Full wwPDB EM Validation Report (i)

Apr 16, 2024 – 03:19 am BST

PDB ID	:	6ZTJ
EMDB ID	:	EMD-11418
Title	:	E. coli 70S-RNAP expressome complex in NusG-coupled state (38 nt intervening mRNA)
Authors	:	Webster, M.W.; Takacs, M.; Weixlbaumer, A.
Deposited on	:	2020-07-20
Resolution	:	3.40 Å(reported)
Based on initial models	:	6ALH, 4YBB

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 (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:

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 3.40 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 (i)

There are 68 unique types of molecules in this entry. The entry contains 176970 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1533	32909	14684	6037	10655	1533	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	226	1765	1116	317	324	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	211	1653	1046	310	293	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	156	1148	715	217	210	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	9	CYS	GLY	conflict	UNP A0A090BZW5

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AG	153	1203	750	231	218	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AI	128	1031	639	207	182	3	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AJ	101	808	504	155	148	1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AL	122	951	588	195	163	5	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	AR	60	494	310	93	91	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	AU	70	590	366	125	98	1	0	0

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	AV	40	849	381	154	274	40	0	0

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
23	AW	77	1645	734	297	536	77	1	0	0

- Molecule 24 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
24	AX	76	1624	724	290	533	76	1	0	0

- Molecule 25 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	AY	89	677	423	112	142	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	BA	2900	62270	27786	11456	20128	2900	0	0

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BC	272	2092	1294	425	366	7	0	0

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	BF	178	1420	905	251	258	6	0	0

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a protein called 50S ribosomal protein L10.

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

- Molecule 35 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	BJ	141	1032	651	179	196	6	0	0

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	BL	123	947	593	181	167	6	0	0

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	BM	144	1052	653	207	190	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	77	VAL	ILE	conflict	UNP P02413

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	BN	136	1075	686	205	178	6	0	0

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	BO	120	960	593	196	166	5	0	0

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BP	117	900	557	179	163	1	0	0

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BU	96	764	484	142	136	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	BV	103	789	498	148	143	0	0

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	BZ	63	509	313	99	95	2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	B1	58	449	281	87	79	2	0	0

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	B2	56	444	269	94	80	1	0	0

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
54	B3	53	436	281	80	75	0	0

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	B4	46	377	228	90	57	2	0	0

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	B5	64	504	323	105	74	2	0	0

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	B6	38	301	185	65	47	4	0	0

- Molecule 58 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	B7	70	549	339	104	100	6	0	0

- Molecule 59 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
59	CN	30	618	294	114	180	30	0	0

- Molecule 60 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
60	CT	30	606	288	105	183	30	0	0

- Molecule 61 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	CA	229	1775	1106	313	350	6	0	0
61	CB	219	1684	1051	295	332	6	0	0

- Molecule 62 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	CC	1320	10415	6535	1815	2021	44	0	0

- Molecule 63 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	CD	1333	10375	6518	1851	1956	50	0	0

- Molecule 64 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	CE	51	399	246	77	75	1	0	0

- Molecule 65 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	CF	161	1283	818	221	237	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CF	121	ALA	LYS	conflict	UNP P0AFG1

- Molecule 66 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
66	AA	148	148	148	0
66	AI	1	1	1	0

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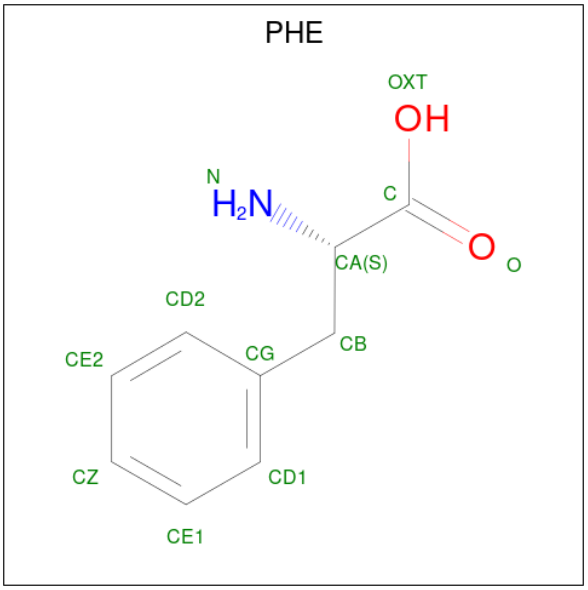
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
66	AW	1	1	1	0
			Total	Mg	
66	AX	1	1	1	0
			Total	Mg	
66	BA	314	314	314	0
			Total	Mg	
66	BB	6	6	6	0
			Total	Mg	
66	BC	3	3	3	0
			Total	Mg	
66	BD	1	1	1	0
			Total	Mg	
66	BE	1	1	1	0
			Total	Mg	
66	BQ	1	1	1	0
			Total	Mg	
66	BT	1	1	1	0
			Total	Mg	
66	CD	1	1	1	0

- Molecule 67 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
67	AX	1	11	9	1	1	0

- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
68	B6	1	1	1	0
68	B7	1	1	1	0
68	CD	2	2	2	0

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, Not provided	
Number of particles used	15327	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

