Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 06:58 am BST

PDB ID	:	7NWT
EMDB ID	:	EMD-12635
Title	:	Initiated 70S ribosome in complex with 2A protein from encephalomyocarditis virus (EMCV)
Authors	:	Hill, C.H.; Napthine, S.; Pekarek, L.; Kibe, A.; Firth, A.E.; Graham, S.C.; Caliskan, N.; Brierley, I.
Deposited on	:	2021-03-17
Resolution	:	2.66 Å(reported)
Based on initial model	:	5MDZ

This is a Full wwPDB EM 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/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	:	FAILED
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

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 2.66 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 149932 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 protein called 50S ribosomal protein L2.

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

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	209	1565	979	288	294	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	94	Total 746	C 470	N 140	O 134	S 2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	U	103	Total 788	C 498	N 148	O 142	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 27 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 29 is a RNA chain called fMet-NH-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	5	76	Total	C	N	O	P	S	0	0
			1622	725	292	528	76	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	8	4SU	G	conflict	GB 1317722521

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 33 is a protein called 50S ribosomal protein L34.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

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

- Molecule 39 is a protein called 30S ribosomal protein S5.

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

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

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

- Molecule 49 is a protein called 30S ribosomal protein S15.

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

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	82	Total 649	C 406	N 128	O 114	S 1	0	0

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	80	Total 648	C 411	N 121	O 113	S 3	0	0

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	66	Total 544	C 344	N 102	O 97	S 1	0	0

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	83	Total 663	C 424	N 126	O 111	S 2	0	0

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	86	Total 669	C 414	N 138	O 114	S 3	0	0

- Molecule 55 is a protein called 30S ribosomal protein S21.

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

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	XX	8	Total	C	N	O	P	0	0
			176	78	34	56	8		

- Molecule 57 is a protein called Protein 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AA	127	Total	C	N	O	S	0	0
			1067	690	192	182	3		
57	BB	130	Total	C	N	O	S	2	0
			1111	716	204	188	3		
57	CC	125	Total	C	N	O	S	0	0
			1048	677	190	178	3		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	144	GLY	-	expression tag	UNP P12296
AA	145	SER	-	expression tag	UNP P12296
AA	146	LYS	-	expression tag	UNP P12296
AA	147	HIS	-	expression tag	UNP P12296
AA	148	HIS	-	expression tag	UNP P12296
AA	149	HIS	-	expression tag	UNP P12296
AA	150	HIS	-	expression tag	UNP P12296
AA	151	HIS	-	expression tag	UNP P12296
AA	152	HIS	-	expression tag	UNP P12296
BB	144	GLY	-	expression tag	UNP P12296
BB	145	SER	-	expression tag	UNP P12296
BB	146	LYS	-	expression tag	UNP P12296
BB	147	HIS	-	expression tag	UNP P12296
BB	148	HIS	-	expression tag	UNP P12296
BB	149	HIS	-	expression tag	UNP P12296
BB	150	HIS	-	expression tag	UNP P12296
BB	151	HIS	-	expression tag	UNP P12296
BB	152	HIS	-	expression tag	UNP P12296
CC	144	GLY	-	expression tag	UNP P12296
CC	145	SER	-	expression tag	UNP P12296
CC	146	LYS	-	expression tag	UNP P12296

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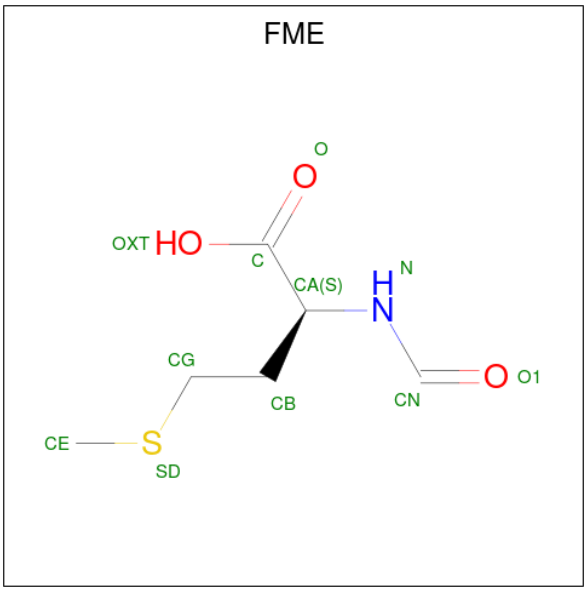
Chain	Residue	Modelled	Actual	Comment	Reference
CC	147	HIS	-	expression tag	UNP P12296
CC	148	HIS	-	expression tag	UNP P12296
CC	149	HIS	-	expression tag	UNP P12296
CC	150	HIS	-	expression tag	UNP P12296
CC	151	HIS	-	expression tag	UNP P12296
CC	152	HIS	-	expression tag	UNP P12296

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
58	B	1	Total Mg 1 1	0
58	C	1	Total Mg 1 1	0
58	M	1	Total Mg 1 1	0
58	N	1	Total Mg 1 1	0
58	Q	1	Total Mg 1 1	0
58	1	290	Total Mg 290 290	0
58	2	128	Total Mg 128 128	0
58	3	8	Total Mg 8 8	0
58	5	3	Total Mg 3 3	0
58	b	1	Total Mg 1 1	0
58	i	1	Total Mg 1 1	0
58	BB	1	Total Mg 1 1	0

