



Full wwPDB EM Validation Report ⓘ

Jun 3, 2024 – 09:29 PM JST

PDB ID : 8H6J
EMDB ID : EMD-34505
Title : Cryo-EM structure of human exon-defined spliceosome in the mature pre-B state.
Authors : Zhang, W.; Zhan, X.; Zhang, X.; Lei, J.; Yan, C.; Shi, Y.
Deposited on : 2022-10-18
Resolution : 3.25 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
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) : 2.36.2

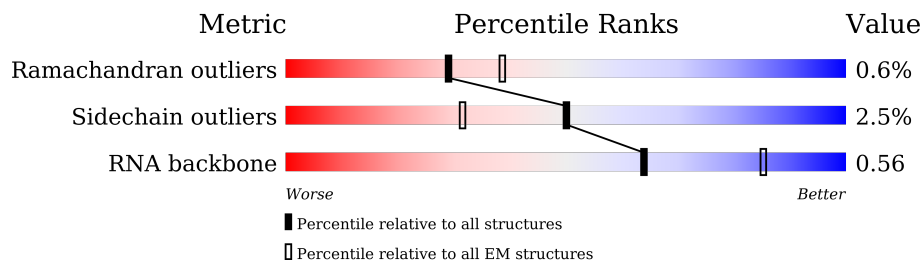
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




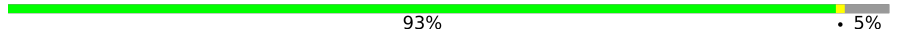



















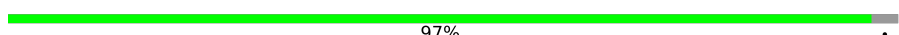
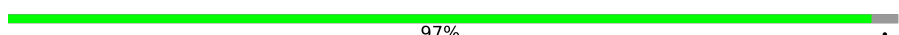


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	144	
2	6A	107	
3	6a	95	
4	6b	102	
5	6c	139	
6	6d	91	
7	6e	80	
8	6f	103	
9	6g	96	

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Mol	Chain	Length	Quality of chain
10	5A	117	 61% 33% . .
11	5B	2335	 93% . 5%
12	5C	972	 86% . 12%
13	5D	2136	 91% . 6%
14	5E	357	 84% . 16%
15	2a	231	 37% 63%
15	4a	231	 35% 65%
15	5a	231	 37% 63%
16	2b	119	 69% 31%
16	4b	119	 68% 32%
16	5b	119	 69% 31%
17	2c	118	 71% . 28%
17	4c	118	 78% 22%
17	5c	118	 81% . 18%
18	2d	86	 86% 14%
18	4d	86	 83% . 16%
18	5d	86	 85% 15%
19	2e	92	 86% 14%
19	4e	92	 82% . 17%
19	5e	92	 86% 14%
20	2f	76	 87% 13%
20	4f	76	 97% .
20	5f	76	 97% .
21	2g	126	 63% 37%
21	4g	126	 66% 34%



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Mol	Chain	Length	Quality of chain
21	5g	126	61% 39%
22	4A	144	67% 19% 13%
23	4B	683	28% 72%
24	4C	522	69% 31%
25	4D	499	54% 46%
26	4E	128	97%
27	4F	142	96%
28	4G	941	81% 17%
29	4R	480	21% 78%
30	4S	800	8% 92%
31	4T	565	80% 19%
32	4U	820	70% 30%
33	4X	155	13% 86%
34	4Y	1007	32% 68%
35	2A	188	33% 21% 42%
36	2B	255	63% 36%
37	2C	225	42% 58%
38	2D	793	15% 84%
39	2E	464	18% 80%
40	2F	501	83% 16%
41	2G	1304	78% 20%
42	2H	895	20% 80%
43	2I	1217	94%
44	2J	424	18% 82%
45	2K	125	83% 14%

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Mol	Chain	Length	Quality of chain
46	2L	110	 81% 19%
47	2M	86	 74% 23%

2 Entry composition i

There are 51 unique types of molecules in this entry. The entry contains 96473 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 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	42	864	387	124	311	42	0	0

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	6A	54	1142	509	206	373	54	0	0

- Molecule 3 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	6a	89	356	178	89	89	0	0

- Molecule 4 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	6b	74	296	148	74	74	0	0

- Molecule 5 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	6c	74	296	148	74	74	0	0

- Molecule 6 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	6d	72	288	144	72	72	0	0

- Molecule 7 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	6e	70	280	140	70	70	0	0

- Molecule 8 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	6f	65	260	130	65	65	0	0

- Molecule 9 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	6g	61	244	122	61	61	0	0

- Molecule 10 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	5A	114	2398	1074	398	812	114	0	0

- Molecule 11 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	5B	2209	18244	11760	3170	3235	79	0	0

- Molecule 12 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	5C	852	6727	4300	1127	1266	34	0	0

- Molecule 13 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	5D	2001	16077	10235	2767	2991	84	0	0

- Molecule 14 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	5E	301	1481	879	301	301	0	0

- Molecule 15 is a protein called Isoform SM-B of Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	5a	86	344	172	86	86	0	0
15	4a	82	405	241	82	82	0	0
15	2a	85	340	170	85	85	0	0

- Molecule 16 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	5b	82	328	164	82	82	0	0
16	4b	81	401	239	81	81	0	0
16	2b	82	328	164	82	82	0	0

- Molecule 17 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	5c	97	388	194	97	97	0	0
17	4c	92	455	271	92	92	0	0
17	2c	85	340	170	85	85	0	0

- Molecule 18 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	5d	73	292	146	73	73	0	0
18	4d	72	351	207	72	72	0	0
18	2d	74	296	148	74	74	0	0

- Molecule 19 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	5e	79	Total	C	N	O	0	0
			316	158	79	79		
19	4e	76	Total	C	N	O	0	0
			376	224	76	76		
19	2e	79	Total	C	N	O	0	0
			316	158	79	79		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	5f	74	Total	C	N	O	0	0
			296	148	74	74		
20	4f	74	Total	C	N	O	0	0
			363	215	74	74		
20	2f	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	5g	77	Total	C	N	O	0	0
			308	154	77	77		
21	4g	83	Total	C	N	O	0	0
			409	243	83	83		
21	2g	80	Total	C	N	O	0	0
			320	160	80	80		

- Molecule 22 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4A	125	Total	C	N	O	P	0	0
			2656	1188	468	876	124		

