Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 02:38 pm BST

PDB ID	:	8CIV
EMDB ID	:	EMD-16684
Title	:	Translocation intermediate 5 (TI-5) of 80S S. cerevisiae ribosome with ligands and eEF2 in the presence of sordarin
Authors	:	Milicevic, N.; Jenner, L.; Myasnikov, A.; Yusupov, M.; Yusupova, G.
Deposited on	:	2023-02-10
Resolution	:	2.47 Å(reported)

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
buster-report	:	1.1.7 (2018)
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 2.47 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 91 unique types of molecules in this entry. The entry contains 207374 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 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	134	1073	676	208	189	0	0

- Molecule 2 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	70	563	360	104	99	0	0

- Molecule 3 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	97	769	475	160	129	5	0	0

- Molecule 4 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	81	610	382	110	113	5	0	0

- Molecule 5 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	63	497	306	99	91	1	0	0

- Molecule 6 is a protein called HLJ1_G0030400.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	49	404	249	86	65	4	0	0

- Molecule 7 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	53	Total	C	N	O	S	0	0
			427	269	88	69	1		

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	318	Total	C	N	O	S	0	0
			2436	1541	418	469	8		

- Molecule 9 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	36	Total	C	N	O	S	0	0
			276	173	54	45	4		

- Molecule 10 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 11 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	3197	Total	C	N	O	P	0	0
			68429	30589	12334	22309	3197		

- Molecule 12 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Aa	816	Total	C	N	O	S	0	0
			6368	4051	1088	1198	31		

- Molecule 13 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	B	154	Total	C	N	O	0	0
			1222	761	237	224		

- Molecule 14 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BB	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 15 is a RNA chain called Transfer RNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Bb	76	Total	C	N	O	P	0	0
			1638	736	294	533	75		

- Molecule 16 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 17 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CC	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 18 is a RNA chain called Transfer RNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Cc	77	Total	C	N	O	P	0	0
			1644	732	298	537	77		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cc	18	C	U	conflict	GB 170517292

- Molecule 19 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	D	176	Total	C	N	O	0	0
			1423	875	308	240		

- Molecule 20 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DD	197	Total	C	N	O	S	0	0
			1531	980	266	281	4		

- Molecule 21 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Dd	6	Total	C	N	O	P	0	0
			125	56	18	45	6		

- Molecule 22 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	E	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 23 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	EE	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 24 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ee	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 25 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 26 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	FF	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 27 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	G	97	Total 770	C 499	N 126	O 145	0	0

- Molecule 28 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	GG	361	Total 2748	C 1729	N 522	O 494	S 3	0	0

- Molecule 29 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H	129	Total 963	C 607	N 180	O 169	S 7	0	0

- Molecule 30 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	HH	296	Total 2375	C 1501	N 414	O 458	S 2	0	0

- Molecule 31 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	63	Total 521	C 336	N 102	O 82	S 1	0	0

- Molecule 32 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	II	155	Total 1230	C 795	N 221	O 213	S 1	0	0

- Molecule 33 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	120	Total 959	C 617	N 168	O 172	S 2	0	0

- Molecule 34 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	JJ	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 35 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	K	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 36 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	KK	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 37 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	L	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 38 is a protein called RPL9A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LL	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 39 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	M	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 40 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	MM	215	Total	C	N	O	S	0	0
			1743	1102	331	303	7		

- Molecule 41 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	N	58	Total 462	C 289	N 100	O 73	0	0

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	NN	169	Total 1353	C 847	N 253	O 249	S 4	0	0

- Molecule 43 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	O	97	Total 742	C 479	N 124	O 138	S 1	0	0

- Molecule 44 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	OO	193	Total 1543	C 962	N 315	O 266	0	0

- Molecule 45 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	P	109	Total 883	C 559	N 167	O 156	S 1	0	0

- Molecule 46 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	PP	136	Total 1053	C 675	N 199	O 177	S 2	0	0

- Molecule 47 is a protein called Polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Pp	2	Total 19	C 14	N 2	O 2	S 1	0	0

- Molecule 48 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Q	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 49 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	QQ	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 50 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	R	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 51 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 52 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	T	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 53 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	U	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 54 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	V	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 55 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	W	77	Total 612	C 391	N 115	O 106	0	0

- Molecule 56 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	50	Total 436	C 272	N 97	O 65	S 2	0	0

- Molecule 57 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Y	52	Total 417	C 259	N 86	O 67	S 5	0	0

- Molecule 58 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Z	25	Total 233	C 142	N 63	O 27	S 1	0	0

- Molecule 59 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	a	102	Total 819	C 514	N 166	O 134	S 5	0	0

- Molecule 60 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	b	91	Total 694	C 429	N 138	O 121	S 6	0	0

- Molecule 61 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	c	1622	Total 34613	C 15487	N 6148	O 11356	P 1622	0	0

- Molecule 62 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	d	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 63 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	e	212	Total	C	N	O	S	0	0
			1689	1073	303	309	4		

- Molecule 64 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	f	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 65 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	g	183	Total	C	N	O	S	0	0
			1412	893	260	253	6		

- Molecule 66 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	h	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 67 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	i	199	Total	C	N	O	S	0	0
			1572	987	290	292	3		

- Molecule 68 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	j	219	Total	C	N	O	S	0	0
			1766	1108	341	314	3		

- Molecule 69 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	k	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 70 is a protein called 40S ribosomal protein S8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	l	184	Total	C	N	O	S	0	0
			1457	906	291	258	2		

- Molecule 71 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	m	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 72 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	n	33	Total	C	N	O	0	0
			300	199	46	55		

- Molecule 73 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	o	142	Total	C	N	O	S	0	0
			1146	735	217	191	3		

- Molecule 74 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	p	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 75 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	q	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 76 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	r	91	Total	C	N	O	S	0	0
			732	469	138	120	5		

- Molecule 77 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
77	s	137	Total	C	N	O	0	0
			1080	692	199	189		

- Molecule 78 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	t	121	Total	C	N	O	S	0	0
			961	599	182	178	2		

- Molecule 79 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	u	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 80 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	v	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 81 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	w	100	Total	C	N	O	S	0	0
			800	509	144	146	1		

- Molecule 82 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	x	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 83 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	y	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 84 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	z	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	2	1	Total	Zn	0
			1	1	
85	5	1	Total	Zn	0
			1	1	
85	8	1	Total	Zn	0
			1	1	
85	S	1	Total	Zn	0
			1	1	
85	V	1	Total	Zn	0
			1	1	
85	Y	1	Total	Zn	0
			1	1	
85	a	1	Total	Zn	0
			1	1	
85	b	1	Total	Zn	0
			1	1	

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	AA	192	Total	Mg	0
			192	192	
86	Aa	1	Total	Mg	0
			1	1	
86	B	1	Total	Mg	0
			1	1	
86	BB	5	Total	Mg	0
			5	5	
86	Bb	1	Total	Mg	0
			1	1	

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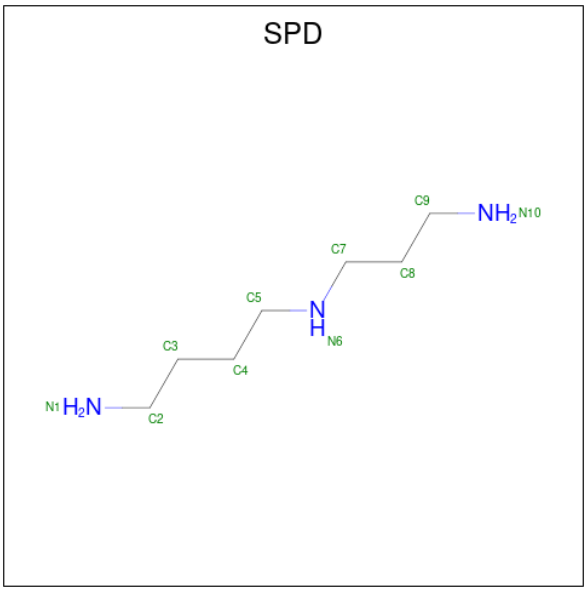
Mol	Chain	Residues	Atoms	AltConf
86	CC	3	Total Mg 3 3	0
86	FF	1	Total Mg 1 1	0
86	H	1	Total Mg 1 1	0
86	MM	1	Total Mg 1 1	0
86	QQ	1	Total Mg 1 1	0
86	c	44	Total Mg 44 44	0

- Molecule 87 is POTASSIUM ION (three-letter code: K) (formula: K).

