



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jun 30, 2019 – 07:56 PM EDT

PDB ID : 6QB8
EMDB ID: : EMD-4489
Title : Human CCT:mLST8 complex
Authors : Cuellar, J.; Santiago, C.; Ludlam, W.G.; Bueno-Carrasco, M.T.; Valpuesta, J.M.; Willardson, B.M.
Deposited on : 2018-12-20
Resolution : 3.97 Å(reported)
Based on PDB ID : 5GW5

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

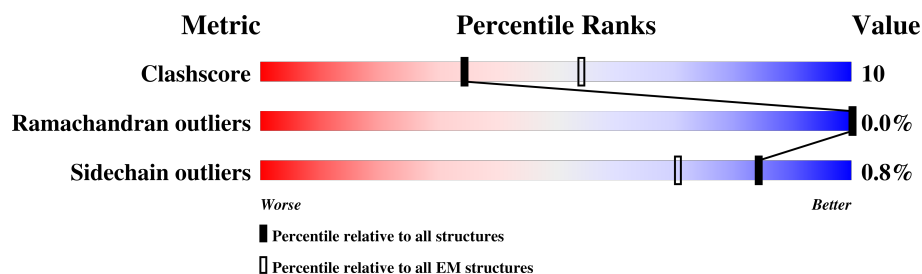
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.97 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	556	50% 38% 11%
1	a	556	87% 12%
2	B	535	54% 37% 8%
2	b	535	89% 11%
3	D	539	54% 36% 10%
3	d	539	90% 9%
4	E	541	52% 40% 7%
4	e	541	93% 7%
5	G	544	53% 36% 11%

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Mol	Chain	Length	Quality of chain
5	g	544	<div><div></div><div>87%</div><div></div><div></div><div>12%</div></div>
6	H	543	<div><div></div><div>69%</div><div></div><div>23%</div><div></div><div>8%</div></div>
6	h	543	<div><div></div><div>91%</div><div></div><div></div><div>8%</div></div>
7	Q	548	<div><div></div><div>61%</div><div></div><div>26%</div><div></div><div>12%</div></div>
7	q	548	<div><div></div><div>84%</div><div></div><div></div><div>12%</div></div>
8	Z	531	<div><div></div><div>52%</div><div></div><div>41%</div><div></div><div>6%</div></div>
8	z	531	<div><div></div><div>95%</div><div></div><div></div><div></div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60035 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	490	Total	C	N	O	S	0	0
			3709	2323	651	713	22		
1	A	494	Total	C	N	O	S	0	0
			3742	2345	656	719	22		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	478	Total	C	N	O	S	0	0
			3590	2248	630	694	18		
2	B	492	Total	C	N	O	S	0	0
			3698	2311	648	720	19		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	489	Total	C	N	O	S	0	0
			3673	2302	636	714	21		
3	D	487	Total	C	N	O	S	0	0
			3655	2292	634	708	21		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	505	Total	C	N	O	S	0	0
			3882	2422	678	752	30		
4	E	503	Total	C	N	O	S	0	0
			3863	2412	672	749	30		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	477	Total	C	N	O	S	0	0
			3678	2295	654	700	29		
5	G	485	Total	C	N	O	S	0	0
			3741	2335	664	713	29		

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	500	Total	C	N	O	S	0	0
			3834	2422	662	727	23		
6	H	499	Total	C	N	O	S	0	0
			3825	2417	661	724	23		

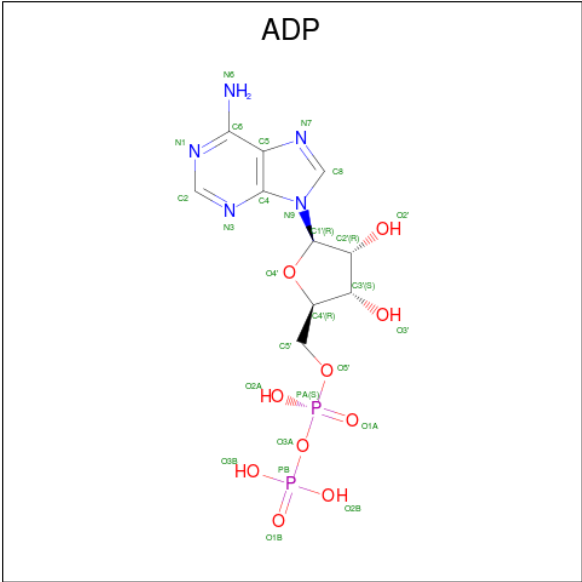
- Molecule 7 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	483	Total	C	N	O	S	0	0
			3692	2327	628	712	25		
7	Q	483	Total	C	N	O	S	0	0
			3692	2327	628	712	25		

- Molecule 8 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	508	Total	C	N	O	S	0	0
			3894	2447	680	747	20		
8	Z	497	Total	C	N	O	S	0	0
			3813	2395	670	728	20		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

