



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:48 AM GMT

PDB ID : 4A93  
Title : RNA Polymerase II elongation complex containing a CPD Lesion  
Authors : Walmacq, C.; Cheung, A.C.M.; Kireeva, M.L.; Lubkowska, L.; Ye, C.; Gotte, D.; Strathern, J.N.; Carell, T.; Cramer, P.; Kashlev, M.  
Deposited on : 2011-11-23  
Resolution : 3.40 Å(reported)

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

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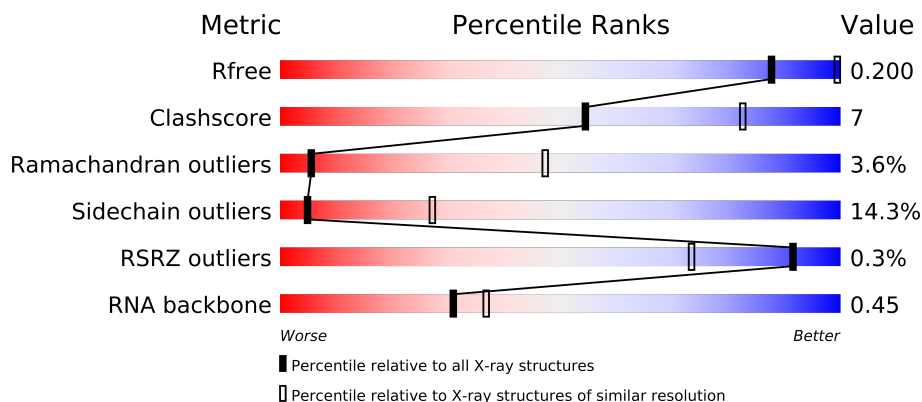
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)
RNA backbone	1838	1002 (4.02-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	1732	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

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Mol	Chain	Length	Quality of chain
13	N	14	
14	P	12	
15	T	25	

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32105 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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	1113	Total	C	N	O	S	0	0	0
			8839	5597	1548	1639	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 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	12	Total	C	N	O	P	0	0	0
			247	118	44	73	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	9	Total	C	N	O	P	0	0	0
			197	88	41	59	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	23	Total	Br	C	N	O	P	0	0
			485	1	234	81	146	23		

- 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).

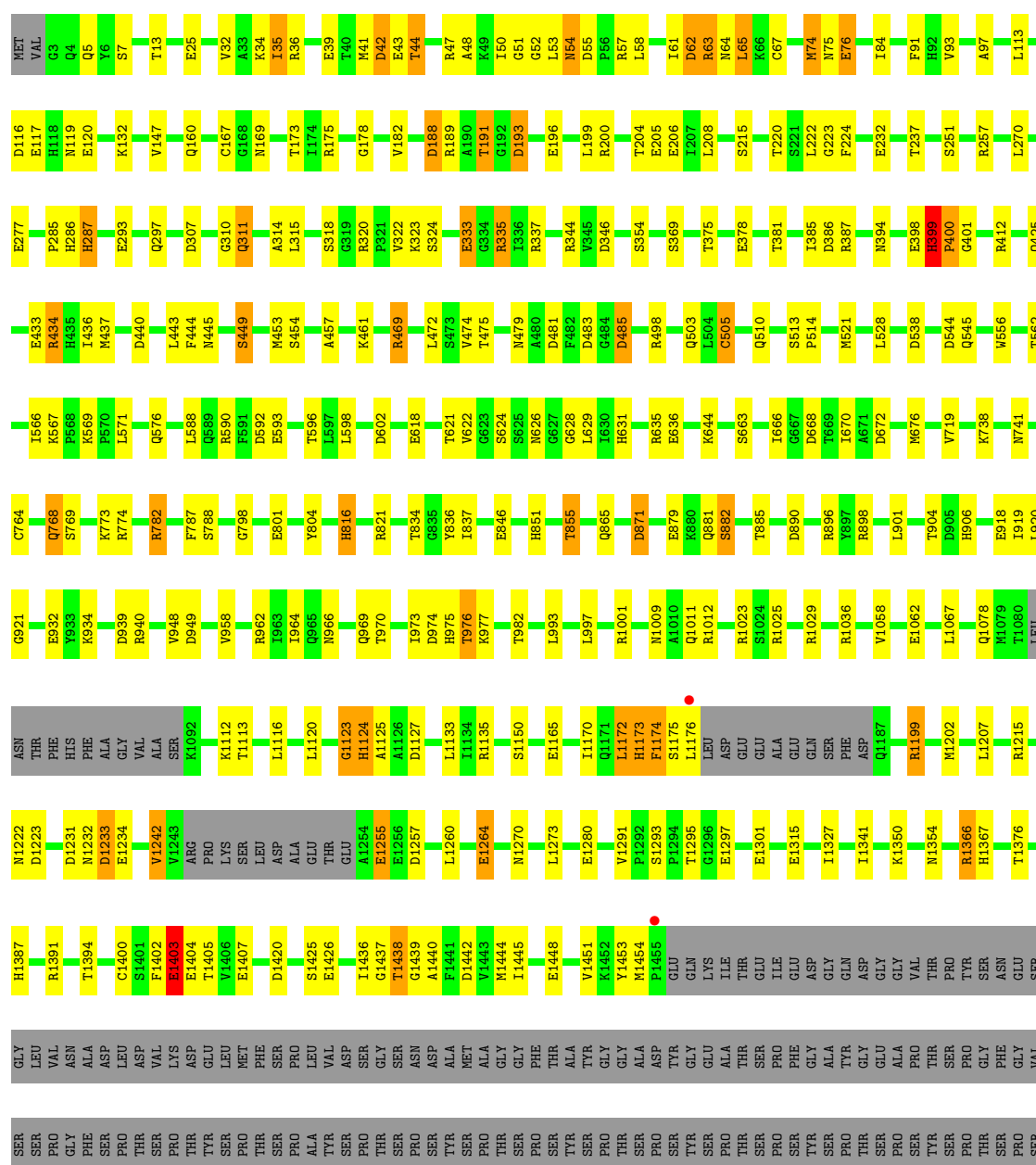
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

