



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:43 AM GMT

PDB ID : 4A1C  
Title : T.THERMOPHILA 60S RIBOSOMAL SUBUNIT IN COMPLEX WITH INITIATION FACTOR 6. THIS FILE CONTAINS 5S RRNA, 5.8S RRNA AND PROTEINS OF MOLECULE 4.  
Authors : Klinge, S.; Voigts-Hoffmann, F.; Leibundgut, M.; Arpagaus, S.; Ban, N.  
Deposited on : 2011-09-14  
Resolution : 3.52 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>

---

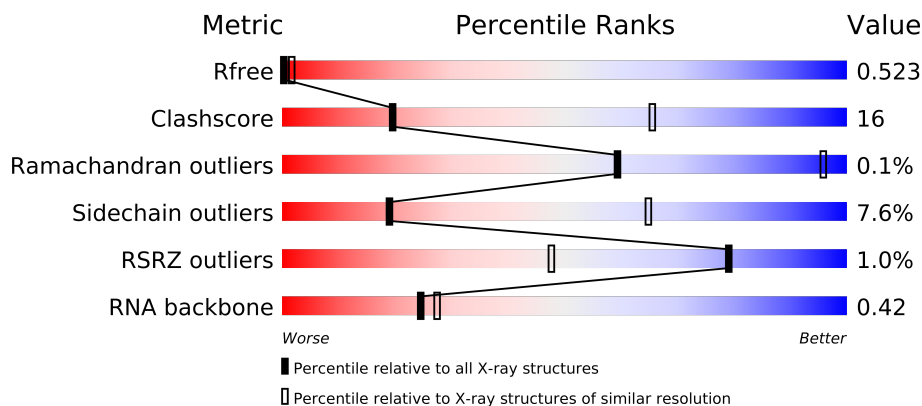
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.52 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.









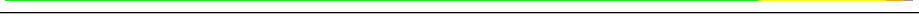

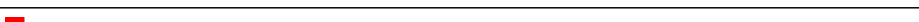







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1256 (3.74-3.30)
Clashscore	79885	1020 (3.68-3.36)
Ramachandran outliers	78287	1082 (3.70-3.34)
Sidechain outliers	78261	1082 (3.70-3.34)
RSRZ outliers	66119	1256 (3.74-3.30)
RNA backbone	1838	1008 (4.26-2.76)

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	2	154	
2	3	120	
3	A	264	
4	B	391	
5	C	410	
6	D	172	
7	E	188	
8	F	255	
9	G	123	
10	H	215	
11	I	198	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
12	J	141	
13	K	149	
14	L	204	
15	M	301	
16	N	181	
17	O	185	
18	P	157	
19	Q	183	
20	R	150	
21	S	135	
22	T	158	
23	U	124	
24	V	239	
25	W	111	
26	X	134	
27	Y	103	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
28	MG	0	197	-	X
28	MG	0	200	-	X
28	MG	0	228	-	X
28	MG	0	325	-	X
28	MG	0	347	-	X

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 43522 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 RNA chain called 5.8S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	154	Total	C	N	O	P	0	0	0
			3300	1475	602	1069	154			

- Molecule 2 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3	120	Total	C	N	O	P	0	0	0
			2566	1145	463	838	120			

- Molecule 3 is a protein called RPL8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	257	Total	C	N	O	S	0	0	0
			1977	1226	400	343	8			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	386	Total	C	N	O	S	0	0	0
			3080	1944	595	530	11			

- Molecule 5 is a protein called RPL4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	409	Total	C	N	O	S	0	0	0
			3172	1975	622	571	4			

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	169	Total	C	N	O	S	0	0	0
			1357	851	254	243	9			

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	186	Total	C	N	O	S	0	0	0
			1481	939	272	264	6			

- Molecule 8 is a protein called RPL7A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	231	Total	C	N	O	S	0	0	0
			1860	1191	341	327	1			

- Molecule 9 is a protein called RPLP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	123	Total	C	N	O	S	0	0	0
			711	465	123	123				

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	201	Total	C	N	O	S	0	0	0
			1620	1027	319	271	3			

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L13A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	198	Total	C	N	O	S	0	0	0
			1594	1019	308	263	4			

- Molecule 12 is a protein called RPL23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	138	Total	C	N	O	S	0	0	0
			1022	643	193	179	7			

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	148	Total	C	N	O	S	0	0	0
			1161	739	234	182	6			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	203	Total	C	N	O	S	0	0	0
			1691	1061	351	275	4			

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	300	Total	C	N	O	S	0	0	0
			2424	1541	447	432	4			

- Molecule 16 is a protein called RPL18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	180	Total	C	N	O	S	0	0	0
			1441	909	280	249	3			

- Molecule 17 is a protein called RPL19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	153	Total	C	N	O	S	0	0	0
			1234	772	256	201	5			

- Molecule 18 is a protein called 60S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	156	Total	C	N	O	S	0	0	0
			1272	804	251	215	2			

- Molecule 19 is a protein called RPL17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	157	Total	C	N	O	S	0	0	0
			1239	771	249	216	3			

- Molecule 20 is a protein called RPL23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	121	Total	C	N	O	S	0	0	0
			965	613	176	173	3			

- Molecule 21 is a protein called RPL26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	126	Total	C	N	O	S	0	0	0
			1013	638	200	173	2			

- Molecule 22 is a protein called RPL24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	61	Total	C	N	O	S	0	0	0
			510	331	100	76	3			

- Molecule 23 is a protein called RPL35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	123	Total	C	N	O	S	0	0	0
			990	629	196	165				

- Molecule 24 is a protein called 60S RIBOSOMAL PROTEIN L7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	234	Total	C	N	O	S	0	0	0
			1910	1221	362	323	4			

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	110	Total	C	N	O	S	0	0	0
			901	563	171	164	3			

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	125	Total	C	N	O	S	0	0	0
			1012	639	205	165	3			

- Molecule 27 is a protein called RPL37A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	102	Total	C	N	O	S	0	0	0
			786	502	148	131	5			

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	0	176	Total	Mg	0	0
			176	176		

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	Y	1	Total	Zn	0	0
			1	1		

- Molecule 30 is water.

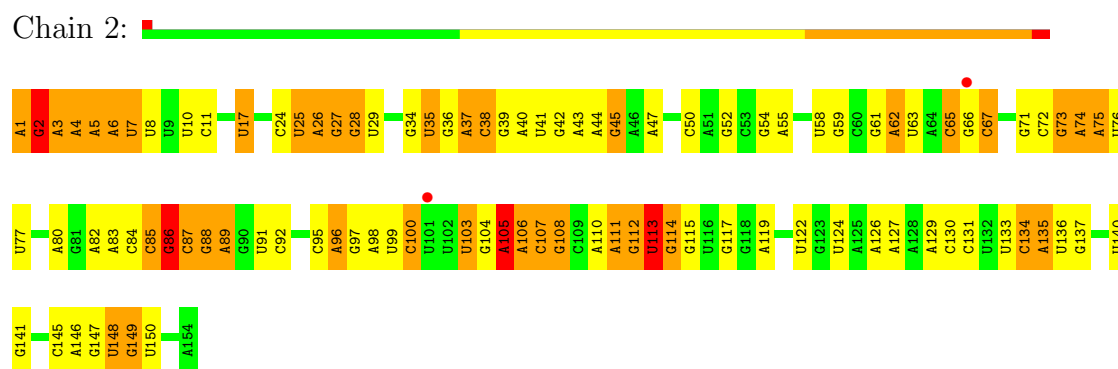
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	0	1056	Total	O	0	0
			1056	1056		



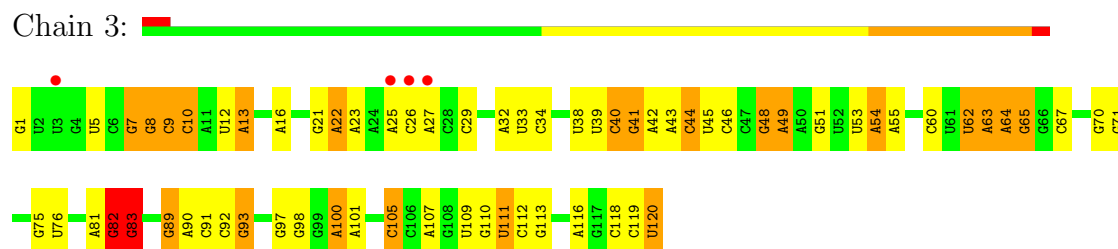
### 3 Residue-property plots

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: 5.8S rRNA



#### • Molecule 2: 5S rRNA

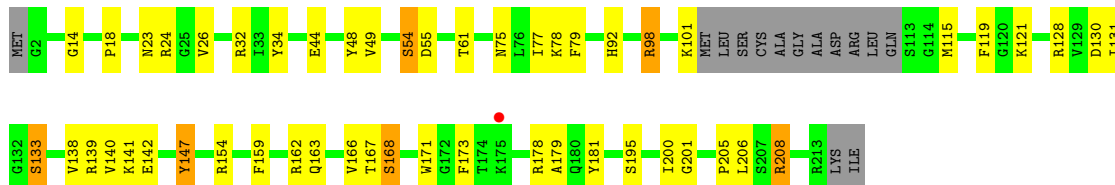






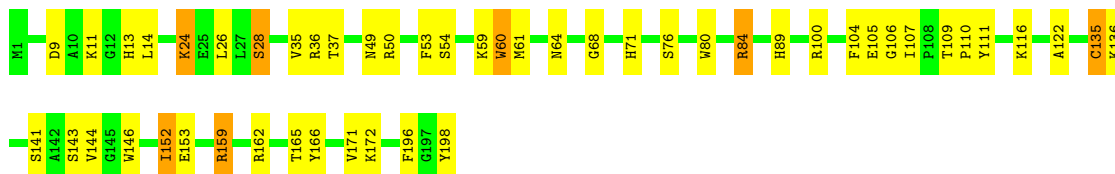
• Molecule 10: 60S RIBOSOMAL PROTEIN L10

Chain H:



• Molecule 11: 60S RIBOSOMAL PROTEIN L13A

Chain I:



• Molecule 12: RPL23

Chain J:



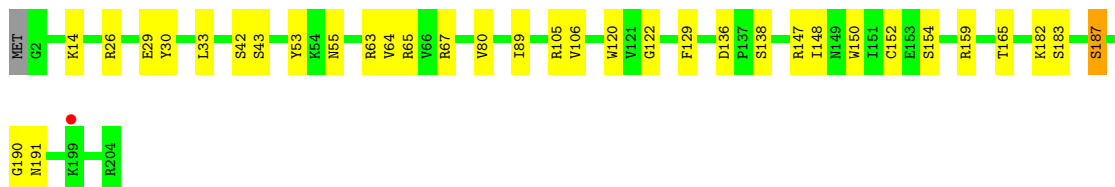
• Molecule 13: 60S RIBOSOMAL PROTEIN L27A

Chain K:



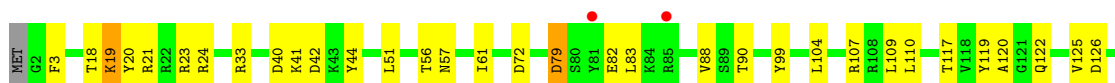
• Molecule 14: RIBOSOMAL PROTEIN L15

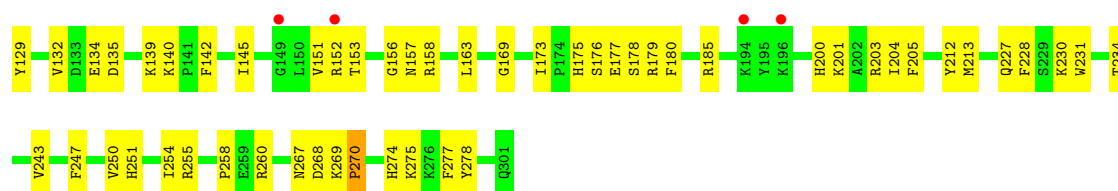
Chain L:



• Molecule 15: 60S RIBOSOMAL PROTEIN L5

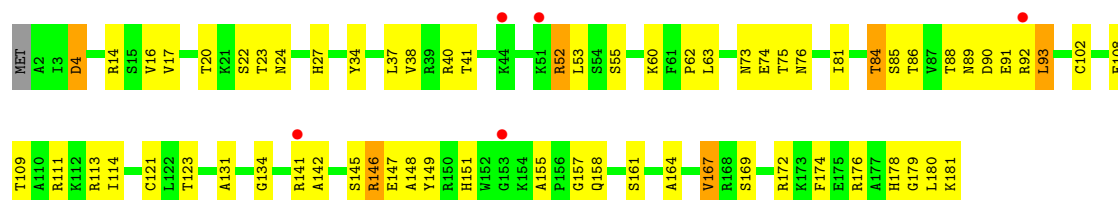
Chain M:





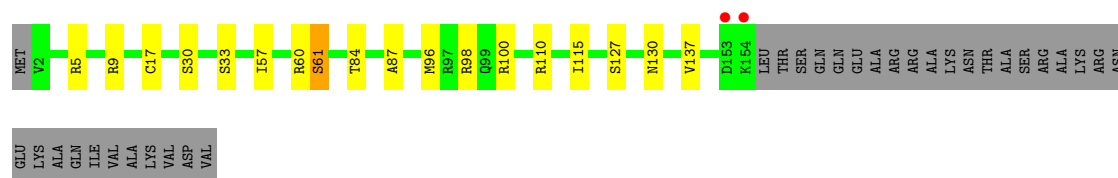
• Molecule 16: RPL18

Chain N:



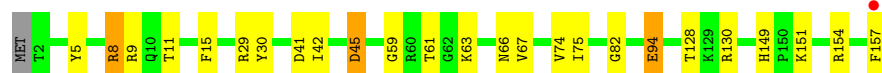
• Molecule 17: RPL19

Chain O:



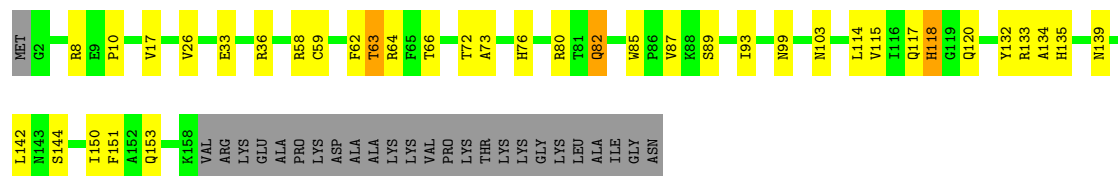
• Molecule 18: 60S RIBOSOMAL PROTEIN L21

Chain P:



• Molecule 19: RPL17

Chain Q:



• Molecule 20: RPL23A

Chain R:

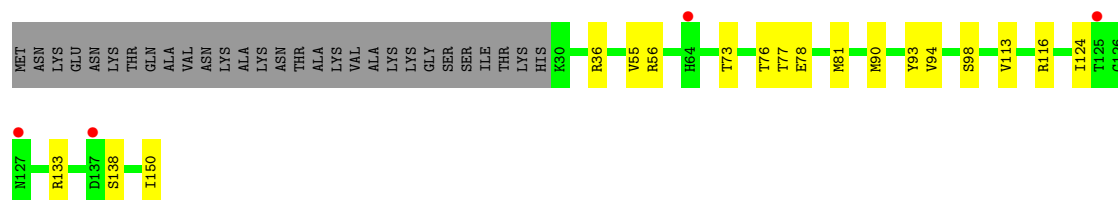


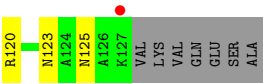
Figure 1: Schematic representation of the 127 amino acids of the protein. The diagram shows a horizontal bar divided into 127 segments, each representing an amino acid. The segments are color-coded: yellow for hydrophobic, red for basic, blue for acidic, green for polar, and grey for non-polar. The amino acids are listed in two rows: D111, K112, S113, R114, Q115, T119, L125, K126, T127, LYS, GLY, GLN, LYS, HIS, LYS, THR, VAL, ALA, MET, K2, T3, H4, V5, E6, R11, R12, H18, S21, H24, L25, R26, H33, R39, M43, V44, R45, S46, R50, K51, V55, L56, R59, K68, V69, T70, Q71, Y72, V73, R74, W77, H80, I84, K88, G91, Q95, A100, L103, and K107.

[illegible]

D162	D163	N163	T164	L170	G171	C177	H183	E184	V188	E194	A195	N196	L199	Y218	G222	D223	N226	R227	E228	L239	MET	SER	LVS	PHE	VAL	P86	E7	R15	R27	R37	E40	W41	Y48	K63	K68	F72	Y73	F82	R85	H93	P94	D95	R98	V99	L100	R101	R104	A112	F113	F114	R115	V116	N117	L121	V127	L128	P129	F130	F133	R138	T141
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

Amino Acid	Relative Abundance (approx.)
MET	100
V2	80
D10	10
N14	10
L15	90
H16	90
K17	10
S23	10
T45	10
R69	10
R73	10
L74	10
C75	10
N79	10
A84	100
Q87	10
T108	10
E111	10

Residue Class	Count
MET	1
ALA	1
I3	3
V6	6
A7	7
H8	8
K14	14
R15	15
K18	18
E25	25
D31	31
S32	32
S33	33
W34	34
R35	35
R36	36
L40	40
D41	41
N42	42
R43	43
V44	44
R45	45
R52	52
I57	57
G58	58
F59	59
D62	62
N71	71
K75	75
F76	76
L77	77
R78	78
R79	79
L84	84
F85	85
I86	86
L87	87
R88	88
L89	89
M89	89
N90	90
N91	91
G96	96
E97	97
I98	98
R113	113



● Molecule 27: RPL37A

Chain Y:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	320.19Å 289.25Å 535.04Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	20.00 – 3.52 39.96 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.52) 99.4 (39.96-3.52)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.216 , 0.244 0.526 , 0.523	Depositor DCC
$R_{free}$ test set	10000 reflections (0.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 76.0	EDS
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 1192534 reflections	Xtriage
$F_o, F_c$ correlation	0.45	EDS
Total number of atoms	43522	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	2	0.86	1/3696 (0.0%)	1.17	24/5761 (0.4%)
2	3	0.63	0/2870	0.98	10/4473 (0.2%)
3	A	0.60	0/2019	0.76	1/2712 (0.0%)
4	B	0.52	0/3144	0.72	0/4213
5	C	0.53	0/3222	0.69	1/4338 (0.0%)
6	D	0.47	0/1376	0.67	0/1833
7	E	0.50	0/1501	0.74	2/2015 (0.1%)
8	F	0.49	0/1893	0.66	0/2548
10	H	0.46	0/1652	0.67	0/2213
11	I	0.87	6/1624 (0.4%)	0.92	7/2176 (0.3%)
12	J	0.68	1/1038 (0.1%)	0.77	2/1394 (0.1%)
13	K	0.58	0/1189	0.74	0/1589
14	L	0.59	0/1727	0.73	0/2308
15	M	0.53	1/2469 (0.0%)	0.72	1/3306 (0.0%)
16	N	0.60	0/1464	0.78	1/1965 (0.1%)
17	O	0.50	0/1250	0.65	0/1660
18	P	0.54	0/1300	0.64	0/1743
19	Q	0.56	0/1259	0.78	1/1693 (0.1%)
20	R	0.52	0/981	0.67	0/1320
21	S	0.50	0/1028	0.63	0/1372
22	T	0.53	0/521	0.70	0/693
23	U	0.51	0/995	0.66	0/1318
24	V	0.49	0/1950	0.66	1/2614 (0.0%)
25	W	0.51	0/913	0.68	0/1222
26	X	0.56	0/1028	0.68	0/1371
27	Y	0.55	0/799	0.75	0/1069
All	All	0.59	9/42908 (0.0%)	0.79	51/58919 (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
8	F	0	1
13	K	0	2
19	Q	0	1
26	X	0	1
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	60	TRP	NE1-CE2	-18.39	1.13	1.37
11	I	60	TRP	CD2-CE2	13.85	1.57	1.41
11	I	60	TRP	CG-CD2	11.72	1.63	1.43
11	I	60	TRP	CD2-CE3	-7.63	1.28	1.40
15	M	117	THR	CA-CB	-7.02	1.35	1.53
12	J	89	TRP	NE1-CE2	-7.00	1.28	1.37
11	I	60	TRP	CD1-NE1	6.29	1.48	1.38
1	2	105	A	N3-C4	5.48	1.38	1.34
11	I	60	TRP	CG-CD1	-5.12	1.29	1.36

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	60	TRP	CE2-CD2-CG	-18.64	92.39	107.30
11	I	60	TRP	NE1-CE2-CZ2	-11.79	117.43	130.40
1	2	95	C	C6-N1-C2	9.96	124.28	120.30
11	I	60	TRP	CD1-NE1-CE2	9.80	117.82	109.00
11	I	60	TRP	CD2-CE2-CZ2	-9.52	110.88	122.30
2	3	83	G	N3-C4-C5	8.54	132.87	128.60
11	I	60	TRP	CB-CG-CD2	-7.91	116.31	126.60
11	I	60	TRP	CG-CD1-NE1	-7.82	102.28	110.10
2	3	83	G	N3-C4-N9	-7.82	121.31	126.00
1	2	86	G	N3-C4-C5	7.56	132.38	128.60
1	2	136	U	C5-C6-N1	-7.09	119.15	122.70
1	2	86	G	C5-C6-N1	-6.56	108.22	111.50
1	2	59	G	C8-N9-C4	6.50	109.00	106.40
1	2	113	U	C5-C6-N1	-6.46	119.47	122.70
7	E	1	MET	CG-SD-CE	6.32	110.31	100.20
3	A	217	HIS	N-CA-C	6.04	127.32	111.00
1	2	136	U	C6-N1-C2	5.95	124.57	121.00
5	C	254	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	2	86	G	N1-C6-O6	5.89	123.43	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	44	C	C6-N1-C2	5.89	122.66	120.30
1	2	105	A	N1-C2-N3	-5.84	126.38	129.30
11	I	60	TRP	CH2-CZ2-CE2	-5.81	111.59	117.40
1	2	2	G	C8-N9-C1'	-5.72	119.56	127.00
1	2	63	U	C5-C6-N1	-5.59	119.91	122.70
2	3	8	G	C8-N9-C4	5.58	108.63	106.40
1	2	5	A	N9-C4-C5	-5.53	103.59	105.80
2	3	93	G	C2-N3-C4	-5.50	109.15	111.90
1	2	86	G	C6-N1-C2	5.49	128.39	125.10
1	2	17	U	C5-C6-N1	-5.42	119.99	122.70
1	2	54	G	C4-C5-N7	5.42	112.97	110.80
1	2	83	A	C8-N9-C4	5.42	107.97	105.80
1	2	96	A	N7-C8-N9	5.38	116.49	113.80
1	2	5	A	C4-C5-N7	5.35	113.37	110.70
24	V	170	LEU	CA-CB-CG	-5.34	103.02	115.30
1	2	86	G	C2-N3-C4	-5.32	109.24	111.90
2	3	92	C	C6-N1-C2	5.27	122.41	120.30
19	Q	114	LEU	CA-CB-CG	-5.22	103.30	115.30
1	2	108	G	C8-N9-C4	5.22	108.49	106.40
1	2	59	G	N3-C4-C5	5.20	131.20	128.60
2	3	93	G	N3-C4-C5	5.17	131.18	128.60
2	3	83	G	C2-N3-C4	-5.16	109.32	111.90
2	3	93	G	N3-C4-N9	-5.14	122.92	126.00
12	J	47	LYS	N-CA-C	-5.13	97.14	111.00
1	2	83	A	N9-C4-C5	-5.13	103.75	105.80
1	2	103	U	C5-C6-N1	-5.09	120.15	122.70
12	J	89	TRP	CE2-CD2-CG	-5.06	103.25	107.30
16	N	22	SER	N-CA-C	-5.05	97.37	111.00
7	E	4	LEU	CA-CB-CG	-5.04	103.71	115.30
15	M	269	LYS	N-CA-C	5.03	124.58	111.00
2	3	82	G	C8-N9-C4	5.03	108.41	106.40
1	2	2	G	C4-N9-C1'	5.01	133.01	126.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	F	174	LYS	Peptide
13	K	23	GLY	Peptide
13	K	58	LEU	Peptide
19	Q	118	HIS	Peptide
26	X	8	HIS	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	2	3300	0	11	72	0
2	3	2566	0	0	73	0
3	A	1977	0	0	41	0
4	B	3080	0	0	59	0
5	C	3172	0	0	68	0
6	D	1357	0	0	22	0
7	E	1481	0	0	14	0
8	F	1860	0	0	33	0
9	G	711	0	0	8	0
10	H	1620	0	0	30	0
11	I	1594	0	0	27	0
12	J	1022	0	0	13	0
13	K	1161	0	0	24	0
14	L	1691	0	0	19	0
15	M	2424	0	0	71	0
16	N	1441	0	0	44	0
17	O	1234	0	0	5	0
18	P	1272	0	0	18	0
19	Q	1239	0	0	18	0
20	R	965	0	0	9	0
21	S	1013	0	0	29	0
22	T	510	0	0	5	0
23	U	990	0	0	9	0
24	V	1910	0	0	28	0
25	W	901	0	0	5	0
26	X	1012	0	0	16	0
27	Y	786	0	0	13	0
28	0	176	0	0	0	0
29	Y	1	0	0	0	0
30	0	1056	0	0	25	0
All	All	43522	0	11	683	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 16.

All (683) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:395:ASP:OD1	18:P:154:ARG:NH2	1.80	1.15
26:X:15:ARG:O	30:0:5447:HOH:O	1.68	1.09
12:J:51:SER:OG	30:0:6869:HOH:O	1.71	1.08
3:A:218:GLN:O	30:0:6118:HOH:O	1.72	1.08
1:2:100:C:OP2	20:R:56:ARG:NH2	1.88	1.07
2:3:12:U:O3'	2:3:109:U:O2'	1.76	1.03
13:K:60:MET:O	16:N:172:ARG:NH1	1.93	1.00
2:3:65:G:OP2	30:0:7222:HOH:O	1.78	0.99
8:F:126:LYS:NZ	8:F:194:THR:OG1	1.97	0.98
2:3:1:G:N3	15:M:274:HIS:NE2	2.10	0.97
27:Y:15:GLY:O	27:Y:23:ARG:NH1	2.02	0.92
1:2:39:G:C2	23:U:90:ARG:NH1	2.38	0.92
4:B:16:PHE:CD2	4:B:273:ARG:NH1	2.38	0.92
6:D:26:SER:OG	6:D:63:GLU:OE2	1.87	0.91
24:V:162:ASP:OD1	24:V:164:THR:N	2.03	0.90
12:J:51:SER:OG	30:0:6867:HOH:O	1.88	0.89
26:X:31:ASP:OD1	26:X:32:SER:N	2.06	0.89
2:3:83:G:OP1	30:0:5525:HOH:O	1.90	0.87
4:B:282:ARG:NH1	4:B:291:ASN:O	2.06	0.87
3:A:119:GLU:N	3:A:123:ASP:OD2	2.08	0.86
1:2:134:C:O2'	1:2:135:A:OP1	1.94	0.85
10:H:18:PRO:O	10:H:23:ASN:ND2	2.10	0.85
1:2:3:A:OP1	1:2:4:A:N7	2.11	0.84
4:B:278:LYS:NZ	4:B:325:CYS:O	2.10	0.83
2:3:13:A:O2'	15:M:24:ARG:NH2	2.12	0.83
19:Q:133:ARG:CD	30:0:6087:HOH:O	2.28	0.82
19:Q:132:TYR:O	30:0:6083:HOH:O	1.96	0.81
2:3:42:A:C8	6:D:72:ARG:NH1	2.48	0.81
24:V:162:ASP:OD1	24:V:163:ASN:N	2.14	0.81
7:E:1:MET:CG	7:E:2:ARG:N	2.43	0.81
5:C:234:ASP:OD2	5:C:254:ARG:NH2	2.14	0.80
2:3:13:A:P	2:3:109:U:O2'	2.40	0.80
1:2:67:C:OP1	23:U:53:LYS:NZ	2.14	0.79
1:2:1:A:H2'	1:2:3:A:C8	2.18	0.79
1:2:77:U:O4	21:S:71:GLN:NE2	2.15	0.79
6:D:50:ALA:O	6:D:62:ASN:N	2.17	0.78
27:Y:7:LYS:O	27:Y:27:LYS:NZ	2.16	0.78
5:C:309:LYS:O	16:N:40:ARG:NH1	2.17	0.78
16:N:158:GLN:CB	30:0:7176:HOH:O	2.31	0.78
17:O:87:ALA:O	30:0:5864:HOH:O	2.02	0.77
18:P:94:GLU:OE1	18:P:94:GLU:N	2.18	0.77
8:F:154:GLU:OE2	14:L:26:ARG:NH2	2.18	0.76
26:X:98:ILE:O	26:X:123:ASN:ND2	2.19	0.76