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

53 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	$\#\|Z\| > 2$
24	7MG	AX	46	24	20,25,27	3.27	10 (50%)	27,37,42	2.22	8 (29%)
24	4SU	AX	8	24	18,21,22	4.12	8 (44%)	26,30,33	2.26	5 (19%)
1	5MC	AA	967	1	18,22,23	3.99	7 (38%)	26,32,35	1.03	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MA6	AA	1518	1	18,26,27	1.34	3 (16%)	19,38,41	4.16	2 (10%)
26	PSU	BA	955	26,66	18,21,22	1.07	2 (11%)	22,30,33	1.74	4 (18%)
23	OMC	AW	32	23	19,22,23	3.03	8 (42%)	26,31,34	0.92	1 (3%)
24	3AU	AX	47	24	18,21,29	3.40	8 (44%)	26,30,43	1.64	4 (15%)
26	2MG	BA	1835	26	18,26,27	2.30	7 (38%)	16,38,41	1.62	4 (25%)
26	PSU	BA	2504	26	18,21,22	1.06	3 (16%)	22,30,33	2.05	6 (27%)
24	H2U	AX	20	24	18,21,22	3.15	5 (27%)	21,30,33	1.95	4 (19%)
26	PSU	BA	2580	26	18,21,22	1.05	2 (11%)	22,30,33	2.07	6 (27%)
26	PSU	BA	2605	26	18,21,22	1.04	1 (5%)	22,30,33	1.96	6 (27%)
23	H2U	AW	20	23	18,21,22	3.07	5 (27%)	21,30,33	1.99	5 (23%)
1	UR3	AA	1498	66,1	19,22,23	2.59	7 (36%)	26,32,35	1.31	1 (3%)
1	G7M	AA	527	1	20,26,27	2.28	8 (40%)	17,39,42	1.22	2 (11%)
23	PSU	AW	55	23	18,21,22	1.04	1 (5%)	22,30,33	1.98	7 (31%)
1	2MG	AA	1516	1	18,26,27	2.28	7 (38%)	16,38,41	1.64	4 (25%)
26	6MZ	BA	1618	26	18,25,26	1.99	3 (16%)	16,36,39	1.86	3 (18%)
26	OMU	BA	2552	26	19,22,23	3.01	7 (36%)	26,31,34	1.71	5 (19%)
1	MA6	AA	1519	1	18,26,27	1.35	3 (16%)	19,38,41	4.12	2 (10%)
26	OMC	BA	2498	26	19,22,23	2.91	8 (42%)	26,31,34	0.87	1 (3%)
23	5MU	AW	54	23	19,22,23	1.41	5 (26%)	28,32,35	2.11	6 (21%)
1	2MG	AA	1207	66,1	18,26,27	2.36	7 (38%)	16,38,41	1.42	4 (25%)
24	PSU	AX	32	66,24	18,21,22	1.09	2 (11%)	22,30,33	1.77	4 (18%)
26	1MG	BA	745	26	18,26,27	2.66	5 (27%)	19,39,42	1.46	3 (15%)
26	H2U	BA	2449	26	18,21,22	2.82	5 (27%)	21,30,33	2.13	5 (23%)
23	4SU	AW	8	23	18,21,22	4.16	8 (44%)	26,30,33	2.28	5 (19%)
26	PSU	BA	2457	26	18,21,22	1.05	1 (5%)	22,30,33	2.00	6 (27%)
26	G7M	BA	2069	26	20,26,27	2.32	7 (35%)	17,39,42	1.18	2 (11%)
26	2MA	BA	2503	26,66	17,25,26	2.62	6 (35%)	17,37,40	1.41	3 (17%)
12	D2T	AL	89	12	7,9,10	1.11	0	6,11,13	2.48	4 (66%)
26	5MC	BA	1962	26	18,22,23	3.97	7 (38%)	26,32,35	1.14	1 (3%)
1	5MC	AA	1407	1	18,22,23	3.89	7 (38%)	26,32,35	0.97	1 (3%)
26	2MG	BA	2445	26,30	18,26,27	2.31	7 (38%)	16,38,41	1.54	4 (25%)
26	PSU	BA	1917	26	18,21,22	0.99	1 (5%)	22,30,33	1.80	5 (22%)
1	2MG	AA	966	1	18,26,27	2.41	7 (38%)	16,38,41	1.74	6 (37%)
1	4OC	AA	1402	1	20,23,24	3.40	9 (45%)	26,32,35	1.01	2 (7%)
39	4D4	BN	81	39	9,11,12	2.41	2 (22%)	8,13,15	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	5MU	AX	54	24	19,22,23	1.34	5 (26%)	28,32,35	2.09	6 (21%)
24	PSU	AX	55	24	18,21,22	1.10	1 (5%)	22,30,33	1.89	5 (22%)
26	6MZ	BA	2030	26	18,25,26	1.93	3 (16%)	16,36,39	2.48	3 (18%)
29	MEQ	BD	150	29	8,9,10	0.86	0	5,10,12	0.92	0
26	3TD	BA	1915	26	18,22,23	4.47	10 (55%)	22,32,35	1.91	4 (18%)
24	MIA	AX	37	24	18,24,32	1.49	3 (16%)	18,35,47	1.53	2 (11%)
26	PSU	BA	746	26,66	18,21,22	1.03	1 (5%)	22,30,33	2.12	8 (36%)
1	PSU	AA	516	1	18,21,22	1.05	2 (11%)	22,30,33	2.04	7 (31%)
26	5MU	BA	747	26	19,22,23	1.41	4 (21%)	28,32,35	2.16	6 (21%)
26	5MU	BA	1939	26	19,22,23	1.42	4 (21%)	28,32,35	2.29	6 (21%)
26	PSU	BA	1911	26	18,21,22	1.07	1 (5%)	22,30,33	1.77	3 (13%)
26	OMG	BA	2251	26,23	18,26,27	2.69	8 (44%)	19,38,41	1.52	4 (21%)
24	H2U	AX	16	24	18,21,22	3.05	5 (27%)	21,30,33	2.01	5 (23%)
24	PSU	AX	39	24	18,21,22	1.14	1 (5%)	22,30,33	1.78	5 (22%)
26	PSU	BA	2604	26	18,21,22	1.01	1 (5%)	22,30,33	1.67	3 (13%)

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
24	7MG	AX	46	24	-	2/7/34/38	0/3/3/3
24	4SU	AX	8	24	-	1/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	1/7/29/30	0/3/3/3
26	PSU	BA	955	26,66	-	0/7/25/26	0/2/2/2
23	OMC	AW	32	23	-	3/9/27/28	0/2/2/2
24	3AU	AX	47	24	-	2/7/25/35	0/2/2/2
26	2MG	BA	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	BA	2504	26	-	0/7/25/26	0/2/2/2
24	H2U	AX	20	24	-	3/7/38/39	0/2/2/2
26	PSU	BA	2580	26	-	0/7/25/26	0/2/2/2
26	PSU	BA	2605	26	-	0/7/25/26	0/2/2/2
23	H2U	AW	20	23	-	7/7/38/39	0/2/2/2
1	UR3	AA	1498	66,1	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	1/3/25/26	0/3/3/3
23	PSU	AW	55	23	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
26	6MZ	BA	1618	26	-	4/5/27/28	0/3/3/3
26	OMU	BA	2552	26	-	2/9/27/28	0/2/2/2
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
26	OMC	BA	2498	26	-	2/9/27/28	0/2/2/2
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	66,1	-	2/5/27/28	0/3/3/3
24	PSU	AX	32	66,24	-	2/7/25/26	0/2/2/2
26	1MG	BA	745	26	-	0/3/25/26	0/3/3/3
26	H2U	BA	2449	26	-	2/7/38/39	0/2/2/2
23	4SU	AW	8	23	-	2/7/25/26	0/2/2/2
26	PSU	BA	2457	26	-	0/7/25/26	0/2/2/2
26	G7M	BA	2069	26	-	2/3/25/26	0/3/3/3
26	2MA	BA	2503	26,66	-	2/3/25/26	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
26	5MC	BA	1962	26	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
26	2MG	BA	2445	26,30	-	2/5/27/28	0/3/3/3
26	PSU	BA	1917	26	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
39	4D4	BN	81	39	-	4/11/12/14	-
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	4/7/25/26	0/2/2/2
26	6MZ	BA	2030	26	-	3/5/27/28	0/3/3/3
29	MEQ	BD	150	29	-	4/8/9/11	-
26	3TD	BA	1915	26	-	3/7/25/26	0/2/2/2
24	MIA	AX	37	24	-	0/3/25/34	0/3/3/3
26	PSU	BA	746	26,66	-	2/7/25/26	0/2/2/2
1	PSU	AA	516	1	-	2/7/25/26	0/2/2/2
26	5MU	BA	747	26	-	0/7/25/26	0/2/2/2
26	5MU	BA	1939	26	-	2/7/25/26	0/2/2/2
26	PSU	BA	1911	26	-	1/7/25/26	0/2/2/2
26	OMG	BA	2251	26,23	-	0/5/27/28	0/3/3/3
24	H2U	AX	16	24	-	4/7/38/39	0/2/2/2
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
26	PSU	BA	2604	26	-	0/7/25/26	0/2/2/2

