Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 01:54 PM EDT

PDB ID	:	4RMO
Title	:	Crystal Structure of the CptIN Type III Toxin-Antitoxin System from Eubacterium rectale
Authors	:	Rao, F.; Voss, J.E.; Short, F.L.; Luisi, B.F.
Deposited on	:	2014-10-21
Resolution	:	2.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

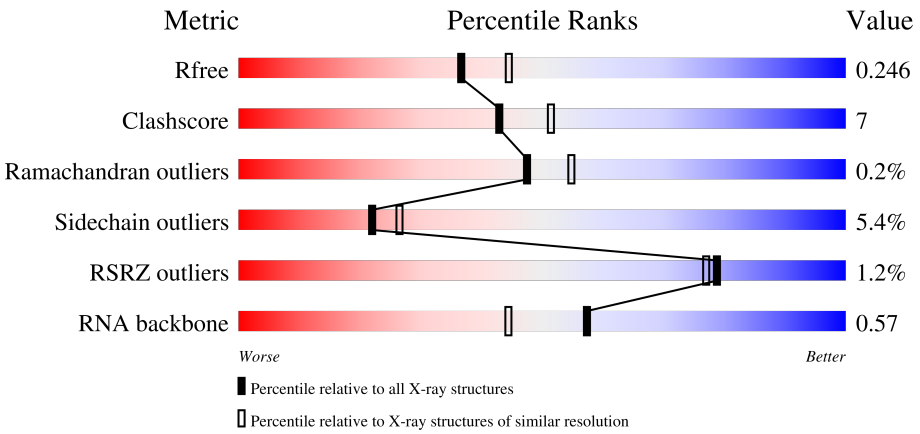
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	155	% 85% 12% •
1	C	155	84% 15% •
1	E	155	81% 15% • •
1	G	155	83% 15% •

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Mol	Chain	Length	Quality of chain
1	I	155	%, 81%, 17%
1	K	155	%, 84%, 12%, 5%
1	M	155	%, 85%, 10%, 5%
1	O	155	6%, 85%, 12%
2	B	45	64%, 27%, 7%
2	D	45	58%, 38%
2	F	45	62%, 33%
2	H	45	62%, 31%
2	J	45	2%, 62%, 29%, 7%
2	L	45	60%, 29%, 9%
2	N	45	58%, 33%, 9%
2	P	45	7%, 42%, 36%, 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19477 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 CptN Toxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	155	1303	832	230	234	2	5	0	1	0
1	C	155	1303	832	230	234	2	5	0	1	0
1	E	155	1303	832	230	234	2	5	0	1	0
1	G	155	1303	832	230	234	2	5	0	1	0
1	I	155	1293	827	226	233	2	5	0	1	0
1	K	155	1303	832	230	234	2	5	0	1	0
1	M	155	1300	830	229	234	2	5	0	1	0
1	O	155	1303	832	230	234	2	5	0	1	0

- Molecule 2 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	45	962	430	171	316	45	0	0	0
2	D	45	962	430	171	316	45	0	0	0
2	F	45	962	430	171	316	45	0	0	0
2	H	45	962	430	171	316	45	0	0	0
2	J	45	962	430	171	316	45	0	0	0
2	L	45	962	430	171	316	45	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	N	45	962	430	171	316	45	0	0	0
			Total	C	N	O	P			
2	P	45	962	430	171	316	45	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0
			Total	Ca		
3	B	5	5	5	0	0
			Total	Ca		
3	C	1	1	1	0	0
			Total	Ca		
3	D	6	6	6	0	0
			Total	Ca		
3	E	1	1	1	0	0
			Total	Ca		
3	F	4	4	4	0	0
			Total	Ca		
3	G	1	1	1	0	0
			Total	Ca		
3	H	6	6	6	0	0
			Total	Ca		
3	I	1	1	1	0	0
			Total	Ca		
3	J	6	6	6	0	0
			Total	Ca		
3	K	1	1	1	0	0
			Total	Ca		
3	L	5	5	5	0	0
			Total	Ca		
3	M	1	1	1	0	0
			Total	Ca		
3	N	5	5	5	0	0
			Total	Ca		
3	O	1	1	1	0	0
			Total	Ca		
3	P	3	3	3	0	0

- Molecule 4 is water.

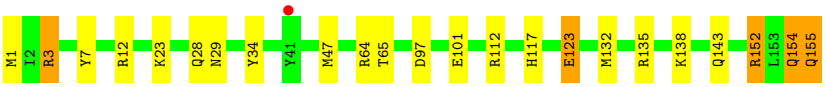
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	82	82	82	0	0
			Total	O		
4	B	99	99	99	0	0
			Total	O		
4	C	88	88	88	0	0
			Total	O		
4	D	98	98	98	0	0
			Total	O		
4	E	53	53	53	0	0
			Total	O		
4	F	67	67	67	0	0
			Total	O		
4	G	112	112	112	0	0
			Total	O		
4	H	100	100	100	0	0
			Total	O		
4	I	81	81	81	0	0
			Total	O		
4	J	100	100	100	0	0
			Total	O		
4	K	89	89	89	0	0
			Total	O		
4	L	85	85	85	0	0
			Total	O		
4	M	54	54	54	0	0
			Total	O		
4	N	83	83	83	0	0
			Total	O		
4	O	67	67	67	0	0
			Total	O		
4	P	64	64	64	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

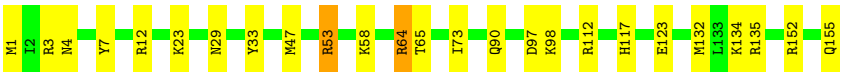
- Molecule 1: CptN Toxin

Chain A:



- Molecule 1: CptN Toxin

Chain C:

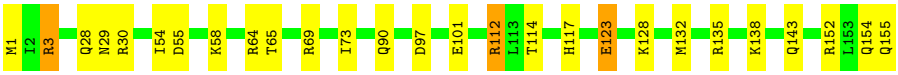


- Molecule 1: CptN Toxin

Chain E:

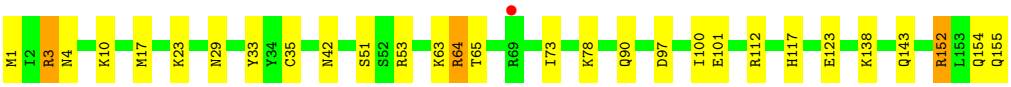
- Molecule 1: CptN Toxin

Chain G:



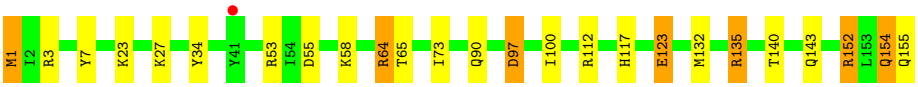
- Molecule 1: CptN Toxin

Chain I:



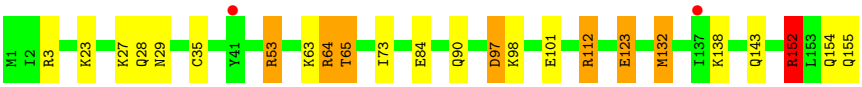
- Molecule 1: CptN Toxin

Chain K:



• Molecule 1: CptN Toxin

Chain M:



• Molecule 1: CptN Toxin

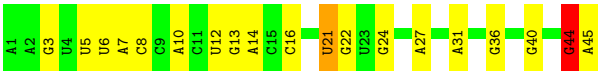
Chain O:

• Molecule 2: RNA (45-MER)

Chain B:

• Molecule 2: RNA (45-MER)

Chain D:

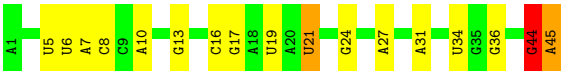


• Molecule 2: RNA (45-MER)

Chain F:

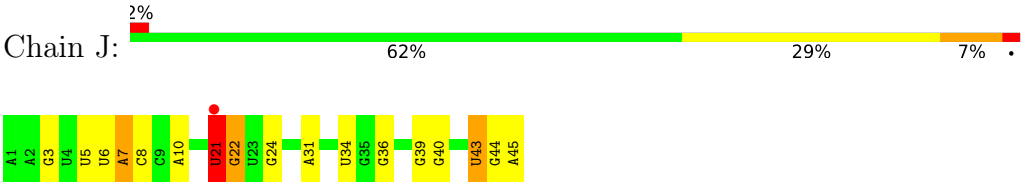
• Molecule 2: RNA (45-MER)

Chain H:



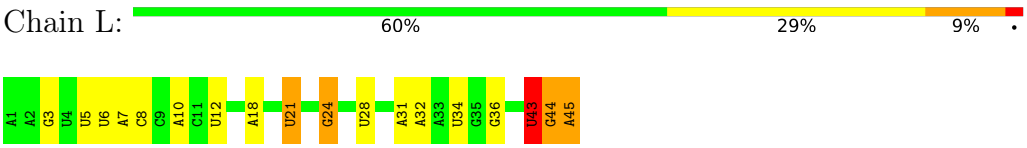
• Molecule 2: RNA (45-MER)

Chain J:



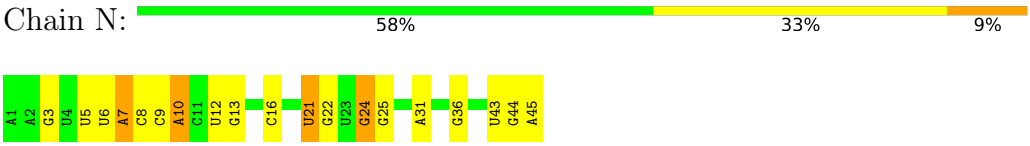
• Molecule 2: RNA (45-MER)

Chain L:



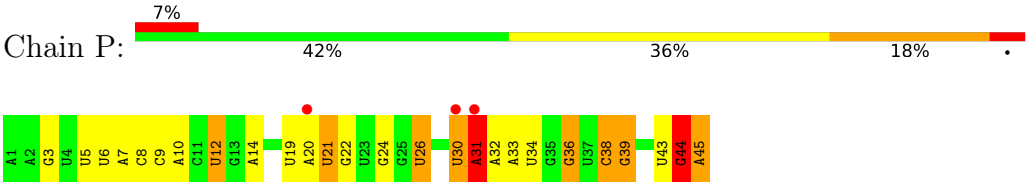
• Molecule 2: RNA (45-MER)

Chain N:



• Molecule 2: RNA (45-MER)

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.11Å 185.89Å 138.78Å 90.00° 92.63° 90.00°	Depositor
Resolution (Å)	63.12 – 2.20 63.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (63.12-2.20) 97.8 (63.04-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.199 , 0.234 0.212 , 0.246	Depositor DCC
R_{free} test set	7919 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19477	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A23, CA

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	0.84	4/1331 (0.3%)	0.92	4/1776 (0.2%)
1	C	0.86	0/1331	1.01	12/1776 (0.7%)
1	E	0.81	2/1331 (0.2%)	0.94	7/1776 (0.4%)
1	G	0.90	5/1331 (0.4%)	0.95	5/1776 (0.3%)
1	I	0.85	0/1321	0.91	3/1764 (0.2%)
1	K	0.90	5/1331 (0.4%)	1.03	8/1776 (0.5%)
1	M	0.87	6/1328 (0.5%)	0.94	7/1773 (0.4%)
1	O	0.80	2/1331 (0.2%)	0.90	7/1776 (0.4%)
2	B	0.67	1/1048 (0.1%)	0.98	3/1632 (0.2%)
2	D	0.60	0/1048	0.92	4/1632 (0.2%)
2	F	0.54	0/1048	0.91	4/1632 (0.2%)
2	H	0.51	0/1048	0.90	3/1632 (0.2%)
2	J	0.72	1/1048 (0.1%)	0.98	6/1632 (0.4%)
2	L	0.58	0/1048	0.92	5/1632 (0.3%)
2	N	0.64	0/1048	0.98	6/1632 (0.4%)
2	P	0.76	3/1048 (0.3%)	1.33	18/1632 (1.1%)
All	All	0.76	29/19019 (0.2%)	0.97	102/27249 (0.4%)

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
1	K	0	1
1	O	0	1
2	B	0	1
2	D	0	1
2	H	0	1
2	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	42	U	O3'-P	-10.66	1.48	1.61
2	P	19	U	O3'-P	8.94	1.71	1.61
2	P	44	G	O5'-C5'	-7.43	1.30	1.42
2	J	40	G	O5'-C5'	-6.01	1.33	1.42
1	M	123[A]	GLU	CD-OE1	5.83	1.32	1.25
1	M	123[B]	GLU	CD-OE1	5.83	1.32	1.25
1	E	123[A]	GLU	CG-CD	5.73	1.60	1.51
1	E	123[B]	GLU	CG-CD	5.73	1.60	1.51
1	G	123[A]	GLU	CG-CD	5.59	1.60	1.51
1	G	123[B]	GLU	CG-CD	5.59	1.60	1.51
1	K	123[A]	GLU	CG-CD	5.49	1.60	1.51
1	K	123[B]	GLU	CG-CD	5.49	1.60	1.51
1	K	55	ASP	CB-CG	-5.35	1.40	1.51
1	A	123[A]	GLU	CG-CD	5.33	1.59	1.51
1	A	123[B]	GLU	CG-CD	5.33	1.59	1.51
1	M	132	MSE	CG-SE	-5.28	1.77	1.95
1	A	123[A]	GLU	CD-OE1	5.27	1.31	1.25
1	A	123[B]	GLU	CD-OE1	5.27	1.31	1.25
1	M	84	GLU	CD-OE2	-5.23	1.19	1.25
1	K	123[A]	GLU	CD-OE1	5.21	1.31	1.25
1	K	123[B]	GLU	CD-OE1	5.21	1.31	1.25
2	P	36	G	P-OP2	-5.19	1.40	1.49
1	G	1	MSE	CG-SE	-5.18	1.77	1.95
1	O	123[A]	GLU	CG-CD	5.11	1.59	1.51
1	O	123[B]	GLU	CG-CD	5.11	1.59	1.51
1	G	123[A]	GLU	CD-OE1	5.06	1.31	1.25
1	G	123[B]	GLU	CD-OE1	5.06	1.31	1.25
1	M	123[A]	GLU	CG-CD	5.03	1.59	1.51
1	M	123[B]	GLU	CG-CD	5.03	1.59	1.51