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
59	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	B	2	Total	O	0
			2	2	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	120749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The contrast transfer function (CTF) was estimated per-image using CtfFind4. All further phase+amplitude correction was performed internally in Relion. Per-particle CTF refinement was done after polishing	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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	$\#\|Z\| > 2$
27	MA6	2	1519	27	18,26,27	1.37	2 (11%)	19,38,41	3.41	2 (10%)
26	OMC	1	2498	58,26	19,22,23	2.69	8 (42%)	26,31,34	0.97	1 (3%)
29	4OC	5	32	29	20,23,24	2.83	8 (40%)	26,32,35	0.97	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PSU	1	955	26	18,21,22	1.15	1 (5%)	22,30,33	2.02	4 (18%)
26	PSU	1	2504	26	18,21,22	1.02	1 (5%)	22,30,33	1.87	4 (18%)
26	6MZ	1	2030	26	18,25,26	1.70	5 (27%)	16,36,39	2.96	5 (31%)
26	OMG	1	2251	29,26	18,26,27	2.34	8 (44%)	19,38,41	1.44	3 (15%)
27	PSU	2	516	58,27	18,21,22	1.08	1 (5%)	22,30,33	1.81	3 (13%)
29	5MU	5	54	29	19,22,23	4.75	7 (36%)	28,32,35	3.65	9 (32%)
27	7MG	2	527	27	22,26,27	3.26	10 (45%)	29,39,42	1.95	8 (27%)
29	4SU	5	8	29	18,21,22	3.64	8 (44%)	26,30,33	2.22	5 (19%)
27	5MC	2	967	27	18,22,23	3.33	7 (38%)	26,32,35	1.06	2 (7%)
27	MA6	2	1518	27	18,26,27	1.37	2 (11%)	19,38,41	3.27	2 (10%)
27	UR3	2	1498	27	19,22,23	2.43	6 (31%)	26,32,35	1.44	2 (7%)
26	2MG	1	2445	3,26	18,26,27	2.25	6 (33%)	16,38,41	1.48	4 (25%)
26	PSU	1	2605	26	18,21,22	1.15	2 (11%)	22,30,33	1.64	4 (18%)
27	2MG	2	1207	27	18,26,27	2.35	7 (38%)	16,38,41	1.47	4 (25%)
27	2MG	2	966	27	18,26,27	2.26	7 (38%)	16,38,41	1.41	3 (18%)
26	2MG	1	1835	26	18,26,27	2.09	7 (38%)	16,38,41	1.41	4 (25%)
26	PSU	1	1917	26	18,21,22	1.02	2 (11%)	22,30,33	1.66	4 (18%)
26	6MZ	1	1618	26	18,25,26	1.77	5 (27%)	16,36,39	1.89	3 (18%)
26	OMU	1	2552	26	19,22,23	2.65	7 (36%)	26,31,34	2.10	7 (26%)
46	0TD	q	89	46	7,9,10	1.47	0	6,11,13	2.30	2 (33%)
26	1MG	1	745	26	18,26,27	2.46	5 (27%)	19,39,42	1.65	4 (21%)
26	PSU	1	746	26	18,21,22	1.09	1 (5%)	22,30,33	1.70	4 (18%)
26	G7M	1	2069	26	20,26,27	1.72	5 (25%)	17,39,42	1.31	3 (17%)
26	PSU	1	2580	58,26	18,21,22	1.31	3 (16%)	22,30,33	1.89	4 (18%)
29	PSU	5	55	29	18,21,22	1.04	1 (5%)	22,30,33	1.78	5 (22%)
26	PSU	1	2457	26	18,21,22	1.15	1 (5%)	22,30,33	2.13	5 (22%)
26	2MA	1	2503	58,26	17,25,26	2.37	5 (29%)	17,37,40	1.35	3 (17%)
29	H2U	5	20	58,29	18,21,22	3.54	3 (16%)	21,30,33	2.02	5 (23%)
27	2MG	2	1516	27	18,26,27	2.21	7 (38%)	16,38,41	1.60	4 (25%)
26	3TD	1	1915	26	18,22,23	4.49	7 (38%)	22,32,35	1.71	3 (13%)
29	8AN	5	76	58,29,59	19,24,25	5.61	8 (42%)	13,35,38	3.10	3 (23%)
26	5MU	1	1939	58,26	19,22,23	4.68	7 (36%)	28,32,35	3.87	12 (42%)
27	5MC	2	1407	27	18,22,23	3.19	7 (38%)	26,32,35	1.12	1 (3%)
26	5MC	1	1962	26	18,22,23	3.23	7 (38%)	26,32,35	1.05	2 (7%)
26	5MU	1	747	26	19,22,23	4.78	7 (36%)	28,32,35	3.41	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	4OC	2	1402	27	20,23,24	2.84	8 (40%)	26,32,35	0.95	1 (3%)
26	PSU	1	1911	26	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	MA6	2	1519	27	-	0/7/29/30	0/3/3/3
26	OMC	1	2498	58,26	-	1/9/27/28	0/2/2/2
29	4OC	5	32	29	-	0/9/29/30	0/2/2/2
26	PSU	1	955	26	-	0/7/25/26	0/2/2/2
26	PSU	1	2504	26	-	0/7/25/26	0/2/2/2
26	6MZ	1	2030	26	-	2/5/27/28	0/3/3/3
26	OMG	1	2251	29,26	-	1/5/27/28	0/3/3/3
27	PSU	2	516	58,27	-	2/7/25/26	0/2/2/2
29	5MU	5	54	29	-	2/7/25/26	0/2/2/2
27	7MG	2	527	27	-	2/7/37/38	0/3/3/3
29	4SU	5	8	29	-	4/7/25/26	0/2/2/2
27	5MC	2	967	27	-	0/7/25/26	0/2/2/2
27	MA6	2	1518	27	-	0/7/29/30	0/3/3/3
27	UR3	2	1498	27	-	0/7/25/26	0/2/2/2
26	2MG	1	2445	3,26	-	2/5/27/28	0/3/3/3
26	PSU	1	2605	26	-	0/7/25/26	0/2/2/2
27	2MG	2	1207	27	-	0/5/27/28	0/3/3/3
27	2MG	2	966	27	-	2/5/27/28	0/3/3/3
26	2MG	1	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	1	1917	26	-	0/7/25/26	0/2/2/2
26	6MZ	1	1618	26	-	2/5/27/28	0/3/3/3
26	OMU	1	2552	26	-	1/9/27/28	0/2/2/2
46	0TD	q	89	46	-	1/7/12/14	-
26	1MG	1	745	26	-	0/3/25/26	0/3/3/3
26	PSU	1	746	26	-	2/7/25/26	0/2/2/2
26	G7M	1	2069	26	-	1/3/25/26	0/3/3/3
26	PSU	1	2580	58,26	-	0/7/25/26	0/2/2/2
29	PSU	5	55	29	-	0/7/25/26	0/2/2/2
26	PSU	1	2457	26	-	0/7/25/26	0/2/2/2
26	2MA	1	2503	58,26	-	2/3/25/26	0/3/3/3
29	H2U	5	20	58,29	-	5/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	2MG	2	1516	27	-	0/5/27/28	0/3/3/3
26	3TD	1	1915	26	-	5/7/25/26	0/2/2/2
29	8AN	5	76	58,29,59	-	3/3/25/26	0/3/3/3
26	5MU	1	1939	58,26	-	0/7/25/26	0/2/2/2
27	5MC	2	1407	27	-	0/7/25/26	0/2/2/2
26	5MC	1	1962	26	-	0/7/25/26	0/2/2/2
26	5MU	1	747	26	-	0/7/25/26	0/2/2/2
27	4OC	2	1402	27	-	2/9/29/30	0/2/2/2
26	PSU	1	1911	26	-	0/7/25/26	0/2/2/2

