



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2016 – 06:10 PM EDT

PDB ID : 4BY7  
Title : elongating RNA Polymerase II-Bye1 TLD complex  
Authors : Kinkelin, K.; Wozniak, G.G.; Rothbart, S.B.; Lidschreiber, M.; Strahl, B.D.; Cramer, P.  
Deposited on : 2013-07-18  
Resolution : 3.15 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
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) : rb-20027790

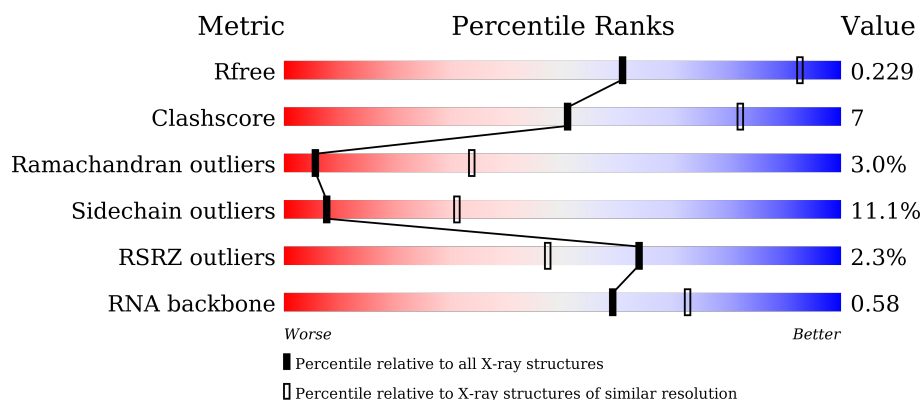
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)
RNA backbone	2183	1046 (3.62-2.70)

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	1733	<div> <div>2%</div> <div>62% 16% 18%</div> </div>
2	B	1224	<div> <div>2%</div> <div>69% 19% 9%</div> </div>
3	C	318	<div> <div></div> <div>61% 20% 16%</div> </div>
4	D	221	<div> <div></div> <div>61% 18% 19%</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	11	
15	T	26	
16	X	146	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	EPE	A	2459	-	-	-	X
19	EPE	G	1172	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 33261 atoms, of which 34 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	1426	Total	C	N	O	S	0	0	0
			11223	7068	1959	2134	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
			1387	860	246	279	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	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- 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	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called 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 , 5'-D(\*DAP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP\*A

P\*GP\*CP\*DTP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	13	Total	C	N	O	P	0	0	0
			269	128	52	76	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	10	Total	C	N	O	P	0	0	0
			215	96	41	68	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	25	Total	Br	C	N	O	P	0	0
			504	1	240	83	155	25		

- Molecule 16 is a protein called TRANSCRIPTION FACTOR BYE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	X	119	Total	C	N	O	S	0	0	0
			977	628	162	184	3			

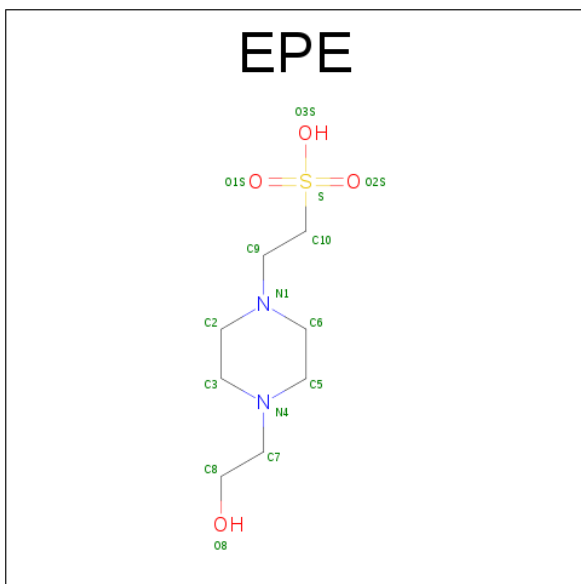
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 1 1	0	0

- Molecule 19 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).

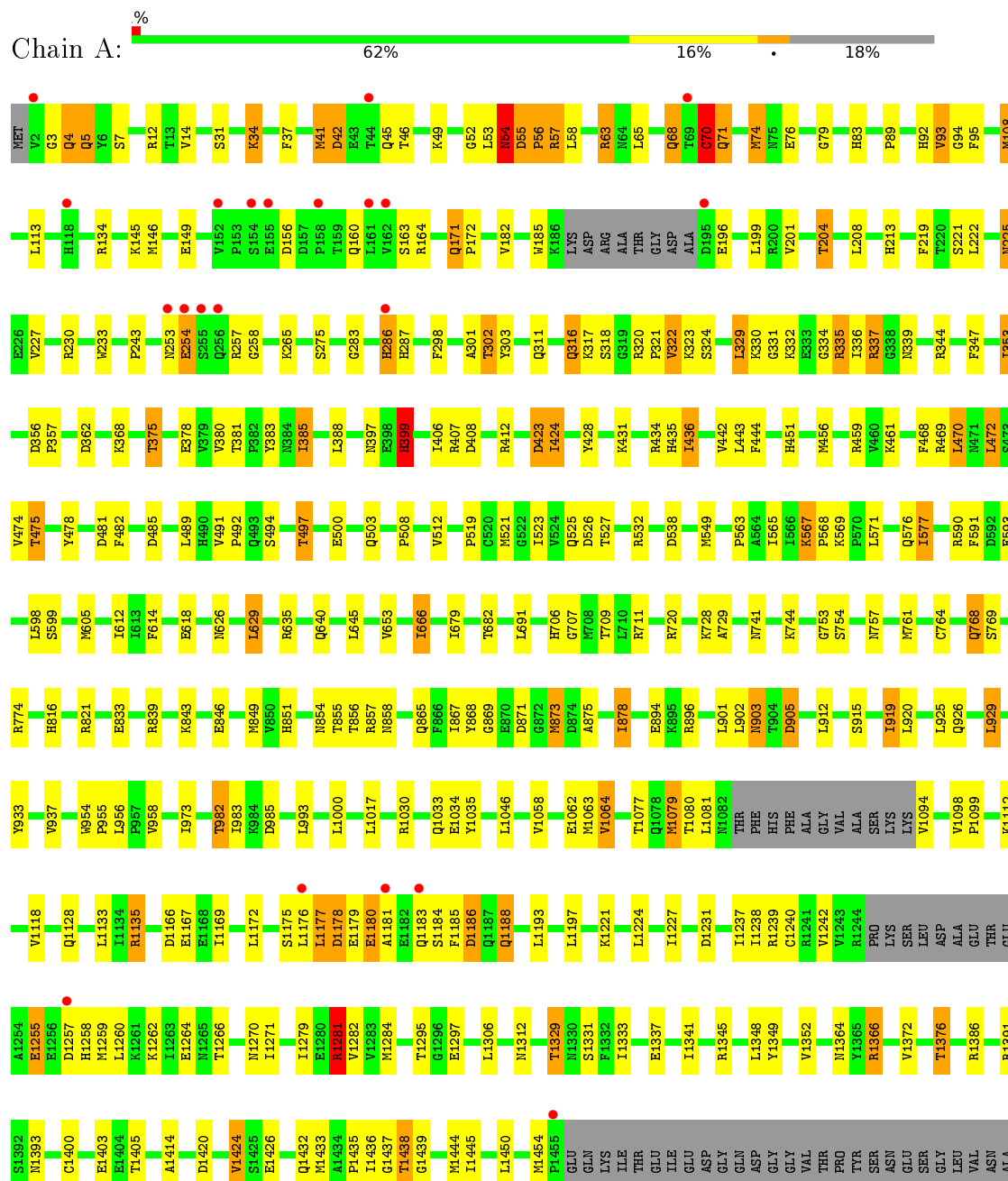


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
19	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
19	G	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

### 3 Residue-property plots

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

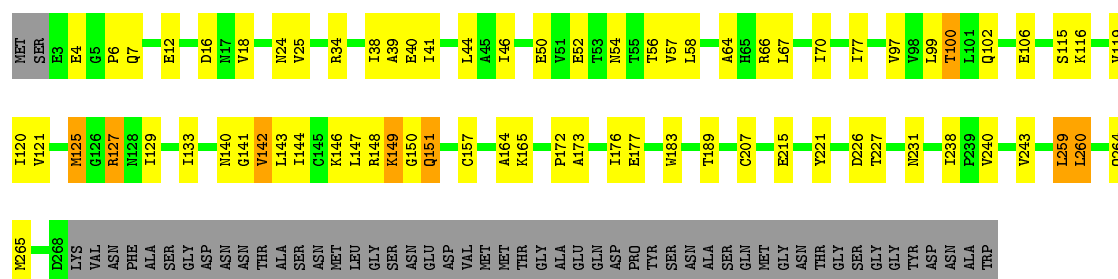
#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1