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	44	G	O5'-P-OP1	-16.77	90.58	110.70
2	B	42	U	C2'-C3'-O3'	14.73	141.91	109.50
2	P	44	G	O5'-P-OP2	11.68	124.71	110.70
2	P	44	G	C5'-C4'-O4'	-11.51	95.29	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	38	C	C2'-C3'-O3'	11.06	133.83	109.50
1	K	55	ASP	N-CA-CB	-10.62	91.48	110.60
2	P	39	G	P-O5'-C5'	-10.54	104.04	120.90
2	P	36	G	O5'-P-OP2	10.26	123.02	110.70
2	P	44	G	C5'-C4'-C3'	-9.74	100.41	116.00
2	P	36	G	C5'-C4'-O4'	9.65	120.69	109.10
2	B	24	G	O5'-P-OP2	-9.44	97.20	105.70
1	C	53	ARG	NE-CZ-NH1	9.26	124.93	120.30
2	D	24	G	O5'-P-OP2	-9.14	97.48	105.70
2	J	24	G	O5'-P-OP2	-9.09	97.52	105.70
2	P	12	U	O5'-P-OP2	-8.84	97.74	105.70
1	G	64	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	K	64	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	C	64	ARG	NE-CZ-NH2	-8.32	116.14	120.30
2	F	24	G	O5'-P-OP2	-8.30	98.23	105.70
1	C	152	ARG	CG-CD-NE	-8.16	94.66	111.80
2	H	24	G	O5'-P-OP2	-8.13	98.38	105.70
2	P	31	A	O5'-P-OP1	-8.02	98.48	105.70
1	M	64	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	53	ARG	NE-CZ-NH2	-7.88	116.36	120.30
2	N	7	A	O3'-P-O5'	-7.83	89.12	104.00
2	J	43	U	O5'-P-OP2	-7.74	98.73	105.70
1	A	64	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	E	64	ARG	NE-CZ-NH2	-7.66	116.47	120.30
2	L	12	U	O5'-P-OP2	-7.60	98.86	105.70
2	N	24	G	O5'-P-OP2	-7.40	99.04	105.70
1	C	112	ARG	NE-CZ-NH1	7.31	123.95	120.30
2	J	40	G	C5'-C4'-C3'	-7.29	104.34	116.00
1	I	35	CYS	N-CA-CB	7.20	123.57	110.60
1	K	64	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	E	135	ARG	NE-CZ-NH2	-7.09	116.75	120.30
2	F	12	U	O5'-P-OP2	-7.02	99.38	105.70
1	I	64	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	L	44	G	O4'-C1'-N9	6.96	113.77	108.20
2	P	44	G	O4'-C1'-N9	6.93	113.75	108.20
1	M	53	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	O	135	ARG	NE-CZ-NH1	6.83	123.71	120.30
2	L	24	G	O5'-P-OP2	-6.80	99.58	105.70
2	P	36	G	P-O5'-C5'	6.77	131.73	120.90
2	N	12	U	O5'-P-OP2	-6.69	99.68	105.70
2	P	24	G	O5'-P-OP2	-6.57	99.79	105.70
1	C	64	ARG	NE-CZ-NH1	6.53	123.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	35	CYS	N-CA-CB	6.51	122.33	110.60
1	K	135	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	C	12	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	H	34	U	O5'-P-OP1	-6.40	99.94	105.70
2	J	21	U	N1-C1'-C2'	6.35	122.25	114.00
1	C	12	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	B	44	G	O4'-C1'-N9	6.18	113.14	108.20
2	L	34	U	O5'-P-OP1	-6.15	100.17	105.70
2	F	44	G	O4'-C1'-N9	6.04	113.03	108.20
1	G	64	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	M	53	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	N	16	C	O5'-P-OP2	-6.00	100.30	105.70
2	H	44	G	O4'-C1'-N9	5.94	112.95	108.20
2	D	40	G	O5'-P-OP2	-5.93	100.36	105.70
1	E	65	THR	N-CA-CB	5.88	121.46	110.30
1	K	55	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	O	64	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	J	39	G	O3'-P-O5'	-5.85	92.88	104.00
1	O	101	GLU	CA-CB-CG	-5.81	100.63	113.40
1	C	152	ARG	NE-CZ-NH2	-5.77	117.42	120.30
2	P	36	G	C5'-C4'-C3'	-5.76	106.78	116.00
1	A	64	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	P	31	A	O5'-P-OP2	5.75	117.60	110.70
1	M	64	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	K	97	ASP	CB-CG-OD1	5.73	123.46	118.30
1	O	135	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	53	ARG	CD-NE-CZ	5.67	131.54	123.60
2	D	44	G	O4'-C1'-N9	5.66	112.73	108.20
2	N	8	C	O5'-P-OP2	5.64	117.46	110.70
1	E	69	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	P	34	U	O5'-P-OP1	-5.63	100.64	105.70
1	G	3	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	155	GLN	N-CA-CB	5.55	120.60	110.60
1	I	64	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	G	55	ASP	CB-CG-OD1	5.52	123.27	118.30
2	P	26	U	O5'-P-OP2	-5.51	100.74	105.70
1	C	112	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	O	64	ARG	CG-CD-NE	5.43	123.21	111.80
2	L	43	U	O5'-P-OP2	-5.42	100.83	105.70
1	K	135	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	O	112	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	12	ARG	NE-CZ-NH1	5.36	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	64	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	J	34	U	O5'-P-OP1	-5.33	100.90	105.70
2	D	16	C	O5'-P-OP2	-5.32	100.92	105.70
2	F	16	C	O5'-P-OP2	-5.28	100.95	105.70
2	N	44	G	O4'-C1'-N9	5.22	112.38	108.20
1	M	97	ASP	CB-CG-OD1	5.21	122.99	118.30
1	E	152	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	M	152	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	58	LYS	CB-CA-C	5.15	120.71	110.40
2	P	44	G	P-O5'-C5'	-5.09	112.75	120.90
1	O	64	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	E	152	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	G	30	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	K	53	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	GLN	Peptide
2	B	44	G	Sidechain
2	D	44	G	Sidechain
2	H	44	G	Sidechain
1	K	154	GLN	Peptide
1	O	154	GLN	Peptide
2	P	44	G	Sidechain

5.2 Too-close contacts (i)

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	1303	0	1315	23	0
1	C	1303	0	1315	18	0
1	E	1303	0	1315	22	0
1	G	1303	0	1315	17	0
1	I	1293	0	1289	22	0
1	K	1303	0	1315	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1300	0	1306	28	0
1	O	1303	0	1315	12	0
2	B	962	0	481	11	0
2	D	962	0	481	13	0
2	F	962	0	481	13	0
2	H	962	0	481	12	0
2	J	962	0	481	12	0
2	L	962	0	481	16	0
2	N	962	0	481	14	0
2	P	962	0	481	20	0
3	A	1	0	0	0	0
3	B	5	0	0	0	0
3	C	1	0	0	0	0
3	D	6	0	0	0	0
3	E	1	0	0	0	0
3	F	4	0	0	0	0
3	G	1	0	0	0	0
3	H	6	0	0	0	0
3	I	1	0	0	0	0
3	J	6	0	0	0	0
3	K	1	0	0	0	0
3	L	5	0	0	0	0
3	M	1	0	0	0	0
3	N	5	0	0	1	0
3	O	1	0	0	0	0
3	P	3	0	0	0	0
4	A	82	0	0	3	1
4	B	99	0	0	2	0
4	C	88	0	0	2	1
4	D	98	0	0	1	0
4	E	53	0	0	1	0
4	F	67	0	0	4	0
4	G	112	0	0	8	0
4	H	100	0	0	4	0
4	I	81	0	0	4	0
4	J	100	0	0	5	0
4	K	89	0	0	4	0
4	L	85	0	0	4	0
4	M	54	0	0	12	0
4	N	83	0	0	9	0
4	O	67	0	0	1	0
4	P	64	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19477	0	14333	221	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 7.

