



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:44 PM GMT

PDB ID : 4PJO
Title : Minimal U1 snRNP
Authors : Kondo, Y.; Oubridge, C.; van Roon, A.M.; Nagai, K.
Deposited on : 2014-05-12
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

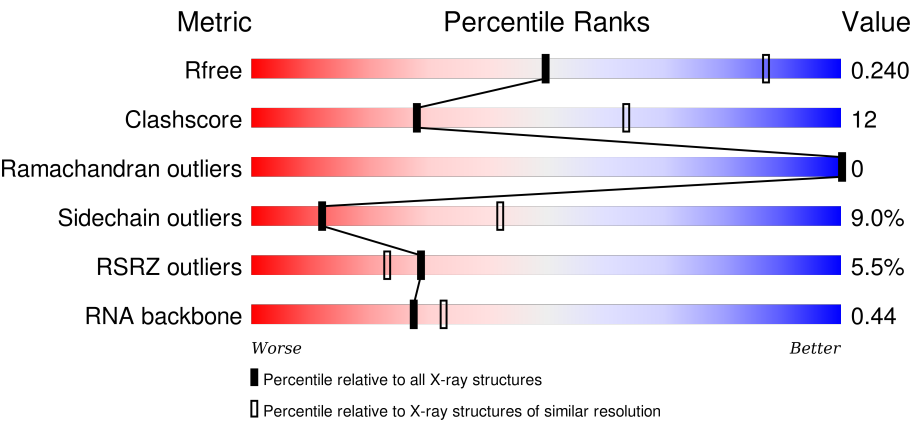
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	126	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>37%24%6%33%</div></div>
1	O	126	<div><div>19%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>41%20%••35%</div></div>
1	a	126	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>60%5%•34%</div></div>
1	o	126	<div><div>11%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>56%6%•36%</div></div>

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Mol	Chain	Length	Quality of chain
2	B	95	
2	P	95	
2	b	95	
2	p	95	
3	C	91	
3	Q	91	
3	c	91	
3	q	91	
4	D	118	
4	R	118	
4	d	118	
4	r	118	
5	E	92	
5	S	92	
5	e	92	
5	s	92	
6	F	75	
6	T	75	
6	f	75	
6	t	75	
7	G	76	
7	U	76	
7	g	76	
7	u	76	
8	K	60	

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Mol	Chain	Length	Quality of chain
8	N	60	
8	k	60	
8	n	60	
9	L	61	
9	M	61	
9	l	61	
9	m	61	
10	1	60	
10	2	60	
10	3	60	
10	4	60	
11	X	10	
11	Y	10	
11	x	10	
11	y	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	EPE	2	201	-	-	-	X
14	MG	2	202	-	-	-	X
17	CL	4	203	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 26921 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	84	Total	C	N	O	S	0	0	0
			657	412	116	123	6			
1	a	83	Total	C	N	O	S	0	0	0
			652	409	115	122	6			
1	O	82	Total	C	N	O	S	0	0	0
			643	403	113	121	6			
1	o	81	Total	C	N	O	S	0	0	0
			637	400	112	119	6			

- Molecule 2 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	S	0	0	0
			673	425	123	118	7			
2	b	78	Total	C	N	O	S	0	0	0
			635	402	114	112	7			
2	P	83	Total	C	N	O	S	0	0	0
			673	425	123	118	7			
2	p	86	Total	C	N	O	S	0	0	0
			692	435	126	124	7			

- Molecule 3 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	86	Total	C	N	O	S	0	0	0
			668	423	117	125	3			
3	c	87	Total	C	N	O	S	0	0	0
			675	428	118	126	3			
3	Q	85	Total	C	N	O	S	0	0	0
			664	421	116	124	3			
3	q	87	Total	C	N	O	S	0	0	0
			674	426	118	127	3			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	linker	UNP P62314
C	-4	SER	-	linker	UNP P62314
C	-3	GLY	-	linker	UNP P62314
C	-2	SER	-	linker	UNP P62314
C	-1	GLY	-	linker	UNP P62314
C	0	SER	-	linker	UNP P62314
C	1	VAL	-	linker	UNP P62314
c	-5	GLY	-	linker	UNP P62314
c	-4	SER	-	linker	UNP P62314
c	-3	GLY	-	linker	UNP P62314
c	-2	SER	-	linker	UNP P62314
c	-1	GLY	-	linker	UNP P62314
c	0	SER	-	linker	UNP P62314
c	1	VAL	-	linker	UNP P62314
Q	-5	GLY	-	linker	UNP P62314
Q	-4	SER	-	linker	UNP P62314
Q	-3	GLY	-	linker	UNP P62314
Q	-2	SER	-	linker	UNP P62314
Q	-1	GLY	-	linker	UNP P62314
Q	0	SER	-	linker	UNP P62314
Q	1	VAL	-	linker	UNP P62314
q	-5	GLY	-	linker	UNP P62314
q	-4	SER	-	linker	UNP P62314
q	-3	GLY	-	linker	UNP P62314
q	-2	SER	-	linker	UNP P62314
q	-1	GLY	-	linker	UNP P62314
q	0	SER	-	linker	UNP P62314
q	1	VAL	-	linker	UNP P62314

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	98	Total	C	N	O	S	0	0	0
			796	498	144	148	6			
4	d	92	Total	C	N	O	S	0	0	0
			753	472	138	138	5			
4	R	96	Total	C	N	O	S	0	1	0
			790	497	141	146	6			
4	r	95	Total	C	N	O	S	0	0	0
			777	486	141	144	6			

- Molecule 5 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
5	e	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
5	S	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
5	s	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			

- Molecule 6 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	73	Total	C	N	O	S	0	0	0
			568	367	94	102	5			
6	f	74	Total	C	N	O	S	0	0	0
			577	373	95	104	5			
6	T	74	Total	C	N	O	S	0	0	0
			577	373	95	104	5			
6	t	74	Total	C	N	O	S	0	0	0
			577	373	95	104	5			

- Molecule 7 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	1	0
			584	369	106	103	6			
7	g	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			
7	U	71	Total	C	N	O	S	0	0	0
			558	353	100	99	6			
7	u	73	Total	C	N	O	S	0	0	0
			568	358	102	102	6			

- Molecule 8 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	58	Total	C	N	O	S	0	0	0
			477	313	82	81	1			
8	k	57	Total	C	N	O	S	0	0	0
			470	309	81	79	1			
8	N	53	Total	C	N	O	S	0	0	0
			431	283	73	74	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	n	58	Total	C	N	O	S	0	0	0
			477	313	82	81	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	GLY	-	expression tag	UNP P08621
k	1	GLY	-	expression tag	UNP P08621
N	1	GLY	-	expression tag	UNP P08621
n	1	GLY	-	expression tag	UNP P08621

- Molecule 9 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L	53	Total	C	N	O	S	0	0	0
			448	280	77	87	4			
9	l	53	Total	C	N	O	S	0	0	0
			448	280	77	87	4			
9	M	53	Total	C	N	O	S	0	0	0
			448	280	77	87	4			
9	m	50	Total	C	N	O	S	0	0	0
			425	266	73	82	4			

- Molecule 10 is a RNA chain called U1 RNA variant (48-MER) with 4-helix junction replaced by kissing loop (HIV-1 (Mal) DIS) and shorter stem-loop 4..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1	48	Total	C	N	O	P	0	0	0
			1036	458	183	345	50			
10	2	48	Total	C	N	O	P	0	0	0
			1036	458	183	345	50			
10	3	47	Total	C	N	O	P	0	0	0
			1013	448	178	338	49			
10	4	49	Total	C	N	O	P	0	0	0
			1059	468	188	352	51			

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*GP*GP*UP*AP*AP*GP*UP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	X	10	Total	C	N	O	P	0	0	0
			212	96	40	67	9			

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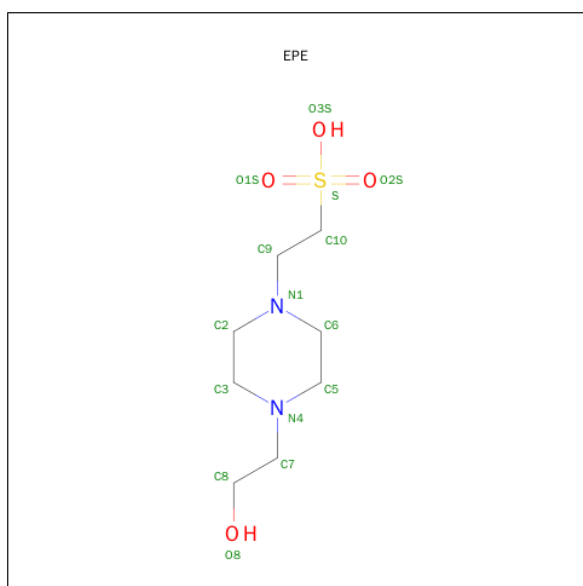
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	x	10	Total	C	N	O	P	0	0	0
			212	96	40	67	9			
11	Y	10	Total	C	N	O	P	0	0	0
			212	96	40	67	9			
11	y	10	Total	C	N	O	P	0	0	0
			212	96	40	67	9			

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	l	1	Total	Zn	0	0
			1	1		
12	m	1	Total	Zn	0	0
			1	1		
12	L	1	Total	Zn	0	0
			1	1		
12	M	1	Total	Zn	0	0
			1	1		

- Molecule 13 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	1	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
13	2	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

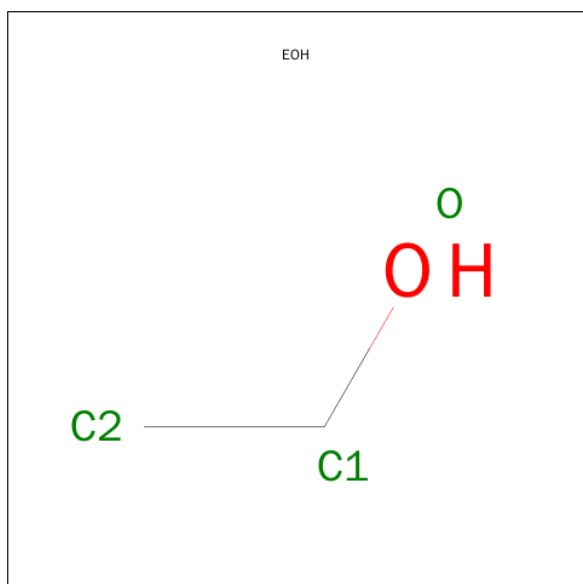
- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	1	8	Total Mg 8 8	0	0
14	4	1	Total Mg 1 1	0	0
14	2	4	Total Mg 4 4	0	0
14	y	2	Total Mg 2 2	0	0
14	1	1	Total Mg 1 1	0	0
14	3	4	Total Mg 4 4	0	0

- Molecule 15 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	b	2	Total K 2 2	0	0
15	1	1	Total K 1 1	0	0
15	Q	1	Total K 1 1	0	0
15	3	2	Total K 2 2	0	0

- Molecule 16 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).

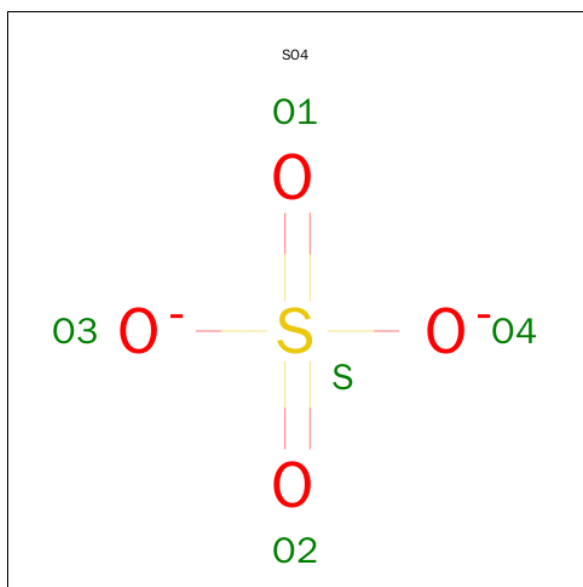


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	4	1	Total C O 3 2 1	0	0

- Molecule 17 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	4	1	Total Cl 1 1	0	0

- Molecule 18 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	y	1	Total O S 5 4 1	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	5	Total O 5 5	0	0
19	G	2	Total O 2 2	0	0
19	K	1	Total O 1 1	0	0
19	1	6	Total O 6 6	0	0

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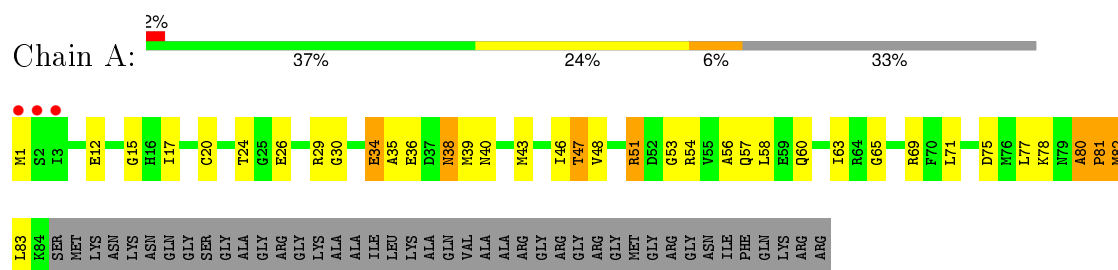
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	a	1	Total O 1 1	0	0
19	b	1	Total O 1 1	0	0
19	c	2	Total O 2 2	0	0
19	d	6	Total O 6 6	0	0
19	g	1	Total O 1 1	0	0
19	2	4	Total O 4 4	0	0
19	P	2	Total O 2 2	0	0
19	R	1	Total O 1 1	0	0
19	S	1	Total O 1 1	0	0
19	T	1	Total O 1 1	0	0
19	N	1	Total O 1 1	0	0
19	3	2	Total O 2 2	0	0
19	Y	1	Total O 1 1	0	0
19	p	1	Total O 1 1	0	0
19	q	2	Total O 2 2	0	0
19	r	1	Total O 1 1	0	0
19	t	1	Total O 1 1	0	0
19	m	1	Total O 1 1	0	0
19	4	4	Total O 4 4	0	0

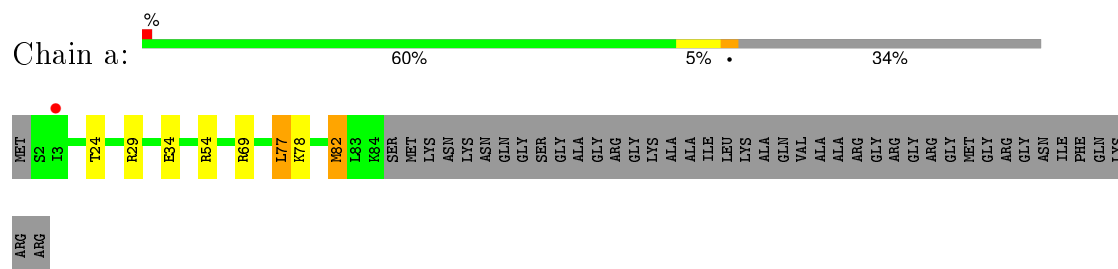
3 Residue-property plots [i](#)

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.