All (248) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1915	3TD	C6-C5	11.99	1.49	1.35
1	AA	967	5MC	C6-C5	10.01	1.51	1.34
1	AA	1407	5MC	C6-C5	9.87	1.50	1.34
24	AX	20	H2U	C2-N1	9.80	1.49	1.35
26	BA	1915	3TD	C2-N1	9.77	1.49	1.37
26	BA	1962	5MC	C6-C5	9.68	1.50	1.34
23	AW	8	4SU	C4-N3	9.40	1.47	1.37
23	AW	20	H2U	C2-N1	9.32	1.48	1.35
24	AX	16	H2U	C2-N1	9.26	1.48	1.35
24	AX	8	4SU	C4-N3	9.09	1.47	1.37
26	BA	2449	H2U	C2-N1	8.17	1.47	1.35
24	AX	8	4SU	C2-N1	7.96	1.51	1.38
26	BA	745	1MG	C2-N3	7.69	1.48	1.34
23	AW	8	4SU	C2-N1	7.69	1.50	1.38
26	BA	1962	5MC	C4-N3	7.57	1.46	1.34
24	AX	47	3AU	C2-N1	7.52	1.50	1.38
1	AA	967	5MC	C4-N3	7.31	1.46	1.34
26	BA	2503	2MA	C2-N3	7.26	1.46	1.31
1	AA	1407	5MC	C4-N3	7.04	1.46	1.34
26	BA	1618	6MZ	C6-N6	7.03	1.46	1.35
24	AX	47	3AU	C6-C5	6.99	1.51	1.35
26	BA	2552	OMU	C2-N3	6.96	1.50	1.38
1	AA	1402	4OC	C4-N3	6.94	1.44	1.32
1	AA	967	5MC	C2-N3	6.87	1.50	1.36
26	BA	1962	5MC	C2-N3	6.78	1.50	1.36
23	AW	8	4SU	C2-N3	6.67	1.49	1.38
24	AX	20	H2U	C2-N3	6.57	1.49	1.38
1	AA	1407	5MC	C2-N3	6.55	1.49	1.36
23	AW	20	H2U	C2-N3	6.54	1.49	1.38
24	AX	16	H2U	C2-N3	6.51	1.49	1.38
26	BA	2030	6MZ	C6-N6	6.50	1.45	1.35
1	AA	1402	4OC	C6-C5	6.48	1.50	1.35
23	AW	32	OMC	C2-N3	6.47	1.49	1.36
24	AX	8	4SU	C2-N3	6.46	1.49	1.38
24	AX	47	3AU	C2-N3	6.45	1.49	1.38
1	AA	1498	UR3	C2-N1	6.26	1.47	1.38
26	BA	2498	OMC	C2-N3	6.16	1.48	1.36
26	BA	1915	3TD	C6-N1	6.15	1.46	1.36
39	BN	81	4D4	CZ-NE	6.11	1.45	1.33
26	BA	2552	OMU	C6-C5	6.11	1.49	1.35
1	AA	1498	UR3	C6-C5	6.09	1.49	1.35
26	BA	2449	H2U	C2-N3	6.05	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	8	4SU	C6-C5	6.04	1.49	1.35
24	AX	8	4SU	C6-C5	6.03	1.49	1.35
23	AW	32	OMC	C6-C5	5.98	1.49	1.35
24	AX	46	7MG	C4-N9	5.96	1.44	1.37
24	AX	46	7MG	C4-N3	5.95	1.48	1.34
1	AA	1402	4OC	C2-N3	5.92	1.48	1.36
24	AX	46	7MG	C2-N3	5.92	1.47	1.33
26	BA	2552	OMU	C2-N1	5.85	1.47	1.38
26	BA	2498	OMC	C6-C5	5.79	1.48	1.35
23	AW	8	4SU	C5-C4	5.63	1.49	1.42
23	AW	8	4SU	C4-S4	-5.49	1.58	1.68
24	AX	8	4SU	C5-C4	5.49	1.49	1.42
24	AX	8	4SU	C4-S4	-5.45	1.58	1.68
26	BA	2251	OMG	C2-N2	5.42	1.47	1.34
1	AA	967	5MC	C4-N4	5.38	1.48	1.34
26	BA	745	1MG	C2-N2	5.37	1.43	1.34
26	BA	2251	OMG	C2-N3	5.36	1.46	1.33
26	BA	1962	5MC	C4-N4	5.36	1.48	1.34
1	AA	967	5MC	C6-N1	5.26	1.47	1.38
23	AW	32	OMC	C4-N3	5.23	1.45	1.34
1	AA	1407	5MC	C4-N4	5.23	1.47	1.34
26	BA	1962	5MC	C6-N1	5.23	1.47	1.38
26	BA	2251	OMG	C4-N3	5.19	1.50	1.37
26	BA	2503	2MA	C4-N3	5.18	1.49	1.37
1	AA	1407	5MC	C6-N1	5.17	1.46	1.38
24	AX	47	3AU	C4-N3	5.14	1.47	1.38
23	AW	20	H2U	C4-N3	5.07	1.46	1.37
26	BA	2498	OMC	C4-N3	5.04	1.44	1.34
26	BA	2069	G7M	C2-N3	5.03	1.45	1.33
24	AX	16	H2U	C4-N3	4.97	1.46	1.37
26	BA	1915	3TD	C1'-C5	-4.94	1.38	1.50
24	AX	20	H2U	C4-N3	4.92	1.46	1.37
23	AW	32	OMC	C4-N4	4.86	1.45	1.33
24	AX	46	7MG	C2-N2	4.81	1.45	1.34
1	AA	1402	4OC	C4-N4	4.78	1.45	1.35
26	BA	2498	OMC	C4-N4	4.78	1.45	1.33
1	AA	527	G7M	C2-N3	4.77	1.44	1.33
1	AA	1402	4OC	O2-C2	-4.70	1.15	1.23
1	AA	966	2MG	C2-N2	4.70	1.43	1.33
26	BA	1962	5MC	C2-N1	4.67	1.50	1.40
1	AA	1498	UR3	C2-N3	4.67	1.48	1.39
