Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jan 25, 2017 – 11:55 AM EST

PDB ID	:	5SYE
EMDB ID:	:	EMD-8321
Title	:	Near-atomic resolution cryo-EM reconstruction of doubly bound Taxol- and p eloruside-stabilized microtubule
Authors	:	Kellogg, E.H.; Nogales, E.
Deposited on	:	2016-08-10
Resolution	:	3.50 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

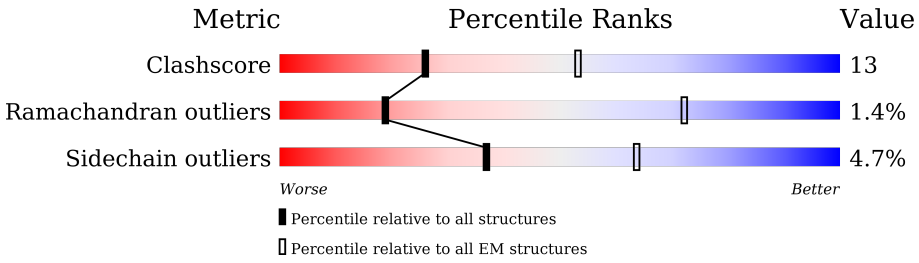
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	437	79% 17% • •
2	B	426	83% 16% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	POU	B	503	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6864 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.

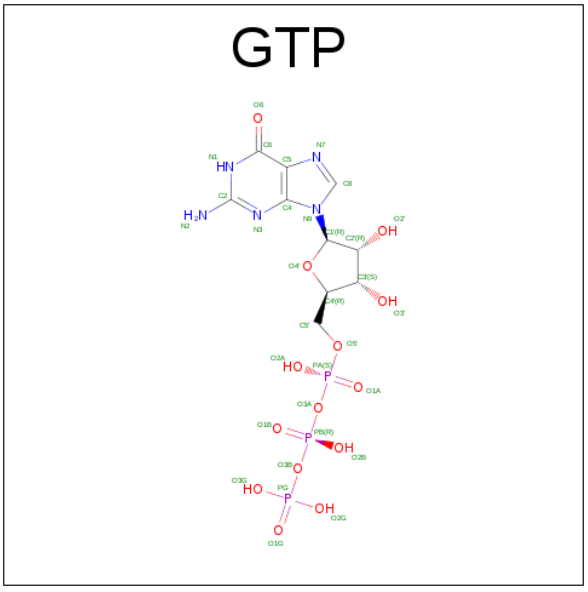
- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	427	3351	2125	570	634	22	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	426	3352	2106	575	645	26	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

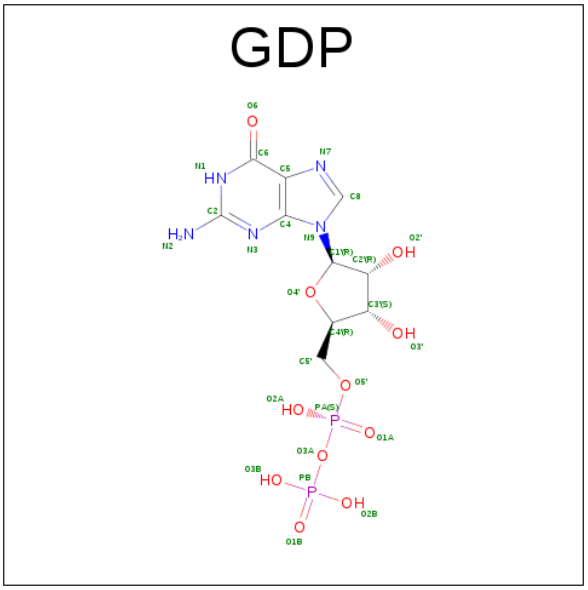


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	32	10	5	14	3	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