- Molecule 23 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	4B	193	Total	C	N	O	0	0
			953	567	193	193		

- Molecule 24 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	4C	359	1765	1047	359	359	0	0

- Molecule 25 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	4D	270	1340	800	270	270	0	0

- Molecule 26 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	4E	124	615	367	124	124	0	0

- Molecule 27 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	4F	141	1169	751	194	214	10	0	0

- Molecule 28 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	4G	784	4539	2745	884	901	9	0	0

- Molecule 29 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	4R	106	874	553	160	157	4	0	0

- Molecule 30 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	4S	61	505	317	94	91	3	0	0

- Molecule 31 is a protein called U4/U6.U5 tri-snRNP-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	4T	456	3749	2427	635	673	14	0	0

- Molecule 32 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	4U	578	3414	2063	682	667	2	1	0

- Molecule 33 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	4X	21	184	115	40	28	1	0	0

- Molecule 34 is a protein called Serine/threonine-protein kinase PRP4 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	4Y	322	1595	951	322	322	0	0

- Molecule 35 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	2A	109	2311	1032	396	774	109	0	0

- Molecule 36 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	2B	162	648	324	162	162	0	0

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	2C	94	376	188	94	94	0	0

- Molecule 38 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	2D	124	Total	C	N	O	0	0
			496	248	124	124		

- Molecule 39 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	2E	94	Total	C	N	O	0	0
			376	188	94	94		

- Molecule 40 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	2F	423	Total	C	N	O	0	0
			1693	847	423	423		

- Molecule 41 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	2G	1048	Total	C	N	O	0	0
			4192	2096	1048	1048		

- Molecule 42 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	2H	182	Total	C	N	O	0	0
			728	364	182	182		

- Molecule 43 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	2I	1168	Total	C	N	O	0	0
			4672	2336	1168	1168		

- Molecule 44 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	2J	78	Total	C	N	O	0	0
			312	156	78	78		

- Molecule 45 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
45	2K	108	432	216	108	108	0	0

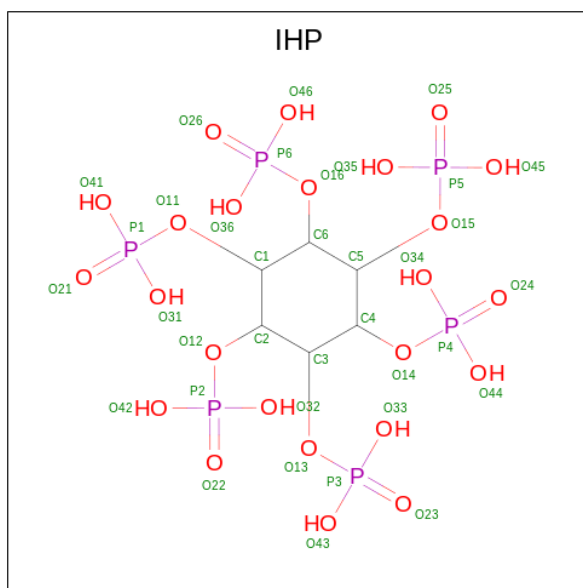
- Molecule 46 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
46	2L	89	356	178	89	89	0	0

- Molecule 47 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
47	2M	66	264	132	66	66	0	0

- Molecule 48 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).

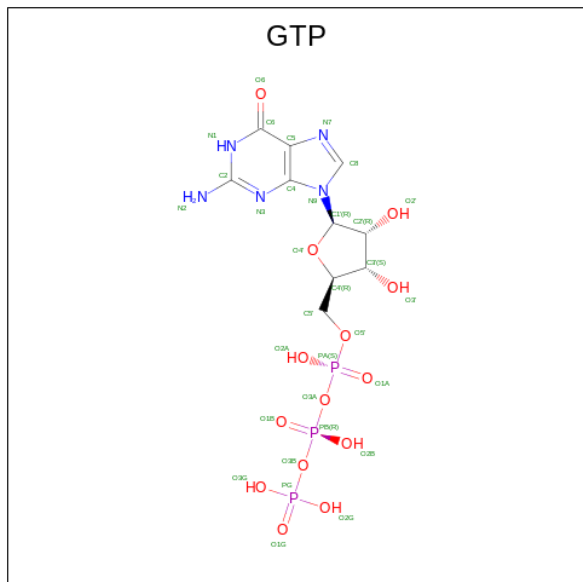


Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
48	5B	1	36	6	24	6	0

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
49	5C	1	1	1	0


- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

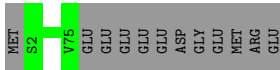


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	5C	1	32	10	5	14	3	0


- Molecule 51 is ZINC ION (three-letter code: ZN) (formula: Zn).

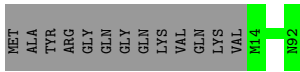
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
51	4T	1	1	1	0

Chain 2d:  86% 14%




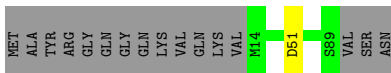
- Molecule 19: Small nuclear ribonucleoprotein E

Chain 5e:  86% 14%




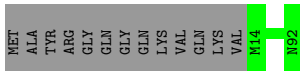
- Molecule 19: Small nuclear ribonucleoprotein E

Chain 4e:  82% 17%



- Molecule 19: Small nuclear ribonucleoprotein E

Chain 2e:  86% 14%



- Molecule 20: Small nuclear ribonucleoprotein G

Chain 5f:  97%




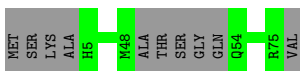
- Molecule 20: Small nuclear ribonucleoprotein G

Chain 4f:  97%




- Molecule 20: Small nuclear ribonucleoprotein G

Chain 2f:  87% 13%




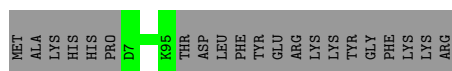
- Molecule 21: Small nuclear ribonucleoprotein Sm D3

Chain 2K:  83% 14%




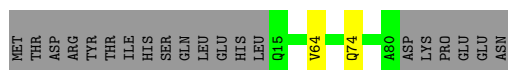
- Molecule 46: PHD finger-like domain-containing protein 5A