### 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

Chain A:







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

Chain I: 



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

Chain J: 



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

Chain K: 



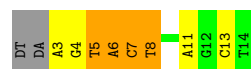
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 



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

Chain N: 



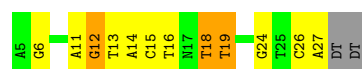
- Molecule 14: 5'-R(\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*AP\*AP)-3'

Chain P: 



- Molecule 15: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*T\*TTP\*TP\*TP\*CP\*CBR UP\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'

Chain T: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.64Å 391.52Å 281.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.09 – 3.40 54.09 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.09-3.40) 99.9 (54.09-3.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.165 , 0.199 0.167 , 0.200	Depositor DCC
$R_{free}$ test set	3291 reflections (1.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	103.5	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 81.8	EDS
Estimated twinning fraction	0.025 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.029 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 167220 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32105	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, BRU, TT

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	0.53	0/11374	0.75	1/15383 (0.0%)
2	B	0.50	0/9010	0.73	3/12149 (0.0%)
3	C	0.49	0/2133	0.67	0/2891
4	D	0.62	2/1444 (0.1%)	0.76	1/1935 (0.1%)
5	E	0.44	0/1788	0.63	0/2406
6	F	0.64	0/691	0.88	1/933 (0.1%)
7	G	0.51	0/1368	0.71	0/1844
8	H	0.39	0/1086	0.63	0/1470
9	I	0.41	0/989	0.63	0/1331
10	J	0.50	0/541	0.79	2/727 (0.3%)
11	K	0.52	0/938	0.68	0/1267
12	L	0.51	0/365	0.83	0/485
13	N	0.94	0/276	1.92	11/424 (2.6%)
14	P	0.69	0/221	1.21	0/343
15	T	0.76	0/475	1.52	12/725 (1.7%)
All	All	0.52	2/32699 (0.0%)	0.77	31/44313 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
4	D	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	187	THR	CB-CG2	9.38	1.83	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	187	THR	CA-CB	8.33	1.75	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	3	DA	O4'-C1'-N9	11.17	115.82	108.00
15	T	18	DT	O4'-C1'-N1	11.08	115.76	108.00
13	N	3	DA	O4'-C1'-C2'	-11.01	97.09	105.90
13	N	3	DA	C1'-O4'-C4'	-9.53	100.57	110.10
4	D	187	THR	CA-CB-CG2	7.69	123.17	112.40
13	N	8	DT	O4'-C1'-N1	7.52	113.27	108.00
15	T	19	DT	N3-C4-O4	6.98	124.09	119.90
15	T	11	DA	O4'-C1'-N9	6.97	112.88	108.00
13	N	7	DC	O4'-C1'-N1	6.87	112.81	108.00
15	T	19	DT	N3-C2-O2	6.80	126.38	122.30
15	T	19	DT	C5-C4-O4	-6.78	120.16	124.90
15	T	18	DT	N3-C4-O4	6.65	123.89	119.90
13	N	6	DA	O4'-C1'-N9	6.36	112.45	108.00
15	T	16	DT	O4'-C1'-N1	6.35	112.44	108.00
13	N	5	DT	N3-C2-O2	-5.90	118.76	122.30
13	N	8	DT	N3-C4-O4	5.83	123.40	119.90
15	T	13	DT	N3-C4-O4	5.75	123.35	119.90
13	N	3	DA	N9-C1'-C2'	5.74	123.51	112.60
13	N	11	DA	O4'-C1'-N9	5.51	111.86	108.00
15	T	24	DG	O4'-C4'-C3'	-5.49	102.30	104.50
1	A	65	LEU	CA-CB-CG	5.47	127.89	115.30
10	J	3	VAL	CB-CA-C	-5.42	101.10	111.40
15	T	18	DT	C5-C4-O4	-5.42	121.11	124.90
15	T	13	DT	C5-C4-O4	-5.40	121.12	124.90
6	F	135	ARG	NE-CZ-NH1	-5.37	117.61	120.30
2	B	1160	VAL	CB-CA-C	-5.34	101.25	111.40
13	N	5	DT	O4'-C1'-N1	5.22	111.66	108.00
2	B	211	VAL	CB-CA-C	-5.11	101.68	111.40
15	T	12	DG	C4'-C3'-C2'	-5.05	98.56	103.10
2	B	446	LEU	CA-CB-CG	5.03	126.88	115.30
10	J	64	ASN	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	34	LYS	Peptide
1	A	399	HIS	Peptide
1	A	55	ASP	Peptide
1	A	63	ARG	Peptide
4	D	25	ALA	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	0	76	0
2	B	8839	0	0	64	0
3	C	2095	0	0	16	0
4	D	1434	0	0	18	0
5	E	1752	0	0	9	0
6	F	679	0	0	6	0
7	G	1340	0	0	5	0
8	H	1068	0	0	6	0
9	I	971	0	0	5	0
10	J	532	0	0	7	0
11	K	920	0	0	5	0
12	L	363	0	0	2	0
13	N	247	0	0	4	0
14	P	197	0	0	15	0
15	T	485	0	0	8	0
16	A	2	0	0	0	0
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	32105	0	0	216	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (216) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:187:THR:CA	4:D:187:THR:CB	1.75	1.60
4:D:187:THR:CG2	4:D:187:THR:CB	1.83	1.55
14:P:11:A:C5'	14:P:11:A:C8	2.30	1.13
3:C:66:ARG:NH2	10:J:3:VAL:O	2.00	0.95
7:G:1:MET:SD	7:G:2:PHE:N	2.45	0.90
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.09	0.85
14:P:10:A:N6	15:T:19:DT:O4	2.14	0.80
14:P:11:A:C3'	14:P:11:A:C8	2.66	0.79
2:B:1037:LEU:O	10:J:47:ARG:NH1	2.17	0.77
13:N:13:DC:N4	15:T:6:DG:O6	2.18	0.76
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.57	0.76
1:A:976:THR:OG1	1:A:977:LYS:N	2.18	0.76
