



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:48 AM UTC

PDB ID : 6ZYX / pdb_00006zyx
EMDB ID : EMD-11579
Title : Outer Dynein Arm-Shulin complex - Shulin region from Tetrahymena thermophila
Authors : Mali, G.R.; Abid Ali, F.; Lau, C.K.; Carter, A.P.
Deposited on : 2020-08-03
Resolution : 4.30 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

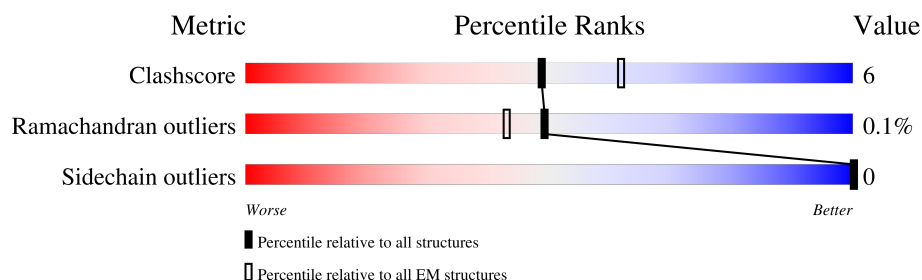
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	C	4620	5% . 94%
2	J	93	78% 12% 10%
3	K	111	81% 5% 14%
4	L	111	70% 17% 13%
5	M	87	90% 9% .
6	N	132	69% 14% 17%
7	O	117	78% 17% 5%
8	Y	1200	80% 9% 11%
9	d	667	12% . 86%

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Mol	Chain	Length	Quality of chain
10	e	670	 6% • 93%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16725 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 Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	278	Total	C	N	O	S	0	0
			2282	1444	396	434	8		

- Molecule 2 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	84	Total	C	N	O	S	0	0
			702	459	114	125	4		

- Molecule 3 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	95	Total	C	N	O	S	0	0
			803	525	134	139	5		

- Molecule 4 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	97	Total	C	N	O	S	0	0
			773	506	131	133	3		

- Molecule 5 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	86	Total	C	N	O	S	0	0
			726	472	122	128	4		

- Molecule 6 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	109	Total	C	N	O	S	0	0
			897	581	154	159	3		

- Molecule 7 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	111	Total	C	N	O	S	0	0
			878	558	143	174	3		

- Molecule 8 is a protein called Shulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	1067	Total	C	N	O	S	0	0
			8476	5503	1397	1550	26		

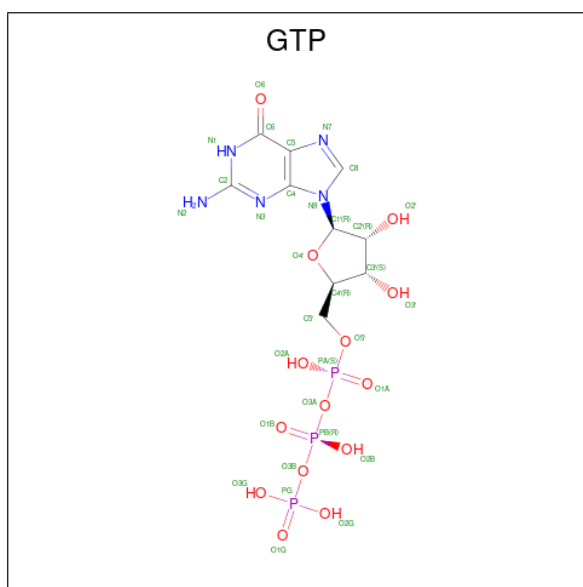
- Molecule 9 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	91	Total	C	N	O	S	0	0
			767	481	133	150	3		

- Molecule 10 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	e	49	Total	C	N	O	0	0
			389	239	72	78		