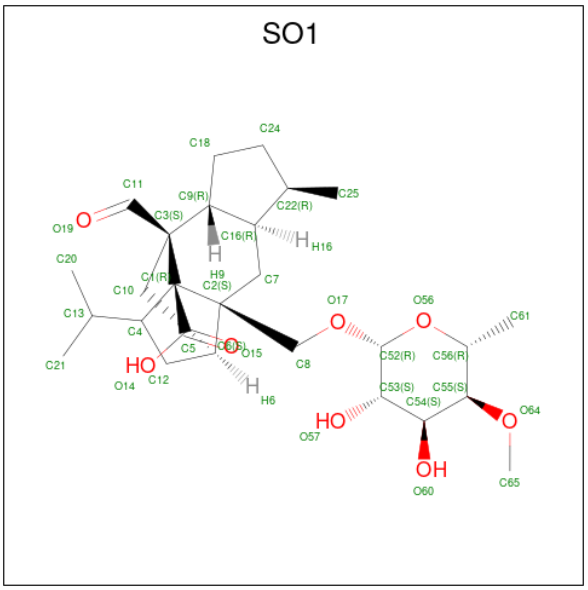
Mol	Chain	Residues	Atoms	AltConf
87	AA	13	Total K 13 13	0
87	EE	1	Total K 1 1	0
87	MM	1	Total K 1 1	0
87	Q	1	Total K 1 1	0
87	S	1	Total K 1 1	0
87	a	1	Total K 1 1	0
87	c	2	Total K 2 2	0
87	q	1	Total K 1 1	0

- Molecule 88 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



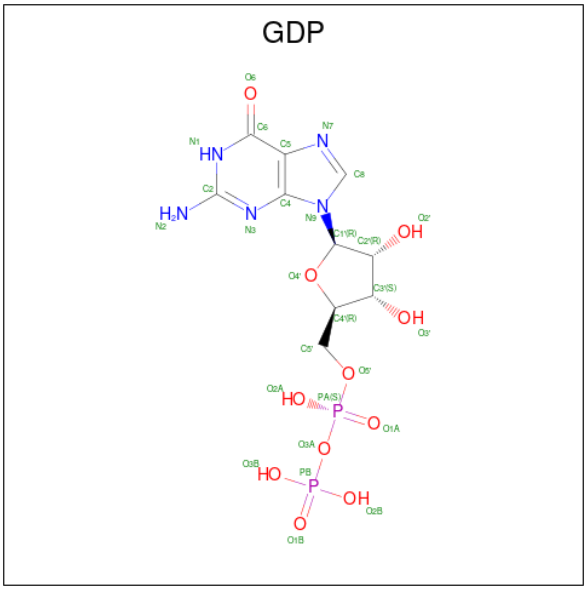
Mol	Chain	Residues	Atoms	AltConf
88	AA	1	Total C N 10 7 3	0
88	AA	1	Total C N 10 7 3	0
88	AA	1	Total C N 10 7 3	0

- Molecule 89 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula: $C_{27}H_{42}O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
89	Aa	1	Total C O 35 27 8	0

- Molecule 90 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
90	Aa	1	Total C N O P 28 10 5 11 2	0

- Molecule 91 is water.

Mol	Chain	Residues	Atoms	AltConf
91	2	2	Total O 2 2	0
91	A	2	Total O 2 2	0
91	AA	748	Total O 748 748	0
91	B	3	Total O 3 3	0
91	BB	12	Total O 12 12	0
91	CC	13	Total O 13 13	0
91	Cc	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
91	D	2	Total O 2 2	0
91	EE	9	Total O 9 9	0
91	F	3	Total O 3 3	0
91	FF	3	Total O 3 3	0
91	GG	2	Total O 2 2	0
91	H	3	Total O 3 3	0
91	HH	1	Total O 1 1	0
91	J	1	Total O 1 1	0
91	JJ	1	Total O 1 1	0
91	M	3	Total O 3 3	0
91	MM	2	Total O 2 2	0
91	N	1	Total O 1 1	0
91	Q	4	Total O 4 4	0
91	QQ	7	Total O 7 7	0
91	V	2	Total O 2 2	0
91	c	116	Total O 116 116	0
91	e	1	Total O 1 1	0
91	h	3	Total O 3 3	0
91	o	1	Total O 1 1	0
91	p	1	Total O 1 1	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	23733	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	270000	Depositor
Image detector	FEI FALCON IV (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

62 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	$\#\|Z\| > 2$
11	OMG	AA	2793	11	18,26,27	1.32	2 (11%)	19,38,41	1.20	3 (15%)
11	OMC	AA	663	11	19,22,23	1.20	2 (10%)	26,31,34	0.84	0
61	A2M	c	796	61	18,25,26	3.63	8 (44%)	18,36,39	3.29	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	OMU	AA	2347	11	19,22,23	1.74	4 (21%)	26,31,34	1.91	5 (19%)
11	A2M	AA	2280	11	18,25,26	0.99	0	18,36,39	1.26	2 (11%)
61	A2M	c	28	61	18,25,26	0.99	0	18,36,39	1.39	3 (16%)
11	OMU	AA	2921	86,11	19,22,23	1.71	4 (21%)	26,31,34	2.17	6 (23%)
12	DDE	Aa	699	12	14,20,21	0.94	0	14,28,30	1.08	1 (7%)
61	A2M	c	436	61	18,25,26	3.62	8 (44%)	18,36,39	3.39	3 (16%)
11	OMG	AA	2922	11	18,26,27	1.48	4 (22%)	19,38,41	1.55	3 (15%)
61	A2M	c	974	61	18,25,26	3.63	8 (44%)	18,36,39	3.44	4 (22%)
61	OMG	c	562	61	18,26,27	1.19	2 (11%)	19,38,41	0.93	1 (5%)
11	OMG	AA	2619	15,11	18,26,27	1.35	2 (11%)	19,38,41	1.22	2 (10%)
61	OMG	c	1126	61	18,26,27	1.20	2 (11%)	19,38,41	0.89	1 (5%)
61	OMC	c	1639	86,61	19,22,23	0.58	0	26,31,34	0.56	0
61	OMC	c	414	61	19,22,23	0.55	0	26,31,34	0.60	0
11	5MC	AA	2278	86,11	18,22,23	1.20	1 (5%)	26,32,35	1.50	5 (19%)
11	5MC	AA	2870	87,11	18,22,23	1.15	2 (11%)	26,32,35	1.61	6 (23%)
11	OMC	AA	1437	86,11	19,22,23	0.85	0	26,31,34	1.04	1 (3%)
61	B8N	c	1191	61	24,29,30	3.03	6 (25%)	29,42,45	1.75	7 (24%)
11	A2M	AA	2256	11	18,25,26	0.95	1 (5%)	18,36,39	1.69	4 (22%)
11	OMU	AA	2729	11	19,22,23	1.70	4 (21%)	26,31,34	1.87	4 (15%)
11	OMC	AA	2197	87,11	19,22,23	1.15	1 (5%)	26,31,34	1.36	3 (11%)
11	1MA	AA	645	86,11	16,25,26	1.50	3 (18%)	18,37,40	1.34	4 (22%)
11	OMU	AA	2421	11	19,22,23	1.73	4 (21%)	26,31,34	2.01	6 (23%)
11	OMU	AA	1888	11	19,22,23	1.67	4 (21%)	26,31,34	2.21	8 (30%)
11	OMC	AA	2948	11	19,22,23	1.18	2 (10%)	26,31,34	1.04	1 (3%)
61	OMC	c	1007	61	19,22,23	0.60	0	26,31,34	0.64	0
61	MA6	c	1782	61	18,26,27	1.03	2 (11%)	19,38,41	3.60	2 (10%)
11	OMC	AA	2959	86,11	19,22,23	1.11	2 (10%)	26,31,34	1.16	2 (7%)
11	A2M	AA	2220	11	18,25,26	0.89	0	18,36,39	1.28	3 (16%)
11	A2M	AA	2640	11	18,25,26	0.99	0	18,36,39	1.36	3 (16%)
11	A2M	AA	1449	86,11	18,25,26	1.10	1 (5%)	18,36,39	1.21	2 (11%)
61	4AC	c	1773	61	21,24,25	3.42	9 (42%)	29,34,37	1.99	6 (20%)
11	A2M	AA	876	11	18,25,26	1.18	1 (5%)	18,36,39	1.34	3 (16%)
11	OMU	AA	2724	11	19,22,23	1.67	5 (26%)	26,31,34	1.75	4 (15%)
11	OMG	AA	2288	11	18,26,27	1.33	1 (5%)	19,38,41	1.26	2 (10%)
11	1MA	AA	2142	86,11	16,25,26	1.52	3 (18%)	18,37,40	1.27	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	OMG	AA	867	87,11	18,26,27	1.45	2 (11%)	19,38,41	1.21	2 (10%)
61	A2M	c	541	61	18,25,26	3.63	8 (44%)	18,36,39	3.38	4 (22%)
61	MA6	c	1781	61	18,26,27	1.05	2 (11%)	19,38,41	3.31	2 (10%)
11	UR3	AA	2634	11	19,22,23	1.17	2 (10%)	26,32,35	1.73	2 (7%)
11	OMG	AA	805	11	18,26,27	1.27	1 (5%)	19,38,41	1.23	3 (15%)
11	A2M	AA	2281	11	18,25,26	0.98	0	18,36,39	1.52	3 (16%)
11	A2M	AA	807	11	18,25,26	0.94	0	18,36,39	1.35	2 (11%)
11	A2M	AA	649	11	18,25,26	1.01	0	18,36,39	1.47	4 (22%)
11	OMG	AA	2815	11	18,26,27	1.39	2 (11%)	19,38,41	1.25	1 (5%)
61	A2M	c	100	86,61	18,25,26	3.61	8 (44%)	18,36,39	3.25	4 (22%)
11	A2M	AA	1133	86,11	18,25,26	1.03	0	18,36,39	1.50	3 (16%)
61	A2M	c	420	61	18,25,26	3.61	8 (44%)	18,36,39	3.46	4 (22%)
11	OMG	AA	908	11	18,26,27	1.46	2 (11%)	19,38,41	1.35	3 (15%)
11	OMC	AA	650	11	19,22,23	1.10	2 (10%)	26,31,34	0.95	1 (3%)
61	A2M	c	619	86,61	18,25,26	0.92	1 (5%)	18,36,39	1.37	2 (11%)
11	OMG	AA	2791	11	18,26,27	1.19	1 (5%)	19,38,41	0.95	1 (5%)
11	OMU	AA	898	11	19,22,23	1.68	4 (21%)	26,31,34	2.03	6 (23%)
11	OMG	AA	1450	11	18,26,27	1.38	2 (11%)	19,38,41	1.29	3 (15%)
11	OMU	AA	2417	11	19,22,23	1.75	4 (21%)	26,31,34	2.08	6 (23%)
61	OMU	c	578	61	19,22,23	3.05	8 (42%)	26,31,34	1.70	5 (19%)
11	A2M	AA	2946	86,11	18,25,26	1.03	0	18,36,39	1.50	4 (22%)
11	A2M	AA	817	86,11	18,25,26	1.11	1 (5%)	18,36,39	1.52	4 (22%)
11	OMC	AA	2337	11	19,22,23	1.24	2 (10%)	26,31,34	0.99	1 (3%)
15	YYG	Bb	37	15	31,42,43	2.22	8 (25%)	33,62,65	1.86	9 (27%)