All (221) 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)
2:L:18:A:N7	4:L:212:HOH:O	1.58	1.32
1:M:53:ARG:CD	4:M:349:HOH:O	1.77	1.28
1:M:53:ARG:NE	4:M:349:HOH:O	1.67	1.21
2:N:10:A:OP2	4:N:261:HOH:O	1.66	1.13
1:A:1:MSE:HE3	1:A:7:TYR:CD2	1.93	1.04
1:C:1:MSE:HE2	1:C:7:TYR:CD1	1.99	0.98
1:A:1:MSE:CE	1:A:7:TYR:CD2	2.48	0.96
2:N:7:A:O2'	4:N:253:HOH:O	1.82	0.96
1:E:1:MSE:HE2	1:E:7:TYR:CD1	2.01	0.96
1:M:65:THR:HG21	4:M:333:HOH:O	1.67	0.94
1:M:53:ARG:CZ	4:M:349:HOH:O	2.01	0.92
2:N:25:G:OP2	4:N:201:HOH:O	1.88	0.90
1:M:53:ARG:HG3	4:M:349:HOH:O	1.69	0.88
1:G:69:ARG:NH1	4:G:409:HOH:O	2.04	0.87
1:A:1:MSE:HE3	1:A:7:TYR:CG	2.12	0.85
1:E:117:HIS:HD2	4:E:321:HOH:O	1.59	0.85
1:G:3:ARG:HD3	4:G:350:HOH:O	1.77	0.84
1:I:63:LYS:CG	4:J:269:HOH:O	2.26	0.83
2:F:11:C:OP1	4:F:264:HOH:O	1.97	0.81
2:J:21:U:C5	4:J:256:HOH:O	2.33	0.81
2:J:21:U:O2'	2:J:22:G:OP2	1.97	0.81
1:G:114:THR:OG1	4:G:307:HOH:O	1.99	0.81
2:J:21:U:C6	4:J:256:HOH:O	2.34	0.80
2:F:32:A:OP2	4:F:255:HOH:O	1.98	0.80
1:K:143:GLN:NE2	4:K:365:HOH:O	2.15	0.76
2:P:12:U:O2	2:P:20:A:N6	2.19	0.76
2:N:24:G:O6	4:N:204:HOH:O	2.03	0.74
1:O:152:ARG:NH2	4:O:314:HOH:O	2.20	0.74
1:O:10:LYS:HG2	1:O:101:GLU:HG3	1.70	0.74
1:O:131:GLY:HA2	2:P:26:U:O2'	1.89	0.73
2:J:21:U:O2'	2:J:22:G:P	2.46	0.73
1:E:10:LYS:HG2	1:E:101:GLU:HG2	1.71	0.72
1:M:53:ARG:CG	4:M:349:HOH:O	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:143:GLN:CG	4:M:321:HOH:O	2.36	0.72
2:H:19:U:O2'	4:H:288:HOH:O	2.07	0.71
2:N:9:C:OP2	4:N:250:HOH:O	2.07	0.71
1:E:154:GLN:O	1:E:155:GLN:HB2	1.91	0.70
1:G:154:GLN:O	1:G:155:GLN:HB2	1.90	0.70
1:I:154:GLN:O	1:I:155:GLN:HB2	1.91	0.70
1:M:154:GLN:O	1:M:155:GLN:HB2	1.90	0.70
3:N:105:CA:CA	4:N:263:HOH:O	1.67	0.70
2:H:16:C:OP2	4:H:266:HOH:O	2.10	0.69
1:A:1:MSE:HE1	1:A:47:MSE:HE1	1.73	0.69
1:I:42:ASN:CB	4:I:335:HOH:O	2.39	0.69
1:M:143:GLN:HG3	4:M:321:HOH:O	1.92	0.68
2:P:9:C:H4'	4:P:227:HOH:O	1.92	0.68
1:E:132:MSE:HE1	2:F:6:U:C1'	2.23	0.68
1:K:140:THR:OG1	4:K:365:HOH:O	2.12	0.68
2:L:28:U:OP2	4:L:245:HOH:O	2.13	0.67
2:N:43:U:OP1	4:N:213:HOH:O	2.12	0.67
1:I:1:MSE:SE	1:I:100:ILE:HG13	2.45	0.67
1:C:1:MSE:HE2	1:C:7:TYR:CG	2.30	0.67
1:K:58:LYS:CE	4:K:332:HOH:O	2.43	0.67
1:I:3:ARG:HD3	4:I:325:HOH:O	1.96	0.65
2:B:44:G:H1'	1:E:29:ASN:HB2	1.79	0.65
2:F:22:G:OP2	4:F:236:HOH:O	2.14	0.65
2:L:24:G:N7	4:L:203:HOH:O	2.30	0.64
1:K:1:MSE:CE	1:K:7:TYR:CG	2.81	0.63
1:C:53:ARG:HD2	2:H:45:A23:O2C	1.98	0.63
1:I:51:SER:CA	2:L:45:A23:H8	2.28	0.63
1:E:1:MSE:HE1	1:E:47:MSE:HE1	1.80	0.63
1:A:1:MSE:CE	1:A:34:TYR:HB2	2.27	0.62
1:C:1:MSE:HE1	1:C:47:MSE:HE1	1.81	0.62
1:E:1:MSE:HE2	1:E:7:TYR:CG	2.34	0.62
2:L:43:U:O2	1:M:27:LYS:NZ	2.24	0.62
1:G:128:LYS:NZ	4:G:381:HOH:O	2.33	0.61
2:N:36:G:OP1	1:O:117:HIS:HE1	1.84	0.61
1:E:1:MSE:HE1	1:E:47:MSE:CE	2.31	0.60
1:A:132:MSE:HE1	2:B:6:U:C1'	2.31	0.60
1:A:135:ARG:HD2	2:B:27:A:N6	2.17	0.60
1:G:54:ILE:HG22	1:G:58:LYS:HD3	1.83	0.60
1:K:1:MSE:HE2	1:K:7:TYR:CG	2.37	0.60
1:A:1:MSE:CE	1:A:7:TYR:CE2	2.85	0.59
2:P:9:C:C5'	4:P:227:HOH:O	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:64:ARG:HD2	2:P:6:U:C5	2.37	0.59
1:A:117:HIS:HE1	2:F:36:G:OP1	1.86	0.59
1:A:1:MSE:HE2	1:A:7:TYR:CE2	2.37	0.59
1:K:58:LYS:NZ	4:K:332:HOH:O	2.29	0.59
1:C:1:MSE:HE1	1:C:47:MSE:CE	2.33	0.59
2:F:21:U:H3'	4:F:236:HOH:O	2.01	0.59
2:H:17:G:H5"	4:H:236:HOH:O	2.03	0.58
1:K:23:LYS:HE2	2:L:3:G:O6	2.04	0.58
1:M:23:LYS:HE2	2:N:3:G:O6	2.03	0.58
1:E:132:MSE:HE1	2:F:6:U:O4'	2.03	0.58
2:B:36:G:OP1	1:E:117:HIS:HE1	1.87	0.58
1:M:28:GLN:NE2	1:M:101:GLU:OE2	2.37	0.58
2:B:14:A:O2'	1:E:112:ARG:NH2	2.37	0.57
1:A:1:MSE:HE1	1:A:34:TYR:HB2	1.86	0.57
1:A:132:MSE:HE1	2:B:6:U:O4'	2.04	0.57
2:N:21:U:O2'	2:N:22:G:H5'	2.05	0.57
1:A:28:GLN:NE2	1:A:101:GLU:OE2	2.37	0.56
1:I:64:ARG:NH2	2:J:6:U:O2'	2.39	0.56
1:A:152:ARG:HD3	4:A:370:HOH:O	2.05	0.56
1:M:152:ARG:HH11	1:M:152:ARG:CG	2.19	0.56
1:K:152:ARG:CG	1:K:152:ARG:HH11	2.19	0.56
1:K:1:MSE:HE1	1:K:7:TYR:CG	2.41	0.55
1:C:29:ASN:HD22	2:H:44:G:H1'	1.71	0.55
1:I:117:HIS:HE1	2:L:36:G:OP1	1.88	0.55
1:E:152:ARG:HH11	1:E:152:ARG:CG	2.19	0.55
1:K:1:MSE:HE2	1:K:7:TYR:CD2	2.42	0.55
1:C:1:MSE:CE	1:C:7:TYR:CG	2.90	0.55
2:N:9:C:P	4:N:250:HOH:O	2.65	0.54
2:P:9:C:H4'	4:P:259:HOH:O	2.06	0.54
1:A:152:ARG:HH11	1:A:152:ARG:CG	2.20	0.54
1:M:53:ARG:NH1	4:M:349:HOH:O	2.30	0.54
1:I:51:SER:C	2:L:45:A23:H8	2.28	0.54
2:J:36:G:OP1	1:K:117:HIS:HE1	1.91	0.54
1:G:138:LYS:NZ	4:G:345:HOH:O	2.41	0.54
1:O:23:LYS:HE2	2:P:3:G:O6	2.08	0.54
1:A:3:ARG:NH1	4:A:333:HOH:O	2.40	0.53
1:G:135:ARG:NH1	4:G:397:HOH:O	2.41	0.53
