



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:12 AM EST

PDB ID : 7M2X  
EMDB ID : EMD-23636  
Title : Open conformation of the Yeast wild-type gamma-TuRC  
Authors : Brilot, A.F.; Lyon, A.S.; Zelter, A.; Viswanath, S.; Maxwell, A.; MacCoss, M.J.; Muller, E.G.; Sali, A.; Davis, T.N.; Agard, D.A.  
Deposited on : 2021-03-17  
Resolution : 3.60 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
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) : 2.31.2

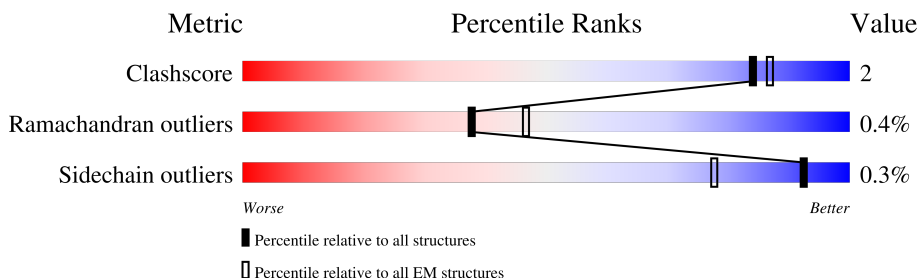
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	473	85% 8% 6%
1	B	473	85% 8% 6%
2	C	823	77% 8% 15%
3	D	846	73% 6% 20%
4	U	220	15% 85%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18704 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 Tubulin gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	444	Total	C	N	O	S	0	0
			3474	2172	588	698	16		
1	B	446	Total	C	N	O	S	0	0
			3486	2179	590	700	17		

- Molecule 2 is a protein called Spindle pole body component SPC97.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	701	Total	C	N	O	S	0	0
			5853	3770	983	1071	29		

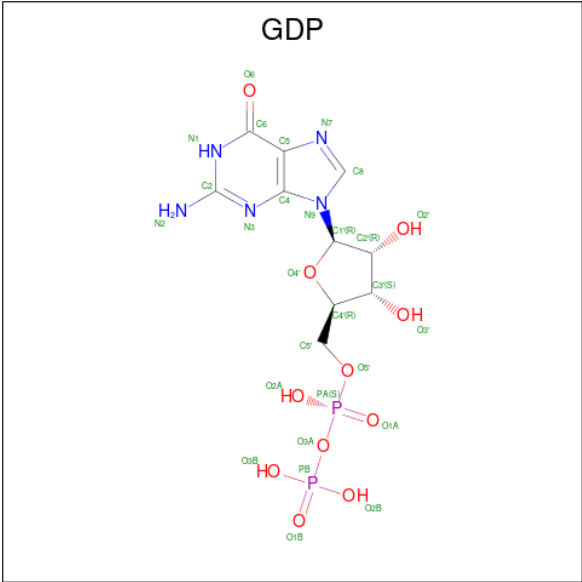
- Molecule 3 is a protein called Spindle pole body component SPC98.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	673	Total	C	N	O	S	0	0
			5560	3595	918	1031	16		

- Molecule 4 is a protein called Spindle pole body component 110.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	33	Total	C	N	O	S	0	0
			275	170	51	52	2		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=0.01 Å, axial sym=C1	Depositor
Number of segments used	36251	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Final reconstruction in cis-TEM	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	47214	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP

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	1.16	18/3546 (0.5%)	0.97	9/4815 (0.2%)
1	B	1.07	6/3558 (0.2%)	0.96	8/4830 (0.2%)
2	C	1.27	28/5969 (0.5%)	1.01	24/8057 (0.3%)
3	D	1.28	33/5679 (0.6%)	0.94	11/7677 (0.1%)
4	U	1.21	1/278 (0.4%)	0.85	0/368
All	All	1.22	86/19030 (0.5%)	0.97	52/25747 (0.2%)

