wwPDB EM Validation Summary Report

May 13, 2024 – 09:27 pm BST

PDB ID	:	8P17
EMDB ID	:	EMD-17347
Title	:	E167K RF2 on E. coli 70S release complex with UGG (Structure II)
Authors	:	Pundir, S.; Larsson, D.S.D.; Selmer, M.; Sanyal, S.
Deposited on	:	2023-05-11
Resolution	:	2.78 Å(reported)
Based on initial models	:	8B0X, 1GQE, 7K00, 5MDV

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

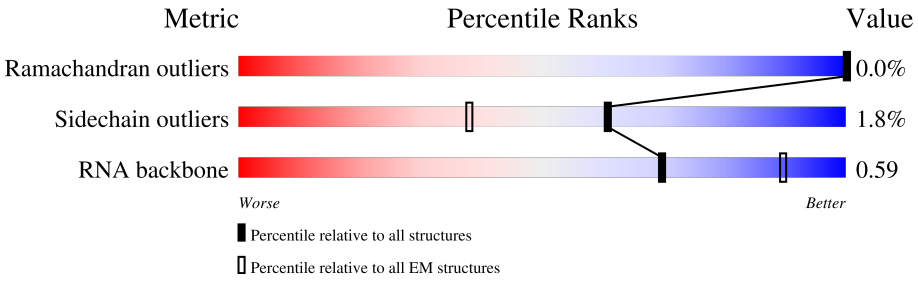
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	2	1542	84% 16%
2	g	241	90% · 7%
3	h	233	88% · 10%
4	i	206	98% ·
5	j	167	93% · 7%
6	k	135	76% · 24%
7	l	179	84% · 14%
8	m	130	98% ··
9	n	130	96% · ·

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Mol	Chain	Length	Quality of chain
10	o	103	92% 5%
11	p	129	89% 9%
12	q	124	98%
13	r	118	97%
14	s	101	99%
15	t	89	97%
16	u	82	99%
17	v	84	90% 6%
18	w	75	88% 12%
19	x	92	91% 9%
20	y	87	98%
21	z	71	99%
22	4	49	37% 16% 47%
23	5	76	62% 38%
24	1	2904	84% 16%
25	3	120	91% 8%
26	B	273	98%
27	C	209	98%
28	D	201	100%
29	E	179	97%
30	F	177	97%
31	J	142	99%
32	K	123	99%
33	L	144	99%
34	M	136	99%

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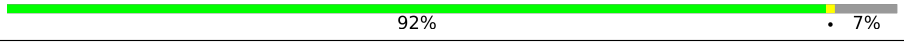
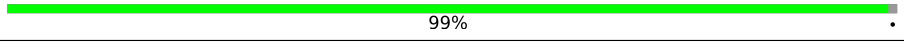
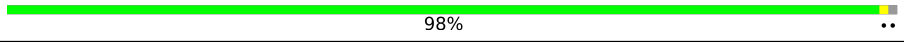
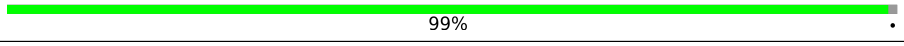
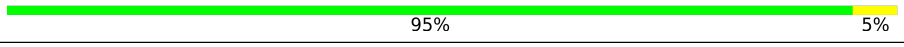
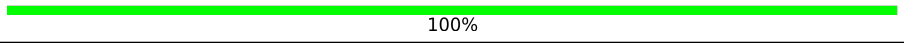
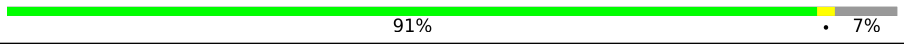
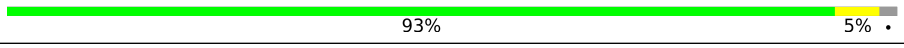
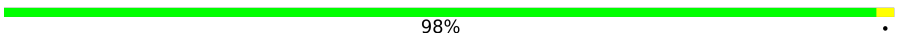
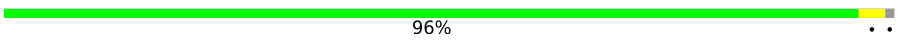
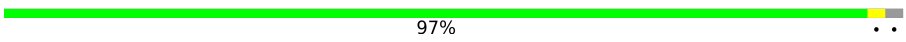
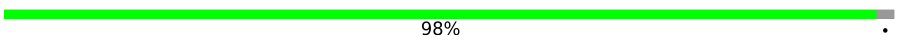
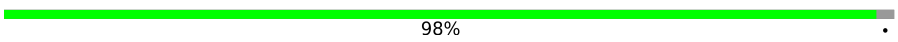
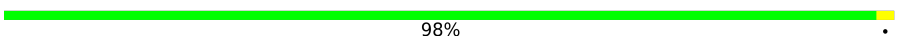
Mol	Chain	Length	Quality of chain
35	N	127	
36	O	117	
37	P	115	
38	Q	118	
39	R	103	
40	S	110	
41	T	100	
42	U	104	
43	V	94	
44	W	85	
45	X	78	
46	Y	63	
47	Z	59	
48	b	57	
49	c	55	
50	d	46	