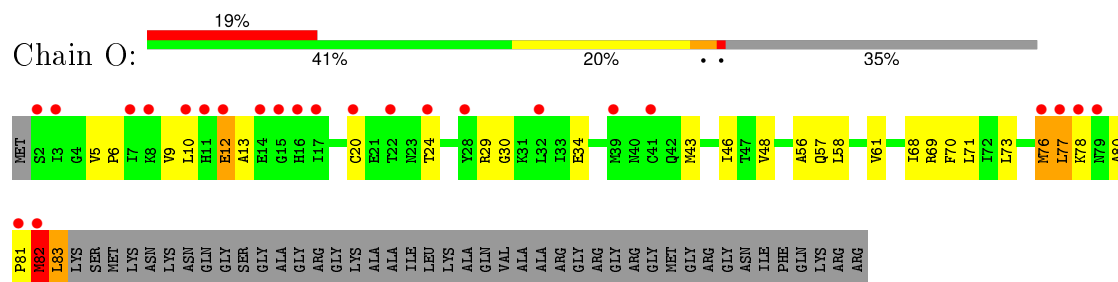
- Molecule 1: Small nuclear ribonucleoprotein Sm D3



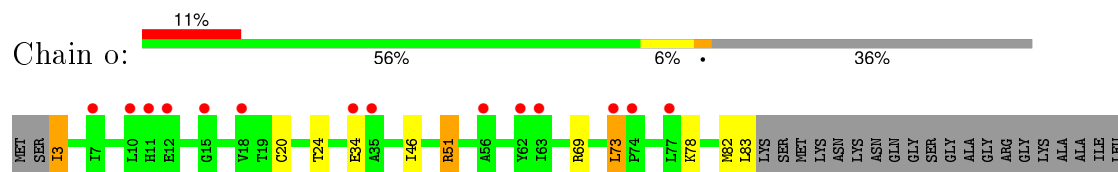
- Molecule 1: Small nuclear ribonucleoprotein Sm D3



- Molecule 1: Small nuclear ribonucleoprotein Sm D3



- Molecule 1: Small nuclear ribonucleoprotein Sm D3



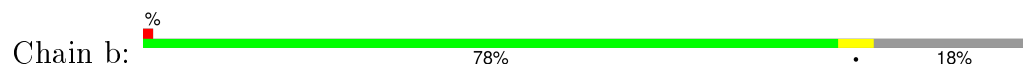
LYS
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GLY
ARG
GLY
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ARG
GLY
ASN
ILE
PHE
GLN
LYS
ARG

- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'



MET THR VAL GLY LYS S6 S7 S8 S9 Q10 Q11 Q12 Q13 Q14 Q15 Q16 Q17 Q18 T30 C43 K50 K51 K52 K53 Q58 Q59 Q60 V78 T81 V82 P86 P87 P88 ASP THR GLY ILE ALA ARG VAL

- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'



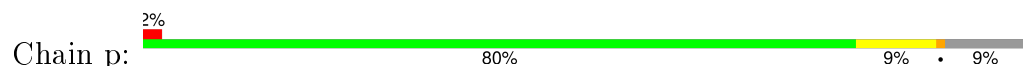
MET THR VAL GLY LYS S6 S7 Q11 Q25 P53 LYS ASN SER LYS GLN ALA P60 L71 M80 P89 THR GLY ILE ALA ARG VAL

- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'



MET THR VAL GLY LYS S6 S7 S8 S9 Q10 Q11 Q12 Q13 Q14 Q15 Q16 Q17 Q18 T30 C43 K50 K51 K52 K53 K54 K55 K56 K57 K58 Q59 Q60 E61 E62 E63 L71 L72 R73 M80 T81 V82 E83 P87 K88 ASP THR GLY ILE ALA ARG VAL

- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'



MET THR VAL GLY LYS S6 S7 H12 H13 D14 R18 K54 K55 K56 K57 Q58 L67 G68 L69 V70 L71 T90 G91 ILE ALA ARG VAL

- Molecule 3: Small nuclear ribonucleoprotein Sm D1



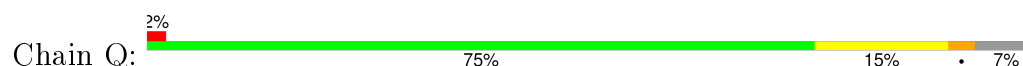
GLY SER G-3 V4 R5 M8 E18 E19 L19 K20 T23 Q24 V25 T30 G31 V32 D33 V34 L40 K41 M45 T46 L47 R50 E51 N63 N64 I65 I66 R66 Y67 V81 D82 VAL GLU PRO

- Molecule 3: Small nuclear ribonucleoprotein Sm D1



GLY SER G-3 V4 S11 L19 M36 K41 A42 M45 R66 V83 GLU PRO

- Molecule 3: Small nuclear ribonucleoprotein Sm D1





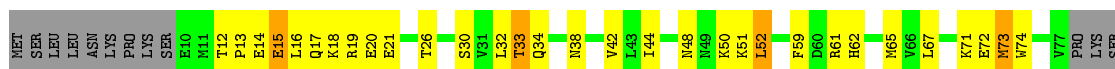
- Molecule 3: Small nuclear ribonucleoprotein Sm D1

Chain q: 87% 7% . .



- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain D:  45% 31% 8% 17%



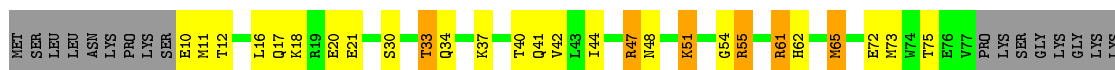
- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain d:  64% 14% • 22%



- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain R:  48% 25% 8% 19%



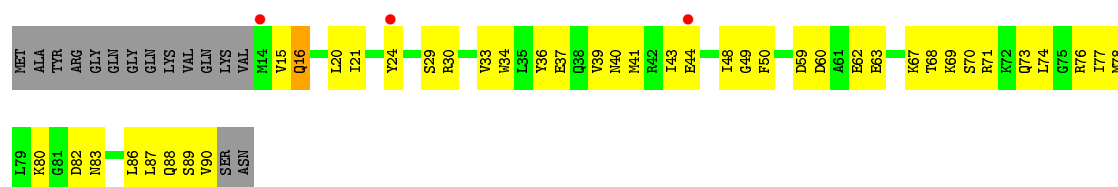
- Molecule 4: Small nuclear ribonucleoprotein Sm D2

Chain r:



- Molecule 5: Small nuclear ribonucleoprotein E

Chain E: 



- Molecule 5: Small nuclear ribonucleoprotein E



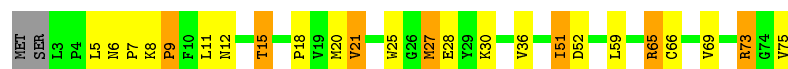
- Molecule 5: Small nuclear ribonucleoprotein E



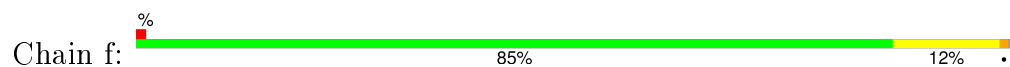
- Molecule 5: Small nuclear ribonucleoprotein E



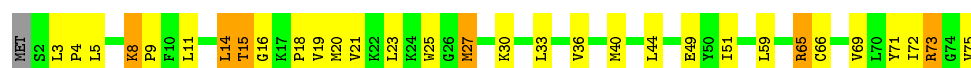
- Molecule 6: Small nuclear ribonucleoprotein F



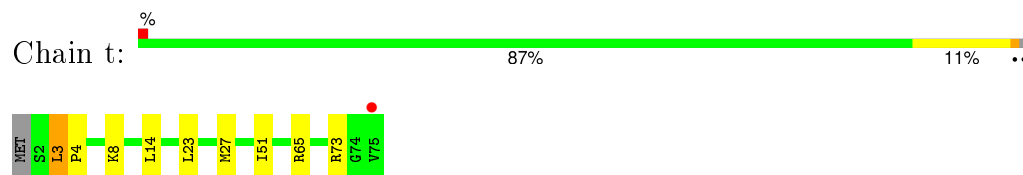
- Molecule 6: Small nuclear ribonucleoprotein F



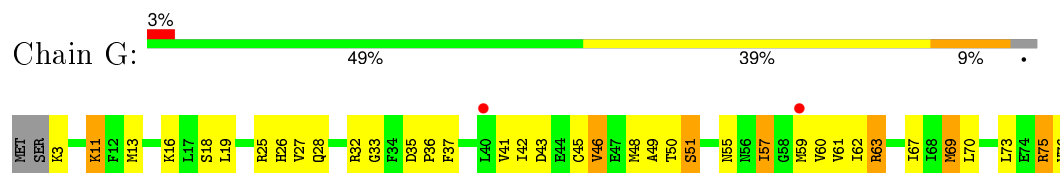
- Molecule 6: Small nuclear ribonucleoprotein F



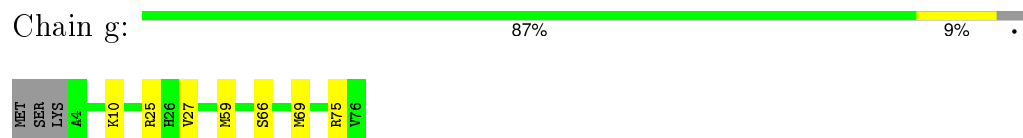
- Molecule 6: Small nuclear ribonucleoprotein F



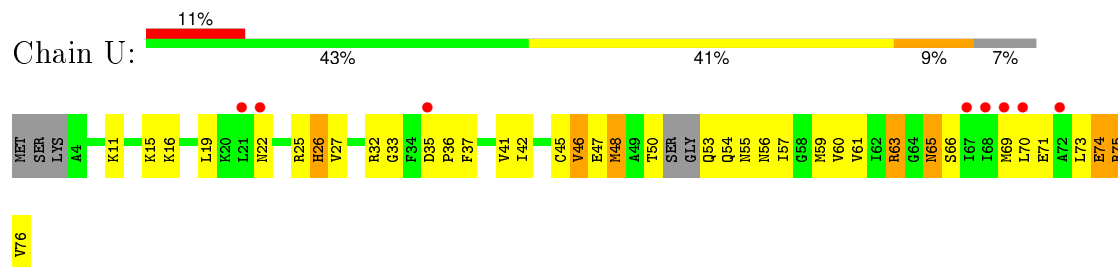
- Molecule 7: Small nuclear ribonucleoprotein G



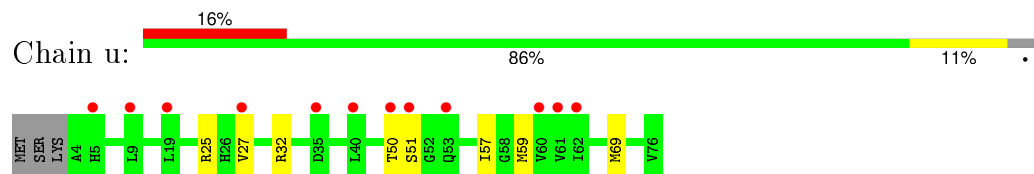
- Molecule 7: Small nuclear ribonucleoprotein G



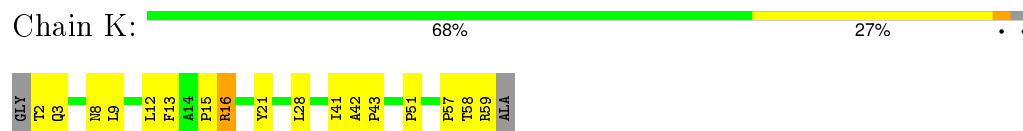
- Molecule 7: Small nuclear ribonucleoprotein G



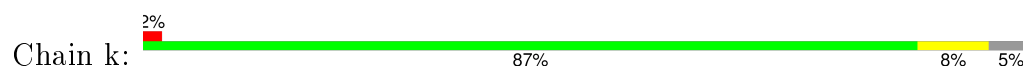
- Molecule 7: Small nuclear ribonucleoprotein G



- Molecule 8: U1 small nuclear ribonucleoprotein 70 kDa

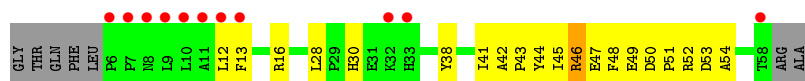


- Molecule 8: U1 small nuclear ribonucleoprotein 70 kDa

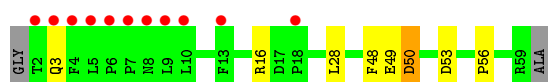
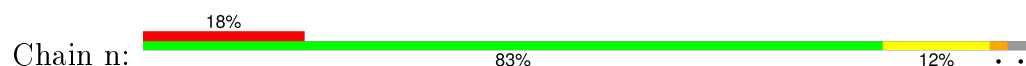




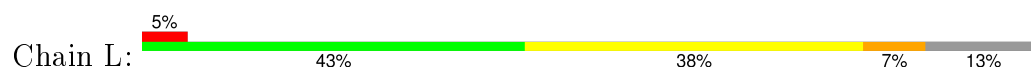
- Molecule 8: U1 small nuclear ribonucleoprotein 70 kDa



- Molecule 8: U1 small nuclear ribonucleoprotein 70 kDa



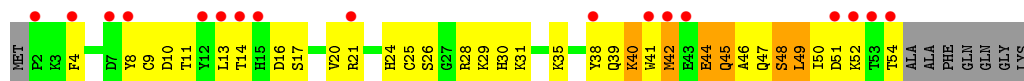
- Molecule 9: U1 small nuclear ribonucleoprotein C



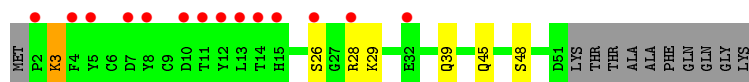
- Molecule 9: U1 small nuclear ribonucleoprotein C



- Molecule 9: U1 small nuclear ribonucleoprotein C



- Molecule 9: U1 small nuclear ribonucleoprotein C



- Molecule 10: U1 RNA variant (48-MER) with 4-helix junction replaced by kissing loop (HIV-1 (Mal) DIS) and shorter stem-loop 4.





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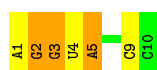
- Molecule 10: U1 RNA variant (48-MER) with 4-helix junction replaced by kissing loop (HIV-1 (Mal) DIS) and shorter stem-loop 4.



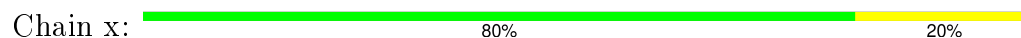
- Molecule 10: U1 RNA variant (48-MER) with 4-helix junction replaced by kissing loop (HIV-1 (Mal) DIS) and shorter stem-loop 4.