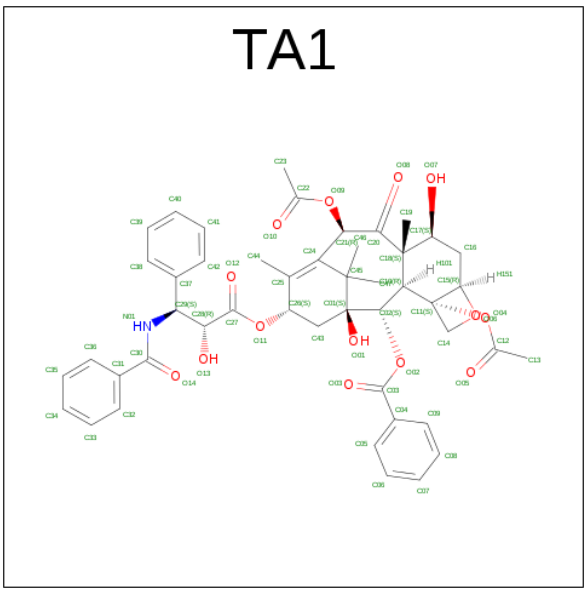
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



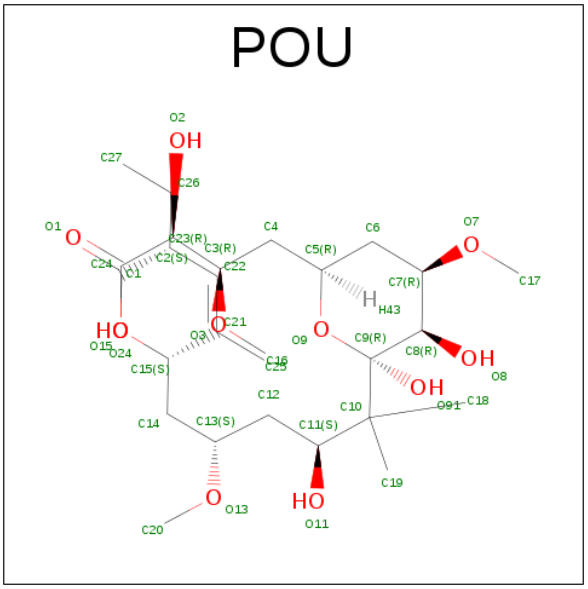
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	B	1	28	10	5	11	2	0

- Molecule 6 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			62	47	1	14	

- Molecule 7 is Peloruside A (three-letter code: POU) (formula: $C_{27}H_{48}O_{11}$).



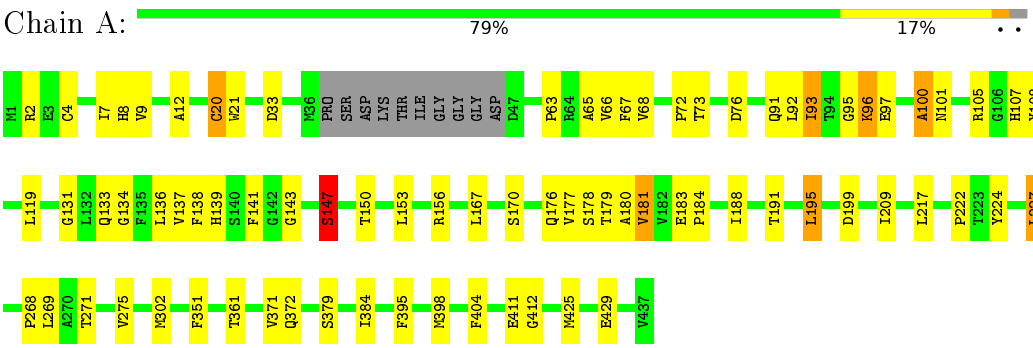
Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	C	O	0
			38	27	11	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