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:K:122:PRO:CA	13:K:142:GLY:O	2.34	0.76
1:2:105:A:C8	1:2:106:A:C8	2.74	0.76
16:N:93:LEU:O	16:N:113:ARG:NH2	2.19	0.76
1:2:100:C:P	20:R:56:ARG:NH2	2.58	0.75
18:P:8:ARG:O	18:P:11:THR:OG1	2.03	0.75
7:E:52:ASN:OD1	7:E:53:VAL:N	2.20	0.74
16:N:158:GLN:NE2	30:0:7174:HOH:O	2.20	0.74
1:2:86:G:N1	21:S:111:ASP:OD2	2.20	0.74
2:3:13:A:N3	15:M:24:ARG:NH2	2.34	0.74
26:X:25:GLU:OE2	26:X:52:ARG:NH2	2.21	0.74
4:B:36:ASP:OD1	4:B:38:SER:N	2.20	0.74
18:P:41:ASP:OD1	18:P:61:THR:OG1	2.07	0.73
4:B:26:ARG:NH1	4:B:176:ILE:O	2.22	0.73
11:I:49:ASN:ND2	11:I:135:CYS:SG	2.62	0.72
3:A:218:GLN:OE1	30:0:6133:HOH:O	2.06	0.72
2:3:8:G:OP1	15:M:33:ARG:NH1	2.22	0.72
4:B:114:THR:CB	4:B:161:HIS:NE2	2.53	0.72
5:C:157:TYR:CD1	5:C:159:PHE:CE1	2.77	0.72
2:3:83:G:OP1	30:0:5527:HOH:O	2.08	0.71
5:C:369:HIS:ND1	24:V:68:LYS:NZ	2.39	0.71
15:M:41:LYS:NZ	18:P:30:TYR:O	2.24	0.71
15:M:180:PHE:CD1	15:M:200:HIS:CE1	2.79	0.70
2:3:70:G:O6	30:0:7444:HOH:O	2.08	0.70
16:N:16:VAL:CG1	16:N:17:VAL:N	2.54	0.70
2:3:64:A:O2'	10:H:205:PRO:CG	2.39	0.70
19:Q:133:ARG:CG	19:Q:139:ASN:ND2	2.56	0.69
1:2:149:G:N7	30:0:5016:HOH:O	2.25	0.69
4:B:192:PHE:O	4:B:195:SER:OG	2.09	0.69
2:3:82:G:N7	30:0:5624:HOH:O	2.26	0.69
5:C:311:ALA:N	16:N:40:ARG:NH2	2.41	0.68
2:3:13:A:OP1	2:3:109:U:O2'	2.12	0.68
16:N:81:ILE:O	16:N:102:CYS:N	2.26	0.68
5:C:152:VAL:CG1	5:C:157:TYR:CE2	2.77	0.68
4:B:58:ARG:NH1	4:B:281:TYR:OH	2.27	0.68
15:M:120:ALA:O	15:M:255:ARG:NH1	2.27	0.68
4:B:162:THR:O	4:B:174:ASN:CB	2.42	0.67
5:C:167:GLU:N	5:C:171:GLN:NE2	2.42	0.67
15:M:129:TYR:CE1	15:M:175:HIS:O	2.48	0.67
1:2:124:U:O2'	1:2:126:A:N7	2.28	0.67
11:I:37:THR:OG1	11:I:104:PHE:O	2.12	0.67
4:B:54:THR:CG2	4:B:55:HIS:N	2.56	0.67
3:A:131:SER:OG	3:A:175:ARG:NH1	2.28	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:N:52:ARG:NH1	16:N:141:ARG:NE	2.43	0.67
8:F:127:TYR:C	8:F:127:TYR:CD1	2.68	0.66
10:H:48:TYR:CE1	10:H:178:ARG:CZ	2.78	0.66
13:K:78:ASP:N	13:K:78:ASP:OD1	2.29	0.66
1:2:41:U:C2	23:U:93:ARG:NH2	2.63	0.66
15:M:33:ARG:NH2	15:M:72:ASP:OD2	2.29	0.66
26:X:87:LEU:O	26:X:91:ASN:N	2.29	0.65
27:Y:45:VAL:CG2	27:Y:45:VAL:O	2.43	0.65
5:C:42:PHE:CZ	5:C:46:ASN:ND2	2.65	0.65
24:V:194:GLU:OE1	24:V:194:GLU:N	2.30	0.65
21:S:51:LYS:O	21:S:69:VAL:O	2.14	0.65
19:Q:33:GLU:OE2	19:Q:64:ARG:N	2.29	0.65
4:B:117:ARG:NH1	4:B:174:ASN:O	2.30	0.65
16:N:151:HIS:ND1	16:N:164:ALA:O	2.29	0.65
15:M:119:TYR:CD1	15:M:132:VAL:CG1	2.80	0.65
3:A:66:ASP:OD1	3:A:68:TYR:N	2.30	0.64
4:B:119:TYR:CD2	4:B:122:TRP:CZ3	2.86	0.64
4:B:282:ARG:NH2	4:B:293:SER:O	2.29	0.64
2:3:49:A:O2'	15:M:230:LYS:NZ	2.31	0.64
1:2:107:C:C4	1:2:135:A:C6	2.86	0.64
8:F:131:HIS:CD2	8:F:135:LEU:CD1	2.80	0.64
14:L:183:SER:CA	14:L:191:ASN:ND2	2.60	0.64
4:B:24:HIS:CE1	4:B:28:ARG:NH1	2.66	0.64
1:2:37:A:C4'	1:2:38:C:OP1	2.45	0.64
13:K:75:VAL:CG2	13:K:109:PHE:CG	2.81	0.64
1:2:88:G:O2'	1:2:89:A:O5'	2.16	0.63
9:G:15:UNK:CG	9:G:65:UNK:CA	2.77	0.63
24:V:226:ASN:O	24:V:226:ASN:OD1	2.16	0.63
10:H:34:TYR:CZ	10:H:92:HIS:ND1	2.67	0.63
3:A:248:ARG:NH2	30:0:6934:HOH:O	2.30	0.63
4:B:113:ASN:CB	4:B:174:ASN:ND2	2.61	0.63
21:S:6:GLU:OE1	21:S:6:GLU:N	2.31	0.63
2:3:83:G:P	30:0:5527:HOH:O	2.56	0.63
3:A:31:ARG:O	3:A:164:ARG:NH1	2.31	0.63
5:C:276:THR:CG2	5:C:277:GLY:N	2.62	0.62
19:Q:73:ALA:O	19:Q:76:HIS:CD2	2.53	0.62
2:3:62:U:O2'	2:3:63:A:OP2	2.17	0.62
1:2:98:A:OP1	23:U:67:ARG:NH1	2.31	0.62
1:2:35:U:O2	1:2:37:A:N6	2.32	0.62
3:A:128:SER:O	3:A:128:SER:OG	2.16	0.62
24:V:98:ARG:CG	24:V:98:ARG:NH1	2.63	0.62
1:2:1:A:H4'	1:2:2:G:OP1	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:3:33:U:C5	15:M:212:TYR:CE1	2.87	0.62
10:H:75:ASN:O	10:H:79:PHE:CD1	2.53	0.62
4:B:19:ARG:O	4:B:271:HIS:CE1	2.52	0.62
15:M:122:GLN:NE2	15:M:126:ASP:OD2	2.32	0.62
1:2:40:A:C8	1:2:42:G:C2	2.88	0.62
1:2:148:U:O2'	8:F:58:ARG:NH1	2.33	0.62
3:A:148:ARG:NH1	3:A:158:THR:OG1	2.32	0.61
2:3:33:U:C4	15:M:212:TYR:CE1	2.87	0.61
26:X:42:ASN:ND2	26:X:45:ARG:N	2.47	0.61
1:2:77:U:C4	21:S:73:TYR:CE2	2.87	0.61
3:A:29:GLN:OE1	3:A:124:ARG:NH2	2.34	0.61
24:V:48:TYR:CE1	24:V:183:HIS:CG	2.89	0.61
10:H:168:SER:OG	18:P:157:PHE:O	2.18	0.61
1:2:110:A:C2	1:2:115:G:C6	2.88	0.61
8:F:127:TYR:CD1	8:F:185:LYS:NZ	2.68	0.60
24:V:72:PHE:CD1	24:V:73:TYR:N	2.69	0.60
17:O:98:ARG:NH1	17:O:130:ASN:OD1	2.34	0.60
13:K:14:HIS:CG	30:O:6230:HOH:O	2.52	0.60
13:K:60:MET:C	16:N:172:ARG:NH1	2.54	0.60
2:3:34:C:O2	15:M:203:ARG:NH1	2.34	0.60
1:2:62:A:OP1	1:2:99:U:O2'	2.19	0.60
5:C:259:THR:CG2	5:C:260:GLU:N	2.64	0.60
15:M:175:HIS:CD2	15:M:180:PHE:CE2	2.90	0.60
5:C:401:GLN:O	10:H:179:ALA:CB	2.49	0.60
18:P:74:VAL:CG1	18:P:75:ILE:N	2.65	0.60
1:2:86:G:C6	21:S:111:ASP:OD2	2.54	0.60
1:2:3:A:C4'	1:2:4:A:OP2	2.49	0.60
3:A:33:TYR:N	3:A:164:ARG:NH2	2.50	0.60
13:K:81:TRP:CZ2	13:K:123:VAL:CG2	2.84	0.60
15:M:212:TYR:CD2	15:M:228:PHE:CZ	2.90	0.59
1:2:112:G:C4'	1:2:113:U:OP1	2.50	0.59
2:3:83:G:N2	2:3:93:G:N2	2.51	0.59
19:Q:33:GLU:OE1	19:Q:62:PHE:CA	2.50	0.59
1:2:58:U:N3	1:2:65:C:C5	2.71	0.59
1:2:1:A:C4'	1:2:2:G:OP1	2.50	0.59
5:C:245:GLN:O	5:C:254:ARG:NH1	2.36	0.59
11:I:80:TRP:CH2	11:I:84:ARG:NH1	2.72	0.58
1:2:111:A:O2'	1:2:112:G:OP1	2.21	0.58
1:2:107:C:C5	1:2:135:A:C5	2.92	0.58
4:B:332:ARG:NH1	4:B:332:ARG:CG	2.67	0.58
3:A:33:TYR:CA	3:A:164:ARG:NH2	2.66	0.58
13:K:89:ARG:O	13:K:121:GLN:NE2	2.36	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:H:130:ASP:OD1	10:H:131:ILE:N	2.36	0.58
26:X:98:ILE:N	26:X:123:ASN:ND2	2.52	0.58
3:A:20:HIS:CD2	3:A:193:LYS:O	2.56	0.58
22:T:22:ARG:NE	22:T:32:PHE:CD2	2.72	0.58
4:B:204:ASP:N	4:B:204:ASP:OD1	2.33	0.58
5:C:163:VAL:O	5:C:166:TYR:CD2	2.57	0.57
1:2:1:A:C5'	1:2:2:G:OP1	2.52	0.57
5:C:369:HIS:CE1	24:V:68:LYS:NZ	2.72	0.57
1:2:7:U:OP1	19:Q:64:ARG:CG	2.52	0.57
3:A:42:ILE:CD1	3:A:43:ARG:N	2.68	0.57
27:Y:32:THR:CG2	27:Y:69:TRP:O	2.53	0.57
21:S:26:ARG:NH1	21:S:74:ARG:O	2.38	0.57
16:N:85:SER:OG	16:N:86:THR:N	2.36	0.57
15:M:274:HIS:O	15:M:278:TYR:CD1	2.58	0.57
5:C:195:ARG:NH1	5:C:204:ARG:CB	2.68	0.57
2:3:33:U:C2	15:M:212:TYR:CD1	2.93	0.57
19:Q:99:ASN:O	19:Q:103:ASN:CB	2.53	0.57
8:F:170:PHE:O	8:F:215:TYR:CD2	2.58	0.57
3:A:48:ASP:O	3:A:61:GLU:N	2.38	0.57
21:S:43:ASN:O	21:S:125:LEU:CD1	2.53	0.57
2:3:46:C:OP1	15:M:158:ARG:CG	2.53	0.57
15:M:125:VAL:O	15:M:201:LYS:NZ	2.38	0.57
5:C:308:VAL:CG1	16:N:40:ARG:NH1	2.68	0.56
2:3:48:G:O2'	15:M:227:GLN:O	2.22	0.56
1:2:28:G:N7	21:S:12:ARG:NH2	2.53	0.56
13:K:48:GLU:CA	13:K:48:GLU:OE1	2.53	0.56
15:M:176:SER:O	15:M:177:GLU:CG	2.54	0.56
2:3:119:C:O2'	15:M:270:PRO:O	2.22	0.56
14:L:120:TRP:CZ2	14:L:122:GLY:CA	2.89	0.56
16:N:114:ILE:CD1	16:N:121:CYS:SG	2.94	0.56
8:F:36:GLN:NE2	8:F:39:ARG:NH2	2.54	0.56
19:Q:33:GLU:OE1	19:Q:63:THR:N	2.39	0.56
26:X:78:ILE:N	26:X:97:GLU:O	2.39	0.56
2:3:81:A:C2'	2:3:82:G:C5'	2.84	0.56
2:3:1:G:OP1	15:M:275:LYS:NZ	2.38	0.56
26:X:25:GLU:OE1	26:X:25:GLU:N	2.39	0.56
3:A:35:PHE:CZ	3:A:39:GLN:OE1	2.59	0.56
1:2:25:U:C4'	1:2:26:A:OP1	2.53	0.56
2:3:83:G:N1	2:3:93:G:N2	2.54	0.56
1:2:1:A:H5''	1:2:2:G:OP1	2.05	0.56
4:B:373:GLU:OE2	22:T:16:TYR:OH	2.24	0.56
7:E:145:GLN:NE2	7:E:186:MET:O	2.39	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:103:THR:CG2	4:B:104:THR:N	2.68	0.56
16:N:155:ALA:CB	16:N:158:GLN:NE2	2.69	0.56
27:Y:10:ILE:CD1	27:Y:30:GLU:CB	2.84	0.55
3:A:210:HIS:CD2	3:A:212:HIS:N	2.75	0.55
24:V:196:ASN:O	24:V:199:LEU:N	2.39	0.55
16:N:53:LEU:O	16:N:60:LYS:NZ	2.39	0.55
14:L:187:SER:O	14:L:190:GLY:N	2.39	0.55
4:B:303:ILE:CD1	4:B:319:PHE:CE1	2.90	0.55
22:T:11:CYS:SG	22:T:13:TYR:CD2	3.00	0.55
1:2:7:U:OP1	19:Q:36:ARG:NH1	2.40	0.55
5:C:328:ASN:OD1	5:C:329:ALA:N	2.40	0.55
16:N:89:ASN:OD1	16:N:90:ASP:N	2.39	0.55
1:2:27:G:OP2	21:S:12:ARG:NH1	2.40	0.55
2:3:90:A:C2	10:H:162:ARG:NH2	2.74	0.55
13:K:117:ARG:NH1	13:K:137:ARG:CZ	2.70	0.54
3:A:46:ILE:O	3:A:86:GLY:N	2.41	0.54
8:F:149:ASP:OD1	8:F:149:ASP:C	2.46	0.54
5:C:133:LEU:O	5:C:136:SER:OG	2.25	0.54
16:N:167:VAL:CG1	16:N:169:SER:O	2.55	0.54
5:C:105:ARG:CG	5:C:105:ARG:NH1	2.71	0.54
3:A:30:TYR:OH	3:A:166:THR:OG1	2.24	0.54
2:3:41:G:N2	2:3:44:C:N3	2.56	0.54
3:A:31:ARG:NH1	3:A:42:ILE:CG1	2.70	0.54
4:B:183:GLY:O	4:B:189:LYS:CE	2.55	0.54
1:2:114:G:C8	1:2:114:G:C3'	2.90	0.54
21:S:18:HIS:O	21:S:21:SER:OG	2.25	0.54
7:E:46:GLN:NE2	7:E:56:GLN:NE2	2.56	0.54
26:X:6:VAL:CG1	26:X:7:ALA:N	2.72	0.54
10:H:171:TRP:CE2	10:H:181:TYR:CE2	2.95	0.54
1:2:75:A:OP2	21:S:51:LYS:CB	2.56	0.53
14:L:30:TYR:CE2	14:L:63:ARG:CD	2.91	0.53
2:3:83:G:C5'	30:0:5527:HOH:O	2.56	0.53
5:C:272:THR:CG2	5:C:273:TYR:N	2.71	0.53
9:G:22:UNK:O	9:G:119:UNK:N	2.40	0.53
15:M:79:ASP:OD1	15:M:79:ASP:N	2.41	0.53
26:X:75:LYS:NZ	26:X:97:GLU:OE1	2.41	0.53
16:N:37:LEU:O	16:N:41:THR:CB	2.57	0.53
4:B:377:PHE:CD2	4:B:378:PHE:CE1	2.96	0.53
4:B:62:ARG:CG	4:B:62:ARG:NH1	2.71	0.53
10:H:48:TYR:CE2	10:H:142:GLU:CG	2.92	0.53
3:A:212:HIS:O	3:A:213:GLY:C	2.45	0.53
5:C:82:PRO:O	5:C:96:ALA:N	2.42	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:129:A:C5	1:2:130:C:C5	2.96	0.53
4:B:55:HIS:N	4:B:55:HIS:CD2	2.76	0.53
12:J:91:ARG:NH2	12:J:141:VAL:O	2.42	0.53
14:L:26:ARG:O	14:L:30:TYR:CD1	2.61	0.53
2:3:63:A:C8	10:H:206:LEU:CD2	2.92	0.53
24:V:37:ARG:O	24:V:40:GLU:N	2.41	0.53
3:A:117:VAL:O	3:A:126:THR:N	2.42	0.53
10:H:14:GLY:O	10:H:128:ARG:NH2	2.42	0.53
2:3:63:A:O5'	10:H:206:LEU:CG	2.57	0.52
1:2:86:G:O6	21:S:113:SER:OG	2.27	0.52
4:B:111:ASP:O	4:B:114:THR:CG2	2.57	0.52
8:F:208:SER:O	8:F:212:LYS:N	2.41	0.52
3:A:48:ASP:OD1	3:A:49:ILE:N	2.43	0.52
18:P:66:ASN:OD1	18:P:67:VAL:N	2.42	0.52