26	BA	2069	G7M	C2-N2	4.63	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1207	2MG	C2-N2	4.59	1.43	1.33
1	AA	527	G7M	C2-N2	4.55	1.45	1.34
26	BA	2449	H2U	C4-N3	4.54	1.45	1.37
26	BA	1835	2MG	C2-N2	4.53	1.43	1.33
26	BA	2445	2MG	C2-N2	4.51	1.43	1.33
26	BA	2069	G7M	C4-N3	4.50	1.48	1.37
26	BA	745	1MG	C4-N3	4.48	1.48	1.37
1	AA	527	G7M	C4-N3	4.48	1.48	1.37
23	AW	32	OMC	C2-N1	4.41	1.49	1.40
1	AA	1516	2MG	C2-N2	4.39	1.43	1.33
1	AA	967	5MC	C2-N1	4.39	1.49	1.40
1	AA	1402	4OC	C5-C4	4.37	1.50	1.40
1	AA	1407	5MC	C2-N1	4.35	1.49	1.40
24	AX	46	7MG	C5-C4	4.31	1.43	1.37
1	AA	966	2MG	C6-N1	4.30	1.44	1.37
1	AA	1207	2MG	C6-N1	4.26	1.44	1.37
1	AA	966	2MG	C2-N1	4.25	1.43	1.36
1	AA	1402	4OC	C2-N1	4.22	1.49	1.40
26	BA	1915	3TD	C2-N3	4.22	1.47	1.38
26	BA	2552	OMU	C4-N3	4.07	1.45	1.38
1	AA	1207	2MG	C2-N1	4.07	1.43	1.36
24	AX	37	MIA	C6-N6	4.07	1.48	1.34
24	AX	46	7MG	C2-N1	4.05	1.47	1.37
24	AX	46	7MG	C5-C6	4.05	1.52	1.42
26	BA	2445	2MG	C4-N3	3.98	1.47	1.37
1	AA	1516	2MG	C6-N1	3.98	1.43	1.37
1	AA	1516	2MG	C2-N1	3.95	1.43	1.36
26	BA	2498	OMC	C2-N1	3.94	1.48	1.40
26	BA	2445	2MG	C2-N1	3.92	1.43	1.36
26	BA	1835	2MG	C4-N3	3.91	1.46	1.37
26	BA	1835	2MG	C6-N1	3.90	1.43	1.37
26	BA	2445	2MG	C6-N1	3.87	1.43	1.37
1	AA	1207	2MG	C4-N3	3.86	1.46	1.37
26	BA	2552	OMU	O4-C4	-3.84	1.17	1.24
1	AA	966	2MG	C4-N3	3.78	1.46	1.37
26	BA	2251	OMG	C6-N1	3.78	1.43	1.37
1	AA	1516	2MG	C4-N3	3.73	1.46	1.37
26	BA	1835	2MG	C2-N1	3.71	1.42	1.36
26	BA	2069	G7M	C6-N1	3.52	1.43	1.37
24	AX	39	PSU	C6-C5	3.52	1.39	1.35
24	AX	46	7MG	O6-C6	-3.50	1.16	1.23
1	AA	527	G7M	C6-N1	3.45	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	55	PSU	C6-C5	3.45	1.39	1.35
26	BA	1835	2MG	O6-C6	-3.43	1.16	1.23
1	AA	1402	4OC	CM4-N4	3.41	1.51	1.45
24	AX	32	PSU	C6-C5	3.39	1.39	1.35
24	AX	46	7MG	C6-N1	3.37	1.45	1.38
26	BA	2503	2MA	C6-N1	3.35	1.45	1.38
1	AA	1516	2MG	O6-C6	-3.35	1.16	1.23
26	BA	2445	2MG	O6-C6	-3.32	1.16	1.23
24	AX	47	3AU	C6-N1	3.28	1.45	1.38
1	AA	966	2MG	O6-C6	-3.21	1.16	1.23
26	BA	2498	OMC	C6-N1	3.19	1.45	1.38
1	AA	1207	2MG	O6-C6	-3.17	1.16	1.23
26	BA	2552	OMU	O2-C2	-3.15	1.17	1.23
1	AA	1402	4OC	C6-N1	3.11	1.45	1.38
26	BA	1939	5MU	C4-N3	-3.11	1.33	1.38
24	AX	8	4SU	C6-N1	3.11	1.45	1.38
24	AX	8	4SU	O2-C2	-3.10	1.17	1.23
23	AW	8	4SU	C6-N1	3.10	1.45	1.38
23	AW	8	4SU	O2-C2	-3.08	1.17	1.23
23	AW	55	PSU	C6-C5	3.07	1.38	1.35
1	AA	1518	MA6	C2-N3	3.04	1.37	1.32
1	AA	966	2MG	C5-C4	-3.04	1.35	1.43
23	AW	32	OMC	C6-N1	3.03	1.45	1.38
26	BA	1911	PSU	C6-C5	3.03	1.38	1.35
26	BA	746	PSU	C6-C5	3.02	1.38	1.35
1	AA	1519	MA6	C2-N3	3.00	1.36	1.32
24	AX	46	7MG	C5-N7	3.00	1.44	1.35
26	BA	1915	3TD	O2-C2	-2.98	1.17	1.23
26	BA	1915	3TD	O4-C4	-2.97	1.16	1.23
26	BA	1915	3TD	C4-N3	2.97	1.46	1.40
26	BA	747	5MU	C4-N3	-2.95	1.33	1.38
26	BA	2030	6MZ	C5-C4	-2.94	1.33	1.40
26	BA	2251	OMG	C5-C6	2.93	1.53	1.47
1	AA	1519	MA6	C5-C4	-2.93	1.33	1.40
26	BA	2604	PSU	C6-C5	2.92	1.38	1.35
24	AX	47	3AU	O4-C4	-2.91	1.18	1.24
26	BA	2251	OMG	C5-C4	-2.90	1.35	1.43
26	BA	2580	PSU	C6-C5	2.90	1.38	1.35
1	AA	966	2MG	C5-C6	2.90	1.53	1.47
26	BA	955	PSU	C6-C5	2.89	1.38	1.35