2:L:32:A:OP2	4:L:225:HOH:O	2.18	0.53
1:G:132:MSE:HE1	2:H:6:U:C1'	2.38	0.53
1:M:29:ASN:HD22	2:P:44:G:H1'	1.74	0.53
2:D:12:U:OP1	4:D:285:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASN:HD22	2:F:44:G:H1'	1.74	0.52
1:K:64:ARG:NH2	2:L:6:U:O2'	2.43	0.52
1:E:23:LYS:HE2	2:F:3:G:O6	2.09	0.52
1:K:1:MSE:HE3	1:K:100:ILE:HG21	1.91	0.52
1:M:98:LYS:HE2	4:M:338:HOH:O	2.08	0.52
2:J:21:U:C1'	4:J:204:HOH:O	2.58	0.51
1:I:10:LYS:HG2	1:I:101:GLU:OE1	2.09	0.51
1:I:23:LYS:HE2	2:J:3:G:O6	2.11	0.51
1:G:28:GLN:NE2	1:G:101:GLU:OE2	2.43	0.51
1:C:23:LYS:HE2	2:D:3:G:O6	2.10	0.51
1:C:132:MSE:HE1	2:D:6:U:O4'	2.11	0.51
1:E:1:MSE:CE	1:E:7:TYR:CG	2.94	0.51
2:D:36:G:OP1	1:G:117:HIS:HE1	1.94	0.51
1:G:135:ARG:HD2	2:H:27:A:N6	2.26	0.51
1:A:117:HIS:HD2	4:A:364:HOH:O	1.94	0.50
1:I:29:ASN:HD22	2:L:44:G:H1'	1.76	0.50
1:C:64:ARG:HD2	2:D:6:U:C4	2.46	0.50
1:C:155:GLN:NE2	1:C:155:GLN:HA	2.26	0.49
1:M:143:GLN:CD	4:M:321:HOH:O	2.50	0.49
2:J:7:A:H2'	2:J:8:C:O4'	2.12	0.49
1:K:1:MSE:HE2	1:K:7:TYR:CD1	2.48	0.48
2:P:20:A:O2'	2:P:21:U:H2'	2.13	0.48
1:C:98:LYS:CE	4:C:367:HOH:O	2.61	0.48
2:D:7:A:H2'	2:D:8:C:O4'	2.13	0.48
1:I:10:LYS:NZ	4:I:352:HOH:O	2.44	0.48
2:P:43:U:C3'	2:P:44:G:H5"	2.42	0.48
2:P:7:A:H2'	2:P:8:C:O4'	2.14	0.48
2:L:7:A:H2'	2:L:8:C:O4'	2.14	0.48
1:M:112:ARG:NH2	2:P:14:A:O2'	2.46	0.48
1:G:73:ILE:HB	1:G:90:GLN:HB3	1.96	0.47
1:I:51:SER:HA	2:L:45:A23:H8	1.96	0.47
2:H:7:A:H2'	2:H:8:C:O4'	2.13	0.47
1:C:73:ILE:HB	1:C:90:GLN:HB3	1.97	0.47
2:D:13:G:C8	4:G:307:HOH:O	2.56	0.46
1:C:117:HIS:HE1	2:H:36:G:OP1	1.99	0.46
2:P:43:U:H2'	2:P:44:G:H5"	1.97	0.46
1:C:132:MSE:HE1	2:D:6:U:C1'	2.46	0.46
1:K:73:ILE:HB	1:K:90:GLN:HB3	1.97	0.46
2:F:7:A:H2'	2:F:8:C:O4'	2.16	0.46
2:B:24:G:N7	4:B:207:HOH:O	2.36	0.45
2:J:21:U:HO2'	2:J:22:G:P	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:LYS:HA	1:G:143:GLN:OE1	2.16	0.45
1:O:64:ARG:CD	2:P:6:U:C4	2.99	0.45
1:E:12:ARG:HG2	1:E:12:ARG:HH11	1.82	0.45
1:I:53:ARG:HG2	1:M:53:ARG:HD3	1.97	0.45
1:I:73:ILE:HB	1:I:90:GLN:HB3	1.97	0.45
1:C:135:ARG:HD2	2:D:27:A:N6	2.32	0.44
1:E:73:ILE:HB	1:E:90:GLN:HB3	1.99	0.44
1:I:3:ARG:NH1	4:I:325:HOH:O	2.43	0.44
2:B:7:A:H2'	2:B:8:C:O4'	2.18	0.44
2:B:14:A:O2'	4:B:229:HOH:O	2.14	0.44
2:P:31:A:H1'	4:P:241:HOH:O	2.17	0.44
2:D:44:G:H8	1:G:29:ASN:HD22	1.66	0.44
1:E:4:ASN:HA	1:E:33:TYR:CE1	2.53	0.44
1:A:1:MSE:HE2	1:A:34:TYR:HB2	1.98	0.43
2:J:21:U:H1'	4:J:204:HOH:O	2.18	0.43
2:L:21:U:O2	2:L:21:U:C2'	2.67	0.43
1:E:132:MSE:CE	2:F:6:U:O4'	2.67	0.43
1:I:53:ARG:HG2	1:M:53:ARG:CD	2.48	0.43
1:M:73:ILE:HB	1:M:90:GLN:HB3	2.01	0.43
1:K:132:MSE:HE1	2:L:6:U:C1'	2.49	0.43
2:L:21:U:O2	2:L:21:U:H2'	2.19	0.43
1:I:4:ASN:HA	1:I:33:TYR:CE1	2.53	0.43
1:K:1:MSE:HB2	1:K:34:TYR:CD2	2.53	0.43
1:I:138:LYS:HA	1:I:143:GLN:OE1	2.19	0.43
2:F:21:U:O2	2:F:21:U:C2'	2.67	0.43
1:M:132:MSE:HE1	2:N:6:U:O4'	2.18	0.43
1:I:17:MSE:SE	1:I:152:ARG:HD2	2.69	0.43
1:A:28:GLN:CD	1:A:101:GLU:OE2	2.57	0.42
1:E:138:LYS:HA	1:E:143:GLN:OE1	2.19	0.42
1:E:41:TYR:CE2	1:E:154:GLN:OE1	2.72	0.42
2:F:21:U:O2	2:F:21:U:H2'	2.19	0.42
1:M:138:LYS:HA	1:M:143:GLN:OE1	2.19	0.42
1:M:138:LYS:HD2	4:N:229:HOH:O	2.19	0.42
2:D:21:U:O2	2:D:21:U:C2'	2.67	0.42
1:O:17:MSE:SE	1:O:152:ARG:HD2	2.70	0.42
1:C:98:LYS:NZ	4:C:367:HOH:O	2.47	0.42
2:P:32:A:H2'	2:P:33:A:C8	2.55	0.42
2:H:21:U:O2	2:H:21:U:H2'	2.20	0.42
1:O:138:LYS:HA	1:O:143:GLN:OE1	2.20	0.41
1:K:152:ARG:HH11	1:K:152:ARG:HG2	1.86	0.41
2:N:21:U:O2	2:N:21:U:H2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:HA	1:A:143:GLN:OE1	2.20	0.41
1:K:1:MSE:HE3	1:K:100:ILE:CG2	2.50	0.41
2:B:21:U:O2	2:B:21:U:C2'	2.68	0.41
2:D:14:A:O2'	1:G:112:ARG:NH2	2.53	0.41
2:D:21:U:O2	2:D:21:U:H2'	2.20	0.41
1:M:53:ARG:HD2	4:M:349:HOH:O	1.82	0.41
1:M:64:ARG:NH2	2:N:6:U:O2'	2.54	0.41
1:M:152:ARG:HH11	1:M:152:ARG:HG2	1.84	0.41
2:N:21:U:O2	2:N:21:U:C2'	2.68	0.41
1:O:131:GLY:CA	2:P:26:U:O2'	2.64	0.41
1:E:152:ARG:HH11	1:E:152:ARG:HG2	1.85	0.41
1:A:132:MSE:CE	2:B:6:U:O4'	2.69	0.40
1:G:3:ARG:CD	4:G:350:HOH:O	2.53	0.40
2:P:43:U:C2'	2:P:44:G:H5"	2.51	0.40
2:H:21:U:O2	2:H:21:U:C2'	2.67	0.40
2:P:30:U:C3'	2:P:31:A:H5'	2.52	0.40
1:I:53:ARG:HG2	1:M:53:ARG:NE	2.37	0.40
2:J:43:U:C5	2:J:44:G:C6	3.10	0.40
1:O:134:LYS:HB2	1:O:134:LYS:HE2	1.86	0.40
2:P:20:A:C6	2:P:22:G:H1'	2.57	0.40
1:C:4:ASN:HA	1:C:33:TYR:CE1	2.57	0.40
1:O:73:ILE:HB	1:O:90:GLN:HB3	2.02	0.40
1:A:23:LYS:HA	1:A:23:LYS:HD2	1.92	0.40
2:H:13:G:OP1	4:H:258:HOH:O	2.22	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)
4:A:326:HOH:O	4:C:377:HOH:O[1_455]	2.13	0.07