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
11	OMG	AA	2793	11	-	0/5/27/28	0/3/3/3
11	OMC	AA	663	11	-	1/9/27/28	0/2/2/2
61	A2M	c	796	61	-	0/5/27/28	0/3/3/3
11	OMU	AA	2347	11	-	0/9/27/28	0/2/2/2
11	A2M	AA	2280	11	-	2/5/27/28	0/3/3/3
61	A2M	c	28	61	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMU	AA	2921	86,11	-	0/9/27/28	0/2/2/2
12	DDE	Aa	699	12	-	0/20/21/23	0/1/1/1
61	A2M	c	436	61	-	0/5/27/28	0/3/3/3
11	OMG	AA	2922	11	-	3/5/27/28	0/3/3/3
61	A2M	c	974	61	-	0/5/27/28	0/3/3/3
61	OMG	c	562	61	-	2/5/27/28	0/3/3/3
11	OMG	AA	2619	15,11	-	2/5/27/28	0/3/3/3
61	OMG	c	1126	61	-	0/5/27/28	0/3/3/3
61	OMC	c	1639	86,61	-	0/9/27/28	0/2/2/2
61	OMC	c	414	61	-	1/9/27/28	0/2/2/2
11	5MC	AA	2278	86,11	-	0/7/25/26	0/2/2/2
11	5MC	AA	2870	87,11	-	4/7/25/26	0/2/2/2
11	OMC	AA	1437	86,11	-	2/9/27/28	0/2/2/2
61	B8N	c	1191	61	-	5/16/34/35	0/2/2/2
11	A2M	AA	2256	11	-	2/5/27/28	0/3/3/3
11	OMU	AA	2729	11	-	0/9/27/28	0/2/2/2
11	OMC	AA	2197	87,11	-	4/9/27/28	0/2/2/2
11	1MA	AA	645	86,11	-	0/3/25/26	0/3/3/3
11	OMU	AA	2421	11	-	0/9/27/28	0/2/2/2
11	OMU	AA	1888	11	-	0/9/27/28	0/2/2/2
11	OMC	AA	2948	11	-	1/9/27/28	0/2/2/2
61	OMC	c	1007	61	-	0/9/27/28	0/2/2/2
61	MA6	c	1782	61	-	2/7/29/30	0/3/3/3
11	OMC	AA	2959	86,11	-	0/9/27/28	0/2/2/2
11	A2M	AA	2220	11	-	3/5/27/28	0/3/3/3
11	A2M	AA	2640	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	1449	86,11	-	1/5/27/28	0/3/3/3
61	4AC	c	1773	61	-	1/11/29/30	0/2/2/2
11	A2M	AA	876	11	-	0/5/27/28	0/3/3/3
11	OMU	AA	2724	11	-	1/9/27/28	0/2/2/2
11	OMG	AA	2288	11	-	0/5/27/28	0/3/3/3
11	1MA	AA	2142	86,11	-	0/3/25/26	0/3/3/3
11	OMG	AA	867	87,11	-	2/5/27/28	0/3/3/3
61	A2M	c	541	61	-	2/5/27/28	0/3/3/3
61	MA6	c	1781	61	-	0/7/29/30	0/3/3/3
11	UR3	AA	2634	11	-	0/7/25/26	0/2/2/2
11	OMG	AA	805	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	2281	11	-	2/5/27/28	0/3/3/3
11	A2M	AA	807	11	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	A2M	AA	649	11	-	1/5/27/28	0/3/3/3
11	OMG	AA	2815	11	-	0/5/27/28	0/3/3/3
61	A2M	c	100	86,61	-	2/5/27/28	0/3/3/3
11	A2M	AA	1133	86,11	-	0/5/27/28	0/3/3/3
61	A2M	c	420	61	-	2/5/27/28	0/3/3/3
11	OMG	AA	908	11	-	2/5/27/28	0/3/3/3
11	OMC	AA	650	11	-	0/9/27/28	0/2/2/2
61	A2M	c	619	86,61	-	3/5/27/28	0/3/3/3
11	OMG	AA	2791	11	-	1/5/27/28	0/3/3/3
11	OMU	AA	898	11	-	0/9/27/28	0/2/2/2
11	OMG	AA	1450	11	-	2/5/27/28	0/3/3/3
11	OMU	AA	2417	11	-	1/9/27/28	0/2/2/2
61	OMU	c	578	61	-	2/9/27/28	0/2/2/2
11	A2M	AA	2946	86,11	-	1/5/27/28	0/3/3/3
11	A2M	AA	817	86,11	-	2/5/27/28	0/3/3/3
11	OMC	AA	2337	11	-	0/9/27/28	0/2/2/2
15	YYG	Bb	37	15	-	12/20/42/43	0/3/4/4