26	BA	2457	PSU	C6-C5	2.89	1.38	1.35
23	AW	32	OMC	O2-C2	-2.88	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1518	MA6	C10-N6	2.88	1.52	1.45
26	BA	2498	OMC	O2-C2	-2.87	1.18	1.23
1	AA	516	PSU	C6-C5	2.87	1.38	1.35
1	AA	1516	2MG	C5-C4	-2.86	1.35	1.43
26	BA	2605	PSU	C6-C5	2.84	1.38	1.35
26	BA	1835	2MG	C5-C4	-2.84	1.35	1.43
1	AA	1519	MA6	C10-N6	2.83	1.52	1.45
26	BA	2445	2MG	C5-C6	2.83	1.53	1.47
1	AA	1207	2MG	C5-C6	2.80	1.53	1.47
26	BA	1835	2MG	C5-C6	2.79	1.53	1.47
26	BA	2445	2MG	C5-C4	-2.77	1.36	1.43
24	AX	47	3AU	C5-C4	2.77	1.49	1.43
24	AX	54	5MU	C4-N3	-2.75	1.33	1.38
1	AA	1207	2MG	C5-C4	-2.75	1.36	1.43
26	BA	2503	2MA	C5-C4	-2.74	1.36	1.43
1	AA	1518	MA6	C5-C4	-2.74	1.33	1.40
26	BA	1917	PSU	C6-C5	2.70	1.38	1.35
26	BA	747	5MU	C6-N1	-2.70	1.33	1.38
26	BA	2069	G7M	C5-C6	2.70	1.52	1.45
1	AA	1498	UR3	C6-N1	2.70	1.44	1.38
23	AW	54	5MU	C4-N3	-2.68	1.33	1.38
26	BA	1939	5MU	C6-N1	-2.66	1.33	1.38
24	AX	37	MIA	C2-N3	2.65	1.36	1.32
26	BA	2251	OMG	C2-N1	2.63	1.44	1.37
26	BA	2069	G7M	C2-N1	2.61	1.44	1.37
26	BA	2503	2MA	CM2-C2	2.61	1.56	1.49
1	AA	527	G7M	C5-C6	2.60	1.52	1.45
26	BA	1618	6MZ	C5-C4	-2.58	1.34	1.40
26	BA	1962	5MC	O2-C2	-2.58	1.18	1.23
23	AW	54	5MU	C6-C5	2.57	1.38	1.34
26	BA	1939	5MU	C2-N3	-2.57	1.33	1.38
1	AA	1516	2MG	C5-C6	2.57	1.52	1.47
26	BA	747	5MU	C6-C5	2.57	1.38	1.34
26	BA	1939	5MU	C6-C5	2.57	1.38	1.34
1	AA	1407	5MC	O2-C2	-2.57	1.19	1.23
26	BA	1915	3TD	C10-N3	2.55	1.51	1.47
1	AA	527	G7M	O6-C6	-2.55	1.18	1.23
39	BN	81	4D4	CZ-NH1	2.55	1.45	1.34
26	BA	1618	6MZ	C2-N3	2.54	1.36	1.32
26	BA	1915	3TD	O4'-C1'	-2.53	1.40	1.43
24	AX	47	3AU	O2-C2	-2.52	1.18	1.23
26	BA	2449	H2U	O2-C2	-2.51	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2504	PSU	C6-C5	2.50	1.38	1.35
1	AA	967	5MC	O2-C2	-2.46	1.19	1.23
1	AA	1498	UR3	O4-C4	-2.46	1.18	1.23
26	BA	2503	2MA	C2-N1	2.45	1.44	1.36
24	AX	20	H2U	O4-C4	-2.43	1.18	1.23
1	AA	527	G7M	C2-N1	2.42	1.43	1.37
24	AX	37	MIA	C5-C4	-2.42	1.34	1.40
23	AW	54	5MU	C6-N1	-2.42	1.33	1.38
26	BA	2552	OMU	C6-N1	2.41	1.43	1.38
26	BA	747	5MU	C2-N3	-2.40	1.33	1.38
24	AX	54	5MU	C6-N1	-2.39	1.34	1.38
23	AW	20	H2U	O2-C2	-2.37	1.18	1.23
1	AA	1498	UR3	O2-C2	-2.37	1.18	1.22
26	BA	2069	G7M	O6-C6	-2.35	1.18	1.23
26	BA	2449	H2U	O4-C4	-2.35	1.18	1.23
24	AX	54	5MU	C2-N3	-2.33	1.33	1.38
24	AX	16	H2U	O2-C2	-2.33	1.18	1.23
24	AX	54	5MU	C6-C5	2.32	1.38	1.34
23	AW	32	OMC	C5-C4	2.31	1.48	1.42
26	BA	2030	6MZ	C2-N3	2.28	1.35	1.32
23	AW	54	5MU	C4-C5	2.27	1.48	1.44
26	BA	745	1MG	C5-C6	2.26	1.54	1.47
24	AX	16	H2U	O4-C4	-2.25	1.18	1.23
24	AX	20	H2U	O2-C2	-2.22	1.19	1.23
26	BA	2251	OMG	O6-C6	-2.17	1.18	1.23
23	AW	20	H2U	O4-C4	-2.16	1.18	1.23
26	BA	745	1MG	C6-N1	2.16	1.43	1.39
23	AW	54	5MU	C2-N3	-2.14	1.34	1.38
26	BA	2498	OMC	C5-C4	2.12	1.47	1.42
26	BA	2504	PSU	O4'-C1'	-2.09	1.40	1.43
1	AA	516	PSU	C4-C5	-2.09	1.38	1.44
26	BA	955	PSU	C4-C5	-2.09	1.38	1.44
26	BA	2580	PSU	C4-C5	-2.04	1.38	1.44
1	AA	527	G7M	C5-C4	-2.04	1.34	1.39
26	BA	2504	PSU	C4-C5	-2.04	1.38	1.44
1	AA	1498	UR3	C5-C4	2.03	1.49	1.43
24	AX	54	5MU	C4-C5	2.02	1.48	1.44
24	AX	32	PSU	C4-C5	-2.01	1.38	1.44