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	583	TYR	CB-CG	-9.07	1.38	1.51
2	C	498	TYR	CB-CG	-8.88	1.38	1.51
1	A	4	GLU	CG-CD	-8.61	1.39	1.51
3	D	267	PHE	CB-CG	-8.38	1.37	1.51
2	C	197	PHE	CB-CG	-8.04	1.37	1.51
1	A	398	PHE	CG-CD1	-7.92	1.26	1.38
2	C	190	TYR	CB-CG	-7.61	1.40	1.51
3	D	400	TYR	CB-CG	-7.54	1.40	1.51
3	D	603	GLU	CG-CD	-7.40	1.40	1.51
3	D	349	TRP	CB-CG	-7.12	1.37	1.50
1	B	294	VAL	CB-CG2	-6.93	1.38	1.52
3	D	445	PHE	CB-CG	-6.88	1.39	1.51
3	D	425	PHE	CB-CG	-6.86	1.39	1.51
2	C	405	PHE	CB-CG	-6.83	1.39	1.51
4	U	134	PHE	CB-CG	-6.74	1.39	1.51
2	C	279	TYR	CB-CG	-6.70	1.41	1.51
1	A	109	TYR	CB-CG	-6.63	1.41	1.51
1	A	362	TYR	CB-CG	-6.60	1.41	1.51
1	A	4	GLU	CD-OE1	-6.54	1.18	1.25
3	D	216	PHE	CB-CG	-6.44	1.40	1.51
3	D	335	PHE	CB-CG	-6.43	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	288	TYR	CB-CG	-6.42	1.42	1.51
3	D	342	TYR	CB-CG	-6.42	1.42	1.51
2	C	324	TYR	CB-CG	-6.41	1.42	1.51
3	D	231	TYR	CB-CG	-6.38	1.42	1.51
2	C	116	TYR	CB-CG	-6.35	1.42	1.51
2	C	558	TYR	CB-CG	-6.32	1.42	1.51
3	D	403	PHE	CB-CG	-6.31	1.40	1.51
1	A	217	PHE	CG-CD1	-6.30	1.29	1.38
2	C	325	PHE	CB-CG	-6.22	1.40	1.51
2	C	647	PHE	CB-CG	-6.21	1.40	1.51
2	C	429	TYR	CB-CG	-6.05	1.42	1.51
3	D	409	TYR	CB-CG	-6.00	1.42	1.51
3	D	411	PHE	CB-CG	-5.95	1.41	1.51
2	C	782	PHE	CB-CG	-5.95	1.41	1.51
3	D	319	PHE	CB-CG	-5.90	1.41	1.51
2	C	403	GLU	CD-OE1	-5.90	1.19	1.25
2	C	657	TYR	CB-CG	-5.88	1.42	1.51
3	D	488	PHE	CB-CG	-5.85	1.41	1.51
1	A	244	PHE	CB-CG	-5.84	1.41	1.51
3	D	187	TYR	CG-CD1	-5.79	1.31	1.39
2	C	298	GLU	CD-OE1	-5.79	1.19	1.25
3	D	784	TYR	CB-CG	-5.76	1.43	1.51
3	D	603	GLU	CD-OE2	-5.73	1.19	1.25
3	D	769	VAL	CB-CG2	-5.69	1.40	1.52
1	B	204	PHE	CB-CG	-5.66	1.41	1.51
1	A	64	PRO	N-CD	-5.66	1.40	1.47
1	B	381	SER	CB-OG	-5.65	1.34	1.42
2	C	558	TYR	CD2-CE2	-5.53	1.31	1.39
3	D	598	TYR	CG-CD1	-5.53	1.31	1.39
1	A	264	GLU	CD-OE2	-5.52	1.19	1.25
3	D	312	PHE	CB-CG	-5.51	1.42	1.51
1	A	28	GLU	CG-CD	-5.49	1.43	1.51
1	A	275	PHE	CB-CG	-5.48	1.42	1.51
1	A	226	HIS	CB-CG	-5.45	1.40	1.50
3	D	174	TYR	CB-CG	-5.42	1.43	1.51
1	A	419	VAL	CB-CG1	-5.42	1.41	1.52
2	C	116	TYR	CG-CD1	-5.41	1.32	1.39
2	C	145	PHE	CB-CG	-5.41	1.42	1.51
2	C	41	PHE	CB-CG	-5.39	1.42	1.51
1	B	437	TYR	CB-CG	-5.38	1.43	1.51
1	B	4	GLU	CG-CD	-5.37	1.43	1.51
2	C	172	GLU	CG-CD	-5.37	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	PHE	CB-CG	-5.34	1.42	1.51
2	C	410	PHE	CB-CG	-5.30	1.42	1.51
3	D	600	TYR	CB-CG	-5.29	1.43	1.51
1	A	126	GLU	CD-OE2	-5.29	1.19	1.25
2	C	778	CYS	CB-SG	-5.28	1.73	1.81
2	C	559	HIS	CB-CG	-5.25	1.40	1.50
3	D	297	TYR	CG-CD1	-5.25	1.32	1.39
3	D	510	TYR	CB-CG	-5.25	1.43	1.51
2	C	232	VAL	CB-CG1	-5.24	1.41	1.52
2	C	150	TYR	CB-CG	-5.22	1.43	1.51
1	B	134	GLU	CB-CG	5.22	1.62	1.52
2	C	168	PHE	CB-CG	-5.16	1.42	1.51
2	C	754	GLU	CD-OE1	-5.12	1.20	1.25
3	D	388	GLU	CD-OE2	-5.11	1.20	1.25
1	A	228	ASN	CB-CG	-5.11	1.39	1.51
1	A	4	GLU	CD-OE2	-5.10	1.20	1.25
1	A	29	HIS	CB-CG	-5.10	1.40	1.50
3	D	363	PHE	CB-CG	-5.07	1.42	1.51
3	D	361	GLU	CD-OE1	-5.05	1.20	1.25
3	D	289	GLU	CD-OE1	-5.05	1.20	1.25
3	D	836	GLU	CD-OE2	-5.03	1.20	1.25
2	C	393	TYR	CB-CG	-5.01	1.44	1.51
3	D	409	TYR	CD2-CE2	-5.01	1.31	1.39