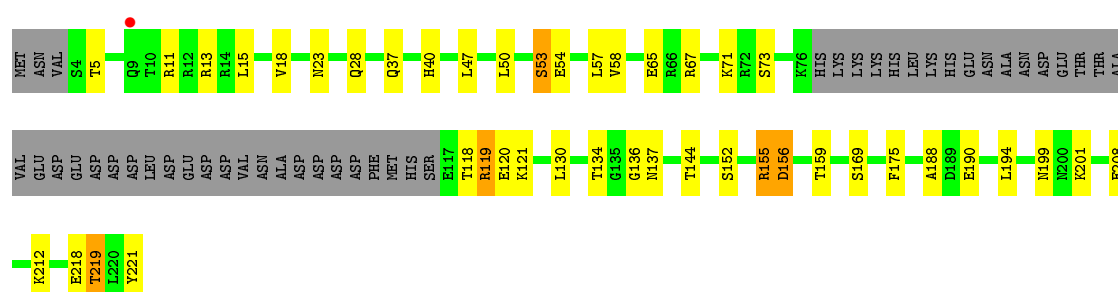


Chain C:  61% 20% • 16%




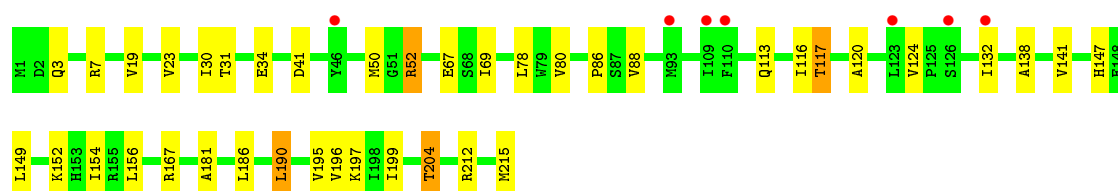
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D:  61% 18% • 19%



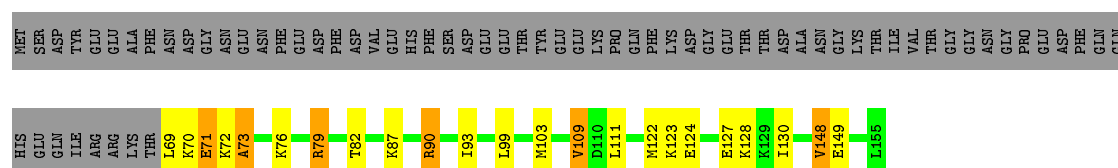
● Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E: 



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

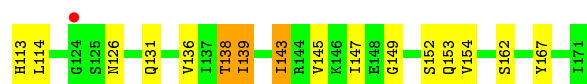
Chain F:  41% 11% . 44%



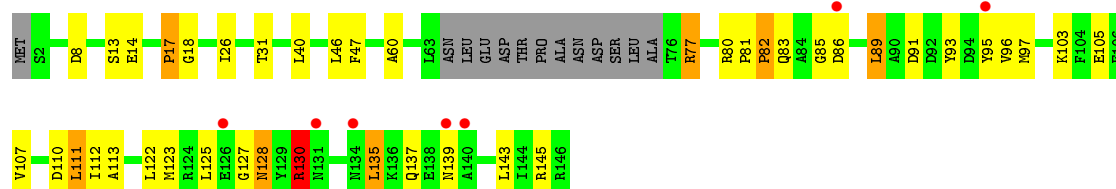
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:  %

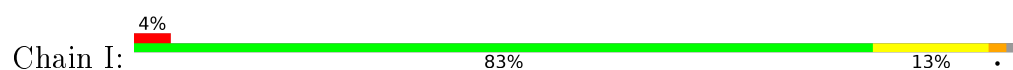




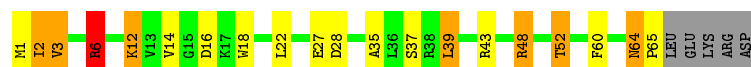
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



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



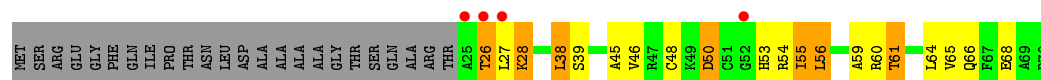
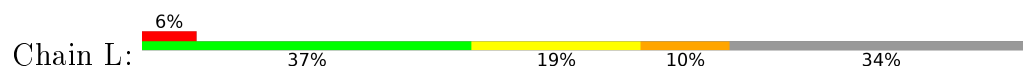
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



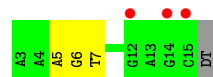
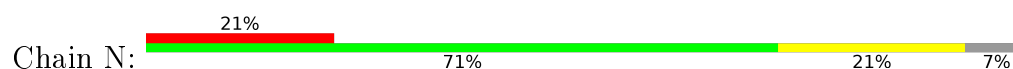
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



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



- Molecule 13: , 5'-D(\*DAP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*DTP)-3'



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

Chain P: 

55%

27%

9%

9%



• Molecule 15: 5'-D(\*DAP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*DAP \*TP\*TP\*CP\*CP\*BP\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'

Chain T: 

8%

62%

31%

.

.



• Molecule 16: TRANSCRIPTION FACTOR BYE1

Chain X: 

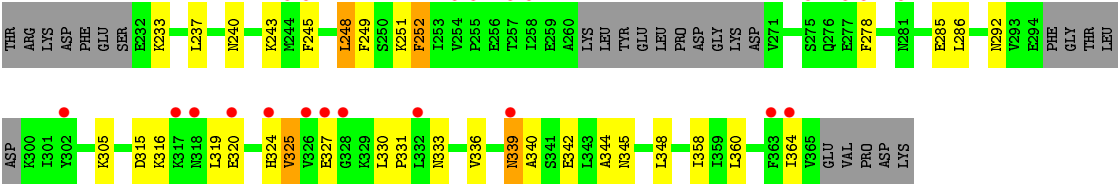
15%

58%

21%

.

18%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.50Å 390.68Å 281.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 – 3.15 48.84 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.84-3.15) 100.0 (48.84-3.15)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.189 , 0.212 0.206 , 0.229	Depositor DCC
$R_{free}$ test set	4003 reflections (1.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.4	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 83.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.003 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	33261	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: ZN, EPE, MG, 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	0.51	1/11424 (0.0%)	0.78	5/15452 (0.0%)
2	B	0.48	0/9030	0.74	4/12174 (0.0%)
3	C	0.46	0/2133	0.74	0/2891
4	D	0.48	0/1397	0.75	0/1878
5	E	0.43	0/1796	0.63	0/2416
6	F	0.55	0/717	0.78	1/967 (0.1%)
7	G	0.47	0/1368	0.78	2/1844 (0.1%)
8	H	0.46	0/1085	0.72	0/1467
9	I	0.45	0/989	0.70	0/1331
10	J	0.49	0/541	0.82	0/727
11	K	0.42	0/938	0.64	0/1267
12	L	0.53	0/364	0.85	0/482
13	N	1.05	0/302	1.03	0/464
14	P	1.10	1/240 (0.4%)	0.94	0/372
15	T	1.22	1/539 (0.2%)	1.11	2/825 (0.2%)
16	X	0.47	0/990	0.70	0/1325
All	All	0.52	3/33853 (0.0%)	0.76	14/45882 (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
15	T	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	24	DA	C3'-O3'	6.30	1.52	1.44
1	A	56	PRO	C-N	5.51	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	3	C	C1'-N1	5.49	1.56	1.48

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1177	LEU	C-N-CA	6.51	137.99	121.70
15	T	24	DA	O4'-C1'-N9	6.48	112.53	108.00
7	G	1	MET	C-N-CA	6.24	137.31	121.70
1	A	399	HIS	N-CA-CB	6.17	121.72	110.60
1	A	56	PRO	C-N-CA	6.05	136.83	121.70
1	A	54	ASN	C-N-CA	6.01	136.73	121.70
1	A	55	ASP	N-CA-CB	5.87	121.17	110.60
7	G	2	PHE	N-CA-C	-5.86	95.17	111.00
6	F	70	LYS	C-N-CA	5.81	136.22	121.70
2	B	1184	GLY	C-N-CA	5.46	135.34	121.70
2	B	1155	SER	C-N-CA	5.30	134.96	121.70
2	B	296	GLU	N-CA-C	-5.28	96.74	111.00
2	B	339	THR	C-N-CA	5.06	134.35	121.70
15	T	11	DC	O4'-C1'-N1	5.05	111.53	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	T	15	DT	Sidechain
15	T	25	DT	Sidechain

## 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	11223	0	11273	187	0
2	B	8859	0	8902	118	0
3	C	2095	0	2051	36	0
4	D	1387	0	1366	20	0
5	E	1760	0	1788	22	0
6	F	705	0	731	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1340	0	1357	33	0
8	H	1068	0	1039	30	0
9	I	971	0	927	6	0
10	J	532	0	542	11	0
11	K	920	0	929	15	0
12	L	363	0	385	7	0
13	N	269	0	147	3	0
14	P	215	0	109	1	0
15	T	504	0	274	4	0
16	X	977	0	996	13	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
19	A	15	17	17	1	0
19	G	15	17	17	0	0
All	All	33227	34	32850	458	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 7.