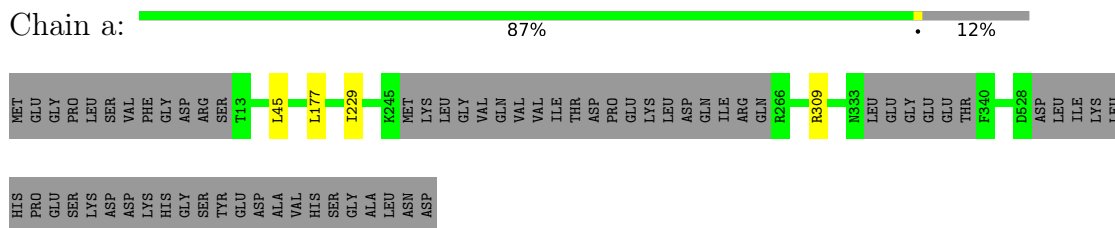


Mol	Chain	Residues	Atoms					AltConf
9	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	

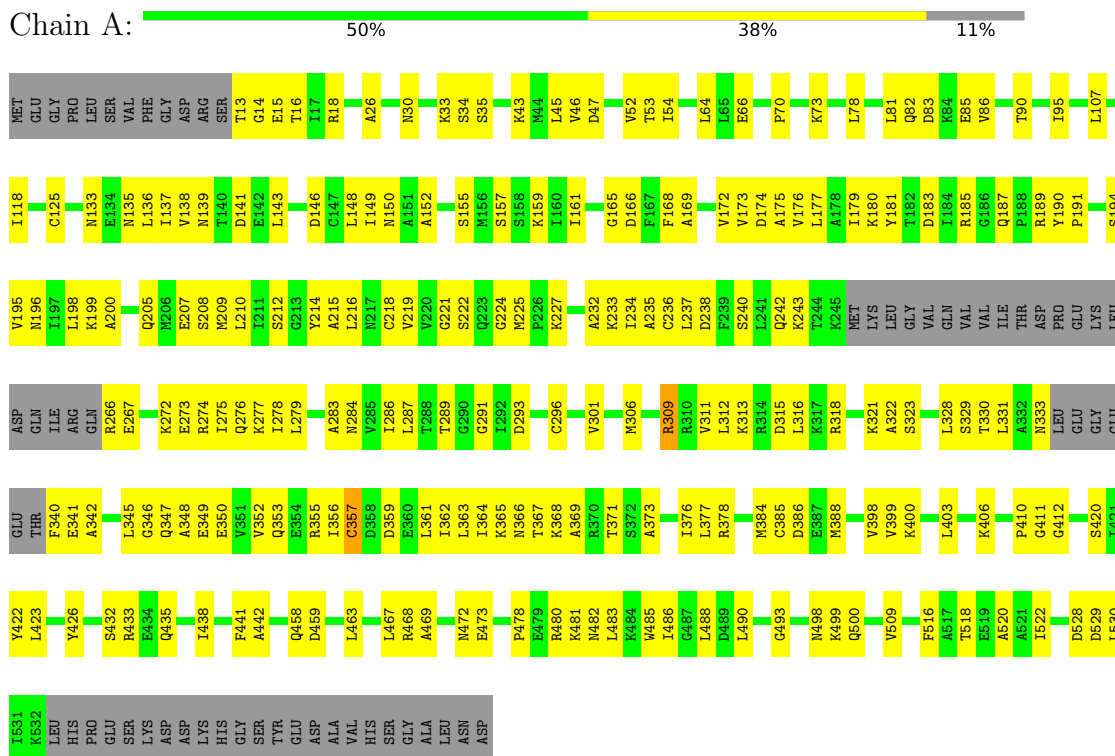
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

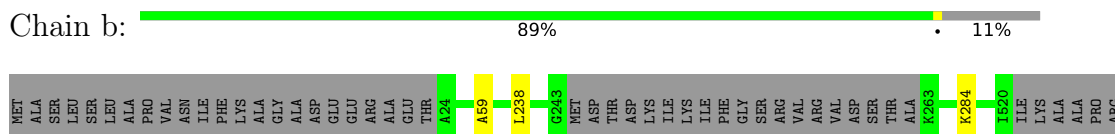
- Molecule 1: T-complex protein 1 subunit alpha