13:K:122:PRO:CB	13:K:142:GLY:O	2.58	0.52
4:B:102:LEU:O	4:B:103:THR:OG1	2.27	0.52
11:I:109:THR:CG2	11:I:110:PRO:CD	2.87	0.52
2:3:7:G:O3'	15:M:33:ARG:NH1	2.43	0.52
24:V:48:TYR:CE1	24:V:183:HIS:CD2	2.97	0.52
2:3:93:G:O5'	2:3:93:G:C8	2.63	0.52
15:M:254:ILE:O	15:M:258:PRO:CD	2.58	0.52
21:S:100:ALA:O	21:S:103:LEU:N	2.42	0.52
8:F:154:GLU:OE1	8:F:154:GLU:N	2.43	0.52
5:C:157:TYR:CE1	5:C:159:PHE:CZ	2.98	0.52
10:H:130:ASP:O	10:H:133:SER:OG	2.28	0.52
15:M:83:LEU:CB	15:M:88:VAL:CG2	2.87	0.52
25:W:10:ASP:OD1	25:W:73:ARG:CG	2.58	0.51
1:2:24:C:OP1	5:C:200:LYS:NZ	2.43	0.51
5:C:233:VAL:O	5:C:234:ASP:OD1	2.28	0.51
1:2:110:A:C2	1:2:115:G:O6	2.64	0.51
8:F:197:ARG:O	8:F:198:ASN:C	2.47	0.51
11:I:9:ASP:O	11:I:13:HIS:CD2	2.63	0.51
15:M:51:LEU:N	15:M:145:ILE:O	2.43	0.51
2:3:8:G:P	15:M:33:ARG:NH1	2.83	0.51
4:B:162:THR:CG2	4:B:175:HIS:CD2	2.93	0.51
11:I:152:ILE:CG2	11:I:153:GLU:N	2.72	0.51
13:K:148:THR:CG2	13:K:149:ALA:N	2.73	0.51
12:J:98:TYR:N	12:J:98:TYR:CD1	2.78	0.51
12:J:23:VAL:CG2	12:J:41:ILE:O	2.59	0.51
11:I:14:LEU:N	11:I:122:ALA:O	2.43	0.51
1:2:61:G:C2'	1:2:100:C:O2'	2.59	0.51
15:M:125:VAL:CG2	15:M:205:PHE:CE1	2.94	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:J:85:GLN:NE2	12:J:87:ARG:O	2.44	0.51
26:X:96:GLY:N	26:X:120:ARG:O	2.44	0.51
5:C:126:ARG:CB	5:C:283:TYR:CE2	2.94	0.51
1:2:134:C:C3'	1:2:134:C:C6	2.94	0.50
5:C:272:THR:O	5:C:275:THR:O	2.29	0.50
4:B:66:ARG:NH1	12:J:13:THR:O	2.44	0.50
13:K:100:PRO:O	13:K:124:VAL:N	2.44	0.50
15:M:56:THR:CG2	15:M:57:ASN:N	2.74	0.50
13:K:123:VAL:O	13:K:144:ALA:N	2.45	0.50
18:P:15:PHE:CD1	18:P:15:PHE:N	2.80	0.50
2:3:13:A:O2'	15:M:24:ARG:CZ	2.60	0.50
24:V:218:TYR:CA	24:V:222:GLY:O	2.59	0.50
17:O:30:SER:O	17:O:33:SER:OG	2.30	0.50
4:B:119:TYR:CE2	4:B:122:TRP:CZ3	3.00	0.50
11:I:84:ARG:NE	11:I:89:HIS:CD2	2.79	0.50
3:A:81:GLU:N	3:A:169:ILE:O	2.44	0.50
1:2:77:U:N3	21:S:73:TYR:CE2	2.79	0.50
24:V:133:PHE:CZ	24:V:226:ASN:CB	2.95	0.50
15:M:90:THR:O	15:M:231:TRP:CZ3	2.65	0.50
1:2:73:G:O2'	1:2:88:G:N2	2.45	0.50
14:L:14:LYS:NZ	14:L:120:TRP:CZ3	2.80	0.50
21:S:24:HIS:CD2	21:S:25:LEU:N	2.80	0.50
7:E:49:THR:O	7:E:51:ASP:N	2.45	0.50
8:F:92:TYR:OH	8:F:200:ASP:OD2	2.30	0.50
13:K:116:GLY:O	13:K:137:ARG:NH1	2.45	0.50
4:B:50:LYS:NZ	4:B:328:GLY:O	2.45	0.50
1:2:76:U:O2	1:2:76:U:O4'	2.29	0.50
20:R:116:ARG:N	20:R:133:ARG:O	2.45	0.49
16:N:89:ASN:ND2	16:N:109:THR:CG2	2.76	0.49
4:B:225:ALA:N	4:B:266:GLY:O	2.45	0.49
16:N:4:ASP:O	24:V:101:ARG:NH2	2.45	0.49
13:K:23:GLY:O	13:K:24:LYS:O	2.30	0.49
10:H:101:LYS:CB	10:H:121:LYS:NZ	2.76	0.49
4:B:210:ASN:ND2	4:B:352:ILE:N	2.60	0.49
5:C:175:PHE:C	5:C:175:PHE:CD1	2.86	0.49
3:A:31:ARG:CB	3:A:37:GLU:OE2	2.61	0.49
15:M:163:LEU:CD1	15:M:173:ILE:CG2	2.91	0.49
5:C:275:THR:CG2	5:C:276:THR:N	2.76	0.49
15:M:110:LEU:CD1	15:M:169:GLY:O	2.61	0.49
1:2:119:A:C2	1:2:133:U:O2	2.66	0.49
5:C:159:PHE:CZ	5:C:179:VAL:CG1	2.96	0.49
8:F:92:TYR:CE1	8:F:200:ASP:OD2	2.66	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:115:LYS:CG	6:D:116:TYR:N	2.75	0.49
11:I:53:PHE:CE2	11:I:144:VAL:CG1	2.96	0.49
19:Q:8:ARG:NH1	19:Q:118:HIS:N	2.60	0.49
6:D:9:MET:O	6:D:134:PRO:CG	2.61	0.49
2:3:75:G:N2	2:3:100:A:OP2	2.46	0.49
16:N:157:GLY:N	16:N:161:SER:OG	2.46	0.49
15:M:243:VAL:CG1	15:M:247:PHE:CD2	2.96	0.49
6:D:7:ASN:C	6:D:9:MET:N	2.65	0.49
1:2:45:G:O6	1:2:104:G:C2	2.66	0.49
16:N:174:PHE:O	16:N:176:ARG:N	2.46	0.49
16:N:178:HIS:ND1	16:N:179:GLY:O	2.46	0.49
8:F:92:TYR:CE2	8:F:123:ILE:CG2	2.96	0.48
1:2:71:G:C5	1:2:72:C:C5	3.01	0.48
24:V:223:ASP:OD1	24:V:223:ASP:N	2.45	0.48
24:V:41:TRP:CD1	24:V:177:CYS:SG	3.06	0.48
15:M:163:LEU:CD2	15:M:175:HIS:CG	2.96	0.48
2:3:43:A:OP1	6:D:137:ARG:CD	2.61	0.48
16:N:24:ASN:OD1	16:N:27:HIS:CB	2.62	0.48
12:J:11:VAL:CG1	12:J:11:VAL:O	2.61	0.48
5:C:394:GLU:OE1	18:P:151:LYS:NZ	2.46	0.48
10:H:98:ARG:NH2	10:H:119:PHE:CZ	2.81	0.48
2:3:111:U:O4	15:M:21:ARG:NH1	2.47	0.48
4:B:21:ARG:NE	4:B:267:GLN:OE1	2.47	0.48
16:N:63:LEU:O	16:N:88:THR:N	2.46	0.48
5:C:70:GLU:O	5:C:82:PRO:CA	2.61	0.48
19:Q:115:VAL:N	19:Q:153:GLN:O	2.47	0.48
14:L:26:ARG:CZ	14:L:43:SER:OG	2.62	0.48
1:2:27:G:OP2	21:S:12:ARG:CD	2.62	0.48
24:V:127:VAL:O	24:V:130:PHE:N	2.46	0.48
4:B:294:THR:CG2	4:B:295:ALA:N	2.77	0.48
13:K:75:VAL:CG2	13:K:109:PHE:CD2	2.97	0.48
14:L:67:ARG:O	30:O:7768:HOH:O	2.20	0.48
14:L:33:LEU:O	14:L:65:ARG:NH1	2.47	0.48
12:J:28:ASN:N	12:J:102:ASN:O	2.46	0.48
2:3:39:U:C2	6:D:46:VAL:CG2	2.96	0.48
16:N:180:LEU:O	16:N:181:LYS:C	2.52	0.48
2:3:45:U:OP1	15:M:151:VAL:CG1	2.62	0.48
12:J:46:ILE:CD1	12:J:54:PRO:CB	2.92	0.48
21:S:18:HIS:CE1	21:S:77:TRP:CH2	3.02	0.48
6:D:133:ARG:CG	6:D:152:GLN:O	2.62	0.48
20:R:73:THR:O	20:R:93:TYR:N	2.47	0.48
4:B:95:THR:CG2	4:B:98:GLY:O	2.62	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:77:U:C4	21:S:73:TYR:CD2	3.02	0.47
18:P:5:TYR:CD1	18:P:5:TYR:N	2.81	0.47
21:S:80:HIS:ND1	21:S:95:GLN:CB	2.76	0.47
3:A:33:TYR:CD1	3:A:164:ARG:NH2	2.82	0.47
27:Y:26:VAL:O	27:Y:27:LYS:C	2.53	0.47
19:Q:10:PRO:CB	19:Q:153:GLN:NE2	2.78	0.47
27:Y:8:VAL:CG1	27:Y:12:ARG:N	2.78	0.47
24:V:184:GLU:O	24:V:188:VAL:N	2.47	0.47
5:C:65:MET:CE	5:C:105:ARG:NH1	2.77	0.47
2:3:29:C:OP1	6:D:134:PRO:O	2.32	0.47
19:Q:66:THR:CG2	19:Q:82:GLN:NE2	2.77	0.47
12:J:10:GLN:CG	12:J:129:ILE:CG2	2.92	0.47
5:C:44:ASP:OD1	5:C:44:ASP:N	2.47	0.47
25:W:14:ASN:ND2	25:W:17:LYS:CE	2.78	0.47
2:3:22:A:C6	15:M:274:HIS:CG	3.03	0.47
3:A:71:LYS:CE	3:A:73:ASN:OD1	2.63	0.47
1:2:3:A:C5'	1:2:4:A:OP2	2.63	0.47
13:K:75:VAL:CG2	13:K:109:PHE:CB	2.92	0.47
5:C:163:VAL:CG2	5:C:175:PHE:CE2	2.97	0.47
19:Q:117:GLN:O	19:Q:151:PHE:O	2.32	0.47
15:M:82:GLU:OE1	15:M:104:LEU:CD2	2.63	0.47
8:F:95:GLU:OE1	8:F:100:LYS:CG	2.63	0.47
5:C:289:LEU:O	16:N:123:THR:OG1	2.32	0.47
9:G:11:UNK:O	9:G:15:UNK:CG	2.62	0.47
10:H:55:ASP:O	10:H:131:ILE:CG1	2.63	0.47
8:F:71:HIS:O	8:F:74:THR:OG1	2.33	0.47
4:B:111:ASP:N	4:B:111:ASP:OD1	2.48	0.47
10:H:159:PHE:CB	10:H:163:GLN:NE2	2.77	0.47
19:Q:85:TRP:O	19:Q:87:VAL:N	2.48	0.47
7:E:23:ARG:NH1	7:E:39:ARG:O	2.48	0.47
5:C:303:GLU:OE1	5:C:303:GLU:N	2.48	0.46
17:O:60:ARG:O	17:O:61:SER:C	2.53	0.46
4:B:35:ASP:OD2	4:B:189:LYS:NZ	2.48	0.46
11:I:165:THR:O	11:I:166:TYR:C	2.53	0.46
3:A:210:HIS:CD2	3:A:211:PRO:CD	2.99	0.46
20:R:76:THR:O	20:R:76:THR:CG2	2.63	0.46
21:S:111:ASP:C	21:S:111:ASP:OD1	2.53	0.46
15:M:228:PHE:CD1	15:M:231:TRP:CD1	3.03	0.46
8:F:196:VAL:CG1	8:F:197:ARG:N	2.78	0.46
7:E:75:ILE:O	7:E:76:LYS:C	2.54	0.46
8:F:19:ASN:CB	8:F:20:PRO:CD	2.94	0.46
2:3:22:A:C6	2:3:23:A:C6	3.04	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:39:G:N3	23:U:90:ARG:NH1	2.63	0.46
24:V:128:LEU:N	24:V:129:PRO:CD	2.79	0.46
5:C:343:GLN:O	5:C:347:ALA:N	2.49	0.46
3:A:186:GLN:OE1	3:A:186:GLN:CA	2.63	0.46
3:A:68:TYR:C	3:A:69:ARG:CG	2.84	0.46
16:N:53:LEU:C	16:N:60:LYS:NZ	2.69	0.46
11:I:11:LYS:O	11:I:13:HIS:CD2	2.68	0.46
14:L:64:VAL:CG2	14:L:106:VAL:CG2	2.94	0.45
1:2:107:C:C5	1:2:135:A:C4	3.05	0.45
1:2:74:A:N6	1:2:88:G:C1'	2.79	0.45
16:N:146:ARG:CB	16:N:149:TYR:CE2	2.99	0.45
18:P:45:ASP:C	18:P:45:ASP:OD1	2.55	0.45
4:B:367:ARG:NH1	22:T:13:TYR:CD1	2.85	0.45
5:C:283:TYR:C	5:C:283:TYR:CD1	2.90	0.45
5:C:316:THR:O	5:C:317:HIS:CD2	2.69	0.45
5:C:287:ARG:CD	16:N:111:ARG:NH1	2.80	0.45
1:2:85:C:C4'	1:2:85:C:OP1	2.65	0.45
10:H:139:ARG:CG	10:H:173:PHE:CE1	2.99	0.45
6:D:133:ARG:CB	6:D:134:PRO:CD	2.95	0.45
5:C:242:ASN:C	5:C:244:LEU:N	2.69	0.45
1:2:6:A:O2'	19:Q:80:ARG:NH2	2.49	0.45
9:G:101:UNK:O	9:G:105:UNK:CG	2.65	0.45
6:D:162:TRP:CH2	6:D:167:PHE:CE2	3.04	0.45
16:N:73:ASN:N	16:N:76:ASN:OD1	2.49	0.45
7:E:22:GLN:OE1	7:E:39:ARG:NH2	2.50	0.45
5:C:33:ILE:CG2	5:C:33:ILE:O	2.65	0.45
4:B:114:THR:CG2	4:B:115:LYS:N	2.79	0.45
15:M:247:PHE:O	15:M:251:HIS:CD2	2.69	0.45
24:V:114:PHE:CD2	24:V:115:ARG:O	2.69	0.45
18:P:82:GLY:CA	30:O:6247:HOH:O	2.64	0.45
13:K:109:PHE:C	13:K:110:PHE:CD1	2.90	0.45
3:A:212:HIS:O	3:A:214:GLY:N	2.50	0.45
3:A:118:GLU:OE1	3:A:122:GLY:N	2.50	0.45
5:C:302:ASN:O	5:C:306:SER:OG	2.35	0.45
1:2:50:C:N4	30:O:5301:HOH:O	2.50	0.45
13:K:102:ILE:N	13:K:124:VAL:O	2.50	0.45
26:X:14:LYS:NZ	26:X:58:GLY:O	2.49	0.45
17:O:96:MET:CE	17:O:100:ARG:NH2	2.80	0.45
7:E:141:THR:CG2	7:E:142:LEU:N	2.80	0.45
14:L:182:LYS:CG	14:L:183:SER:N	2.80	0.44
19:Q:134:ALA:O	19:Q:135:HIS:CB	2.65	0.44
23:U:35:ALA:O	23:U:36:LYS:C	2.54	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:74:PRO:N	27:Y:75:PRO:CD	2.80	0.44
4:B:56:ILE:CG2	4:B:57:LEU:N	2.80	0.44
8:F:136:ILE:O	8:F:166:ASN:ND2	2.50	0.44
1:2:28:G:C5	1:2:29:U:C5	3.05	0.44
25:W:14:ASN:ND2	25:W:69:ARG:CZ	2.80	0.44
5:C:330:LEU:O	5:C:334:ASN:N	2.50	0.44
15:M:119:TYR:OH	15:M:139:LYS:O	2.35	0.44
14:L:120:TRP:CE2	14:L:122:GLY:CA	3.01	0.44
24:V:117:ASN:O	24:V:121:LEU:N	2.49	0.44
1:2:10:U:C4	1:2:11:C:N4	2.85	0.44
5:C:395:ASP:CG	18:P:154:ARG:NH2	2.63	0.44
3:A:218:GLN:CD	30:0:6133:HOH:O	2.54	0.44
2:3:70:G:C2	2:3:71:G:C8	3.06	0.44
3:A:117:VAL:CG1	3:A:118:GLU:N	2.80	0.44
15:M:99:TYR:CG	15:M:204:ILE:CG2	3.00	0.44
27:Y:55:TRP:CZ2	27:Y:70:GLU:C	2.91	0.44
8:F:183:VAL:O	8:F:183:VAL:CG1	2.66	0.44
2:3:33:U:C6	15:M:212:TYR:CE1	3.05	0.44
5:C:65:MET:CE	5:C:105:ARG:CG	2.95	0.44
10:H:139:ARG:CD	10:H:173:PHE:CE1	3.01	0.44
15:M:156:GLY:N	15:M:179:ARG:O	2.50	0.44
21:S:88:LYS:O	21:S:91:GLY:N	2.50	0.44
2:3:89:G:C6	2:3:90:A:C6	3.05	0.44
11:I:109:THR:O	11:I:110:PRO:C	2.54	0.44
8:F:232:GLN:O	8:F:233:LYS:C	2.52	0.44
5:C:333:LEU:CD2	24:V:161:THR:O	2.65	0.44
21:S:55:VAL:CG1	21:S:56:LEU:N	2.81	0.44
15:M:135:ASP:O	15:M:135:ASP:OD1	2.35	0.44