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 148609 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1536	32966	14711	6044	10675	1536	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	g	224	1753	1109	315	321	8	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	h	210	1648	1043	309	292	4	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	i	205	1643	1026	315	298	4	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	j	156	1152	717	217	212	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	k	103	839	530	151	151	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	o	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	p	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	119	IAS	ASN	variant	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	r	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	s	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	t	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	u	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	v	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	x	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	y	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4	26	Total	C	N	O	P	0	0
			562	251	104	181	26		

- Molecule 23 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5	76	Total	C	N	O	P	2	0
			1665	742	302	543	78		

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	E	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	82	MS6	MET	variant	UNP P0ADY7

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	c	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 50 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	d	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	e	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	a	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 54 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	I	68	Total	C	N	O	S	0	0
			484	298	89	94	3		

- Molecule 55 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	361	Total	C	N	O	S	0	0
			2855	1757	501	587	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	167	LYS	GLU	engineered mutation	UNP P07012

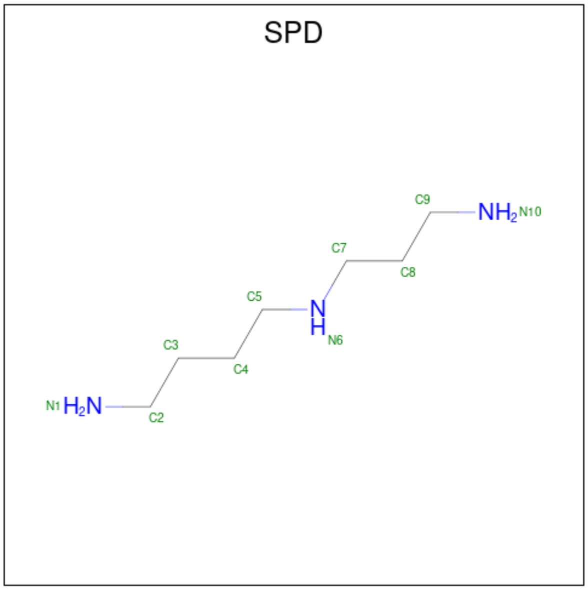
- Molecule 56 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	2	93	Total	Mg	0
			93	93	
57	s	1	Total	Mg	0
			1	1	
57	4	1	Total	Mg	0
			1	1	
57	5	2	Total	Mg	0
			2	2	
57	1	222	Total	Mg	0
			222	222	
57	3	4	Total	Mg	0
			4	4	
57	C	1	Total	Mg	0
			1	1	
57	b	1	Total	Mg	0
			1	1	

- Molecule 58 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

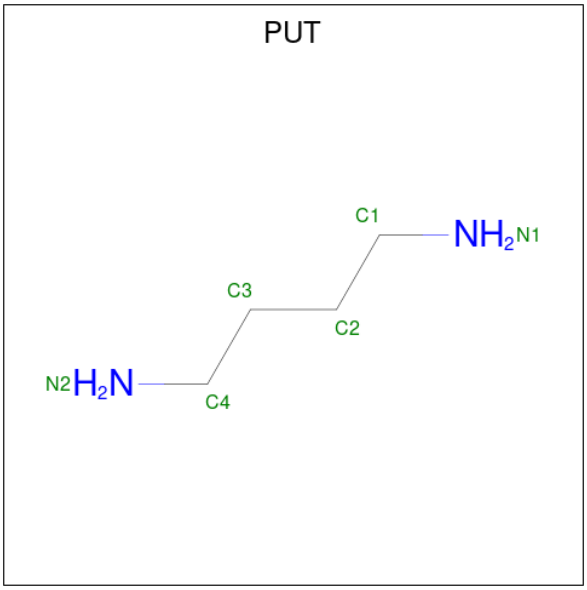


Mol	Chain	Residues	Atoms			AltConf
58	2	1	Total 10	C 7	N 3	0
58	2	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0
58	1	1	Total 10	C 7	N 3	0