1:A:200:ARG:NH2	1:A:206:GLU:OE2	2.20	0.74
2:B:642:ASP:O	2:B:644:GLU:N	2.22	0.73
13:N:8:DT:O2	15:T:12:DG:N2	2.22	0.73
4:D:4:SER:OG	4:D:5:THR:N	2.20	0.72
2:B:322:PHE:O	2:B:325:GLN:NE2	2.23	0.72
2:B:429:PHE:O	2:B:433:GLN:NE2	2.23	0.71
14:P:11:A:C4'	14:P:11:A:C8	2.72	0.71
1:A:469:ARG:NH2	2:B:991:GLY:O	2.24	0.70
2:B:996:ARG:NH2	3:C:174:ALA:O	2.24	0.70
2:B:339:THR:OG1	2:B:351:TYR:OH	2.11	0.69
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.26	0.69
14:P:3:G:O2'	14:P:4:A:OP1	2.11	0.68
2:B:328:GLU:OE1	2:B:328:GLU:N	2.26	0.68
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.26	0.68
2:B:890:TYR:OH	2:B:936:ASP:OD2	2.11	0.67
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.27	0.67
1:A:42:ASP:O	1:A:44:THR:N	2.28	0.67
3:C:184:ASN:ND2	3:C:189:THR:O	2.28	0.67
1:A:544:ASP:OD1	1:A:545:GLN:N	2.27	0.67
2:B:531:GLN:NE2	15:T:18:DT:O4	2.28	0.67
14:P:10:A:C2'	14:P:11:A:OP1	2.44	0.66
8:H:62:SER:OG	8:H:63:LEU:N	2.28	0.66
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.28	0.66
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.29	0.66
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.30	0.65
2:B:801:LYS:O	10:J:52:THR:OG1	2.15	0.65
3:C:183:TRP:O	3:C:185:LYS:N	2.30	0.64
2:B:904:ARG:NH1	12:L:66:GLN:O	2.31	0.63
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.32	0.63
2:B:822:ASN:O	10:J:48:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:481:ASP:OD1	1:A:481:ASP:N	2.30	0.62
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.33	0.62
4:D:23:ASN:N	4:D:23:ASN:OD1	2.33	0.61
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.34	0.60
1:A:485:ASP:OD1	1:A:485:ASP:N	2.30	0.60
2:B:169:ARG:N	2:B:454:THR:OG1	2.34	0.60
2:B:221:ASN:N	2:B:241:ARG:O	2.34	0.60
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.33	0.60
4:D:26:THR:O	4:D:26:THR:OG1	2.18	0.60
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.35	0.60
2:B:1182:CYS:SG	2:B:1185:CYS:CB	2.90	0.59
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.35	0.59
1:A:1437:GLY:O	1:A:1440:ALA:N	2.35	0.59
8:H:82:PRO:O	8:H:84:ALA:N	2.36	0.59
2:B:363:HIS:O	2:B:365:THR:N	2.36	0.58
2:B:936:ASP:OD1	2:B:937:ALA:N	2.36	0.58
4:D:15:LEU:O	4:D:17:LYS:N	2.37	0.58
1:A:882:SER:O	1:A:1025:ARG:NH2	2.36	0.58
1:A:483:ASP:C	1:A:483:ASP:OD1	2.42	0.57
8:H:13:SER:N	8:H:27:GLU:O	2.38	0.57
2:B:936:ASP:OD1	2:B:938:SER:N	2.38	0.57
1:A:1437:GLY:O	1:A:1439:GLY:N	2.38	0.56
8:H:56:THR:OG1	8:H:146:ARG:NH1	2.38	0.56
3:C:165:LYS:O	11:K:6:ARG:NH1	2.39	0.56
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.37	0.56
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.38	0.56
1:A:285:PRO:O	1:A:287:HIS:N	2.39	0.56
4:D:118:THR:O	4:D:120:GLU:N	2.39	0.55
2:B:642:ASP:N	2:B:642:ASP:OD1	2.39	0.55
4:D:52:LEU:O	4:D:53:SER:OG	2.24	0.55
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.40	0.54
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.40	0.54
1:A:636:GLU:OE1	1:A:962:ARG:NH1	2.40	0.54
10:J:9:SER:OG	10:J:48:ARG:NH2	2.41	0.54
9:I:77:LYS:O	9:I:79:HIS:N	2.40	0.54
2:B:707:PRO:O	2:B:710:LEU:N	2.41	0.54
2:B:460:ALA:O	2:B:464:GLY:N	2.41	0.54
2:B:287:ARG:NH1	2:B:324:ILE:O	2.41	0.54
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.40	0.54
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.41	0.53
5:E:76:GLY:N	5:E:106:GLN:OE1	2.41	0.53
2:B:1165:ILE:O	2:B:1217:TYR:OH	2.26	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:590:ARG:NH1	1:A:592:ASP:OD2	2.41	0.53
14:P:10:A:C2	14:P:11:A:C2	2.97	0.53
2:B:861:ASP:OD1	2:B:862:GLN:N	2.42	0.53
1:A:119:ASN:OD1	1:A:120:GLU:N	2.42	0.52
2:B:979:LYS:NZ	14:P:11:A:OP2	2.41	0.52
5:E:29:PHE:N	5:E:63:ASN:O	2.41	0.52
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.43	0.52
1:A:346:ASP:N	2:B:1154:ALA:O	2.43	0.52
7:G:90:THR:O	7:G:102:GLN:N	2.43	0.51
1:A:62:ASP:O	1:A:64:ASN:N	2.43	0.51
1:A:53:LEU:CD2	1:A:54:ASN:N	2.73	0.51
5:E:46:TYR:O	5:E:54:GLN:N	2.43	0.51
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.44	0.51
1:A:437:MET:N	1:A:440:ASP:OD2	2.44	0.51
1:A:1172:LEU:O	1:A:1174:PHE:N	2.43	0.50
1:A:483:ASP:OD1	14:P:11:A:O3'	2.30	0.50
1:A:483:ASP:OD2	14:P:11:A:O3'	2.30	0.50
1:A:483:ASP:OD1	1:A:485:ASP:OD1	2.30	0.50
4:D:39:ASN:O	4:D:42:GLY:N	2.44	0.50
1:A:481:ASP:OD2	1:A:483:ASP:OD2	2.30	0.50
3:C:246:ARG:O	3:C:250:THR:N	2.45	0.50
4:D:14:ARG:O	4:D:16:LYS:N	2.45	0.50
1:A:297:GLN:O	1:A:297:GLN:NE2	2.45	0.50
1:A:974:ASP:O	1:A:976:THR:N	2.45	0.50
3:C:76:ASP:OD2	3:C:128:ASN:N	2.45	0.49
8:H:83:GLN:O	8:H:86:ASP:N	2.45	0.49
1:A:399:HIS:CG	1:A:400:PRO:N	2.78	0.49
6:F:81:THR:OG1	6:F:144:GLU:OE1	2.31	0.49
1:A:25:GLU:N	1:A:25:GLU:OE1	2.45	0.49
3:C:194:GLU:N	3:C:200:GLU:OE1	2.46	0.49
1:A:481:ASP:O	1:A:485:ASP:OD2	2.30	0.49
2:B:635:ARG:NH1	2:B:742:GLU:OE1	2.45	0.49
4:D:135:GLY:O	4:D:137:ASN:N	2.45	0.49
14:P:10:A:O2'	14:P:11:A:OP1	2.30	0.49
14:P:10:A:O2'	14:P:11:A:P	2.70	0.49
2:B:371:GLU:N	2:B:371:GLU:OE1	2.46	0.49
