91,91,91	0
16	ZN	I	1121	1/1	1.00	0.12	-0.52	136,136,136,136	0
16	ZN	J	1066	1/1	1.00	0.25	-0.87	101,101,101,101	0
16	ZN	C	1269	1/1	1.00	0.12	-1.02	96,96,96,96	0
16	ZN	A	2457	1/1	1.00	0.14	-1.57	81,81,81,81	0
16	ZN	L	1071	1/1	0.93	0.06	-1.70	201,201,201,201	0
16	ZN	I	1122	1/1	0.98	0.03	-1.77	201,201,201,201	0
16	ZN	A	2456	1/1	0.98	0.06	-2.35	155,155,155,155	0
17	MG	A	2458	1/1	0.75	0.32	-	281,281,281,281	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.