All (200) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	76	8AN	C2'-C1'	-15.41	1.30	1.53
29	5	76	8AN	O4'-C1'	15.38	1.62	1.41
26	1	1915	3TD	C6-C5	14.20	1.51	1.35
29	5	20	H2U	C2-N1	12.18	1.53	1.35
29	5	54	5MU	C2-N1	10.92	1.56	1.38
26	1	747	5MU	C2-N1	10.79	1.55	1.38
26	1	747	5MU	C6-N1	10.50	1.56	1.38
29	5	54	5MU	C6-N1	10.25	1.55	1.38
26	1	1939	5MU	C2-N1	10.15	1.54	1.38
29	5	54	5MU	C4-C5	9.75	1.61	1.44
26	1	1939	5MU	C4-C5	9.49	1.60	1.44
26	1	1939	5MU	C4-N3	-9.13	1.21	1.38
26	1	1939	5MU	C6-N1	9.05	1.53	1.38
26	1	747	5MU	C4-C5	9.01	1.59	1.44
26	1	1962	5MC	C6-C5	8.70	1.48	1.34
26	1	1915	3TD	C2-N1	8.60	1.48	1.37
27	2	967	5MC	C6-C5	8.51	1.48	1.34
27	2	1407	5MC	C6-C5	8.42	1.48	1.34
26	1	747	5MU	C4-N3	-8.22	1.23	1.38
29	5	76	8AN	O4'-C4'	-7.98	1.27	1.45
29	5	8	4SU	C4-N3	7.95	1.46	1.37
29	5	54	5MU	C4-N3	-7.94	1.24	1.38
27	2	527	7MG	C8-N9	7.83	1.50	1.46
27	2	527	7MG	C5-N7	7.44	1.44	1.35
26	1	2503	2MA	C2-N3	7.01	1.46	1.31
29	5	8	4SU	C2-N3	6.74	1.50	1.38
29	5	20	H2U	C2-N3	6.50	1.49	1.38
29	5	8	4SU	C2-N1	6.09	1.48	1.38
27	2	1402	4OC	C4-N3	6.08	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	5	32	4OC	C4-N3	6.05	1.43	1.32
26	1	2552	OMU	C2-N3	6.05	1.48	1.38
26	1	2552	OMU	C2-N1	5.93	1.48	1.38
27	2	1402	4OC	C6-C5	5.91	1.48	1.35
26	1	747	5MU	C6-C5	5.89	1.44	1.34
27	2	1498	UR3	C2-N1	5.84	1.46	1.38
26	1	1915	3TD	C2-N3	5.81	1.51	1.38
27	2	967	5MC	C4-N3	5.80	1.43	1.34
29	5	32	4OC	C6-C5	5.77	1.48	1.35
27	2	967	5MC	C2-N3	5.64	1.47	1.36
29	5	8	4SU	C6-C5	5.57	1.48	1.35
29	5	54	5MU	C6-C5	5.54	1.43	1.34
26	1	745	1MG	C2-N2	5.51	1.44	1.34
26	1	2498	OMC	C6-C5	5.42	1.47	1.35
26	1	1962	5MC	C4-N3	5.40	1.43	1.34
26	1	745	1MG	C2-N3	5.40	1.44	1.34
27	2	1407	5MC	C4-N3	5.36	1.43	1.34
26	1	1939	5MU	C6-C5	5.35	1.43	1.34
29	5	20	H2U	C4-N3	5.34	1.46	1.37
29	5	32	4OC	C2-N3	5.27	1.47	1.36
26	1	2552	OMU	C6-C5	5.25	1.47	1.35
27	2	1498	UR3	C6-C5	5.24	1.47	1.35
27	2	966	2MG	C2-N2	5.21	1.45	1.33
26	1	1962	5MC	C2-N3	5.17	1.46	1.36
27	2	1407	5MC	C2-N3	5.15	1.46	1.36
27	2	1402	4OC	C2-N3	5.08	1.46	1.36
26	1	1915	3TD	C6-N1	5.06	1.44	1.36
26	1	2498	OMC	C2-N3	5.05	1.46	1.36
27	2	1207	2MG	C2-N2	5.00	1.44	1.33
29	5	8	4SU	C4-S4	-4.99	1.58	1.68
27	2	527	7MG	C2-N3	4.86	1.44	1.33
26	1	1618	6MZ	C6-N6	4.83	1.43	1.35
27	2	527	7MG	C4-N3	4.81	1.45	1.34
27	2	966	2MG	C4-N3	4.62	1.48	1.37
26	1	2445	2MG	C2-N2	4.57	1.43	1.33
26	1	2498	OMC	C4-N3	4.54	1.43	1.34
26	1	2251	OMG	C2-N3	4.49	1.44	1.33
27	2	1516	2MG	C2-N2	4.47	1.43	1.33