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
59	2	38	Total K 38 38	0
59	1	90	Total K 90 90	0

- Molecule 60 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms	AltConf
60	2	1	Total C N 6 4 2	0
60	2	1	Total C N 6 4 2	0
60	1	1	Total C N 6 4 2	0
60	1	1	Total C N 6 4 2	0
60	1	1	Total C N 6 4 2	0
60	1	1	Total C N 6 4 2	0
60	1	1	Total C N 6 4 2	0
60	1	1	Total C N 6 4 2	0
60	1	1	Total C N 6 4 2	0
60	1	1	Total C N 6 4 2	0

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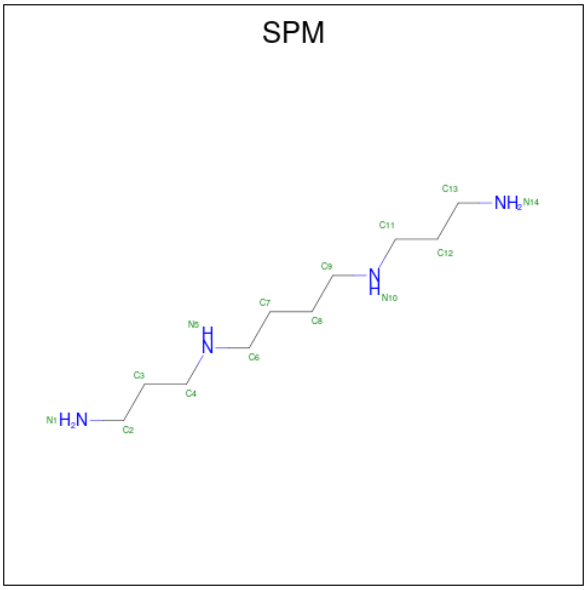
Mol	Chain	Residues	Atoms	AltConf
60	1	1	Total C N 6 4 2	0
60	1	1	Total C N 6 4 2	0
60	1	1	Total C N 6 4 2	0

- Molecule 61 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
61	1	1	Total C N 14 10 4	0

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
62	f	1	Total Zn 1 1	0
62	a	1	Total Zn 1 1	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	AltConf
63	1	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
63	6	1	Total	O	0
			1	1	