15:M:19:LYS:O	15:M:24:ARG:NH1	2.51	0.44
11:I:11:LYS:CD	11:I:36:ARG:NH1	2.80	0.44
23:U:92:ILE:O	23:U:95:LYS:CG	2.66	0.44
4:B:25:HIS:CD2	4:B:270:TYR:OH	2.71	0.44
10:H:201:GLY:O	10:H:208:ARG:NH2	2.51	0.44
12:J:32:ASN:ND2	12:J:117:GLN:N	2.65	0.44
8:F:161:GLN:OE1	8:F:164:ARG:NH1	2.51	0.44
5:C:205:ARG:NH2	21:S:11:ARG:NH1	2.65	0.44
1:2:2:G:O2'	1:2:3:A:P	2.76	0.44
15:M:173:ILE:O	15:M:175:HIS:ND1	2.51	0.44
4:B:24:HIS:CE1	4:B:28:ARG:CD	3.00	0.44
15:M:212:TYR:CD2	15:M:228:PHE:CE2	3.06	0.44
2:3:120:U:OP2	15:M:270:PRO:CB	2.66	0.44
5:C:65:MET:CE	5:C:97:PHE:CB	2.96	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:227:LEU:O	5:C:228:ARG:C	2.55	0.44
22:T:27:ASP:N	22:T:27:ASP:OD1	2.47	0.44
10:H:44:GLU:CD	10:H:181:TYR:OH	2.56	0.44
11:I:35:VAL:CG1	11:I:36:ARG:N	2.81	0.44
10:H:54:SER:OG	10:H:54:SER:O	2.36	0.44
5:C:369:HIS:O	5:C:372:GLY:N	2.51	0.43
21:S:3:THR:CG2	21:S:3:THR:O	2.64	0.43
11:I:107:ILE:CG1	11:I:159:ARG:NH1	2.80	0.43
2:3:21:G:C4'	15:M:277:PHE:CD1	3.01	0.43
4:B:85:THR:O	4:B:161:HIS:N	2.51	0.43
15:M:231:TRP:CZ2	15:M:243:VAL:CG2	3.01	0.43
10:H:44:GLU:OE2	10:H:181:TYR:OH	2.37	0.43
3:A:151:LEU:O	3:A:154:GLY:N	2.50	0.43
11:I:24:LYS:O	11:I:28:SER:OG	2.36	0.43
21:S:84:ILE:CG2	21:S:84:ILE:O	2.66	0.43
16:N:174:PHE:C	16:N:176:ARG:N	2.68	0.43
5:C:127:HIS:CE1	5:C:286:GLN:OE1	2.72	0.43
7:E:58:TRP:O	7:E:59:GLN:C	2.57	0.43
20:R:113:VAL:CG1	20:R:138:SER:OG	2.66	0.43
1:2:75:A:N3	1:2:89:A:O2'	2.51	0.43
4:B:367:ARG:NE	4:B:368:PHE:CZ	2.86	0.43
27:Y:55:TRP:N	27:Y:55:TRP:CD1	2.86	0.43
25:W:79:ASN:N	25:W:87:GLN:O	2.51	0.43
20:R:77:THR:O	20:R:78:GLU:C	2.57	0.43
16:N:73:ASN:OD1	16:N:74:GLU:OE1	2.36	0.43
12:J:21:LEU:O	12:J:56:ALA:N	2.52	0.43
5:C:8:HIS:N	5:C:154:GLU:OE2	2.52	0.43
2:3:43:A:C5	2:3:44:C:C4	3.07	0.43
6:D:101:ASN:OD1	6:D:131:LEU:N	2.52	0.43
5:C:95:ALA:CB	5:C:101:CYS:SG	3.07	0.43
4:B:371:VAL:CG1	4:B:382:ARG:CZ	2.97	0.43
2:3:16:A:C6	2:3:64:A:C6	3.06	0.43
4:B:208:ALA:N	4:B:211:GLU:OE1	2.50	0.43
15:M:157:ASN:OD1	15:M:158:ARG:N	2.52	0.43
4:B:330:LYS:O	4:B:331:LYS:CB	2.66	0.43
4:B:375:ASP:CB	4:B:380:ARG:O	2.67	0.43
11:I:59:LYS:O	11:I:71:HIS:CE1	2.71	0.43
1:2:87:C:O4'	1:2:87:C:O2	2.35	0.43
16:N:146:ARG:CB	16:N:149:TYR:CD2	3.02	0.43
8:F:45:VAL:CG1	8:F:46:ARG:N	2.81	0.43
20:R:55:VAL:N	23:U:83:ASP:OD2	2.52	0.43
15:M:153:THR:CG2	15:M:153:THR:O	2.67	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:H:34:TYR:CE1	10:H:92:HIS:CE1	3.07	0.42
11:I:35:VAL:CG1	11:I:106:GLY:O	2.66	0.42
10:H:140:VAL:CG1	10:H:141:LYS:N	2.82	0.42
10:H:166:VAL:CG1	10:H:167:THR:N	2.81	0.42
10:H:147:TYR:CD1	10:H:147:TYR:N	2.87	0.42
16:N:34:TYR:O	16:N:38:VAL:CG2	2.66	0.42
2:3:8:G:C5	2:3:9:C:C5	3.07	0.42
24:V:133:PHE:CE1	24:V:226:ASN:CB	3.01	0.42
2:3:26:C:OP1	15:M:56:THR:CG2	2.67	0.42
2:3:75:G:O2'	2:3:76:U:OP2	2.37	0.42
4:B:47:THR:OG1	4:B:177:LEU:CD1	2.67	0.42
14:L:136:ASP:OD1	14:L:138:SER:OG	2.38	0.42
4:B:49:PHE:CD1	4:B:49:PHE:N	2.87	0.42
15:M:274:HIS:CA	15:M:277:PHE:CD2	3.02	0.42
1:2:147:G:O2'	1:2:149:G:OP1	2.36	0.42
16:N:52:ARG:CB	16:N:84:THR:CG2	2.97	0.42
2:3:40:C:C5'	2:3:41:G:OP2	2.67	0.42
2:3:40:C:C2'	2:3:40:C:O2	2.68	0.42
27:Y:17:ARG:C	27:Y:18:TYR:CD2	2.92	0.42
13:K:128:LYS:C	13:K:129:TYR:CD1	2.93	0.42
8:F:66:VAL:N	8:F:226:GLY:O	2.52	0.42
4:B:235:HIS:CD2	4:B:235:HIS:O	2.72	0.42
13:K:141:VAL:CG1	13:K:141:VAL:O	2.67	0.42
3:A:30:TYR:CB	3:A:164:ARG:NH1	2.83	0.42
5:C:34:ARG:NE	16:N:24:ASN:CB	2.83	0.42
2:3:39:U:N1	6:D:46:VAL:CG2	2.82	0.42
16:N:147:GLU:O	16:N:148:ALA:C	2.58	0.42
5:C:19:THR:CG2	5:C:20:ALA:N	2.81	0.42
3:A:90:TYR:N	3:A:101:ASN:OD1	2.52	0.42
8:F:170:PHE:CD1	8:F:216:ASN:OD1	2.73	0.42
16:N:90:ASP:OD1	16:N:92:ARG:CG	2.67	0.42
2:3:44:C:O2'	15:M:152:ARG:CD	2.67	0.42
15:M:250:VAL:O	15:M:254:ILE:CG1	2.67	0.42
11:I:144:VAL:CG1	11:I:144:VAL:O	2.68	0.42
6:D:25:GLU:O	6:D:30:LEU:CD1	2.67	0.42
8:F:142:LYS:NZ	8:F:201:LYS:NZ	2.68	0.42
4:B:33:PRO:CD	4:B:44:THR:CG2	2.97	0.42
2:3:105:C:C5'	2:3:105:C:C6	3.03	0.42
18:P:11:THR:CG2	18:P:15:PHE:CD2	3.03	0.42
5:C:163:VAL:CA	5:C:166:TYR:CD2	3.02	0.42
6:D:92:ARG:N	6:D:95:ASN:ND2	2.66	0.42
10:H:77:ILE:CG1	10:H:78:LYS:N	2.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:3:83:G:C2	2:3:93:G:N2	2.88	0.42
18:P:11:THR:CG2	18:P:15:PHE:CG	3.03	0.42
1:2:103:U:C4	1:2:104:G:C6	3.08	0.42
24:V:82:PHE:CD1	24:V:112:ALA:O	2.73	0.42
6:D:19:ILE:CG2	6:D:125:MET:CE	2.97	0.42
5:C:348:ALA:C	5:C:350:ALA:N	2.72	0.42
21:S:115:GLN:O	21:S:119:THR:OG1	2.37	0.42
24:V:170:LEU:O	24:V:171:GLY:C	2.57	0.42
4:B:50:LYS:NZ	4:B:326:CYS:O	2.53	0.42
4:B:60:VAL:CG2	4:B:67:HIS:O	2.68	0.42
3:A:206:ASN:O	3:A:208:VAL:N	2.53	0.42
15:M:212:TYR:CE2	15:M:227:GLN:NE2	2.88	0.42
2:3:39:U:O2'	6:D:44:GLU:O	2.37	0.42
13:K:129:TYR:N	13:K:129:TYR:CD1	2.87	0.42
3:A:114:VAL:CG1	3:A:165:ALA:CB	2.98	0.42
24:V:85:ARG:CZ	24:V:100:LEU:CD1	2.97	0.42
8:F:126:LYS:CE	8:F:194:THR:OG1	2.66	0.41
4:B:275:GLU:OE2	4:B:278:LYS:NZ	2.53	0.41
7:E:43:VAL:CG1	7:E:44:ASP:N	2.83	0.41
5:C:31:ALA:O	5:C:134:ALA:CB	2.68	0.41
9:G:33:UNK:CG	9:G:36:UNK:CG	2.98	0.41
8:F:68:PRO:CD	8:F:225:TRP:NE1	2.83	0.41
2:3:12:U:OP2	2:3:67:C:O2'	2.38	0.41
14:L:147:ARG:O	14:L:150:TRP:CD1	2.72	0.41
26:X:44:VAL:O	26:X:45:ARG:C	2.59	0.41
7:E:49:THR:C	7:E:51:ASP:N	2.74	0.41
15:M:109:LEU:CD2	15:M:142:PHE:CD2	3.03	0.41
5:C:157:TYR:CE1	5:C:179:VAL:CG1	3.04	0.41
5:C:34:ARG:CZ	16:N:24:ASN:CB	2.99	0.41
11:I:141:SER:O	11:I:146:TRP:N	2.53	0.41
26:X:57:ILE:C	26:X:59:PHE:N	2.72	0.41
11:I:61:MET:CE	11:I:68:GLY:CA	2.99	0.41
5:C:152:VAL:CG1	5:C:157:TYR:CD2	3.04	0.41
2:3:81:A:C3'	2:3:82:G:C5'	2.99	0.41
1:2:73:G:C2	1:2:88:G:C2	3.09	0.41
21:S:70:THR:N	21:S:80:HIS:O	2.53	0.41
1:2:52:G:C6	1:2:80:A:C2	3.09	0.41
7:E:38:PHE:CE2	7:E:71:ILE:CG2	3.03	0.41
13:K:79:LYS:O	13:K:82:SER:OG	2.38	0.41
8:F:220:GLU:O	8:F:224:THR:N	2.53	0.41
5:C:298:ILE:O	5:C:304:VAL:CG2	2.68	0.41
2:3:42:A:N9	6:D:72:ARG:NH1	2.69	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:272:THR:O	5:C:275:THR:N	2.53	0.41
2:3:116:A:C4'	15:M:260:ARG:NH2	2.83	0.41
4:B:230:ARG:NH2	4:B:267:GLN:O	2.54	0.41
9:G:28:UNK:N	9:G:112:UNK:O	2.53	0.41
26:X:71:ASN:OD1	26:X:71:ASN:C	2.58	0.41
14:L:129:PHE:CD1	14:L:129:PHE:N	2.88	0.41
2:3:1:G:C2	15:M:274:HIS:NE2	2.85	0.41
1:2:107:C:C5	1:2:135:A:C6	3.09	0.41
23:U:78:SER:O	23:U:79:LEU:CB	2.68	0.41
6:D:12:VAL:CG2	6:D:162:TRP:CD1	3.04	0.41
7:E:38:PHE:CD1	7:E:38:PHE:N	2.89	0.41
3:A:172:GLY:N	27:Y:66:GLY:O	2.53	0.41
14:L:53:TYR:OH	14:L:55:ASN:OD1	2.39	0.41
24:V:93:HIS:CD2	24:V:95:ASP:CB	3.04	0.41
27:Y:57:CYS:SG	27:Y:59:PRO:CG	3.09	0.41
16:N:62:PRO:O	16:N:142:ALA:CB	2.69	0.41
9:G:85:UNK:O	9:G:85:UNK:CG	2.65	0.41
5:C:108:ALA:O	5:C:109:PRO:C	2.58	0.41
4:B:213:LEU:O	4:B:214:ASP:OD1	2.39	0.41
1:2:87:C:O2'	1:2:88:G:C5'	2.69	0.41
8:F:170:PHE:CE1	8:F:216:ASN:OD1	2.74	0.41
2:3:54:A:O2'	6:D:152:GLN:NE2	2.54	0.41
8:F:142:LYS:N	8:F:193:LEU:O	2.54	0.41
20:R:94:VAL:CG1	20:R:98:SER:OG	2.68	0.41
11:I:196:PHE:O	11:I:196:PHE:CD1	2.74	0.41
2:3:32:A:C2	2:3:41:G:C5	3.09	0.40
11:I:9:ASP:O	11:I:13:HIS:NE2	2.54	0.40
11:I:159:ARG:CD	11:I:162:ARG:NH2	2.84	0.40
15:M:40:ASP:C	15:M:42:ASP:N	2.74	0.40
9:G:5:UNK:C	9:G:7:UNK:N	2.81	0.40
2:3:10:C:C2	15:M:20:TYR:CD1	3.09	0.40
11:I:26:LEU:O	11:I:100:ARG:NH1	2.54	0.40
8:F:126:LYS:CE	8:F:135:LEU:CD1	2.99	0.40
25:W:10:ASP:OD1	25:W:108:THR:CG2	2.70	0.40
2:3:116:A:O3'	15:M:260:ARG:NH2	2.54	0.40
15:M:267:ASN:OD1	15:M:268:ASP:N	2.55	0.40
21:S:33:HIS:NE2	21:S:39:ARG:NH2	2.69	0.40
4:B:365:HIS:CE1	30:0:6710:HOH:O	2.74	0.40
16:N:131:ALA:O	16:N:134:GLY:N	2.54	0.40
2:3:13:A:OP1	2:3:109:U:C2'	2.69	0.40
14:L:26:ARG:O	14:L:29:GLU:N	2.55	0.40
11:I:171:VAL:O	11:I:172:LYS:C	2.58	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:284:GLN:CG	16:N:108:GLU:OE2	2.70	0.40
15:M:18:THR:O	15:M:18:THR:CG2	2.69	0.40
18:P:42:ILE:O	18:P:59:GLY:N	2.54	0.40
18:P:11:THR:O	18:P:11:THR:CG2	2.68	0.40
3:A:210:HIS:CE1	3:A:236:VAL:CG1	3.04	0.40
5:C:81:ILE:CG2	5:C:82:PRO:O	2.69	0.40
2:3:75:G:O2'	2:3:76:U:P	2.80	0.40
14:L:148:ILE:O	14:L:148:ILE:CG2	2.69	0.40
11:I:111:TYR:N	11:I:111:TYR:CD1	2.90	0.40
6:D:120:THR:O	6:D:120:THR:CG2	2.70	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	
3	A	255/264 (97%)	237 (93%)	18 (7%)	0	100	100
4	B	384/391 (98%)	370 (96%)	14 (4%)	0	100	100
5	C	407/410 (99%)	386 (95%)	21 (5%)	0	100	100
6	D	167/172 (97%)	156 (93%)	11 (7%)	0	100	100
7	E	184/188 (98%)	171 (93%)	13 (7%)	0	100	100
8	F	229/255 (90%)	219 (96%)	10 (4%)	0	100	100
10	H	197/215 (92%)	186 (94%)	11 (6%)	0	100	100
11	I	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
12	J	136/141 (96%)	132 (97%)	4 (3%)	0	100	100
13	K	146/149 (98%)	135 (92%)	8 (6%)	3 (2%)	11	62
14	L	201/204 (98%)	193 (96%)	7 (4%)	1 (0%)	38	87
15	M	298/301 (99%)	285 (96%)	12 (4%)	1 (0%)	50	92
16	N	178/181 (98%)	168 (94%)	10 (6%)	0	100	100
17	O	151/185 (82%)	143 (95%)	8 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	P	154/157 (98%)	147 (96%)	7 (4%)	0	100	100
19	Q	155/183 (85%)	147 (95%)	8 (5%)	0	100	100
20	R	119/150 (79%)	114 (96%)	5 (4%)	0	100	100
21	S	124/135 (92%)	118 (95%)	6 (5%)	0	100	100
22	T	59/158 (37%)	57 (97%)	2 (3%)	0	100	100
23	U	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
24	V	232/239 (97%)	216 (93%)	15 (6%)	1 (0%)	43	90
25	W	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
26	X	123/134 (92%)	117 (95%)	6 (5%)	0	100	100
27	Y	100/103 (97%)	90 (90%)	10 (10%)	0	100	100
All	All	4424/4748 (93%)	4190 (95%)	228 (5%)	6 (0%)	59	96