All (458) 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:53:LEU:HD23	1:A:54:ASN:H	1.23	1.02
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.45	0.94
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.49	0.94
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.83	0.93
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.52	0.92
1:A:567:LYS:HB3	8:H:96:VAL:H	1.34	0.91
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.37	0.90
4:D:53:SER:HB3	4:D:152:SER:HB2	1.54	0.89
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.19	0.88
1:A:1177:LEU:HB3	1:A:1179:GLU:H	1.37	0.87
3:C:56:THR:HG22	3:C:58:LEU:H	1.38	0.87
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.58	0.86
1:A:869:GLY:O	5:E:204:THR:HG21	1.77	0.85
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:654:ARG:H	2:B:657:HIS:HD2	1.28	0.82
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.63	0.80
16:X:316:LYS:HG2	16:X:320:GLU:HB3	1.62	0.80
11:K:65:HIS:HD2	11:K:67:PHE:H	1.29	0.80
1:A:68:GLN:OE1	1:A:70:CYS:HB3	1.82	0.78
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.65	0.78
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.65	0.77
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.13	0.77
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.67	0.76
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.67	0.75
2:B:277:LYS:H	2:B:338:GLY:HA3	1.51	0.75
2:B:345:LYS:HA	2:B:348:ARG:HD3	1.69	0.75
11:K:65:HIS:CD2	11:K:67:PHE:H	2.05	0.74
1:A:53:LEU:HD23	1:A:54:ASN:N	2.00	0.73
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.54	0.73
1:A:567:LYS:HB3	8:H:96:VAL:N	2.03	0.72
3:C:100:THR:HG22	3:C:119:VAL:HB	1.69	0.71
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.20	0.70
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.21	0.70
6:F:99:LEU:HG	6:F:103:MET:HE1	1.74	0.70
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.20	0.69
1:A:494:SER:HB3	1:A:497:THR:HB	1.73	0.69
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.75	0.69
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.90	0.68
1:A:903:ASN:HD22	1:A:905:ASP:H	1.42	0.66
2:B:273:LEU:H	2:B:276:ILE:HD11	1.60	0.66
1:A:741:ASN:HD22	1:A:744:LYS:H	1.42	0.66
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.79	0.66
2:B:744:HIS:HD2	2:B:746:SER:H	1.43	0.66
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.78	0.66
1:A:1364:ASN:HD22	1:A:1366:ARG:HD2	1.60	0.66
4:D:155:ARG:HB2	4:D:219:THR:HG21	1.78	0.66
4:D:23:ASN:HA	4:D:28:GLN:O	1.96	0.66
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.76	0.66
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.76	0.65
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.61	0.65
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.78	0.65
2:B:705:MET:H	2:B:710:LEU:HD12	1.62	0.65
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.79	0.65
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.80	0.64
2:B:882:THR:HG1	2:B:935:ARG:N	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.79	0.64
4:D:119:ARG:HH21	4:D:120:GLU:HB2	1.63	0.64
1:A:57:ARG:O	1:A:68:GLN:HG2	1.98	0.64
2:B:363:HIS:O	2:B:364:ILE:HB	1.98	0.63
1:A:298:PHE:O	1:A:302:THR:HB	1.98	0.62
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.81	0.62
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.81	0.62
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.82	0.62
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.81	0.61
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.47	0.61
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.82	0.61
1:A:65:LEU:HD23	1:A:71:GLN:HB2	1.83	0.61
7:G:1:MET:HE1	7:G:79:PHE:HA	1.82	0.60
3:C:46:ILE:HG12	3:C:157:CYS:HB3	1.83	0.60
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.84	0.60
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.15	0.60
2:B:711:GLU:H	2:B:712:PRO:HD3	1.66	0.60
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.67	0.60
1:A:225:ASN:HD22	1:A:227:VAL:H	1.49	0.60
1:A:565:ILE:HG23	1:A:567:LYS:HG3	1.83	0.60
7:G:14:HIS:CD2	7:G:16:SER:H	2.20	0.60
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.83	0.60
2:B:333:PHE:O	2:B:337:ARG:HG2	2.02	0.59
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.85	0.59
1:A:1424:VAL:HG13	1:A:1436:ILE:HG12	1.83	0.59
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.30	0.59
5:E:31:THR:HG23	5:E:34:GLU:H	1.67	0.59
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.33	0.59
1:A:55:ASP:N	1:A:56:PRO:HD3	2.18	0.58
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.51	0.58
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.97	0.58
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.84	0.58
1:A:1177:LEU:HB3	1:A:1179:GLU:N	2.13	0.58
7:G:1:MET:HE2	7:G:2:PHE:H	1.68	0.58
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.39	0.58
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.84	0.58
1:A:4:GLN:O	1:A:5:GLN:HB3	2.04	0.57
2:B:1013:ASN:OD1	2:B:1015:HIS:HD2	1.87	0.57
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.85	0.57
7:G:1:MET:CE	7:G:80:LYS:H	2.17	0.57
3:C:142:VAL:H	10:J:16:ASP:HB3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:111:THR:HG22	7:G:113:HIS:H	1.70	0.57
1:A:1176:LEU:HB3	16:X:240:ASN:HB3	1.87	0.57
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.88	0.56
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.37	0.56
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.89	0.56
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.88	0.56
6:F:109:VAL:HG13	6:F:123:LYS:HE3	1.88	0.56
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.36	0.56
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.88	0.56
8:H:130:ARG:H	8:H:130:ARG:HD2	1.71	0.56
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.89	0.55
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.22	0.55
1:A:321:PRO:O	1:A:322:VAL:HB	2.07	0.55
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.88	0.55
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.41	0.55
1:A:353:ILE:HD12	1:A:482:PHE:HD1	1.72	0.55
1:A:563:PRO:HA	1:A:576:GLN:HE22	1.71	0.55
1:A:754:SER:H	1:A:757:ASN:HD22	1.55	0.55
2:B:1013:ASN:OD1	2:B:1015:HIS:CD2	2.60	0.55
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.88	0.54
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.87	0.54
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.88	0.54
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.43	0.54
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.89	0.54
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.89	0.54
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.90	0.54
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.90	0.54
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.90	0.54
1:A:472:LEU:O	1:A:475:THR:HB	2.08	0.53
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.89	0.53
2:B:515:HIS:H	2:B:518:HIS:CD2	2.26	0.53
1:A:709:THR:HG22	1:A:711:ARG:H	1.72	0.53
1:A:92:HIS:HD2	1:A:94:GLY:H	1.56	0.53
2:B:685:LEU:HD12	2:B:690:VAL:HG13	1.91	0.53
2:B:792:MET:HA	2:B:856:PHE:O	2.09	0.53
2:B:344:LYS:O	2:B:347:LYS:HG2	2.07	0.53
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.74	0.53
3:C:148:ARG:HD3	3:C:149:LYS:HE3	1.90	0.53
1:A:933:TYR:O	1:A:937:VAL:HG23	2.10	0.52
2:B:1096:ARG:HH11	2:B:1096:ARG:HB2	1.73	0.52
2:B:449:ASN:HD22	2:B:452:THR:HG23	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.90	0.52
1:A:567:LYS:CB	1:A:568:PRO:CD	2.83	0.52
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.91	0.52
1:A:92:HIS:HE1	2:B:1210:MET:O	1.93	0.52
4:D:73:SER:HB2	7:G:21:ARG:HH12	1.74	0.52
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.92	0.52
1:A:362:ASP:OD2	1:A:459:ARG:HD3	2.10	0.52
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.92	0.52
1:A:982:THR:H	1:A:985:ASP:HB2	1.75	0.52
3:C:56:THR:HG22	3:C:57:VAL:N	2.25	0.52
16:X:248:LEU:O	16:X:252:PHE:HB3	2.10	0.52
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.92	0.52
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.75	0.52
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.92	0.52
1:A:1081:LEU:HD12	1:A:1099:PRO:HD3	1.92	0.51
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.10	0.51
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.92	0.51
3:C:54:ASN:OD1	3:C:56:THR:HB	2.10	0.51
6:F:99:LEU:HG	6:F:103:MET:CE	2.40	0.51
1:A:63:ARG:HG3	1:A:74:MET:HE3	1.93	0.51
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.92	0.51
6:F:128:LYS:HE2	6:F:148:VAL:O	2.10	0.51
1:A:41:MET:HB3	1:A:49:LYS:HA	1.92	0.51
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.93	0.51
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.92	0.51
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.46	0.51
1:A:549:MET:SD	1:A:577:ILE:HD11	2.50	0.51
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.92	0.51
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.93	0.51
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.92	0.50
7:G:1:MET:HE2	7:G:2:PHE:N	2.26	0.50
2:B:323:VAL:HG23	2:B:324:ILE:HD12	1.93	0.50
8:H:111:LEU:HA	8:H:127:GLY:O	2.10	0.50
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.93	0.50
1:A:929:LEU:HD21	1:A:983:ILE:HG12	1.94	0.50
1:A:42:ASP:HA	1:A:46:THR:O	2.11	0.50
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.17	0.50
3:C:66:ARG:HH21	10:J:2:ILE:HG23	1.77	0.50
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.94	0.50
7:G:102:GLN:HE22	7:G:107:LYS:HE2	1.76	0.50
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.93	0.50
1:A:1178:ASP:C	1:A:1180:GLU:H	2.15	0.50
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.47	0.50
1:A:903:ASN:ND2	1:A:905:ASP:H	2.09	0.50
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.94	0.50
3:C:4:GLU:H	3:C:7:GLN:HE22	1.60	0.50
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.94	0.50
2:B:1100:ASP:HA	2:B:1103:ILE:HG22	1.94	0.49
1:A:590:ARG:O	1:A:591:PHE:HB2	2.12	0.49
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.94	0.49
3:C:66:ARG:NH2	10:J:2:ILE:HG23	2.27	0.49
7:G:14:HIS:HD2	7:G:16:SER:H	1.59	0.49
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.76	0.49
5:E:147:HIS:CD2	5:E:149:LEU:H	2.30	0.49
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.94	0.49
1:A:856:THR:HB	1:A:865:GLN:HB2	1.95	0.49
2:B:654:ARG:H	2:B:657:HIS:CD2	2.19	0.49
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.94	0.49
2:B:542:MET:HE1	2:B:743:ILE:HB	1.95	0.49
5:E:23:VAL:HG23	5:E:30:ILE:HD13	1.94	0.49
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.60	0.49
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.13	0.49
1:A:567:LYS:CB	8:H:96:VAL:H	2.13	0.49
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.48	0.48
1:A:709:THR:HG23	9:I:94:ASP:HA	1.95	0.48
9:I:8:ARG:O	9:I:9:ASP:HB2	2.13	0.48
1:A:149:GLU:HB3	1:A:164:ARG:HD3	1.95	0.48
1:A:225:ASN:ND2	1:A:227:VAL:H	2.12	0.48
2:B:653:VAL:HG13	2:B:689:LEU:HB3	1.95	0.48
7:G:1:MET:HE1	7:G:80:LYS:H	1.79	0.48
2:B:193:LYS:HE3	10:J:65:PRO:HD2	1.95	0.48
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.95	0.48
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.95	0.48
1:A:134:ARG:HD2	1:A:221:SER:O	2.13	0.48
15:T:9:DT:H2'	15:T:10:DA:C8	2.48	0.48
5:E:147:HIS:HD2	5:E:149:LEU:H	1.59	0.48
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.96	0.48
1:A:925:LEU:HD23	1:A:983:ILE:HB	1.96	0.48
3:C:50:GLU:HG3	12:L:66:GLN:HG3	1.96	0.48
2:B:310:MET:O	2:B:313:MET:HB2	2.13	0.48
2:B:792:MET:H	2:B:857:ARG:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:MET:O	2:B:993:THR:HA	2.13	0.47
4:D:134:THR:HG23	4:D:136:GLY:H	1.79	0.47
10:J:6:ARG:HA	10:J:12:LYS:O	2.14	0.47
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.97	0.47
4:D:37:GLN:HE22	7:G:5:LYS:HE3	1.79	0.47
16:X:305:LYS:HE2	16:X:339:ASN:HD22	1.79	0.47