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22082	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38.14	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, MG, 6MZ, PUT, D2T, PSU, SPM, OMC, SPD, 1MG, 3TD, K, MEQ, 4OC, 5MC, 2MA, MS6, MA6, 4D4, 5MU, IAS, G7M, UR3, OMU, ZN, H2U, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	2	0.51	0/36631	0.81	11/57136 (0.0%)
2	g	0.28	0/1784	0.48	0/2403
3	h	0.30	0/1675	0.52	0/2256
4	i	0.30	0/1665	0.52	0/2227
5	j	0.31	0/1165	0.52	0/1568
6	k	0.30	0/858	0.51	0/1160
7	l	0.27	0/1230	0.52	0/1649
8	m	0.31	0/989	0.51	0/1326
9	n	0.29	0/1034	0.56	0/1375
10	o	0.29	0/796	0.56	0/1077
11	p	0.30	0/884	0.55	0/1191
12	q	0.33	0/960	0.59	0/1286
13	r	0.27	0/900	0.56	0/1204
14	s	0.29	0/817	0.53	0/1088
15	t	0.28	0/722	0.53	0/964
16	u	0.30	0/653	0.56	0/877
17	v	0.29	0/650	0.52	0/871
18	w	0.32	0/553	0.53	0/742
19	x	0.29	0/685	0.50	0/922
20	y	0.28	0/676	0.47	0/895
21	z	0.32	0/597	0.56	0/792
22	4	0.41	0/630	0.88	0/981
23	5	0.49	0/1859	0.83	0/2894
24	1	0.56	0/69147	0.80	9/107869 (0.0%)
25	3	0.45	0/2850	0.79	0/4444
26	B	0.35	0/2121	0.57	0/2852
27	C	0.33	0/1576	0.52	0/2119
28	D	0.31	0/1571	0.51	0/2113
29	E	0.29	0/1434	0.51	0/1926
30	F	0.30	0/1333	0.52	0/1805
31	J	0.33	0/1152	0.50	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	K	0.33	0/955	0.57	0/1279
33	L	0.31	0/1062	0.56	0/1413
34	M	0.33	0/1073	0.55	0/1433
35	N	0.32	0/958	0.57	0/1281
36	O	0.30	0/902	0.54	0/1209
37	P	0.33	0/929	0.55	0/1242
38	Q	0.36	0/960	0.52	0/1278
39	R	0.34	0/829	0.58	0/1107
40	S	0.31	0/864	0.53	0/1156
41	T	0.29	0/744	0.51	0/994
42	U	0.30	0/787	0.51	0/1051
43	V	0.31	0/766	0.50	0/1025
44	W	0.33	0/589	0.54	0/779
45	X	0.33	0/635	0.57	0/848
46	Y	0.27	0/502	0.49	0/667
47	Z	0.29	0/453	0.56	0/605
48	b	0.32	0/450	0.57	0/599
49	c	0.33	0/424	0.51	0/565
50	d	0.31	0/380	0.64	0/498
51	e	0.31	0/513	0.54	0/676
52	f	0.33	0/303	0.57	0/397
53	a	0.29	0/488	0.50	0/649
54	I	0.25	0/486	0.50	0/650
55	6	0.29	0/2884	0.48	0/3885
56	G	0.32	0/1122	0.61	0/1515
All	All	0.48	0/159655	0.74	20/238364 (0.0%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	2096	C	N1-C2-O2	-9.63	113.12	118.90
24	1	2096	C	C2-N3-C4	-8.09	115.86	119.90
1	2	507	C	N1-C2-O2	-6.80	114.82	118.90
1	2	1535	C	N1-C2-O2	-6.66	114.90	118.90
1	2	597	G	N3-C2-N2	-6.46	115.38	119.90

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 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 PDB entries followed by that with respect to all EM entries.

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	
2	g	222/241 (92%)	216 (97%)	6 (3%)	0	100	100
3	h	208/233 (89%)	204 (98%)	4 (2%)	0	100	100
4	i	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	j	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
6	k	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
7	l	152/179 (85%)	145 (95%)	7 (5%)	0	100	100
8	m	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	n	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	o	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	15	41
11	p	113/129 (88%)	110 (97%)	3 (3%)	0	100	100
12	q	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
13	r	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
14	s	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
15	t	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	u	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
17	v	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
18	w	64/75 (85%)	64 (100%)	0	0	100	100
19	x	82/92 (89%)	82 (100%)	0	0	100	100
20	y	84/87 (97%)	84 (100%)	0	0	100	100
21	z	68/71 (96%)	68 (100%)	0	0	100	100
26	B	269/273 (98%)	266 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	C	206/209 (99%)	202 (98%)	3 (2%)	1 (0%)	29	58
28	D	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
29	E	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
30	F	173/177 (98%)	165 (95%)	8 (5%)	0	100	100
31	J	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
32	K	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
33	L	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
34	M	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
35	N	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
36	O	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
37	P	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
38	Q	115/118 (98%)	115 (100%)	0	0	100	100
39	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
40	S	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
41	T	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
42	U	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
43	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
44	W	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
45	X	75/78 (96%)	75 (100%)	0	0	100	100
46	Y	60/63 (95%)	60 (100%)	0	0	100	100
47	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
48	b	54/57 (95%)	54 (100%)	0	0	100	100
49	c	49/55 (89%)	49 (100%)	0	0	100	100
50	d	44/46 (96%)	44 (100%)	0	0	100	100
51	e	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
52	f	36/38 (95%)	36 (100%)	0	0	100	100
53	a	56/70 (80%)	54 (96%)	2 (4%)	0	100	100
54	I	66/142 (46%)	64 (97%)	2 (3%)	0	100	100
55	6	358/365 (98%)	355 (99%)	3 (1%)	0	100	100
56	G	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	22	50
All	All	6015/6420 (94%)	5871 (98%)	141 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	o	57	VAL
27	C	149	ASN
56	G	76	GLU

4.3.2 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 PDB entries followed by that with respect to all EM entries.