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	K	24	LYS
13	K	15	VAL
13	K	46	LEU
14	L	187	SER
24	V	228	GLU
15	M	270	PRO

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	196/198 (99%)	165 (84%)	31 (16%)	4	23
4	B	330/334 (99%)	306 (93%)	24 (7%)	20	66
5	C	325/326 (100%)	300 (92%)	25 (8%)	18	64
6	D	146/149 (98%)	136 (93%)	10 (7%)	22	70
7	E	163/165 (99%)	157 (96%)	6 (4%)	45	86
8	F	201/222 (90%)	194 (96%)	7 (4%)	48	88

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	169/180 (94%)	153 (90%)	16 (10%)	12	51
11	I	166/166 (100%)	150 (90%)	16 (10%)	12	51
12	J	107/108 (99%)	99 (92%)	8 (8%)	19	65
13	K	120/121 (99%)	110 (92%)	10 (8%)	16	59
14	L	174/175 (99%)	166 (95%)	8 (5%)	37	82
15	M	253/254 (100%)	240 (95%)	13 (5%)	33	80
16	N	159/160 (99%)	146 (92%)	13 (8%)	17	60
17	O	127/159 (80%)	117 (92%)	10 (8%)	18	62
18	P	134/135 (99%)	125 (93%)	9 (7%)	23	70
19	Q	128/148 (86%)	115 (90%)	13 (10%)	11	47
20	R	108/132 (82%)	103 (95%)	5 (5%)	37	82
21	S	113/120 (94%)	104 (92%)	9 (8%)	17	62
22	T	52/130 (40%)	46 (88%)	6 (12%)	8	39
23	U	105/106 (99%)	96 (91%)	9 (9%)	15	58
24	V	197/202 (98%)	187 (95%)	10 (5%)	33	80
25	W	100/101 (99%)	96 (96%)	4 (4%)	42	85
26	X	104/111 (94%)	88 (85%)	16 (15%)	4	24
27	Y	79/80 (99%)	73 (92%)	6 (8%)	19	65
All	All	3756/3982 (94%)	3472 (92%)	284 (8%)	19	65