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	154/155 (99%)	148 (96%)	5 (3%)	1 (1%)	25	26
1	C	154/155 (99%)	150 (97%)	4 (3%)	0	100	100
1	E	154/155 (99%)	149 (97%)	5 (3%)	0	100	100
1	G	154/155 (99%)	149 (97%)	5 (3%)	0	100	100
1	I	154/155 (99%)	151 (98%)	3 (2%)	0	100	100
1	K	154/155 (99%)	149 (97%)	4 (3%)	1 (1%)	25	26
1	M	154/155 (99%)	150 (97%)	4 (3%)	0	100	100
1	O	154/155 (99%)	149 (97%)	5 (3%)	0	100	100
All	All	1232/1240 (99%)	1195 (97%)	35 (3%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	K	154	GLN

5.3.2 Protein sidechains (i)

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	143/137 (104%)	135 (94%)	8 (6%)	21	25
1	C	143/137 (104%)	137 (96%)	6 (4%)	30	38
1	E	143/137 (104%)	132 (92%)	11 (8%)	13	13
1	G	143/137 (104%)	137 (96%)	6 (4%)	30	38
1	I	139/137 (102%)	131 (94%)	8 (6%)	20	23
1	K	143/137 (104%)	132 (92%)	11 (8%)	13	13
1	M	142/137 (104%)	134 (94%)	8 (6%)	21	25
1	O	143/137 (104%)	132 (92%)	11 (8%)	13	13
All	All	1139/1096 (104%)	1070 (94%)	69 (6%)	22	21

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	65	THR
1	A	97	ASP
1	A	112	ARG
1	A	123[A]	GLU
1	A	123[B]	GLU
1	A	152	ARG
1	A	155	GLN
1	C	3	ARG
1	C	65	THR
1	C	97	ASP
1	C	123[A]	GLU
1	C	123[B]	GLU
1	C	134	LYS
1	E	3	ARG
1	E	12	ARG
1	E	25	ASN
1	E	52	SER
1	E	69	ARG
1	E	97	ASP
1	E	101	GLU
1	E	112	ARG
1	E	123[A]	GLU
1	E	123[B]	GLU
1	E	152	ARG
1	G	65	THR
1	G	97	ASP
1	G	112	ARG
1	G	123[A]	GLU
1	G	123[B]	GLU
1	G	152	ARG
1	I	3	ARG
1	I	65	THR
1	I	78	LYS
1	I	97	ASP
1	I	112	ARG
1	I	123[A]	GLU
1	I	123[B]	GLU
1	I	152	ARG
1	K	1	MSE
1	K	3	ARG
1	K	27	LYS