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	541	A2M	C3'-C4'	-9.14	1.29	1.53
61	c	420	A2M	C3'-C4'	-8.97	1.30	1.53
61	c	974	A2M	C3'-C4'	-8.95	1.30	1.53
61	c	100	A2M	C3'-C4'	-8.92	1.30	1.53
61	c	796	A2M	C3'-C4'	-8.92	1.30	1.53
61	c	436	A2M	C3'-C4'	-8.85	1.30	1.53
61	c	1191	B8N	C6-N1	7.80	1.55	1.36
61	c	1191	B8N	C4-N3	-7.76	1.26	1.40
61	c	796	A2M	O4'-C4'	7.73	1.62	1.45
61	c	1773	4AC	C4-N3	7.70	1.46	1.32
61	c	420	A2M	O4'-C4'	7.62	1.62	1.45
61	c	436	A2M	O4'-C4'	7.58	1.61	1.45
61	c	100	A2M	O4'-C4'	7.55	1.61	1.45
61	c	974	A2M	O4'-C4'	7.50	1.61	1.45
61	c	541	A2M	O4'-C4'	7.35	1.61	1.45
61	c	436	A2M	O4'-C1'	-7.28	1.30	1.41
61	c	541	A2M	O4'-C1'	-7.24	1.31	1.41
61	c	974	A2M	O4'-C1'	-7.24	1.31	1.41
15	Bb	37	YYG	C21-N20	7.23	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	100	A2M	O4'-C1'	-7.10	1.31	1.41
61	c	578	OMU	C2-N1	7.09	1.49	1.38
61	c	796	A2M	O4'-C1'	-7.01	1.31	1.41
61	c	420	A2M	O4'-C1'	-7.00	1.31	1.41
61	c	578	OMU	C2-N3	6.78	1.50	1.38
61	c	1773	4AC	C6-C5	6.06	1.49	1.35
61	c	1191	B8N	C2-N1	5.86	1.56	1.39
61	c	1773	4AC	C2-N3	5.81	1.48	1.36
61	c	578	OMU	C6-C5	5.73	1.48	1.35
15	Bb	37	YYG	O23-C21	5.40	1.43	1.34
61	c	1191	B8N	C6-C5	5.31	1.42	1.34
61	c	1773	4AC	C2-N1	5.26	1.51	1.40
61	c	1773	4AC	C4-N4	4.64	1.46	1.39
61	c	1773	4AC	C7-N4	4.56	1.45	1.37
11	AA	2815	OMG	C6-N1	-4.45	1.31	1.37
11	AA	2921	OMU	C4-N3	-4.25	1.31	1.38
61	c	578	OMU	C4-N3	4.21	1.46	1.38
11	AA	908	OMG	C6-N1	-4.21	1.31	1.37
11	AA	867	OMG	C6-N1	-4.20	1.31	1.37
11	AA	2729	OMU	C4-N3	-4.20	1.31	1.38
11	AA	2417	OMU	C4-N3	-4.20	1.31	1.38
11	AA	1888	OMU	C4-N3	-4.17	1.31	1.38
11	AA	1450	OMG	C6-N1	-4.16	1.31	1.37
11	AA	2347	OMU	C4-N3	-4.08	1.31	1.38
11	AA	2619	OMG	C6-N1	-4.01	1.31	1.37
15	Bb	37	YYG	O18-C16	4.00	1.43	1.33
11	AA	2922	OMG	C6-N1	-3.98	1.31	1.37
11	AA	2793	OMG	C6-N1	-3.94	1.32	1.37
61	c	1773	4AC	CM7-C7	3.93	1.58	1.50
11	AA	805	OMG	C6-N1	-3.89	1.32	1.37
11	AA	2421	OMU	C2-N3	-3.88	1.31	1.38
11	AA	2417	OMU	C2-N3	-3.87	1.31	1.38
11	AA	2347	OMU	C2-N3	-3.83	1.31	1.38
11	AA	2421	OMU	C4-N3	-3.72	1.31	1.38
11	AA	2729	OMU	C2-N3	-3.69	1.31	1.38
11	AA	2724	OMU	C2-N3	-3.69	1.31	1.38
11	AA	2791	OMG	C6-N1	-3.67	1.32	1.37
11	AA	2921	OMU	C2-N3	-3.67	1.31	1.38
11	AA	898	OMU	C4-N3	-3.63	1.32	1.38
11	AA	2288	OMG	C6-N1	-3.60	1.32	1.37
11	AA	2724	OMU	C4-N3	-3.60	1.32	1.38
61	c	1191	B8N	C1'-C5	3.47	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Bb	37	YYG	O6-C6	-3.47	1.17	1.22
61	c	1773	4AC	C5-C4	3.46	1.48	1.40
11	AA	898	OMU	C2-N3	-3.37	1.32	1.38
11	AA	1888	OMU	C2-N3	-3.32	1.32	1.38
11	AA	645	1MA	C2-N3	3.30	1.33	1.29
61	c	1773	4AC	O7-C7	-3.18	1.16	1.23
11	AA	2142	1MA	C2-N3	3.14	1.32	1.29
11	AA	2278	5MC	C6-N1	-3.13	1.32	1.38
61	c	420	A2M	C6-N6	3.12	1.45	1.34
61	c	541	A2M	C6-N6	3.10	1.45	1.34
61	c	796	A2M	C6-N6	3.09	1.45	1.34
61	c	974	A2M	C6-N6	3.07	1.45	1.34
61	c	436	A2M	C6-N6	3.07	1.45	1.34
61	c	100	A2M	C6-N6	3.05	1.45	1.34
15	Bb	37	YYG	C4-N3	-3.00	1.34	1.40
61	c	562	OMG	C8-N7	-2.97	1.30	1.35
61	c	578	OMU	O4-C4	-2.91	1.18	1.24
61	c	1126	OMG	C8-N7	-2.90	1.30	1.35
61	c	578	OMU	C6-N1	2.89	1.45	1.38
61	c	436	A2M	O3'-C3'	2.87	1.49	1.43
11	AA	2921	OMU	C5-C4	-2.87	1.37	1.43
15	Bb	37	YYG	C13-C12	2.87	1.58	1.50
61	c	796	A2M	O2'-C2'	-2.85	1.35	1.42
61	c	1781	MA6	C5-C4	-2.83	1.33	1.40
11	AA	2724	OMU	C5-C4	-2.82	1.37	1.43
11	AA	2417	OMU	C5-C4	-2.81	1.37	1.43
61	c	100	A2M	C5-C4	-2.80	1.33	1.40
61	c	796	A2M	O3'-C3'	2.79	1.49	1.43
61	c	974	A2M	C5-C4	-2.79	1.33	1.40
61	c	541	A2M	O3'-C3'	2.79	1.49	1.43
61	c	420	A2M	O3'-C3'	2.79	1.49	1.43
11	AA	2347	OMU	C5-C4	-2.78	1.37	1.43
11	AA	2870	5MC	C6-N1	-2.77	1.33	1.38
11	AA	2729	OMU	C5-C4	-2.76	1.37	1.43
11	AA	2421	OMU	C5-C4	-2.75	1.37	1.43
61	c	974	A2M	O3'-C3'	2.74	1.49	1.43
61	c	796	A2M	C5-C4	-2.73	1.33	1.40
61	c	436	A2M	C5-C4	-2.73	1.33	1.40
61	c	541	A2M	C5-C4	-2.73	1.33	1.40
61	c	100	A2M	O3'-C3'	2.73	1.49	1.43
61	c	974	A2M	O2'-C2'	-2.73	1.35	1.42
61	c	1782	MA6	C5-C4	-2.70	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	541	A2M	O2'-C2'	-2.69	1.35	1.42
61	c	436	A2M	O2'-C2'	-2.67	1.35	1.42
61	c	420	A2M	O2'-C2'	-2.64	1.35	1.42
61	c	100	A2M	O2'-C2'	-2.64	1.35	1.42
11	AA	898	OMU	C5-C4	-2.64	1.37	1.43
11	AA	663	OMC	C5-C4	-2.63	1.36	1.42
61	c	420	A2M	C5-C4	-2.60	1.34	1.40
15	Bb	37	YYG	C2-N1	-2.57	1.32	1.37
11	AA	2142	1MA	C6-N6	2.55	1.34	1.27
11	AA	1888	OMU	C5-C4	-2.53	1.38	1.43
61	c	1126	OMG	C5-C6	-2.53	1.42	1.47
15	Bb	37	YYG	C10-C11	2.52	1.54	1.50
61	c	578	OMU	C5-C4	2.50	1.49	1.43
11	AA	2142	1MA	C2'-C1'	-2.44	1.50	1.53
61	c	562	OMG	C5-C6	-2.44	1.42	1.47
11	AA	663	OMC	C6-N1	-2.42	1.32	1.38
11	AA	645	1MA	C6-N6	2.40	1.33	1.27
11	AA	2347	OMU	C6-N1	-2.40	1.32	1.38
11	AA	1450	OMG	C2-N1	-2.39	1.31	1.37
11	AA	898	OMU	C6-N1	-2.39	1.32	1.38
11	AA	2959	OMC	C5-C4	-2.39	1.37	1.42
11	AA	2815	OMG	C2-N1	-2.36	1.31	1.37
11	AA	1888	OMU	C6-N1	-2.35	1.32	1.38
11	AA	650	OMC	C5-C4	-2.35	1.37	1.42
11	AA	2922	OMG	O4'-C4'	-2.34	1.39	1.45
11	AA	2634	UR3	C6-N1	-2.34	1.32	1.38
11	AA	650	OMC	C6-N1	-2.33	1.32	1.38
61	c	578	OMU	O2-C2	-2.33	1.18	1.23
11	AA	645	1MA	C2'-C1'	-2.33	1.50	1.53
11	AA	2421	OMU	C6-N1	-2.32	1.32	1.38
11	AA	2922	OMG	O5'-C5'	-2.32	1.39	1.44
11	AA	2724	OMU	C6-N1	-2.32	1.32	1.38
11	AA	2337	OMC	C6-N1	-2.32	1.32	1.38
11	AA	2619	OMG	C2-N1	-2.28	1.32	1.37
11	AA	2197	OMC	C6-N1	-2.27	1.32	1.38
11	AA	2921	OMU	C6-N1	-2.27	1.32	1.38
61	c	1781	MA6	C2-N3	2.27	1.35	1.32
11	AA	2634	UR3	C5-C4	-2.26	1.38	1.43
11	AA	2337	OMC	C5-C4	-2.26	1.37	1.42
11	AA	2256	A2M	C5-C4	2.21	1.46	1.40
11	AA	2417	OMU	C6-N1	-2.20	1.32	1.38
11	AA	908	OMG	C2-N1	-2.20	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	c	420	A2M	C2-N3	2.19	1.35	1.32
61	c	1782	MA6	C2-N3	2.17	1.35	1.32
11	AA	2793	OMG	C2-N1	-2.17	1.32	1.37
11	AA	2959	OMC	C6-N1	-2.15	1.32	1.38
11	AA	876	A2M	C5-N7	-2.15	1.31	1.39
11	AA	867	OMG	C2-N1	-2.14	1.32	1.37
61	c	619	A2M	C5-C4	2.13	1.46	1.40
61	c	100	A2M	C2-N3	2.12	1.35	1.32
11	AA	2729	OMU	C6-N1	-2.12	1.32	1.38
11	AA	2870	5MC	C6-C5	2.11	1.38	1.34
61	c	1191	B8N	O4-C4	-2.10	1.18	1.23
11	AA	2922	OMG	C2-N1	-2.08	1.32	1.37
11	AA	817	A2M	O4'-C4'	-2.07	1.40	1.45
61	c	541	A2M	C2-N3	2.07	1.35	1.32
11	AA	2948	OMC	C6-N1	-2.07	1.33	1.38
11	AA	2948	OMC	C5-C4	-2.05	1.38	1.42
61	c	796	A2M	C2-N3	2.04	1.35	1.32
61	c	436	A2M	C2-N3	2.04	1.35	1.32
61	c	974	A2M	C2-N3	2.03	1.35	1.32
11	AA	1449	A2M	C5-N7	-2.01	1.32	1.39
11	AA	2724	OMU	O4'-C4'	-2.00	1.40	1.45