Chain 2L:  81% 19%



- Molecule 47: Splicing factor 3B subunit 5

Chain 2M:  74% 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, IHP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.73	3/956 (0.3%)	0.92	0/1481
2	6A	0.36	0/1274	0.90	5/1976 (0.3%)
3	6a	0.43	0/355	0.67	0/442
4	6b	0.47	0/294	0.75	0/364
5	6c	0.34	0/294	0.61	0/364
6	6d	0.43	0/286	0.59	0/354
7	6e	0.43	0/279	0.72	0/347
8	6f	0.39	0/258	0.61	0/319
9	6g	0.41	0/242	0.64	0/299
10	5A	0.27	0/2673	0.94	11/4156 (0.3%)
11	5B	0.25	0/18748	0.49	0/25452
12	5C	0.25	0/6879	0.50	0/9344
13	5D	0.25	0/16393	0.49	0/22174
14	5E	0.28	0/1480	0.57	0/2056
15	2a	0.50	0/339	0.69	0/422
15	4a	0.30	0/404	0.60	0/561
15	5a	0.51	0/343	0.69	0/427
16	2b	0.56	0/327	0.68	0/407
16	4b	0.29	0/400	0.61	0/556
16	5b	0.57	0/327	0.67	0/407
17	2c	0.71	0/338	0.73	0/419
17	4c	0.32	0/454	0.63	0/631
17	5c	0.69	0/387	0.72	0/482
18	2d	0.78	0/295	0.76	0/367
18	4d	0.36	0/350	0.64	0/483
18	5d	0.78	0/291	0.76	0/362
19	2e	0.64	0/315	0.75	0/392
19	4e	0.30	0/375	0.66	0/521
19	5e	0.64	0/315	0.74	0/392
20	2f	0.55	0/262	0.63	0/324
20	4f	0.31	0/362	0.65	0/501
20	5f	0.54	0/295	0.61	0/367

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	2g	0.47	0/318	0.56	0/394
21	4g	0.29	0/408	0.58	0/566
21	5g	0.46	0/307	0.55	0/382
22	4A	0.47	2/2963 (0.1%)	0.89	7/4603 (0.2%)
23	4B	0.25	0/948	0.45	0/1312
24	4C	0.24	0/1764	0.48	0/2450
25	4D	0.24	0/1336	0.40	0/1858
26	4E	0.23	0/614	0.43	0/855
27	4F	0.25	0/1198	0.50	0/1620
28	4G	0.29	1/4561 (0.0%)	0.52	5/6271 (0.1%)
29	4R	0.25	0/891	0.55	0/1188
30	4S	0.26	0/512	0.55	0/673
31	4T	0.25	0/3845	0.49	0/5208
32	4U	0.40	0/3422	0.59	0/4659
33	4X	0.27	0/187	0.65	0/245
34	4Y	0.32	0/1592	0.53	0/2215
35	2A	0.86	11/2576 (0.4%)	1.43	56/4003 (1.4%)
36	2B	0.63	0/647	1.42	0/807
37	2C	0.61	0/375	1.20	0/467
38	2D	0.23	0/493	0.42	0/611
39	2E	0.22	0/373	0.58	1/461 (0.2%)
40	2F	0.25	0/1688	0.47	0/2102
41	2G	1.04	4/4184 (0.1%)	0.83	2/5216 (0.0%)
42	2H	0.74	0/722	0.72	0/892
43	2I	0.85	0/4664	0.76	0/5816
44	2J	0.62	0/311	0.65	0/387
45	2K	0.79	0/431	0.79	0/537
46	2L	0.74	0/355	0.68	0/442
47	2M	1.01	0/263	0.77	0/327
All	All	0.45	21/98538 (0.0%)	0.65	87/133716 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	4a	0	1
17	2c	0	1
17	5c	0	1
18	4d	0	1
19	4e	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	4A	0	1
24	4C	0	1
28	4G	0	2
40	2F	0	1
41	2G	0	11
42	2H	0	3
43	2I	0	11
45	2K	0	1
47	2M	0	1
All	All	0	37

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2G	407	MET	N-CA	12.40	1.71	1.46
22	4A	87	C	O3'-P	11.49	1.75	1.61
41	2G	406	ALA	C-N	7.96	1.52	1.34
35	2A	142	C	C1'-N1	7.25	1.59	1.48
41	2G	1243	PRO	N-CA	-7.10	1.35	1.47
35	2A	182	U	C1'-N1	6.89	1.59	1.48
35	2A	150	U	C1'-N1	6.81	1.58	1.48
35	2A	151	C	C1'-N1	6.51	1.58	1.48
35	2A	141	C	C1'-N1	6.40	1.58	1.48
35	2A	97	G	C1'-N9	-6.36	1.38	1.46
35	2A	184	C	C1'-N1	6.34	1.58	1.48
35	2A	148	C	C1'-N1	6.33	1.58	1.48
41	2G	944	SER	N-CA	-5.76	1.34	1.46
35	2A	48	A	C1'-N9	-5.54	1.39	1.46
35	2A	65	U	C1'-N1	5.50	1.56	1.48
22	4A	91	A	O3'-P	-5.48	1.54	1.61
28	4G	571	PRO	N-CA	5.31	1.56	1.47
1	A	8	U	C1'-N1	5.15	1.56	1.48
1	A	9	U	C1'-N1	5.14	1.56	1.48
35	2A	110	A	C1'-N9	-5.14	1.39	1.46
1	A	7	U	C1'-N1	5.12	1.56	1.48