26	1	2498	OMC	C4-N4	4.45	1.44	1.33
26	1	1835	2MG	C2-N2	4.45	1.43	1.33
26	1	2445	2MG	C4-N3	4.44	1.48	1.37
26	1	2503	2MA	C4-N3	4.44	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	1207	2MG	C4-N3	4.42	1.48	1.37
29	5	32	4OC	C4-N4	4.41	1.45	1.35
26	1	2069	G7M	C4-N3	4.32	1.47	1.37
26	1	1939	5MU	O2-C2	-4.31	1.15	1.23
26	1	2251	OMG	C2-N2	4.31	1.44	1.34
26	1	2030	6MZ	C6-N6	4.29	1.42	1.35
27	2	1207	2MG	C2-N1	4.28	1.43	1.36
27	2	527	7MG	C2-N2	4.23	1.44	1.34
27	2	1402	4OC	C4-N4	4.23	1.44	1.35
27	2	967	5MC	C6-N1	4.23	1.45	1.38
26	1	745	1MG	C4-N3	4.20	1.47	1.37
27	2	1498	UR3	C2-N3	4.17	1.47	1.39
26	1	2251	OMG	C4-N3	4.15	1.47	1.37
26	1	1962	5MC	C6-N1	4.13	1.45	1.38
26	1	2498	OMC	C2-N1	4.13	1.48	1.40
26	1	1835	2MG	C4-N3	4.10	1.47	1.37
27	2	967	5MC	C4-N4	4.06	1.44	1.34
27	2	1407	5MC	C6-N1	4.04	1.45	1.38
29	5	8	4SU	C5-C4	3.99	1.47	1.42
27	2	1516	2MG	C4-N3	3.93	1.46	1.37
27	2	1516	2MG	C2-N1	3.83	1.42	1.36
27	2	966	2MG	C2-N1	3.80	1.42	1.36
27	2	1407	5MC	C4-N4	3.77	1.43	1.34
27	2	527	7MG	C4-N9	3.74	1.42	1.37
26	1	1962	5MC	C4-N4	3.73	1.43	1.34
27	2	967	5MC	C2-N1	3.73	1.48	1.40
27	2	1519	MA6	C5-C4	-3.66	1.31	1.40
26	1	2251	OMG	C5-C4	-3.63	1.33	1.43
27	2	1407	5MC	C2-N1	3.56	1.47	1.40
27	2	1402	4OC	C5-C4	3.54	1.48	1.40
27	2	1518	MA6	C5-C4	-3.51	1.31	1.40
29	5	76	8AN	C5-C4	-3.50	1.31	1.40
29	5	32	4OC	C2-N1	3.50	1.47	1.40
27	2	1402	4OC	O2-C2	-3.48	1.17	1.23
26	1	1962	5MC	O2-C2	-3.47	1.17	1.23
27	2	1516	2MG	C5-C4	-3.47	1.34	1.43
29	5	32	4OC	C5-C4	3.44	1.48	1.40
26	1	747	5MU	O4-C4	-3.40	1.17	1.23
26	1	2251	OMG	O6-C6	-3.35	1.16	1.23
26	1	2445	2MG	C5-C4	-3.34	1.34	1.43
26	1	2445	2MG	O6-C6	-3.33	1.16	1.23
27	2	1402	4OC	C2-N1	3.28	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	745	1MG	C5-C4	-3.28	1.34	1.43
26	1	1835	2MG	C2-N1	3.27	1.42	1.36
27	2	527	7MG	O6-C6	-3.26	1.17	1.23
27	2	1407	5MC	O2-C2	-3.23	1.17	1.23
27	2	967	5MC	O2-C2	-3.22	1.17	1.23
27	2	1207	2MG	C5-C4	-3.21	1.34	1.43
29	5	8	4SU	C6-N1	3.19	1.45	1.38
26	1	2552	OMU	C4-N3	3.15	1.44	1.38
26	1	1939	5MU	O4-C4	-3.14	1.17	1.23
26	1	1962	5MC	C2-N1	3.13	1.46	1.40
26	1	2069	G7M	C2-N2	3.13	1.41	1.34
26	1	2030	6MZ	C5-C4	-3.13	1.32	1.40
26	1	1835	2MG	O6-C6	-3.11	1.17	1.23
26	1	2498	OMC	C6-N1	3.09	1.45	1.38
26	1	2503	2MA	C5-C4	-3.09	1.35	1.43
26	1	1618	6MZ	C5-C4	-3.08	1.32	1.40
27	2	527	7MG	C2-N1	3.08	1.45	1.37
26	1	1915	3TD	O2-C2	-3.07	1.17	1.23
27	2	527	7MG	C5-C6	3.07	1.51	1.43
26	1	1835	2MG	C5-C4	-3.06	1.35	1.43
29	5	76	8AN	C6-N6	3.06	1.45	1.34