12:L:28:LYS:H	12:L:39:SER:HA	1.79	0.47
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.97	0.47
1:A:497:THR:HG21	2:B:1149:GLU:OE2	2.15	0.47
2:B:1022:THR:HG23	2:B:1022:THR:O	2.15	0.47
8:H:89:LEU:C	8:H:91:ASP:H	2.18	0.47
2:B:1107:ALA:O	2:B:1108:ARG:HB2	2.14	0.47
7:G:83:LYS:HD2	7:G:149:GLY:HA2	1.96	0.47
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.79	0.47
1:A:868:TYR:CZ	1:A:1064:VAL:HG22	2.50	0.47
5:E:50:MET:HB2	5:E:52:ARG:HD2	1.96	0.47
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.80	0.47
1:A:512:VAL:HA	1:A:519:PRO:HA	1.97	0.47
1:A:31:SER:OG	1:A:83:HIS:HD2	1.98	0.47
1:A:851:HIS:CD2	1:A:857:ARG:HB2	2.49	0.47
1:A:3:GLY:HA3	2:B:1159:ARG:HB3	1.96	0.47
1:A:567:LYS:CB	8:H:95:TYR:HA	2.44	0.47
1:A:1227:ILE:HG13	1:A:1239:ARG:HB2	1.97	0.47
1:A:230:ARG:HD2	1:A:233:TRP:CZ2	2.49	0.47
1:A:182:VAL:HG22	1:A:201:VAL:HG22	1.96	0.46
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.30	0.46
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.97	0.46
3:C:99:LEU:HD13	3:C:120:ILE:HG13	1.96	0.46
1:A:399:HIS:O	1:A:435:HIS:CD2	2.68	0.46
6:F:128:LYS:HG3	6:F:149:GLU:HA	1.97	0.46
1:A:337:ARG:HD2	2:B:1132:GLU:OE2	2.15	0.46
2:B:744:HIS:CD2	2:B:746:SER:H	2.27	0.46
10:J:48:ARG:O	10:J:52:THR:HG22	2.16	0.46
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.99	0.46
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.65	0.46
1:A:92:HIS:HD2	1:A:94:GLY:N	2.14	0.46
2:B:1188:LYS:H	2:B:1189:ILE:HD12	1.80	0.46
11:K:12:LEU:HD22	11:K:16:GLU:HB3	1.97	0.46
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.98	0.46
5:E:156:LEU:HD13	5:E:195:VAL:HG12	1.98	0.46
8:H:95:TYR:HE1	8:H:97:MET:CG	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:GLY:HA3	1:A:1281:ARG:HD2	1.98	0.46
16:X:245:PHE:HA	16:X:248:LEU:HD23	1.97	0.46
3:C:6:PRO:HA	3:C:24:ASN:HB3	1.97	0.46
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.51	0.46
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.96	0.45
1:A:89:PRO:HG2	1:A:204:THR:HB	1.98	0.45
1:A:915:SER:O	1:A:919:ILE:HB	2.15	0.45
2:B:516:ASN:HD22	2:B:516:ASN:H	1.64	0.45
16:X:325:VAL:HB	16:X:330:LEU:HD22	1.98	0.45
1:A:1177:LEU:HD11	16:X:237:LEU:HB3	1.98	0.45
1:A:565:ILE:HG12	1:A:567:LYS:HE2	1.98	0.45
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.57	0.45
1:A:1329:THR:HG22	1:A:1331:SER:H	1.80	0.45
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.98	0.45
7:G:1:MET:HE3	7:G:80:LYS:H	1.81	0.45
3:C:64:ALA:HA	3:C:67:LEU:HD12	1.98	0.45
12:L:38:LEU:HD13	12:L:56:LEU:HD21	1.98	0.45
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.97	0.45
8:H:47:PHE:CD2	8:H:95:TYR:HD2	2.34	0.45
13:N:5:DA:H2''	13:N:6:DG:H8	1.80	0.45
1:A:55:ASP:C	1:A:57:ARG:H	2.19	0.45
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.98	0.45
8:H:47:PHE:HB3	8:H:95:TYR:HD2	1.82	0.45
9:I:68:LEU:HB3	9:I:84:VAL:HG22	1.98	0.45
1:A:855:THR:HG22	1:A:857:ARG:HG3	1.99	0.45
3:C:173:ALA:HB2	3:C:243:VAL:HG11	1.99	0.45
6:F:76:LYS:HA	6:F:79:ARG:CD	2.47	0.45
13:N:6:DG:H2'	13:N:7:DT:C6	2.52	0.45
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.52	0.45
1:A:456:MET:HB2	1:A:478:TYR:OH	2.17	0.45
2:B:766:ARG:CZ	2:B:1020:ARG:HD3	2.47	0.45
1:A:1266:THR:HG23	1:A:1270:ASN:HD22	1.82	0.44
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.98	0.44
2:B:620:ARG:HG3	9:I:57:GLY:HA3	1.99	0.44
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.17	0.44
1:A:55:ASP:CG	1:A:55:ASP:O	2.55	0.44
2:B:745:PRO:O	2:B:748:ILE:HG12	2.17	0.44
3:C:147:LEU:HB3	3:C:151:GLN:HB3	1.99	0.44
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.99	0.44
1:A:1135:ARG:HD3	1:A:1282:VAL:HB	2.00	0.44
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:CD	1:A:58:LEU:HG	2.41	0.44
2:B:652:LYS:HD2	2:B:688:GLY:O	2.17	0.44
1:A:329:LEU:HA	1:A:335:ARG:H	1.82	0.44
1:A:492:PRO:CB	1:A:497:THR:HG23	2.47	0.44
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.18	0.44
11:K:51:LEU:HD13	11:K:59:ALA:HB3	2.00	0.44
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.83	0.44
2:B:464:GLY:HA2	2:B:480:SER:HB3	2.00	0.44
4:D:144:THR:HG21	7:G:46:LEU:HD13	2.00	0.44
9:I:8:ARG:O	9:I:9:ASP:CB	2.64	0.44
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	2.00	0.44
6:F:109:VAL:HB	6:F:124:GLU:HG2	2.00	0.44
6:F:69:LEU:C	6:F:71:GLU:H	2.21	0.44
16:X:285:GLU:HB3	16:X:336:VAL:HG21	1.99	0.44
1:A:55:ASP:OD2	1:A:55:ASP:O	2.36	0.43
2:B:126:SER:OG	2:B:172:ILE:HD11	2.18	0.43
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.00	0.43
2:B:957:ASN:HB3	2:B:961:LEU:HB2	2.00	0.43
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.53	0.43
2:B:889:THR:HG22	2:B:891:ASP:H	1.83	0.43
3:C:70:ILE:HD11	3:C:144:ILE:HG12	2.00	0.43
2:B:884:ARG:HD2	2:B:935:ARG:HB2	1.99	0.43
4:D:54:GLU:O	4:D:58:VAL:HG23	2.19	0.43
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	2.00	0.43
1:A:629:LEU:HD13	1:A:645:LEU:HD21	2.01	0.43
2:B:470:LYS:HD2	2:B:472:ALA:HB2	2.00	0.43
7:G:50:ASP:OD2	7:G:53:ASN:HB2	2.18	0.43
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.99	0.43
7:G:131:GLN:HG2	7:G:136:VAL:HG22	2.00	0.43
1:A:316:GLN:HB3	1:A:322:VAL:HG23	2.01	0.43
2:B:117:ALA:HA	2:B:122:LEU:HB2	2.00	0.43
5:E:156:LEU:HD11	5:E:197:LYS:HB2	2.01	0.43
2:B:901:PRO:HD2	12:L:59:ALA:C	2.39	0.43
1:A:901:LEU:H	1:A:926:GLN:NE2	2.16	0.43
2:B:1158:PHE:CE2	2:B:1160:VAL:HG13	2.54	0.43
2:B:460:ALA:HB2	2:B:468:GLU:HG3	2.00	0.43
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.84	0.43
2:B:877:PRO:HA	2:B:934:LYS:HE3	2.00	0.43
7:G:138:THR:HG22	7:G:139:ILE:H	1.83	0.43
3:C:18:VAL:CG1	11:K:109:TRP:HZ3	2.32	0.43
2:B:331:LEU:HB3	2:B:349:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:683:SER:O	2:B:687:GLU:HB2	2.19	0.42
16:X:286:LEU:HD12	16:X:336:VAL:HG13	2.01	0.42
1:A:527:THR:HG23	1:A:653:VAL:HB	2.01	0.42
1:A:55:ASP:N	1:A:56:PRO:CD	2.82	0.42
4:D:194:LEU:HD22	7:G:86:VAL:HG11	2.00	0.42
1:A:53:LEU:CD2	1:A:54:ASN:H	2.12	0.42
1:A:982:THR:HB	1:A:985:ASP:H	1.85	0.42
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.20	0.42
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	2.01	0.42
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.84	0.42
8:H:80:ARG:HG2	11:K:57:LEU:HD22	2.01	0.42
1:A:1035:TYR:N	1:A:1035:TYR:CD1	2.88	0.42
1:A:854:ASN:HB3	1:A:867:ILE:HD11	1.99	0.42
1:A:92:HIS:CD2	1:A:94:GLY:H	2.35	0.42
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.02	0.42
2:B:276:ILE:HD13	2:B:280:ILE:HD12	2.02	0.42
1:A:219:PHE:HA	1:A:222:LEU:HD12	2.01	0.42
2:B:269:ILE:HD11	2:B:386:LEU:HD21	2.02	0.42
2:B:468:GLU:HG2	2:B:468:GLU:O	2.19	0.42
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.55	0.42
4:D:67:ARG:HH11	4:D:71:LYS:NZ	2.17	0.42
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.53	0.42
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.01	0.42
2:B:41:LYS:O	2:B:45:SER:HB3	2.20	0.42
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.48	0.42
9:I:17:ARG:HB2	9:I:28:GLU:HG2	2.00	0.42
10:J:35:ALA:O	10:J:39:LEU:HD22	2.20	0.42
4:D:156:ASP:HB2	4:D:159:THR:OG1	2.20	0.42
16:X:249:PHE:HA	16:X:252:PHE:CD1	2.55	0.42
1:A:1279:ILE:HD11	1:A:1312:ASN:HB3	2.01	0.42
1:A:380:VAL:HG13	1:A:385:ILE:HG12	2.02	0.42
3:C:125:MET:HG3	3:C:127:ARG:HH21	1.84	0.42
3:C:259:LEU:HD12	3:C:259:LEU:HA	1.89	0.42
8:H:135:LEU:C	8:H:137:GLN:H	2.22	0.42
2:B:882:THR:HG22	2:B:883:LEU:N	2.34	0.42
4:D:130:LEU:O	4:D:134:THR:HG22	2.18	0.42
7:G:143:ILE:HG22	7:G:145:VAL:HG13	2.02	0.42
3:C:142:VAL:H	10:J:16:ASP:CB	2.32	0.42
16:X:345:ASN:HD22	16:X:348:LEU:HD12	1.85	0.42
1:A:330:LYS:O	1:A:334:GLY:HA3	2.20	0.42
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.20	0.42
1:A:336:ILE:HD11	2:B:1203:LEU:HD13	2.01	0.42
2:B:467:GLY:HA3	2:B:471:LYS:HD3	2.02	0.42
16:X:233:LYS:O	16:X:237:LEU:HG	2.20	0.42
1:A:912:LEU:HD22	1:A:1033:GLN:HA	2.02	0.41
4:D:190:GLU:HG3	7:G:167:TYR:CD1	2.55	0.41
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.01	0.41
2:B:237:VAL:HG11	2:B:255:GLN:HE21	1.85	0.41
5:E:117:THR:HB	5:E:120:ALA:H	1.86	0.41
4:D:50:LEU:HD11	7:G:4:ILE:HG13	2.01	0.41
1:A:1062:GLU:HB3	1:A:1064:VAL:HG23	2.01	0.41
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.01	0.41
2:B:976:ILE:O	2:B:990:ILE:O	2.38	0.41
3:C:260:LEU:HD23	3:C:264:GLN:HE22	1.85	0.41
1:A:871:ASP:CB	5:E:204:THR:HG23	2.49	0.41
13:N:5:DA:H2"	13:N:6:DG:C8	2.55	0.41
1:A:1186:ASP:HA	1:A:1188:GLN:HE21	1.85	0.41
1:A:442:VAL:HG21	1:A:489:LEU:HD11	2.03	0.41
2:B:291:ILE:HD12	2:B:291:ILE:N	2.35	0.41
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.85	0.41
7:G:65:ASP:OD1	7:G:67:SER:HB2	2.19	0.41
8:H:135:LEU:HD13	8:H:137:GLN:HE21	1.86	0.41
1:A:93:VAL:HG13	1:A:301:ALA:HB1	2.03	0.41
6:F:103:MET:HE3	7:G:15:PRO:HG2	2.03	0.41
1:A:526:ASP:OD2	2:B:832:GLY:HA2	2.21	0.41
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.19	0.41
2:B:251:ILE:HG13	2:B:251:ILE:H	1.66	0.41
2:B:899:ILE:HD12	2:B:911:ILE:HG22	2.03	0.41
5:E:190:LEU:HD11	5:E:196:VAL:HG13	2.02	0.41
7:G:14:HIS:HD2	7:G:16:SER:OG	2.04	0.41
11:K:7:PHE:HB2	11:K:11:LEU:HD22	2.02	0.41
1:A:399:HIS:O	1:A:435:HIS:HD2	2.02	0.41
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.50	0.41
5:E:154:ILE:O	5:E:196:VAL:HA	2.20	0.41
8:H:125:LEU:HG	8:H:130:ARG:NH2	2.33	0.41
1:A:108:MET:H	1:A:171:GLN:NE2	2.18	0.41
1:A:1424:VAL:HG11	2:B:1139:ILE:HG12	2.02	0.41
2:B:756:ILE:O	2:B:759:PRO:HD3	2.21	0.41
1:A:34:LYS:HB3	19:A:2459:EPE:O2S	2.20	0.41
1:A:380:VAL:HG12	1:A:428:TYR:HA	2.02	0.41
2:B:336:ARG:HH12	2:B:345:LYS:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.03	0.41
15:T:23:DC:H2''	15:T:24:DA:O5'	2.20	0.41
1:A:1079:MET:HB3	1:A:1098:VAL:HG23	2.01	0.41
1:A:406:ILE:HG13	1:A:412:ARG:HG2	2.01	0.41
2:B:339:THR:HG22	2:B:341:LEU:HD11	2.02	0.41
3:C:40:GLU:HG2	3:C:165:LYS:HD2	2.02	0.41
5:E:152:LYS:HD2	5:E:199:ILE:HB	2.03	0.41
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.91	0.41
1:A:605:MET:HE1	1:A:612:ILE:HG23	2.03	0.41
1:A:954:TRP:HA	1:A:955:PRO:HD3	1.97	0.41
3:C:149:LYS:HD2	3:C:150:GLY:H	1.86	0.41
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.02	0.40
1:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.85	0.40
11:K:33:ILE:HD13	11:K:87:LEU:HD22	2.04	0.40
16:X:249:PHE:HA	16:X:252:PHE:HD1	1.86	0.40
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.01	0.40
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.86	0.40
1:A:753:GLY:HA2	1:A:757:ASN:HD22	1.85	0.40
2:B:1106:ARG:CZ	2:B:1118:PRO:HB3	2.50	0.40
2:B:1167:GLY:HA3	2:B:1216:LEU:H	1.86	0.40
2:B:336:ARG:HG2	2:B:348:ARG:HH21	1.86	0.40
2:B:476:ARG:HH22	14:P:6:C:H5'	1.87	0.40
4:D:37:GLN:NE2	7:G:5:LYS:HE3	2.36	0.40
15:T:5:DC:H2''	15:T:6:DA:C8	2.56	0.40
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	2.03	0.40
2:B:1043:ASP:OD1	2:B:1045:SER:HB2	2.21	0.40
6:F:69:LEU:HD23	6:F:73:ALA:H	1.86	0.40
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.04	0.40
1:A:1030:ARG:O	1:A:1034:GLU:HB2	2.21	0.40
3:C:77:ILE:HA	3:C:77:ILE:HD12	1.96	0.40
12:L:60:ARG:HH21	12:L:65:VAL:HG21	1.85	0.40
15:T:24:DA:N3	15:T:24:DA:H2'	2.36	0.40
2:B:70:ILE:HD12	2:B:429:PHE:HE1	1.87	0.40
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.55	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	1418/1733 (82%)	1274 (90%)	96 (7%)	48 (3%)	5	29
2	B	1097/1224 (90%)	981 (89%)	84 (8%)	32 (3%)	6	35
3	C	264/318 (83%)	246 (93%)	14 (5%)	4 (2%)	13	53
4	D	174/221 (79%)	156 (90%)	11 (6%)	7 (4%)	4	25
5	E	213/215 (99%)	209 (98%)	4 (2%)	0	100	100
6	F	85/155 (55%)	79 (93%)	4 (5%)	2 (2%)	7	41
7	G	169/171 (99%)	153 (90%)	12 (7%)	4 (2%)	7	41
8	H	128/146 (88%)	103 (80%)	15 (12%)	10 (8%)	1	7
9	I	117/122 (96%)	102 (87%)	13 (11%)	2 (2%)	11	50
10	J	63/70 (90%)	55 (87%)	5 (8%)	3 (5%)	3	20
11	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
12	L	42/70 (60%)	32 (76%)	5 (12%)	5 (12%)	0	2
16	X	113/146 (77%)	101 (89%)	8 (7%)	4 (4%)	4	29
All	All	3996/4711 (85%)	3603 (90%)	272 (7%)	121 (3%)	5	34