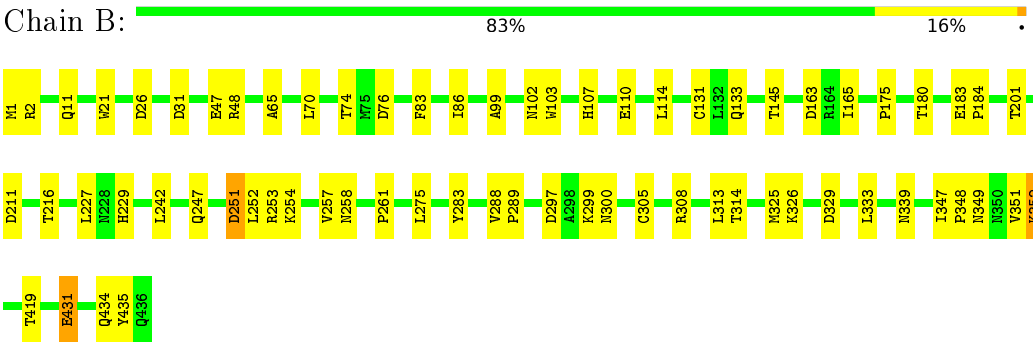
- Molecule 1: Tubulin alpha chain

Chain A:



- Molecule 2: Tubulin beta chain

Chain B:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	17069	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	27500	Depositor
Image detector	Not provided	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, GTP, MG, POU, TA1

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	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	A	0.40	0/3427	0.67	0/4650
2	B	0.44	0/3427	0.65	0/4641
All	All	0.42	0/6854	0.66	0/9291

There are no bond length outliers.

There are no bond angle outliers.

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	3351	0	3265	114	0
2	B	3352	0	3237	144	0
3	A	32	0	12	1	0
4	A	1	0	0	0	0
5	B	28	0	12	0	0
6	B	62	0	51	12	0
7	B	38	0	48	23	0
All	All	6864	0	6625	181	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 13.