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	c	1782	MA6	N1-C6-N6	-14.48	101.81	117.06
61	c	1781	MA6	N1-C6-N6	-13.15	103.21	117.06
61	c	974	A2M	C5-C6-N6	10.85	136.84	120.35
61	c	420	A2M	C5-C6-N6	10.82	136.80	120.35
61	c	436	A2M	C5-C6-N6	10.58	136.44	120.35
61	c	541	A2M	C5-C6-N6	10.50	136.30	120.35
61	c	796	A2M	C5-C6-N6	10.34	136.06	120.35
61	c	100	A2M	C5-C6-N6	10.11	135.72	120.35
61	c	420	A2M	N6-C6-N1	-7.46	103.08	118.57
61	c	974	A2M	N6-C6-N1	-7.36	103.30	118.57
61	c	436	A2M	N6-C6-N1	-7.28	103.46	118.57
61	c	1773	4AC	N4-C4-N3	7.25	126.02	113.85
61	c	541	A2M	N6-C6-N1	-7.15	103.73	118.57
61	c	100	A2M	N6-C6-N1	-6.93	104.20	118.57
61	c	796	A2M	N6-C6-N1	-6.92	104.20	118.57
11	AA	2634	UR3	C4-N3-C2	-6.79	118.17	124.56
61	c	436	A2M	N3-C2-N1	-5.60	119.92	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	c	974	A2M	N3-C2-N1	-5.58	119.96	128.68
11	AA	1888	OMU	C4-N3-C2	-5.57	119.23	126.58
61	c	541	A2M	N3-C2-N1	-5.55	120.01	128.68
61	c	420	A2M	N3-C2-N1	-5.52	120.05	128.68
61	c	1781	MA6	N3-C2-N1	-5.52	120.05	128.68
61	c	100	A2M	N3-C2-N1	-5.51	120.06	128.68
61	c	1782	MA6	N3-C2-N1	-5.49	120.10	128.68
61	c	796	A2M	N3-C2-N1	-5.39	120.26	128.68
15	Bb	37	YYG	O23-C21-N20	5.31	120.12	110.80
11	AA	898	OMU	C4-N3-C2	-5.30	119.59	126.58
11	AA	2921	OMU	C4-N3-C2	-5.28	119.62	126.58
61	c	578	OMU	C4-N3-C2	-5.28	119.62	126.58
11	AA	1888	OMU	N3-C2-N1	5.27	121.88	114.89
61	c	1191	B8N	C5-C4-N3	5.19	125.78	116.17
11	AA	2421	OMU	C4-N3-C2	-5.15	119.79	126.58
11	AA	898	OMU	N3-C2-N1	5.14	121.72	114.89
11	AA	2417	OMU	N3-C2-N1	5.11	121.68	114.89
11	AA	2417	OMU	C4-N3-C2	-5.06	119.90	126.58
11	AA	2347	OMU	C4-N3-C2	-4.86	120.16	126.58
11	AA	2724	OMU	C4-N3-C2	-4.81	120.23	126.58
11	AA	2921	OMU	N3-C2-N1	4.79	121.25	114.89
61	c	1191	B8N	C4-N3-C2	-4.76	119.44	125.46
11	AA	2421	OMU	N3-C2-N1	4.76	121.20	114.89
61	c	1773	4AC	C5-C4-N4	-4.64	114.86	122.92
11	AA	2347	OMU	N3-C2-N1	4.48	120.84	114.89
11	AA	2921	OMU	C5-C4-N3	4.48	121.54	114.84
11	AA	2724	OMU	C5-C4-N3	4.42	121.45	114.84
11	AA	2417	OMU	C5-C4-N3	4.33	121.32	114.84
11	AA	2729	OMU	C4-N3-C2	-4.31	120.90	126.58
11	AA	2729	OMU	N3-C2-N1	4.29	120.58	114.89
11	AA	2421	OMU	C5-C4-N3	4.21	121.14	114.84
11	AA	2921	OMU	C2'-C1'-N1	-4.10	106.27	114.22
11	AA	2347	OMU	C5-C4-N3	4.08	120.94	114.84
11	AA	1888	OMU	C5-C4-N3	4.05	120.90	114.84
11	AA	2870	5MC	C5-C6-N1	-4.05	119.17	123.34
11	AA	1888	OMU	C2'-C1'-N1	-4.01	106.44	114.22
11	AA	2729	OMU	C5-C4-N3	3.93	120.72	114.84
61	c	28	A2M	N3-C2-N1	-3.86	122.64	128.68
61	c	578	OMU	N3-C2-N1	3.86	120.01	114.89
11	AA	2281	A2M	N3-C2-N1	-3.83	122.69	128.68
11	AA	807	A2M	N3-C2-N1	-3.79	122.76	128.68
11	AA	2724	OMU	N3-C2-N1	3.74	119.86	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	898	OMU	C5-C4-N3	3.73	120.42	114.84
11	AA	2278	5MC	C5-C6-N1	-3.69	119.54	123.34
11	AA	2922	OMG	C5'-C4'-C3'	-3.65	101.52	115.18
11	AA	1133	A2M	N3-C2-N1	-3.64	122.98	128.68
11	AA	2417	OMU	C2'-C1'-N1	-3.64	107.16	114.22
11	AA	2256	A2M	N3-C2-N1	-3.63	123.01	128.68
11	AA	649	A2M	N3-C2-N1	-3.48	123.23	128.68
11	AA	2640	A2M	N3-C2-N1	-3.44	123.31	128.68
11	AA	2220	A2M	N3-C2-N1	-3.42	123.34	128.68
15	Bb	37	YYG	O23-C21-O22	-3.39	119.59	124.58
11	AA	817	A2M	N3-C2-N1	-3.38	123.39	128.68
11	AA	2946	A2M	N3-C2-N1	-3.35	123.44	128.68
15	Bb	37	YYG	O18-C16-C15	3.35	120.08	111.52
11	AA	2815	OMG	C5-C6-N1	3.33	119.83	113.95
11	AA	2421	OMU	O4-C4-C5	-3.32	119.32	125.16
61	c	578	OMU	C5-C4-N3	3.26	119.72	114.84
11	AA	876	A2M	N3-C2-N1	-3.25	123.60	128.68
11	AA	2640	A2M	C4-C5-N7	-3.18	106.08	109.40
11	AA	1449	A2M	N3-C2-N1	-3.18	123.71	128.68
11	AA	2619	OMG	C5-C6-N1	3.15	119.51	113.95
15	Bb	37	YYG	C5-C6-N1	3.14	118.65	113.96
11	AA	2724	OMU	O4-C4-C5	-3.13	119.65	125.16
11	AA	898	OMU	O2-C2-N1	-3.12	118.64	122.79
61	c	619	A2M	N3-C2-N1	-3.12	123.81	128.68
61	c	1773	4AC	CM7-C7-N4	3.10	120.66	115.29
11	AA	805	OMG	C5-C6-N1	2.99	119.23	113.95
11	AA	1133	A2M	O4'-C4'-C3'	-2.99	99.21	105.11
11	AA	817	A2M	C4-C5-N7	-2.97	106.30	109.40
11	AA	2278	5MC	C3'-C2'-C1'	2.97	107.07	101.43
11	AA	2921	OMU	O4-C4-C5	-2.97	119.94	125.16
11	AA	1450	OMG	C5-C6-N1	2.95	119.17	113.95
11	AA	2870	5MC	O2-C2-N3	-2.94	117.55	122.33