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	57	ARG
1	A	76	GLU
1	A	253	ASN
1	A	257	ARG
1	A	311	GLN
1	A	322	VAL
1	A	332	LYS
1	A	525	GLN
1	A	567	LYS

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Mol	Chain	Res	Type
1	A	706	HIS
1	A	1188	GLN
2	B	67	SER
2	B	344	LYS
2	B	469	GLN
2	B	477	ALA
2	B	712	PRO
2	B	731	VAL
2	B	880	THR
2	B	881	ASN
2	B	1046	PRO
2	B	1176	ASN
2	B	1181	GLU
2	B	1185	CYS
4	D	18	VAL
4	D	169	SER
7	G	2	PHE
9	I	9	ASP
10	J	2	ILE
16	X	315	ASP
16	X	339	ASN
1	A	254	GLU
1	A	318	SER
1	A	331	GLY
1	A	399	HIS
1	A	423	ASP
1	A	593	GLU
1	A	1178	ASP
1	A	1184	SER
1	A	1221	LYS
1	A	1271	ILE
1	A	1281	ARG
2	B	262	GLU
2	B	339	THR
2	B	707	PRO
2	B	737	THR
2	B	772	ALA
2	B	907	GLY
3	C	141	GLY
3	C	215	GLU
3	C	227	THR
4	D	11	ARG