- Molecule 11 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

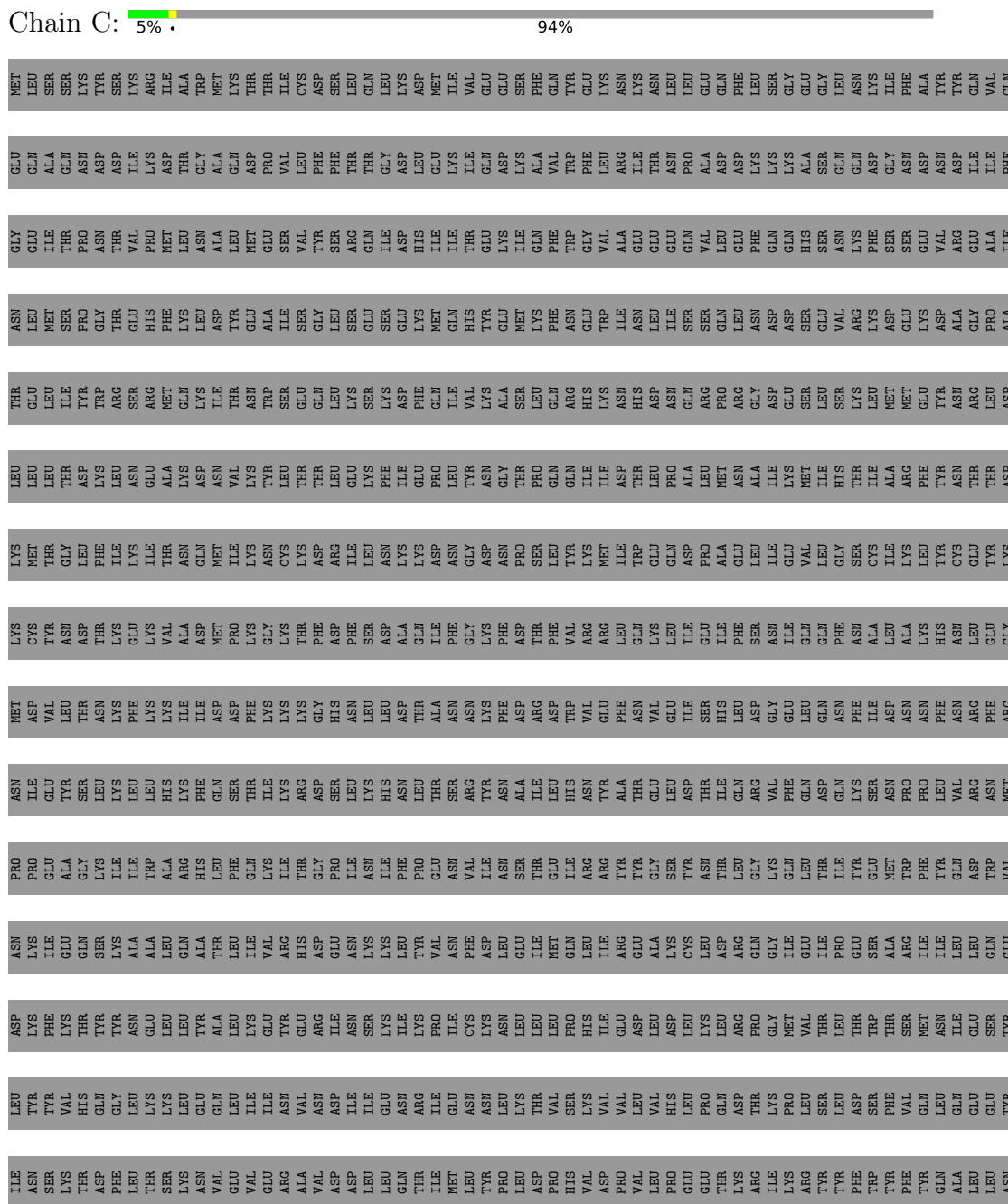


Mol	Chain	Residues	Atoms					AltConf
11	Y	1	Total	C	N	O	P	0
			32	10	5	14	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Dynein heavy chain, outer arm protein







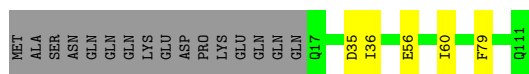
- Molecule 2: Dynein light chain

Chain J:  78% 12% 10%



- Molecule 3: Dynein light chain

Chain K:  81% 5% 14%

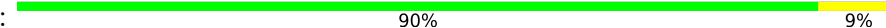


- Molecule 4: Dynein light chain

Chain L:  70% 17% 13%



- Molecule 5: Dynein light chain

Chain M:  90% 9% .