- Molecule 1: T-complex protein 1 subunit alpha



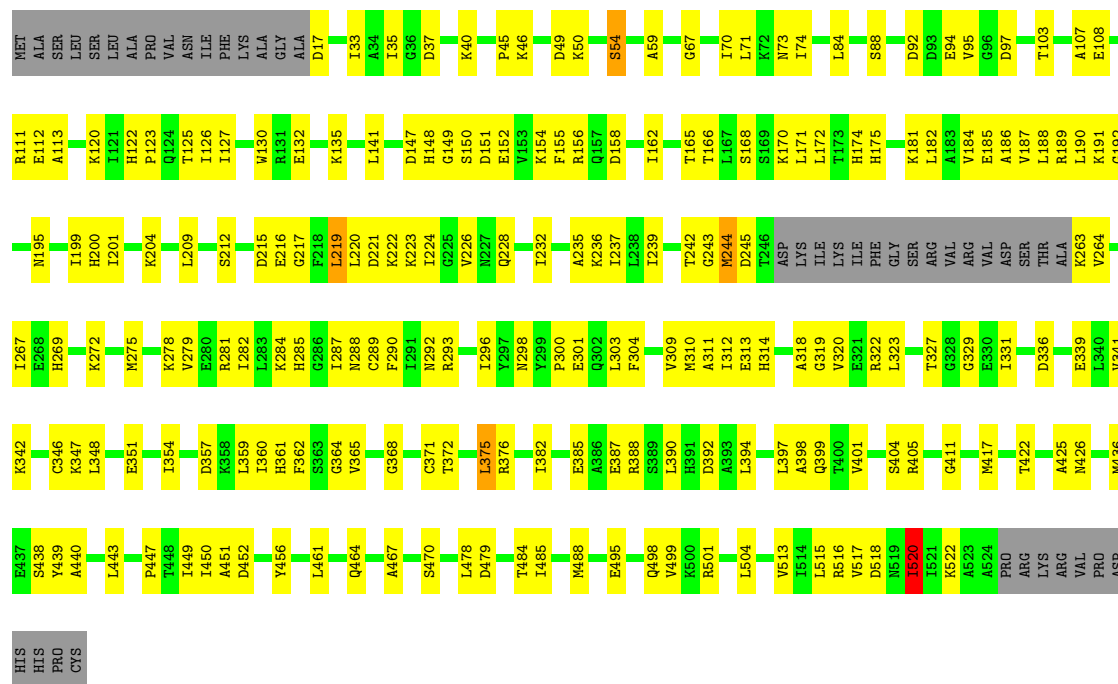
- Molecule 2: T-complex protein 1 subunit beta



LYS
ARG
VAL
PRO
SER
ASP
HIS
HIS
PRO
CYS

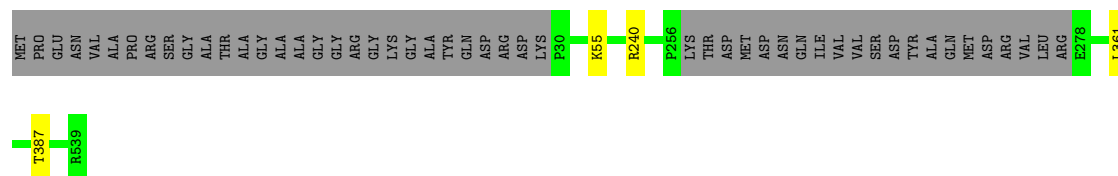
• Molecule 2: T-complex protein 1 subunit beta

Chain B: 54% 37% 8%



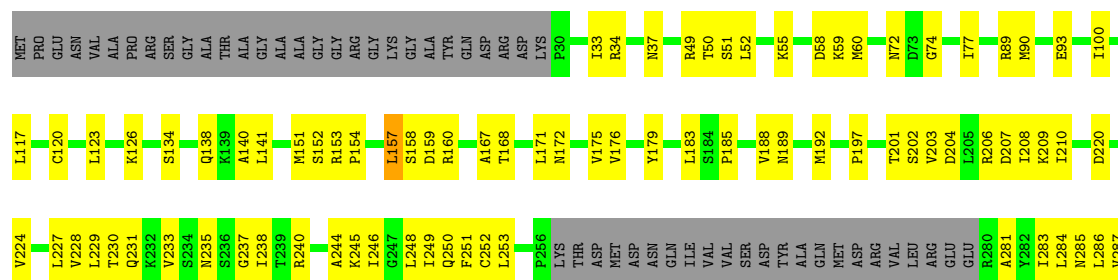
• Molecule 3: T-complex protein 1 subunit delta