11	AA	2948	OMC	O2-C2-N3	-2.93	117.56	122.33
11	AA	2870	5MC	C5-C4-N3	-2.93	118.51	121.67
11	AA	2280	A2M	N3-C2-N1	-2.93	124.10	128.68
61	c	1191	B8N	N3-C2-N1	2.91	120.87	116.76
11	AA	2256	A2M	C4-C5-N7	-2.91	106.37	109.40
11	AA	2959	OMC	C2'-C1'-N1	-2.91	108.58	114.22
11	AA	898	OMU	O4-C4-C5	-2.89	120.08	125.16
61	c	1773	4AC	C6-C5-C4	2.89	120.50	116.96
11	AA	2870	5MC	C3'-C2'-C1'	2.84	106.83	101.43
15	Bb	37	YYG	C8-N7-C5	2.83	108.39	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	2922	OMG	C5-C6-N1	2.81	118.92	113.95
11	AA	908	OMG	C5-C6-N1	2.80	118.89	113.95
15	Bb	37	YYG	O22-C21-N20	-2.78	120.29	124.85
11	AA	650	OMC	C2'-C1'-N1	-2.76	108.86	114.22
61	c	578	OMU	O4-C4-C5	-2.76	120.31	125.16
11	AA	2946	A2M	C4-C5-N7	-2.75	106.53	109.40
11	AA	867	OMG	C5-C6-N1	2.74	118.80	113.95
11	AA	908	OMG	O6-C6-C5	-2.72	119.06	124.37
11	AA	2421	OMU	C2'-C1'-N1	-2.72	108.95	114.22
11	AA	649	A2M	O2'-C2'-C1'	-2.70	103.75	109.09
11	AA	2278	5MC	C5-C4-N3	-2.70	118.77	121.67
11	AA	2347	OMU	O4-C4-C5	-2.65	120.51	125.16
11	AA	1437	OMC	C2'-C1'-N1	-2.63	109.11	114.22
11	AA	2793	OMG	C5-C6-N1	2.61	118.57	113.95
12	Aa	699	DDE	CBW-CBI-NAD	2.59	118.58	115.28
15	Bb	37	YYG	O6-C6-C5	-2.59	119.58	124.17
61	c	619	A2M	C4-C5-N7	-2.58	106.71	109.40
61	c	1773	4AC	C1'-N1-C2	2.57	124.16	118.42
61	c	1191	B8N	C31-N3-C2	2.57	121.53	117.67
11	AA	2281	A2M	C4-C5-N7	-2.56	106.73	109.40
11	AA	2959	OMC	O2-C2-N3	-2.56	118.17	122.33
11	AA	2197	OMC	O4'-C1'-C2'	-2.55	102.09	106.57
11	AA	2288	OMG	C5-C6-N1	2.54	118.43	113.95
11	AA	898	OMU	C2'-C1'-N1	-2.52	109.33	114.22
11	AA	2870	5MC	N1-C2-N3	2.51	123.37	118.81
11	AA	805	OMG	O6-C6-C5	-2.50	119.49	124.37
11	AA	1133	A2M	C4-C5-N7	-2.50	106.80	109.40
11	AA	908	OMG	O3'-C3'-C4'	-2.50	103.83	111.05
11	AA	2946	A2M	O4'-C4'-C3'	-2.49	100.18	105.11
61	c	541	A2M	C1'-N9-C4	2.48	131.00	126.64
11	AA	645	1MA	C5-C6-N1	2.46	117.57	113.90
11	AA	645	1MA	N1-C2-N3	-2.45	123.17	126.02
11	AA	2142	1MA	C8-N7-C5	2.43	107.62	102.99
11	AA	2946	A2M	C2-N1-C6	2.42	122.89	118.75
11	AA	2729	OMU	O4-C4-C5	-2.42	120.91	125.16
11	AA	2417	OMU	O4-C4-C5	-2.42	120.91	125.16
11	AA	2288	OMG	C8-N7-C5	2.41	107.58	102.99
11	AA	2197	OMC	O3'-C3'-C4'	-2.40	104.11	111.05
11	AA	2347	OMU	C2'-C1'-N1	-2.37	109.62	114.22
61	c	1191	B8N	O4-C4-N3	-2.35	115.98	119.98
61	c	562	OMG	O6-C6-C5	2.34	128.94	124.37
15	Bb	37	YYG	C14-C13-C12	2.34	117.95	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	649	A2M	C4-C5-N7	-2.34	106.96	109.40
11	AA	2634	UR3	C3U-N3-C4	2.33	121.22	117.89
61	c	100	A2M	C1'-N9-C4	2.33	130.74	126.64
11	AA	2142	1MA	C5-C6-N1	2.32	117.35	113.90
61	c	1126	OMG	O6-C6-C5	2.32	128.90	124.37
11	AA	2142	1MA	O4'-C1'-C2'	-2.31	103.55	106.93
11	AA	2280	A2M	C4-C5-N7	-2.31	106.99	109.40
11	AA	867	OMG	C8-N7-C5	2.30	107.38	102.99
11	AA	2256	A2M	C2-N1-C6	2.30	122.69	118.75
11	AA	2417	OMU	O2-C2-N1	-2.28	119.75	122.79
11	AA	1888	OMU	O4-C4-C5	-2.27	121.16	125.16
11	AA	649	A2M	O4'-C1'-C2'	-2.27	102.65	106.59
11	AA	645	1MA	C8-N7-C5	2.26	107.29	102.99
61	c	420	A2M	C1'-N9-C4	2.25	130.60	126.64
11	AA	2421	OMU	O2-C2-N1	-2.25	119.80	122.79
15	Bb	37	YYG	C3-N3-C4	2.23	120.67	116.71
61	c	796	A2M	C1'-N9-C4	2.22	130.55	126.64
61	c	28	A2M	O2'-C2'-C1'	-2.22	104.70	109.09
11	AA	2278	5MC	O2-C2-N3	-2.20	118.75	122.33
11	AA	2870	5MC	O4'-C1'-N1	2.20	113.40	108.36
11	AA	805	OMG	C8-N7-C5	2.20	107.17	102.99
61	c	578	OMU	O2-C2-N1	-2.19	119.87	122.79
11	AA	1888	OMU	O4'-C1'-N1	2.17	113.33	108.36
11	AA	2256	A2M	O2'-C2'-C1'	2.17	113.40	109.09
11	AA	2791	OMG	C5-C6-N1	2.17	117.79	113.95
11	AA	2278	5MC	CM5-C5-C6	-2.16	119.96	122.85
11	AA	2220	A2M	C2-N1-C6	2.16	122.45	118.75
11	AA	2619	OMG	C8-N7-C5	2.16	107.10	102.99
11	AA	2197	OMC	C1'-N1-C6	2.16	125.54	120.84
61	c	1773	4AC	C5-C4-N3	-2.16	119.12	122.59
11	AA	2921	OMU	O2-C2-N1	-2.15	119.93	122.79
11	AA	2793	OMG	C8-N7-C5	2.15	107.08	102.99
11	AA	817	A2M	O3'-C3'-C4'	-2.15	104.84	111.05
11	AA	645	1MA	O4'-C1'-C2'	-2.14	103.79	106.93
11	AA	807	A2M	C2-N1-C6	2.14	122.41	118.75
11	AA	1449	A2M	C4-C5-N7	-2.13	107.18	109.40
11	AA	1888	OMU	O2-C2-N3	-2.10	117.59	121.50
61	c	28	A2M	C4-C5-N7	-2.10	107.21	109.40
11	AA	1888	OMU	C5-C6-N1	-2.09	118.30	121.81
11	AA	2220	A2M	C4-C5-N7	-2.09	107.22	109.40