All (284) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	ARG
3	A	14	ASN
3	A	19	SER
3	A	29	GLN
3	A	31	ARG
3	A	32	VAL
3	A	33	TYR
3	A	42	ILE
3	A	43	ARG
3	A	45	CYS
3	A	93	LEU
3	A	108	ILE
3	A	128	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	A	145	ASP
3	A	180	ILE
3	A	186	GLN
3	A	192	ARG
3	A	194	ARG
3	A	196	SER
3	A	206	ASN
3	A	217	HIS
3	A	220	ILE
3	A	225	THR
3	A	226	VAL
3	A	227	SER
3	A	231	SER
3	A	236	VAL
3	A	238	LEU
3	A	239	ARG
3	A	243	ARG
3	A	244	THR
4	B	4	ARG
4	B	29	CYS
4	B	55	HIS
4	B	58	ARG
4	B	60	VAL
4	B	61	ASP
4	B	62	ARG
4	B	68	ASN
4	B	76	VAL
4	B	95	THR
4	B	97	ARG
4	B	120	LYS
4	B	162	THR
4	B	204	ASP
4	B	250	ILE
4	B	257	ARG
4	B	262	VAL
4	B	278	LYS
4	B	327	VAL
4	B	332	ARG
4	B	337	ARG
4	B	339	SER
4	B	367	ARG
4	B	370	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	C	36	ASP
5	C	44	ASP
5	C	74	THR
5	C	81	ILE
5	C	83	ARG
5	C	87	SER
5	C	97	PHE
5	C	99	ASN
5	C	100	GLN
5	C	143	PHE
5	C	145	ARG
5	C	157	TYR
5	C	161	ASP
5	C	169	THR
5	C	187	ARG
5	C	209	ARG
5	C	223	LEU
5	C	240	ARG
5	C	265	LYS
5	C	304	VAL
5	C	306	SER
5	C	328	ASN
5	C	330	LEU
5	C	377	ILE
5	C	382	LYS
6	D	10	ARG
6	D	20	ASN
6	D	26	SER
6	D	48	SER
6	D	49	ARG
6	D	56	SER
6	D	89	MET
6	D	108	GLU
6	D	114	MET
6	D	146	SER
7	E	35	LYS
7	E	62	ARG
7	E	70	SER
7	E	113	LYS
7	E	168	LYS
7	E	171	ARG
8	F	50	TYR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
8	F	53	LEU
8	F	74	THR
8	F	103	ARG
8	F	149	ASP
8	F	156	VAL
8	F	197	ARG
10	H	24	ARG
10	H	26	VAL
10	H	32	ARG
10	H	49	VAL
10	H	54	SER
10	H	61	THR
10	H	98	ARG
10	H	115	MET
10	H	133	SER
10	H	138	VAL
10	H	147	TYR
10	H	154	ARG
10	H	168	SER
10	H	195	SER
10	H	200	ILE
10	H	208	ARG
11	I	24	LYS
11	I	28	SER
11	I	50	ARG
11	I	54	SER
11	I	60	TRP
11	I	64	ASN
11	I	76	SER
11	I	84	ARG
11	I	105	GLU
11	I	116	LYS
11	I	135	CYS
11	I	136	LYS
11	I	143	SER
11	I	152	ILE
11	I	159	ARG
11	I	198	TYR
12	J	23	VAL
12	J	47	LYS
12	J	50	LEU
12	J	61	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	J	70	SER
12	J	92	ARG
12	J	116	SER
12	J	126	CYS
13	K	12	ARG
13	K	17	HIS
13	K	48	GLU
13	K	58	LEU
13	K	60	MET
13	K	70	LEU
13	K	78	ASP
13	K	79	LYS
13	K	129	TYR
13	K	137	ARG
14	L	42	SER
14	L	80	VAL
14	L	89	ILE
14	L	105	ARG
14	L	152	CYS
14	L	154	SER
14	L	159	ARG
14	L	165	THR
15	M	3	PHE
15	M	19	LYS
15	M	23	ARG
15	M	44	TYR
15	M	61	ILE
15	M	79	ASP
15	M	107	ARG
15	M	134	GLU
15	M	140	LYS
15	M	178	SER
15	M	185	ARG
15	M	213	MET
15	M	234	THR
16	N	4	ASP
16	N	14	ARG
16	N	20	THR
16	N	23	THR
16	N	52	ARG
16	N	55	SER
16	N	75	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	N	84	THR
16	N	91	GLU
16	N	93	LEU
16	N	145	SER
16	N	146	ARG
16	N	167	VAL
17	O	5	ARG
17	O	9	ARG
17	O	17	CYS
17	O	57	ILE
17	O	61	SER
17	O	84	THR
17	O	110	ARG
17	O	115	ILE
17	O	127	SER
17	O	137	VAL
18	P	8	ARG
18	P	9	ARG
18	P	29	ARG
18	P	45	ASP
18	P	63	LYS
18	P	94	GLU
18	P	128	THR
18	P	130	ARG
18	P	149	HIS
19	Q	17	VAL
19	Q	26	VAL
19	Q	58	ARG
19	Q	59	CYS
19	Q	63	THR
19	Q	72	THR
19	Q	82	GLN
19	Q	89	SER
19	Q	93	ILE
19	Q	120	GLN
19	Q	142	LEU
19	Q	144	SER
19	Q	150	ILE
20	R	36	ARG
20	R	81	MET
20	R	90	MET
20	R	124	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	R	150	ILE
21	S	12	ARG
21	S	45	ARG
21	S	46	SER
21	S	50	ARG
21	S	51	LYS
21	S	59	ARG
21	S	68	LYS
21	S	107	LYS
21	S	111	ASP
22	T	27	ASP
22	T	39	LYS
22	T	42	SER
22	T	52	THR
22	T	57	ARG
22	T	60	LEU
23	U	14	THR
23	U	28	GLU
23	U	41	THR
23	U	43	ASN
23	U	48	ILE
23	U	83	ASP
23	U	93	ARG
23	U	109	GLN
23	U	120	PHE
24	V	15	ARG
24	V	27	ARG
24	V	63	LYS
24	V	98	ARG
24	V	104	ARG
24	V	121	LEU
24	V	138	ARG
24	V	161	THR
24	V	223	ASP
24	V	227	ARG
25	W	16	HIS
25	W	23	SER
25	W	45	THR
25	W	75	CYS
26	X	32	SER
26	X	33	SER
26	X	35	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	X	36	ARG
26	X	40	ILE
26	X	52	ARG
26	X	57	ILE
26	X	62	ASP
26	X	75	LYS
26	X	77	LEU
26	X	79	ARG
26	X	84	LEU
26	X	86	ILE
26	X	89	MET
26	X	113	ARG
26	X	125	ASN
27	Y	4	ARG
27	Y	7	LYS
27	Y	16	THR
27	Y	60	CYS
27	Y	71	LEU
27	Y	73	THR

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	154/154 (100%)	60 (38%)	13 (8%)
2	3	119/120 (99%)	38 (31%)	1 (0%)
All	All	273/274 (99%)	98 (35%)	14 (5%)

All (98) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	G
1	2	3	A
1	2	4	A
1	2	5	A
1	2	6	A
1	2	7	U
1	2	8	U
1	2	17	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2	26	A
1	2	27	G
1	2	28	G
1	2	34	G
1	2	35	U
1	2	36	G
1	2	38	C
1	2	43	A
1	2	44	A
1	2	45	G
1	2	47	A
1	2	55	A
1	2	62	A
1	2	65	C
1	2	66	G
1	2	67	C
1	2	73	G
1	2	74	A
1	2	75	A
1	2	82	A
1	2	84	C
1	2	85	C
1	2	86	G
1	2	87	C
1	2	88	G
1	2	89	A
1	2	91	U
1	2	92	C
1	2	96	A
1	2	97	G
1	2	100	C
1	2	105	A
1	2	106	A
1	2	107	C
1	2	108	G
1	2	112	G
1	2	113	U
1	2	114	G
1	2	117	G
1	2	122	U
1	2	127	A
1	2	131	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2	134	C
1	2	135	A
1	2	137	G
1	2	140	U
1	2	141	G
1	2	145	C
1	2	146	A
1	2	148	U
1	2	149	G
1	2	150	U
2	3	5	U
2	3	7	G
2	3	9	C
2	3	10	C
2	3	13	A
2	3	22	A
2	3	25	A
2	3	27	A
2	3	38	U
2	3	40	C
2	3	41	G
2	3	48	G
2	3	49	A
2	3	51	G
2	3	53	U
2	3	54	A
2	3	55	A
2	3	60	C
2	3	62	U
2	3	63	A
2	3	64	A
2	3	65	G
2	3	82	G
2	3	83	G
2	3	89	G
2	3	91	C
2	3	97	G
2	3	98	G
2	3	100	A
2	3	101	A
2	3	105	C
2	3	107	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	3	110	G
2	3	111	U
2	3	112	C
2	3	113	G
2	3	118	C
2	3	120	U

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1	A
1	2	2	G
1	2	3	A
1	2	25	U
1	2	37	A
1	2	43	A
1	2	88	G
1	2	91	U
1	2	96	A
1	2	107	C
1	2	111	A
1	2	112	G
1	2	134	C
2	3	62	U