Chain d: 90% 9%



• Molecule 3: T-complex protein 1 subunit delta

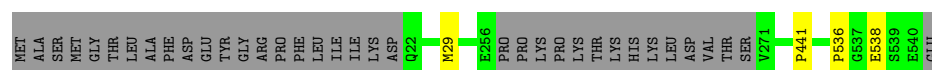
Chain D: 54% 36% 10%





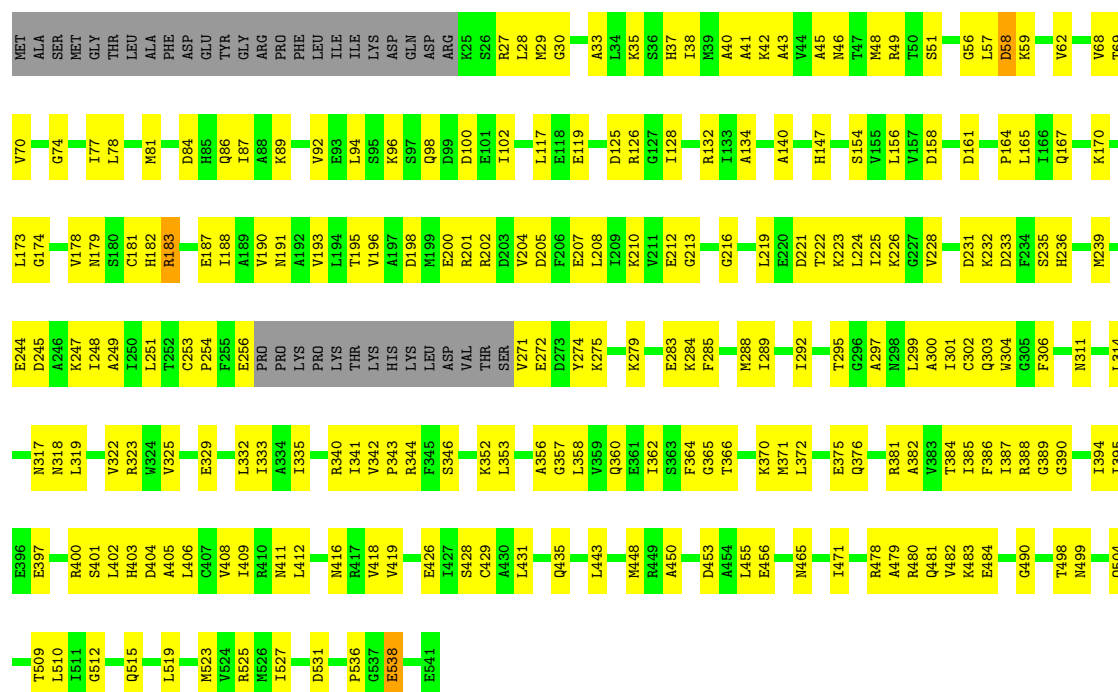
- Molecule 4: T-complex protein 1 subunit epsilon

Chain e: 93% • 7%



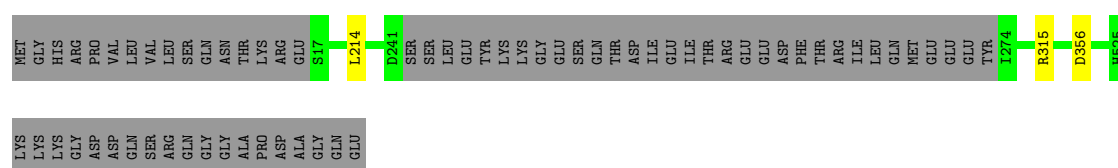
- Molecule 4: T-complex protein 1 subunit epsilon