- Molecule 6: Dynein light chain 2A

Chain N:  69% 14% 17%



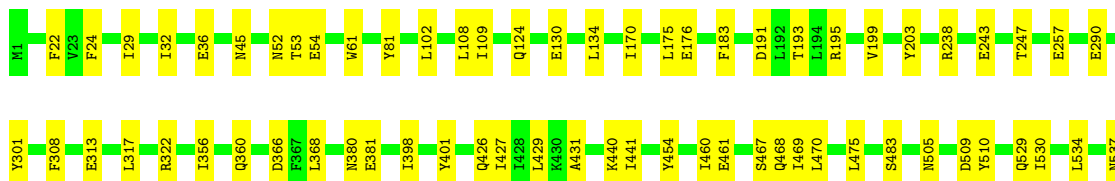
- Molecule 7: Dynein light chain tctex-type 1 protein

Chain O:  78% 17% 5%



- Molecule 8: Shulin

Chain Y:  80% 9% 11%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43338	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
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: GTP

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	C	0.54	2/2320 (0.1%)	0.71	3/3111 (0.1%)
2	J	0.43	1/723 (0.1%)	0.60	0/966
3	K	0.35	0/828	0.60	0/1114
4	L	0.38	0/790	0.70	0/1063
5	M	0.33	0/743	0.57	0/996
6	N	0.35	0/915	0.64	1/1229 (0.1%)
7	O	0.23	0/891	0.42	0/1209
8	Y	0.32	0/8641	0.56	2/11670 (0.0%)
9	d	0.36	0/781	0.68	0/1050
10	e	0.36	0/394	0.58	0/536
All	All	0.37	3/17026 (0.0%)	0.60	6/22944 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1091	GLU	C-N	-5.49	1.26	1.33
2	J	30	LYS	CE-NZ	-5.47	1.32	1.49
1	C	1304	ILE	C-N	5.27	1.41	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	1106	PRO	N-CA-CB	7.53	111.16	103.25
8	Y	723	PRO	N-CA-CB	7.20	110.81	103.25
1	C	1051	GLN	N-CA-CB	5.92	118.83	110.12
6	N	59	LEU	CA-CB-CG	5.17	134.40	116.30
1	C	1304	ILE	CA-C-N	-5.00	112.71	120.31
1	C	1304	ILE	C-N-CA	-5.00	112.71	120.31

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	C	2282	0	2236	36	0
2	J	702	0	671	26	0
3	K	803	0	766	3	0
4	L	773	0	806	14	0
5	M	726	0	726	7	0
6	N	897	0	911	15	0
7	O	878	0	868	17	0
8	Y	8476	0	8421	70	0
9	d	767	0	747	36	0
10	e	389	0	357	14	0
11	Y	32	0	12	2	0
All	All	16725	0	16521	191	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 6.