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	5A	78	U	P-O3'-C3'	-14.15	102.72	119.70
10	5A	58	U	P-O3'-C3'	-12.85	104.29	119.70
35	2A	167	U	C5-C4-O4	11.56	132.84	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	5A	57	G	P-O3'-C3'	-11.33	106.11	119.70
41	2G	406	ALA	C-N-CA	10.26	147.35	121.70
35	2A	164	C	N1-C2-O2	-10.18	112.79	118.90
28	4G	571	PRO	N-CA-CB	-10.05	91.24	103.30
10	5A	80	U	P-O3'-C3'	-9.62	108.16	119.70
22	4A	56	U	P-O3'-C3'	-9.62	108.16	119.70
22	4A	55	U	P-O3'-C3'	-9.53	108.27	119.70
10	5A	78	U	C3'-C2'-C1'	-9.21	94.13	101.50
35	2A	162	U	N3-C2-O2	-8.92	115.96	122.20
28	4G	569	VAL	O-C-N	-8.29	109.44	122.70
35	2A	164	C	C5'-C4'-O4'	-8.26	99.19	109.10
35	2A	169	C	P-O3'-C3'	8.25	129.60	119.70
35	2A	166	G	O4'-C1'-N9	8.10	114.68	108.20
22	4A	87	C	O3'-P-O5'	8.08	119.35	104.00
35	2A	167	U	N3-C4-O4	-7.91	113.86	119.40
35	2A	164	C	P-O3'-C3'	7.51	128.72	119.70
10	5A	56	C	P-O3'-C3'	-7.46	110.75	119.70
35	2A	167	U	N1-C2-O2	7.45	128.02	122.80
35	2A	164	C	N3-C2-O2	7.39	127.08	121.90
35	2A	149	A	OP2-P-O3'	7.27	121.19	105.20
35	2A	113	G	OP2-P-O3'	7.26	121.17	105.20
35	2A	114	A	OP2-P-O3'	7.25	121.15	105.20
35	2A	182	U	OP2-P-O3'	7.24	121.12	105.20
35	2A	183	G	OP2-P-O3'	7.24	121.12	105.20
35	2A	141	C	OP2-P-O3'	7.23	121.11	105.20
2	6A	31	U	N1-C2-O2	7.23	127.86	122.80
22	4A	87	C	P-O3'-C3'	-7.22	111.03	119.70
35	2A	150	U	OP2-P-O3'	7.22	121.08	105.20
35	2A	181	G	OP2-P-O3'	7.22	121.08	105.20
35	2A	180	G	OP2-P-O3'	7.21	121.05	105.20
35	2A	148	C	OP2-P-O3'	7.18	120.99	105.20
35	2A	168	A	P-O5'-C5'	-7.15	109.45	120.90
10	5A	77	G	P-O3'-C3'	-7.14	111.13	119.70
35	2A	167	U	N3-C2-O2	-7.04	117.27	122.20
35	2A	149	A	O3'-P-O5'	-6.83	91.02	104.00
41	2G	406	ALA	CA-C-O	-6.82	105.77	120.10
35	2A	180	G	O3'-P-O5'	-6.81	91.07	104.00
35	2A	182	U	O3'-P-O5'	-6.80	91.08	104.00
35	2A	183	G	O3'-P-O5'	-6.80	91.08	104.00
35	2A	148	C	O3'-P-O5'	-6.78	91.12	104.00
2	6A	31	U	N3-C2-O2	-6.77	117.46	122.20
35	2A	155	C	P-O3'-C3'	6.77	127.82	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	2A	141	C	O3'-P-O5'	-6.76	91.15	104.00
35	2A	181	G	O3'-P-O5'	-6.76	91.16	104.00
35	2A	114	A	O3'-P-O5'	-6.75	91.18	104.00
35	2A	113	G	O3'-P-O5'	-6.74	91.19	104.00
35	2A	150	U	O3'-P-O5'	-6.74	91.20	104.00
22	4A	87	C	OP2-P-O3'	-6.69	90.49	105.20
28	4G	571	PRO	N-CA-C	6.67	129.45	112.10
10	5A	23	C	C2-N1-C1'	6.60	126.06	118.80
35	2A	165	A	O4'-C1'-N9	-6.27	103.18	108.20
2	6A	58	G	P-O3'-C3'	-6.25	112.20	119.70
35	2A	166	G	C8-N9-C4	-6.16	103.94	106.40
2	6A	56	A	P-O3'-C3'	-6.14	112.33	119.70
35	2A	166	G	N9-C4-C5	6.09	107.84	105.40
35	2A	162	U	N1-C2-O2	6.05	127.03	122.80
35	2A	166	G	N3-C4-C5	-5.99	125.61	128.60
35	2A	168	A	C5'-C4'-C3'	-5.94	106.50	116.00
28	4G	707	ASP	C-N-CA	5.90	136.46	121.70
35	2A	156	U	P-O3'-C3'	-5.82	112.71	119.70
35	2A	172	C	P-O3'-C3'	5.82	126.68	119.70
28	4G	572	SER	CA-C-O	-5.79	107.94	120.10
35	2A	164	C	C5-C4-N4	-5.78	116.16	120.20
35	2A	167	U	O3'-P-O5'	-5.76	93.05	104.00
39	2E	146	MET	C-N-CA	5.76	146.19	122.00
22	4A	130	U	N3-C2-O2	-5.59	118.29	122.20
35	2A	157	G	O4'-C1'-N9	-5.49	103.81	108.20
2	6A	31	U	C2-N1-C1'	5.42	124.21	117.70
35	2A	166	G	C6-N1-C2	-5.42	121.85	125.10
35	2A	106	G	O5'-P-OP1	5.39	117.16	110.70
10	5A	59	G	P-O3'-C3'	-5.38	113.24	119.70
22	4A	1	A	OP1-P-OP2	5.36	127.64	119.60
35	2A	156	U	OP2-P-O3'	5.27	116.79	105.20
35	2A	160	A	P-O5'-C5'	-5.26	112.49	120.90
35	2A	170	C	N3-C4-C5	-5.22	119.81	121.90
35	2A	170	C	O4'-C1'-C2'	-5.22	100.58	105.80
35	2A	157	G	P-O5'-C5'	-5.17	112.63	120.90
35	2A	164	C	C6-N1-C2	5.09	122.34	120.30
35	2A	176	G	N9-C4-C5	5.07	107.43	105.40
35	2A	156	U	C4'-C3'-C2'	5.06	107.66	102.60
35	2A	176	G	N3-C4-C5	-5.06	126.07	128.60
10	5A	23	C	N1-C2-O2	5.04	121.92	118.90
10	5A	78	U	C4'-C3'-C2'	-5.01	97.58	102.60
35	2A	162	U	C2-N3-C4	-5.01	123.99	127.00