Chain E: 52% 40% • 7%

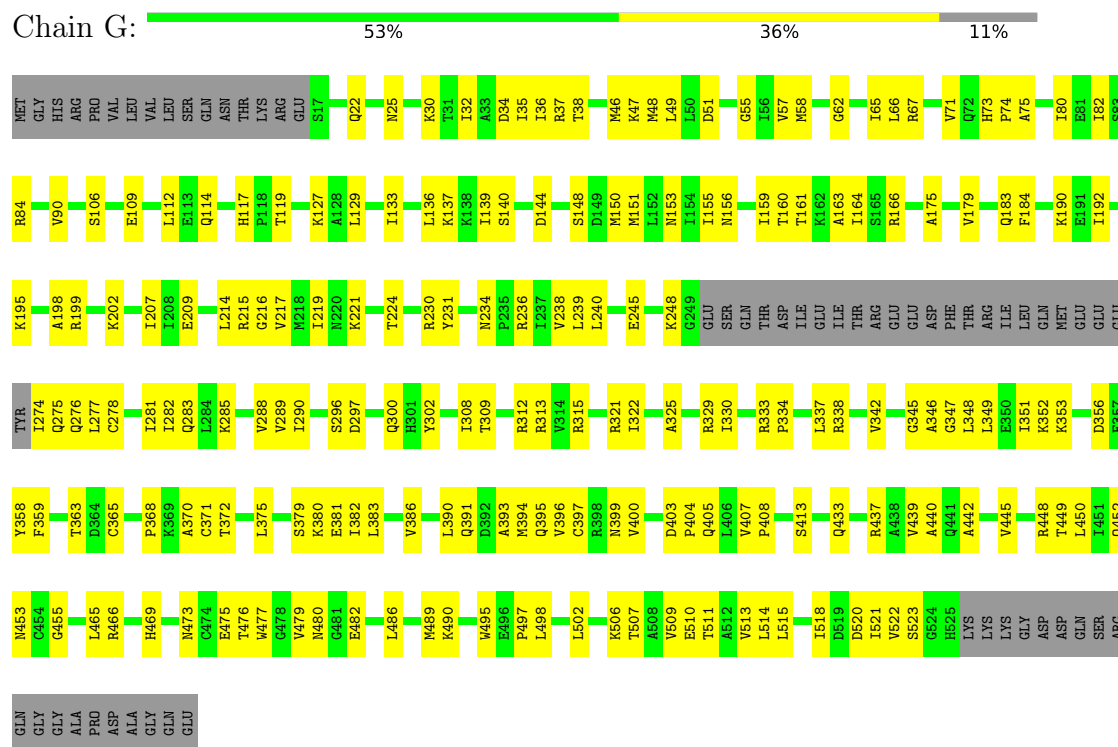


- Molecule 5: T-complex protein 1 subunit gamma

Chain g: 87% • 12%

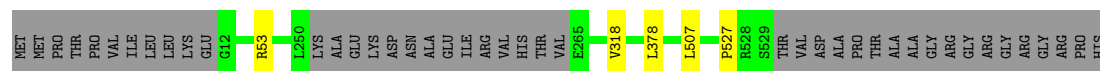


- Molecule 5: T-complex protein 1 subunit gamma



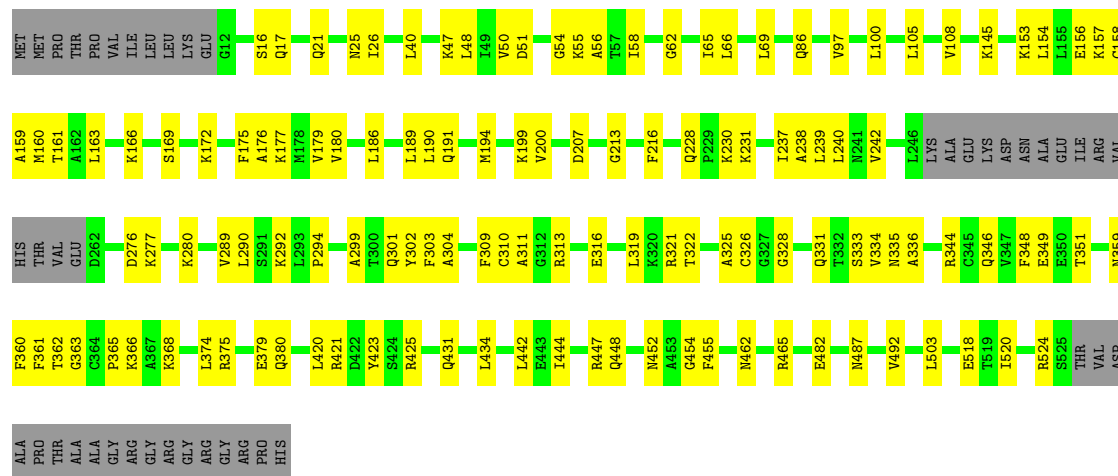
- Molecule 6: T-complex protein 1 subunit eta

Chain h: 91% • 8%



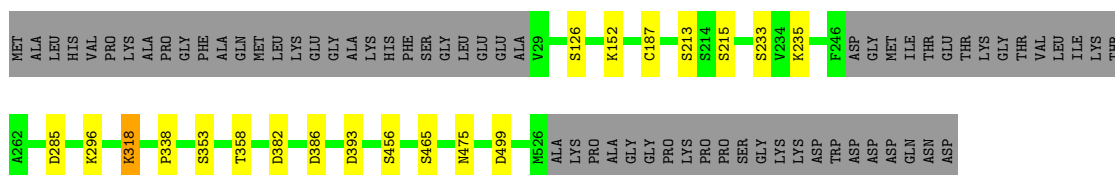
- Molecule 6: T-complex protein 1 subunit eta

Chain H:  69% 23% 8%



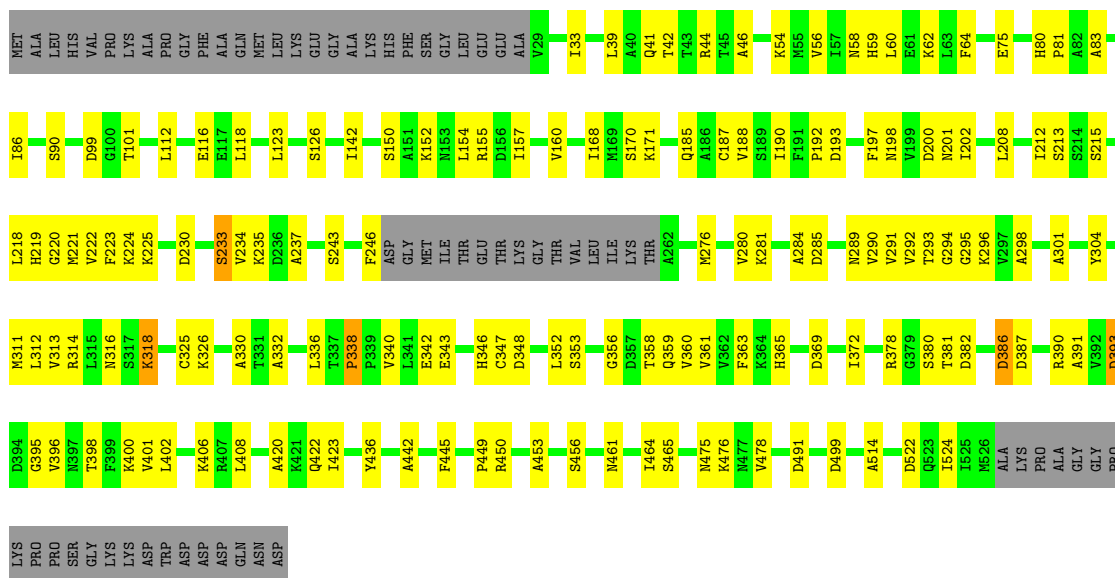
- Molecule 7: T-complex protein 1 subunit theta