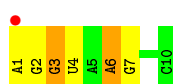
- Molecule 11: RNA (5'-R(*AP*GP*GP*UP*AP*AP*GP*UP*CP*C)-3')



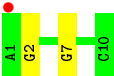
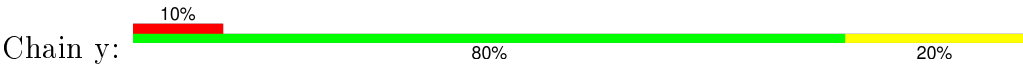
- Molecule 11: RNA (5'-R(*AP*GP*GP*UP*AP*AP*GP*UP*CP*C)-3')



- Molecule 11: RNA (5'-R(*AP*GP*GP*UP*AP*AP*GP*UP*CP*C)-3')



- Molecule 11: RNA (5'-R(*AP*GP*GP*UP*AP*AP*GP*UP*CP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.36Å 172.63Å 256.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.30 69.67 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (70.00-3.30) 97.4 (69.67-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.255 0.196 , 0.240	Depositor DCC
R_{free} test set	4038 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	86.2	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 78932 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	26921	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, K, EOH, ZN, GTP, SO4, EPE

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	0.74	1/665 (0.2%)	1.04	4/896 (0.4%)
1	O	0.52	0/651	1.15	5/878 (0.6%)
1	a	0.71	0/660	1.18	8/889 (0.9%)
1	o	0.53	0/645	1.19	6/870 (0.7%)
2	B	0.77	0/683	1.08	2/910 (0.2%)
2	P	0.65	0/683	1.08	1/910 (0.1%)
2	b	0.75	0/644	1.10	1/858 (0.1%)
2	p	0.63	0/702	1.16	3/936 (0.3%)
3	C	0.87	0/676	1.19	6/914 (0.7%)
3	Q	0.74	0/672	1.19	6/909 (0.7%)
3	c	0.84	0/683	1.28	4/924 (0.4%)
3	q	0.67	0/682	1.22	7/922 (0.8%)
4	D	0.75	1/805 (0.1%)	1.15	6/1081 (0.6%)
4	R	0.80	0/803	1.32	8/1079 (0.7%)
4	d	0.76	0/762	1.18	5/1022 (0.5%)
4	r	0.69	0/786	1.14	2/1055 (0.2%)
5	E	0.67	0/646	0.98	2/867 (0.2%)
5	S	0.64	0/646	1.30	6/867 (0.7%)
5	e	0.71	0/646	1.13	4/867 (0.5%)
5	s	0.62	0/646	1.27	5/867 (0.6%)
6	F	0.81	1/580 (0.2%)	1.17	3/783 (0.4%)
6	T	0.69	0/589	1.16	3/795 (0.4%)
6	f	0.77	0/589	1.24	4/795 (0.5%)
6	t	0.66	1/589 (0.2%)	1.18	4/795 (0.5%)
7	G	0.76	0/595	1.28	5/794 (0.6%)
7	U	0.57	0/564	1.06	1/752 (0.1%)
7	g	0.77	1/575 (0.2%)	1.27	4/768 (0.5%)
7	u	0.59	0/575	1.17	4/768 (0.5%)
8	K	0.76	0/499	1.10	1/688 (0.1%)
8	N	0.61	0/452	1.11	1/624 (0.2%)
8	k	0.77	0/492	1.10	2/678 (0.3%)
8	n	0.63	0/499	1.09	4/688 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	L	0.60	0/460	1.00	2/618 (0.3%)
9	M	0.61	0/460	1.12	6/618 (1.0%)
9	l	0.58	0/460	0.96	0/618
9	m	0.56	0/437	1.16	4/587 (0.7%)
10	1	0.62	0/1122	1.21	12/1747 (0.7%)
10	2	0.58	0/1122	1.16	7/1747 (0.4%)
10	3	0.49	0/1096	1.09	6/1706 (0.4%)
10	4	0.49	0/1148	1.10	7/1788 (0.4%)
11	X	0.44	0/237	1.33	5/368 (1.4%)
11	Y	0.43	0/237	1.26	4/368 (1.1%)
11	x	0.44	0/237	1.11	2/368 (0.5%)
11	y	0.40	0/237	0.94	0/368
All	All	0.67	5/27637 (0.0%)	1.16	182/38350 (0.5%)

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	1
2	P	0	1
3	C	0	1
3	c	0	1
4	R	0	1
4	r	0	1
6	T	0	1
8	k	0	1
8	n	0	1
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	89	PRO	N-CD	5.34	1.55	1.47
1	A	81	PRO	N-CD	5.18	1.55	1.47
6	F	9	PRO	N-CD	5.13	1.55	1.47
7	g	66	SER	CB-OG	-5.13	1.35	1.42
6	t	4	PRO	N-CD	5.04	1.54	1.47