All (181) 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:A:398:MET:CE	2:B:348:PRO:HD2	1.07	1.53
1:A:398:MET:HE2	2:B:348:PRO:CD	1.43	1.45
2:B:165:ILE:CD1	2:B:253:ARG:HG3	1.50	1.37
1:A:73:THR:HA	2:B:48:ARG:NH2	1.42	1.33
1:A:398:MET:CE	2:B:348:PRO:CD	2.02	1.32
1:A:404:PHE:CE2	2:B:261:PRO:HB3	1.65	1.31
2:B:165:ILE:HD11	2:B:253:ARG:CG	1.60	1.29
2:B:163:ASP:O	2:B:253:ARG:NH2	1.66	1.25
1:A:404:PHE:CD2	2:B:261:PRO:HA	1.72	1.25
2:B:297:ASP:OD1	7:B:503:POU:C2	1.90	1.18
2:B:299:LYS:NZ	7:B:503:POU:H34	1.54	1.18
1:A:404:PHE:CE2	2:B:261:PRO:CB	2.28	1.16
2:B:297:ASP:OD1	7:B:503:POU:O2	1.61	1.15
2:B:229:HIS:NE2	6:B:502:TA1:O14	1.81	1.13
1:A:404:PHE:CE2	2:B:261:PRO:CA	2.32	1.12
2:B:26:ASP:OD2	6:B:502:TA1:H331	1.54	1.07
1:A:224:TYR:CE1	2:B:325:MET:HG3	1.88	1.06
1:A:398:MET:HE3	2:B:348:PRO:HD2	1.06	1.05
1:A:404:PHE:CE2	2:B:261:PRO:HA	1.92	1.03
1:A:178:SER:HB3	2:B:349:ASN:ND2	1.76	1.01
1:A:100:ALA:HB1	2:B:254:LYS:HA	1.43	0.97
1:A:404:PHE:HE2	2:B:261:PRO:CB	1.80	0.94
1:A:404:PHE:CZ	2:B:261:PRO:HB3	2.03	0.94
1:A:181:VAL:CG2	2:B:349:ASN:O	2.16	0.94
2:B:308:ARG:HH11	7:B:503:POU:C16	1.82	0.92
1:A:105:ARG:HH22	2:B:253:ARG:NH1	1.68	0.92
1:A:7:ILE:HD12	1:A:137:VAL:HG22	1.52	0.91
2:B:297:ASP:OD1	7:B:503:POU:H44	1.68	0.91
1:A:73:THR:HA	2:B:48:ARG:HH21	1.07	0.89
2:B:299:LYS:HZ3	7:B:503:POU:H34	1.38	0.89
2:B:308:ARG:NH1	7:B:503:POU:O3	2.06	0.89
2:B:299:LYS:NZ	7:B:503:POU:C6	2.36	0.88
1:A:404:PHE:HE2	2:B:261:PRO:CA	1.79	0.87
1:A:404:PHE:HD2	2:B:261:PRO:HA	1.35	0.85
1:A:398:MET:HE1	2:B:347:ILE:HG23	1.59	0.85
1:A:73:THR:CA	2:B:48:ARG:NH2	2.35	0.84
1:A:105:ARG:HH22	2:B:253:ARG:HH11	1.24	0.82
1:A:398:MET:HE3	2:B:348:PRO:CD	1.90	0.82
1:A:398:MET:HE2	2:B:348:PRO:HD2	0.82	0.82
2:B:299:LYS:HZ1	7:B:503:POU:H34	1.41	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:ASP:CG	7:B:503:POU:H44	2.01	0.81
1:A:73:THR:HA	2:B:48:ARG:HH22	1.42	0.80
1:A:73:THR:CA	2:B:48:ARG:HH21	1.93	0.80
1:A:181:VAL:N	2:B:258:ASN:OD1	2.14	0.80
1:A:180:ALA:HB1	2:B:258:ASN:HD21	1.45	0.80
1:A:398:MET:HE2	2:B:347:ILE:HA	1.63	0.80
2:B:229:HIS:HE1	6:B:502:TA1:H132	1.47	0.80
1:A:100:ALA:HB1	2:B:254:LYS:CA	2.11	0.80
1:A:95:GLY:O	2:B:1:MET:CE	2.26	0.78
2:B:165:ILE:CD1	2:B:253:ARG:CG	2.38	0.78
1:A:181:VAL:CG2	2:B:351:VAL:O	2.31	0.78
1:A:224:TYR:CD1	2:B:325:MET:HG3	2.19	0.77
2:B:70:LEU:HD23	2:B:114:LEU:HD22	1.66	0.76
1:A:181:VAL:HG21	2:B:349:ASN:O	1.84	0.76
2:B:165:ILE:HD11	2:B:253:ARG:HG3	0.76	0.75
1:A:181:VAL:CG1	2:B:349:ASN:O	2.34	0.75
1:A:72:PRO:HD2	2:B:2:ARG:NH1	2.03	0.74
1:A:72:PRO:HG2	2:B:2:ARG:NH1	2.03	0.74
1:A:139:HIS:HB3	1:A:150:THR:HG21	1.69	0.73
2:B:165:ILE:HG13	2:B:253:ARG:HE	1.52	0.73
1:A:76:ASP:OD2	2:B:48:ARG:NH1	2.21	0.73
1:A:181:VAL:HG23	2:B:351:VAL:O	1.89	0.71
1:A:178:SER:OG	2:B:349:ASN:HB3	1.91	0.70
1:A:181:VAL:HG22	2:B:349:ASN:O	1.91	0.69