All (191) 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)
2:J:65:HIS:NE2	9:d:188:GLU:CA	1.69	1.50
2:J:65:HIS:CE1	9:d:188:GLU:HA	1.65	1.31
2:J:65:HIS:CD2	9:d:187:THR:O	1.90	1.24
2:J:65:HIS:NE2	9:d:188:GLU:HA	0.73	1.06
2:J:65:HIS:CD2	9:d:188:GLU:HA	2.00	0.96
2:J:72:TYR:OH	9:d:183:ARG:NH2	2.04	0.89
2:J:65:HIS:HD2	9:d:187:THR:O	1.64	0.77
8:Y:301:TYR:OH	8:Y:475:LEU:O	2.01	0.77
4:L:52:ASP:OD1	4:L:56:ASN:ND2	2.18	0.77
8:Y:635:TYR:O	8:Y:639:ASN:ND2	2.19	0.75
2:J:65:HIS:CD2	9:d:187:THR:C	2.64	0.74
8:Y:895:ASN:OD1	11:Y:1301:GTP:O2'	2.06	0.74
1:C:1158:GLU:CD	9:d:181:ARG:HH22	1.96	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:99:GLN:NE2	7:O:100:CYS:O	2.21	0.73
8:Y:826:ARG:NH2	8:Y:906:LEU:O	2.21	0.72
6:N:96:ARG:NH1	7:O:44:ASN:OD1	2.23	0.72
6:N:57:ASN:O	6:N:60:SER:OG	2.08	0.70
1:C:1035:ILE:HG21	1:C:1095:GLN:HG2	1.72	0.70
1:C:1042:GLY:N	1:C:1043:PRO:HD3	2.07	0.69
8:Y:427:ILE:HD12	8:Y:460:ILE:HG22	1.75	0.69
7:O:96:SER:OG	10:e:26:ARG:NH2	2.26	0.69
8:Y:313:GLU:OE2	8:Y:322:ARG:NH2	2.27	0.68
8:Y:426:GLN:NE2	8:Y:461:GLU:OE1	2.27	0.68
8:Y:29:ILE:HD11	8:Y:61:TRP:HZ3	1.58	0.67
7:O:89:GLN:N	7:O:89:GLN:OE1	2.28	0.67
4:L:75:GLN:OE1	4:L:110:SER:OG	2.06	0.67
10:e:48:ILE:HD12	10:e:50:LEU:HD11	1.75	0.67
4:L:50:GLU:OE2	5:M:62:GLY:N	2.28	0.66
8:Y:862:LEU:HD23	8:Y:892:ILE:HD12	1.78	0.66
1:C:1127:LYS:O	1:C:1131:SER:N	2.29	0.65
8:Y:429:LEU:O	8:Y:440:LYS:NZ	2.29	0.65
1:C:1227:ARG:NH2	1:C:1286:THR:OG1	2.29	0.64
8:Y:777:TYR:O	8:Y:781:LEU:HD12	1.97	0.64
6:N:102:LEU:HD21	7:O:55:ILE:HD12	1.77	0.64
10:e:39:GLN:N	10:e:39:GLN:OE1	2.32	0.62
10:e:37:ILE:N	10:e:39:GLN:OE1	2.32	0.62
2:J:65:HIS:NE2	9:d:188:GLU:N	2.44	0.61
10:e:58:GLU:O	10:e:59:HIS:ND1	2.33	0.61
5:M:60:ASN:ND2	9:d:177:ASN:OD1	2.34	0.61
8:Y:767:ASN:OD1	8:Y:768:GLU:N	2.33	0.61
6:N:102:LEU:HD21	7:O:55:ILE:CD1	2.30	0.60
1:C:1112:THR:CG2	1:C:1182:LEU:HD23	2.31	0.60
1:C:1158:GLU:HB2	9:d:181:ARG:HH12	1.66	0.60
4:L:78:ILE:HD12	4:L:105:ILE:HG22	1.84	0.59
6:N:68:ARG:NH1	7:O:87:ALA:O	2.35	0.59
8:Y:36:GLU:OE2	8:Y:195:ARG:NH1	2.36	0.58
2:J:65:HIS:NE2	9:d:188:GLU:CB	2.63	0.57
2:J:72:TYR:CZ	9:d:183:ARG:NH2	2.69	0.57
8:Y:366:ASP:OD2	8:Y:610:SER:OG	2.23	0.56
4:L:74:TRP:CE3	4:L:107:LEU:HD11	2.40	0.56
9:d:86:ILE:HG23	10:e:55:GLU:OE2	2.06	0.56
2:J:65:HIS:CE1	9:d:188:GLU:CA	2.48	0.55
1:C:1120:THR:O	1:C:1124:LYS:N	2.40	0.55
1:C:1158:GLU:CD	9:d:181:ARG:NH2	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:583:GLU:N	8:Y:583:GLU:OE1	2.39	0.55
5:M:4:GLU:N	5:M:4:GLU:OE1	2.39	0.55
4:L:74:TRP:CZ3	4:L:107:LEU:HD11	2.42	0.55
8:Y:257:GLU:OE1	8:Y:317:LEU:N	2.38	0.55
2:J:65:HIS:NE2	9:d:187:THR:C	2.65	0.55
8:Y:834:ILE:HD13	8:Y:876:LEU:HD13	1.89	0.55
2:J:77:PHE:HB3	9:d:183:ARG:HH22	1.72	0.54
8:Y:534:LEU:HD12	8:Y:560:TYR:HB2	1.90	0.54
2:J:65:HIS:CE1	9:d:188:GLU:CB	2.90	0.54
1:C:1090:LYS:O	1:C:1094:LEU:HD23	2.08	0.54
8:Y:175:LEU:HD23	8:Y:176:GLU:N	2.23	0.54
10:e:38:ASN:N	10:e:39:GLN:OE1	2.41	0.53
6:N:101:CYS:O	6:N:102:LEU:HD22	2.08	0.53
8:Y:743:LYS:NZ	11:Y:1301:GTP:O2B	2.40	0.53
8:Y:381:GLU:OE1	8:Y:401:TYR:OH	2.26	0.53
1:C:1158:GLU:OE1	9:d:181:ARG:NH2	2.41	0.53
8:Y:431:ALA:HB1	8:Y:454:TYR:CE2	2.44	0.53
4:L:73:GLU:OE1	4:L:74:TRP:N	2.41	0.52
