



## wwPDB EM Validation Summary Report ⓘ

Apr 6, 2026 – 01:54 AM UTC

PDB ID : 9NRF / pdb\_00009nrf  
EMDB ID : EMD-49731  
Title : CCT G beta 5 G257E complex state 6  
Authors : Mack, D.C.; Shen, P.S.  
Deposited on : 2025-03-14  
Resolution : 3.10 Å(reported)

This is a wwPDB EM Validation Summary 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.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

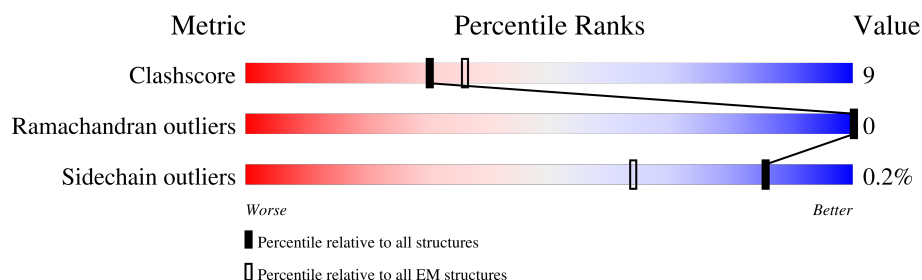
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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.











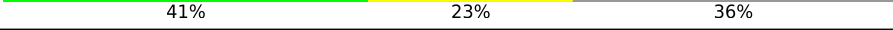
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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  $\geq 3$ , 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	N	441	18% 6% 76%
2	A	556	74% 22% .
2	a	556	72% 24% .
3	B	535	84% 15% .
3	b	535	82% 16% .
4	D	539	80% 16% .
4	d	539	78% 19% .
5	E	541	77% 21% .
5	e	541	78% 21%

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Mol	Chain	Length	Quality of chain
6	G	545	 73% 24% .
6	g	545	 71% 25% .
7	H	543	 78% 19% .
7	h	543	 77% 20% .
8	Q	548	 79% 19% .
8	q	548	 78% 20% .
9	Z	531	 77% 21% .
9	z	531	 77% 22% .
10	P	326	 41% 23% 36%

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
13	AF3	D	603	-	-	X	-
13	AF3	G	603	-	-	X	-
13	AF3	H	603	-	-	X	-
13	AF3	Q	603	-	-	X	-
13	AF3	Z	603	-	-	X	-
13	AF3	g	603	-	-	X	-
13	AF3	h	603	-	-	X	-
13	AF3	z	603	-	-	X	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 67578 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 Guanine nucleotide-binding protein subunit beta-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	105	Total	C	N	O	S	0	0
			794	492	132	161	9		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-31	MET	-	initiating methionine	UNP O14775
N	-30	TRP	-	expression tag	UNP O14775
N	-29	SER	-	expression tag	UNP O14775
N	-28	HIS	-	expression tag	UNP O14775
N	-27	PRO	-	expression tag	UNP O14775
N	-26	GLN	-	expression tag	UNP O14775
N	-25	PHE	-	expression tag	UNP O14775
N	-24	GLU	-	expression tag	UNP O14775
N	-23	LYS	-	expression tag	UNP O14775
N	-22	GLY	-	expression tag	UNP O14775
N	-21	GLY	-	expression tag	UNP O14775
N	-20	GLY	-	expression tag	UNP O14775
N	-19	SER	-	expression tag	UNP O14775
N	-18	GLY	-	expression tag	UNP O14775
N	-17	GLY	-	expression tag	UNP O14775
N	-16	GLY	-	expression tag	UNP O14775
N	-15	SER	-	expression tag	UNP O14775
N	-14	GLY	-	expression tag	UNP O14775
N	-13	GLY	-	expression tag	UNP O14775
N	-12	SER	-	expression tag	UNP O14775
N	-11	SER	-	expression tag	UNP O14775
N	-10	ALA	-	expression tag	UNP O14775
N	-9	TRP	-	expression tag	UNP O14775
N	-8	SER	-	expression tag	UNP O14775
N	-7	HIS	-	expression tag	UNP O14775
N	-6	PRO	-	expression tag	UNP O14775
N	-5	GLN	-	expression tag	UNP O14775
N	-4	PHE	-	expression tag	UNP O14775

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-3	GLU	-	expression tag	UNP O14775
N	-2	LYS	-	expression tag	UNP O14775
N	-1	ALA	-	expression tag	UNP O14775
N	0	ALA	-	expression tag	UNP O14775
N	257	GLU	GLY	engineered mutation	UNP O14775
N	396	GLY	-	expression tag	UNP O14775
N	397	GLY	-	expression tag	UNP O14775
N	398	GLU	-	expression tag	UNP O14775
N	399	ASP	-	expression tag	UNP O14775
N	400	GLN	-	expression tag	UNP O14775
N	401	VAL	-	expression tag	UNP O14775
N	402	ASP	-	expression tag	UNP O14775
N	403	PRO	-	expression tag	UNP O14775
N	404	ARG	-	expression tag	UNP O14775
N	405	LEU	-	expression tag	UNP O14775
N	406	ILE	-	expression tag	UNP O14775
N	407	ASP	-	expression tag	UNP O14775
N	408	GLY	-	expression tag	UNP O14775
N	409	LYS	-	expression tag	UNP O14775