2:B:275:LEU:HD12	2:B:300:ASN:OD1	1.92	0.69
1:A:176:GLN:HB3	2:B:333:LEU:HD11	1.73	0.68
1:A:398:MET:HE2	2:B:348:PRO:N	2.08	0.68
2:B:229:HIS:HE2	6:B:502:TA1:C30	2.05	0.67
1:A:398:MET:CE	2:B:347:ILE:HG23	2.24	0.67
1:A:224:TYR:CE1	2:B:325:MET:CG	2.72	0.66
2:B:2:ARG:HH22	2:B:48:ARG:CZ	2.08	0.66
1:A:72:PRO:CG	2:B:2:ARG:NH1	2.58	0.66
1:A:72:PRO:CG	2:B:2:ARG:HH12	2.08	0.66
1:A:177:VAL:CG2	2:B:329:ASP:OD2	2.42	0.66
1:A:12:ALA:HB2	3:A:501:GTP:C8	2.32	0.65
2:B:165:ILE:HD11	2:B:253:ARG:CD	2.26	0.65
2:B:299:LYS:HZ2	7:B:503:POU:C5	2.10	0.65
1:A:100:ALA:HA	2:B:254:LYS:HE3	1.77	0.65
1:A:398:MET:HE2	2:B:347:ILE:CA	2.28	0.64
1:A:76:ASP:OD2	2:B:48:ARG:NH2	2.30	0.64
2:B:308:ARG:NH1	7:B:503:POU:C16	2.58	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:SER:CB	2:B:349:ASN:ND2	2.59	0.64
1:A:96:LYS:HG2	2:B:131:CYS:CB	2.28	0.62
1:A:95:GLY:O	2:B:1:MET:HE2	1.99	0.62
2:B:299:LYS:HZ2	7:B:503:POU:H43	1.66	0.61
2:B:369:ARG:HB2	6:B:502:TA1:O13	2.00	0.61
2:B:369:ARG:CB	6:B:502:TA1:O13	2.48	0.61
6:B:502:TA1:H261	6:B:502:TA1:H463	1.82	0.61
2:B:165:ILE:CG1	2:B:253:ARG:HE	2.13	0.60
1:A:398:MET:HE1	2:B:347:ILE:CG2	2.30	0.60
1:A:177:VAL:HG21	2:B:329:ASP:OD2	2.02	0.60
1:A:72:PRO:HG2	2:B:2:ARG:HH12	1.67	0.59
1:A:72:PRO:CD	2:B:2:ARG:NH1	2.65	0.59
1:A:7:ILE:HG23	1:A:66:VAL:HB	1.85	0.58
2:B:297:ASP:OD1	7:B:503:POU:C1	2.51	0.58
1:A:180:ALA:HB1	2:B:258:ASN:ND2	2.16	0.57
1:A:404:PHE:HE2	2:B:261:PRO:N	2.02	0.57
2:B:247:GLN:OE1	2:B:325:MET:CE	2.54	0.55
1:A:181:VAL:HG11	2:B:349:ASN:O	2.04	0.55
1:A:217:LEU:HG	1:A:275:VAL:HG12	1.88	0.55
1:A:95:GLY:O	2:B:1:MET:HE1	1.89	0.55
2:B:11:GLN:HA	2:B:74:THR:HG21	1.88	0.55
2:B:133:GLN:HG3	2:B:252:LEU:HD12	1.88	0.54
1:A:76:ASP:OD2	2:B:48:ARG:CZ	2.56	0.54
2:B:133:GLN:NE2	2:B:251:ASP:OD2	2.40	0.54
1:A:209:ILE:HG21	1:A:227:LEU:HD13	1.90	0.54
1:A:404:PHE:CD2	2:B:261:PRO:CA	2.58	0.54
1:A:139:HIS:CB	1:A:150:THR:HG21	2.38	0.53
2:B:308:ARG:HD3	7:B:503:POU:H15	1.90	0.53
1:A:269:LEU:HD21	1:A:384:ILE:HG12	1.91	0.53
1:A:178:SER:HB3	2:B:349:ASN:CG	2.28	0.52
2:B:299:LYS:NZ	7:B:503:POU:C5	2.70	0.52
6:B:502:TA1:H171	6:B:502:TA1:H442	1.91	0.52
1:A:199:ASP:OD1	1:A:256:GLN:NE2	2.43	0.51
2:B:308:ARG:HH11	7:B:503:POU:H7	1.72	0.51
2:B:247:GLN:OE1	2:B:325:MET:SD	2.68	0.51
1:A:181:VAL:HG13	2:B:349:ASN:O	2.11	0.50
1:A:2:ARG:HG2	1:A:133:GLN:HE21	1.76	0.50
1:A:4:CYS:SG	1:A:134:GLY:N	2.85	0.50
1:A:72:PRO:HD2	2:B:2:ARG:HH11	1.77	0.49
1:A:178:SER:OG	2:B:349:ASN:CB	2.60	0.49
2:B:297:ASP:OD2	7:B:503:POU:H43	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HB2	2:B:2:ARG:HH12	1.77	0.49
1:A:72:PRO:CB	2:B:2:ARG:HH12	2.26	0.48
2:B:165:ILE:CG1	2:B:253:ARG:CG	2.92	0.48
6:B:502:TA1:H101	6:B:502:TA1:C25	2.44	0.48
1:A:21:TRP:HZ2	1:A:65:ALA:HB2	1.79	0.48
1:A:63:PRO:O	1:A:91:GLN:NE2	2.31	0.47
1:A:398:MET:HE3	2:B:348:PRO:CG	2.42	0.47