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	87	LEU	CB-CG-CD2	13.57	134.07	111.00
9	m	28	ARG	NE-CZ-NH1	12.22	126.41	120.30
6	f	73	ARG	NE-CZ-NH1	-10.81	114.89	120.30
4	d	32	LEU	CB-CG-CD2	10.65	129.10	111.00
10	2	136	G	C4'-C3'-O3'	-10.48	87.40	109.40
4	D	73	MET	CG-SD-CE	-10.37	83.61	100.20
1	o	73	LEU	CB-CG-CD2	10.19	128.32	111.00
4	R	94	ARG	NE-CZ-NH1	10.05	125.32	120.30
6	t	73	ARG	NE-CZ-NH1	-10.04	115.28	120.30
4	D	102	ARG	NE-CZ-NH1	-9.75	115.42	120.30
3	c	19	LEU	CB-CG-CD1	9.69	127.46	111.00
11	X	3	G	O5'-P-OP2	-9.67	97.00	105.70
5	s	59	ASP	CB-CG-OD2	9.41	126.77	118.30
3	Q	19	LEU	CB-CG-CD1	9.24	126.71	111.00
10	4	128	U	O5'-P-OP1	-8.88	97.70	105.70
10	2	128	U	O5'-P-OP1	-8.75	97.83	105.70
11	X	3	G	O5'-P-OP1	8.70	121.14	110.70
5	s	71	ARG	NE-CZ-NH2	-8.53	116.03	120.30
3	c	36	MET	CG-SD-CE	-8.53	86.56	100.20
6	f	73	ARG	NE-CZ-NH2	8.53	124.56	120.30
4	R	102	ARG	NE-CZ-NH1	-8.41	116.09	120.30
6	t	73	ARG	NE-CZ-NH2	8.39	124.50	120.30
10	1	137	U	O5'-P-OP1	-8.33	98.20	105.70
2	p	18	ARG	NE-CZ-NH2	-8.00	116.30	120.30
8	N	52	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	o	51	ARG	NE-CZ-NH2	7.92	124.26	120.30
3	q	56	GLU	OE1-CD-OE2	-7.92	113.80	123.30
3	C	45	MET	CG-SD-CE	-7.91	87.55	100.20
1	o	69	ARG	NE-CZ-NH1	7.90	124.25	120.30
9	M	10	ASP	CB-CG-OD2	-7.89	111.20	118.30
3	Q	45	MET	CG-SD-CE	-7.72	87.85	100.20
2	p	14	ASP	CB-CG-OD2	-7.69	111.38	118.30
11	X	5	A	O5'-P-OP2	7.62	119.84	110.70
10	1	138	G	O5'-P-OP1	7.52	119.72	110.70
4	R	94	ARG	NE-CZ-NH2	-7.47	116.57	120.30
3	c	45	MET	CG-SD-CE	-7.40	88.35	100.20
10	1	138	G	O5'-P-OP2	-7.39	99.05	105.70
5	s	86	LEU	CA-CB-CG	7.38	132.26	115.30
6	f	3	LEU	CA-CB-CG	7.37	132.24	115.30
10	1	128	U	O5'-P-OP1	-7.32	99.11	105.70
11	Y	6	A	O5'-P-OP2	-7.22	99.20	105.70
1	o	51	ARG	NE-CZ-NH1	-7.14	116.73	120.30
10	1	124	U	O5'-P-OP1	-7.13	99.28	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	2	124	U	O5'-P-OP1	-7.12	99.29	105.70
8	K	16	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	a	69	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	a	54	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	O	12	GLU	OE1-CD-OE2	6.96	131.65	123.30
3	q	66	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	O	76	MET	CB-CG-SD	6.90	133.09	112.40
3	q	45	MET	CG-SD-CE	-6.88	89.19	100.20
10	1	137	U	N1-C1'-C2'	-6.87	104.45	112.00
10	3	126	A	O5'-P-OP1	-6.87	99.52	105.70
7	G	13	MET	CG-SD-CE	-6.85	89.23	100.20
9	M	10	ASP	CB-CG-OD1	6.84	124.46	118.30
10	2	126	A	O5'-P-OP1	-6.84	99.54	105.70
4	R	47	ARG	NE-CZ-NH2	-6.83	116.89	120.30
4	R	20	GLU	OE1-CD-OE2	-6.83	115.10	123.30
1	a	54	ARG	NE-CZ-NH2	-6.83	116.89	120.30
9	m	28	ARG	NE-CZ-NH2	-6.75	116.92	120.30
11	Y	4	U	O5'-P-OP2	6.75	118.80	110.70
8	k	16	ARG	NE-CZ-NH1	6.74	123.67	120.30
3	Q	66	ARG	CG-CD-NE	6.74	125.95	111.80
10	4	124	U	O5'-P-OP1	-6.70	99.67	105.70
7	u	32	ARG	NE-CZ-NH2	6.69	123.65	120.30
10	3	128	U	O5'-P-OP1	-6.69	99.68	105.70
1	A	69	ARG	NE-CZ-NH1	6.64	123.62	120.30
11	x	3	G	O5'-P-OP2	-6.55	99.81	105.70
7	g	25	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	O	77	LEU	CA-CB-CG	6.45	130.14	115.30
7	G	63	ARG	NE-CZ-NH1	6.45	123.52	120.30
10	1	126	A	O5'-P-OP1	-6.38	99.95	105.70
6	T	14	LEU	CB-CG-CD1	6.38	121.84	111.00
4	d	102	ARG	NE-CZ-NH1	-6.38	117.11	120.30
4	r	99	MET	CG-SD-CE	-6.37	90.01	100.20
10	1	137	U	O5'-P-OP2	6.37	118.34	110.70
9	M	40	LYS	CD-CE-NZ	6.36	126.33	111.70
9	m	3	LYS	CB-CG-CD	6.34	128.07	111.60
7	u	25	ARG	NE-CZ-NH2	-6.29	117.16	120.30
4	R	99	MET	CG-SD-CE	-6.27	90.16	100.20
9	M	42	MET	CG-SD-CE	6.26	110.22	100.20
2	B	18	ARG	NE-CZ-NH2	-6.25	117.17	120.30
11	X	4	U	O5'-P-OP2	6.16	118.10	110.70
8	k	46	ARG	NE-CZ-NH2	-6.16	117.22	120.30
5	S	74	LEU	N-CA-C	-6.13	94.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	51	GLU	OE1-CD-OE2	-6.12	115.95	123.30
1	A	54	ARG	NE-CZ-NH2	-6.10	117.25	120.30
5	S	58	LEU	CB-CG-CD1	-6.09	100.65	111.00
10	1	136	G	C4'-C3'-O3'	6.09	125.17	113.00
4	D	99	MET	CG-SD-CE	-6.07	90.48	100.20
3	C	66	ARG	CG-CD-NE	6.07	124.55	111.80
7	g	75	ARG	NE-CZ-NH1	6.07	123.33	120.30
6	t	3	LEU	C-N-CD	6.06	141.13	128.40
11	Y	4	U	O5'-P-OP1	-6.05	100.25	105.70
4	R	55	ARG	NE-CZ-NH1	6.04	123.32	120.30
9	L	21	ARG	NE-CZ-NH1	6.01	123.31	120.30
8	n	50	ASP	CB-CG-OD1	-6.01	112.89	118.30
10	4	136	G	C4'-C3'-O3'	6.00	125.00	113.00
6	T	15	THR	CA-C-N	6.00	128.19	116.20
10	2	123	A	C2'-C3'-O3'	5.97	123.25	113.70
3	C	50	ARG	NE-CZ-NH1	5.95	123.28	120.30
10	4	126	A	O5'-P-OP1	-5.95	100.35	105.70
1	a	77	LEU	CB-CG-CD2	-5.94	100.91	111.00
3	q	19	LEU	CB-CG-CD2	5.93	121.08	111.00
7	G	57	ILE	N-CA-C	-5.91	95.04	111.00
1	a	82	MET	CG-SD-CE	5.89	109.62	100.20
5	e	30	ARG	NE-CZ-NH2	-5.89	117.36	120.30
5	E	16	GLN	C-N-CD	5.88	140.75	128.40
10	3	124	U	O5'-P-OP1	-5.88	100.41	105.70
3	q	33	ASP	CB-CG-OD2	-5.87	113.02	118.30
4	R	65	MET	CG-SD-CE	-5.86	90.83	100.20
5	e	74	LEU	CB-CG-CD1	5.84	120.93	111.00
3	c	66	ARG	CG-CD-NE	5.84	124.06	111.80
7	G	25	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	P	18	ARG	NE-CZ-NH2	-5.79	117.41	120.30
11	X	2	G	O4'-C4'-C3'	-5.78	98.22	104.00
1	a	77	LEU	CB-CG-CD1	5.78	120.83	111.00
3	C	19	LEU	CB-CG-CD2	5.77	120.81	111.00
4	d	93	ASP	CB-CG-OD1	5.76	123.48	118.30
7	u	25	ARG	NE-CZ-NH1	5.75	123.18	120.30
4	d	60	ASP	CB-CG-OD2	5.73	123.46	118.30
11	x	5	A	O5'-P-OP1	5.72	117.56	110.70
1	A	51	ARG	NE-CZ-NH2	-5.71	117.44	120.30
6	F	15	THR	N-CA-CB	5.71	121.16	110.30
3	Q	66	ARG	NE-CZ-NH1	-5.71	117.45	120.30
10	3	126	A	O5'-P-OP2	5.71	117.55	110.70
3	q	66	ARG	CG-CD-NE	5.70	123.77	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	75	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	O	82	MET	CG-SD-CE	5.68	109.29	100.20
11	Y	6	A	O5'-P-OP1	5.67	117.51	110.70
7	G	25	ARG	NE-CZ-NH2	-5.65	117.47	120.30
6	F	8	LYS	C-N-CD	5.63	140.22	128.40
5	S	76	ARG	NE-CZ-NH1	-5.61	117.50	120.30
5	S	75	GLY	N-CA-C	-5.58	99.14	113.10
9	L	10	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	80	ALA	C-N-CD	5.58	140.12	128.40
4	d	65	MET	CG-SD-CE	-5.57	91.30	100.20
9	m	28	ARG	CD-NE-CZ	5.56	131.38	123.60
7	U	25	ARG	NE-CZ-NH2	-5.56	117.52	120.30
5	s	74	LEU	CB-CG-CD1	5.55	120.44	111.00
4	D	88	LYS	C-N-CD	5.54	140.04	128.40
3	Q	18	GLU	OE1-CD-OE2	5.50	129.90	123.30
10	4	2	G	O5'-P-OP1	-5.50	100.75	105.70
10	3	136	G	C4'-C3'-O3'	5.49	123.99	113.00
2	p	7	SER	CA-CB-OG	5.46	125.93	111.20
9	M	31	LYS	CD-CE-NZ	5.44	124.21	111.70
5	E	74	LEU	CB-CG-CD1	5.41	120.20	111.00
10	1	126	A	O5'-P-OP2	5.40	117.18	110.70
10	4	126	A	O5'-P-OP2	5.36	117.14	110.70
9	M	44	GLU	CB-CA-C	5.36	121.12	110.40
10	2	126	A	O5'-P-OP2	5.32	117.08	110.70
1	o	3	ILE	CA-CB-CG2	5.31	121.52	110.90
4	D	102	ARG	NE-CZ-NH2	5.31	122.95	120.30
7	g	25	ARG	NE-CZ-NH1	5.31	122.95	120.30
3	q	82	ASP	CB-CG-OD1	5.30	123.07	118.30
6	F	21	VAL	CB-CA-C	-5.29	101.35	111.40
8	n	49	GLU	OE1-CD-OE2	-5.27	116.98	123.30
7	u	32	ARG	NE-CZ-NH1	-5.26	117.67	120.30
3	C	18	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	a	29	ARG	NE-CZ-NH2	-5.25	117.67	120.30
6	T	73	ARG	CA-CB-CG	5.25	124.95	113.40
4	r	102	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	a	77	LEU	CA-CB-CG	5.20	127.26	115.30
10	1	2	G	O5'-P-OP1	-5.20	101.02	105.70
1	o	73	LEU	CB-CG-CD1	-5.17	102.21	111.00
6	t	73	ARG	CG-CD-NE	5.15	122.61	111.80
1	O	69	ARG	NE-CZ-NH1	5.13	122.86	120.30
5	S	36	TYR	N-CA-C	5.12	124.83	111.00
10	4	137	U	N1-C1'-C2'	5.11	120.65	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	25	ARG	NE-CZ-NH2	-5.08	117.76	120.30
4	D	15	GLU	N-CA-C	5.07	124.68	111.00
3	Q	33	ASP	CB-CG-OD2	-5.07	113.74	118.30
6	f	73	ARG	CG-CD-NE	5.07	122.44	111.80
8	n	16	ARG	NE-CZ-NH1	5.05	122.83	120.30
5	e	14	MET	CG-SD-CE	5.05	108.28	100.20
10	l	136	G	P-O3'-C3'	5.05	125.76	119.70
5	s	73	GLN	CA-CB-CG	5.05	124.51	113.40
5	e	76	ARG	NE-CZ-NH1	-5.04	117.78	120.30
10	3	137	U	N1-C1'-C2'	5.02	120.53	114.00
10	2	26	A	P-O5'-C5'	-5.02	112.87	120.90
8	n	53	ASP	CB-CG-OD2	5.02	122.81	118.30
2	B	9	MET	CG-SD-CE	5.00	108.20	100.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
3	C	81	VAL	Peptide
2	P	87	PRO	Peptide
4	R	17	GLN	Peptide
6	T	16	GLY	Peptide
3	c	42	ALA	Peptide
8	k	57	PRO	Peptide
8	n	56	PRO	Peptide
4	r	17	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	657	0	675	33	0
1	O	643	0	657	31	0
1	a	652	0	670	0	0
1	o	637	0	652	0	0
2	B	673	0	703	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	673	0	703	25	0
2	b	635	0	656	0	0
2	p	692	0	717	0	0
3	C	668	0	709	25	0
3	Q	664	0	705	14	0
3	c	675	0	718	0	0
3	q	674	0	714	0	0
4	D	796	0	821	68	0
4	R	790	0	813	38	0
4	d	753	0	779	0	0
4	r	777	0	800	0	0
5	E	638	0	657	60	1
5	S	638	0	657	79	0
5	e	638	0	657	0	1
5	s	638	0	657	0	0
6	F	568	0	575	23	0
6	T	577	0	589	30	0
6	f	577	0	589	0	0
6	t	577	0	589	0	0
7	G	584	0	610	43	0
7	U	558	0	581	52	0
7	g	568	0	590	0	0
7	u	568	0	590	0	0
8	K	477	0	466	23	0
8	N	431	0	419	29	0
8	k	470	0	459	0	0
8	n	477	0	466	0	0
9	L	448	0	420	33	0
9	M	448	0	420	19	0
9	l	448	0	421	0	0
9	m	425	0	393	0	0
10	1	1036	0	515	15	0
10	2	1036	0	516	11	0
10	3	1013	0	505	10	0
10	4	1059	0	527	19	0
11	X	212	0	110	7	0
11	Y	212	0	110	6	0
11	x	212	0	110	0	0
11	y	212	0	110	0	0
12	L	1	0	0	0	0
12	M	1	0	0	0	0
12	l	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	m	1	0	0	0	0
13	1	15	0	18	1	0
13	2	15	0	18	1	0
14	1	8	0	0	0	0
14	2	4	0	0	0	0
14	3	4	0	0	0	0
14	4	1	0	0	0	0
14	l	1	0	0	0	0
14	y	2	0	0	0	0
15	1	1	0	0	0	0
15	3	2	0	0	0	0
15	Q	1	0	0	0	0
15	b	2	0	0	0	0
16	4	3	0	6	0	0
17	4	1	0	0	4	0
18	y	5	0	0	0	0
19	1	6	0	0	2	0
19	2	4	0	0	0	0
19	3	2	0	0	0	0
19	4	4	0	0	1	0
19	D	5	0	0	5	0
19	G	2	0	0	0	0
19	K	1	0	0	0	0
19	N	1	0	0	0	0
19	P	2	0	0	3	0
19	R	1	0	0	1	0
19	S	1	0	0	0	0
19	T	1	0	0	0	0
19	Y	1	0	0	0	0
19	a	1	0	0	0	0
19	b	1	0	0	0	0
19	c	2	0	0	0	0
19	d	6	0	0	0	0
19	g	1	0	0	0	0
19	m	1	0	0	0	0
19	p	1	0	0	0	0
19	q	2	0	0	0	0
19	r	1	0	0	0	0
19	t	1	0	0	0	0
All	All	26921	0	24842	594	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (594) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:65:ASN:HD21	10:3:127:U:C1'	1.49	1.23
2:P:8:LYS:O	2:P:12:HIS:NE2	3.81	1.23
2:B:17:MET:CE	2:B:82:VAL:HA	1.75	1.16
5:E:69:LYS:HA	5:E:69:LYS:HE3	4.99	1.11
2:B:17:MET:HE3	2:B:82:VAL:HG22	1.28	1.11
5:E:88:GLN:HG3	7:G:57:ILE:CG2	2.92	1.07
3:C:5:ARG:HD3	3:C:8:MET:CE	1.84	1.07
5:S:81:GLY:O	7:U:63:ARG:NH1	1.88	1.06
5:S:85:THR:HG23	7:U:66:SER:OG	1.92	1.06
5:E:88:GLN:HG3	7:G:57:ILE:HG23	3.89	1.05
7:U:65:ASN:ND2	10:3:127:U:C1'	2.20	1.04
7:U:65:ASN:ND2	10:3:127:U:H1'	1.76	1.00
4:D:50:LYS:HG2	4:D:74:TRP:HB3	1.47	0.95
5:E:68:THR:HG22	5:E:70:SER:HB2	2.76	0.94
2:B:17:MET:HE2	2:B:82:VAL:HA	1.48	0.94
2:B:17:MET:CE	2:B:82:VAL:CA	2.45	0.94
2:B:17:MET:HE3	2:B:82:VAL:CG2	1.96	0.93
4:D:16:LEU:HD12	4:D:19:ARG:HH11	12.87	0.91
7:U:65:ASN:ND2	10:3:127:U:O4'	2.04	0.89
5:S:88:GLN:HG3	7:U:57:ILE:HG12	4.53	0.89
2:B:17:MET:HE3	2:B:82:VAL:HA	1.53	0.88
2:B:17:MET:CE	2:B:82:VAL:HG22	2.04	0.87
4:R:112:ASN:OD1	8:N:47:GLU:HG2	10.24	0.87
10:4:137:U:N3	17:4:203:CL:CL	2.45	0.86
7:G:28:GLN:OE1	7:G:48:MET:HE3	2.54	0.86
7:G:28:GLN:OE1	7:G:48:MET:CE	3.09	0.85
4:D:72:GLU:OE1	4:D:94:ARG:HD3	1.76	0.85
9:L:49:LEU:HA	9:L:52:LYS:HD3	1.57	0.83
1:A:36:GLU:O	1:A:38:ASN:O	1.95	0.83
9:L:49:LEU:HA	9:L:52:LYS:CD	2.07	0.83
5:S:81:GLY:C	7:U:63:ARG:NH1	2.32	0.83
7:G:28:GLN:CD	7:G:48:MET:CE	3.28	0.83
4:D:17:GLN:OE1	4:D:17:GLN:N	3.85	0.82
9:L:49:LEU:HD12	9:L:50:ILE:HD13	1.59	0.82
1:O:58:LEU:HD22	7:U:71:GLU:OE1	2.85	0.82
5:E:78:MET:HE2	6:F:11:LEU:HD11	1.62	0.81
4:D:114:LEU:HD22	8:K:51:PRO:HB3	1.62	0.81
9:L:41:TRP:O	9:L:44:GLU:HB3	1.80	0.81
2:B:17:MET:CE	2:B:82:VAL:CG2	2.56	0.81
5:S:81:GLY:C	7:U:63:ARG:HH12	1.84	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ALA:HB1	1:A:82:MET:HE1	1.62	0.81
3:C:5:ARG:HD3	3:C:8:MET:HE1	1.64	0.79
5:E:59:ASP:OD2	5:E:76:ARG:NH1	4.36	0.78
5:S:48:ILE:HD11	5:S:59:ASP:CB	2.99	0.77
1:A:43:MET:HB3	1:A:46:ILE:HD11	1.66	0.77
6:T:19:VAL:HG11	6:T:72:ILE:HD11	2.97	0.77
2:P:53:PRO:HG3	2:P:58:GLN:O	2.53	0.77
5:S:37:GLU:OE2	8:N:30:HIS:HB3	2.52	0.76
2:B:9:MET:CE	2:B:9:MET:HA	4.04	0.76
2:P:8:LYS:O	2:P:12:HIS:CD2	4.41	0.76
1:A:80:ALA:HB1	1:A:82:MET:CE	2.16	0.76
4:D:16:LEU:HD12	4:D:19:ARG:NH1	13.73	0.75
4:D:65:MET:HE2	4:D:67:LEU:HD21	1.67	0.75
9:L:49:LEU:CB	9:L:52:LYS:HE3	2.17	0.75
5:E:78:MET:CE	6:F:11:LEU:HD11	2.16	0.75
1:A:24:THR:OG1	1:A:26:GLU:OE1	2.01	0.75
2:B:7:SER:O	2:B:11:GLN:HG2	4.36	0.75
4:D:14:GLU:HA	4:D:17:GLN:HG2	6.74	0.75
10:1:17:G:O6	19:1:303:HOH:O	2.05	0.75
5:S:33:VAL:HG12	5:S:87:LEU:CD2	3.75	0.75
9:L:49:LEU:CD1	9:L:50:ILE:HD13	2.17	0.74
4:D:104:ASP:OD2	19:D:202:HOH:O	2.06	0.74
5:E:33:VAL:HG12	5:E:87:LEU:CD2	2.18	0.74
6:F:18:PRO:HG2	6:F:75:VAL:HG12	1.68	0.74
5:E:69:LYS:CE	5:E:69:LYS:HA	4.98	0.73
9:L:49:LEU:HB3	9:L:52:LYS:CE	2.18	0.73
5:E:48:ILE:HD11	5:E:59:ASP:CB	4.96	0.72
5:S:48:ILE:HD11	5:S:59:ASP:CG	3.46	0.72
5:E:68:THR:CG2	5:E:70:SER:HB2	3.60	0.72
10:1:26:A:OP2	13:1:201:EPE:H52	1.90	0.72
7:G:62:ILE:HG21	7:G:67:ILE:HD11	2.44	0.72
4:D:51:LYS:HD2	8:K:41:ILE:HG22	1.71	0.72
9:L:49:LEU:CA	9:L:52:LYS:HD3	2.18	0.72
8:N:53:ASP:OD1	8:N:54:ALA:N	5.12	0.71
5:E:88:GLN:HG3	7:G:57:ILE:HG21	2.61	0.71
4:D:51:LYS:HE3	8:K:41:ILE:CG2	2.20	0.71
7:U:55:ASN:OD1	7:U:56:ASN:N	2.24	0.70
11:X:2:G:H2'	11:X:3:G:C8	2.26	0.70
5:S:88:GLN:CG	7:U:57:ILE:HG12	5.37	0.69
4:D:52:LEU:HD21	19:D:205:HOH:O	1.92	0.69
1:O:46:ILE:HD11	1:O:61:VAL:HG21	3.29	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:42:ILE:HD11	7:U:45:CYS:SG	7.25	0.69
2:P:52:LYS:NZ	2:P:54:LYS:H	1.90	0.69
6:F:6:ASN:O	6:F:9:PRO:HG2	1.92	0.69
9:L:46:ALA:O	9:L:49:LEU:HG	1.93	0.68
8:K:9:LEU:O	8:K:12:LEU:HD12	2.72	0.68
8:N:45:ILE:N	8:N:45:ILE:HD12	3.68	0.68
7:U:27:VAL:CG1	7:U:45:CYS:SG	2.82	0.68
11:X:2:G:H2'	11:X:3:G:H8	1.57	0.68
6:F:7:PRO:O	6:F:11:LEU:HD12	1.93	0.68
3:C:5:ARG:HA	3:C:8:MET:HE2	1.76	0.67
4:D:114:LEU:O	19:D:201:HOH:O	2.12	0.67
2:P:58:GLN:HG3	2:P:59:ALA:N	5.21	0.67
2:P:17:MET:HE3	2:P:82:VAL:HA	1.77	0.67
1:O:13:ALA:HB2	1:O:77:LEU:HD21	1.76	0.66
1:A:78:LYS:HA	1:A:83:LEU:HD12	1.76	0.66
2:B:13:ILE:O	2:B:14:ASP:HB2	2.24	0.66
5:S:80:LYS:HD3	6:T:69:VAL:CG1	4.93	0.66
4:D:113:PRO:O	4:D:115:ILE:HD13	1.96	0.66
5:S:20:LEU:HD13	7:U:61:VAL:HG23	1.78	0.65
4:D:14:GLU:CA	4:D:17:GLN:HG2	5.86	0.65
4:D:13:PRO:O	4:D:16:LEU:HB3	9.34	0.65
10:1:137:U:H3'	10:1:138:G:H5'	1.77	0.65
5:S:36:TYR:N	5:S:83:ASN:O	2.40	0.65
5:S:88:GLN:HG3	7:U:57:ILE:CG1	3.75	0.65
10:1:137:U:H3'	10:1:138:G:C5'	2.26	0.65
6:F:66:CYS:O	6:F:69:VAL:HG12	4.93	0.65
5:E:80:LYS:HD3	6:F:69:VAL:HG13	4.45	0.65
4:R:112:ASN:CG	8:N:47:GLU:HG2	10.77	0.64
6:T:66:CYS:O	6:T:69:VAL:HG12	1.97	0.64
4:D:16:LEU:O	4:D:19:ARG:HB2	5.38	0.64
4:R:41:GLN:OE1	8:N:48:PHE:CD1	3.20	0.64
4:R:62:HIS:O	6:T:65:ARG:NH1	2.29	0.64
9:M:47:GLN:OE1	9:M:50:ILE:HD12	2.49	0.64
5:E:20:LEU:HD12	7:G:41:VAL:HG13	5.77	0.64
4:D:62:HIS:O	6:F:65:ARG:NH1	2.49	0.64
5:S:81:GLY:CA	7:U:63:ARG:HH12	2.11	0.64
4:D:18:LYS:O	4:D:21:GLU:HG3	5.30	0.64
6:T:15:THR:O	6:T:33:LEU:O	2.15	0.64
5:E:88:GLN:CG	7:G:57:ILE:HG23	4.43	0.63
7:G:18:SER:HG	7:G:26[A]:HIS:HE2	1.42	0.63
2:P:12:HIS:CD2	2:P:12:HIS:H	3.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:68:THR:HG22	5:E:70:SER:CB	2.84	0.63
4:D:51:LYS:HE3	8:K:41:ILE:HG22	1.79	0.63
9:L:49:LEU:HA	9:L:52:LYS:HB2	1.79	0.63
4:D:51:LYS:CD	8:K:41:ILE:HG22	2.27	0.63
4:D:14:GLU:HB2	4:D:15:GLU:OE1	7.99	0.63
1:A:43:MET:CB	1:A:46:ILE:HD11	2.27	0.63
2:P:10:LEU:O	2:P:13:ILE:HG22	2.20	0.63
4:D:96:ILE:HG21	4:D:99:MET:HE2	1.81	0.62
5:S:59:ASP:OD2	5:S:76:ARG:NH1	2.43	0.62
6:T:25:TRP:HB2	6:T:27:MET:CE	2.30	0.62
2:P:52:LYS:HZ1	2:P:54:LYS:H	1.48	0.61
5:E:80:LYS:HD3	6:F:69:VAL:CG1	3.49	0.61
10:1:1:GTP:O1A	10:1:1:GTP:O4'	2.18	0.61
4:D:30:SER:HA	4:D:33:THR:OG1	2.00	0.61
10:4:135:A:N6	17:4:203:CL:CL	2.71	0.61
5:E:48:ILE:CG2	5:E:59:ASP:HB2	2.31	0.61
11:Y:2:G:H2'	11:Y:3:G:C8	2.54	0.61
1:A:15:GLY:HA3	8:K:3:GLN:HG3	1.83	0.61
4:D:14:GLU:C	4:D:17:GLN:HG2	5.05	0.61
4:R:61:ARG:HG3	4:R:62:HIS:CD2	2.50	0.61
9:M:9:CYS:HB2	9:M:11:THR:HG22	1.82	0.61
1:A:36:GLU:C	1:A:38:ASN:O	2.37	0.61
8:N:48:PHE:HE2	8:N:53:ASP:HA	15.80	0.61
8:N:45:ILE:HG22	8:N:45:ILE:O	2.47	0.61
3:Q:66:ARG:NH1	10:3:132:G:O6	2.34	0.61
5:E:44:GLU:OE2	5:E:71:ARG:NH1	2.34	0.60
5:S:36:TYR:HA	5:S:85:THR:OG1	2.00	0.60
1:A:29:ARG:NH2	8:K:16:ARG:O	2.39	0.60
9:L:49:LEU:HA	9:L:52:LYS:CG	2.30	0.60
9:L:9:CYS:HB2	9:L:11:THR:HG22	1.84	0.60
5:S:88:GLN:OE1	7:U:57:ILE:HG21	3.32	0.60
1:O:43:MET:HB3	1:O:46:ILE:HD11	1.84	0.60
9:L:45:GLN:O	9:L:48:SER:HB3	2.02	0.60
1:A:75:ASP:O	1:A:78:LYS:HG2	2.01	0.60
5:S:68:THR:OG1	5:S:70:SER:HB2	2.35	0.60
4:D:42:VAL:CG1	4:D:109:VAL:HG13	2.31	0.60
6:T:3:LEU:HD23	6:T:4:PRO:HD2	6.54	0.59
9:L:49:LEU:CB	9:L:52:LYS:CE	2.78	0.59
3:Q:66:ARG:NH2	4:R:48:ASN:HB3	2.17	0.59
5:E:34:TRP:CE2	5:E:86:LEU:HD22	2.39	0.59
1:O:76:MET:HG3	8:N:12:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:74:LEU:HD22	5:S:77:ILE:HD11	1.84	0.59
5:S:67:LYS:HG2	5:S:68:THR:N	2.17	0.59
4:D:14:GLU:O	4:D:17:GLN:HG2	3.83	0.59
4:D:13:PRO:HB3	4:D:16:LEU:CD2	13.11	0.59
4:D:51:LYS:CE	8:K:41:ILE:HG22	2.32	0.59
5:S:80:LYS:HD3	6:T:69:VAL:HG13	4.39	0.58
4:D:87:SER:OG	4:D:88:LYS:N	2.27	0.58
3:C:20:LYS:HE2	3:C:63:ASN:O	2.03	0.58
4:R:96:ILE:HG21	4:R:99:MET:HE2	1.84	0.58
1:O:5:VAL:O	1:O:9:VAL:HG12	2.04	0.58
10:4:137:U:C4	17:4:203:CL:CL	2.94	0.58
4:D:104:ASP:HB2	10:1:132:G:H5"	1.84	0.58
7:G:32:ARG:NH2	7:G:43:ASP:OD2	2.36	0.58
3:C:33:ASP:OD1	3:C:34:VAL:N	2.36	0.58
5:S:36:TYR:O	7:U:22:ASN:OD1	2.22	0.58
5:E:48:ILE:CG1	5:E:59:ASP:HB2	3.85	0.58