1:A:1199:ARG:NH2	1:A:1231:ASP:O	2.46	0.49
1:A:782:ARG:NH1	1:A:787:PHE:O	2.46	0.49
2:B:552:MET:SD	2:B:552:MET:N	2.87	0.48
1:A:836:TYR:OH	1:A:1403:GLU:OE1	2.32	0.48
2:B:554:ILE:O	2:B:558:LEU:N	2.47	0.48
1:A:1202:MET:O	1:A:1207:LEU:N	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:515:HIS:ND1	2:B:517:THR:OG1	2.47	0.48
2:B:1197:PRO:O	2:B:1200:ALA:N	2.47	0.48
1:A:966:ASN:O	1:A:970:THR:N	2.47	0.47
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.47	0.47
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.47	0.47
2:B:1065:GLN:OE1	2:B:1067:ARG:N	2.47	0.47
2:B:852:ARG:NH2	12:L:70:ARG:O	2.48	0.47
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.47	0.47
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.48	0.47
1:A:399:HIS:O	1:A:400:PRO:C	2.53	0.47
3:C:145:CYS:SG	3:C:146:LYS:N	2.88	0.47
1:A:457:ALA:N	1:A:505:CYS:O	2.48	0.46
1:A:485:ASP:OD1	14:P:11:A:O2'	2.30	0.46
1:A:399:HIS:O	1:A:401:GLY:N	2.48	0.46
1:A:949:ASP:N	1:A:949:ASP:OD1	2.49	0.46
1:A:663:SER:OG	2:B:827:ILE:O	2.33	0.46
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.48	0.46
2:B:773:MET:O	2:B:776:GLN:N	2.49	0.46
1:A:378:GLU:OE1	1:A:434:ARG:NH1	2.50	0.46
9:I:45:ARG:NH2	9:I:47:GLU:OE1	2.48	0.46
2:B:1156:ASP:OD1	2:B:1198:TYR:N	2.49	0.45
1:A:503:GLN:OE1	6:F:90:ARG:NH2	2.50	0.45
2:B:368:GLU:O	2:B:370:PHE:N	2.50	0.45
3:C:44:LEU:N	3:C:74:SER:OG	2.49	0.45
6:F:99:LEU:O	6:F:102:SER:OG	2.35	0.45
1:A:514:PRO:O	1:A:1367:HIS:NE2	2.49	0.44
1:A:483:ASP:CG	14:P:11:A:O3'	2.55	0.44
2:B:189:LEU:O	2:B:192:LEU:N	2.51	0.44
4:D:186:ASP:O	4:D:187:THR:C	2.55	0.44
1:A:562:THR:O	1:A:576:GLN:NE2	2.51	0.44
1:A:1402:PHE:O	1:A:1404:GLU:N	2.50	0.44
15:T:26:DC:N3	15:T:27:DA:N6	2.66	0.44
11:K:65:HIS:CE1	11:K:67:PHE:CG	3.05	0.44
4:D:167:LEU:O	4:D:169:SER:N	2.51	0.44
1:A:222:LEU:O	1:A:224:PHE:N	2.51	0.44
1:A:1009:ASN:OD1	1:A:1012:ARG:NH1	2.50	0.44
5:E:35:VAL:O	5:E:37:LEU:N	2.51	0.43
4:D:158:GLU:N	4:D:158:GLU:OE1	2.51	0.43
15:T:18:DT:C2	15:T:19:DT:O4	2.71	0.43
4:D:217:LEU:O	4:D:219:THR:N	2.52	0.43
5:E:163:GLU:OE2	5:E:167:ARG:NE	2.51	0.43
9:I:101:PHE:N	9:I:110:PHE:O	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:92:CYS:O	3:C:96:SER:OG	2.35	0.43
6:F:80:ALA:N	6:F:144:GLU:OE2	2.52	0.43
1:A:205:GLU:OE1	1:A:205:GLU:N	2.52	0.43
7:G:1:MET:CG	7:G:2:PHE:N	2.82	0.43
6:F:140:ASP:OD1	6:F:142:SER:OG	2.37	0.42
2:B:125:SER:O	2:B:169:ARG:NH1	2.52	0.42
1:A:624:SER:OG	1:A:624:SER:O	2.36	0.42
1:A:846:GLU:OE2	1:A:1425:SER:OG	2.37	0.42
5:E:211:TYR:CD1	5:E:211:TYR:N	2.87	0.42
1:A:768:GLN:N	1:A:798:GLY:O	2.52	0.42
8:H:118:PHE:N	8:H:121:LEU:O	2.52	0.42
3:C:69:LEU:O	10:J:6:ARG:NH1	2.52	0.42
1:A:74:MET:O	1:A:76:GLU:N	2.52	0.42
1:A:91:PHE:N	1:A:297:GLN:OE1	2.53	0.42
9:I:7:CYS:SG	9:I:10:CYS:N	2.93	0.42
14:P:6:C:C2	14:P:7:A:C8	3.08	0.42
2:B:944:THR:OG1	2:B:1122:ARG:NH2	2.53	0.41
13:N:6:DA:C2	13:N:7:DC:C2	3.08	0.41
1:A:116:ASP:OD1	1:A:116:ASP:N	2.53	0.41
3:C:185:LYS:NZ	3:C:211:ASP:O	2.53	0.41
2:B:26:THR:OG1	2:B:27:ALA:N	2.54	0.41
4:D:148:LEU:O	4:D:152:SER:OG	2.39	0.41
1:A:7:SER:OG	2:B:1161:HIS:NE2	2.53	0.41
15:T:26:DC:C4	15:T:27:DA:N6	2.89	0.41
13:N:4:DG:N2	13:N:5:DT:C2	2.88	0.41
2:B:519:TRP:C	2:B:519:TRP:CD1	2.93	0.41
2:B:788:ARG:NH2	2:B:790:ASP:OD2	2.52	0.41
7:G:14:HIS:ND1	7:G:16:SER:OG	2.53	0.41
2:B:880:THR:O	2:B:882:THR:N	2.53	0.41
1:A:1150:SER:OG	1:A:1264:GLU:OE1	2.38	0.41
1:A:481:ASP:O	1:A:485:ASP:CG	2.59	0.41
1:A:901:LEU:O	1:A:921:GLY:N	2.54	0.41
4:D:150:ASN:O	7:G:142:ARG:NH2	2.53	0.41
1:A:626:ASN:O	1:A:631:HIS:CD2	2.74	0.41
2:B:604:ARG:NH2	2:B:697:GLU:OE2	2.53	0.41
6:F:118:LEU:O	6:F:122:MET:N	2.54	0.41
2:B:198:ASP:OD2	2:B:202:TYR:OH	2.38	0.41
1:A:1123:GLY:O	1:A:1125:ALA:N	2.54	0.41
2:B:744:HIS:ND1	2:B:746:SER:OG	2.53	0.40
5:E:10:SER:O	5:E:14:ARG:N	2.54	0.40
4:D:41:GLN:N	4:D:41:GLN:OE1	2.54	0.40
2:B:610:ASN:O	2:B:613:VAL:N	2.54	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:198:ILE:N	5:E:210:SER:O	2.53	0.40
1:A:668:ASP:O	1:A:741:ASN:ND2	2.53	0.40
3:C:234:SER:OG	3:C:238:ILE:O	2.39	0.40
2:B:598:GLU:O	2:B:602:THR:OG1	2.39	0.40
15:T:14:DA:C2	15:T:15:DC:C2	3.10	0.40
9:I:7:CYS:SG	9:I:10:CYS:CB	3.09	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	1414/1732 (82%)	1209 (86%)	145 (10%)	60 (4%)	4	41
2	B	1096/1224 (90%)	945 (86%)	120 (11%)	31 (3%)	8	54
3	C	264/318 (83%)	237 (90%)	23 (9%)	4 (2%)	15	68
4	D	174/221 (79%)	146 (84%)	15 (9%)	13 (8%)	2	22
5	E	212/215 (99%)	193 (91%)	14 (7%)	5 (2%)	9	58
6	F	82/155 (53%)	74 (90%)	7 (8%)	1 (1%)	19	74
7	G	169/171 (99%)	153 (90%)	13 (8%)	3 (2%)	13	65
8	H	129/146 (88%)	102 (79%)	19 (15%)	8 (6%)	2	27
9	I	117/122 (96%)	100 (86%)	12 (10%)	5 (4%)	4	40
10	J	63/70 (90%)	56 (89%)	4 (6%)	3 (5%)	4	36
11	K	113/120 (94%)	104 (92%)	9 (8%)	0	100	100
12	L	44/70 (63%)	31 (70%)	6 (14%)	7 (16%)	0	4
All	All	3877/4564 (85%)	3350 (86%)	387 (10%)	140 (4%)	5	47