7:O:101:TYR:CZ	7:O:103:ILE:HD11	2.44	0.52
8:Y:529:GLN:NE2	8:Y:530:ILE:O	2.42	0.52
1:C:1116:LYS:HG3	1:C:1182:LEU:HD21	1.90	0.52
4:L:93:LEU:HD21	10:e:48:ILE:HD11	1.91	0.52
4:L:93:LEU:CD2	10:e:48:ILE:HD11	2.39	0.52
1:C:1356:TYR:O	1:C:1359:SER:HB2	2.10	0.52
2:J:69:TYR:CD1	9:d:184:GLY:HA3	2.44	0.52
3:K:56:GLU:OE2	3:K:60:ILE:HD11	2.10	0.52
7:O:101:TYR:OH	7:O:103:ILE:HD11	2.10	0.51
7:O:32:SER:O	7:O:36:ILE:N	2.43	0.51
8:Y:380:ASN:OD1	8:Y:381:GLU:N	2.44	0.51
8:Y:561:TYR:O	8:Y:567:LEU:HD12	2.11	0.51
8:Y:467:SER:OG	8:Y:468:GLN:N	2.43	0.51
7:O:90:ASP:OD2	7:O:92:ASN:N	2.44	0.51
1:C:1145:GLU:O	1:C:1149:ILE:HD12	2.10	0.50
1:C:1035:ILE:HD13	1:C:1095:GLN:HG2	1.92	0.50
8:Y:52:ASN:OD1	8:Y:53:THR:N	2.44	0.50
8:Y:124:GLN:N	8:Y:124:GLN:OE1	2.45	0.50
1:C:1293:LEU:HD21	1:C:1347:TRP:CZ2	2.47	0.49
2:J:39:GLU:OE2	10:e:62:ASN:ND2	2.45	0.49
2:J:65:HIS:NE2	9:d:187:THR:O	2.30	0.49
2:J:77:PHE:HD2	9:d:183:ARG:HH12	1.60	0.49
9:d:117:TRP:CH2	10:e:39:GLN:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:117:SER:HB3	6:N:120:VAL:HG22	1.94	0.49
8:Y:953:ARG:HA	8:Y:956:ILE:HG22	1.93	0.49
8:Y:560:TYR:HB3	8:Y:567:LEU:HD11	1.94	0.49
8:Y:806:THR:OG1	8:Y:927:TYR:OH	2.07	0.49
8:Y:943:PHE:HE2	8:Y:947:ILE:HD11	1.78	0.49
8:Y:534:LEU:O	8:Y:537:ASN:ND2	2.45	0.49
9:d:117:TRP:HA	9:d:117:TRP:CE3	2.48	0.48
8:Y:817:GLU:N	8:Y:817:GLU:OE1	2.46	0.48
1:C:1300:TYR:CD1	1:C:1353:LEU:HD13	2.48	0.48
1:C:1035:ILE:CD1	1:C:1095:GLN:HG2	2.44	0.48
9:d:87:THR:HG21	10:e:58:GLU:HG2	1.95	0.48
1:C:1032:GLN:OE1	1:C:1095:GLN:CD	2.46	0.48
1:C:1246:MET:SD	1:C:1246:MET:N	2.87	0.47
4:L:95:PHE:CD1	4:L:106:LEU:HD13	2.50	0.47
1:C:1142:ILE:O	1:C:1146:GLN:N	2.47	0.47
8:Y:45:ASN:ND2	8:Y:81:TYR:O	2.47	0.47
1:C:1300:TYR:HD1	1:C:1353:LEU:HD13	1.79	0.47
8:Y:130:GLU:O	8:Y:134:LEU:HD23	2.15	0.47
8:Y:750:ARG:O	8:Y:750:ARG:NH1	2.48	0.47
8:Y:769:MET:SD	8:Y:801:PRO:HG3	2.55	0.47
8:Y:830:THR:OG1	8:Y:861:LEU:HD12	2.15	0.47
1:C:1035:ILE:HG21	1:C:1095:GLN:CG	2.41	0.47
1:C:1116:LYS:CG	1:C:1182:LEU:HD21	2.45	0.46
4:L:26:MET:HE3	4:L:94:ALA:HB2	1.96	0.46
4:L:74:TRP:CD1	4:L:109:LYS:HZ2	2.33	0.46
3:K:35:ASP:OD1	3:K:36:ILE:N	2.48	0.46
8:Y:22:PHE:CD2	8:Y:108:LEU:HD12	2.51	0.46
8:Y:238:ARG:NH1	8:Y:505:ASN:O	2.45	0.46
2:J:69:TYR:CD1	9:d:184:GLY:CA	2.99	0.46
8:Y:32:ILE:HD11	8:Y:199:VAL:HG21	1.97	0.46
2:J:47:LYS:NZ	2:J:58:TRP:O	2.49	0.46
8:Y:356:ILE:HG22	8:Y:360:GLN:HE22	1.82	0.45
4:L:18:PRO:HG2	4:L:99:LEU:HD21	1.98	0.45
5:M:57:VAL:HG13	5:M:82:LEU:CD2	2.47	0.45
1:C:1253:GLU:HA	1:C:1256:TYR:CE1	2.52	0.45
5:M:16:MET:HA	5:M:16:MET:HE3	1.98	0.45
8:Y:53:THR:OG1	8:Y:54:GLU:OE2	2.34	0.45
8:Y:22:PHE:CG	8:Y:108:LEU:HD12	2.52	0.45
8:Y:426:GLN:O	8:Y:427:ILE:HD13	2.17	0.45
1:C:1292:ASN:OD1	1:C:1293:LEU:N	2.50	0.44
2:J:79:PHE:CD2	9:d:185:VAL:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:1025:ARG:HB3	8:Y:1034:LEU:CD2	2.48	0.44
1:C:1055:PHE:CE2	1:C:1093:LYS:NZ	2.85	0.44
1:C:1158:GLU:CG	9:d:181:ARG:HH22	2.30	0.44
5:M:69:THR:HG21	9:d:166:PHE:HE1	1.83	0.44
7:O:24:VAL:HG11	7:O:50:ILE:HD13	2.00	0.44
7:O:68:CYS:SG	7:O:69:VAL:N	2.91	0.44
1:C:1345:LYS:HG2	1:C:1346:GLU:N	2.33	0.43
2:J:77:PHE:CD2	9:d:183:ARG:NH1	2.84	0.43
1:C:1055:PHE:HE2	1:C:1093:LYS:NZ	2.16	0.43