26	1	746	PSU	C6-C5	3.06	1.38	1.35
29	5	32	4OC	O2-C2	-3.06	1.18	1.23
26	1	2552	OMU	O4-C4	-3.05	1.18	1.24
26	1	747	5MU	O2-C2	-3.05	1.17	1.23
29	5	55	PSU	C6-C5	3.04	1.38	1.35
27	2	1207	2MG	C6-N1	3.02	1.42	1.37
26	1	2445	2MG	C2-N1	3.01	1.41	1.36
27	2	1516	2MG	O6-C6	-3.01	1.17	1.23
27	2	1498	UR3	O2-C2	-2.97	1.17	1.22
27	2	1402	4OC	C6-N1	2.94	1.45	1.38
26	1	745	1MG	O6-C6	-2.93	1.16	1.22
27	2	1498	UR3	O4-C4	-2.92	1.17	1.23
29	5	8	4SU	O2-C2	-2.92	1.17	1.23
26	1	1911	PSU	C6-C5	2.89	1.38	1.35
27	2	966	2MG	C5-C4	-2.85	1.35	1.43
27	2	1207	2MG	C5-C6	2.82	1.53	1.47
27	2	516	PSU	C6-C5	2.80	1.38	1.35
26	1	2498	OMC	O2-C2	-2.78	1.18	1.23
26	1	2445	2MG	C5-C6	2.76	1.53	1.47
29	5	76	8AN	C3'-N3'	-2.74	1.43	1.47
29	5	54	5MU	O4-C4	-2.73	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	966	2MG	C6-N1	2.70	1.41	1.37
26	1	2069	G7M	C5-C4	-2.67	1.33	1.39
27	2	1516	2MG	C6-N1	2.66	1.41	1.37
26	1	1917	PSU	C6-C5	2.66	1.38	1.35
26	1	2030	6MZ	C9-N6	-2.66	1.40	1.45
26	1	2580	PSU	O4'-C1'	-2.65	1.40	1.43
29	5	32	4OC	C6-N1	2.62	1.44	1.38
26	1	2504	PSU	C6-C5	2.58	1.38	1.35
26	1	1915	3TD	O4-C4	-2.58	1.17	1.23
27	2	966	2MG	O6-C6	-2.58	1.18	1.23
27	2	1498	UR3	C6-N1	2.55	1.44	1.38
26	1	1915	3TD	C4-N3	2.52	1.45	1.40
27	2	1207	2MG	O6-C6	-2.50	1.18	1.23
26	1	2457	PSU	C6-C5	2.47	1.38	1.35
29	5	54	5MU	O2-C2	-2.47	1.18	1.23
27	2	1516	2MG	C5-C6	2.43	1.52	1.47
26	1	2251	OMG	C5-C6	2.43	1.52	1.47
26	1	1618	6MZ	C6-N1	-2.43	1.30	1.34
26	1	2069	G7M	C2-N3	2.42	1.39	1.33
26	1	2030	6MZ	C5-N7	-2.42	1.31	1.39
26	1	2251	OMG	C2-N1	2.42	1.43	1.37
26	1	2580	PSU	C6-C5	2.41	1.38	1.35
26	1	2605	PSU	C6-C5	2.39	1.38	1.35
29	5	76	8AN	C2-N3	2.39	1.35	1.32
26	1	2503	2MA	C2-N1	2.35	1.43	1.36
26	1	2503	2MA	C6-N1	2.30	1.43	1.38
27	2	527	7MG	C6-N1	2.27	1.43	1.38
26	1	2552	OMU	O2-C2	-2.27	1.18	1.23
26	1	2580	PSU	C4-C5	-2.27	1.37	1.44
29	5	76	8AN	O2'-C2'	2.26	1.48	1.43
27	2	1518	MA6	C2-N3	2.25	1.35	1.32
26	1	1618	6MZ	C9-N6	-2.25	1.41	1.45
27	2	966	2MG	C5-C6	2.24	1.51	1.47
26	1	2069	G7M	C6-N1	2.22	1.41	1.37
26	1	2030	6MZ	C4-N3	-2.17	1.32	1.35
27	2	1519	MA6	C2-N3	2.17	1.35	1.32
26	1	2552	OMU	C6-N1	2.16	1.43	1.38
26	1	2498	OMC	C5-C4	2.16	1.47	1.42
26	1	1618	6MZ	C5-N7	-2.15	1.31	1.39
26	1	2605	PSU	C4-C5	-2.11	1.38	1.44
26	1	1835	2MG	C5-C6	2.11	1.51	1.47
26	1	2251	OMG	C6-N1	2.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	1835	2MG	C6-N1	2.04	1.40	1.37
26	1	1917	PSU	C4-C5	-2.04	1.38	1.44
26	1	955	PSU	O4'-C1'	-2.00	1.41	1.43