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU

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Mol	Chain	Res	Type
1	A	48	ALA
1	A	57	ARG
1	A	58	LEU
1	A	74	MET
1	A	76	GLU
1	A	169	ASN
1	A	193	ASP
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	399	HIS
1	A	556	TRP
1	A	885	THR
1	A	1403	GLU
1	A	1438	THR
2	B	340	ALA
2	B	343	ILE
2	B	367	LEU
2	B	476	ARG
2	B	643	ASP
2	B	707	PRO
2	B	731	VAL
2	B	879	ARG
2	B	881	ASN
2	B	959	ASP
2	B	1046	PRO
2	B	1170	THR
4	D	13	ARG
4	D	15	LEU
4	D	16	LYS
4	D	18	VAL
4	D	53	SER
4	D	119	ARG
4	D	169	SER
4	D	198	LEU
7	G	154	VAL
8	H	83	GLN
9	I	95	THR
10	J	2	ILE
10	J	6	ARG
12	L	39	SER
1	A	97	ALA

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Mol	Chain	Res	Type
1	A	167	CYS
1	A	178	GLY
1	A	223	GLY
1	A	310	GLY
1	A	314	ALA
1	A	318	SER
1	A	628	GLY
1	A	774	ARG
1	A	855	THR
1	A	1123	GLY
1	A	1124	HIS
1	A	1173	HIS
1	A	1175	SER
1	A	1232	ASN
1	A	1233	ASP
1	A	1405	THR
2	B	108	VAL
2	B	867	GLY
2	B	937	ALA
2	B	1155	SER
2	B	1176	ASN
2	B	1181	GLU
3	C	136	ASP
3	C	184	ASN
4	D	218	GLU
5	E	36	GLU
5	E	45	LYS
8	H	81	PRO
8	H	82	PRO
9	I	9	ASP
9	I	78	CYS
9	I	79	HIS
12	L	56	LEU
1	A	51	GLY
1	A	63	ARG
1	A	75	ASN
1	A	189	ARG
1	A	333	GLU
1	A	400	PRO
1	A	449	SER
1	A	958	VAL
1	A	975	HIS