6:N:97:ILE:HG22	7:O:72:ILE:HG23	1.99	0.43
8:Y:203:TYR:CE2	8:Y:454:TYR:HA	2.54	0.43
4:L:66:GLU:OE1	4:L:66:GLU:N	2.49	0.43
1:C:1047:ASN:O	1:C:1051:GLN:OE1	2.35	0.43
6:N:108:ASP:OD1	6:N:130:TYR:N	2.46	0.43
8:Y:769:MET:HA	8:Y:772:LEU:HD23	2.01	0.43
7:O:20:SER:O	7:O:24:VAL:HG23	2.18	0.43
8:Y:441:ILE:HG13	8:Y:441:ILE:O	2.19	0.43
8:Y:792:ASN:OD1	8:Y:793:THR:N	2.52	0.42
2:J:40:ASN:OD1	10:e:62:ASN:ND2	2.49	0.42
8:Y:102:LEU:CD1	8:Y:109:ILE:HD11	2.49	0.42
9:d:86:ILE:O	9:d:99:ASP:N	2.52	0.42
8:Y:469:ILE:HG23	8:Y:470:LEU:HG	2.02	0.42
6:N:84:GLN:NE2	6:N:85:VAL:O	2.52	0.42
8:Y:766:LEU:HA	8:Y:769:MET:HB3	2.02	0.42
9:d:117:TRP:N	9:d:119:GLU:OE1	2.52	0.42
1:C:1042:GLY:N	1:C:1043:PRO:CD	2.79	0.42
8:Y:24:PHE:HA	8:Y:697:LEU:HD11	2.01	0.42
8:Y:243:GLU:O	8:Y:247:THR:HG22	2.20	0.42
8:Y:356:ILE:HG22	8:Y:360:GLN:OE1	2.20	0.42
8:Y:862:LEU:HD23	8:Y:892:ILE:CD1	2.48	0.42
10:e:57:SER:OG	10:e:58:GLU:N	2.53	0.42
6:N:60:SER:O	6:N:64:VAL:HG23	2.20	0.41
8:Y:483:SER:O	8:Y:483:SER:OG	2.37	0.41
1:C:1044:THR:O	1:C:1047:ASN:HB2	2.20	0.41
6:N:114:THR:HG21	9:d:109:PHE:HB2	2.01	0.41
6:N:121:TYR:OH	7:O:81:ILE:HD13	2.20	0.41
8:Y:398:ILE:H	8:Y:398:ILE:HD12	1.84	0.41
1:C:1115:THR:HG21	1:C:1183:LEU:HD23	2.01	0.41
2:J:61:VAL:HG21	3:K:79:PHE:CE2	2.55	0.41
2:J:69:TYR:HD1	9:d:184:GLY:CA	2.34	0.41
6:N:101:CYS:C	6:N:102:LEU:HD22	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:691:SER:OG	8:Y:922:LYS:NZ	2.53	0.41
5:M:15:ASP:OD1	5:M:15:ASP:N	2.53	0.41
8:Y:308:PHE:CE2	8:Y:368:LEU:HD23	2.55	0.41
8:Y:427:ILE:HG23	8:Y:460:ILE:HG22	2.03	0.41
8:Y:509:ASP:OD1	8:Y:510:TYR:N	2.51	0.41
1:C:1351:ARG:O	1:C:1355:ASN:ND2	2.53	0.41
8:Y:642:LYS:HA	8:Y:642:LYS:HE2	2.02	0.41
6:N:86:VAL:HG13	7:O:81:ILE:HD11	2.02	0.40
8:Y:290:GLU:OE1	8:Y:290:GLU:N	2.54	0.40
8:Y:170:ILE:HG23	8:Y:183:PHE:HB3	2.03	0.40
8:Y:803:PHE:CE1	8:Y:804:ILE:HG23	2.56	0.40
8:Y:191:ASP:OD1	8:Y:193:THR:OG1	2.34	0.40
8:Y:29:ILE:HD11	8:Y:61:TRP:CZ3	2.46	0.40
1:C:1167:LEU:O	1:C:1167:LEU:HD23	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	C	272/4620 (6%)	256 (94%)	16 (6%)	0	100	100
2	J	82/93 (88%)	77 (94%)	5 (6%)	0	100	100
3	K	93/111 (84%)	83 (89%)	10 (11%)	0	100	100
4	L	95/111 (86%)	90 (95%)	5 (5%)	0	100	100
5	M	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
6	N	107/132 (81%)	100 (94%)	7 (6%)	0	100	100
7	O	109/117 (93%)	99 (91%)	10 (9%)	0	100	100
8	Y	1059/1200 (88%)	1013 (96%)	44 (4%)	2 (0%)	43	77
9	d	87/667 (13%)	79 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	e	47/670 (7%)	41 (87%)	6 (13%)	0	100	100
All	All	2035/7808 (26%)	1915 (94%)	118 (6%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	Y	723	PRO
8	Y	1106	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	C	241/4196 (6%)	241 (100%)	0	100	100
2	J	74/82 (90%)	74 (100%)	0	100	100
3	K	81/97 (84%)	81 (100%)	0	100	100
4	L	86/99 (87%)	86 (100%)	0	100	100
5	M	77/78 (99%)	77 (100%)	0	100	100
6	N	96/119 (81%)	96 (100%)	0	100	100
7	O	98/104 (94%)	98 (100%)	0	100	100
8	Y	903/1102 (82%)	903 (100%)	0	100	100
9	d	86/609 (14%)	86 (100%)	0	100	100
10	e	42/597 (7%)	42 (100%)	0	100	100
All	All	1784/7083 (25%)	1784 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1266	ASN