9:L:44:GLU:OE1	9:L:45:GLN:N	2.37	0.57
2:B:7:SER:O	2:B:11:GLN:CG	3.83	0.57
6:F:25:TRP:HB2	6:F:27:MET:CE	2.40	0.57
5:E:48:ILE:HD11	5:E:59:ASP:OD2	6.44	0.57
5:E:62:GLU:HG2	5:E:73:GLN:NE2	2.19	0.57
10:4:137:U:C2	17:4:203:CL:CL	2.94	0.57
8:N:42:ALA:O	8:N:45:ILE:HD13	3.67	0.57
5:S:20:LEU:HD12	7:U:41:VAL:HG13	1.86	0.57
5:E:33:VAL:HG12	5:E:87:LEU:HD23	1.86	0.57
4:D:104:ASP:HB2	10:2:132:G:H5"	67.59	0.57
2:B:17:MET:HE3	2:B:82:VAL:CA	2.21	0.57
5:E:39:VAL:O	5:E:39:VAL:HG12	2.05	0.56
3:C:66:ARG:NH2	10:1:132:G:O6	2.39	0.56
3:C:66:ARG:NH1	4:D:48:ASN:HB3	2.20	0.56
7:U:50:THR:O	7:U:53:GLN:N	2.38	0.56
6:T:49:GLU:HB2	6:T:59:LEU:HD11	1.87	0.56
4:D:34:GLN:HB3	4:D:111:ARG:NH1	2.24	0.56
1:O:82:MET:C	1:O:83:LEU:HD23	2.25	0.56
3:C:5:ARG:HA	3:C:8:MET:CE	2.35	0.56
4:R:55:ARG:HH22	8:N:49:GLU:CD	2.08	0.56
4:D:12:THR:O	4:D:12:THR:HG22	2.05	0.56
5:S:48:ILE:HD13	5:S:76:ARG:NH2	7.00	0.56
4:R:30:SER:HA	4:R:33:THR:OG1	2.46	0.56
9:L:48:SER:O	9:L:51:ASP:HB2	2.06	0.56
4:D:115:ILE:O	4:D:116:ALA:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:LEU:HD13	7:G:61:VAL:HG23	5.49	0.56
3:Q:20:LYS:HE2	3:Q:63:ASN:O	2.07	0.56
7:U:27:VAL:HG11	7:U:45:CYS:SG	2.45	0.56
5:E:15:VAL:O	7:G:33:GLY:HA3	2.49	0.56
2:P:12:HIS:N	2:P:12:HIS:CD2	3.44	0.56
2:B:17:MET:HE1	2:B:82:VAL:CG2	2.36	0.56
5:S:80:LYS:O	5:S:83:ASN:ND2	4.18	0.56
10:4:22:G:OP2	19:4:304:HOH:O	2.18	0.56
5:E:87:LEU:O	7:G:60:VAL:CG2	4.59	0.55
2:P:16:ARG:NH2	19:P:102:HOH:O	2.39	0.55
10:1:18:A:H4'	10:1:19:G:O5'	2.07	0.55
5:S:80:LYS:HG3	6:T:69:VAL:HG13	1.88	0.55
9:L:49:LEU:HB2	9:L:52:LYS:HE3	1.87	0.55
5:S:78:MET:CE	6:T:40:MET:SD	2.95	0.55
1:O:71:LEU:HD12	1:O:71:LEU:N	3.06	0.55
10:3:18:A:H4'	10:3:19:G:O5'	2.07	0.55
9:M:28:ARG:NH2	11:Y:6:A:OP1	2.40	0.55
3:C:5:ARG:HD3	3:C:8:MET:HE3	1.78	0.55
1:O:43:MET:CB	1:O:46:ILE:HD11	2.37	0.55
2:B:9:MET:HE1	2:B:9:MET:HA	4.30	0.55
1:A:12:GLU:HB3	1:A:77:LEU:HD22	1.89	0.55
3:C:5:ARG:CD	3:C:8:MET:CE	2.73	0.55
5:S:48:ILE:HD11	5:S:59:ASP:OD2	3.06	0.55
4:D:26:THR:O	19:D:204:HOH:O	17.52	0.55
5:E:87:LEU:O	7:G:60:VAL:HG23	4.96	0.54
9:L:49:LEU:HA	9:L:52:LYS:CB	2.37	0.54
9:L:49:LEU:HB3	9:L:52:LYS:HE2	1.87	0.54
5:E:48:ILE:HG23	5:E:59:ASP:HB2	1.90	0.54
7:U:42:ILE:CD1	7:U:45:CYS:SG	6.72	0.54
2:B:53:PRO:HG3	2:B:58:GLN:O	2.07	0.54
5:S:65:HIS:HB3	5:S:67:LYS:CE	2.38	0.54
2:B:50:LYS:HB3	2:B:60:GLU:OE2	2.07	0.54
4:R:54:GLY:HA2	19:R:201:HOH:O	8.30	0.54
4:D:20:GLU:HG3	4:D:21:GLU:N	3.26	0.54
5:S:78:MET:HE2	6:T:40:MET:SD	2.48	0.54
5:S:48:ILE:CG1	5:S:59:ASP:HB2	2.65	0.54
5:S:48:ILE:CG2	6:T:5:LEU:HB3	2.40	0.54
3:C:66:ARG:NH2	4:D:48:ASN:HB3	3.90	0.54
1:O:12:GLU:HB3	1:O:77:LEU:HD22	4.45	0.53
4:R:34:GLN:HB3	4:R:111:ARG:NH1	2.25	0.53
5:S:80:LYS:O	5:S:83:ASN:OD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:ILE:HD11	4:D:65:MET:HE1	2.19	0.53
7:U:26:HIS:O	7:U:47:GLU:O	2.25	0.53
10:4:138:G:C6	10:4:139:G:C2	2.96	0.53
3:C:66:ARG:HG2	10:2:136:G:O6	62.39	0.53
8:N:49:GLU:C	8:N:51:PRO:HD2	4.43	0.53
10:4:18:A:H4'	10:4:19:G:O5'	2.07	0.53
4:D:114:LEU:CD2	8:K:51:PRO:HB3	2.38	0.53
5:S:87:LEU:N	5:S:87:LEU:HD12	2.24	0.53
7:U:48:MET:SD	7:U:54:GLN:HG3	5.61	0.53
2:B:12:HIS:O	2:B:15:TYR:HB2	2.08	0.53
6:F:25:TRP:HB2	6:F:27:MET:HE3	1.91	0.53
4:R:44:ILE:HD11	4:R:65:MET:HE1	1.89	0.53
2:B:17:MET:CE	2:B:82:VAL:N	2.72	0.53
5:S:36:TYR:HB2	5:S:83:ASN:O	2.33	0.53
1:A:30:GLY:HA3	1:A:46:ILE:HD13	1.90	0.53
5:S:87:LEU:O	7:U:60:VAL:HG23	2.09	0.53
3:C:66:ARG:NH1	10:2:132:G:O6	57.23	0.53
8:N:42:ALA:N	8:N:43:PRO:CD	2.79	0.53
8:K:2:THR:HG21	8:K:13:PHE:CZ	2.44	0.53
5:E:21:ILE:HG22	5:E:50:PHE:CE2	3.47	0.53
4:D:13:PRO:HB3	4:D:16:LEU:HD22	13.77	0.53
5:S:33:VAL:HG12	5:S:87:LEU:HD23	3.71	0.53
7:G:45:CYS:O	7:G:57:ILE:O	2.26	0.53
7:G:49:ALA:O	7:G:51:SER:O	5.00	0.53
5:E:77:ILE:HG22	6:F:73:ARG:HB2	1.91	0.53
1:A:75:ASP:OD2	8:K:16:ARG:NH2	2.36	0.52
10:2:18:A:H4'	10:2:19:G:O5'	2.08	0.52
4:D:51:LYS:HE3	8:K:41:ILE:HG23	1.90	0.52
9:L:16:ASP:OD2	9:L:21:ARG:NH1	2.41	0.52
5:E:48:ILE:HD11	5:E:59:ASP:CG	5.48	0.52
7:U:46:VAL:HA	7:U:55:ASN:O	2.10	0.52
8:N:45:ILE:N	8:N:45:ILE:CD1	3.20	0.52
1:O:83:LEU:N	1:O:83:LEU:HD23	2.24	0.52
1:A:48:VAL:CG1	1:A:56:ALA:HB3	2.40	0.52
5:S:56:LEU:HB3	5:S:58:LEU:HD11	1.90	0.52
7:G:28:GLN:OE1	7:G:48:MET:HE1	3.73	0.52
5:S:48:ILE:HD11	5:S:59:ASP:CA	4.28	0.52
2:B:7:SER:HA	2:B:10:LEU:HB2	2.33	0.52
4:D:42:VAL:CG1	4:D:109:VAL:CG1	2.88	0.52
3:C:67:TYR:HE2	19:D:205:HOH:O	1.92	0.52
5:S:68:THR:OG1	5:S:70:SER:N	2.95	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:61:ALA:HB3	5:S:77:ILE:HD12	1.92	0.52
4:R:51:LYS:HG3	8:N:44:TYR:CE2	2.97	0.52
5:E:48:ILE:HD11	5:E:59:ASP:HB2	4.33	0.52
5:E:24:TYR:OH	7:G:59:MET:O	2.24	0.52
7:U:26:HIS:CD2	7:U:26:HIS:N	2.78	0.52
6:F:11:LEU:HD13	6:F:36:VAL:HG11	2.87	0.51
7:U:63:ARG:HD3	7:U:65:ASN:OD1	2.10	0.51
2:B:17:MET:HE1	2:B:82:VAL:N	2.26	0.51
5:E:36:TYR:N	5:E:83:ASN:O	2.42	0.51
7:G:43:ASP:CG	7:G:59:MET:CE	2.91	0.51
5:S:23:ARG:HD3	5:S:27:ASN:OD1	5.20	0.51
9:L:49:LEU:HD12	9:L:50:ILE:N	2.25	0.51
7:G:63:ARG:NH2	10:1:127:U:C6	2.79	0.51
6:T:21:VAL:CG1	6:T:69:VAL:HG23	2.41	0.51
7:G:18:SER:OG	7:G:26[A]:HIS:NE2	2.34	0.51
5:S:65:HIS:HB3	5:S:67:LYS:HE2	1.93	0.51
3:C:30:THR:CG2	3:C:41:LYS:HB2	4.33	0.51
4:R:115:ILE:O	4:R:115:ILE:HD12	2.11	0.51
5:E:62:GLU:HG2	5:E:73:GLN:HE22	1.74	0.51
5:S:62:GLU:OE1	5:S:71:ARG:HD3	2.10	0.51
7:G:37:PHE:CD2	10:2:127:U:C4	72.68	0.51
3:Q:5:ARG:HA	3:Q:8:MET:HE2	2.00	0.51
5:S:85:THR:CG2	7:U:66:SER:OG	2.79	0.51
5:S:86:LEU:HD12	5:S:87:LEU:N	5.11	0.51
3:C:66:ARG:NH2	10:2:136:G:N7	56.19	0.51
6:T:11:LEU:HD13	6:T:36:VAL:HG11	1.92	0.51
2:P:73:ARG:NH2	19:P:101:HOH:O	27.22	0.50
2:B:17:MET:HE2	2:B:81:THR:O	2.10	0.50
2:B:17:MET:HE3	2:B:82:VAL:CB	2.41	0.50
11:Y:1:A:H1'	10:4:26:A:H5'	74.20	0.50
9:L:13:LEU:HD23	9:L:20:VAL:HG12	1.94	0.50
5:S:20:LEU:O	5:S:20:LEU:HD12	5.49	0.50
8:N:46:ARG:CG	8:N:47:GLU:N	3.69	0.50
5:S:59:ASP:OD2	5:S:76:ARG:CZ	3.14	0.50
5:E:20:LEU:HD21	7:G:59:MET:HG3	1.93	0.50
4:R:104:ASP:HB2	10:4:132:G:H5''	76.64	0.50
2:B:17:MET:HE1	2:B:82:VAL:HG23	1.94	0.50
7:G:57:ILE:O	7:G:57:ILE:HG22	4.94	0.50
3:C:5:ARG:CD	3:C:8:MET:HE1	2.40	0.50
4:D:115:ILE:H	4:D:115:ILE:HD13	1.76	0.50
3:Q:5:ARG:HA	3:Q:8:MET:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:42:ALA:N	8:K:43:PRO:CD	2.83	0.50
4:D:18:LYS:C	4:D:20:GLU:N	2.61	0.50
1:A:80:ALA:CB	1:A:82:MET:HE2	2.42	0.50
2:P:58:GLN:HG3	2:P:59:ALA:H	5.23	0.50
5:S:86:LEU:C	5:S:87:LEU:HD12	2.32	0.50
4:D:71:LYS:HE2	4:D:73:MET:HE3	1.94	0.50
9:M:47:GLN:HG3	9:M:47:GLN:O	2.12	0.49
5:S:74:LEU:CD2	6:T:71:TYR:CZ	2.95	0.49
1:O:68:ILE:HG21	1:O:71:LEU:HD11	2.68	0.49
7:G:57:ILE:HD12	7:G:60:VAL:HG11	1.95	0.49
4:D:16:LEU:CD1	4:D:19:ARG:NH1	14.06	0.49
1:O:6:PRO:HA	1:O:9:VAL:CG1	2.42	0.49
5:S:15:VAL:O	7:U:33:GLY:HA3	2.15	0.49
6:T:18:PRO:HG2	6:T:75:VAL:HG22	2.45	0.49
4:D:72:GLU:OE1	4:D:94:ARG:CD	2.55	0.49
5:S:67:LYS:HG2	5:S:68:THR:HG23	1.94	0.49
6:T:3:LEU:CG	6:T:4:PRO:HD2	4.99	0.49
9:L:49:LEU:N	9:L:52:LYS:HD3	2.28	0.49
5:S:84:ILE:HG21	5:S:87:LEU:HD11	1.94	0.49
5:E:80:LYS:O	5:E:83:ASN:ND2	2.45	0.49
5:E:30:ARG:HE	5:E:44:GLU:CD	2.16	0.49
7:G:62:ILE:HG21	7:G:67:ILE:CD1	3.08	0.49
11:X:5:A:C2	10:2:7:A:C2	84.55	0.49
1:O:6:PRO:O	1:O:9:VAL:HG13	2.13	0.49
7:G:35:ASP:HB2	7:G:36:PRO:CD	2.46	0.49
5:E:48:ILE:HD11	5:E:59:ASP:CA	4.73	0.49
2:P:11:GLN:HG2	2:P:12:HIS:CD2	3.18	0.48
2:P:53:PRO:CG	2:P:58:GLN:O	3.14	0.48
1:O:83:LEU:N	1:O:83:LEU:HD12	4.76	0.48
7:U:15:LYS:HD2	7:U:74:GLU:HG2	1.95	0.48
1:A:40:ASN:HD21	10:1:128:U:H3	1.60	0.48
4:D:13:PRO:HB3	4:D:16:LEU:HB2	11.38	0.48
5:S:87:LEU:O	7:U:60:VAL:CG2	2.61	0.48
6:F:21:VAL:CG1	6:F:69:VAL:HG23	4.06	0.48
8:N:50:ASP:N	8:N:51:PRO:HD2	4.04	0.48
6:T:3:LEU:CD2	6:T:4:PRO:HD2	6.27	0.48
7:U:37:PHE:CD2	10:3:127:U:C4	3.01	0.48
5:S:58:LEU:N	5:S:58:LEU:CD1	2.77	0.48
4:R:51:LYS:HD2	8:N:41:ILE:HG22	1.95	0.48
7:G:63:ARG:NH2	10:2:127:U:C6	69.76	0.48
5:E:48:ILE:CG2	6:F:5:LEU:HB3	4.85	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:13:ALA:HB2	1:O:77:LEU:HD11	2.77	0.48
3:C:32:VAL:HG12	3:C:33:ASP:N	2.29	0.48
5:S:21:ILE:HG22	5:S:50:PHE:CE2	2.49	0.48
7:U:65:ASN:ND2	10:3:127:U:C4'	2.77	0.48
1:A:34:GLU:HG3	1:A:35:ALA:N	2.28	0.48
1:A:47:THR:HG23	1:A:57:GLN:OE1	2.14	0.48
1:O:76:MET:HG3	8:N:13:PHE:CE1	4.80	0.48
3:C:41:LYS:HE3	4:R:115:ILE:HG21	93.33	0.48
7:G:35:ASP:HB2	7:G:36:PRO:HD2	2.00	0.48
19:P:101:HOH:O	10:4:128:U:H1'	90.82	0.48
9:M:13:LEU:HD23	9:M:20:VAL:HG12	1.96	0.48
7:U:46:VAL:CG1	7:U:55:ASN:O	2.61	0.47
7:U:19:LEU:HD22	7:U:70:LEU:HB3	1.95	0.47
4:R:112:ASN:HA	8:N:47:GLU:OE2	12.87	0.47
7:G:28:GLN:CD	7:G:48:MET:HE2	2.80	0.47
5:S:20:LEU:HD13	7:U:61:VAL:CG2	2.44	0.47
9:M:24:HIS:C	9:M:24:HIS:CD2	2.87	0.47
11:X:1:A:O4'	10:2:26:A:H5'	99.42	0.47
1:O:70:PHE:C	1:O:71:LEU:HD12	3.65	0.47
1:O:20:CYS:HB2	1:O:71:LEU:HD23	1.95	0.47
7:U:57:ILE:CG1	7:U:57:ILE:O	3.43	0.47
4:D:104:ASP:HB2	10:1:132:G:C5'	2.44	0.47
5:S:74:LEU:HD21	6:T:71:TYR:OH	2.14	0.47
11:Y:1:A:H2'	11:Y:2:G:H8	2.19	0.47
4:D:32:LEU:HB3	4:D:59:PHE:CD2	2.69	0.47
4:D:104:ASP:HB2	10:2:132:G:C5'	67.23	0.47
1:A:75:ASP:CG	8:K:16:ARG:HH21	2.15	0.47
5:S:61:ALA:CB	5:S:77:ILE:HD12	2.44	0.47
10:1:7:A:C2	11:X:5:A:C2	3.02	0.47
8:K:58:THR:O	8:K:59:ARG:C	2.53	0.47
9:L:49:LEU:HB3	9:L:52:LYS:HE3	1.84	0.47
1:A:17:ILE:HB	8:K:15:PRO:HB3	2.07	0.47
3:Q:82:ASP:OD1	3:Q:82:ASP:N	2.97	0.47
11:Y:1:A:H2'	11:Y:2:G:C8	2.71	0.46
4:R:104:ASP:HB2	10:3:132:G:H5''	1.97	0.46
1:A:40:ASN:HA	1:A:63:ILE:O	2.16	0.46
6:T:19:VAL:HG11	6:T:72:ILE:CD1	3.86	0.46
7:U:16:LYS:HG2	7:U:73:LEU:HD12	1.96	0.46
3:Q:18:GLU:OE1	4:R:94:ARG:NH2	4.77	0.46
7:G:46:VAL:HA	7:G:55:ASN:O	2.15	0.46
4:R:10:GLU:OE1	4:R:10:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:16:LYS:HG2	7:G:73:LEU:HD12	1.97	0.46
1:O:10:LEU:HD13	1:O:71:LEU:HD22	3.15	0.46
7:G:11:LYS:O	7:G:76:VAL:HG13	4.47	0.46
7:U:63:ARG:NH2	10:4:127:U:C6	47.97	0.46
6:T:21:VAL:HG23	6:T:21:VAL:O	4.24	0.46
5:E:20:LEU:CD2	5:E:24:TYR:CZ	4.43	0.46
1:A:40:ASN:OD1	1:A:65:GLY:N	2.30	0.46
4:D:13:PRO:HB3	4:D:16:LEU:CB	11.68	0.46
5:S:23:ARG:O	5:S:27:ASN:OD1	4.80	0.46
5:S:80:LYS:HE2	5:S:80:LYS:HB3	4.45	0.46
7:U:35:ASP:HB2	7:U:36:PRO:HD2	1.98	0.46
7:G:19:LEU:HD22	7:G:70:LEU:HB3	1.98	0.46
5:S:48:ILE:HD11	5:S:59:ASP:HA	4.79	0.46
5:S:27:ASN:OD1	5:S:27:ASN:N	4.38	0.46
9:M:41:TRP:O	9:M:44:GLU:HB3	4.64	0.46
3:Q:53:VAL:HG12	3:Q:55:LEU:CD1	4.31	0.46
1:A:51:ARG:CZ	8:K:28:LEU:HD13	2.54	0.46
4:R:115:ILE:O	4:R:116:ALA:HB2	2.16	0.46
5:S:16:GLN:HG2	5:S:19:ASN:OD1	2.17	0.46
6:F:20:MET:HE2	6:F:30:LYS:HB2	1.99	0.46
9:M:4:PHE:CE2	9:M:21:ARG:HD3	2.51	0.46
4:D:16:LEU:HD12	4:D:19:ARG:HD3	12.59	0.45
10:4:138:G:N3	10:4:138:G:H2'	2.31	0.45
4:R:113:PRO:O	4:R:114:LEU:HD12	4.65	0.45
4:R:96:ILE:HD12	4:R:99:MET:HE2	1.97	0.45
3:C:25:VAL:HG11	3:C:40:LEU:HD13	2.15	0.45
5:S:36:TYR:CB	5:S:83:ASN:O	2.86	0.45
5:S:48:ILE:HG22	6:T:5:LEU:HB3	2.01	0.45
4:D:42:VAL:HG11	4:D:109:VAL:CG1	2.46	0.45
4:R:34:GLN:HB3	4:R:111:ARG:HH12	1.82	0.45
9:L:24:HIS:CD2	9:L:24:HIS:C	2.90	0.45
7:U:57:ILE:HD12	7:U:57:ILE:O	4.12	0.45
5:S:48:ILE:CD1	5:S:59:ASP:OD2	3.69	0.45
4:D:88:LYS:N	4:D:89:PRO:CD	4.62	0.45
4:R:72:GLU:OE1	4:R:94:ARG:NH1	2.49	0.45
7:U:35:ASP:OD1	7:U:36:PRO:HD2	3.65	0.45
7:U:35:ASP:HB2	7:U:36:PRO:CD	2.47	0.45
8:N:48:PHE:CE2	8:N:53:ASP:HA	14.96	0.45
6:F:25:TRP:HB2	6:F:27:MET:HE2	3.21	0.45
3:Q:68:PHE:HB2	4:R:100:PHE:HB3	2.03	0.45
5:E:40:ASN:HB3	5:E:67:LYS:HD2	6.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:14:GLU:HA	4:D:17:GLN:CG	6.66	0.45
2:P:12:HIS:H	2:P:12:HIS:HD2	4.06	0.45
5:E:20:LEU:HD11	7:G:59:MET:HG2	1.99	0.45
4:D:42:VAL:HG11	4:D:109:VAL:HG13	1.97	0.45
2:B:51:ILE:O	2:B:60:GLU:HB3	4.79	0.45
1:A:20:CYS:HB2	1:A:71:LEU:HD23	1.98	0.45
1:A:80:ALA:HB1	1:A:81:PRO:HD2	2.39	0.45
1:O:80:ALA:HB1	1:O:81:PRO:HD2	1.99	0.45
4:D:38:ASN:HA	8:K:57:PRO:HB3	1.99	0.45
1:A:80:ALA:HB1	1:A:82:MET:HE2	1.95	0.45
2:P:54:LYS:C	2:P:54:LYS:HD2	2.38	0.44
5:S:74:LEU:N	5:S:74:LEU:HD12	2.32	0.44
6:F:51:ILE:O	6:F:52:ASP:OD1	2.36	0.44
1:A:80:ALA:CB	1:A:82:MET:CE	2.91	0.44
5:E:36:TYR:HB2	5:E:83:ASN:O	2.17	0.44
4:R:62:HIS:CD2	4:R:62:HIS:N	2.92	0.44
9:M:46:ALA:O	9:M:50:ILE:HG13	2.20	0.44
13:2:201:EPE:H82	13:2:201:EPE:H52	1.86	0.44
3:C:5:ARG:HD3	3:C:8:MET:HE2	1.88	0.44
2:P:17:MET:HE3	2:P:82:VAL:CA	2.46	0.44
5:E:62:GLU:OE1	5:E:71:ARG:HD3	3.02	0.44
5:S:78:MET:HE1	6:T:40:MET:SD	2.58	0.44
9:L:8:TYR:HH	9:L:38:TYR:HH	1.66	0.44
5:E:48:ILE:HG21	5:E:59:ASP:HB2	1.99	0.44
5:S:33:VAL:HG22	5:S:43:ILE:O	2.18	0.44
5:E:36:TYR:O	5:E:37:GLU:HB2	2.17	0.44
1:O:82:MET:HB2	1:O:83:LEU:HD12	6.33	0.44
2:B:16:ARG:HH11	2:B:16:ARG:HG3	1.83	0.44
6:T:25:TRP:HB2	6:T:27:MET:HE2	1.98	0.44
5:E:33:VAL:HG22	5:E:43:ILE:O	2.18	0.44
10:4:138:G:O4'	10:4:138:G:OP1	2.36	0.44
9:L:49:LEU:C	9:L:49:LEU:HD12	2.37	0.44
4:R:104:ASP:HB2	10:4:132:G:C5'	75.92	0.44
4:D:34:GLN:HB3	4:D:111:ARG:HH12	1.85	0.44
1:O:29:ARG:NH2	8:N:16:ARG:O	2.51	0.44
9:L:25:CYS:HA	9:L:30:HIS:CD2	2.53	0.44
9:M:25:CYS:HA	9:M:30:HIS:CD2	2.52	0.44
5:E:20:LEU:HD22	5:E:24:TYR:CZ	5.34	0.43
7:G:75:ARG:HD2	7:G:75:ARG:HA	3.03	0.43
5:S:65:HIS:O	5:S:69:LYS:HA	2.18	0.43
9:L:49:LEU:CA	9:L:52:LYS:HB2	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:LYS:HA	4:D:88:LYS:HD3	1.74	0.43
5:S:65:HIS:CB	5:S:67:LYS:CE	2.96	0.43
9:L:16:ASP:OD1	9:L:17:SER:N	2.52	0.43
2:B:17:MET:HE2	2:B:82:VAL:CA	2.28	0.43
3:Q:66:ARG:NH2	10:4:136:G:N7	91.99	0.43
4:D:17:GLN:O	4:D:20:GLU:HG3	5.03	0.43
11:X:1:A:C1'	10:2:26:A:H5'	98.15	0.43
8:K:9:LEU:HD23	9:L:42:MET:SD	2.59	0.43
1:O:48:VAL:CG1	1:O:56:ALA:HB3	2.50	0.43
2:P:18:ARG:HD2	2:P:83:GLU:OE1	4.23	0.43
1:O:46:ILE:HG12	1:O:58:LEU:HB2	3.68	0.43
6:T:14:LEU:HD22	6:T:19:VAL:HG12	2.01	0.43
4:R:73:MET:SD	8:N:47:GLU:HG3	2.59	0.43
1:A:38:ASN:O	1:A:39:MET:HB2	4.59	0.43
1:O:46:ILE:CD1	1:O:61:VAL:HG21	3.51	0.43
5:E:48:ILE:HD11	5:E:59:ASP:HA	4.03	0.43
5:S:67:LYS:HG2	5:S:68:THR:H	1.83	0.43
5:S:67:LYS:HG3	5:S:68:THR:N	3.56	0.43
9:M:52:LYS:O	9:M:52:LYS:HD3	2.19	0.43
7:G:42:ILE:HB	7:G:60:VAL:HG12	6.12	0.43
1:O:9:VAL:HG12	1:O:73:LEU:HD23	9.54	0.43
4:R:55:ARG:NH2	8:N:49:GLU:OE1	2.45	0.43
5:E:48:ILE:CD1	5:E:59:ASP:HB2	3.77	0.42
3:C:66:ARG:NH1	10:1:136:G:N7	2.63	0.42
4:R:62:HIS:H	4:R:62:HIS:CD2	2.41	0.42
6:T:25:TRP:HB2	6:T:27:MET:HE1	2.06	0.42
4:R:40:THR:HG21	4:R:111:ARG:HH21	1.84	0.42
5:E:41:MET:SD	5:E:63:GLU:HG2	2.59	0.42
10:1:17:G:H1'	19:1:304:HOH:O	2.19	0.42
3:Q:66:ARG:NH1	10:4:132:G:O6	84.35	0.42
7:U:57:ILE:HG13	7:U:57:ILE:O	2.96	0.42
4:R:114:LEU:HD22	8:N:48:PHE:HB2	2.01	0.42
1:O:30:GLY:HA3	1:O:46:ILE:HD13	2.02	0.42
7:U:59:MET:O	7:U:60:VAL:HG13	5.28	0.42
1:A:57:GLN:O	1:A:58:LEU:HD23	2.19	0.42
9:M:45:GLN:O	9:M:48:SER:HB3	4.21	0.42
5:E:89:SER:O	5:E:90:VAL:HG12	2.87	0.42
4:D:19:ARG:CZ	4:D:19:ARG:HB3	5.05	0.42
10:4:137:U:H5''	10:4:138:G:OP1	2.19	0.42
5:E:49:GLY:HA3	6:F:5:LEU:O	2.41	0.42
9:L:4:PHE:CE2	9:L:21:ARG:HD3	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:42:MET:O	9:M:45:GLN:HB2	2.20	0.42
5:E:48:ILE:HG22	6:F:5:LEU:HB3	5.32	0.42
3:Q:49:ASN:ND2	10:4:138:G:C8	107.67	0.42
4:D:15:GLU:O	4:D:18:LYS:HB2	8.13	0.42
2:B:9:MET:HE2	2:B:9:MET:HA	4.29	0.42
5:S:20:LEU:CD2	5:S:24:TYR:CZ	3.03	0.42
9:M:46:ALA:O	9:M:49:LEU:HG	6.41	0.42
6:F:20:MET:CE	6:F:30:LYS:HB2	2.50	0.42
8:N:50:ASP:N	8:N:51:PRO:CD	4.10	0.42
5:E:87:LEU:O	7:G:60:VAL:HG22	5.13	0.42
4:D:50:LYS:CG	4:D:74:TRP:HB3	2.33	0.42
5:S:57:VAL:C	5:S:58:LEU:HD12	2.40	0.42
4:R:47:ARG:HD2	8:N:38:TYR:OH	2.19	0.42
2:P:60:GLU:HG2	2:P:60:GLU:O	4.88	0.42
2:P:13:ILE:O	2:P:14:ASP:HB2	2.20	0.41
6:T:3:LEU:HG	6:T:4:PRO:HD2	5.28	0.41
9:M:8:TYR:HH	9:M:38:TYR:HH	1.69	0.41
6:T:8:LYS:N	6:T:9:PRO:HD2	2.35	0.41
4:D:15:GLU:OE2	4:D:18:LYS:HG3	13.05	0.41
6:F:65:ARG:NH2	10:1:132:G:OP2	2.53	0.41
5:E:80:LYS:HE2	5:E:80:LYS:HB3	1.79	0.41
11:Y:1:A:C1'	10:4:26:A:H5'	74.24	0.41
8:N:46:ARG:HG3	8:N:47:GLU:N	3.02	0.41
1:O:57:GLN:O	1:O:58:LEU:HD23	2.21	0.41
7:U:76:VAL:O	7:U:76:VAL:HG12	2.23	0.41
8:K:8:ASN:OD1	8:K:9:LEU:N	2.53	0.41
9:M:40:LYS:HE3	9:M:40:LYS:HA	5.07	0.41
7:U:63:ARG:NE	7:U:65:ASN:OD1	2.53	0.41
5:S:85:THR:HG23	7:U:66:SER:CB	2.50	0.41
2:B:14:ASP:O	2:B:86:PRO:HB3	2.25	0.41
7:G:62:ILE:CG2	7:G:67:ILE:HD11	2.76	0.41
4:D:14:GLU:O	4:D:17:GLN:HB2	5.25	0.41
2:P:52:LYS:NZ	2:P:53:PRO:HD2	2.36	0.41
7:U:74:GLU:C	7:U:75:ARG:HG3	2.40	0.41
2:P:52:LYS:HZ2	2:P:53:PRO:HD2	1.86	0.41
11:X:1:A:C2	11:X:2:G:C4	3.52	0.41
2:B:30:THR:HB	2:B:43:CYS:HB2	2.03	0.41
2:P:52:LYS:HZ2	2:P:54:LYS:H	1.67	0.41
1:O:83:LEU:N	1:O:83:LEU:CD1	4.36	0.41
4:R:40:THR:HG21	4:R:111:ARG:NH2	2.36	0.41
9:M:16:ASP:OD1	9:M:17:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:17:SER:O	9:M:21:ARG:HG2	5.50	0.41
7:U:11:LYS:O	7:U:76:VAL:HG13	7.23	0.41
6:T:20:MET:HE2	6:T:30:LYS:HB2	2.02	0.41
1:A:60:GLN:HG3	7:G:76:VAL:HG23	3.44	0.41
4:R:18:LYS:HG3	4:R:21:GLU:OE1	2.21	0.41
7:G:69:MET:HG2	7:G:70:LEU:N	2.44	0.40
1:A:24:THR:HG22	8:K:28:LEU:HD11	2.74	0.40
3:Q:48:LYS:HA	3:Q:48:LYS:HD2	1.95	0.40
2:P:30:THR:HB	2:P:43:CYS:HB2	2.03	0.40
2:B:78:VAL:HA	3:C:64:ASN:ND2	3.59	0.40
6:F:12:ASN:HA	6:F:15:THR:HG23	2.08	0.40
9:L:44:GLU:OE1	9:L:45:GLN:HG2	2.21	0.40
5:E:20:LEU:HD13	7:G:61:VAL:CG2	6.21	0.40
1:O:73:LEU:CD1	1:O:73:LEU:N	4.34	0.40
4:R:115:ILE:HA	8:N:51:PRO:HG3	2.04	0.40
3:Q:33:ASP:OD1	3:Q:33:ASP:C	2.64	0.40
5:S:20:LEU:HD22	5:S:24:TYR:CE2	2.57	0.40
3:C:33:ASP:OD1	3:C:33:ASP:C	2.88	0.40
3:C:23:THR:OG1	3:C:47:LEU:HD23	2.21	0.40
1:A:53:GLY:HA2	8:K:21:TYR:CE1	2.64	0.40
9:M:14:THR:HG23	10:3:27:C:OP1	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:62:GLU:OE2	5:e:28:ARG:NH1[4_445]	1.93	0.27