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	2F	443	THR	Peptide
41	2G	1025	LYS	Peptide
41	2G	1122	THR	Peptide
41	2G	1127	THR	Peptide
41	2G	1179	ASP	Peptide
41	2G	1199	VAL	Peptide
41	2G	220	GLN	Peptide
41	2G	415	LEU	Peptide,Mainchain
41	2G	689	ILE	Peptide
41	2G	941	ASN	Peptide
41	2G	944	SER	Peptide
42	2H	553	MET	Peptide
42	2H	558	ARG	Peptide
42	2H	571	LEU	Peptide
43	2I	261	PHE	Peptide
43	2I	366	ASP	Peptide
43	2I	468	ASP	Peptide
43	2I	530	ASP	Peptide
43	2I	534	ASN	Peptide
43	2I	552	ARG	Peptide
43	2I	670	GLN	Peptide
43	2I	678	VAL	Peptide
43	2I	74	THR	Peptide
43	2I	980	LYS	Peptide
43	2I	986	ILE	Peptide
45	2K	29	LYS	Peptide
47	2M	74	GLN	Peptide
17	2c	112	ASN	Peptide
22	4A	90	G	Sidechain
24	4C	459	PRO	Peptide
28	4G	569	VAL	Mainchain
28	4G	572	SER	Mainchain
15	4a	53	PRO	Peptide
18	4d	40	MET	Peptide
19	4e	51	ASP	Peptide
17	5c	112	ASN	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	6a	87/95 (92%)	76 (87%)	7 (8%)	4 (5%)	2	15
4	6b	70/102 (69%)	64 (91%)	3 (4%)	3 (4%)	2	16
5	6c	70/139 (50%)	64 (91%)	5 (7%)	1 (1%)	11	40
6	6d	68/91 (75%)	63 (93%)	4 (6%)	1 (2%)	10	39
7	6e	68/80 (85%)	64 (94%)	2 (3%)	2 (3%)	4	25
8	6f	61/103 (59%)	56 (92%)	5 (8%)	0	100	100
9	6g	57/96 (59%)	52 (91%)	4 (7%)	1 (2%)	8	35
11	5B	2195/2335 (94%)	2099 (96%)	96 (4%)	0	100	100
12	5C	850/972 (87%)	823 (97%)	27 (3%)	0	100	100
13	5D	1989/2136 (93%)	1912 (96%)	77 (4%)	0	100	100
14	5E	299/357 (84%)	280 (94%)	17 (6%)	2 (1%)	22	56
15	2a	83/231 (36%)	81 (98%)	2 (2%)	0	100	100
15	4a	80/231 (35%)	71 (98%)	9 (11%)	0	100	100
15	5a	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
16	2b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
16	4b	79/119 (66%)	75 (95%)	4 (5%)	0	100	100
16	5b	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
17	2c	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
17	4c	90/118 (76%)	84 (93%)	6 (7%)	0	100	100
17	5c	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
18	2d	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
18	4d	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
18	5d	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
19	2e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
19	4e	74/92 (80%)	71 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	5e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
20	2f	62/76 (82%)	60 (97%)	2 (3%)	0	100	100
20	4f	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
20	5f	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
21	2g	76/126 (60%)	74 (97%)	2 (3%)	0	100	100
21	4g	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
21	5g	75/126 (60%)	73 (97%)	2 (3%)	0	100	100
23	4B	183/683 (27%)	177 (97%)	6 (3%)	0	100	100
24	4C	357/522 (68%)	333 (93%)	24 (7%)	0	100	100
25	4D	262/499 (52%)	252 (96%)	10 (4%)	0	100	100
26	4E	122/128 (95%)	114 (93%)	8 (7%)	0	100	100
27	4F	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
28	4G	776/941 (82%)	739 (95%)	33 (4%)	4 (0%)	29	62
29	4R	104/480 (22%)	93 (89%)	11 (11%)	0	100	100
30	4S	59/800 (7%)	57 (97%)	2 (3%)	0	100	100
31	4T	454/565 (80%)	425 (94%)	29 (6%)	0	100	100
32	4U	559/820 (68%)	541 (97%)	17 (3%)	1 (0%)	47	77
33	4X	19/155 (12%)	19 (100%)	0	0	100	100
34	4Y	316/1007 (31%)	294 (93%)	18 (6%)	4 (1%)	12	41
36	2B	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12	41
37	2C	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
38	2D	118/793 (15%)	106 (90%)	6 (5%)	6 (5%)	2	13
39	2E	88/464 (19%)	63 (72%)	16 (18%)	9 (10%)	0	3
40	2F	413/501 (82%)	367 (89%)	41 (10%)	5 (1%)	13	43
41	2G	1032/1304 (79%)	845 (82%)	165 (16%)	22 (2%)	7	32
42	2H	170/895 (19%)	151 (89%)	15 (9%)	4 (2%)	6	28
43	2I	1152/1217 (95%)	1053 (91%)	89 (8%)	10 (1%)	17	50
44	2J	76/424 (18%)	75 (99%)	1 (1%)	0	100	100
45	2K	106/125 (85%)	85 (80%)	18 (17%)	3 (3%)	5	25
46	2L	87/110 (79%)	75 (86%)	12 (14%)	0	100	100
47	2M	64/86 (74%)	55 (86%)	8 (12%)	1 (2%)	9	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	14353/22191 (65%)	13407 (93%)	861 (6%)	85 (1%)	29 59

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	6a	55	LEU
4	6b	84	MET
6	6d	70	ASP
7	6e	52	VAL
7	6e	55	GLN
14	5E	59	ILE
28	4G	136	PRO
28	4G	571	PRO
28	4G	573	LYS
34	4Y	697	VAL
38	2D	301	PRO
39	2E	139	PRO
39	2E	141	ILE
39	2E	146	MET
39	2E	162	PRO
39	2E	165	ARG
39	2E	218	PRO
40	2F	284	ARG
41	2G	208	PRO
41	2G	416	PRO
41	2G	418	PRO
41	2G	456	VAL
41	2G	717	THR
41	2G	941	ASN
41	2G	1107	GLN
43	2I	405	SER
43	2I	919	SER
45	2K	99	GLN
45	2K	105	LYS
3	6a	74	ALA
4	6b	97	PRO
5	6c	12	ASN
34	4Y	851	VAL
36	2B	160	LYS
38	2D	223	LYS
38	2D	280	VAL
40	2F	277	THR

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Mol	Chain	Res	Type
41	2G	113	ALA
41	2G	1110	VAL
42	2H	597	PHE
43	2I	917	PRO
32	4U	582	ALA
40	2F	177	ARG
40	2F	393	PRO
41	2G	437	PRO
42	2H	510	TYR
4	6b	96	ALA
14	5E	58	PRO
34	4Y	699	SER
36	2B	32	PRO
38	2D	300	THR
41	2G	112	ILE
41	2G	523	ALA
41	2G	909	VAL
41	2G	1006	MET
42	2H	463	ALA
42	2H	574	ALA
43	2I	529	ALA
43	2I	578	THR
3	6a	73	PRO
28	4G	569	VAL
34	4Y	722	ASN
39	2E	147	PRO
39	2E	217	PRO
41	2G	1047	ALA
41	2G	1075	ARG
41	2G	1186	GLN
43	2I	95	SER
43	2I	229	GLU
45	2K	75	ASP
9	6g	34	ILE
39	2E	220	PRO
41	2G	326	THR
41	2G	932	ILE
43	2I	918	ARG
43	2I	1138	HIS
41	2G	417	PRO
38	2D	221	PRO
41	2G	223	THR