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
2	g	186/199 (94%)	178 (96%)	8 (4%)	29 59
3	h	172/190 (90%)	166 (96%)	6 (4%)	36 67
4	i	172/173 (99%)	168 (98%)	4 (2%)	50 79
5	j	119/126 (94%)	118 (99%)	1 (1%)	81 93
6	k	90/116 (78%)	89 (99%)	1 (1%)	73 90
7	l	127/147 (86%)	124 (98%)	3 (2%)	49 78
8	m	104/105 (99%)	103 (99%)	1 (1%)	76 91
9	n	105/107 (98%)	103 (98%)	2 (2%)	57 83
10	o	86/90 (96%)	84 (98%)	2 (2%)	50 79
11	p	89/98 (91%)	88 (99%)	1 (1%)	73 90
12	q	102/103 (99%)	102 (100%)	0	100 100
13	r	93/96 (97%)	92 (99%)	1 (1%)	73 90
14	s	83/84 (99%)	83 (100%)	0	100 100
15	t	76/77 (99%)	74 (97%)	2 (3%)	46 76
16	u	65/65 (100%)	65 (100%)	0	100 100
17	v	73/78 (94%)	70 (96%)	3 (4%)	30 61
18	w	57/65 (88%)	57 (100%)	0	100 100
19	x	72/79 (91%)	72 (100%)	0	100 100
20	y	65/66 (98%)	64 (98%)	1 (2%)	65 87
21	z	60/61 (98%)	60 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	B	216/218 (99%)	213 (99%)	3 (1%)	67 87
27	C	163/163 (100%)	159 (98%)	4 (2%)	47 77
28	D	165/165 (100%)	164 (99%)	1 (1%)	86 95
29	E	148/150 (99%)	145 (98%)	3 (2%)	55 82
30	F	136/138 (99%)	132 (97%)	4 (3%)	42 73
31	J	116/116 (100%)	115 (99%)	1 (1%)	78 92
32	K	104/104 (100%)	103 (99%)	1 (1%)	76 91
33	L	103/103 (100%)	102 (99%)	1 (1%)	76 91
34	M	107/107 (100%)	107 (100%)	0	100 100
35	N	98/103 (95%)	97 (99%)	1 (1%)	76 91
36	O	86/87 (99%)	86 (100%)	0	100 100
37	P	99/100 (99%)	98 (99%)	1 (1%)	76 91
38	Q	89/90 (99%)	89 (100%)	0	100 100
39	R	84/84 (100%)	79 (94%)	5 (6%)	19 45
40	S	93/93 (100%)	93 (100%)	0	100 100
41	T	80/84 (95%)	78 (98%)	2 (2%)	47 77
42	U	83/85 (98%)	78 (94%)	5 (6%)	19 45
43	V	78/78 (100%)	76 (97%)	2 (3%)	46 76
44	W	58/63 (92%)	58 (100%)	0	100 100
45	X	67/68 (98%)	65 (97%)	2 (3%)	41 72
46	Y	54/55 (98%)	53 (98%)	1 (2%)	57 83
47	Z	48/49 (98%)	48 (100%)	0	100 100
48	b	47/48 (98%)	47 (100%)	0	100 100
49	c	46/49 (94%)	44 (96%)	2 (4%)	29 59
50	d	38/38 (100%)	37 (97%)	1 (3%)	46 76
51	e	51/52 (98%)	50 (98%)	1 (2%)	55 82
52	f	34/34 (100%)	34 (100%)	0	100 100
53	a	55/62 (89%)	55 (100%)	0	100 100
54	I	50/110 (46%)	49 (98%)	1 (2%)	55 82
55	6	305/310 (98%)	297 (97%)	8 (3%)	46 76
56	G	114/114 (100%)	108 (95%)	6 (5%)	22 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5011/5245 (96%)	4919 (98%)	92 (2%)	61 84

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	R	26	ASP
45	X	54	LYS
39	R	48	LYS
42	U	49	VAL
50	d	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
46	Y	39	GLN
55	6	322	GLN
51	e	31	HIS
55	6	280	GLN
56	G	20	ASN

4.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1531/1542 (99%)	235 (15%)	5 (0%)
22	4	25/49 (51%)	7 (28%)	1 (4%)
23	5	73/76 (96%)	29 (39%)	0
24	1	2893/2904 (99%)	437 (15%)	6 (0%)
25	3	118/120 (98%)	10 (8%)	0
All	All	4640/4691 (98%)	718 (15%)	12 (0%)

5 of 718 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	7	A
1	2	9	G
1	2	22	G
1	2	23	C