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	2	1519	MA6	N1-C6-N6	-13.54	102.81	117.06
27	2	1518	MA6	N1-C6-N6	-12.74	103.65	117.06
29	5	54	5MU	C5-C4-N3	12.27	125.79	115.31
26	1	747	5MU	C5-C4-N3	11.28	124.94	115.31
26	1	1939	5MU	C5-C4-N3	11.27	124.93	115.31
26	1	1939	5MU	C5-C6-N1	-10.71	112.32	123.34
29	5	54	5MU	C5-C6-N1	-9.98	113.08	123.34
26	1	747	5MU	C5-C6-N1	-8.71	114.38	123.34
29	5	76	8AN	C5-C6-N6	7.56	131.84	120.35
29	5	8	4SU	C4-N3-C2	-7.07	120.47	127.34
26	1	2030	6MZ	N3-C2-N1	-7.05	117.65	128.68
29	5	20	H2U	C4-N3-C2	-7.03	119.96	125.79
26	1	2552	OMU	C4-N3-C2	-6.41	118.13	126.58
26	1	2030	6MZ	C2-N1-C6	6.24	121.94	116.59
26	1	747	5MU	O4-C4-C5	-6.18	117.73	124.90
26	1	1939	5MU	N3-C2-N1	6.11	123.00	114.89
29	5	76	8AN	N3-C2-N1	-6.07	119.19	128.68
27	2	1518	MA6	N3-C2-N1	-5.96	119.37	128.68
26	1	2457	PSU	N1-C2-N3	5.83	121.74	115.13
26	1	2030	6MZ	C1'-N9-C4	-5.79	116.48	126.64
27	2	1498	UR3	C4-N3-C2	-5.69	119.21	124.56
26	1	1939	5MU	C4-N3-C2	-5.66	120.03	127.35
26	1	1618	6MZ	N3-C2-N1	-5.63	119.87	128.68
27	2	1519	MA6	N3-C2-N1	-5.46	120.15	128.68
26	1	2504	PSU	C4-N3-C2	-5.44	118.51	126.34
26	1	1915	3TD	N1-C2-N3	5.42	120.42	116.14
26	1	2457	PSU	C4-N3-C2	-5.41	118.54	126.34
26	1	955	PSU	C4-N3-C2	-5.40	118.56	126.34
26	1	955	PSU	N1-C2-N3	5.32	121.16	115.13
29	5	8	4SU	C5-C4-N3	5.29	119.59	114.69
29	5	54	5MU	O4-C4-C5	-5.19	118.89	124.90
26	1	747	5MU	N3-C2-N1	5.09	121.64	114.89
27	2	527	7MG	C5-C6-N1	5.01	119.81	110.99
26	1	2580	PSU	N1-C2-N3	4.95	120.74	115.13
26	1	1939	5MU	C5M-C5-C6	-4.94	116.25	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	2552	OMU	C5-C4-N3	4.83	122.06	114.84
27	2	516	PSU	C4-N3-C2	-4.81	119.40	126.34
26	1	2580	PSU	C4-N3-C2	-4.66	119.62	126.34
26	1	2605	PSU	C4-N3-C2	-4.60	119.71	126.34
29	5	54	5MU	C4-N3-C2	-4.57	121.43	127.35
26	1	746	PSU	C4-N3-C2	-4.57	119.76	126.34
29	5	76	8AN	N6-C6-N1	-4.56	109.12	118.57
29	5	55	PSU	N1-C2-N3	4.51	120.25	115.13
26	1	2504	PSU	N1-C2-N3	4.47	120.20	115.13
29	5	55	PSU	C4-N3-C2	-4.45	119.92	126.34
26	1	746	PSU	N1-C2-N3	4.39	120.11	115.13
26	1	1911	PSU	N1-C2-N3	4.39	120.10	115.13
46	q	89	0TD	OD2-CG-CB	4.36	122.56	113.15
26	1	747	5MU	C4-N3-C2	-4.34	121.73	127.35
26	1	1917	PSU	C4-N3-C2	-4.32	120.11	126.34
29	5	54	5MU	C5M-C5-C4	4.29	123.49	118.77
27	2	516	PSU	N1-C2-N3	4.29	119.98	115.13
26	1	1911	PSU	C4-N3-C2	-4.25	120.22	126.34
26	1	745	1MG	C5-C6-N1	4.23	120.27	113.90
27	2	527	7MG	C2-N3-C4	4.22	119.81	112.30
29	5	54	5MU	C5M-C5-C6	-4.15	117.31	122.85
26	1	1917	PSU	N1-C2-N3	4.12	119.80	115.13
27	2	1407	5MC	C5-C6-N1	-4.12	119.10	123.34
26	1	1915	3TD	C4-N3-C2	-3.97	120.30	124.61
26	1	2503	2MA	C5-C6-N1	3.95	120.84	114.02
26	1	2605	PSU	N1-C2-N3	3.95	119.60	115.13
29	5	54	5MU	N3-C2-N1	3.93	120.11	114.89
27	2	1516	2MG	C5-C6-N1	3.86	120.77	113.95
26	1	1939	5MU	C5M-C5-C4	3.83	122.98	118.77
26	1	2445	2MG	C5-C6-N1	3.75	120.58	113.95
26	1	2552	OMU	N3-C2-N1	3.75	119.87	114.89
26	1	1939	5MU	O4-C4-C5	-3.75	120.56	124.90
27	2	967	5MC	C5-C6-N1	-3.69	119.54	123.34
26	1	1962	5MC	C5-C6-N1	-3.65	119.58	123.34
29	5	8	4SU	N3-C2-N1	3.64	119.72	114.89
27	2	966	2MG	C5-C6-N1	3.63	120.36	113.95
26	1	1835	2MG	C5-C6-N1	3.62	120.35	113.95
27	2	1207	2MG	C5-C6-N1	3.54	120.20	113.95
27	2	527	7MG	C5-C4-N3	-3.48	121.51	128.13
29	5	8	4SU	C1'-N1-C2	3.46	123.83	117.57
27	2	527	7MG	C5-C4-N9	3.38	110.73	106.35
26	1	747	5MU	C6-N1-C2	-3.38	117.88	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	1618	6MZ	C2-N1-C6	3.34	119.45	116.59