11	AA	876	A2M	N6-C6-N1	2.09	122.91	118.57
11	AA	2281	A2M	C2-N1-C6	2.08	122.31	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	2142	1MA	N1-C2-N3	-2.08	123.60	126.02
61	c	1191	B8N	O36-C34-C33	2.07	120.44	113.38
11	AA	817	A2M	C1'-N9-C4	-2.05	123.03	126.64
61	c	1191	B8N	O36-C34-O35	-2.05	119.42	124.09
61	c	974	A2M	C1'-N9-C4	2.05	130.25	126.64
11	AA	2337	OMC	C2'-C1'-N1	-2.04	110.25	114.22
11	AA	2793	OMG	O6-C6-C5	-2.03	120.41	124.37
11	AA	2922	OMG	C8-N7-C5	2.03	106.86	102.99
11	AA	1450	OMG	C2-N1-C6	-2.02	121.37	125.10
11	AA	1450	OMG	C8-N7-C5	2.02	106.85	102.99
11	AA	876	A2M	C4-C5-N7	-2.01	107.30	109.40
11	AA	2640	A2M	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AA	663	OMC	C1'-C2'-O2'-CM2
11	AA	908	OMG	C3'-C4'-C5'-O5'
11	AA	1437	OMC	C1'-C2'-O2'-CM2
11	AA	1450	OMG	O4'-C4'-C5'-O5'
11	AA	2197	OMC	C2'-C1'-N1-C2
11	AA	2197	OMC	C2'-C1'-N1-C6
11	AA	2220	A2M	C1'-C2'-O2'-CM'
11	AA	2256	A2M	C1'-C2'-O2'-CM'
11	AA	2281	A2M	O4'-C4'-C5'-O5'
11	AA	2281	A2M	C3'-C4'-C5'-O5'
11	AA	2417	OMU	C1'-C2'-O2'-CM2
11	AA	2619	OMG	C1'-C2'-O2'-CM2
11	AA	2791	OMG	C1'-C2'-O2'-CM2
11	AA	2922	OMG	C3'-C4'-C5'-O5'
11	AA	2946	A2M	C1'-C2'-O2'-CM'
11	AA	2948	OMC	C1'-C2'-O2'-CM2
15	Bb	37	YYG	N1-C12-C13-C14
15	Bb	37	YYG	C11-C12-C13-C14
15	Bb	37	YYG	C12-C13-C14-C15
15	Bb	37	YYG	C16-C15-N20-C21
15	Bb	37	YYG	O23-C21-N20-C15
61	c	414	OMC	C1'-C2'-O2'-CM2
61	c	541	A2M	C3'-C4'-C5'-O5'
61	c	562	OMG	C3'-C4'-C5'-O5'
61	c	578	OMU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
61	c	578	OMU	O4'-C4'-C5'-O5'
61	c	619	A2M	C1'-C2'-O2'-CM'
61	c	1191	B8N	C2'-C1'-C5-C6
61	c	1191	B8N	C2'-C1'-C5-C4
15	Bb	37	YYG	O17-C16-O18-C19
15	Bb	37	YYG	C15-C16-O18-C19
15	Bb	37	YYG	O22-C21-N20-C15
61	c	1191	B8N	C32-C31-N3-C4
11	AA	867	OMG	C3'-C4'-C5'-O5'
11	AA	908	OMG	O4'-C4'-C5'-O5'
11	AA	1450	OMG	C3'-C4'-C5'-O5'
61	c	619	A2M	O4'-C4'-C5'-O5'
61	c	619	A2M	C3'-C4'-C5'-O5'
11	AA	2922	OMG	O4'-C4'-C5'-O5'
61	c	100	A2M	O4'-C4'-C5'-O5'
61	c	541	A2M	O4'-C4'-C5'-O5'
61	c	562	OMG	O4'-C4'-C5'-O5'
61	c	1191	B8N	C32-C31-N3-C2
15	Bb	37	YYG	C13-C14-C15-N20
11	AA	867	OMG	O4'-C4'-C5'-O5'
11	AA	2220	A2M	O4'-C4'-C5'-O5'
11	AA	2220	A2M	C3'-C4'-C5'-O5'
15	Bb	37	YYG	C13-C14-C15-C16
11	AA	2870	5MC	C2'-C1'-N1-C6
61	c	420	A2M	C1'-C2'-O2'-CM'
61	c	1782	MA6	C4'-C5'-O5'-P
11	AA	2197	OMC	O4'-C1'-N1-C2
15	Bb	37	YYG	N20-C15-C16-O17
61	c	1773	4AC	N3-C4-N4-C7
11	AA	817	A2M	C4'-C5'-O5'-P
61	c	1191	B8N	N3-C31-C32-C33
11	AA	2197	OMC	O4'-C1'-N1-C6
11	AA	2280	A2M	O4'-C4'-C5'-O5'
61	c	420	A2M	O4'-C4'-C5'-O5'
11	AA	2870	5MC	O4'-C1'-N1-C6
15	Bb	37	YYG	N20-C15-C16-O18
11	AA	1449	A2M	C3'-C2'-O2'-CM'
11	AA	2280	A2M	C3'-C2'-O2'-CM'
11	AA	2619	OMG	C3'-C4'-C5'-O5'
11	AA	2922	OMG	C3'-C2'-O2'-CM2
11	AA	2870	5MC	O4'-C1'-N1-C2
11	AA	649	A2M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
61	c	28	A2M	O4'-C4'-C5'-O5'
61	c	100	A2M	C3'-C4'-C5'-O5'
11	AA	2724	OMU	C1'-C2'-O2'-CM2
11	AA	807	A2M	C3'-C2'-O2'-CM'
61	c	1782	MA6	C3'-C4'-C5'-O5'
11	AA	2870	5MC	C2'-C1'-N1-C2
11	AA	2256	A2M	O4'-C4'-C5'-O5'
11	AA	817	A2M	O4'-C4'-C5'-O5'
11	AA	1437	OMC	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 285 ligands modelled in this entry, 280 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
88	SPD	AA	3605	-	9,9,9	0.31	0	8,8,8	0.97	0
88	SPD	AA	3606	-	9,9,9	0.31	0	8,8,8	0.72	0
90	GDP	Aa	1102	-	24,30,30	0.92	1 (4%)	30,47,47	1.33	4 (13%)
89	SO1	Aa	1101	-	35,39,39	1.13	2 (5%)	39,64,64	1.05	2 (5%)
88	SPD	AA	3608	-	9,9,9	0.33	0	8,8,8	0.82	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
88	SPD	AA	3605	-	-	0/7/7/7	-
88	SPD	AA	3606	-	-	1/7/7/7	-
90	GDP	Aa	1102	-	-	7/12/32/32	0/3/3/3
89	SO1	Aa	1101	-	-	11/21/104/104	0/7/5/5
88	SPD	AA	3608	-	-	2/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	Aa	1101	SO1	C2-C6	-3.89	1.49	1.55
90	Aa	1102	GDP	C6-N1	-2.45	1.34	1.37
89	Aa	1101	SO1	C16-C22	-2.36	1.51	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
90	Aa	1102	GDP	PA-O3A-PB	-3.44	121.04	132.83
90	Aa	1102	GDP	C3'-C2'-C1'	3.30	105.94	100.98
89	Aa	1101	SO1	C12-C6-C10	-2.55	105.89	107.91
90	Aa	1102	GDP	C8-N7-C5	2.36	107.48	102.99
90	Aa	1102	GDP	C5-C6-N1	2.31	118.03	113.95
89	Aa	1101	SO1	C7-C2-C6	2.08	116.11	112.17