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	NE-CZ-NH2	-8.66	115.97	120.30
2	C	108	ARG	NE-CZ-NH2	-8.48	116.06	120.30
2	C	9	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	B	65	ARG	NE-CZ-NH2	-8.21	116.19	120.30
2	C	594	TYR	CB-CG-CD1	-8.21	116.08	121.00
2	C	229	ARG	NE-CZ-NH2	-8.11	116.24	120.30
2	C	137	ARG	NE-CZ-NH2	-7.92	116.34	120.30
2	C	9	ARG	NE-CZ-NH1	7.80	124.20	120.30
3	D	544	ARG	NE-CZ-NH2	-7.67	116.46	120.30
2	C	318	ARG	NE-CZ-NH2	-7.51	116.55	120.30
2	C	687	ARG	NE-CZ-NH2	-7.26	116.67	120.30
2	C	52	ARG	NE-CZ-NH2	-7.19	116.71	120.30
3	D	389	ARG	NE-CZ-NH1	7.18	123.89	120.30
3	D	187	TYR	CB-CG-CD1	-7.11	116.73	121.00
3	D	633	ARG	NE-CZ-NH2	-7.09	116.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	77	TYR	CB-CG-CD1	-7.07	116.76	121.00
2	C	76	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	C	429	TYR	CB-CG-CD1	-6.97	116.82	121.00
2	C	160	ARG	NE-CZ-NH2	-6.96	116.82	120.30
3	D	533	ARG	NE-CZ-NH2	-6.70	116.95	120.30
2	C	617	TYR	CB-CG-CD2	6.56	124.93	121.00
2	C	704	TYR	CB-CG-CD1	-6.36	117.19	121.00
2	C	657	TYR	CB-CG-CD2	-6.30	117.22	121.00
2	C	617	TYR	CB-CG-CD1	-6.24	117.26	121.00
2	C	262	ARG	NE-CZ-NH2	-6.21	117.19	120.30
3	D	342	TYR	CB-CG-CD1	-6.16	117.30	121.00
1	A	398	PHE	CB-CG-CD1	-6.14	116.50	120.80
3	D	598	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	B	315	TYR	N-CA-C	6.01	127.22	111.00
1	B	437	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	B	162	TYR	CB-CG-CD2	-5.86	117.48	121.00
2	C	74	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	A	55	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	398	PHE	CB-CG-CD2	5.60	124.72	120.80
2	C	752	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	316	PHE	CB-CG-CD2	5.54	124.68	120.80
1	B	319	TYR	CB-CG-CD2	-5.51	117.70	121.00
2	C	190	TYR	CB-CG-CD1	-5.44	117.74	121.00
2	C	62	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	46	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	65	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	427	ARG	NE-CZ-NH2	-5.31	117.64	120.30
3	D	389	ARG	NE-CZ-NH2	-5.30	117.65	120.30
3	D	236	TYR	CB-CG-CD1	-5.29	117.83	121.00
3	D	510	TYR	CB-CG-CD1	-5.29	117.83	121.00
2	C	393	TYR	CB-CG-CD1	-5.22	117.86	121.00
1	B	247	TYR	CB-CG-CD2	-5.21	117.87	121.00