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 177 ligands modelled in this entry, 177 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	2	154/154 (100%)	-0.03	2 (1%) 74 41	98, 146, 182, 210	0
2	3	120/120 (100%)	0.29	4 (3%) 44 21	95, 138, 175, 235	0
3	A	257/264 (97%)	-0.03	2 (0%) 83 53	60, 106, 157, 242	0
4	B	386/391 (98%)	-0.07	0 100 100	51, 82, 132, 217	0
5	C	409/410 (99%)	-0.01	3 (0%) 84 56	77, 143, 195, 252	0
6	D	169/172 (98%)	0.12	4 (2%) 56 27	96, 139, 182, 216	0
7	E	186/188 (98%)	-0.18	0 100 100	53, 91, 135, 220	0
8	F	231/255 (90%)	-0.06	1 (0%) 90 71	112, 166, 210, 233	0
9	G	0/123	-	-	-	-
10	H	201/215 (93%)	-0.03	1 (0%) 88 65	71, 118, 171, 203	0
11	I	198/198 (100%)	-0.17	0 100 100	53, 91, 151, 195	0
12	J	138/141 (97%)	-0.02	0 100 100	30, 60, 98, 186	0
13	K	148/149 (99%)	-0.08	1 (0%) 84 56	78, 129, 181, 208	0
14	L	203/204 (99%)	-0.10	1 (0%) 88 65	89, 133, 165, 205	0
15	M	300/301 (99%)	0.20	6 (2%) 62 31	98, 157, 204, 233	0
16	N	180/181 (99%)	0.04	5 (2%) 50 24	94, 139, 188, 248	0
17	O	153/185 (82%)	-0.21	2 (1%) 74 41	67, 109, 153, 262	0
18	P	156/157 (99%)	-0.02	1 (0%) 86 60	69, 122, 163, 222	0
19	Q	157/183 (85%)	0.00	0 100 100	60, 106, 157, 200	0
20	R	121/150 (80%)	0.12	4 (3%) 44 21	97, 138, 175, 191	0
21	S	126/135 (93%)	0.02	3 (2%) 56 27	101, 143, 186, 218	0
22	T	61/158 (38%)	-0.16	0 100 100	42, 76, 115, 138	0
23	U	123/124 (99%)	-0.06	3 (2%) 56 27	113, 157, 193, 233	0
24	V	234/239 (97%)	0.02	1 (0%) 90 71	75, 121, 173, 239	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	110/111 (99%)	-0.06	2 (1%) 65 34	63, 102, 183, 216	0
26	X	125/134 (93%)	-0.04	2 (1%) 68 36	73, 117, 162, 215	0
27	Y	102/103 (99%)	-0.36	0 100 100	53, 102, 189, 222	0
All	All	4748/5145 (92%)	-0.02	48 (1%) 79 48	30, 125, 186, 262	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	O	154	LYS	8.9
6	D	4	LYS	5.6
17	O	153	ASP	5.1
1	2	101	U	4.8
21	S	4	HIS	3.8
15	M	85	ARG	3.6
1	2	66	G	3.4
16	N	92	ARG	3.4
21	S	2	LYS	3.4
2	3	26	C	3.3
6	D	55	ARG	3.3
23	U	2	ASP	3.3
2	3	3	U	3.3
20	R	64	HIS	3.0
5	C	3	SER	3.0
5	C	2	THR	2.9
23	U	118	ARG	2.8
18	P	157	PHE	2.7
16	N	141	ARG	2.7
20	R	137	ASP	2.7
15	M	149	GLY	2.7
3	A	142	GLU	2.6
25	W	84	ALA	2.6
13	K	149	ALA	2.5
2	3	25	A	2.5
16	N	44	LYS	2.5
3	A	47	ARG	2.4
26	X	127	LYS	2.4
26	X	18	LYS	2.3
8	F	19	ASN	2.3
23	U	40	GLY	2.3
14	L	199	LYS	2.2
6	D	5	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
20	R	127	ASN	2.2
15	M	194	LYS	2.2
15	M	196	LYS	2.2
20	R	125	THR	2.2
25	W	2	VAL	2.2
15	M	152	ARG	2.2
6	D	153	MET	2.1
10	H	175	LYS	2.1
2	3	27	A	2.1
21	S	73	TYR	2.1
5	C	370	LYS	2.1
16	N	153	GLY	2.1
24	V	7	GLU	2.1
15	M	81	TYR	2.1
16	N	51	LYS	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
28	MG	0	197	1/1	0.51	23.36	174,174,174,174	0
28	MG	0	347	1/1	0.28	12.71	171,171,171,171	0
28	MG	0	325	1/1	0.57	11.36	143,143,143,143	0
28	MG	0	228	1/1	0.23	7.00	114,114,114,114	0
28	MG	0	200	1/1	0.25	2.89	137,137,137,137	0
28	MG	0	70	1/1	0.18	0.45	181,181,181,181	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	MG	0	135	1/1	0.19	0.39	73,73,73,73	0
28	MG	0	204	1/1	0.15	0.31	86,86,86,86	0
28	MG	0	1	1/1	0.16	0.08	141,141,141,141	0
28	MG	0	345	1/1	0.21	-0.25	146,146,146,146	0
28	MG	0	100	1/1	0.20	-0.38	119,119,119,119	0
28	MG	0	145	1/1	0.21	-0.55	141,141,141,141	0
28	MG	0	8	1/1	0.19	-0.97	146,146,146,146	0
28	MG	0	63	1/1	0.11	-1.10	122,122,122,122	0
29	ZN	Y	104	1/1	0.06	-1.17	116,116,116,116	0
28	MG	0	314	1/1	0.18	-1.51	114,114,114,114	0
28	MG	0	359	1/1	0.09	-2.42	114,114,114,114	0
28	MG	0	74	1/1	0.09	-2.61	62,62,62,62	0
28	MG	0	66	1/1	0.12	-2.61	112,112,112,112	0
28	MG	0	117	1/1	0.15	-5.00	136,136,136,136	0
28	MG	0	373	1/1	0.08	-5.43	113,113,113,113	0
28	MG	0	140	1/1	0.09	-5.72	142,142,142,142	0
28	MG	0	183	1/1	0.14	-5.75	134,134,134,134	0
28	MG	0	277	1/1	0.07	-5.97	69,69,69,69	0
28	MG	0	174	1/1	0.05	-7.34	102,102,102,102	0
28	MG	0	94	1/1	0.24	-147.00	96,96,96,96	0
28	MG	0	317	1/1	0.16	-	212,212,212,212	0
28	MG	0	366	1/1	0.23	-	124,124,124,124	0
28	MG	0	244	1/1	0.18	-	104,104,104,104	0
28	MG	0	35	1/1	0.27	-	173,173,173,173	0
28	MG	0	300	1/1	0.26	-	121,121,121,121	0
28	MG	0	342	1/1	0.38	-	221,221,221,221	0
28	MG	0	242	1/1	0.32	-	166,166,166,166	0
28	MG	0	287	1/1	0.16	-	80,80,80,80	0
28	MG	0	233	1/1	0.17	-	81,81,81,81	0
28	MG	0	356	1/1	0.28	-	154,154,154,154	0
28	MG	0	202	1/1	0.41	-	121,121,121,121	0
28	MG	0	263	1/1	0.17	-	79,79,79,79	0
28	MG	0	371	1/1	0.55	-	131,131,131,131	0
28	MG	0	172	1/1	0.07	-	97,97,97,97	0
28	MG	0	12	1/1	0.25	-	111,111,111,111	0
28	MG	0	309	1/1	0.69	-	151,151,151,151	0
28	MG	0	272	1/1	0.10	-	82,82,82,82	0
28	MG	0	271	1/1	0.23	-	75,75,75,75	0
28	MG	0	60	1/1	0.12	-	114,114,114,114	0
28	MG	0	132	1/1	0.20	-	120,120,120,120	0
28	MG	0	285	1/1	0.07	-	64,64,64,64	0
28	MG	0	129	1/1	0.26	-	146,146,146,146	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	MG	0	376	1/1	0.16	-	123,123,123,123	0
28	MG	0	335	1/1	0.12	-	119,119,119,119	0
28	MG	0	362	1/1	0.12	-	156,156,156,156	0
28	MG	0	331	1/1	0.46	-	99,99,99,99	0
28	MG	0	14	1/1	0.16	-	132,132,132,132	0
28	MG	0	101	1/1	0.15	-	87,87,87,87	0
28	MG	0	141	1/1	0.23	-	157,157,157,157	0
28	MG	0	330	1/1	0.10	-	94,94,94,94	0
28	MG	0	11	1/1	0.09	-	118,118,118,118	0
28	MG	0	337	1/1	0.16	-	154,154,154,154	0
28	MG	0	320	1/1	0.12	-	107,107,107,107	0
28	MG	0	303	1/1	0.13	-	87,87,87,87	0
28	MG	0	217	1/1	0.12	-	123,123,123,123	0
28	MG	0	224	1/1	0.07	-	70,70,70,70	0
28	MG	0	166	1/1	0.34	-	147,147,147,147	0
28	MG	0	338	1/1	0.21	-	157,157,157,157	0
28	MG	0	99	1/1	0.16	-	77,77,77,77	0
28	MG	0	259	1/1	0.17	-	111,111,111,111	0
28	MG	0	239	1/1	0.08	-	162,162,162,162	0
28	MG	0	279	1/1	0.09	-	95,95,95,95	0
28	MG	0	96	1/1	0.06	-	108,108,108,108	0
28	MG	0	108	1/1	0.22	-	94,94,94,94	0
28	MG	0	374	1/1	0.44	-	146,146,146,146	0
28	MG	0	264	1/1	0.09	-	56,56,56,56	0
28	MG	0	316	1/1	0.37	-	123,123,123,123	0
28	MG	0	54	1/1	0.16	-	133,133,133,133	0
28	MG	0	241	1/1	0.05	-	108,108,108,108	0
28	MG	0	255	1/1	0.18	-	206,206,206,206	0
28	MG	0	227	1/1	0.12	-	103,103,103,103	0
28	MG	0	256	1/1	0.09	-	122,122,122,122	0
28	MG	0	308	1/1	0.66	-	110,110,110,110	0
28	MG	0	143	1/1	0.10	-	68,68,68,68	0
28	MG	0	193	1/1	0.17	-	107,107,107,107	0
28	MG	0	192	1/1	0.09	-	109,109,109,109	0
28	MG	0	273	1/1	0.06	-	110,110,110,110	0
28	MG	0	229	1/1	0.25	-	132,132,132,132	0
28	MG	0	247	1/1	0.07	-	105,105,105,105	0
28	MG	0	37	1/1	0.27	-	117,117,117,117	0
28	MG	0	350	1/1	0.48	-	174,174,174,174	0
28	MG	0	80	1/1	0.10	-	151,151,151,151	0
28	MG	0	270	1/1	0.12	-	60,60,60,60	0
28	MG	0	329	1/1	0.11	-	157,157,157,157	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	MG	0	162	1/1	0.05	-	111,111,111,111	0
28	MG	0	361	1/1	0.24	-	146,146,146,146	0
28	MG	0	153	1/1	0.12	-	78,78,78,78	0
28	MG	0	50	1/1	0.35	-	169,169,169,169	0
28	MG	0	363	1/1	0.18	-	120,120,120,120	0
28	MG	0	195	1/1	0.07	-	95,95,95,95	0
28	MG	0	321	1/1	0.29	-	167,167,167,167	0
28	MG	0	191	1/1	0.22	-	143,143,143,143	0
28	MG	0	112	1/1	0.20	-	132,132,132,132	0
28	MG	0	364	1/1	0.14	-	175,175,175,175	0
28	MG	0	268	1/1	0.30	-	141,141,141,141	0
28	MG	0	351	1/1	0.36	-	140,140,140,140	0
28	MG	0	64	1/1	0.11	-	141,141,141,141	0
28	MG	0	190	1/1	0.04	-	108,108,108,108	0
28	MG	0	328	1/1	0.43	-	139,139,139,139	0
28	MG	0	160	1/1	0.09	-	66,66,66,66	0
28	MG	0	92	1/1	0.37	-	98,98,98,98	0
28	MG	0	148	1/1	0.29	-	110,110,110,110	0
28	MG	0	226	1/1	0.04	-	52,52,52,52	0
28	MG	0	276	1/1	0.17	-	91,91,91,91	0
28	MG	0	150	1/1	0.17	-	98,98,98,98	0
28	MG	0	251	1/1	0.12	-	122,122,122,122	0
28	MG	0	137	1/1	0.15	-	102,102,102,102	0
28	MG	0	348	1/1	0.19	-	168,168,168,168	0
28	MG	0	340	1/1	0.31	-	162,162,162,162	0
28	MG	0	144	1/1	0.15	-	120,120,120,120	0
28	MG	0	211	1/1	0.32	-	124,124,124,124	0
28	MG	0	336	1/1	0.17	-	214,214,214,214	0
28	MG	0	307	1/1	0.15	-	79,79,79,79	0
28	MG	0	261	1/1	0.15	-	96,96,96,96	0
28	MG	0	354	1/1	0.07	-	128,128,128,128	0
28	MG	0	184	1/1	0.11	-	131,131,131,131	0
28	MG	0	25	1/1	0.25	-	193,193,193,193	0
28	MG	0	304	1/1	0.04	-	66,66,66,66	0
28	MG	0	163	1/1	0.06	-	113,113,113,113	0
28	MG	0	21	1/1	0.17	-	111,111,111,111	0
28	MG	0	267	1/1	0.10	-	65,65,65,65	0
28	MG	0	305	1/1	0.06	-	73,73,73,73	0
28	MG	0	102	1/1	0.24	-	82,82,82,82	0
28	MG	0	278	1/1	0.27	-	111,111,111,111	0
28	MG	0	152	1/1	0.06	-	156,156,156,156	0
28	MG	0	119	1/1	0.21	-	93,93,93,93	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
28	MG	0	34	1/1	0.32	-	120,120,120,120	0
28	MG	0	19	1/1	0.17	-	105,105,105,105	0
28	MG	0	130	1/1	0.24	-	93,93,93,93	0
28	MG	0	16	1/1	0.15	-	101,101,101,101	0
28	MG	0	139	1/1	0.09	-	79,79,79,79	0
28	MG	0	133	1/1	0.23	-	75,75,75,75	0
28	MG	0	97	1/1	0.20	-	105,105,105,105	0
28	MG	0	165	1/1	0.48	-	145,145,145,145	0
28	MG	0	142	1/1	0.11	-	65,65,65,65	0
28	MG	0	358	1/1	0.21	-	183,183,183,183	0
28	MG	0	56	1/1	0.39	-	113,113,113,113	0
28	MG	0	349	1/1	0.30	-	152,152,152,152	0
28	MG	0	181	1/1	0.09	-	69,69,69,69	0
28	MG	0	298	1/1	0.24	-	140,140,140,140	0
28	MG	0	306	1/1	0.45	-	129,129,129,129	0
28	MG	0	369	1/1	0.24	-	202,202,202,202	0
28	MG	0	274	1/1	0.05	-	82,82,82,82	0
28	MG	0	78	1/1	0.22	-	97,97,97,97	0
28	MG	0	252	1/1	0.13	-	108,108,108,108	0
28	MG	0	215	1/1	0.07	-	104,104,104,104	0
28	MG	0	346	1/1	0.13	-	150,150,150,150	0
28	MG	0	151	1/1	0.29	-	118,118,118,118	0
28	MG	0	154	1/1	0.07	-	108,108,108,108	0
28	MG	0	77	1/1	0.23	-	113,113,113,113	0
28	MG	0	222	1/1	0.28	-	123,123,123,123	0
28	MG	0	171	1/1	0.14	-	90,90,90,90	0
28	MG	0	269	1/1	0.18	-	50,50,50,50	0
28	MG	0	120	1/1	0.09	-	116,116,116,116	0
28	MG	0	208	1/1	0.18	-	140,140,140,140	0
28	MG	0	291	1/1	0.30	-	143,143,143,143	0
28	MG	0	98	1/1	0.13	-	83,83,83,83	0
28	MG	0	375	1/1	0.20	-	128,128,128,128	0
28	MG	0	110	1/1	0.06	-	91,91,91,91	0
28	MG	0	368	1/1	0.17	-	152,152,152,152	0
28	MG	0	186	1/1	0.15	-	78,78,78,78	0
28	MG	0	294	1/1	0.09	-	120,120,120,120	0
28	MG	0	357	1/1	0.18	-	137,137,137,137	0
28	MG	0	206	1/1	0.17	-	119,119,119,119	0
28	MG	0	18	1/1	0.08	-	143,143,143,143	0
28	MG	0	280	1/1	0.11	-	75,75,75,75	0
28	MG	0	341	1/1	0.20	-	153,153,153,153	0
28	MG	0	355	1/1	0.17	-	136,136,136,136	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	MG	0	33	1/1	0.45	-	192,192,192,192	0
28	MG	0	236	1/1	0.17	-	134,134,134,134	0
28	MG	0	365	1/1	0.33	-	188,188,188,188	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.