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	Aa	1101	SO1	C20-C13-C4-C1
89	Aa	1101	SO1	C21-C13-C4-C1
89	Aa	1101	SO1	C20-C13-C4-C12
89	Aa	1101	SO1	C21-C13-C4-C12
89	Aa	1101	SO1	O19-C11-C3-C1
89	Aa	1101	SO1	O19-C11-C3-C10
90	Aa	1102	GDP	C5'-O5'-PA-O1A
90	Aa	1102	GDP	C5'-O5'-PA-O2A
90	Aa	1102	GDP	O4'-C4'-C5'-O5'
90	Aa	1102	GDP	C3'-C4'-C5'-O5'
88	AA	3608	SPD	C7-C8-C9-N10
89	Aa	1101	SO1	C3-C1-C5-O14
88	AA	3606	SPD	N1-C2-C3-C4
90	Aa	1102	GDP	C5'-O5'-PA-O3A

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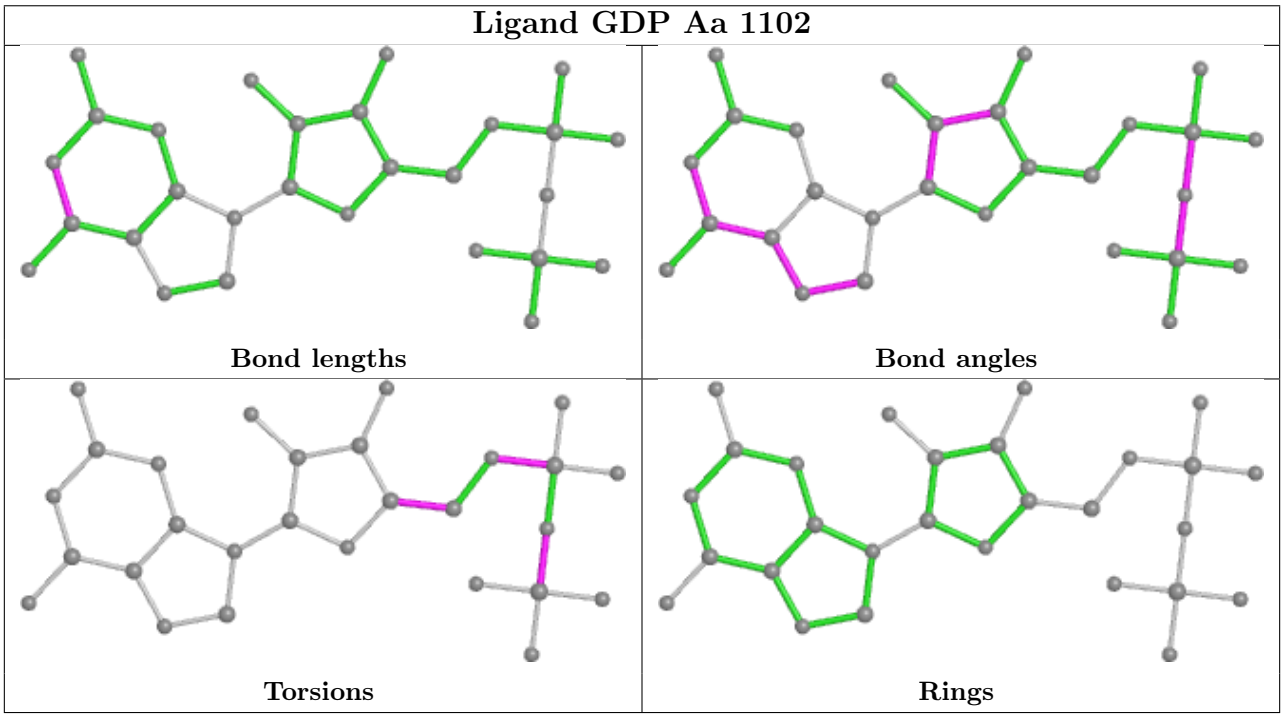
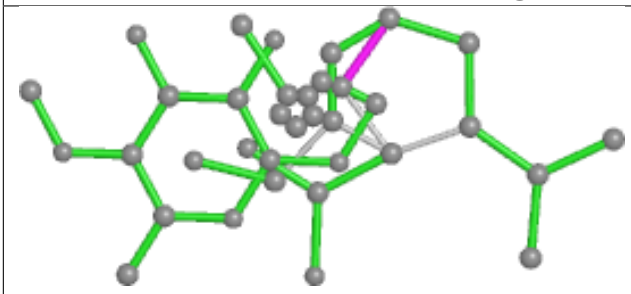
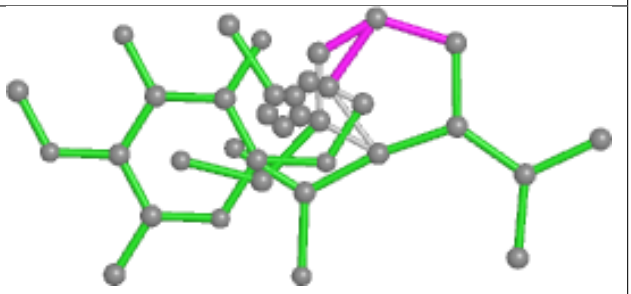
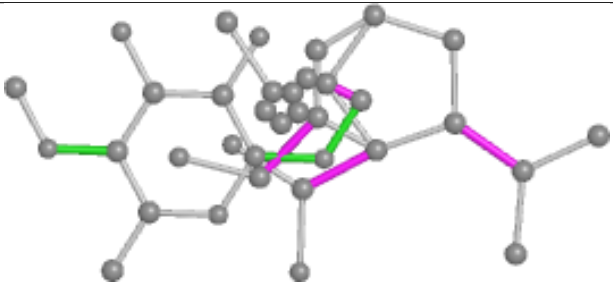
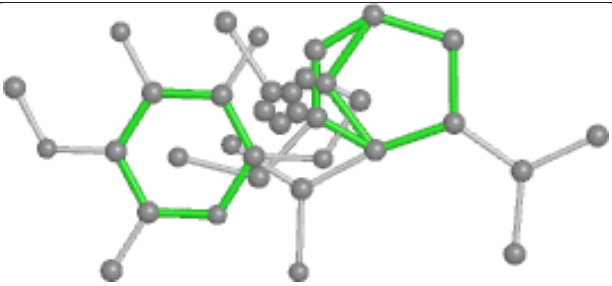
Mol	Chain	Res	Type	Atoms
89	Aa	1101	SO1	C2-C1-C5-O14
89	Aa	1101	SO1	C3-C1-C5-O15
89	Aa	1101	SO1	C2-C1-C5-O15
88	AA	3608	SPD	N1-C2-C3-C4
90	Aa	1102	GDP	PA-O3A-PB-O1B
90	Aa	1102	GDP	PA-O3A-PB-O3B
89	Aa	1101	SO1	C1-C2-C8-O17

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand SO1 Aa 1101	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-16684. 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.