Chain q: 84% • 12%



- Molecule 7: T-complex protein 1 subunit theta

Chain Q:  61% 26% • 12%



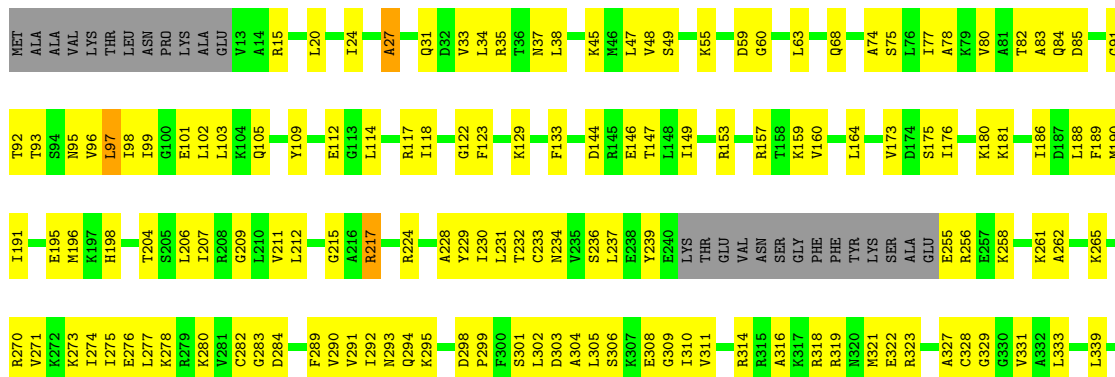
- Molecule 8: T-complex protein 1 subunit zeta

Chain z: 95% . .



- Molecule 8: T-complex protein 1 subunit zeta

Chain Z: 52% 41% • 6%



C343	D442	I521
L344	I446	H522
G345	GLY	R523
H346	ALA	
A347	MET	
G348	K449	
L349	SER	
V350	SER	
V351	LEU	
E352	LYS	
Y353	GLY	
K359	D458	
F360	L459	
T361	Q460	
F362	E461	
T363	T462	
E364	L463	
K365	V464	
C366	K465	
N367	I466	
	Q467	
R370	A468	
S371	E469	
V372	H470	
T373	S471	
L374		
L375	G474	
I376	Q475	
K377		
G378	D480	
L384	T483	
I387	P486	
L395	V492	
	G493	
V398	V494	
I402	N497	
	Y498	
V408	C499	
	V500	
V414	K501	
E415	R502	
V416	Q503	
A417	L504	
A421	S507	
L422	G508	
	T509	
H425	V510	
K426		
	T513	
K430	L517	
G431	V518	
R432	D519	
	E520	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	452000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	105000	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: ADP

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	0.28	0/3775	0.53	1/5093 (0.0%)
1	a	0.28	0/3742	0.55	2/5049 (0.0%)
2	B	0.29	0/3736	0.58	3/5036 (0.1%)
2	b	0.28	0/3628	0.57	1/4891 (0.0%)
3	D	0.28	0/3684	0.57	3/4972 (0.1%)
3	d	0.29	0/3702	0.55	1/4996 (0.0%)
4	E	0.29	0/3904	0.56	0/5256
4	e	0.28	0/3923	0.55	0/5281
5	G	0.29	0/3783	0.54	1/5104 (0.0%)
5	g	0.29	0/3719	0.56	2/5020 (0.0%)
6	H	0.29	0/3878	0.53	0/5232
6	h	0.29	0/3887	0.54	1/5244 (0.0%)
7	Q	0.29	0/3742	0.54	1/5059 (0.0%)
7	q	0.29	0/3742	0.55	1/5059 (0.0%)
8	Z	0.29	0/3855	0.54	3/5197 (0.1%)
8	z	0.30	0/3938	0.57	3/5309 (0.1%)
All	All	0.29	0/60638	0.55	23/81798 (0.0%)

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
1	a	0	1
2	B	0	3
2	b	0	1
3	d	0	1
4	E	0	2
4	e	0	5
6	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	h	0	3
7	Q	0	2
7	q	0	2
8	Z	0	2
8	z	0	1
All	All	0	24