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	1	504	A
24	1	784	G
24	1	2162	G
24	1	827	U
1	2	1026	G

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

40 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	$\#\|Z\| > 2$
1	PSU	2	516	1,57	18,21,22	0.58	0	22,30,33	0.60	1 (4%)
24	5MU	1	1939	59,24	19,22,23	0.56	0	28,32,35	0.90	3 (10%)
24	PSU	1	2457	24	18,21,22	0.60	0	22,30,33	0.57	0
24	3TD	1	1915	24	19,22,23	0.53	0	21,32,35	0.74	0
24	PSU	1	746	24,57	18,21,22	0.62	0	22,30,33	0.38	0
24	PSU	1	2604	24	18,21,22	0.54	0	22,30,33	0.62	0
24	5MC	1	1962	59,24	18,22,23	0.32	0	26,32,35	0.43	0
24	PSU	1	2504	59,24	18,21,22	0.57	0	22,30,33	0.62	0
1	MA6	2	1518	1	18,26,27	0.77	0	19,38,41	0.76	0
24	PSU	1	1911	24	18,21,22	0.53	0	22,30,33	0.56	0
24	2MG	1	2445	24	18,26,27	1.11	3 (16%)	16,38,41	0.63	0
1	UR3	2	1498	1	19,22,23	0.33	0	26,32,35	0.35	0
24	H2U	1	2449	24	18,21,22	0.32	0	21,30,33	0.46	0
24	5MU	1	747	24	19,22,23	0.35	0	28,32,35	0.32	0
11	IAS	p	119	11	6,7,8	0.95	0	6,8,10	1.24	1 (16%)
24	6MZ	1	2030	24	18,25,26	0.79	0	16,36,39	0.78	1 (6%)
24	6MZ	1	1618	24	18,25,26	0.75	0	16,36,39	0.81	1 (6%)
24	2MG	1	1835	24	18,26,27	1.04	3 (16%)	16,38,41	0.64	0
1	G7M	2	527	59,1	20,26,27	0.61	0	17,39,42	0.52	0
24	PSU	1	2580	24	18,21,22	0.63	1 (5%)	22,30,33	0.67	1 (4%)
24	1MG	1	745	24	18,26,27	0.98	2 (11%)	19,39,42	0.44	0
24	OMG	1	2251	59,24,23	18,26,27	1.03	3 (16%)	19,38,41	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	4OC	2	1402	1,57	20,23,24	0.37	0	26,32,35	0.63	0
1	2MG	2	1516	1	18,26,27	0.99	3 (16%)	16,38,41	0.69	0
24	PSU	1	2605	24	18,21,22	0.55	0	22,30,33	0.61	0
34	4D4	M	81	34	9,11,12	0.65	0	8,13,15	1.93	3 (37%)
1	MA6	2	1519	1	18,26,27	0.78	0	19,38,41	0.80	0
27	MEQ	C	150	27	8,9,10	0.84	0	5,10,12	0.51	0
24	G7M	1	2069	59,24	20,26,27	0.62	0	17,39,42	0.49	0
24	OMU	1	2552	24,57	19,22,23	0.33	0	26,31,34	0.42	0
1	2MG	2	966	1	18,26,27	1.04	3 (16%)	16,38,41	0.66	0
55	MEQ	6	252	55	8,9,10	0.93	0	5,10,12	0.58	0
24	OMC	1	2498	24,57	19,22,23	0.36	0	26,31,34	0.43	0
1	5MC	2	1407	1	18,22,23	0.35	0	26,32,35	0.45	0
24	2MA	1	2503	59,24,57	17,25,26	0.88	2 (11%)	17,37,40	0.59	0