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.50	0.47
2:B:165:ILE:HD13	2:B:253:ARG:HG3	1.74	0.47
6:B:502:TA1:H381	6:B:502:TA1:H131	1.96	0.47
1:A:136:LEU:HD23	1:A:167:LEU:HB2	1.97	0.47
2:B:83:PHE:O	2:B:86:ILE:HG12	2.14	0.47
1:A:68:VAL:HG13	1:A:93:ILE:HG21	1.98	0.46
1:A:143:GLY:O	1:A:147:SER:HB2	2.16	0.46
1:A:178:SER:CB	2:B:349:ASN:CG	2.84	0.46
2:B:103:TRP:CH2	2:B:107:HIS:CG	3.03	0.46
2:B:70:LEU:HD12	2:B:145:THR:HG22	1.98	0.46
2:B:183:GLU:N	2:B:184:PRO:HD2	2.31	0.46
1:A:115:ILE:HD11	1:A:153:LEU:HA	1.96	0.46
1:A:7:ILE:HG22	1:A:9:VAL:HG23	1.97	0.46
1:A:7:ILE:N	1:A:136:LEU:O	2.44	0.46
1:A:67:PHE:CB	1:A:92:LEU:HD23	2.46	0.45
2:B:308:ARG:HG2	7:B:503:POU:H15	1.98	0.45
1:A:179:THR:O	2:B:352:LYS:HA	2.17	0.45
6:B:502:TA1:C26	6:B:502:TA1:H463	2.47	0.45
1:A:67:PHE:HB3	1:A:92:LEU:HD23	1.99	0.45
1:A:68:VAL:HG13	1:A:93:ILE:CG2	2.47	0.45
1:A:97:GLU:OE1	2:B:131:CYS:SG	2.75	0.44
2:B:253:ARG:O	2:B:257:VAL:HG23	2.18	0.44
2:B:229:HIS:CE1	6:B:502:TA1:O14	2.60	0.44
7:B:503:POU:H27	7:B:503:POU:O15	2.18	0.44
1:A:224:TYR:HE1	2:B:325:MET:SD	2.41	0.44
1:A:398:MET:CE	2:B:347:ILE:HA	2.43	0.43
1:A:224:TYR:CD1	2:B:325:MET:CG	2.97	0.43
2:B:2:ARG:HD2	2:B:242:LEU:HD22	2.00	0.43
1:A:271:THR:HA	1:A:302:MET:HG3	2.00	0.43
2:B:99:ALA:O	2:B:102:ASN:HB3	2.19	0.43
2:B:209:LEU:HB3	2:B:227:LEU:HD22	2.00	0.43
1:A:115:ILE:HD11	1:A:153:LEU:CA	2.48	0.42
1:A:101:ASN:OD1	2:B:254:LYS:HE2	2.19	0.42
1:A:181:VAL:CA	2:B:258:ASN:OD1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HD12	1:A:395:PHE:HB2	2.02	0.42
2:B:313:LEU:HD21	2:B:435:TYR:HB3	2.02	0.42
1:A:119:LEU:HD21	1:A:156:ARG:HB3	2.02	0.42
1:A:224:TYR:CE1	2:B:325:MET:SD	3.13	0.41
1:A:398:MET:HE2	2:B:347:ILE:C	2.40	0.41
1:A:96:LYS:HG2	2:B:131:CYS:HB3	2.01	0.41
2:B:299:LYS:NZ	7:B:503:POU:H31	2.36	0.41
1:A:191:THR:HG21	1:A:425:MET:CE	2.50	0.41
2:B:299:LYS:HZ1	7:B:503:POU:C6	2.20	0.41
2:B:431:GLU:O	2:B:434:GLN:HB2	2.21	0.41
1:A:8:HIS:CE1	1:A:138:PHE:CD1	3.09	0.41
2:B:70:LEU:HD13	2:B:110:GLU:HG3	2.02	0.41
7:B:503:POU:H12	7:B:503:POU:H45	1.85	0.41
2:B:165:ILE:HD13	2:B:252:LEU:HB2	2.02	0.41
1:A:222:PRO:HG2	2:B:326:LYS:HB2	2.03	0.41
2:B:288:VAL:N	2:B:289:PRO:HD2	2.36	0.40
1:A:183:GLU:N	1:A:184:PRO:CD	2.84	0.40
1:A:20:CYS:SG	1:A:235:VAL:HG11	2.61	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	423/437 (97%)	378 (89%)	35 (8%)	10 (2%)	7 47
2	B	424/426 (100%)	409 (96%)	13 (3%)	2 (0%)	34 78
All	All	847/863 (98%)	787 (93%)	48 (6%)	12 (1%)	19 58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	LEU
2	B	369	ARG
1	A	113	GLU
1	A	141	PHE
1	A	147	SER
1	A	100	ALA
1	A	108	TYR
1	A	412	GLY
1	A	131	GLY
2	B	358	ILE
1	A	181	VAL
1	A	268	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
1	A	360/368 (98%)	344 (96%)	16 (4%)	35 73
2	B	367/367 (100%)	349 (95%)	18 (5%)	31 70
All	All	727/735 (99%)	693 (95%)	34 (5%)	37 72