2	C	627	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	161	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	109	TYR	CB-CG-CD1	-5.07	117.96	121.00
3	D	583	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	B	333	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3474	0	3329	20	0
1	B	3486	0	3344	42	0
2	C	5853	0	5914	15	0
3	D	5560	0	5575	10	0
4	U	275	0	280	0	0
5	A	28	0	12	0	0
5	B	28	0	12	0	0
All	All	18704	0	18466	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:PHE:HB2	1:B:379:ASN:O	1.46	1.14
1:B:315:TYR:HB3	1:B:343:LYS:O	1.52	1.08
1:B:316:PHE:CB	1:B:379:ASN:O	2.04	1.04
1:B:180:VAL:HG13	1:B:393:THR:HG21	1.40	1.04
1:A:188:ILE:HD12	1:A:394:PHE:CD1	2.02	0.93
1:A:188:ILE:CD1	1:A:394:PHE:CD1	2.56	0.87
1:B:184:SER:HB2	1:B:394:PHE:HB3	1.56	0.86
1:B:259:LEU:HA	1:B:317:ASN:ND2	1.90	0.85
1:B:180:VAL:HG13	1:B:393:THR:CG2	2.07	0.85
1:B:315:TYR:O	1:B:380:MET:HG2	1.86	0.76
1:B:180:VAL:CG1	1:B:393:THR:HG21	2.16	0.73
1:A:188:ILE:HD13	1:A:394:PHE:CG	2.24	0.72
1:A:188:ILE:CD1	1:A:394:PHE:CG	2.71	0.72
1:A:188:ILE:HD13	1:A:394:PHE:CD1	2.29	0.65
2:C:581:LYS:NZ	2:C:681:THR:OG1	2.30	0.63
1:B:387:PHE:O	1:B:391:CYS:SG	2.52	0.63
1:B:394:PHE:HE1	1:B:427:ARG:NE	1.97	0.61
1:B:180:VAL:HG22	1:B:393:THR:HG21	1.81	0.60
3:D:471:ARG:NH2	3:D:671:THR:OG1	2.35	0.60
1:B:258:THR:O	1:B:317:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:PHE:HB3	1:B:379:ASN:O	2.00	0.59
1:B:259:LEU:HA	1:B:317:ASN:HD21	1.68	0.59
1:B:246:SER:OG	1:B:247:TYR:N	2.35	0.58
1:A:246:SER:OG	1:A:247:TYR:N	2.39	0.56
2:C:459:ASP:N	2:C:459:ASP:OD1	2.38	0.55
1:B:316:PHE:HB2	1:B:380:MET:HA	1.88	0.55
3:D:163:SER:OG	3:D:164:SER:N	2.41	0.54
1:A:188:ILE:HD12	1:A:394:PHE:HD1	1.66	0.54
2:C:618:SER:OG	2:C:619:HIS:N	2.42	0.52
1:B:180:VAL:HG22	1:B:393:THR:CG2	2.40	0.52
1:B:394:PHE:CE1	1:B:427:ARG:CD	2.93	0.51
2:C:18:ASN:OD1	2:C:18:ASN:N	2.37	0.51
2:C:128:ASP:OD1	2:C:129:THR:N	2.43	0.51
2:C:663:TYR:O	2:C:665:ASN:N	2.44	0.51
1:B:394:PHE:HE1	1:B:427:ARG:CD	2.25	0.50
3:D:498:ASP:N	3:D:498:ASP:OD1	2.41	0.50
1:A:188:ILE:HG22	1:A:189:LEU:HD12	1.93	0.50
1:B:394:PHE:C	1:B:394:PHE:CD1	2.85	0.50
1:B:452:ASP:OD2	3:D:630:LYS:NZ	2.44	0.50
1:B:223:ASP:OD1	1:B:224:LEU:N	2.45	0.50
1:A:188:ILE:CD1	1:A:394:PHE:CB	2.89	0.50
1:B:394:PHE:CE1	1:B:427:ARG:HD3	2.47	0.49
1:A:61:LYS:NZ	1:A:85:GLY:O	2.46	0.49