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	82/126 (65%)	80 (98%)	2 (2%)	0	100	100
1	O	80/126 (64%)	74 (92%)	6 (8%)	0	100	100
1	a	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
1	o	79/126 (63%)	75 (95%)	4 (5%)	0	100	100
2	B	81/95 (85%)	80 (99%)	1 (1%)	0	100	100
2	P	81/95 (85%)	80 (99%)	1 (1%)	0	100	100
2	b	74/95 (78%)	73 (99%)	1 (1%)	0	100	100
2	p	84/95 (88%)	82 (98%)	2 (2%)	0	100	100
3	C	84/91 (92%)	79 (94%)	5 (6%)	0	100	100
3	Q	83/91 (91%)	81 (98%)	2 (2%)	0	100	100
3	c	85/91 (93%)	81 (95%)	4 (5%)	0	100	100
3	q	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
4	D	94/118 (80%)	90 (96%)	4 (4%)	0	100	100
4	R	93/118 (79%)	87 (94%)	6 (6%)	0	100	100
4	d	88/118 (75%)	86 (98%)	2 (2%)	0	100	100
4	r	91/118 (77%)	85 (93%)	6 (7%)	0	100	100
5	E	75/92 (82%)	71 (95%)	4 (5%)	0	100	100
5	S	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
5	e	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
5	s	75/92 (82%)	70 (93%)	5 (7%)	0	100	100
6	F	71/75 (95%)	67 (94%)	4 (6%)	0	100	100
6	T	72/75 (96%)	68 (94%)	4 (6%)	0	100	100
6	f	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
6	t	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
7	G	73/76 (96%)	69 (94%)	4 (6%)	0	100	100
7	U	67/76 (88%)	64 (96%)	3 (4%)	0	100	100
7	g	71/76 (93%)	68 (96%)	3 (4%)	0	100	100
7	u	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
8	K	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
8	N	51/60 (85%)	47 (92%)	4 (8%)	0	100	100
8	k	55/60 (92%)	53 (96%)	2 (4%)	0	100	100
8	n	56/60 (93%)	47 (84%)	9 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	L	51/61 (84%)	48 (94%)	3 (6%)	0	100	100
9	M	51/61 (84%)	47 (92%)	4 (8%)	0	100	100
9	l	51/61 (84%)	48 (94%)	3 (6%)	0	100	100
9	m	48/61 (79%)	47 (98%)	1 (2%)	0	100	100
All	All	2633/3176 (83%)	2509 (95%)	124 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	73/101 (72%)	69 (94%)	4 (6%)	27	66
1	O	72/101 (71%)	67 (93%)	5 (7%)	19	57
1	a	73/101 (72%)	68 (93%)	5 (7%)	20	57
1	o	71/101 (70%)	61 (86%)	10 (14%)	4	20
2	B	76/85 (89%)	73 (96%)	3 (4%)	39	75
2	P	76/85 (89%)	71 (93%)	5 (7%)	21	59
2	b	72/85 (85%)	69 (96%)	3 (4%)	36	73
2	p	78/85 (92%)	70 (90%)	8 (10%)	9	34
3	C	79/83 (95%)	78 (99%)	1 (1%)	76	89
3	Q	79/83 (95%)	77 (98%)	2 (2%)	55	82
3	c	80/83 (96%)	77 (96%)	3 (4%)	40	75
3	q	80/83 (96%)	76 (95%)	4 (5%)	30	68
4	D	93/110 (84%)	88 (95%)	5 (5%)	27	66
4	R	92/110 (84%)	82 (89%)	10 (11%)	8	32
4	d	88/110 (80%)	75 (85%)	13 (15%)	4	17
4	r	91/110 (83%)	83 (91%)	8 (9%)	12	44
5	E	72/84 (86%)	68 (94%)	4 (6%)	26	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	72/84 (86%)	61 (85%)	11 (15%)	3	16
5	e	72/84 (86%)	57 (79%)	15 (21%)	1	6
5	s	72/84 (86%)	61 (85%)	11 (15%)	3	16
6	F	61/64 (95%)	55 (90%)	6 (10%)	10	37
6	T	63/64 (98%)	56 (89%)	7 (11%)	8	31
6	f	63/64 (98%)	54 (86%)	9 (14%)	4	19
6	t	63/64 (98%)	56 (89%)	7 (11%)	8	31
7	G	65/66 (98%)	57 (88%)	8 (12%)	6	25
7	U	62/66 (94%)	53 (86%)	9 (14%)	4	18
7	g	63/66 (96%)	59 (94%)	4 (6%)	22	60
7	u	63/66 (96%)	57 (90%)	6 (10%)	11	38
8	K	53/53 (100%)	53 (100%)	0	100	100
8	N	48/53 (91%)	46 (96%)	2 (4%)	36	73
8	k	52/53 (98%)	50 (96%)	2 (4%)	40	75
8	n	53/53 (100%)	49 (92%)	4 (8%)	17	52
9	L	51/56 (91%)	45 (88%)	6 (12%)	6	27
9	M	51/56 (91%)	42 (82%)	9 (18%)	2	10
9	l	51/56 (91%)	45 (88%)	6 (12%)	6	27
9	m	48/56 (86%)	42 (88%)	6 (12%)	6	24
All	All	2471/2808 (88%)	2250 (91%)	221 (9%)	12	43