26	1	1939	5MU	O2-C2-N1	-3.34	118.35	122.79
27	2	1516	2MG	CM2-N2-C2	-3.32	116.53	123.86
29	5	8	4SU	C5-C4-S4	-3.32	120.19	124.47
26	1	955	PSU	O2-C2-N1	-3.29	119.17	122.79
26	1	1939	5MU	C6-C5-C4	3.27	120.76	118.03
26	1	747	5MU	O2-C2-N1	-3.25	118.46	122.79
26	1	745	1MG	O6-C6-C5	-3.18	118.56	124.19
26	1	2552	OMU	O4-C4-C5	-3.12	119.67	125.16
29	5	20	H2U	N3-C2-N1	3.08	119.91	116.65
26	1	2251	OMG	C5-C6-N1	3.07	119.37	113.95
26	1	745	1MG	C8-N7-C5	3.04	108.78	102.99
26	1	2457	PSU	O2-C2-N1	-3.04	119.44	122.79
29	5	20	H2U	C5-C4-N3	2.93	119.94	116.65
26	1	1939	5MU	O4-C4-N3	-2.93	114.50	120.12
26	1	1939	5MU	C1'-N1-C2	2.85	122.73	117.57
27	2	527	7MG	C4-C5-N7	2.81	109.43	105.53
26	1	2069	G7M	C2-N1-C6	-2.78	119.98	125.10
26	1	2552	OMU	O2-C2-N1	-2.78	119.10	122.79
26	1	745	1MG	C2-N1-C6	-2.77	118.69	120.95
26	1	2251	OMG	C8-N7-C5	2.76	108.26	102.99
26	1	2457	PSU	C6-N1-C2	-2.76	119.86	122.68
26	1	2552	OMU	C2'-C1'-N1	-2.75	108.88	114.22
27	2	1207	2MG	C8-N7-C5	2.75	108.22	102.99
26	1	2498	OMC	O2-C2-N3	-2.74	117.87	122.33
26	1	1962	5MC	CM5-C5-C6	-2.65	119.31	122.85
27	2	527	7MG	O6-C6-C5	-2.64	121.06	127.54
26	1	1917	PSU	O2-C2-N1	-2.63	119.89	122.79
29	5	55	PSU	O2-C2-N1	-2.62	119.90	122.79
26	1	2504	PSU	O2-C2-N1	-2.62	119.91	122.79
26	1	2030	6MZ	C4-C5-N7	-2.61	106.68	109.40
26	1	2069	G7M	N2-C2-N1	2.61	122.27	116.71
29	5	20	H2U	C5-C6-N1	2.59	120.16	111.61
27	2	527	7MG	C2-N1-C6	-2.59	120.38	125.10
27	2	1207	2MG	CM2-N2-C2	-2.58	118.16	123.86
27	2	1402	4OC	CM4-N4-C4	-2.58	117.41	122.45
29	5	32	4OC	CM4-N4-C4	-2.55	117.46	122.45
26	1	2030	6MZ	C9-N6-C6	-2.55	120.67	122.87
29	5	54	5MU	O4-C4-N3	-2.50	115.32	120.12
27	2	1516	2MG	O6-C6-C5	-2.46	119.56	124.37
27	2	966	2MG	O6-C6-C5	-2.42	119.64	124.37
29	5	55	PSU	C6-N1-C2	-2.42	120.21	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	2580	PSU	O4'-C1'-C2'	2.42	108.55	105.14
26	1	2552	OMU	CM2-O2'-C2'	-2.41	108.21	114.52
26	1	2445	2MG	CM2-N2-C2	-2.36	118.64	123.86
26	1	1835	2MG	C8-N7-C5	2.35	107.47	102.99
26	1	2503	2MA	C8-N7-C5	2.33	107.44	102.99
26	1	2445	2MG	C8-N7-C5	2.33	107.43	102.99
26	1	2580	PSU	C6-N1-C2	-2.33	120.30	122.68
26	1	1939	5MU	C6-N1-C2	-2.33	118.94	121.30
26	1	746	PSU	O2-C2-N1	-2.32	120.24	122.79
27	2	967	5MC	CM5-C5-C6	-2.31	119.76	122.85
29	5	20	H2U	O2-C2-N1	-2.31	120.21	123.11
27	2	966	2MG	C8-N7-C5	2.31	107.38	102.99
27	2	1498	UR3	C3U-N3-C4	2.30	121.18	117.89
27	2	1516	2MG	C8-N7-C5	2.30	107.37	102.99
26	1	1835	2MG	O6-C6-C5	-2.30	119.88	124.37
29	5	55	PSU	C6-C5-C4	2.30	119.80	118.20
26	1	2251	OMG	C2-N1-C6	-2.29	120.89	125.10
46	q	89	0TD	OD1-CG-CB	-2.28	117.67	122.44
29	5	32	4OC	C6-C5-C4	2.25	119.72	116.96
26	1	2605	PSU	O2-C2-N3	-2.23	117.61	121.82
26	1	2504	PSU	C5-C4-N3	2.22	121.61	116.58
26	1	2457	PSU	C6-C5-C4	2.22	119.75	118.20
26	1	747	5MU	C5M-C5-C6	-2.21	119.90	122.85
29	5	54	5MU	C1'-N1-C2	2.21	121.56	117.57
26	1	746	PSU	C6-N1-C2	-2.20	120.43	122.68
26	1	2445	2MG	O6-C6-C5	-2.19	120.10	124.37
26	1	1911	PSU	C6-N1-C2	-2.19	120.45	122.68
26	1	1618	6MZ	C9-N6-C6	-2.16	121.01	122.87
26	1	1915	3TD	C6-C5-C4	2.16	119.71	118.22
26	1	1917	PSU	C6-N1-C2	-2.15	120.49	122.68
27	2	1207	2MG	O6-C6-C5	-2.12	120.24	124.37
26	1	2503	2MA	CM2-C2-N1	2.11	120.92	116.23
26	1	1911	PSU	O2-C2-N1	-2.10	120.48	122.79
26	1	1835	2MG	CM2-N2-C2	-2.09	119.24	123.86
26	1	955	PSU	C6-N1-C2	-2.07	120.56	122.68
27	2	516	PSU	C5-C4-N3	2.05	121.23	116.58
26	1	2069	G7M	CN7-N7-C8	-2.05	115.56	125.43
27	2	527	7MG	C6-C5-C4	-2.04	118.41	122.62
26	1	2605	PSU	C5-C4-N3	2.00	121.11	116.58