All (209) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1518	MA6	N1-C6-N6	-17.13	99.03	117.06
1	AA	1519	MA6	N1-C6-N6	-16.81	99.37	117.06
23	AW	8	4SU	C4-N3-C2	-8.08	119.49	127.34
24	AX	8	4SU	C4-N3-C2	-7.83	119.73	127.34
24	AX	46	7MG	C5-C4-N3	-7.48	120.08	127.80
26	BA	2449	H2U	C4-N3-C2	-7.25	119.78	125.79
24	AX	16	H2U	C4-N3-C2	-6.94	120.03	125.79
24	AX	20	H2U	C4-N3-C2	-6.81	120.14	125.79
23	AW	20	H2U	C4-N3-C2	-6.78	120.17	125.79
26	BA	2030	6MZ	C9-N6-C6	-6.59	117.20	122.87
26	BA	1915	3TD	N1-C2-N3	5.84	120.75	116.14
26	BA	1939	5MU	C4-N3-C2	-5.84	119.79	127.35
26	BA	2030	6MZ	N3-C2-N1	-5.69	119.79	128.68
26	BA	1939	5MU	N3-C2-N1	5.62	122.35	114.89
1	AA	1519	MA6	N3-C2-N1	-5.58	119.96	128.68
23	AW	8	4SU	C5-C4-N3	5.55	119.83	114.69
24	AX	8	4SU	C5-C4-N3	5.40	119.70	114.69
26	BA	747	5MU	C4-N3-C2	-5.39	120.37	127.35
26	BA	1618	6MZ	N3-C2-N1	-5.39	120.25	128.68
26	BA	747	5MU	N3-C2-N1	5.29	121.92	114.89
24	AX	37	MIA	N3-C2-N1	-5.27	120.44	128.68
1	AA	1518	MA6	N3-C2-N1	-5.27	120.44	128.68
23	AW	54	5MU	C4-N3-C2	-5.20	120.62	127.35
24	AX	54	5MU	C4-N3-C2	-5.19	120.64	127.35
26	BA	2552	OMU	C4-N3-C2	-5.19	119.74	126.58
1	AA	1498	UR3	C4-N3-C2	-4.96	119.89	124.56
23	AW	54	5MU	N3-C2-N1	4.95	121.46	114.89
26	BA	2504	PSU	N1-C2-N3	4.91	120.69	115.13
24	AX	47	3AU	C4-N3-C2	-4.90	120.12	126.58
26	BA	2605	PSU	C4-N3-C2	-4.88	119.31	126.34
26	BA	2457	PSU	C4-N3-C2	-4.88	119.31	126.34
26	BA	2504	PSU	C4-N3-C2	-4.84	119.37	126.34
24	AX	54	5MU	N3-C2-N1	4.77	121.22	114.89
24	AX	55	PSU	C4-N3-C2	-4.76	119.48	126.34
26	BA	746	PSU	C4-N3-C2	-4.76	119.49	126.34
24	AX	55	PSU	N1-C2-N3	4.71	120.46	115.13
26	BA	1939	5MU	C5-C4-N3	4.70	119.32	115.31
26	BA	2605	PSU	N1-C2-N3	4.69	120.44	115.13
26	BA	1911	PSU	C4-N3-C2	-4.69	119.59	126.34
26	BA	1939	5MU	C5-C6-N1	-4.66	118.54	123.34
24	AX	54	5MU	C5-C4-N3	4.65	119.28	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1917	PSU	C4-N3-C2	-4.64	119.66	126.34
26	BA	2457	PSU	N1-C2-N3	4.60	120.34	115.13
26	BA	2580	PSU	C4-N3-C2	-4.60	119.72	126.34
26	BA	955	PSU	C4-N3-C2	-4.57	119.75	126.34
24	AX	39	PSU	C4-N3-C2	-4.56	119.76	126.34
26	BA	2604	PSU	C4-N3-C2	-4.52	119.83	126.34
1	AA	516	PSU	C4-N3-C2	-4.52	119.83	126.34
24	AX	32	PSU	C4-N3-C2	-4.51	119.85	126.34
26	BA	2580	PSU	N1-C2-N3	4.48	120.20	115.13
24	AX	46	7MG	C2-N3-C4	4.48	120.28	112.30
26	BA	747	5MU	C5-C4-N3	4.45	119.11	115.31
24	AX	32	PSU	N1-C2-N3	4.42	120.14	115.13
26	BA	746	PSU	N1-C2-N3	4.41	120.13	115.13
26	BA	1917	PSU	N1-C2-N3	4.41	120.13	115.13
23	AW	55	PSU	C4-N3-C2	-4.40	120.00	126.34
26	BA	1911	PSU	N1-C2-N3	4.39	120.11	115.13
26	BA	747	5MU	O4-C4-C5	-4.39	119.82	124.90
24	AX	39	PSU	N1-C2-N3	4.36	120.07	115.13
23	AW	55	PSU	N1-C2-N3	4.31	120.02	115.13
23	AW	54	5MU	C5-C4-N3	4.31	118.99	115.31
26	BA	1915	3TD	C4-N3-C2	-4.22	120.03	124.61
26	BA	2030	6MZ	C2-N1-C6	4.20	120.19	116.59
1	AA	516	PSU	N1-C2-N3	4.20	119.89	115.13
26	BA	2604	PSU	N1-C2-N3	4.15	119.83	115.13
24	AX	54	5MU	O4-C4-C5	-4.14	120.10	124.90
26	BA	955	PSU	N1-C2-N3	4.09	119.76	115.13
26	BA	745	1MG	C5-C6-N1	4.03	119.96	113.90
12	AL	89	D2T	CB1-SB-CB	4.02	109.71	102.44
24	AX	47	3AU	N3-C2-N1	3.95	120.13	114.89
24	AX	8	4SU	N3-C2-N1	3.94	120.12	114.89
26	BA	1939	5MU	O4-C4-C5	-3.84	120.45	124.90
23	AW	54	5MU	C5-C6-N1	-3.84	119.39	123.34
23	AW	8	4SU	N3-C2-N1	3.83	119.98	114.89
23	AW	54	5MU	O4-C4-C5	-3.80	120.50	124.90
26	BA	2552	OMU	N3-C2-N1	3.74	119.86	114.89
24	AX	54	5MU	C5-C6-N1	-3.74	119.49	123.34
26	BA	1835	2MG	C5-C6-N1	3.74	120.56	113.95
26	BA	1618	6MZ	C2-N1-C6	3.73	119.78	116.59
26	BA	747	5MU	C5-C6-N1	-3.70	119.53	123.34
26	BA	1962	5MC	C5-C6-N1	-3.58	119.65	123.34
26	BA	2503	2MA	C5-C6-N1	3.53	120.11	114.02
26	BA	2251	OMG	C5-C6-N1	3.52	120.16	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	8	4SU	C5-C4-S4	-3.51	119.95	124.47
26	BA	1939	5MU	O2-C2-N1	-3.50	118.13	122.79
1	AA	1516	2MG	CM2-N2-C2	-3.48	116.16	123.86
1	AA	1407	5MC	C5-C6-N1	-3.45	119.79	123.34
1	AA	966	2MG	C5-C6-N1	3.42	119.99	113.95
1	AA	1516	2MG	C5-C6-N1	3.41	119.97	113.95
24	AX	8	4SU	C5-C4-S4	-3.40	120.09	124.47
26	BA	2445	2MG	C5-C6-N1	3.40	119.95	113.95
24	AX	46	7MG	O6-C6-C5	-3.37	119.52	127.24
1	AA	1207	2MG	C5-C6-N1	3.33	119.84	113.95
26	BA	2552	OMU	C5-C4-N3	3.31	119.80	114.84
24	AX	20	H2U	C5-C4-N3	3.28	120.34	116.65
24	AX	47	3AU	C5-C4-N3	3.27	119.74	114.84
26	BA	746	PSU	O2'-C2'-C3'	3.27	122.40	111.82
26	BA	2449	H2U	C5-C4-N3	3.17	120.21	116.65
24	AX	16	H2U	N3-C2-N1	3.12	119.95	116.65
1	AA	516	PSU	O4'-C1'-C2'	3.09	109.50	105.14
23	AW	20	H2U	N3-C2-N1	3.06	119.89	116.65
23	AW	55	PSU	O2-C2-N1	-3.05	119.43	122.79
26	BA	2251	OMG	C2-N1-C6	-3.04	119.50	125.10
24	AX	46	7MG	C2-N1-C6	-3.01	119.61	125.10
24	AX	46	7MG	N9-C4-N3	3.00	129.96	125.47