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	38	ASN
1	A	47	THR
1	A	82	MET
2	B	13	ILE
2	B	16	ARG
2	B	17	MET
3	C	4	VAL
4	D	33	THR
4	D	52	LEU
4	D	61	ARG

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Mol	Chain	Res	Type
4	D	94	ARG
4	D	115	ILE
5	E	16	GLN
5	E	29	SER
5	E	60	ASP
5	E	82	ASP
6	F	27	MET
6	F	28	GLU
6	F	51	ILE
6	F	59	LEU
6	F	65	ARG
6	F	73	ARG
7	G	3	LYS
7	G	11	LYS
7	G	27	VAL
7	G	46	VAL
7	G	50	THR
7	G	51	SER
7	G	69	MET
7	G	75	ARG
9	L	29	LYS
9	L	42	MET
9	L	44	GLU
9	L	48	SER
9	L	53	THR
9	L	54	THR
1	a	24	THR
1	a	34	GLU
1	a	77	LEU
1	a	78	LYS
1	a	82	MET
2	b	11	GLN
2	b	71	LEU
2	b	80	MET
3	c	4	VAL
3	c	11	SER
3	c	41	LYS
4	d	15	GLU
4	d	17	GLN
4	d	20	GLU
4	d	21	GLU
4	d	22	GLU

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Mol	Chain	Res	Type
4	d	32	LEU
4	d	33	THR
4	d	37	LYS
4	d	42	VAL
4	d	51	LYS
4	d	61	ARG
4	d	75	THR
4	d	94	ARG
5	e	14	MET
5	e	20	LEU
5	e	25	LEU
5	e	29	SER
5	e	38	GLN
5	e	60	ASP
5	e	62	GLU
5	e	63	GLU
5	e	67	LYS
5	e	69	LYS
5	e	70	SER
5	e	79	LEU
5	e	80	LYS
5	e	82	ASP
5	e	89	SER
6	f	3	LEU
6	f	8	LYS
6	f	14	LEU
6	f	23	LEU
6	f	27	MET
6	f	44	LEU
6	f	51	ILE
6	f	59	LEU
6	f	65	ARG
7	g	10	LYS
7	g	27	VAL
7	g	59	MET
7	g	69	MET
8	k	10	LEU
8	k	52	ARG
9	l	29	LYS
9	l	35	LYS
9	l	48	SER
9	l	52	LYS

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Mol	Chain	Res	Type
9	I	53	THR
9	I	54	THR
1	O	24	THR
1	O	34	GLU
1	O	78	LYS
1	O	82	MET
1	O	83	LEU
2	P	11	GLN
2	P	13	ILE
2	P	71	LEU
2	P	80	MET
2	P	88	LYS
3	Q	4	VAL
3	Q	11	SER
4	R	11	MET
4	R	12	THR
4	R	16	LEU
4	R	33	THR
4	R	37	LYS
4	R	42	VAL
4	R	51	LYS
4	R	61	ARG
4	R	75	THR
4	R	114	LEU
5	S	20	LEU
5	S	25	LEU
5	S	38	GLN
5	S	59	ASP
5	S	60	ASP
5	S	62	GLU
5	S	63	GLU
5	S	67	LYS
5	S	69	LYS
5	S	78	MET
5	S	82	ASP
6	T	8	LYS
6	T	23	LEU
6	T	27	MET
6	T	44	LEU
6	T	51	ILE
6	T	65	ARG
6	T	73	ARG

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Mol	Chain	Res	Type
7	U	26	HIS
7	U	32	ARG
7	U	46	VAL
7	U	48	MET
7	U	63	ARG
7	U	65	ASN
7	U	69	MET
7	U	74	GLU
7	U	75	ARG
8	N	28	LEU
8	N	46	ARG
9	M	26	SER
9	M	29	LYS
9	M	35	LYS
9	M	39	GLN
9	M	45	GLN
9	M	48	SER
9	M	49	LEU
9	M	51	ASP
9	M	54	THR
1	o	3	ILE
1	o	20	CYS
1	o	24	THR
1	o	34	GLU
1	o	46	ILE
1	o	51	ARG
1	o	73	LEU
1	o	78	LYS
1	o	82	MET
1	o	83	LEU
2	p	7	SER
2	p	12	HIS
2	p	54	LYS
2	p	56	SER
2	p	57	LYS
2	p	58	GLN
2	p	67	LEU
2	p	71	LEU
3	q	4	VAL
3	q	11	SER
3	q	19	LEU
3	q	82	ASP

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Mol	Chain	Res	Type
4	r	20	GLU
4	r	37	LYS
4	r	42	VAL
4	r	51	LYS
4	r	61	ARG
4	r	75	THR
4	r	94	ARG
4	r	114	LEU
5	s	14	MET
5	s	25	LEU
5	s	27	ASN
5	s	60	ASP
5	s	62	GLU
5	s	63	GLU
5	s	68	THR
5	s	70	SER
5	s	80	LYS
5	s	82	ASP
5	s	86	LEU
6	t	3	LEU
6	t	8	LYS
6	t	14	LEU
6	t	23	LEU
6	t	27	MET
6	t	51	ILE
6	t	65	ARG
7	u	27	VAL
7	u	50	THR
7	u	51	SER
7	u	57	ILE
7	u	59	MET
7	u	69	MET
8	n	3	GLN
8	n	28	LEU
8	n	48	PHE
8	n	50	ASP
9	m	3	LYS
9	m	26	SER
9	m	29	LYS
9	m	39	GLN
9	m	45	GLN
9	m	48	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	73	GLN
6	F	43	GLN
2	P	11	GLN
7	U	26	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	1	46/60 (76%)	14 (30%)	4 (8%)
10	2	46/60 (76%)	14 (30%)	3 (6%)
10	3	45/60 (75%)	14 (31%)	3 (6%)
10	4	47/60 (78%)	16 (34%)	4 (8%)
11	X	9/10 (90%)	1 (11%)	0
11	Y	9/10 (90%)	2 (22%)	0
11	x	9/10 (90%)	0	0
11	y	9/10 (90%)	2 (22%)	0
All	All	220/280 (78%)	63 (28%)	14 (6%)