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Mol	Chain	Res	Type
1	K	65	THR
1	K	97	ASP
1	K	112	ARG
1	K	123[A]	GLU
1	K	123[B]	GLU
1	K	135	ARG
1	K	152	ARG
1	K	155	GLN
1	M	3	ARG
1	M	63	LYS
1	M	65	THR
1	M	97	ASP
1	M	112	ARG
1	M	123[A]	GLU
1	M	123[B]	GLU
1	M	152	ARG
1	O	12	ARG
1	O	63	LYS
1	O	65	THR
1	O	82	SER
1	O	97	ASP
1	O	101	GLU
1	O	123[A]	GLU
1	O	123[B]	GLU
1	O	134	LYS
1	O	152	ARG
1	O	155	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	29	ASN
1	A	117	HIS
1	C	29	ASN
1	C	117	HIS
1	C	155	GLN
1	E	117	HIS
1	G	25	ASN
1	G	29	ASN
1	G	117	HIS
1	I	25	ASN

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Mol	Chain	Res	Type
1	I	29	ASN
1	I	117	HIS
1	K	25	ASN
1	K	29	ASN
1	K	117	HIS
1	K	155	GLN
1	M	25	ASN
1	M	29	ASN
1	O	117	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	44/45 (97%)	6 (13%)	2 (4%)
2	D	44/45 (97%)	5 (11%)	1 (2%)
2	F	44/45 (97%)	4 (9%)	1 (2%)
2	H	44/45 (97%)	4 (9%)	1 (2%)
2	J	44/45 (97%)	6 (13%)	1 (2%)
2	L	44/45 (97%)	5 (11%)	1 (2%)
2	N	44/45 (97%)	5 (11%)	0
2	P	44/45 (97%)	10 (22%)	1 (2%)
All	All	352/360 (97%)	45 (12%)	8 (2%)

All (45) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	5	U
2	B	10	A
2	B	21	U
2	B	22	G
2	B	31	A
2	B	43	U
2	D	5	U
2	D	10	A
2	D	21	U
2	D	22	G
2	D	31	A
2	F	5	U
2	F	10	A
2	F	21	U
2	F	31	A

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Mol	Chain	Res	Type
2	H	5	U
2	H	10	A
2	H	21	U
2	H	31	A
2	J	5	U
2	J	7	A
2	J	10	A
2	J	21	U
2	J	22	G
2	J	31	A
2	L	5	U
2	L	10	A
2	L	21	U
2	L	31	A
2	L	43	U
2	N	5	U
2	N	10	A
2	N	13	G
2	N	21	U
2	N	31	A
2	P	5	U
2	P	10	A
2	P	21	U
2	P	30	U
2	P	31	A
2	P	36	G
2	P	38	C
2	P	39	G
2	P	44	G
2	P	45	A23

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	21	U
2	B	42	U
2	D	21	U
2	F	21	U
2	H	21	U
2	J	21	U
2	L	21	U
2	P	38	C

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A23	J	45	2	19,28,29	0.95	1 (5%)	19,43,46	1.57	5 (26%)
2	A23	P	45	2	19,28,29	1.04	1 (5%)	19,43,46	1.75	3 (15%)
2	A23	L	45	2	19,28,29	1.71	4 (21%)	19,43,46	2.82	9 (47%)
2	A23	D	45	2	19,28,29	1.28	3 (15%)	19,43,46	1.50	3 (15%)
2	A23	F	45	2	19,28,29	1.03	0	19,43,46	1.39	4 (21%)
2	A23	N	45	2	19,28,29	1.20	2 (10%)	19,43,46	1.85	5 (26%)
2	A23	H	45	2	19,28,29	0.88	0	19,43,46	1.51	3 (15%)
2	A23	B	45	2	19,28,29	1.57	5 (26%)	19,43,46	1.83	6 (31%)