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Mol	Chain	Res	Type
4	D	53	SER
4	D	199	ASN
6	F	71	GLU
6	F	73	ALA
8	H	82	PRO
8	H	139	ASN
10	J	6	ARG
12	L	45	ALA
12	L	55	ILE
12	L	56	LEU
16	X	340	ALA
1	A	4	GLN
1	A	42	ASP
1	A	1175	SER
1	A	1180	GLU
1	A	1181	ALA
1	A	1183	GLN
1	A	1255	GLU
1	A	1257	ASP
1	A	1403	GLU
1	A	1405	THR
2	B	250	PHE
2	B	472	ALA
2	B	645	SER
2	B	711	GLU
2	B	713	ALA
2	B	792	MET
2	B	883	LEU
2	B	1155	SER
4	D	13	ARG
7	G	63	PRO
7	G	154	VAL
8	H	17	PRO
8	H	77	ARG
8	H	89	LEU
1	A	5	GLN
1	A	196	GLU
1	A	283	GLY
1	A	286	HIS
1	A	317	LYS
1	A	599	SER
2	B	282	ILE

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Mol	Chain	Res	Type
2	B	338	GLY
2	B	364	ILE
2	B	1173	ALA
3	C	142	VAL
4	D	218	GLU
8	H	130	ARG
10	J	64	ASN
1	A	41	MET
1	A	108	MET
1	A	258	GLY
1	A	424	ILE
1	A	626	ASN
1	A	958	VAL
1	A	1185	PHE
1	A	1437	GLY
8	H	60	ALA
8	H	85	GLY
12	L	26	THR
12	L	50	ASP
1	A	70	CYS
8	H	18	GLY
8	H	128	ASN
9	I	95	THR
16	X	344	ALA
2	B	108	VAL
7	G	139	ILE
2	B	992	ILE

### 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	1248/1520 (82%)	1115 (89%)	133 (11%)	8	32
2	B	966/1061 (91%)	860 (89%)	106 (11%)	8	31
3	C	234/274 (85%)	212 (91%)	22 (9%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	147/200 (74%)	132 (90%)	15 (10%)	9	35
5	E	197/197 (100%)	186 (94%)	11 (6%)	26	66
6	F	77/137 (56%)	66 (86%)	11 (14%)	4	19
7	G	152/152 (100%)	133 (88%)	19 (12%)	6	25
8	H	117/128 (91%)	100 (86%)	17 (14%)	4	18
9	I	113/116 (97%)	103 (91%)	10 (9%)	12	43
10	J	60/65 (92%)	48 (80%)	12 (20%)	1	8
11	K	99/102 (97%)	89 (90%)	10 (10%)	9	35
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	1
16	X	109/136 (80%)	93 (85%)	16 (15%)	4	18
All	All	3559/4145 (86%)	3165 (89%)	394 (11%)	8	31

All (394) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	45	GLN
1	A	63	ARG
1	A	68	GLN
1	A	70	CYS
1	A	71	GLN
1	A	74	MET
1	A	93	VAL
1	A	113	LEU
1	A	145	LYS
1	A	146	MET
1	A	156	ASP
1	A	160	GLN
1	A	163	SER
1	A	171	GLN
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	213	HIS
1	A	225	ASN
1	A	254	GLU
1	A	265	LYS
1	A	275	SER