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	2	516	PSU	O4'-C1'-C5-C4
27	2	516	PSU	O4'-C1'-C5-C6
29	5	20	H2U	O4'-C1'-N1-C6
46	q	89	0TD	CG-CB-SB-CSB
26	1	746	PSU	C2'-C1'-C5-C4
26	1	1915	3TD	O4'-C1'-C5-C4
26	1	1915	3TD	C2'-C1'-C5-C6
26	1	1915	3TD	O4'-C1'-C5-C6
26	1	1915	3TD	C3'-C4'-C5'-O5'
26	1	1915	3TD	O4'-C4'-C5'-O5'
26	1	2251	OMG	C1'-C2'-O2'-CM2
26	1	2445	2MG	C3'-C4'-C5'-O5'
26	1	2030	6MZ	O4'-C4'-C5'-O5'
26	1	2030	6MZ	C3'-C4'-C5'-O5'
29	5	76	8AN	C3'-C4'-C5'-O5'
29	5	54	5MU	C3'-C4'-C5'-O5'
29	5	54	5MU	O4'-C4'-C5'-O5'
26	1	1618	6MZ	O4'-C4'-C5'-O5'
26	1	1618	6MZ	C3'-C4'-C5'-O5'
29	5	76	8AN	C4'-C5'-O5'-P
29	5	20	H2U	O4'-C4'-C5'-O5'
29	5	20	H2U	C3'-C4'-C5'-O5'
26	1	2445	2MG	O4'-C4'-C5'-O5'
27	2	966	2MG	C3'-C4'-C5'-O5'
27	2	1402	4OC	O4'-C4'-C5'-O5'
29	5	76	8AN	O4'-C4'-C5'-O5'
26	1	2552	OMU	C3'-C2'-O2'-CM2
27	2	966	2MG	O4'-C4'-C5'-O5'
29	5	8	4SU	C2'-C1'-N1-C6
29	5	8	4SU	O4'-C1'-N1-C6
29	5	20	H2U	O4'-C1'-N1-C2
27	2	527	7MG	C3'-C4'-C5'-O5'
27	2	1402	4OC	C3'-C4'-C5'-O5'
27	2	527	7MG	C4'-C5'-O5'-P
26	1	746	PSU	O4'-C1'-C5-C6
29	5	8	4SU	C2'-C1'-N1-C2
26	1	2503	2MA	C4'-C5'-O5'-P
29	5	8	4SU	O4'-C1'-N1-C2
26	1	2069	G7M	O4'-C4'-C5'-O5'
29	5	20	H2U	C2'-C1'-N1-C2
26	1	2503	2MA	O4'-C4'-C5'-O5'
26	1	2498	OMC	C4'-C5'-O5'-P

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 440 ligands modelled in this entry, 439 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
59	FME	5	104	29	8,9,10	0.88	0	7,9,11	1.82	1 (14%)

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
59	FME	5	104	29	-	4/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	5	104	FME	CA-N-CN	4.05	129.05	122.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	5	104	FME	CB-CA-N-CN
59	5	104	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
59	5	104	FME	CB-CG-SD-CE
59	5	104	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	147:G	O3'	148:G	P	3.01
1	2	1276:G	O3'	1277:C	P	2.98

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-12635. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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.