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Mol	Chain	Res	Type
43	2I	1204	VAL
40	2F	229	TRP
38	2D	298	PRO
41	2G	1031	VAL
47	2M	64	VAL
3	6a	52	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	5B	1978/2108 (94%)	1943 (98%)	35 (2%)	59	77
12	5C	754/866 (87%)	738 (98%)	16 (2%)	53	75
13	5D	1779/1908 (93%)	1730 (97%)	49 (3%)	43	69
27	4F	129/130 (99%)	124 (96%)	5 (4%)	32	61
28	4G	185/792 (23%)	172 (93%)	13 (7%)	15	43
29	4R	94/369 (26%)	88 (94%)	6 (6%)	17	47
30	4S	54/681 (8%)	53 (98%)	1 (2%)	57	76
31	4T	418/511 (82%)	412 (99%)	6 (1%)	67	81
32	4U	133/721 (18%)	129 (97%)	4 (3%)	41	67
33	4X	19/144 (13%)	18 (95%)	1 (5%)	22	53
All	All	5543/8230 (67%)	5407 (98%)	136 (2%)	50	71

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	5B	68	LYS
11	5B	86	ARG
11	5B	106	MET
11	5B	227	ARG
11	5B	258	PHE
11	5B	294	ASN
11	5B	322	ASN

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Mol	Chain	Res	Type
11	5B	345	PRO
11	5B	579	GLN
11	5B	627	CYS
11	5B	654	ASN
11	5B	707	ARG
11	5B	871	TYR
11	5B	883	ARG
11	5B	955	TRP
11	5B	1022	MET
11	5B	1160	ARG
11	5B	1200	CYS
11	5B	1321	GLU
11	5B	1330	MET
11	5B	1341	ARG
11	5B	1378	GLU
11	5B	1400	ASN
11	5B	1402	ARG
11	5B	1414	ARG
11	5B	1469	ASN
11	5B	1759	THR
11	5B	1791	HIS
11	5B	1914	MET
11	5B	1925	LYS
11	5B	1958	LYS
11	5B	2096	ASP
11	5B	2200	MET
11	5B	2203	ASN
11	5B	2249	LYS
12	5C	116	MET
12	5C	154	HIS
12	5C	308	CYS
12	5C	313	GLN
12	5C	323	PHE
12	5C	331	PHE
12	5C	339	PHE
12	5C	379	LYS
12	5C	403	LEU
12	5C	485	ASP
12	5C	645	ARG
12	5C	735	PHE
12	5C	835	GLU
12	5C	910	ASP

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Mol	Chain	Res	Type
12	5C	919	ARG
12	5C	953	PHE
13	5D	52	MET
13	5D	62	GLN
13	5D	74	ARG
13	5D	97	MET
13	5D	111	GLU
13	5D	154	ARG
13	5D	217	TYR
13	5D	243	ASN
13	5D	278	ASP
13	5D	300	ARG
13	5D	406	ARG
13	5D	423	MET
13	5D	483	ARG
13	5D	527	MET
13	5D	719	ASN
13	5D	751	PHE
13	5D	789	MET
13	5D	794	ARG
13	5D	848	ASP
13	5D	902	ASN
13	5D	943	LEU
13	5D	974	LYS
13	5D	992	TYR
13	5D	1018	PHE
13	5D	1025	LYS
13	5D	1031	GLU
13	5D	1101	ASN
13	5D	1141	LYS
13	5D	1145	LYS
13	5D	1148	PHE
13	5D	1152	ARG
13	5D	1289	LEU
13	5D	1305	GLN
13	5D	1325	PHE
13	5D	1376	CYS
13	5D	1402	ASN
13	5D	1553	HIS
13	5D	1568	GLN
13	5D	1580	CYS
13	5D	1595	LYS

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Mol	Chain	Res	Type
13	5D	1713	PHE
13	5D	1736	PHE
13	5D	1808	MET
13	5D	1817	MET
13	5D	1841	LYS
13	5D	1928	ASP
13	5D	1967	THR
13	5D	1983	PHE
13	5D	2014	TYR
27	4F	4	MET
27	4F	53	LYS
27	4F	79	CYS
27	4F	110	GLN
27	4F	120	TYR
28	4G	94	TYR
28	4G	116	ARG
28	4G	131	TYR
28	4G	133	MET
28	4G	134	GLU
28	4G	135	ARG
28	4G	137	LYS
28	4G	138	ILE
28	4G	239	ASP
28	4G	242	LYS
28	4G	251	MET
28	4G	253	MET
28	4G	338	MET
29	4R	390	ASN
29	4R	429	PHE
29	4R	440	ARG
29	4R	446	TYR
29	4R	458	MET
29	4R	460	LYS
30	4S	741	MET
31	4T	149	LYS
31	4T	257	ASP
31	4T	318	ASP
31	4T	324	SER
31	4T	453	CYS
31	4T	463	PHE
32	4U	243	LYS
32	4U	248	HIS

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Mol	Chain	Res	Type
32	4U	277	ASP
32	4U	287	ASN
33	4X	151	LEU

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

Mol	Chain	Res	Type
11	5B	434	HIS
11	5B	884	HIS
11	5B	1766	GLN
11	5B	1823	HIS
11	5B	2203	ASN
12	5C	856	HIS
12	5C	903	HIS
12	5C	905	GLN
13	5D	785	HIS
13	5D	824	HIS
13	5D	1388	GLN
13	5D	1727	HIS
13	5D	2102	HIS
27	4F	32	HIS
28	4G	139	GLN
28	4G	305	ASN
28	4G	307	HIS
31	4T	362	HIS
31	4T	520	HIS
31	4T	540	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	41/144 (28%)	27 (65%)	9 (21%)
10	5A	113/117 (96%)	38 (33%)	6 (5%)
2	6A	50/107 (46%)	8 (16%)	3 (6%)
22	4A	119/144 (82%)	21 (17%)	2 (1%)
35	2A	105/188 (55%)	22 (20%)	3 (2%)
All	All	428/700 (61%)	116 (27%)	23 (5%)