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Mol	Chain	Res	Type
1	A	286	HIS
1	A	287	HIS
1	A	302	THR
1	A	303	TYR
1	A	316	GLN
1	A	320	ARG
1	A	323	LYS
1	A	324	SER
1	A	329	LEU
1	A	335	ARG
1	A	337	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	383	TYR
1	A	385	ILE
1	A	397	ASN
1	A	407	ARG
1	A	408	ASP
1	A	423	ASP
1	A	424	ILE
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	451	HIS
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	481	ASP
1	A	485	ASP
1	A	497	THR
1	A	521	MET
1	A	523	ILE
1	A	532	ARG
1	A	538	ASP
1	A	577	ILE
1	A	598	LEU
1	A	618	GLU

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Mol	Chain	Res	Type
1	A	629	LEU
1	A	640	GLN
1	A	666	ILE
1	A	691	LEU
1	A	720	ARG
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	774	ARG
1	A	821	ARG
1	A	833	GLU
1	A	849	MET
1	A	858	ASN
1	A	873	MET
1	A	878	ILE
1	A	894	GLU
1	A	896	ARG
1	A	903	ASN
1	A	905	ASP
1	A	919	ILE
1	A	920	LEU
1	A	929	LEU
1	A	973	ILE
1	A	982	THR
1	A	1000	LEU
1	A	1058	VAL
1	A	1064	VAL
1	A	1077	THR
1	A	1079	MET
1	A	1080	THR
1	A	1094	VAL
1	A	1112	LYS
1	A	1128	GLN
1	A	1133	LEU
1	A	1135	ARG
1	A	1167	GLU
1	A	1172	LEU
1	A	1186	ASP
1	A	1224	LEU
1	A	1231	ASP
1	A	1237	ILE
1	A	1242	VAL

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Mol	Chain	Res	Type
1	A	1255	GLU
1	A	1258	HIS
1	A	1260	LEU
1	A	1264	GLU
1	A	1281	ARG
1	A	1284	MET
1	A	1295	THR
1	A	1297	GLU
1	A	1329	THR
1	A	1333	ILE
1	A	1337	GLU
1	A	1341	ILE
1	A	1366	ARG
1	A	1376	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1420	ASP
1	A	1424	VAL
1	A	1426	GLU
1	A	1438	THR
1	A	1444	MET
1	A	1445	ILE
1	A	1450	LEU
1	A	1454	MET
2	B	25	ILE
2	B	46	GLN
2	B	94	LYS
2	B	101	MET
2	B	102	VAL
2	B	109	THR
2	B	128	LEU
2	B	134	LYS
2	B	167	ILE
2	B	178	ASN
2	B	211	VAL
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	251	ILE
2	B	261	ARG

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Mol	Chain	Res	Type
2	B	272	THR
2	B	273	LEU
2	B	277	LYS
2	B	278	GLN
2	B	294	ASP
2	B	310	MET
2	B	312	GLU
2	B	313	MET
2	B	324	ILE
2	B	331	LEU
2	B	345	LYS
2	B	348	ARG
2	B	354	ASP
2	B	384	ARG
2	B	387	LEU
2	B	398	ARG
2	B	423	LYS
2	B	429	PHE
2	B	446	LEU
2	B	461	LEU
2	B	466	TRP
2	B	468	GLU
2	B	471	LYS
2	B	482	VAL
2	B	485	ARG
2	B	489	SER
2	B	543	SER
2	B	547	VAL
2	B	549	THR
2	B	563	MET
2	B	570	VAL
2	B	592	ASN
2	B	603	LEU
2	B	616	ILE
2	B	617	ARG
2	B	620	ARG
2	B	628	THR
2	B	629	ASP
2	B	635	ARG
2	B	644	GLU
2	B	653	VAL
2	B	658	ILE

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Mol	Chain	Res	Type
2	B	678	GLU
2	B	682	SER
2	B	687	GLU
2	B	696	GLU
2	B	714	GLU
2	B	722	ASP
2	B	731	VAL
2	B	776	GLN
2	B	790	ASP
2	B	815	ARG
2	B	857	ARG
2	B	868	MET
2	B	873	THR
2	B	875	GLU
2	B	878	GLN
2	B	882	THR
2	B	889	THR
2	B	904	ARG
2	B	943	SER
2	B	944	THR
2	B	953	LEU
2	B	970	THR
2	B	976	ILE
2	B	983	ARG
2	B	996	ARG
2	B	997	GLU
2	B	1007	VAL
2	B	1010	LEU
2	B	1022	THR
2	B	1045	SER
2	B	1049	ASP
2	B	1060	ARG
2	B	1065	GLN
2	B	1067	ARG
2	B	1135	ARG
2	B	1145	SER
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP
2	B	1160	VAL
2	B	1175	LEU
2	B	1179	GLN

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Mol	Chain	Res	Type
2	B	1183	LYS
2	B	1188	LYS
2	B	1202	LEU
2	B	1220	ARG
2	B	1222	ARG
2	B	1223	ASP
3	C	12	GLU
3	C	16	ASP
3	C	25	VAL
3	C	34	ARG
3	C	52	GLU
3	C	100	THR
3	C	102	GLN
3	C	106	GLU
3	C	115	SER
3	C	121	VAL
3	C	125	MET
3	C	127	ARG
3	C	133	ILE
3	C	149	LYS
3	C	151	GLN
3	C	189	THR
3	C	226	ASP
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	260	LEU
3	C	265	MET
4	D	5	THR
4	D	15	LEU
4	D	47	LEU
4	D	57	LEU
4	D	65	GLU
4	D	118	THR
4	D	119	ARG
4	D	121	LYS
4	D	137	ASN
4	D	155	ARG
4	D	156	ASP
4	D	201	LYS
4	D	212	LYS
4	D	219	THR

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Mol	Chain	Res	Type
4	D	221	TYR
5	E	3	GLN
5	E	7	ARG
5	E	41	ASP
5	E	52	ARG
5	E	67	GLU
5	E	69	ILE
5	E	78	LEU
5	E	117	THR
5	E	190	LEU
5	E	204	THR
5	E	215	MET
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	87	LYS
6	F	90	ARG
6	F	93	ILE
6	F	109	VAL
6	F	111	LEU
6	F	122	MET
6	F	127	GLU
6	F	148	VAL
7	G	2	PHE
7	G	5	LYS
7	G	13	LEU
7	G	26	LEU
7	G	29	LYS
7	G	33	GLU
7	G	39	THR
7	G	60	ARG
7	G	61	ILE
7	G	63	PRO
7	G	83	LYS
7	G	93	SER
7	G	114	LEU
7	G	126	ASN
7	G	138	THR
7	G	143	ILE
7	G	152	SER
7	G	153	GLN
7	G	162	SER

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Mol	Chain	Res	Type
8	H	8	ASP
8	H	13	SER
8	H	14	GLU
8	H	17	PRO
8	H	26	ILE
8	H	31	THR
8	H	77	ARG
8	H	83	GLN
8	H	86	ASP
8	H	103	LYS
8	H	107	VAL
8	H	110	ASP
8	H	111	LEU
8	H	112	ILE
8	H	128	ASN
8	H	130	ARG
8	H	135	LEU
9	I	8	ARG
9	I	21	GLU
9	I	31	THR
9	I	35	VAL
9	I	50	THR
9	I	61	ASP
9	I	72	ASP
9	I	74	GLU
9	I	83	ASN
9	I	116	ASN
10	J	3	VAL
10	J	6	ARG
10	J	12	LYS
10	J	14	VAL
10	J	22	LEU
10	J	27	GLU
10	J	28	ASP
10	J	37	SER
10	J	39	LEU
10	J	43	ARG
10	J	48	ARG
10	J	52	THR
11	K	1	MET
11	K	11	LEU
11	K	20	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	K	25	THR
11	K	31	VAL
11	K	37	LYS
11	K	42	LEU
11	K	51	LEU
11	K	74	ARG
11	K	79	GLU
12	L	26	THR
12	L	27	LEU
12	L	28	LYS
12	L	38	LEU
12	L	46	VAL
12	L	50	ASP
12	L	53	HIS
12	L	54	ARG
12	L	55	ILE
12	L	61	THR
12	L	64	LEU
12	L	68	GLU
16	X	243	LYS
16	X	248	LEU
16	X	251	LYS
16	X	252	PHE
16	X	278	PHE
16	X	292	ASN
16	X	319	LEU
16	X	324	HIS
16	X	325	VAL
16	X	327	GLU
16	X	331	PRO
16	X	333	ASN
16	X	342	GLU
16	X	358	ILE
16	X	360	LEU
16	X	364	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	83	HIS
1	A	92	HIS
1	A	118	HIS