24	AX	55	PSU	O2-C2-N1	-3.00	119.49	122.79
26	BA	2552	OMU	O4-C4-C5	-2.98	119.92	125.16
26	BA	2069	G7M	C2-N1-C6	-2.98	119.62	125.10
26	BA	2449	H2U	N3-C2-N1	2.97	119.79	116.65
26	BA	2251	OMG	C8-N7-C5	2.96	108.63	102.99
1	AA	527	G7M	C2-N1-C6	-2.95	119.66	125.10
26	BA	1835	2MG	CM2-N2-C2	-2.93	117.38	123.86
12	AL	89	D2T	O-C-CA	-2.93	117.10	124.78
26	BA	2503	2MA	C8-N7-C5	2.89	108.50	102.99
26	BA	2580	PSU	O4'-C1'-C2'	2.88	109.20	105.14
1	AA	966	2MG	C8-N7-C5	2.87	108.46	102.99
24	AX	54	5MU	O2-C2-N1	-2.87	118.98	122.79
26	BA	746	PSU	C3'-C2'-C1'	2.86	104.97	101.64
26	BA	2449	H2U	O2-C2-N1	-2.85	119.53	123.11
26	BA	2504	PSU	O2-C2-N1	-2.84	119.66	122.79
26	BA	2605	PSU	O2-C2-N1	-2.81	119.69	122.79
26	BA	1835	2MG	C8-N7-C5	2.81	108.34	102.99
24	AX	47	3AU	O4-C4-C5	-2.81	120.22	125.16
24	AX	20	H2U	C5-C6-N1	2.77	120.75	111.61
26	BA	2445	2MG	C8-N7-C5	2.77	108.27	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	516	PSU	C3'-C2'-C1'	2.77	104.86	101.64
26	BA	2449	H2U	C5-C6-N1	2.74	120.66	111.61
23	AW	20	H2U	C5-C6-N1	2.74	120.64	111.61
26	BA	2580	PSU	O2-C2-N1	-2.73	119.78	122.79
26	BA	2580	PSU	C3'-C2'-C1'	2.73	104.82	101.64
1	AA	967	5MC	C5-C6-N1	-2.73	120.53	123.34
26	BA	745	1MG	C8-N7-C5	2.72	108.16	102.99
26	BA	1917	PSU	O2-C2-N1	-2.71	119.80	122.79
23	AW	20	H2U	C5-C4-N3	2.71	119.70	116.65
24	AX	16	H2U	C5-C4-N3	2.71	119.69	116.65
24	AX	16	H2U	C5-C6-N1	2.70	120.50	111.61
1	AA	966	2MG	O3'-C3'-C4'	2.68	118.81	111.05
1	AA	1516	2MG	C8-N7-C5	2.65	108.03	102.99
26	BA	2445	2MG	CM2-N2-C2	-2.64	118.02	123.86
1	AA	1207	2MG	C8-N7-C5	2.62	107.98	102.99
26	BA	2504	PSU	C6-N1-C2	-2.62	120.01	122.68
24	AX	46	7MG	C5-C6-N1	2.61	120.10	112.31
1	AA	1402	4OC	CM4-N4-C4	-2.61	117.36	122.45
23	AW	55	PSU	C3'-C2'-C1'	2.60	104.66	101.64
24	AX	16	H2U	O2-C2-N1	-2.59	119.85	123.11
23	AW	54	5MU	O2-C2-N1	-2.57	119.36	122.79
23	AW	20	H2U	O2-C2-N1	-2.56	119.89	123.11
26	BA	2457	PSU	O2-C2-N1	-2.56	119.97	122.79
26	BA	747	5MU	O2-C2-N1	-2.55	119.40	122.79
26	BA	746	PSU	O2-C2-N1	-2.50	120.04	122.79
23	AW	55	PSU	C6-N1-C2	-2.50	120.13	122.68
1	AA	516	PSU	O2-C2-N1	-2.48	120.06	122.79
24	AX	55	PSU	C6-C5-C4	2.44	119.91	118.20
24	AX	20	H2U	N3-C2-N1	2.42	119.22	116.65
1	AA	516	PSU	C6-N1-C2	-2.41	120.22	122.68
26	BA	1917	PSU	C6-N1-C2	-2.39	120.24	122.68
1	AA	1207	2MG	O6-C6-C5	-2.38	119.73	124.37
1	AA	1516	2MG	O6-C6-C5	-2.37	119.74	124.37
24	AX	46	7MG	C5-C4-N9	2.36	109.97	106.68
26	BA	746	PSU	C6-C5-C4	2.34	119.83	118.20
23	AW	55	PSU	O2'-C2'-C3'	2.33	119.35	111.82
26	BA	2457	PSU	O4'-C1'-C2'	2.32	108.42	105.14
26	BA	1835	2MG	O6-C6-C5	-2.32	119.84	124.37
24	AX	32	PSU	C6-N1-C2	-2.31	120.32	122.68
1	AA	966	2MG	CM2-N2-C2	-2.31	118.76	123.86
26	BA	2504	PSU	C6-C5-C4	2.30	119.81	118.20
1	AA	1402	4OC	C6-C5-C4	2.30	119.78	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	AL	89	D2T	OD2-CG-CB	2.30	118.11	113.15
1	AA	966	2MG	O6-C6-C5	-2.30	119.89	124.37
26	BA	2580	PSU	C6-N1-C2	-2.30	120.34	122.68
26	BA	2605	PSU	C6-N1-C2	-2.28	120.35	122.68
26	BA	2498	OMC	O3'-C3'-C2'	2.28	117.65	111.17
26	BA	1618	6MZ	C9-N6-C6	-2.27	120.92	122.87
24	AX	37	MIA	C5-C6-N6	2.27	123.80	120.35
1	AA	527	G7M	N2-C2-N1	2.26	121.52	116.71
24	AX	55	PSU	C6-N1-C2	-2.23	120.40	122.68
26	BA	2504	PSU	O2'-C2'-C3'	2.23	119.04	111.82
23	AW	32	OMC	O2-C2-N3	-2.22	118.71	122.33
23	AW	8	4SU	O2-C2-N1	-2.22	119.83	122.79
26	BA	1911	PSU	O2-C2-N1	-2.21	120.36	122.79
24	AX	39	PSU	O4'-C1'-C2'	2.21	108.25	105.14
24	AX	46	7MG	C4-C5-N7	2.21	110.43	106.13
24	AX	32	PSU	O2-C2-N1	-2.19	120.38	122.79
26	BA	1917	PSU	O4'-C1'-C2'	2.19	108.23	105.14
24	AX	39	PSU	O2-C2-N1	-2.18	120.39	122.79
24	AX	8	4SU	C1'-N1-C2	2.18	121.52	117.57
26	BA	2604	PSU	O2-C2-N1	-2.17	120.40	122.79
1	AA	1207	2MG	CM2-N2-C2	-2.17	119.06	123.86
26	BA	955	PSU	C6-N1-C2	-2.17	120.46	122.68
26	BA	2445	2MG	O6-C6-C5	-2.17	120.13	124.37
26	BA	2251	OMG	O6-C6-C5	-2.16	120.16	124.37
26	BA	955	PSU	O2-C2-N1	-2.15	120.42	122.79
26	BA	2503	2MA	CM2-C2-N1	2.14	120.99	116.23
24	AX	39	PSU	C6-N1-C2	-2.12	120.52	122.68
26	BA	745	1MG	O6-C6-C5	-2.12	120.44	124.19
23	AW	55	PSU	O4'-C1'-C2'	2.10	108.11	105.14
26	BA	2605	PSU	C6-C5-C4	2.10	119.67	118.20
26	BA	1915	3TD	C6-C5-C4	2.09	119.66	118.22
26	BA	746	PSU	O2'-C2'-C1'	2.08	116.20	111.23
12	AL	89	D2T	CB-CA-N	2.08	113.53	109.10
26	BA	2605	PSU	O4'-C1'-C2'	2.05	108.03	105.14
26	BA	2069	G7M	N2-C2-N1	2.04	121.06	116.71
26	BA	746	PSU	C6-N1-C2	-2.03	120.61	122.68
26	BA	2457	PSU	C6-C5-C4	2.02	119.61	118.20
26	BA	2552	OMU	C1'-N1-C2	2.02	121.23	117.57
1	AA	516	PSU	O2'-C2'-C3'	2.02	118.36	111.82
26	BA	1915	3TD	O4'-C1'-C2'	2.01	107.98	105.14
1	AA	966	2MG	O4'-C4'-C3'	-2.01	101.13	105.11
26	BA	2457	PSU	C6-N1-C2	-2.00	120.64	122.68