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Mol	Chain	Res	Type
2	B	249	ARG
2	B	363	HIS
2	B	711	GLU
2	B	772	ALA
2	B	883	LEU
2	B	943	SER
2	B	1108	ARG
2	B	1156	ASP
4	D	40	HIS
4	D	138	ASN
4	D	168	LYS
5	E	113	GLN
8	H	128	ASN
12	L	45	ALA
12	L	64	LEU
1	A	44	THR
1	A	65	LEU
1	A	196	GLU
1	A	569	LYS
1	A	1255	GLU
2	B	667	GLN
2	B	708	GLU
2	B	713	ALA
3	C	4	GLU
3	C	214	ASN
4	D	10	THR
5	E	43	LYS
8	H	17	PRO
8	H	60	ALA
8	H	77	ARG
8	H	132	LEU
9	I	47	GLU
12	L	26	THR
12	L	59	ALA
1	A	188	ASP
1	A	191	THR
1	A	510	GLN
1	A	1127	ASP
5	E	140	LEU
6	F	73	ALA
7	G	57	GLN
10	J	64	ASN

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Mol	Chain	Res	Type
12	L	42	ARG
1	A	42	ASP
1	A	54	ASN
1	A	453	MET
1	A	567	LYS
1	A	1448	GLU
7	G	63	PRO
1	A	35	ILE
1	A	1242	VAL
2	B	263	GLY
1	A	52	GLY
1	A	61	ILE
2	B	369	GLY

### 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%)	1057 (85%)	183 (15%)	4	25
2	B	964/1061 (91%)	816 (85%)	148 (15%)	4	23
3	C	234/274 (85%)	206 (88%)	28 (12%)	7	35
4	D	160/200 (80%)	136 (85%)	24 (15%)	4	25
5	E	196/197 (100%)	178 (91%)	18 (9%)	13	52
6	F	74/137 (54%)	65 (88%)	9 (12%)	7	34
7	G	152/152 (100%)	128 (84%)	24 (16%)	4	22
8	H	117/128 (91%)	100 (86%)	17 (14%)	5	26
9	I	113/116 (97%)	101 (89%)	12 (11%)	10	43
10	J	60/65 (92%)	53 (88%)	7 (12%)	8	37
11	K	99/102 (97%)	88 (89%)	11 (11%)	9	40
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	3
All	All	3449/4008 (86%)	2956 (86%)	493 (14%)	5	27

All (493) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	32	VAL
1	A	35	ILE
1	A	36	ARG
1	A	39	GLU
1	A	41	MET
1	A	47	ARG
1	A	50	ILE
1	A	62	ASP
1	A	67	CYS
1	A	84	ILE
1	A	93	VAL
1	A	113	LEU
1	A	117	GLU
1	A	132	LYS
1	A	147	VAL
1	A	160	GLN
1	A	173	THR
1	A	175	ARG
1	A	182	VAL
1	A	188	ASP
1	A	191	THR
1	A	193	ASP
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	215	SER
1	A	220	THR
1	A	232	GLU
1	A	237	THR
1	A	251	SER
1	A	270	LEU
1	A	277	GLU
1	A	287	HIS
1	A	293	GLU
1	A	307	ASP
1	A	315	LEU
1	A	320	ARG
1	A	322	VAL
1	A	323	LYS
1	A	324	SER
1	A	333	GLU
1	A	335	ARG

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Mol	Chain	Res	Type
1	A	337	ARG
1	A	344	ARG
1	A	354	SER
1	A	369	SER
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	394	ASN
1	A	398	GLU
1	A	412	ARG
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	444	PHE
1	A	445	ASN
1	A	449	SER
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	479	ASN
1	A	485	ASP
1	A	498	ARG
1	A	505	CYS
1	A	513	SER
1	A	521	MET
1	A	528	LEU
1	A	538	ASP
1	A	566	ILE
1	A	571	LEU
1	A	588	LEU
1	A	593	GLU
1	A	596	THR
1	A	598	LEU
1	A	602	ASP
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU

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Mol	Chain	Res	Type
1	A	635	ARG
1	A	644	LYS
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	676	MET
1	A	719	VAL
1	A	738	LYS
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	782	ARG
1	A	788	SER
1	A	801	GLU
1	A	816	HIS
1	A	821	ARG
1	A	834	THR
1	A	837	ILE
1	A	851	HIS
1	A	855	THR
1	A	865	GLN
1	A	871	ASP
1	A	881	GLN
1	A	882	SER
1	A	896	ARG
1	A	904	THR
1	A	906	HIS
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	932	GLU
1	A	934	LYS
1	A	948	VAL
1	A	964	ILE
1	A	969	GLN
1	A	973	ILE
1	A	976	THR
1	A	982	THR
1	A	993	LEU
1	A	1001	ARG
1	A	1036	ARG

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Mol	Chain	Res	Type
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1112	LYS
1	A	1113	THR
1	A	1116	LEU
1	A	1120	LEU
1	A	1124	HIS
1	A	1133	LEU
1	A	1135	ARG
1	A	1165	GLU
1	A	1170	ILE
1	A	1172	LEU
1	A	1173	HIS
1	A	1174	PHE
1	A	1176	LEU
1	A	1199	ARG
1	A	1215	ARG
1	A	1222	ASN
1	A	1223	ASP
1	A	1234	GLU
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1270	ASN
1	A	1273	LEU
1	A	1280	GLU
1	A	1291	VAL
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1301	GLU
1	A	1315	GLU
1	A	1327	ILE
1	A	1341	ILE
1	A	1366	ARG
1	A	1376	THR
1	A	1387	HIS
1	A	1391	ARG

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Mol	Chain	Res	Type
1	A	1394	THR
1	A	1400	CYS
1	A	1403	GLU
1	A	1407	GLU
1	A	1420	ASP
1	A	1426	GLU
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1453	TYR
1	A	1454	MET
2	B	44	VAL
2	B	46	GLN
2	B	66	ASP
2	B	101	MET
2	B	102	VAL
2	B	105	SER
2	B	112	LEU
2	B	131	ASP
2	B	134	LYS
2	B	165	VAL
2	B	185	THR
2	B	211	VAL
2	B	217	ARG
2	B	218	SER
2	B	225	VAL
2	B	228	LYS
2	B	248	SER
2	B	251	ILE
2	B	261	ARG
2	B	265	SER
2	B	272	THR
2	B	278	GLN
2	B	313	MET
2	B	325	GLN
2	B	337	ARG
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU

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Mol	Chain	Res	Type
2	B	348	ARG
2	B	350	GLN
2	B	357	GLN
2	B	361	LEU
2	B	365	THR
2	B	367	LEU
2	B	371	GLU
2	B	387	LEU
2	B	394	ASP
2	B	401	PHE
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	425	THR
2	B	429	PHE
2	B	430	ARG
2	B	434	ARG
2	B	448	ILE
2	B	453	ILE
2	B	455	SER
2	B	470	LYS
2	B	475	SER
2	B	476	ARG
2	B	480	SER
2	B	481	GLN
2	B	485	ARG
2	B	490	SER
2	B	498	THR
2	B	502	ILE
2	B	529	GLU
2	B	552	MET
2	B	559	SER
2	B	570	VAL
2	B	574	SER
2	B	598	GLU
2	B	603	LEU
2	B	608	ASP
2	B	613	VAL
2	B	615	MET
2	B	620	ARG
2	B	628	THR
2	B	641	GLU

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Mol	Chain	Res	Type
2	B	642	ASP
2	B	648	HIS
2	B	653	VAL
2	B	658	ILE
2	B	678	GLU
2	B	690	VAL
2	B	706	GLN
2	B	722	ASP
2	B	730	ARG
2	B	734	HIS
2	B	737	THR
2	B	754	SER
2	B	764	SER
2	B	766	ARG
2	B	773	MET
2	B	786	ASN
2	B	788	ARG
2	B	790	ASP
2	B	830	TYR
2	B	831	SER
2	B	835	GLN
2	B	837	ASP
2	B	843	GLN
2	B	844	SER
2	B	857	ARG
2	B	858	SER
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	884	ARG
2	B	887	HIS
2	B	889	THR
2	B	904	ARG
2	B	915	THR
2	B	916	THR
2	B	944	THR
2	B	945	GLU
2	B	953	LEU
2	B	956	THR
2	B	959	ASP
2	B	964	VAL
2	B	970	THR

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Mol	Chain	Res	Type
2	B	986	GLN
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1045	SER
2	B	1048	THR
2	B	1050	ILE
2	B	1051	THR
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1106	ARG
2	B	1112	GLN
2	B	1122	ARG
2	B	1129	ARG
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1166	CYS
2	B	1169	MET
2	B	1170	THR
2	B	1172	ILE
2	B	1175	LEU
2	B	1182	CYS
2	B	1183	LYS
2	B	1188	LYS
2	B	1196	ILE
2	B	1202	LEU
2	B	1220	ARG
2	B	1221	SER
3	C	16	ASP
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	27	LEU
3	C	50	GLU

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Mol	Chain	Res	Type
3	C	55	THR
3	C	56	THR
3	C	57	VAL
3	C	81	GLU
3	C	89	GLU
3	C	108	GLU
3	C	111	THR
3	C	119	VAL
3	C	124	LEU
3	C	127	ARG
3	C	129	ILE
3	C	136	ASP
3	C	148	ARG
3	C	200	GLU
3	C	204	SER
3	C	215	GLU
3	C	224	GLN
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	11	ARG
4	D	17	LYS
4	D	18	VAL
4	D	23	ASN
4	D	34	GLN
4	D	51	ASN
4	D	52	LEU
4	D	63	LEU
4	D	73	SER
4	D	118	THR
4	D	121	LYS
4	D	126	ILE
4	D	139	LYS
4	D	141	LEU
4	D	146	GLN
4	D	159	THR
4	D	186	ASP
4	D	187	THR

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Mol	Chain	Res	Type
4	D	197	SER
4	D	213	GLU
4	D	217	LEU
4	D	219	THR
5	E	2	ASP
5	E	5	ASN
5	E	6	GLU
5	E	10	SER
5	E	18	THR
5	E	31	THR
5	E	49	SER
5	E	65	THR
5	E	72	PHE
5	E	84	ASP
5	E	95	THR
5	E	114	ASN
5	E	131	THR
5	E	173	SER
5	E	174	GLN
5	E	191	LYS
5	E	192	ARG
5	E	203	GLU
6	F	72	LYS
6	F	82	THR
6	F	92	ARG
6	F	109	VAL
6	F	111	LEU
6	F	115	THR
6	F	128	LYS
6	F	148	VAL
6	F	153	VAL
7	G	2	PHE
7	G	13	LEU
7	G	22	MET
7	G	34	VAL
7	G	37	SER
7	G	60	ARG
7	G	64	THR
7	G	75	ARG
7	G	83	LYS
7	G	92	VAL
7	G	95	SER

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Mol	Chain	Res	Type
7	G	106	MET
7	G	114	LEU
7	G	118	ASP
7	G	134	GLU
7	G	135	ASP
7	G	136	VAL
7	G	143	ILE
7	G	145	VAL
7	G	151	ILE
7	G	152	SER
7	G	154	VAL
7	G	155	SER
7	G	162	SER
8	H	14	GLU
8	H	26	ILE
8	H	32	THR
8	H	42	ILE
8	H	46	LEU
8	H	76	THR
8	H	86	ASP
8	H	89	LEU
8	H	91	ASP
8	H	106	GLU
8	H	107	VAL
8	H	108	SER
8	H	114	VAL
8	H	124	ARG
8	H	130	ARG
8	H	138	GLU
8	H	145	ARG
9	I	5	ARG
9	I	7	CYS
9	I	8	ARG
9	I	31	THR
9	I	43	VAL
9	I	50	THR
9	I	55	THR
9	I	62	ILE
9	I	94	ASP
9	I	111	THR
9	I	113	ASP
9	I	120	GLN