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	356	ASP	CB-CG-OD2	8.33	125.79	118.30
8	z	34	LEU	CA-CB-CG	-7.70	97.59	115.30
3	D	157	LEU	CA-CB-CG	7.05	131.52	115.30
2	B	219	LEU	CA-CB-CG	7.00	131.40	115.30
7	Q	318	LYS	CD-CE-NZ	6.18	125.92	111.70

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	229	ILE	Peptide
2	b	59	ALA	Peptide
3	d	387	THR	Peptide
4	e	29	MET	Peptide
4	e	441	PRO	Peptide

5.2 Too-close contacts [i](#)

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	3742	0	3898	174	0
1	a	3709	0	3859	0	0
2	B	3698	0	3792	155	0
2	b	3590	0	3691	0	0
3	D	3655	0	3874	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	d	3673	0	3886	0	0
4	E	3863	0	3960	176	0
4	e	3882	0	3979	0	0
5	G	3741	0	3880	142	0
5	g	3678	0	3815	0	0
6	H	3825	0	3914	81	0
6	h	3834	0	3920	0	0
7	Q	3692	0	3746	94	0
7	q	3692	0	3746	0	0
8	Z	3813	0	3951	169	0
8	z	3894	0	4021	0	0
9	Q	27	0	12	5	0
9	q	27	0	12	0	0
All	All	60035	0	61956	1095	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 10.

The worst 5 of 1095 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)
8:Z:204:THR:HA	8:Z:375:LEU:O	1.74	0.88
5:G:352:LYS:O	5:G:359:PHE:HB2	1.86	0.85
1:A:275:ILE:O	1:A:279:LEU:HB2	3.14	0.80
1:A:355:ARG:HA	1:A:359:ASP:O	1.84	0.76
3:D:210:ILE:H	3:D:385:THR:HG23	2.09	0.75

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	488/556 (88%)	453 (93%)	35 (7%)	0	100	100
1	a	484/556 (87%)	450 (93%)	34 (7%)	0	100	100
2	B	488/535 (91%)	447 (92%)	41 (8%)	0	100	100
2	b	474/535 (89%)	432 (91%)	42 (9%)	0	100	100
3	D	483/539 (90%)	440 (91%)	43 (9%)	0	100	100
3	d	485/539 (90%)	452 (93%)	33 (7%)	0	100	100
4	E	499/541 (92%)	448 (90%)	51 (10%)	0	100	100
4	e	501/541 (93%)	448 (89%)	53 (11%)	0	100	100
5	G	481/544 (88%)	443 (92%)	38 (8%)	0	100	100
5	g	473/544 (87%)	438 (93%)	35 (7%)	0	100	100
6	H	495/543 (91%)	453 (92%)	42 (8%)	0	100	100
6	h	496/543 (91%)	452 (91%)	44 (9%)	0	100	100
7	Q	479/548 (87%)	441 (92%)	38 (8%)	0	100	100
7	q	479/548 (87%)	441 (92%)	38 (8%)	0	100	100
8	Z	493/531 (93%)	453 (92%)	39 (8%)	1 (0%)	49	83
8	z	504/531 (95%)	471 (94%)	33 (6%)	0	100	100
All	All	7802/8674 (90%)	7162 (92%)	639 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	Z	430	LYS

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	409/463 (88%)	407 (100%)	2 (0%)	90	95
1	a	405/463 (88%)	404 (100%)	1 (0%)	94	97
2	B	391/427 (92%)	390 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	380/427 (89%)	379 (100%)	1 (0%)	93	96
3	D	413/452 (91%)	412 (100%)	1 (0%)	94	97
3	d	415/452 (92%)	413 (100%)	2 (0%)	90	95
4	E	422/456 (92%)	421 (100%)	1 (0%)	94	97
4	e	424/456 (93%)	424 (100%)	0	100	100
5	G	416/468 (89%)	415 (100%)	1 (0%)	94	97
5	g	409/468 (87%)	408 (100%)	1 (0%)	94	97
6	H	408/443 (92%)	406 (100%)	2 (0%)	90	95
6	h	409/443 (92%)	407 (100%)	2 (0%)	90	95
7	Q	402/452 (89%)	384 (96%)	18 (4%)	30	62
7	q	402/452 (89%)	384 (96%)	18 (4%)	30	62
8	Z	416/442 (94%)	414 (100%)	2 (0%)	90	95
8	z	425/442 (96%)	424 (100%)	1 (0%)	94	97
All	All	6546/7206 (91%)	6492 (99%)	54 (1%)	84	92

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	q	499	ASP
4	E	183	ARG
7	Q	456	SER
8	z	381	LYS
1	A	400	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
8	z	84	GLN
1	A	242	GLN
7	Q	306	ASN
8	z	346	HIS
1	A	135	ASN

5.3.3 RNA ⓘ

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](#)