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
24	AX	32	PSU	C2'-C1'-C5-C4
24	AX	46	7MG	O4'-C4'-C5'-O5'
39	BN	81	4D4	O-C-CA-CB
39	BN	81	4D4	CA-CB-CG-CD
23	AW	20	H2U	O4'-C1'-N1-C6
23	AW	20	H2U	C2'-C1'-N1-C2
23	AW	20	H2U	C2'-C1'-N1-C6
23	AW	32	OMC	C1'-C2'-O2'-CM2
26	BA	746	PSU	C2'-C1'-C5-C6
26	BA	746	PSU	O4'-C1'-C5-C6
26	BA	1618	6MZ	N1-C6-N6-C9
26	BA	1618	6MZ	O4'-C4'-C5'-O5'
26	BA	1618	6MZ	C3'-C4'-C5'-O5'
26	BA	1915	3TD	O4'-C1'-C5-C4
26	BA	1915	3TD	C2'-C1'-C5-C6
26	BA	1915	3TD	O4'-C1'-C5-C6
26	BA	2552	OMU	O4'-C4'-C5'-O5'
1	AA	967	5MC	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
24	AX	46	7MG	C3'-C4'-C5'-O5'
24	AX	55	PSU	O4'-C4'-C5'-O5'
23	AW	8	4SU	C3'-C4'-C5'-O5'
23	AW	55	PSU	C3'-C4'-C5'-O5'
26	BA	1917	PSU	C3'-C4'-C5'-O5'
26	BA	1917	PSU	O4'-C4'-C5'-O5'
26	BA	2030	6MZ	O4'-C4'-C5'-O5'
26	BA	2503	2MA	O4'-C4'-C5'-O5'
26	BA	2552	OMU	C3'-C4'-C5'-O5'
29	BD	150	MEQ	CA-CB-CG-CD
1	AA	516	PSU	C3'-C4'-C5'-O5'
1	AA	967	5MC	C3'-C4'-C5'-O5'
24	AX	55	PSU	C3'-C4'-C5'-O5'
23	AW	8	4SU	O4'-C4'-C5'-O5'
23	AW	20	H2U	C3'-C4'-C5'-O5'
23	AW	55	PSU	O4'-C4'-C5'-O5'
26	BA	2449	H2U	O4'-C4'-C5'-O5'
26	BA	2449	H2U	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
26	BA	2498	OMC	C3'-C4'-C5'-O5'
29	BD	150	MEQ	NE2-CD-CG-CB
29	BD	150	MEQ	OE1-CD-CG-CB
1	AA	1207	2MG	O4'-C4'-C5'-O5'
26	BA	2498	OMC	O4'-C4'-C5'-O5'
39	BN	81	4D4	OB-CB-CG-CD
23	AW	20	H2U	O4'-C4'-C5'-O5'
26	BA	2445	2MG	C3'-C4'-C5'-O5'
26	BA	2030	6MZ	C3'-C4'-C5'-O5'
26	BA	2030	6MZ	N1-C6-N6-C9
29	BD	150	MEQ	C-CA-CB-CG
24	AX	16	H2U	C2'-C1'-N1-C6
1	AA	1518	MA6	C5-C6-N6-C10
26	BA	2503	2MA	C3'-C4'-C5'-O5'
24	AX	20	H2U	C2'-C1'-N1-C2
23	AW	20	H2U	C4'-C5'-O5'-P
24	AX	20	H2U	C2'-C1'-N1-C6
26	BA	1618	6MZ	C5-C6-N6-C9
26	BA	2445	2MG	O4'-C4'-C5'-O5'
24	AX	47	3AU	C4'-C5'-O5'-P
26	BA	1911	PSU	O4'-C4'-C5'-O5'
26	BA	1939	5MU	O4'-C4'-C5'-O5'
1	AA	527	G7M	C4'-C5'-O5'-P
23	AW	20	H2U	O4'-C1'-N1-C2
26	BA	2069	G7M	C4'-C5'-O5'-P
24	AX	47	3AU	O4'-C4'-C5'-O5'
24	AX	16	H2U	O4'-C1'-N1-C2
24	AX	16	H2U	C2'-C1'-N1-C2
24	AX	55	PSU	O4'-C1'-C5-C4
39	BN	81	4D4	N-CA-CB-CG
1	AA	1519	MA6	C4'-C5'-O5'-P
1	AA	1207	2MG	C3'-C4'-C5'-O5'
23	AW	55	PSU	C4'-C5'-O5'-P
12	AL	89	D2T	CG-CB-SB-CB1
24	AX	32	PSU	O4'-C1'-C5-C6
24	AX	55	PSU	O4'-C1'-C5-C6
23	AW	32	OMC	C2'-C1'-N1-C2
26	BA	1939	5MU	C3'-C4'-C5'-O5'
24	AX	8	4SU	C2'-C1'-N1-C2
1	AA	516	PSU	O4'-C4'-C5'-O5'
26	BA	2069	G7M	O4'-C4'-C5'-O5'
1	AA	967	5MC	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
24	AX	16	H2U	C4'-C5'-O5'-P
24	AX	20	H2U	C4'-C5'-O5'-P
23	AW	32	OMC	C2'-C1'-N1-C6

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 484 ligands modelled in this entry, 483 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	$\#\|Z\| > 2$
67	PHE	AX	101	24	10,11,12	0.49	0	10,13,15	0.32	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
67	PHE	AX	101	24	-	2/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
67	AX	101	PHE	CA-CB-CG-CD1
67	AX	101	PHE	CA-CB-CG-CD2

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
63	CD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	1357:ILE	C	1358:PRO	N	1.15

5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11418. 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 (i)

This section was not generated.

5.2 Central slices (i)

This section was not generated.

5.3 Largest variance slices (i)

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

5.5 Orthogonal surface views (i)

This section was not generated.

5.6 Mask visualisation (i)

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

6 Map analysis (i)

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

6.1 Map-value distribution (i)

This section was not generated.

6.2 Volume estimate versus contour level (i)

This section was not generated.

6.3 Rotationally averaged power spectrum (i)

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 (i)

This section was not generated.