24	PSU	1	955	24	18,21,22	0.57	0	22,30,33	0.57	0
24	PSU	1	1917	24	18,21,22	0.56	0	22,30,33	0.56	0
12	D2T	q	89	12	7,9,10	0.89	0	6,11,13	1.74	2 (33%)
1	5MC	2	967	1	18,22,23	0.32	0	26,32,35	0.41	0
1	2MG	2	1207	59,1	18,26,27	0.96	2 (11%)	16,38,41	0.68	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
1	PSU	2	516	1,57	-	0/7/25/26	0/2/2/2
24	5MU	1	1939	59,24	-	2/7/25/26	0/2/2/2
24	PSU	1	2457	24	-	0/7/25/26	0/2/2/2
24	3TD	1	1915	24	-	3/7/25/26	0/2/2/2
24	PSU	1	746	24,57	-	2/7/25/26	0/2/2/2
24	PSU	1	2604	24	-	0/7/25/26	0/2/2/2
24	5MC	1	1962	59,24	-	0/7/25/26	0/2/2/2
24	PSU	1	2504	59,24	-	0/7/25/26	0/2/2/2
1	MA6	2	1518	1	-	0/7/29/30	0/3/3/3
24	PSU	1	1911	24	-	0/7/25/26	0/2/2/2
24	2MG	1	2445	24	-	2/5/27/28	0/3/3/3
1	UR3	2	1498	1	-	0/7/25/26	0/2/2/2
24	H2U	1	2449	24	-	0/7/38/39	0/2/2/2
24	5MU	1	747	24	-	0/7/25/26	0/2/2/2
11	IAS	p	119	11	-	1/7/7/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	6MZ	1	2030	24	-	2/5/27/28	0/3/3/3
24	6MZ	1	1618	24	-	0/5/27/28	0/3/3/3
24	2MG	1	1835	24	-	0/5/27/28	0/3/3/3
1	G7M	2	527	59,1	-	3/3/25/26	0/3/3/3
24	PSU	1	2580	24	-	0/7/25/26	0/2/2/2
24	1MG	1	745	24	-	0/3/25/26	0/3/3/3
24	OMG	1	2251	59,24,23	-	1/5/27/28	0/3/3/3
1	4OC	2	1402	1,57	-	0/9/29/30	0/2/2/2
1	2MG	2	1516	1	-	0/5/27/28	0/3/3/3
24	PSU	1	2605	24	-	0/7/25/26	0/2/2/2
34	4D4	M	81	34	-	3/11/12/14	-
1	MA6	2	1519	1	-	1/7/29/30	0/3/3/3
27	MEQ	C	150	27	-	3/8/9/11	-
24	G7M	1	2069	59,24	-	1/3/25/26	0/3/3/3
24	OMU	1	2552	24,57	-	0/9/27/28	0/2/2/2
1	2MG	2	966	1	-	2/5/27/28	0/3/3/3
55	MEQ	6	252	55	-	2/8/9/11	-
24	OMC	1	2498	24,57	-	0/9/27/28	0/2/2/2
1	5MC	2	1407	1	-	0/7/25/26	0/2/2/2
24	2MA	1	2503	59,24,57	-	2/3/25/26	0/3/3/3
24	PSU	1	955	24	-	0/7/25/26	0/2/2/2
24	PSU	1	1917	24	-	0/7/25/26	0/2/2/2
12	D2T	q	89	12	-	3/7/12/14	-
1	5MC	2	967	1	-	0/7/25/26	0/2/2/2
1	2MG	2	1207	59,1	-	0/5/27/28	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	966	2MG	C5-C6	-2.89	1.41	1.47
24	1	2445	2MG	C5-C6	-2.87	1.41	1.47
24	1	1835	2MG	C5-C6	-2.76	1.41	1.47
24	1	745	1MG	C5-C4	-2.68	1.36	1.43
24	1	2251	OMG	C5-C6	-2.64	1.42	1.47