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Mol	Chain	Res	Type
2	J	45	HIS
5	M	33	GLN
5	M	36	GLN
5	M	64	HIS
7	O	84	GLN
8	Y	537	ASN
8	Y	639	ASN
8	Y	868	ASN
9	d	164	ASN
10	e	44	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	GTP	Y	1301	-	33,34,34	0.89	2 (6%)	50,54,54	1.61	8 (16%)

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	GTP	Y	1301	-	-	6/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	1301	GTP	C5-N7	-2.24	1.34	1.39
11	Y	1301	GTP	C2-N3	2.17	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	1301	GTP	C5-C4-N3	-5.22	120.08	128.39
11	Y	1301	GTP	C2-N3-C4	4.66	120.33	112.30
11	Y	1301	GTP	C2-N1-C6	-3.20	119.31	125.11
11	Y	1301	GTP	N9-C4-N3	3.14	132.23	125.95
11	Y	1301	GTP	C5-C6-N1	2.63	119.94	113.25
11	Y	1301	GTP	O6-C6-C5	-2.47	120.00	126.53
11	Y	1301	GTP	N9-C8-N7	-2.44	108.88	113.40
11	Y	1301	GTP	C8-N7-C5	2.34	108.42	104.26

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	Y	1301	GTP	C5'-O5'-PA-O3A
11	Y	1301	GTP	O4'-C4'-C5'-O5'
11	Y	1301	GTP	C3'-C4'-C5'-O5'
11	Y	1301	GTP	C5'-O5'-PA-O1A
11	Y	1301	GTP	PB-O3A-PA-O5'
11	Y	1301	GTP	PG-O3B-PB-O2B