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	CYS
1	A	33	ASP
1	A	93	ILE
1	A	96	LYS
1	A	107	HIS
1	A	147	SER
1	A	170	SER
1	A	195	LEU
1	A	227	LEU
1	A	351	PHE
1	A	361	THR
1	A	371	VAL

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Mol	Chain	Res	Type
1	A	372	GLN
1	A	379	SER
1	A	411	GLU
1	A	429	GLU
2	B	31	ASP
2	B	47	GLU
2	B	76	ASP
2	B	175	PRO
2	B	180	THR
2	B	201	THR
2	B	205	ASP
2	B	211	ASP
2	B	216	THR
2	B	251	ASP
2	B	283	TYR
2	B	305	CYS
2	B	314	THR
2	B	339	ASN
2	B	352	LYS
2	B	369	ARG
2	B	419	THR
2	B	431	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	136	GLN
2	B	349	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	GTP	A	501	4	26,34,34	1.27	2 (7%)	29,54,54	1.88	5 (17%)
5	GDP	B	501	-	24,30,30	1.25	2 (8%)	26,47,47	2.38	5 (19%)
6	TA1	B	502	-	68,68,68	1.79	14 (20%)	102,105,105	1.31	12 (11%)
7	POU	B	503	-	35,39,39	2.18	6 (17%)	29,57,57	2.39	10 (34%)