All (63) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	1	10	U
10	1	18	A
10	1	19	G
10	1	20	G
10	1	124	U
10	1	126	A
10	1	128	U
10	1	130	G
10	1	132	G
10	1	133	G
10	1	135	A
10	1	136	G
10	1	137	U
10	1	138	G
11	X	9	C
10	2	10	U
10	2	18	A
10	2	19	G
10	2	20	G

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Mol	Chain	Res	Type
10	2	124	U
10	2	126	A
10	2	128	U
10	2	130	G
10	2	131	U
10	2	132	G
10	2	133	G
10	2	135	A
10	2	137	U
10	2	138	G
10	3	10	U
10	3	18	A
10	3	19	G
10	3	20	G
10	3	124	U
10	3	126	A
10	3	128	U
10	3	130	G
10	3	131	U
10	3	132	G
10	3	133	G
10	3	135	A
10	3	136	G
10	3	137	U
11	Y	3	G
11	Y	7	G
10	4	10	U
10	4	18	A
10	4	19	G
10	4	20	G
10	4	124	U
10	4	126	A
10	4	128	U
10	4	130	G
10	4	131	U
10	4	132	G
10	4	133	G
10	4	135	A
10	4	136	G
10	4	137	U
10	4	138	G
10	4	139	G

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Mol	Chain	Res	Type
11	y	2	G
11	y	7	G

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	1	126	A
10	1	128	U
10	1	136	G
10	1	137	U
10	2	126	A
10	2	128	U
10	2	137	U
10	3	126	A
10	3	128	U
10	3	136	G
10	4	126	A
10	4	128	U
10	4	136	G
10	4	138	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 31 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	EPE	1	201	-	14,15,15	0.75	0	18,20,20	2.56	5 (27%)
13	EPE	2	201	-	14,15,15	0.88	0	18,20,20	2.46	9 (50%)
16	EOH	4	201	-	2,2,2	0.54	0	1,1,1	0.16	0
18	SO4	y	103	-	4,4,4	0.48	0	6,6,6	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	EPE	1	201	-	-	0/9/19/19	0/1/1/1
13	EPE	2	201	-	-	0/9/19/19	0/1/1/1
16	EOH	4	201	-	-	0/0/0/0	0/0/0/0
18	SO4	y	103	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	201	EPE	O2S-S-O1S	-3.21	101.77	113.48
13	2	201	EPE	C2-C3-N4	-2.42	106.29	110.63
13	2	201	EPE	O2S-S-O1S	-2.39	104.76	113.48
13	2	201	EPE	C6-N1-C2	2.27	113.81	108.90
13	2	201	EPE	C5-C6-N1	2.40	114.93	110.63
13	2	201	EPE	O8-C8-C7	2.54	122.92	111.28
13	2	201	EPE	C7-N4-C3	2.81	118.48	111.27
13	1	201	EPE	C2-C3-N4	3.03	116.05	110.63
13	2	201	EPE	C3-C2-N1	3.08	116.13	110.63
13	1	201	EPE	C3-C2-N1	3.78	117.40	110.63
13	1	201	EPE	C6-N1-C2	3.81	117.14	108.90
13	2	201	EPE	O1S-S-C10	4.87	111.06	106.91
13	2	201	EPE	C6-C5-N4	5.55	120.56	110.63
13	1	201	EPE	O1S-S-C10	7.74	113.51	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1	201	EPE	1	0
13	2	201	EPE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th 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 ²)	Q<0.9
1	A	84/126 (66%)	0.21	3 (3%) 46 39	50, 68, 102, 155	0
1	O	82/126 (65%)	1.33	24 (29%) 1 1	96, 125, 152, 182	0
1	a	83/126 (65%)	-0.20	1 (1%) 81 76	46, 70, 103, 123	0
1	o	81/126 (64%)	0.87	14 (17%) 2 2	87, 137, 161, 176	0
2	B	83/95 (87%)	0.66	3 (3%) 46 39	41, 65, 189, 219	0
2	P	83/95 (87%)	1.01	14 (16%) 2 2	68, 111, 178, 219	0
2	b	78/95 (82%)	0.08	1 (1%) 79 74	45, 70, 135, 185	0
2	p	86/95 (90%)	0.10	2 (2%) 64 57	75, 122, 185, 221	0
3	C	86/91 (94%)	-0.08	0 100 100	39, 56, 120, 139	0
3	Q	85/91 (93%)	0.09	2 (2%) 62 55	55, 77, 125, 140	0
3	c	87/91 (95%)	0.06	0 100 100	42, 60, 124, 139	0
3	q	87/91 (95%)	-0.20	0 100 100	57, 82, 131, 150	0
4	D	98/118 (83%)	0.04	0 100 100	38, 62, 151, 181	0
4	R	96/118 (81%)	0.16	0 100 100	49, 73, 157, 176	0
4	d	92/118 (77%)	-0.03	0 100 100	41, 63, 154, 176	0
4	r	95/118 (80%)	-0.04	1 (1%) 82 78	63, 85, 173, 233	0
5	E	77/92 (83%)	0.56	3 (3%) 43 36	49, 75, 113, 134	0
5	S	77/92 (83%)	-0.28	2 (2%) 59 53	75, 117, 159, 177	0
5	e	77/92 (83%)	0.67	2 (2%) 59 53	52, 81, 126, 150	0
5	s	77/92 (83%)	0.26	4 (5%) 31 25	86, 115, 155, 171	0
6	F	73/75 (97%)	-0.01	0 100 100	45, 64, 95, 133	0
6	T	74/75 (98%)	-0.07	0 100 100	59, 88, 136, 175	0
6	f	74/75 (98%)	0.39	1 (1%) 78 73	52, 76, 101, 129	0
6	t	74/75 (98%)	0.31	1 (1%) 78 73	73, 100, 144, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	G	74/76 (97%)	0.66	2 (2%) 58 51	51, 80, 120, 137	0
7	U	71/76 (93%)	0.36	8 (11%) 7 5	95, 130, 165, 178	0
7	g	73/76 (96%)	0.01	0 100 100	55, 83, 123, 168	0
7	u	73/76 (96%)	0.76	12 (16%) 2 2	98, 133, 171, 188	0
8	K	58/60 (96%)	-0.11	0 100 100	52, 83, 139, 159	0
8	N	53/60 (88%)	1.08	11 (20%) 1 1	57, 121, 162, 171	0
8	k	57/60 (95%)	-0.16	1 (1%) 71 65	52, 90, 130, 155	0
8	n	58/60 (96%)	1.01	11 (18%) 2 1	80, 140, 185, 196	0
9	L	53/61 (86%)	0.29	3 (5%) 27 22	72, 106, 180, 197	0
9	M	53/61 (86%)	1.53	17 (32%) 1 1	102, 140, 194, 199	0
9	l	53/61 (86%)	0.30	3 (5%) 27 22	70, 112, 177, 202	0
9	m	50/61 (81%)	1.36	14 (28%) 1 1	116, 157, 210, 217	0
10	1	47/60 (78%)	-0.37	0 100 100	46, 93, 150, 176	0
10	2	47/60 (78%)	-0.21	0 100 100	47, 99, 158, 175	0
10	3	46/60 (76%)	-0.20	0 100 100	72, 127, 151, 178	0
10	4	48/60 (80%)	-0.02	0 100 100	77, 129, 173, 196	0
11	X	10/10 (100%)	-0.75	0 100 100	88, 119, 157, 164	0
11	Y	10/10 (100%)	-0.06	1 (10%) 9 8	114, 143, 162, 164	0
11	x	10/10 (100%)	-0.04	0 100 100	89, 118, 165, 176	0
11	y	10/10 (100%)	0.61	1 (10%) 9 8	130, 152, 171, 177	0
All	All	2943/3456 (85%)	0.29	162 (5%) 29 23	38, 95, 165, 233	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	56	SER	18.1
8	n	2	THR	9.7
2	P	55	ASN	8.7
8	n	3	GLN	7.5
2	P	57	LYS	7.1
8	n	10	LEU	7.1
8	N	9	LEU	7.0
9	m	14	THR	7.0
8	N	8	ASN	6.9
8	N	10	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
8	N	13	PHE	6.5
1	O	12	GLU	6.4
8	n	7	PRO	5.7
2	P	58	GLN	5.6
6	t	75	VAL	5.6
7	u	50	THR	5.5
1	o	35	ALA	5.5
1	O	77	LEU	5.4
9	m	13	LEU	5.3
9	M	2	PRO	5.1
8	N	12	LEU	5.1
9	M	8	TYR	5.0
8	n	4	PHE	5.0
9	M	4	PHE	4.9
1	o	34	GLU	4.7
9	M	38	TYR	4.6
1	O	15	GLY	4.6
9	m	12	TYR	4.6
8	N	7	PRO	4.4
9	m	11	THR	4.4
9	M	13	LEU	4.4
9	m	15	HIS	4.2
8	N	6	PRO	4.2
1	O	79	ASN	4.2
8	N	11	ALA	4.2
1	O	76	MET	4.1
9	l	12	TYR	4.1
1	A	1	MET	4.0
2	P	53	PRO	4.0
1	O	2	SER	3.9
8	n	5	LEU	3.9
9	M	7	ASP	3.8
9	M	12	TYR	3.8
2	B	59	ALA	3.7
2	P	60	GLU	3.7
1	O	81	PRO	3.7
1	o	10	LEU	3.6
1	A	2	SER	3.6
2	P	51	ILE	3.6
7	u	51	SER	3.6
1	O	3	ILE	3.5
8	n	8	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	O	16	HIS	3.5
2	P	54	LYS	3.5
2	P	52	LYS	3.4
9	l	2	PRO	3.4
2	B	14	ASP	3.4
8	n	6	PRO	3.3
2	P	61	ARG	3.3
9	M	14	THR	3.3
7	U	68	ILE	3.3
9	M	51	ASP	3.2
8	n	9	LEU	3.1
1	O	82	MET	3.1
8	N	33	HIS	3.1
9	M	53	THR	3.1
1	o	18	VAL	3.1
1	O	7	ILE	3.1
7	u	35	ASP	3.1
7	u	5	HIS	3.0
7	U	69	MET	3.0
1	o	63	ILE	3.0
9	l	11	THR	3.0
2	B	60	GLU	2.9
2	P	63	GLU	2.9
2	p	90	THR	2.9
9	M	21	ARG	2.9
8	n	13	PHE	2.9
9	m	5	TYR	2.9
5	s	88	GLN	2.9
3	Q	-2	SER	2.9
9	M	43	GLU	2.8
9	m	2	PRO	2.8
7	u	27	VAL	2.8
5	e	78	MET	2.8
1	O	10	LEU	2.8
1	o	74	PRO	2.8
1	O	11	HIS	2.8
3	Q	82	ASP	2.7
5	s	14	MET	2.7
1	O	17	ILE	2.7
7	u	9	LEU	2.7
7	U	21	LEU	2.7
1	O	8	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
9	M	15	HIS	2.7
1	o	56	ALA	2.7
5	S	37	GLU	2.7
1	o	77	LEU	2.6
9	m	26	SER	2.6
9	M	54	THR	2.6
1	o	73	LEU	2.6
1	O	41	CYS	2.6
2	p	69	LEU	2.6
5	E	14	MET	2.6
7	G	59	MET	2.6
5	S	36	TYR	2.6
9	m	4	PHE	2.6
1	A	3	ILE	2.6
2	b	7	SER	2.6
2	P	59	ALA	2.6
7	U	72	ALA	2.6
1	O	78	LYS	2.5
5	e	56	LEU	2.5
7	u	53	GLN	2.5
5	s	87	LEU	2.5
6	f	2	SER	2.5
1	O	39	MET	2.5
9	m	10	ASP	2.5
9	m	7	ASP	2.5
5	s	56	LEU	2.4
2	P	50	LYS	2.4
1	O	20	CYS	2.4
1	O	28	TYR	2.4
7	u	40	LEU	2.4
7	u	60	VAL	2.4
11	y	1	A	2.4
5	E	44	GLU	2.4
7	U	70	LEU	2.3
1	O	32	LEU	2.3
1	O	14	GLU	2.3
7	u	62	ILE	2.3
7	u	61	VAL	2.2
9	m	8	TYR	2.2
1	o	7	ILE	2.2
1	o	11	HIS	2.2
1	a	3	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	24	TYR	2.2
7	U	22	ASN	2.2
9	m	28	ARG	2.2
2	P	62	GLU	2.2
8	n	18	PRO	2.2
8	N	32	LYS	2.2
7	U	67	ILE	2.2
9	L	53	THR	2.2
9	m	32	GLU	2.2
4	r	12	THR	2.1
1	O	22	THR	2.1
9	L	5	TYR	2.1
8	N	58	THR	2.1
1	O	24	THR	2.1
7	G	40	LEU	2.1
7	U	35	ASP	2.1
9	L	14	THR	2.1
9	M	41	TRP	2.1
1	o	62	TYR	2.0
9	M	52	LYS	2.0
9	M	42	MET	2.0
11	Y	1	A	2.0
7	u	19	LEU	2.0
1	o	12	GLU	2.0
1	o	15	GLY	2.0
8	k	45	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	MG	2	202	1/1	0.92	0.36	12.31	69,69,69,69	0
13	EPE	2	201	15/15	0.81	0.43	3.02	92,116,141,146	0
13	EPE	1	201	15/15	0.77	0.35	1.93	131,146,150,162	0
14	MG	2	203	1/1	0.35	0.18	1.18	87,87,87,87	0
14	MG	y	102	1/1	0.88	0.21	-0.72	100,100,100,100	0
12	ZN	l	201	1/1	0.99	0.11	-1.11	98,98,98,98	0
12	ZN	L	201	1/1	0.99	0.13	-1.54	83,83,83,83	0
14	MG	3	201	1/1	0.89	0.15	-1.82	75,75,75,75	0
15	K	Q	101	1/1	0.93	0.13	-2.41	97,97,97,97	0
17	CL	4	203	1/1	0.95	0.11	-3.16	111,111,111,111	0
14	MG	1	204	1/1	0.95	0.15	-5.05	64,64,64,64	0
14	MG	3	203	1/1	0.90	0.12	-	80,80,80,80	0
16	EOH	4	201	3/3	0.43	1.09	-	112,112,115,119	0
14	MG	l	202	1/1	0.44	0.94	-	106,106,106,106	0
14	MG	1	203	1/1	0.87	0.20	-	52,52,52,52	0
14	MG	1	209	1/1	0.65	0.27	-	95,95,95,95	0
14	MG	2	204	1/1	0.60	0.27	-	94,94,94,94	0
14	MG	y	101	1/1	0.89	0.30	-	100,100,100,100	0
12	ZN	M	201	1/1	0.97	0.10	-	126,126,126,126	0
15	K	3	206	1/1	0.88	0.41	-	125,125,125,125	0
15	K	1	210	1/1	0.95	0.09	-	91,91,91,91	0
14	MG	1	205	1/1	0.70	0.30	-	71,71,71,71	0
15	K	b	101	1/1	0.88	0.33	-	105,105,105,105	0
14	MG	3	204	1/1	0.81	0.25	-	97,97,97,97	0
18	SO4	y	103	5/5	0.39	0.59	-	192,193,205,208	0
14	MG	1	207	1/1	0.80	0.18	-	82,82,82,82	0
14	MG	1	202	1/1	0.80	0.27	-	100,100,100,100	0
14	MG	4	202	1/1	0.78	0.31	-	86,86,86,86	0
15	K	b	102	1/1	0.89	0.24	-	124,124,124,124	0
12	ZN	m	201	1/1	0.98	0.09	-	136,136,136,136	0
14	MG	3	202	1/1	0.48	0.13	-	91,91,91,91	0
14	MG	1	206	1/1	0.86	0.27	-	86,86,86,86	0
14	MG	2	205	1/1	0.87	0.26	-	61,61,61,61	0
14	MG	1	208	1/1	0.72	0.27	-	75,75,75,75	0
15	K	3	205	1/1	0.44	0.23	-	122,122,122,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.