All (116) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	10	C
1	A	11	C
1	A	12	U
1	A	13	U
1	A	15	A
1	A	20	U
1	A	21	U
1	A	22	C
1	A	25	G
1	A	29	A
1	A	30	C
1	A	31	C
1	A	32	C
1	A	33	U
1	A	34	G
1	A	35	U
1	A	36	C
1	A	37	C
1	A	39	U
1	A	41	U
1	A	42	U
1	A	44	U
1	A	46	U
1	A	47	C
1	A	48	C
2	6A	48	A
2	6A	49	G
2	6A	58	G
2	6A	59	G
2	6A	77	C
2	6A	78	A
2	6A	103	U
2	6A	104	U
10	5A	5	U
10	5A	6	C
10	5A	21	A
10	5A	22	U
10	5A	24	G
10	5A	25	C
10	5A	28	A
10	5A	36	C

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Mol	Chain	Res	Type
10	5A	37	G
10	5A	38	C
10	5A	40	U
10	5A	41	U
10	5A	43	U
10	5A	44	A
10	5A	47	A
10	5A	48	A
10	5A	55	C
10	5A	58	U
10	5A	59	G
10	5A	66	A
10	5A	67	A
10	5A	69	A
10	5A	70	A
10	5A	75	G
10	5A	79	C
10	5A	80	U
10	5A	81	U
10	5A	83	A
10	5A	88	A
10	5A	89	U
10	5A	90	U
10	5A	92	U
10	5A	93	U
10	5A	94	U
10	5A	95	G
10	5A	96	A
10	5A	97	G
10	5A	109	G
22	4A	2	G
22	4A	18	G
22	4A	25	A
22	4A	26	G
22	4A	37	C
22	4A	38	U
22	4A	39	A
22	4A	40	U
22	4A	45	G
22	4A	53	U
22	4A	57	G
22	4A	68	A

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Mol	Chain	Res	Type
22	4A	69	C
22	4A	114	U
22	4A	115	G
22	4A	121	U
22	4A	122	U
22	4A	123	U
22	4A	125	G
22	4A	126	A
22	4A	140	G
35	2A	31	G
35	2A	37	U
35	2A	40	C
35	2A	45	C
35	2A	47	U
35	2A	51	A
35	2A	65	U
35	2A	112	G
35	2A	143	A
35	2A	147	G
35	2A	152	G
35	2A	153	A
35	2A	154	C
35	2A	156	U
35	2A	157	G
35	2A	164	C
35	2A	165	A
35	2A	168	A
35	2A	169	C
35	2A	177	A
35	2A	178	A
35	2A	179	C

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	21	U
1	A	28	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	38	C

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Mol	Chain	Res	Type
1	A	40	U
1	A	41	U
2	6A	47	A
2	6A	48	A
2	6A	77	C
10	5A	58	U
10	5A	59	G
10	5A	78	U
10	5A	79	C
10	5A	94	U
10	5A	96	A
22	4A	68	A
22	4A	114	U
35	2A	156	U
35	2A	164	C
35	2A	168	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
50	GTP	5C	1002	49	26,34,34	1.14	2 (7%)	32,54,54	1.65	6 (18%)
48	IHP	5B	2401	-	36,36,36	0.74	0	54,60,60	1.19	3 (5%)

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
50	GTP	5C	1002	49	-	5/18/38/38	0/3/3/3
48	IHP	5B	2401	-	-	4/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	5C	1002	GTP	C5-C6	-4.08	1.39	1.47
50	5C	1002	GTP	C2-N3	2.08	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	5C	1002	GTP	PA-O3A-PB	-4.22	118.36	132.83
50	5C	1002	GTP	PB-O3B-PG	-4.15	118.59	132.83
50	5C	1002	GTP	C5-C6-N1	3.44	120.02	113.95
48	5B	2401	IHP	C5-C4-C3	3.36	117.76	110.41
50	5C	1002	GTP	C2-N1-C6	-2.97	119.64	125.10
50	5C	1002	GTP	C8-N7-C5	2.84	108.40	102.99
48	5B	2401	IHP	C6-C5-C4	2.63	116.16	110.41
48	5B	2401	IHP	C4-C3-C2	2.31	115.46	110.41
50	5C	1002	GTP	O6-C6-C5	-2.19	120.10	124.37

There are no chirality outliers.

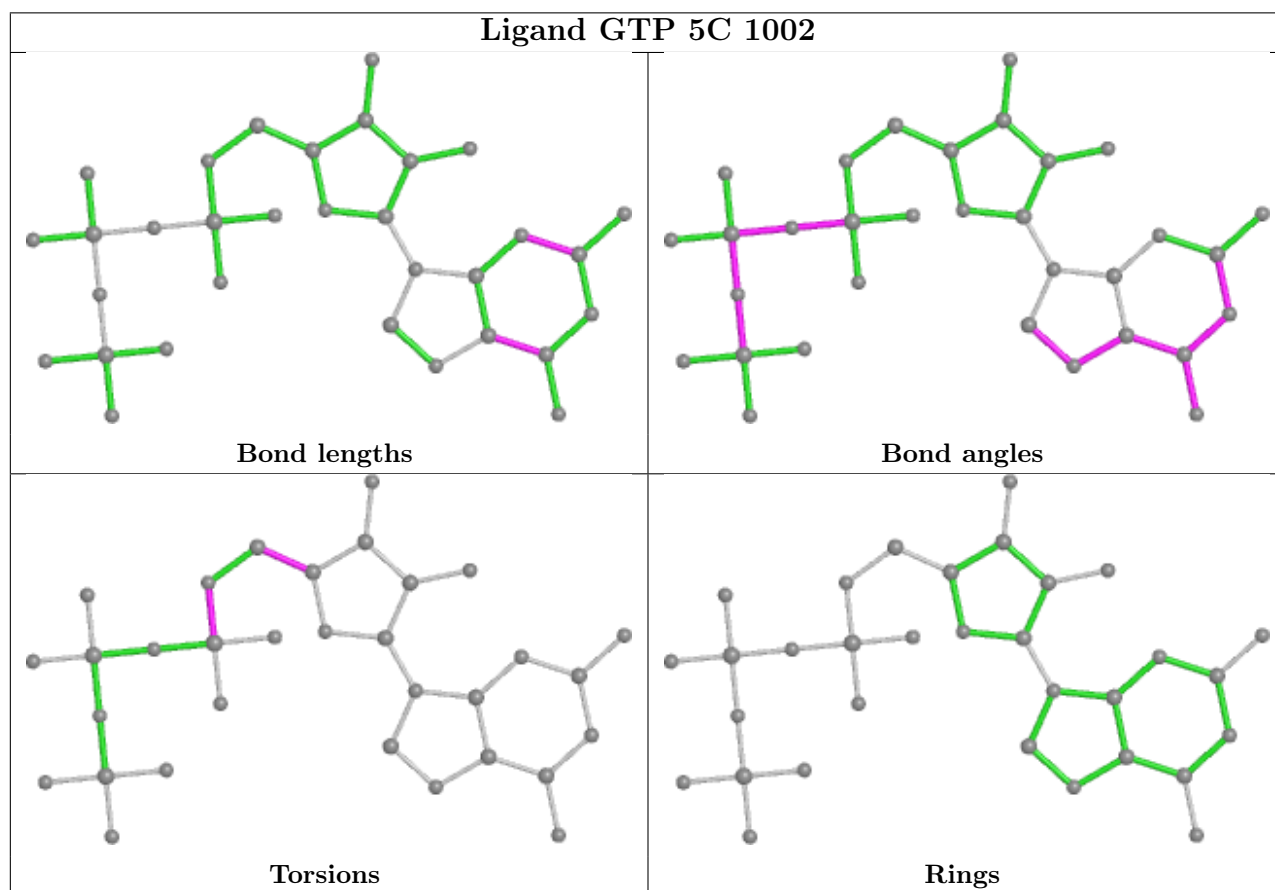
All (9) torsion outliers are listed below:

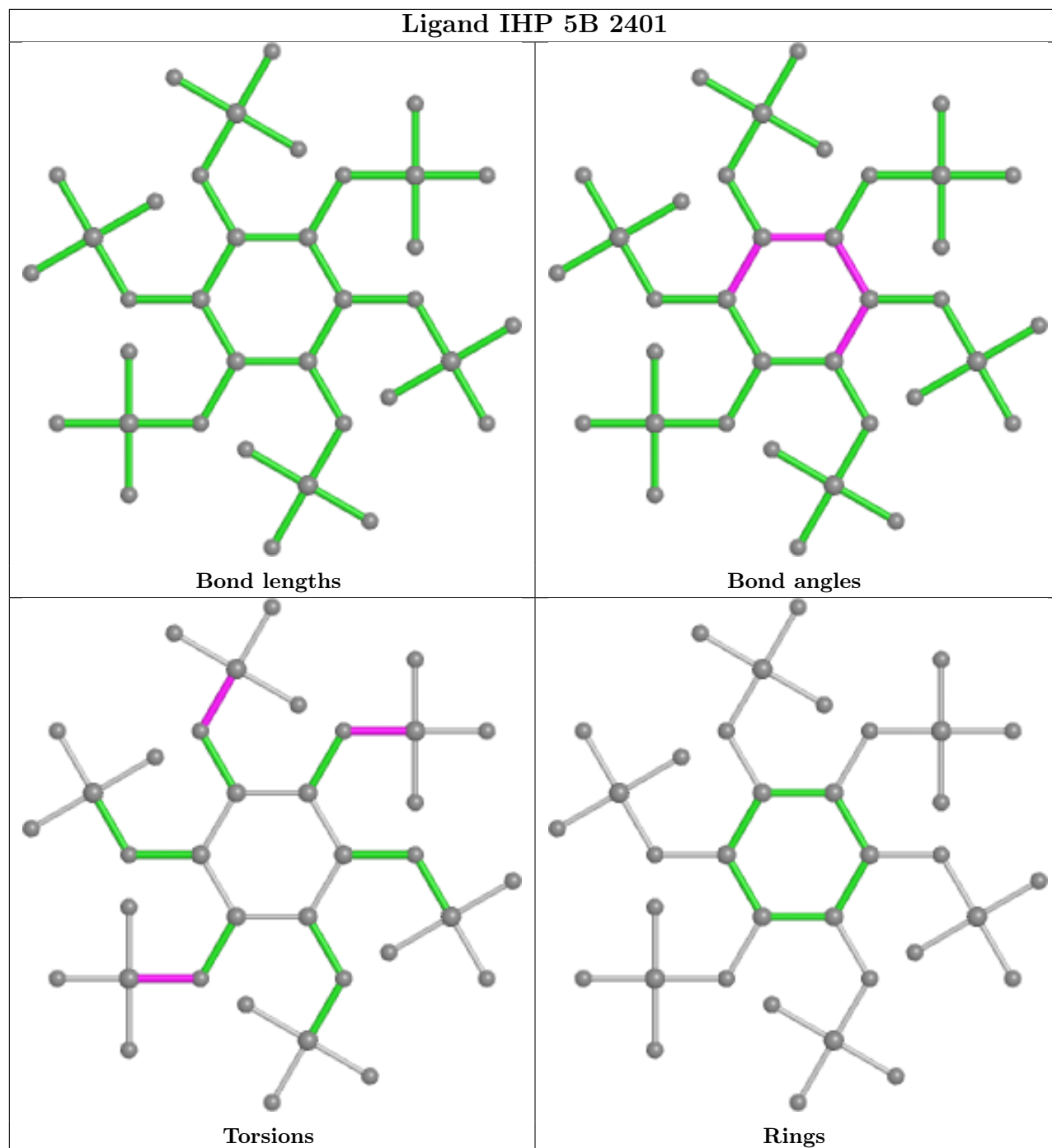
Mol	Chain	Res	Type	Atoms
48	5B	2401	IHP	C1-O11-P1-O41
50	5C	1002	GTP	C5'-O5'-PA-O3A
50	5C	1002	GTP	O4'-C4'-C5'-O5'
50	5C	1002	GTP	C3'-C4'-C5'-O5'
48	5B	2401	IHP	C3-O13-P3-O43
48	5B	2401	IHP	C4-O14-P4-O44
50	5C	1002	GTP	C5'-O5'-PA-O2A
48	5B	2401	IHP	C3-O13-P3-O33
50	5C	1002	GTP	C5'-O5'-PA-O1A

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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.