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
2	A23	J	45	2	-	0/3/35/36	0/4/4/4
2	A23	P	45	2	-	0/3/35/36	0/4/4/4
2	A23	L	45	2	-	0/3/35/36	0/4/4/4
2	A23	D	45	2	-	0/3/35/36	0/4/4/4
2	A23	F	45	2	-	0/3/35/36	0/4/4/4
2	A23	N	45	2	-	0/3/35/36	0/4/4/4
2	A23	H	45	2	-	0/3/35/36	0/4/4/4
2	A23	B	45	2	-	0/3/35/36	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	45	A23	C4-N3	-3.74	1.30	1.35
2	L	45	A23	C5-C4	3.32	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	45	A23	C2-N3	-3.31	1.26	1.32
2	B	45	A23	C5-C4	2.76	1.48	1.40
2	B	45	A23	O2'-C2'	-2.72	1.39	1.45
2	B	45	A23	O4'-C1'	2.62	1.44	1.41
2	D	45	A23	C5-C4	2.45	1.47	1.40
2	L	45	A23	C8-N7	2.27	1.38	1.34
2	N	45	A23	C4-N3	2.17	1.38	1.35
2	D	45	A23	C2-N3	2.16	1.35	1.32
2	P	45	A23	O3'-C3'	-2.15	1.40	1.45
2	B	45	A23	O3'-C3'	-2.13	1.40	1.45
2	N	45	A23	C5-C4	2.11	1.46	1.40
2	J	45	A23	C5-N7	-2.09	1.32	1.39
2	D	45	A23	O4'-C1'	-2.06	1.38	1.41
2	B	45	A23	C2-N3	2.02	1.35	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	45	A23	C2-N1-C6	7.39	131.40	118.75
2	L	45	A23	C5-C6-N6	4.56	127.28	120.35
2	L	45	A23	C5-C6-N1	-4.50	110.14	120.35
2	P	45	A23	O2C-PC-O1C	4.50	124.41	109.89
2	N	45	A23	N3-C2-N1	-3.87	122.63	128.68
2	N	45	A23	O2C-PC-O1C	3.58	121.46	109.89
2	L	45	A23	C4-C5-N7	3.52	113.07	109.40
2	H	45	A23	O2C-PC-O1C	3.51	121.24	109.89
2	J	45	A23	O2C-PC-O1C	3.47	121.09	109.89
2	N	45	A23	C1'-N9-C4	-3.44	120.59	126.64
2	F	45	A23	O2C-PC-O1C	3.38	120.80	109.89
2	J	45	A23	O3'-PC-O1C	-3.38	106.85	115.76
2	B	45	A23	C4-C5-N7	-3.36	105.90	109.40
2	H	45	A23	C4-C5-N7	-3.36	105.90	109.40
2	B	45	A23	O2C-PC-O1C	3.32	120.61	109.89
2	L	45	A23	O2C-PC-O1C	3.29	120.51	109.89
2	P	45	A23	O3'-PC-O1C	-3.27	107.13	115.76
2	D	45	A23	O2C-PC-O1C	3.17	120.13	109.89
2	L	45	A23	C1'-N9-C4	-3.10	121.19	126.64
2	B	45	A23	N3-C2-N1	-3.06	123.89	128.68
2	D	45	A23	C4-C5-N7	-2.99	106.28	109.40
2	P	45	A23	N3-C2-N1	-2.97	124.03	128.68
2	N	45	A23	C2-N1-C6	2.78	123.52	118.75
2	B	45	A23	C5-C6-N6	2.74	124.52	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	45	A23	N6-C6-N1	2.53	123.83	118.57
2	D	45	A23	O3'-PC-O1C	-2.51	109.14	115.76
2	L	45	A23	O4'-C1'-C2'	-2.47	102.31	106.59
2	F	45	A23	O3'-PC-O1C	-2.46	109.26	115.76
2	B	45	A23	O3'-PC-O1C	-2.46	109.28	115.76
2	J	45	A23	N3-C2-N1	-2.41	124.91	128.68
2	L	45	A23	O3'-PC-O1C	-2.40	109.43	115.76
2	F	45	A23	N3-C2-N1	-2.35	125.00	128.68
2	F	45	A23	C4-C5-N7	-2.31	106.99	109.40
2	B	45	A23	C2-N1-C6	2.30	122.69	118.75
2	N	45	A23	O3'-PC-O1C	-2.25	109.82	115.76
2	L	45	A23	N3-C2-N1	-2.22	125.21	128.68
2	H	45	A23	N3-C2-N1	-2.19	125.25	128.68
2	J	45	A23	C5-C6-N6	-2.05	117.24	120.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	45	A23	3	0
2	H	45	A23	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	150/155 (96%)	-0.21	1 (0%)	87	86	21, 33, 62, 74	0
1	C	150/155 (96%)	-0.11	0	100	100	21, 34, 66, 89	0
1	E	150/155 (96%)	0.01	0	100	100	27, 47, 77, 94	0
1	G	150/155 (96%)	-0.01	0	100	100	18, 30, 57, 76	0
1	I	150/155 (96%)	-0.02	1 (0%)	87	86	20, 35, 67, 104	0
1	K	150/155 (96%)	-0.06	1 (0%)	87	86	21, 32, 61, 67	0
1	M	150/155 (96%)	0.03	2 (1%)	77	75	24, 40, 70, 90	0
1	O	150/155 (96%)	0.36	9 (6%)	21	20	25, 48, 97, 134	0
2	B	44/45 (97%)	-0.50	0	100	100	26, 32, 46, 86	0
2	D	44/45 (97%)	-0.29	0	100	100	22, 34, 49, 89	0
2	F	44/45 (97%)	-0.37	0	100	100	26, 40, 63, 98	0
2	H	44/45 (97%)	-0.36	0	100	100	24, 41, 60, 93	0
2	J	44/45 (97%)	-0.31	1 (2%)	60	58	23, 34, 48, 97	0
2	L	44/45 (97%)	-0.21	0	100	100	28, 39, 75, 102	0
2	N	44/45 (97%)	-0.21	0	100	100	24, 39, 65, 96	0
2	P	44/45 (97%)	0.44	3 (6%)	17	16	27, 55, 88, 111	0
All	All	1552/1600 (97%)	-0.05	18 (1%)	79	77	18, 38, 73, 134	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	67	LYS	5.7
1	K	41	TYR	4.2
1	M	41	TYR	3.7
1	O	129	VAL	3.0
1	O	66	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	41	TYR	2.8
1	O	150	TYR	2.8
2	P	20	A	2.8
1	I	69	ARG	2.7
1	O	65	THR	2.7
1	O	133	LEU	2.7
1	O	69	ARG	2.6
2	P	31	A	2.2
1	O	137	ILE	2.2
1	O	64	ARG	2.1
2	P	30	U	2.1
1	M	137	ILE	2.1
2	J	21	U	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å^2)	Q<0.9
2	A23	B	45	25/26	0.94	0.12	40,47,53,58	0
2	A23	L	45	25/26	0.96	0.15	24,29,39,50	0
2	A23	J	45	25/26	0.98	0.15	20,23,26,28	0
2	A23	F	45	25/26	0.98	0.12	20,23,27,27	0
2	A23	N	45	25/26	0.98	0.10	27,32,36,40	0
2	A23	P	45	25/26	0.98	0.12	23,27,31,34	0
2	A23	D	45	25/26	0.99	0.15	18,21,24,28	0
2	A23	H	45	25/26	0.99	0.11	24,25,28,29	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	CA	P	103	1/1	0.53	0.11	87,87,87,87	0
3	CA	G	201	1/1	0.80	0.30	44,44,44,44	0
3	CA	J	104	1/1	0.84	0.39	110,110,110,110	0
3	CA	D	104	1/1	0.86	0.45	100,100,100,100	0
3	CA	L	105	1/1	0.88	0.09	78,78,78,78	0
3	CA	F	101	1/1	0.90	0.10	70,70,70,70	0
3	CA	L	104	1/1	0.90	0.06	68,68,68,68	0
3	CA	P	102	1/1	0.92	0.07	65,65,65,65	0
3	CA	J	102	1/1	0.92	0.08	58,58,58,58	0
3	CA	H	103	1/1	0.93	0.06	63,63,63,63	0
3	CA	P	101	1/1	0.93	0.06	62,62,62,62	0
3	CA	L	101	1/1	0.93	0.06	66,66,66,66	0
3	CA	H	102	1/1	0.93	0.06	61,61,61,61	0
3	CA	N	103	1/1	0.94	0.39	72,72,72,72	0
3	CA	N	104	1/1	0.94	0.05	51,51,51,51	0
3	CA	J	105	1/1	0.94	0.11	70,70,70,70	0
3	CA	F	102	1/1	0.94	0.07	62,62,62,62	0
3	CA	N	102	1/1	0.94	0.06	45,45,45,45	0
3	CA	L	102	1/1	0.95	0.11	64,64,64,64	0
3	CA	B	104	1/1	0.95	0.04	61,61,61,61	0
3	CA	D	102	1/1	0.95	0.05	51,51,51,51	0
3	CA	J	106	1/1	0.96	0.05	58,58,58,58	0
3	CA	H	101	1/1	0.96	0.04	61,61,61,61	0
3	CA	D	106	1/1	0.96	0.06	64,64,64,64	0
3	CA	B	102	1/1	0.96	0.06	55,55,55,55	0
3	CA	H	104	1/1	0.96	0.03	66,66,66,66	0
3	CA	H	106	1/1	0.96	0.07	55,55,55,55	0
3	CA	I	201	1/1	0.96	0.09	44,44,44,44	0
3	CA	J	101	1/1	0.96	0.10	52,52,52,52	0
3	CA	D	103	1/1	0.96	0.06	38,38,38,38	0
3	CA	F	104	1/1	0.96	0.09	49,49,49,49	0
3	CA	D	101	1/1	0.96	0.05	63,63,63,63	0
3	CA	M	201	1/1	0.97	0.08	41,41,41,41	0
3	CA	B	105	1/1	0.97	0.06	69,69,69,69	0
3	CA	N	105	1/1	0.97	0.08	63,63,63,63	0
3	CA	C	201	1/1	0.98	0.07	40,40,40,40	0
3	CA	D	105	1/1	0.98	0.06	47,47,47,47	0
3	CA	B	103	1/1	0.98	0.10	41,41,41,41	0
3	CA	B	101	1/1	0.98	0.06	50,50,50,50	0
3	CA	O	201	1/1	0.98	0.11	34,34,34,34	0
3	CA	A	201	1/1	0.98	0.09	33,33,33,33	0
3	CA	F	103	1/1	0.98	0.07	53,53,53,53	0
3	CA	N	101	1/1	0.98	0.06	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	E	201	1/1	0.99	0.11	29,29,29,29	0
3	CA	H	105	1/1	0.99	0.06	43,43,43,43	0
3	CA	L	103	1/1	0.99	0.06	65,65,65,65	0
3	CA	J	103	1/1	0.99	0.06	36,36,36,36	0
3	CA	K	201	1/1	0.99	0.10	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.