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	169	ASN
1	A	171	GLN
1	A	225	ASN
1	A	253	ASN
1	A	281	HIS
1	A	339	ASN
1	A	435	HIS
1	A	447	GLN
1	A	503	GLN
1	A	517	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	851	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	965	GLN
1	A	975	HIS
1	A	1124	HIS
1	A	1140	HIS
1	A	1188	GLN
1	A	1270	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	103	ASN
2	B	121	ASN
2	B	215	GLN
2	B	224	GLN
2	B	255	GLN
2	B	278	GLN
2	B	357	GLN
2	B	366	GLN
2	B	449	ASN
2	B	516	ASN
2	B	518	HIS
2	B	590	HIS
2	B	592	ASN
2	B	744	HIS
2	B	776	GLN
2	B	862	GLN

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Mol	Chain	Res	Type
2	B	957	ASN
2	B	975	GLN
2	B	986	GLN
2	B	1015	HIS
2	B	1040	ASN
2	B	1065	GLN
2	B	1084	GLN
2	B	1112	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1176	ASN
2	B	1179	GLN
3	C	7	GLN
3	C	73	GLN
3	C	102	GLN
3	C	112	ASN
3	C	264	GLN
4	D	23	ASN
4	D	37	GLN
5	E	146	HIS
5	E	147	HIS
7	G	14	HIS
7	G	71	ASN
7	G	102	GLN
7	G	126	ASN
7	G	131	GLN
8	H	133	ASN
8	H	137	GLN
9	I	12	ASN
9	I	108	HIS
9	I	114	GLN
11	K	52	ASN
11	K	65	HIS
16	X	312	ASN
16	X	339	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/11 (81%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	3	C
14	P	5	A
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	19	15,14	12,21,22	2.36	1 (8%)	16,30,33	2.73	3 (18%)

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	19	15,14	-	0/3/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	19	BRU	C4-C5	7.89	1.48	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	19	BRU	C5-C4-N3	-5.26	118.38	124.00
15	T	19	BRU	O4'-C1'-N1	2.77	112.55	107.71
15	T	19	BRU	C4-N3-C2	9.06	122.72	115.16

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 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	$\# Z  > 2$
19	EPE	A	2459	-	15,15,15	0.94	1 (6%)	19,20,20	0.65	0
19	EPE	G	1172	-	15,15,15	1.14	1 (6%)	19,20,20	0.52	0

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
19	EPE	A	2459	-	-	0/9/19/19	0/1/1/1
19	EPE	G	1172	-	-	0/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	1172	EPE	C10-S	-4.35	1.71	1.77
19	A	2459	EPE	C10-S	-3.54	1.72	1.77

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	2459	EPE	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	1426/1733 (82%)	-0.07	21 (1%) 76 62	60, 98, 157, 213	0
2	B	1115/1224 (91%)	0.04	20 (1%) 71 56	61, 107, 165, 198	0
3	C	266/318 (83%)	-0.16	0 100 100	74, 96, 135, 164	0
4	D	178/221 (80%)	-0.15	1 (0%) 90 84	79, 111, 157, 183	0
5	E	215/215 (100%)	0.06	7 (3%) 50 33	80, 134, 176, 192	0
6	F	87/155 (56%)	-0.24	0 100 100	67, 81, 116, 141	0
7	G	171/171 (100%)	-0.07	1 (0%) 90 84	77, 99, 135, 155	0
8	H	133/146 (91%)	0.31	7 (5%) 30 16	103, 140, 180, 198	0
9	I	119/122 (97%)	0.12	5 (4%) 40 24	108, 139, 175, 194	0
10	J	65/70 (92%)	-0.19	0 100 100	82, 96, 138, 151	0
11	K	115/120 (95%)	-0.04	2 (1%) 73 59	68, 98, 135, 156	0
12	L	46/70 (65%)	1.06	4 (8%) 13 6	77, 172, 184, 191	0
13	N	13/14 (92%)	0.84	3 (23%) 1 1	150, 182, 258, 261	0
14	P	10/11 (90%)	-0.34	0 100 100	85, 108, 157, 162	0
15	T	24/26 (92%)	0.18	2 (8%) 14 6	98, 147, 265, 267	0
16	X	119/146 (81%)	0.82	22 (18%) 2 1	160, 190, 211, 222	0
All	All	4102/4762 (86%)	0.01	95 (2%) 64 47	60, 106, 177, 267	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	25	ALA	8.7
11	K	115	ALA	8.4
12	L	26	THR	7.9
2	B	250	PHE	6.1
1	A	69	THR	5.7

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Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	4.9
2	B	467	GLY	4.8
2	B	709	ASP	4.7
1	A	1455	PRO	4.6
2	B	883	LEU	4.4
16	X	317	LYS	4.1
11	K	114	LEU	3.8
16	X	324	HIS	3.8
5	E	110	PHE	3.6
1	A	44	THR	3.4
16	X	257	THR	3.3
2	B	715	ALA	3.3
16	X	339	ASN	3.3
16	X	318	ASN	3.3
2	B	469	GLN	3.3
1	A	161	LEU	3.2
1	A	195	ASP	3.2
2	B	468	GLU	3.2
16	X	254	VAL	3.1
5	E	123	LEU	3.1
8	H	139	ASN	3.0
16	X	326	VAL	3.0
1	A	1176	LEU	2.9
8	H	86	ASP	2.9
2	B	882	THR	2.9
1	A	256	GLN	2.8
16	X	327	GLU	2.8
2	B	130	VAL	2.8
2	B	262	GLU	2.7
5	E	93	MET	2.7
16	X	302	TYR	2.7
1	A	158	PRO	2.7
1	A	1181	ALA	2.7
8	H	131	ASN	2.6
16	X	281	ASN	2.5
13	N	14	DG	2.5
1	A	1183	GLN	2.5
2	B	708	GLU	2.5
2	B	723	VAL	2.5
5	E	46	TYR	2.5
13	N	15	DC	2.5
1	A	253	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
8	H	140	ALA	2.4
8	H	126	GLU	2.4
9	I	117	LYS	2.4
1	A	2	VAL	2.4
16	X	275	SER	2.4
5	E	126	SER	2.4
4	D	9	GLN	2.4
2	B	866	TYR	2.4
2	B	132	VAL	2.4
16	X	255	PRO	2.4
16	X	277	GLU	2.4
1	A	152	VAL	2.3
1	A	162	VAL	2.3
1	A	255	SER	2.3
5	E	132	ILE	2.3
15	T	2	DG	2.3
5	E	109	ILE	2.3
2	B	339	THR	2.2
16	X	364	ILE	2.2
13	N	12	DG	2.2
9	I	119	THR	2.2
1	A	1257	ASP	2.2
1	A	118	HIS	2.2
16	X	328	GLY	2.2
9	I	76	PRO	2.2
1	A	155	GLU	2.2
12	L	52	GLY	2.1
16	X	245	PHE	2.1
16	X	258	ILE	2.1
9	I	26	LEU	2.1
2	B	473	MET	2.1
2	B	340	ALA	2.1
7	G	124	GLY	2.1
16	X	332	LEU	2.1
1	A	154	SER	2.1
16	X	363	PHE	2.1
2	B	869	SER	2.1
16	X	278	PHE	2.1
16	X	320	GLU	2.1
1	A	286	HIS	2.1
1	A	254	GLU	2.1
15	T	3	DC	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	167	ILE	2.0
2	B	346	GLU	2.0
8	H	134	ASN	2.0
9	I	118	ARG	2.0
16	X	244	MET	2.0
8	H	95	TYR	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. 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	19	20/21	0.96	0.13	-	91,98,105,114	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(Å <sup>2</sup> )	Q<0.9
19	EPE	A	2459	15/15	0.24	1.15	21.37	249,261,272,273	0
19	EPE	G	1172	15/15	0.37	0.85	12.47	217,230,230,231	0
17	ZN	B	2225	1/1	1.00	0.22	0.54	87,87,87,87	0
17	ZN	I	1121	1/1	0.99	0.15	0.33	117,117,117,117	0
17	ZN	A	2457	1/1	0.99	0.19	-0.45	80,80,80,80	0
17	ZN	J	1066	1/1	1.00	0.22	-0.97	84,84,84,84	0
17	ZN	C	1269	1/1	1.00	0.11	-1.14	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
17	ZN	A	2456	1/1	0.99	0.08	-1.61	124,124,124,124	0
17	ZN	I	1122	1/1	0.95	0.04	-2.07	191,191,191,191	0
17	ZN	L	1071	1/1	0.97	0.04	-5.65	193,193,193,193	0
18	MG	A	2458	1/1	0.92	0.12	-	275,275,275,275	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.