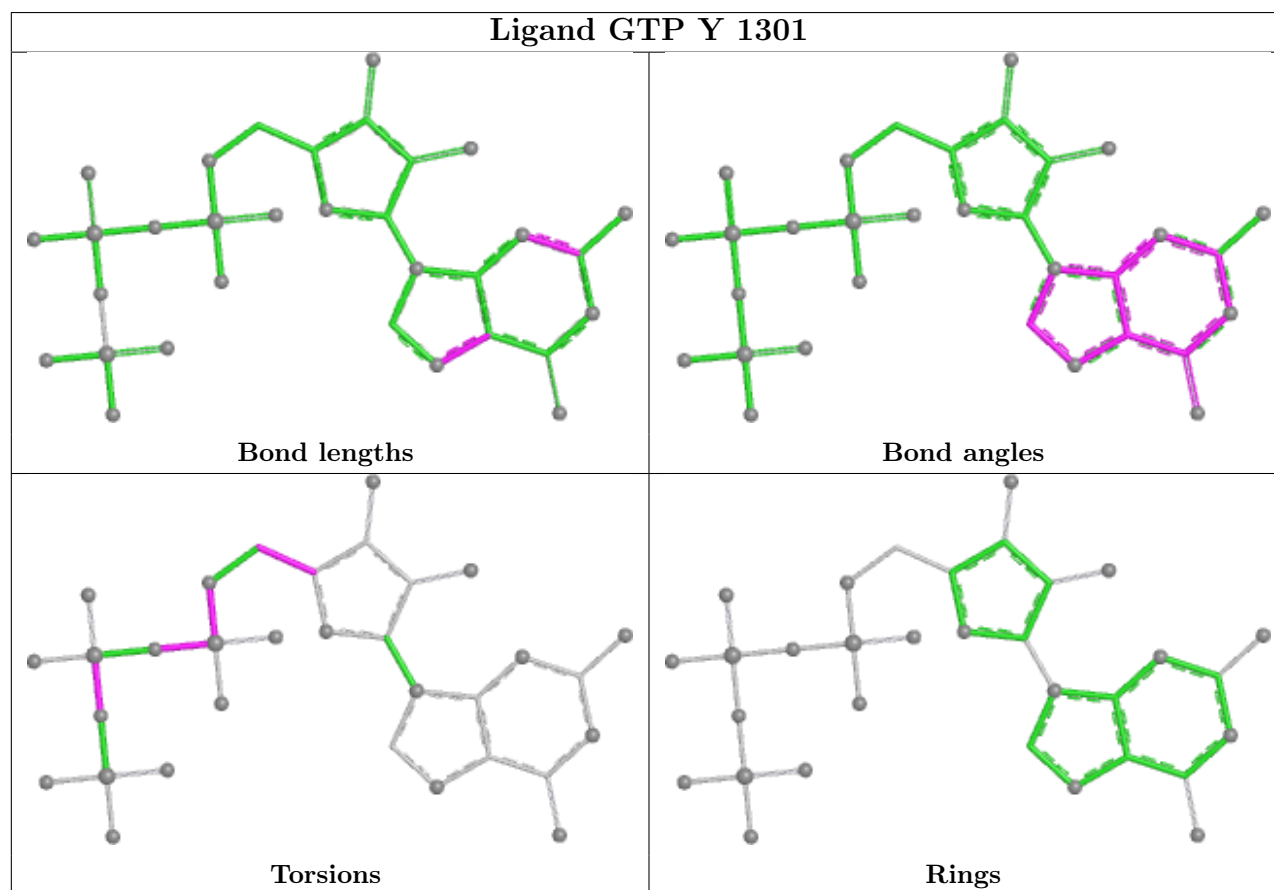
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Y	1301	GTP	2	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	1110:GLN	C	1177:LYS	N	10.60

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11579. 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.

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 standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 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.