2:C:183:ASN:OD1	2:C:183:ASN:N	2.45	0.48
3:D:498:ASP:OD2	3:D:511:LYS:NZ	2.40	0.48
1:B:41:ASP:OD1	1:B:41:ASP:N	2.46	0.48
1:B:180:VAL:HG22	1:B:393:THR:CB	2.43	0.48
1:B:315:TYR:HE1	1:B:441:GLU:HA	1.79	0.47
1:B:391:CYS:HA	1:B:394:PHE:CZ	2.49	0.46
3:D:685:ASN:OD1	3:D:685:ASN:N	2.46	0.46
3:D:250:LYS:NZ	3:D:361:GLU:OE2	2.49	0.46
1:A:29:HIS:O	1:A:31:ILE:N	2.49	0.46
1:A:188:ILE:CD1	1:A:394:PHE:HB2	2.46	0.46
1:B:180:VAL:CG2	1:B:393:THR:HG21	2.44	0.45
1:B:180:VAL:C	1:B:393:THR:HG21	2.37	0.45
1:B:319:TYR:OH	1:B:355:ASN:ND2	2.49	0.45
1:B:391:CYS:HA	1:B:394:PHE:CE2	2.51	0.45
1:B:394:PHE:C	1:B:394:PHE:HD1	2.19	0.45
2:C:123:TYR:CD2	2:C:123:TYR:C	2.90	0.45
1:B:209:LEU:HB3	1:B:227:THR:CG2	2.47	0.45
1:B:47:ASP:OD1	1:B:47:ASP:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:PHE:HB2	1:B:379:ASN:C	2.29	0.44
2:C:702:ILE:HG23	2:C:706:PHE:CZ	2.53	0.43
2:C:501:ILE:O	2:C:502:TYR:C	2.55	0.43
1:A:41:ASP:N	1:A:41:ASP:OD1	2.44	0.43
2:C:710:ILE:O	2:C:711:LYS:HB2	2.19	0.43
1:A:34:ASP:N	1:A:34:ASP:OD1	2.47	0.43
2:C:788:THR:O	2:C:789:GLU:C	2.56	0.42
1:A:449:VAL:HG22	2:C:623:ARG:HB3	2.00	0.42
1:B:51:LYS:N	1:B:52:PRO:HD2	2.34	0.42
1:B:184:SER:CB	1:B:394:PHE:HB3	2.39	0.41
1:A:131:ASP:OD1	1:A:131:ASP:N	2.53	0.41
1:A:344:PHE:HB2	1:A:345:PRO:HD2	2.02	0.41
3:D:409:TYR:CD2	3:D:409:TYR:C	2.94	0.41
1:A:127:ILE:O	1:A:130:THR:OG1	2.38	0.41
1:B:330:GLN:N	1:B:330:GLN:OE1	2.53	0.41
2:C:300:MET:O	2:C:301:THR:CB	2.68	0.41
3:D:247:SER:HA	3:D:248:PRO:HD3	1.96	0.41
1:A:83:PHE:HB3	1:A:86:PHE:HB3	2.03	0.41
1:B:316:PHE:HZ	1:B:440:ALA:HB3	1.86	0.41
1:A:444:SER:O	1:A:445:TYR:C	2.60	0.41
1:B:34:ASP:N	1:B:34:ASP:OD1	2.45	0.41
1:B:180:VAL:HG22	1:B:393:THR:HB	2.02	0.41
3:D:443:THR:O	3:D:446:PHE:N	2.52	0.40
2:C:300:MET:O	2:C:301:THR:HB	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	440/473 (93%)	433 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	442/473 (93%)	425 (96%)	15 (3%)	2 (0%)	29	68
2	C	689/823 (84%)	672 (98%)	14 (2%)	3 (0%)	34	71
3	D	669/846 (79%)	656 (98%)	10 (2%)	3 (0%)	34	71
4	U	31/220 (14%)	31 (100%)	0	0	100	100
All	All	2271/2835 (80%)	2217 (98%)	46 (2%)	8 (0%)	38	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	315	TYR
2	C	664	ARG
3	D	798	SER
2	C	301	THR
2	C	753	GLN
3	D	560	LEU
1	B	317	ASN
3	D	835	ASP