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Mol	Chain	Res	Type
10	J	7	CYS
10	J	13	VAL
10	J	14	VAL
10	J	23	ASN
10	J	34	THR
10	J	42	LYS
10	J	48	ARG
11	K	6	ARG
11	K	12	LEU
11	K	18	LYS
11	K	22	ASP
11	K	25	THR
11	K	41	THR
11	K	47	ARG
11	K	51	LEU
11	K	95	ILE
11	K	101	LEU
11	K	107	THR
12	L	27	LEU
12	L	37	LYS
12	L	38	LEU
12	L	44	ASP
12	L	50	ASP
12	L	51	CYS
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	64	LEU
12	L	65	VAL
12	L	68	GLU

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/12 (75%)	2 (22%)	2 (22%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	4	A
14	P	11	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	3	G
14	P	10	A

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

2 non-standard protein/DNA/RNA residues are 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	TT	T	17	15	41,43,44	1.35	5 (12%)	66,69,72	2.20	16 (24%)
15	BRU	T	22	15,14	19,21,22	1.84	4 (21%)	22,30,33	1.90	4 (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	TT	T	17	15	-	0/19/105/106	0/0/6/6
15	BRU	T	22	15,14	-	0/5/21/22	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C4-C5	4.64	1.47	1.39
15	T	17	TT	P-O2P	4.39	1.51	1.46
15	T	22	BRU	P-OP1	4.11	1.51	1.46
15	T	22	BRU	C2-N1	3.46	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	17	TT	C2-N3	-3.08	1.32	1.38
15	T	17	TT	C1R-N1T	2.88	1.49	1.45
15	T	17	TT	C4-N3	-2.84	1.32	1.37
15	T	17	TT	C2-N1	2.76	1.42	1.36
15	T	22	BRU	C4-N3	-2.24	1.33	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	17	TT	C1'-N1-C2	-8.07	105.61	117.72
15	T	17	TT	O4R-C1R-N1T	7.56	118.19	108.76
15	T	17	TT	C4-N3-C2	-5.58	116.98	126.84
15	T	22	BRU	N3-C2-N1	5.55	120.61	115.97
15	T	22	BRU	C2'-C1'-N1	-4.11	103.41	114.08
15	T	17	TT	O4T-C4T-C5T	-4.08	119.66	122.92
15	T	17	TT	O4-C4-C5	-3.87	119.83	122.92
15	T	17	TT	C2'-C1'-N1	-3.67	110.39	115.68
15	T	17	TT	C6-N1-C2	-3.65	113.44	121.99
15	T	17	TT	C2R-C1R-N1T	-2.80	111.66	115.68
15	T	17	TT	N3T-C2T-N1T	2.72	119.64	116.74
15	T	17	TT	C1'-N1-C6	-2.67	109.68	118.59
15	T	17	TT	C4T-N3T-C2T	-2.66	122.15	126.84
15	T	22	BRU	C4-N3-C2	-2.44	120.37	125.39
15	T	22	BRU	C6-N1-C2	-2.44	121.71	122.41
15	T	17	TT	O2-C2-N1	-2.42	119.58	123.45
15	T	17	TT	C5'-C4'-C3'	-2.30	108.95	114.41
15	T	17	TT	O4R-C4R-C5R	2.29	117.52	109.36
15	T	17	TT	O5R-C5R-C4R	2.28	114.84	109.21
15	T	17	TT	O2T-C2T-N1T	-2.05	120.18	123.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1422/1732 (82%)	-0.15	2 (0%) 93 82	56, 101, 162, 298	0
2	B	1113/1224 (90%)	-0.07	5 (0%) 90 68	53, 113, 185, 237	0
3	C	266/318 (83%)	-0.19	0 100 100	72, 102, 141, 189	0
4	D	178/221 (80%)	-0.11	0 100 100	80, 116, 180, 211	0
5	E	214/215 (99%)	-0.11	1 (0%) 88 61	77, 137, 188, 195	0
6	F	84/155 (54%)	-0.31	0 100 100	59, 80, 109, 134	0
7	G	171/171 (100%)	-0.13	0 100 100	63, 100, 139, 166	0
8	H	133/146 (91%)	0.18	0 100 100	106, 151, 194, 218	0
9	I	119/122 (97%)	-0.09	3 (2%) 54 22	107, 141, 182, 219	0
10	J	65/70 (92%)	-0.21	0 100 100	77, 106, 146, 157	0
11	K	115/120 (95%)	-0.17	1 (0%) 81 47	66, 101, 137, 163	0
12	L	46/70 (65%)	0.02	0 100 100	91, 154, 198, 202	0
13	N	12/14 (85%)	-0.62	0 100 100	164, 177, 260, 301	0
14	P	9/12 (75%)	-0.36	0 100 100	132, 150, 197, 204	0
15	T	23/25 (92%)	-0.49	0 100 100	125, 178, 286, 307	0
All	All	3970/4615 (86%)	-0.12	12 (0%) 91 73	53, 110, 179, 307	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	3.7
9	I	120	GLN	3.0
2	B	468	GLU	2.8
9	I	118	ARG	2.8
1	A	1455	PRO	2.7
9	I	119	THR	2.5
11	K	115	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	93	MET	2.2
2	B	708	GLU	2.2
2	B	715	ALA	2.1
2	B	340	ALA	2.1
1	A	1176	LEU	2.1

## 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	TT	T	17	38/39	0.22	1.00	112,230,240,242	0
15	BRU	T	22	20/21	0.14	-0.43	161,193,214,215	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
16	ZN	J	1066	1/1	0.21	0.27	90,90,90,90	0
16	ZN	I	1121	1/1	0.12	0.08	120,120,120,120	0
16	ZN	C	1269	1/1	0.13	-0.47	75,75,75,75	0
16	ZN	B	2225	1/1	0.18	-0.60	75,75,75,75	0
16	ZN	A	2457	1/1	0.14	-0.79	70,70,70,70	0
16	ZN	I	1122	1/1	0.06	-1.22	196,196,196,196	0
16	ZN	L	1071	1/1	0.07	-1.59	187,187,187,187	0
17	MG	A	2458	1/1	0.09	-3.18	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	ZN	A	2456	1/1	0.05	-3.57	127,127,127,127	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.