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
3	GTP	A	501	4	-	0/18/38/38	0/3/3/3
5	GDP	B	501	-	-	0/12/32/32	0/3/3/3
6	TA1	B	502	-	-	0/41/127/127	0/5/7/7
7	POU	B	503	-	-	1/54/76/76	0/0/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	TA1	C08-C07	-5.14	1.25	1.38
7	B	503	POU	C2-C1	-4.94	1.38	1.52
3	A	501	GTP	PG-O3G	-2.86	1.44	1.54
6	B	502	TA1	C04-C03	-2.65	1.43	1.49
6	B	502	TA1	C11-C10	2.01	1.61	1.55
6	B	502	TA1	C41-C42	2.09	1.43	1.38
7	B	503	POU	C14-C13	2.17	1.57	1.52
7	B	503	POU	O11-C11	2.23	1.47	1.43
7	B	503	POU	C23-C22	2.32	1.53	1.50
6	B	502	TA1	C43-C26	2.36	1.58	1.52
5	B	501	GDP	C6-C5	2.46	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GTP	C6-C5	2.47	1.46	1.41
6	B	502	TA1	C25-C24	2.48	1.38	1.34
7	B	503	POU	O91-C9	2.53	1.44	1.39
6	B	502	TA1	C45-C24	2.63	1.59	1.54
6	B	502	TA1	C43-C01	2.68	1.60	1.54
6	B	502	TA1	C46-C45	2.92	1.60	1.53
6	B	502	TA1	O02-C03	3.12	1.41	1.34
6	B	502	TA1	C36-C31	3.49	1.45	1.39
6	B	502	TA1	C18-C10	3.93	1.68	1.57
5	B	501	GDP	O4'-C1'	4.04	1.47	1.41
6	B	502	TA1	C05-C04	4.18	1.46	1.39
6	B	502	TA1	C06-C05	5.55	1.49	1.38
7	B	503	POU	C22-C21	9.82	1.55	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	503	POU	C13-C12-C11	-8.01	103.99	114.39
5	B	501	GDP	C1'-N9-C4	-6.14	119.95	126.81
6	B	502	TA1	C06-C05-C04	-4.79	114.64	120.35
5	B	501	GDP	C6-C5-C4	-4.52	115.69	120.86
3	A	501	GTP	C5-C6-N1	-4.40	117.77	123.52
5	B	501	GDP	C5-C6-N1	-3.93	118.38	123.52
5	B	501	GDP	N3-C2-N1	-3.76	122.44	127.56
6	B	502	TA1	C05-C04-C03	-3.75	111.94	120.38
3	A	501	GTP	C6-C5-C4	-3.59	116.75	120.86
3	A	501	GTP	N3-C2-N1	-3.27	123.10	127.56
3	A	501	GTP	C1'-N9-C4	-3.24	123.19	126.81
7	B	503	POU	C3-C4-C5	-2.92	107.68	114.93
7	B	503	POU	C7-C6-C5	-2.41	107.17	111.07
6	B	502	TA1	O04-C11-C14	-2.30	102.24	108.08
7	B	503	POU	C25-C21-C22	-2.26	117.73	123.66
6	B	502	TA1	C38-C37-C29	-2.14	117.29	120.79
6	B	502	TA1	C31-C30-N01	-2.10	113.31	116.98
6	B	502	TA1	C08-C09-C04	-2.02	117.94	120.35
7	B	503	POU	O9-C5-C6	2.01	112.98	108.83
7	B	503	POU	C14-C13-C12	2.08	116.09	112.76
6	B	502	TA1	O11-C27-O12	2.08	127.91	123.88
7	B	503	POU	O9-C5-C4	2.12	109.69	106.00
6	B	502	TA1	C17-C18-C20	2.45	109.49	102.14
6	B	502	TA1	O01-C01-C43	2.57	113.53	106.82
6	B	502	TA1	C45-C01-C02	2.75	114.81	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	503	POU	O15-C15-C21	2.89	117.80	109.69
6	B	502	TA1	C09-C04-C03	3.31	127.83	120.38
7	B	503	POU	O15-C15-C14	3.95	114.44	106.28
7	B	503	POU	C15-O15-C1	4.62	126.48	116.81
6	B	502	TA1	C07-C08-C09	5.25	127.50	120.20
3	A	501	GTP	C6-N1-C2	5.53	122.37	115.88
5	B	501	GDP	C6-N1-C2	6.33	123.30	115.88

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	503	POU	C23-C22-C21-C15

There are no ring outliers.

3 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GTP	1	0
6	B	502	TA1	12	0
7	B	503	POU	23	0

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.