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	$\# Z > 2$
9	ADP	Q	5000	-	24,29,29	0.93	1 (4%)	25,45,45	1.65	4 (16%)
9	ADP	q	5000	-	24,29,29	0.94	1 (4%)	25,45,45	1.65	4 (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
9	ADP	Q	5000	-	-	2/12/32/32	0/3/3/3
9	ADP	q	5000	-	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	5000	ADP	C5-C4	2.82	1.46	1.40
9	q	5000	ADP	C5-C4	2.80	1.46	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	5000	ADP	PA-O3A-PB	-4.31	118.87	132.57
9	q	5000	ADP	PA-O3A-PB	-4.30	118.90	132.57
9	Q	5000	ADP	N3-C2-N1	-3.34	123.29	128.68
9	q	5000	ADP	N3-C2-N1	-3.30	123.36	128.68
9	q	5000	ADP	C4'-O4'-C1'	-2.83	106.88	109.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

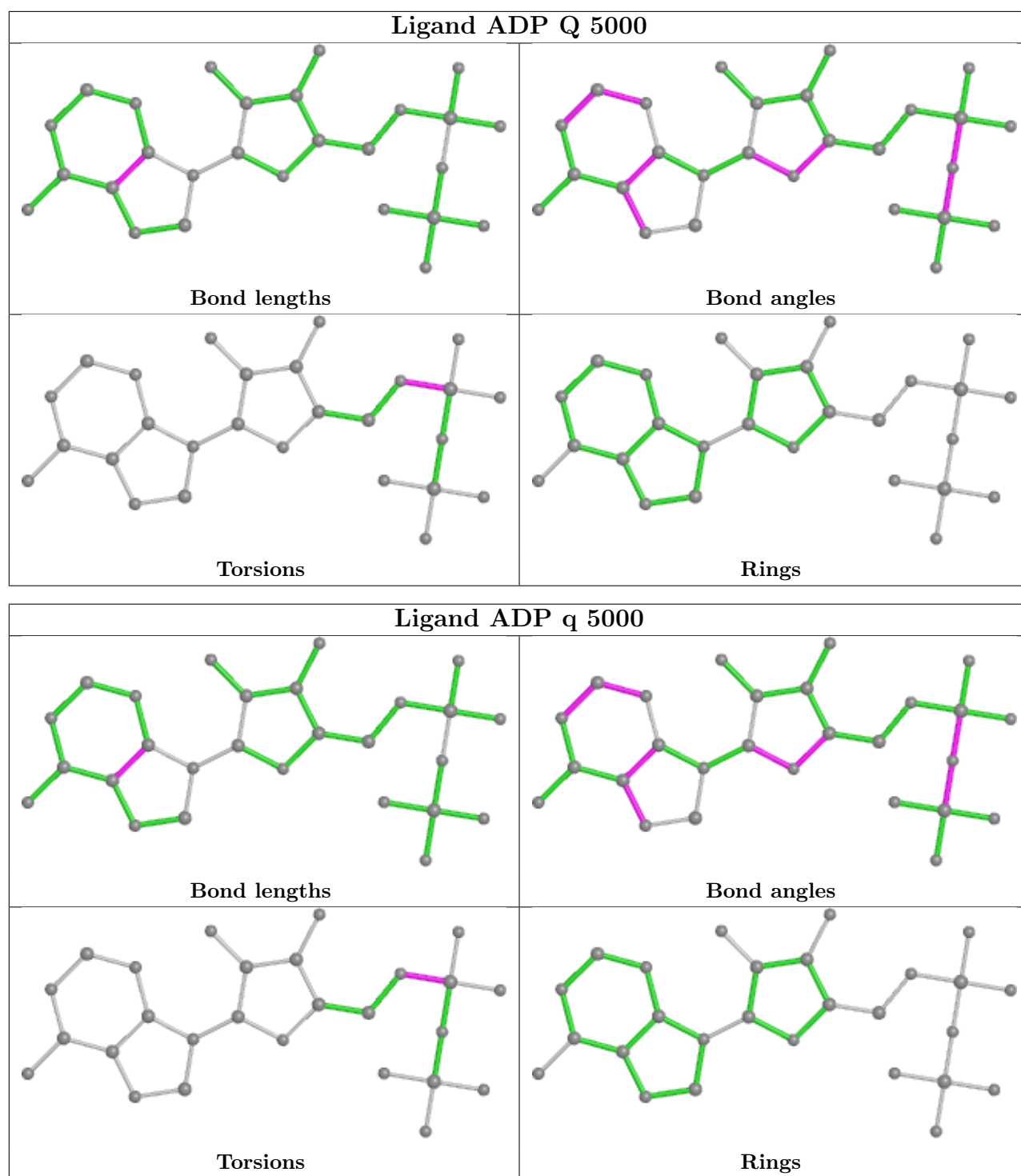
Mol	Chain	Res	Type	Atoms
9	q	5000	ADP	C5'-O5'-PA-O2A
9	q	5000	ADP	C5'-O5'-PA-O3A
9	Q	5000	ADP	C5'-O5'-PA-O3A
9	Q	5000	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	5000	ADP	5	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.