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	M	81	4D4	NE-CZ-NH2	3.72	127.24	120.70
34	M	81	4D4	O-C-CA	-3.03	116.85	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	q	89	D2T	O-C-CA	-2.82	117.39	124.78
24	1	1939	5MU	O4'-C1'-N1	2.50	114.08	108.36
34	M	81	4D4	NH1-CZ-NE	-2.49	113.45	119.19

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	C	150	MEQ	O-C-CA-CB
24	1	746	PSU	C2'-C1'-C5-C4
24	1	1915	3TD	O4'-C4'-C5'-O5'
24	1	1939	5MU	O4'-C4'-C5'-O5'
24	1	2030	6MZ	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 482 ligands modelled in this entry, 455 are monoatomic - leaving 27 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	$\#\|Z\| > 2$
60	PUT	1	3330	-	5,5,5	0.09	0	4,4,4	0.19	0
60	PUT	2	1734	-	5,5,5	0.14	0	4,4,4	0.15	0
60	PUT	1	3331	-	5,5,5	0.11	0	4,4,4	0.14	0
58	SPD	1	3209	-	9,9,9	0.08	0	8,8,8	0.33	0
58	SPD	2	1690	-	9,9,9	0.10	0	8,8,8	0.22	0
60	PUT	2	1733	-	5,5,5	0.10	0	4,4,4	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
58	SPD	1	3208	-	9,9,9	0.08	0	8,8,8	0.17	0
58	SPD	1	3333	-	9,9,9	0.11	0	8,8,8	0.15	0
58	SPD	1	3207	-	9,9,9	0.07	0	8,8,8	0.16	0
60	PUT	1	3323	-	5,5,5	0.06	0	4,4,4	0.18	0
60	PUT	1	3324	-	5,5,5	0.11	0	4,4,4	0.15	0
60	PUT	1	3326	-	5,5,5	0.09	0	4,4,4	0.18	0
60	PUT	1	3335	-	5,5,5	0.09	0	4,4,4	0.18	0
58	SPD	1	3204	-	9,9,9	0.09	0	8,8,8	0.24	0
58	SPD	1	3205	-	9,9,9	0.12	0	8,8,8	0.11	0
58	SPD	2	1689	-	9,9,9	0.09	0	8,8,8	0.19	0
60	PUT	1	3327	-	5,5,5	0.11	0	4,4,4	0.16	0
60	PUT	1	3329	-	5,5,5	0.09	0	4,4,4	0.21	0
60	PUT	1	3332	-	5,5,5	0.12	0	4,4,4	0.15	0
58	SPD	1	3210	-	9,9,9	0.07	0	8,8,8	0.15	0
58	SPD	1	3203	-	9,9,9	0.07	0	8,8,8	0.16	0
60	PUT	1	3325	-	5,5,5	0.08	0	4,4,4	0.18	0
60	PUT	1	3328	-	5,5,5	0.12	0	4,4,4	0.17	0
58	SPD	1	3211	-	9,9,9	0.06	0	8,8,8	0.18	0
58	SPD	1	3212	-	9,9,9	0.12	0	8,8,8	0.15	0
61	SPM	1	3213	-	13,13,13	0.35	0	12,12,12	0.96	0
58	SPD	1	3206	-	9,9,9	0.12	0	8,8,8	0.14	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
60	PUT	1	3330	-	-	1/3/3/3	-
60	PUT	2	1734	-	-	2/3/3/3	-
60	PUT	1	3331	-	-	1/3/3/3	-
58	SPD	1	3209	-	-	3/7/7/7	-
58	SPD	2	1690	-	-	3/7/7/7	-
60	PUT	2	1733	-	-	0/3/3/3	-
58	SPD	1	3208	-	-	2/7/7/7	-
58	SPD	1	3333	-	-	2/7/7/7	-
58	SPD	1	3207	-	-	5/7/7/7	-
60	PUT	1	3323	-	-	1/3/3/3	-
60	PUT	1	3324	-	-	2/3/3/3	-
60	PUT	1	3326	-	-	1/3/3/3	-
60	PUT	1	3335	-	-	3/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SPD	1	3204	-	-	2/7/7/7	-
58	SPD	1	3205	-	-	2/7/7/7	-
58	SPD	2	1689	-	-	2/7/7/7	-
60	PUT	1	3327	-	-	1/3/3/3	-
60	PUT	1	3329	-	-	1/3/3/3	-
60	PUT	1	3332	-	-	2/3/3/3	-
58	SPD	1	3210	-	-	4/7/7/7	-
58	SPD	1	3203	-	-	1/7/7/7	-
60	PUT	1	3325	-	-	2/3/3/3	-
60	PUT	1	3328	-	-	0/3/3/3	-
58	SPD	1	3211	-	-	0/7/7/7	-
58	SPD	1	3212	-	-	4/7/7/7	-
61	SPM	1	3213	-	-	7/11/11/11	-
58	SPD	1	3206	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	1	3327	PUT	C1-C2-C3-C4
58	1	3209	SPD	C3-C4-C5-N6
58	1	3210	SPD	C3-C4-C5-N6
61	1	3213	SPM	C7-C8-C9-N10
58	1	3208	SPD	N6-C7-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-17347. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections

This section was not generated.

5.2 Central slices

This section was not generated.

5.3 Largest variance slices

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

5.5 Orthogonal surface views

This section was not generated.

5.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

6 Map analysis

This section contains the results of statistical analysis of the map.

6.1 Map-value distribution

This section was not generated.

6.2 Volume estimate versus contour level

This section was not generated.

6.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

8 Map-model fit

This section was not generated.