### 5.3.2 Protein sidechains ⓘ

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	
1	A	396/420 (94%)	395 (100%)	1 (0%)	92	97
1	B	397/420 (94%)	393 (99%)	4 (1%)	76	88
2	C	657/766 (86%)	656 (100%)	1 (0%)	93	98
3	D	627/787 (80%)	627 (100%)	0	100	100
4	U	31/206 (15%)	31 (100%)	0	100	100
All	All	2108/2599 (81%)	2102 (100%)	6 (0%)	92	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	B	55	ARG
1	B	161	ARG
1	B	315	TYR
1	B	394	PHE
2	C	617	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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](#)

2 ligands 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	$\# Z  > 2$
5	GDP	A	1400	-	24,30,30	1.41	4 (16%)	30,47,47	1.37	5 (16%)
5	GDP	B	501	-	24,30,30	1.23	2 (8%)	30,47,47	1.61	7 (23%)

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
5	GDP	A	1400	-	-	3/12/32/32	0/3/3/3
5	GDP	B	501	-	-	8/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1400	GDP	O4'-C1'	3.91	1.46	1.41
5	A	1400	GDP	C8-N7	-3.37	1.29	1.35
5	B	501	GDP	C8-N7	-2.88	1.30	1.35
5	B	501	GDP	O4'-C1'	2.36	1.44	1.41
5	A	1400	GDP	C2'-C1'	2.22	1.57	1.53
5	A	1400	GDP	C5'-C4'	2.01	1.57	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	O4'-C1'-C2'	-3.78	101.40	106.93
5	B	501	GDP	C8-N7-C5	3.37	109.41	102.99
5	A	1400	GDP	C5-C6-N1	3.17	119.55	113.95
5	A	1400	GDP	C8-N7-C5	3.01	108.72	102.99
5	B	501	GDP	C5-C6-N1	2.98	119.22	113.95
5	B	501	GDP	O2B-PB-O3A	2.77	113.92	104.64
5	B	501	GDP	C2-N1-C6	-2.35	120.77	125.10
5	A	1400	GDP	O4'-C1'-C2'	-2.25	103.64	106.93
5	A	1400	GDP	C2-N1-C6	-2.16	121.11	125.10
5	A	1400	GDP	C3'-C2'-C1'	2.16	104.23	100.98
5	B	501	GDP	O3B-PB-O3A	2.12	111.73	104.64
5	B	501	GDP	C3'-C2'-C1'	2.05	104.07	100.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1400	GDP	O4'-C4'-C5'-O5'
5	A	1400	GDP	C3'-C4'-C5'-O5'
5	B	501	GDP	C5'-O5'-PA-O3A
5	B	501	GDP	C5'-O5'-PA-O2A
5	B	501	GDP	C4'-C5'-O5'-PA
5	A	1400	GDP	C4'-C5'-O5'-PA

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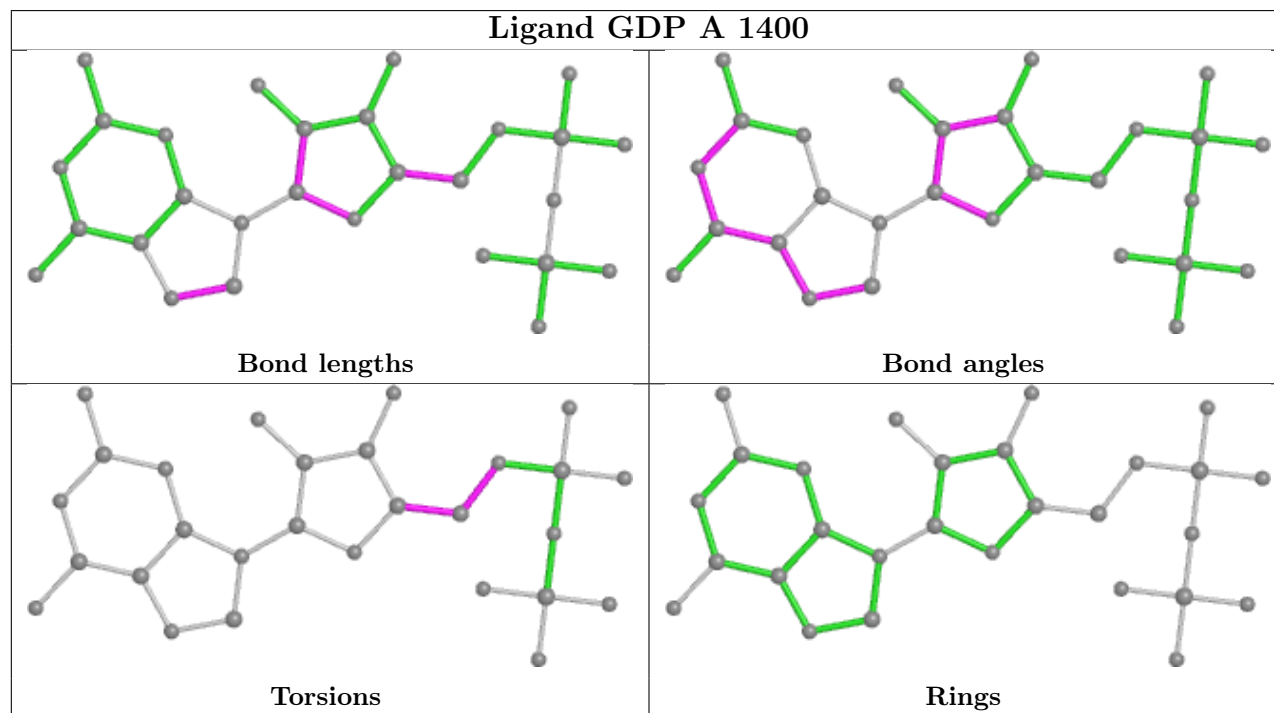
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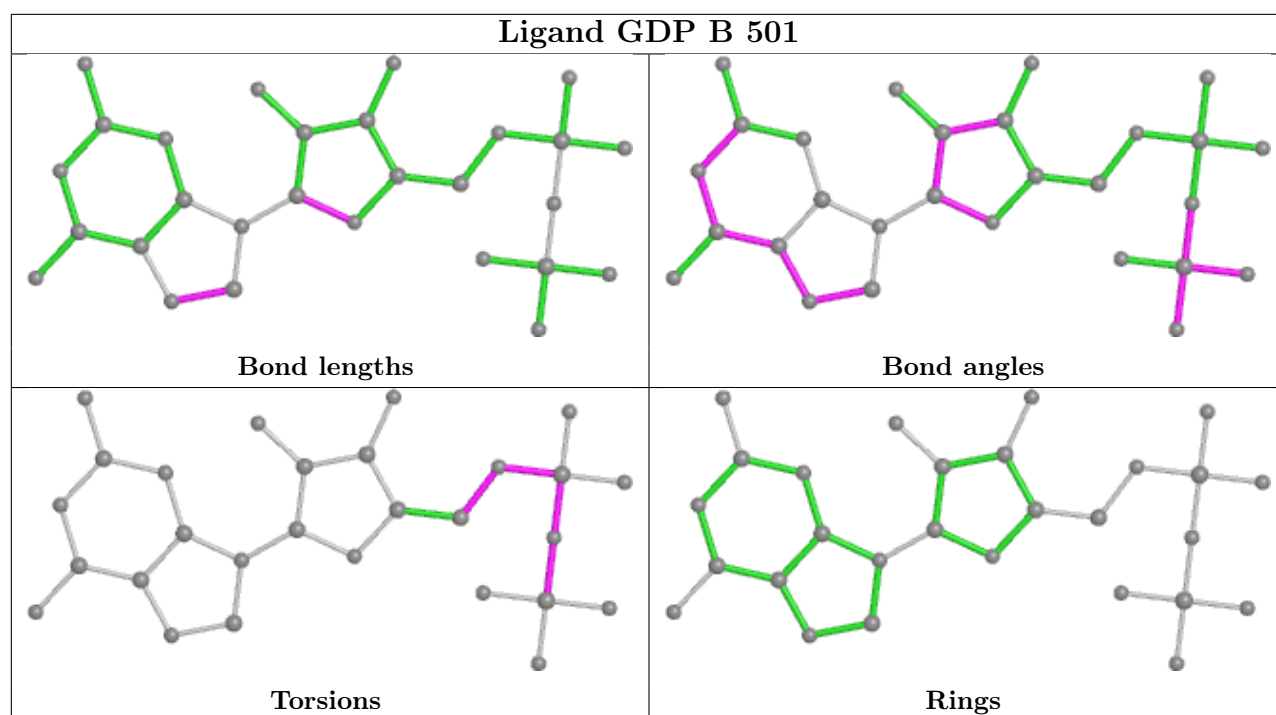
Mol	Chain	Res	Type	Atoms
5	B	501	GDP	C5'-O5'-PA-O1A
5	B	501	GDP	PA-O3A-PB-O1B
5	B	501	GDP	PA-O3A-PB-O2B
5	B	501	GDP	PA-O3A-PB-O3B
5	B	501	GDP	PB-O3A-PA-O2A

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.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23636. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal surface views

This section was not generated.

### 6.5 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

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

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.