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	536	Total	C	N	O	S	0	0
			4069	2548	711	787	23		
2	a	532	Total	C	N	O	S	0	0
			4041	2533	707	778	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	526	Total	C	N	O	S	0	0
			3952	2473	696	764	19		
3	b	525	Total	C	N	O	S	0	0
			3943	2467	694	763	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	520	Total	C	N	O	S	0	0
			3923	2453	683	764	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	520	Total	C	N	O	S	0	0
			3917	2450	680	764	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	535	Total	C	N	O	S	1	0
			4132	2590	719	792	31		
5	e	540	Total	C	N	O	S	1	0
			4169	2610	724	804	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	526	Total	C	N	O	S	0	0
			4089	2548	726	785	30		
6	g	526	Total	C	N	O	S	0	0
			4088	2548	725	785	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	528	Total	C	N	O	S	0	0
			4054	2561	699	769	25		
7	h	525	Total	C	N	O	S	0	0
			4032	2548	696	763	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	538	Total	C	N	O	S	0	0
			4086	2579	696	784	27		
8	q	533	Total	C	N	O	S	0	0
			4053	2558	690	778	27		

- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	525	Total	C	N	O	S	0	0
			4022	2528	704	769	21		
9	z	527	Total	C	N	O	S	0	0
			4033	2534	706	772	21		

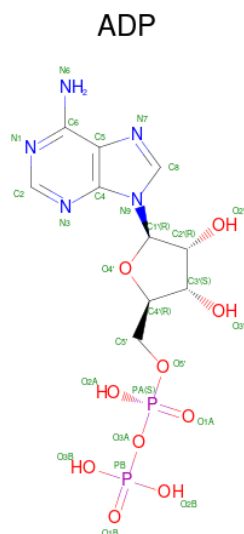
- Molecule 10 is a protein called Phosducin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	209	Total	C	N	O	S	0	0
			1650	1034	278	325	13		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	302	ALA	-	expression tag	UNP Q13371
P	303	LEU	-	expression tag	UNP Q13371
P	304	GLU	-	expression tag	UNP Q13371
P	305	GLY	-	expression tag	UNP Q13371
P	306	PRO	-	expression tag	UNP Q13371
P	307	ARG	-	expression tag	UNP Q13371
P	308	PHE	-	expression tag	UNP Q13371
P	309	GLU	-	expression tag	UNP Q13371
P	310	GLN	-	expression tag	UNP Q13371
P	311	LYS	-	expression tag	UNP Q13371
P	312	LEU	-	expression tag	UNP Q13371
P	313	ILE	-	expression tag	UNP Q13371
P	314	SER	-	expression tag	UNP Q13371
P	315	GLU	-	expression tag	UNP Q13371
P	316	GLU	-	expression tag	UNP Q13371
P	317	ASP	-	expression tag	UNP Q13371
P	318	LEU	-	expression tag	UNP Q13371
P	319	ASN	-	expression tag	UNP Q13371
P	320	MET	-	expression tag	UNP Q13371
P	321	HIS	-	expression tag	UNP Q13371
P	322	HIS	-	expression tag	UNP Q13371
P	323	HIS	-	expression tag	UNP Q13371
P	324	HIS	-	expression tag	UNP Q13371
P	325	HIS	-	expression tag	UNP Q13371
P	326	HIS	-	expression tag	UNP Q13371

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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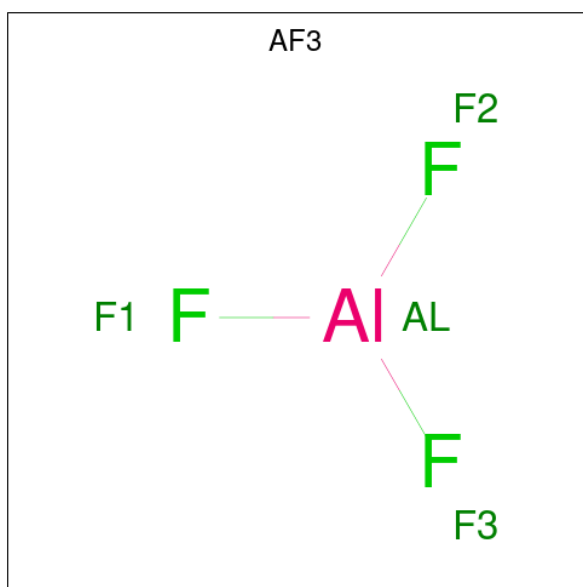
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Mol	Chain	Residues	Atoms					AltConf
11	q	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	z	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Mg	0
			1	1	
12	B	1	Total	Mg	0
			1	1	
12	D	1	Total	Mg	0
			1	1	
12	E	1	Total	Mg	0
			1	1	
12	G	1	Total	Mg	0
			1	1	
12	H	1	Total	Mg	0
			1	1	
12	Q	1	Total	Mg	0
			1	1	
12	Z	1	Total	Mg	0
			1	1	
12	a	1	Total	Mg	0
			1	1	
12	b	1	Total	Mg	0
			1	1	
12	d	1	Total	Mg	0
			1	1	
12	e	1	Total	Mg	0
			1	1	
12	g	1	Total	Mg	0
			1	1	
12	h	1	Total	Mg	0
			1	1	
12	q	1	Total	Mg	0
			1	1	
12	z	1	Total	Mg	0
			1	1	

- Molecule 13 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	Al	F	0
			4	1	3	
13	B	1	Total	Al	F	0
			4	1	3	
13	D	1	Total	Al	F	0
			4	1	3	
13	E	1	Total	Al	F	0
			4	1	3	
13	G	1	Total	Al	F	0
			4	1	3	
13	H	1	Total	Al	F	0
			4	1	3	
13	Q	1	Total	Al	F	0
			4	1	3	
13	Z	1	Total	Al	F	0
			4	1	3	
13	a	1	Total	Al	F	0
			4	1	3	
13	b	1	Total	Al	F	0
			4	1	3	
13	d	1	Total	Al	F	0
			4	1	3	
13	e	1	Total	Al	F	0
			4	1	3	
13	g	1	Total	Al	F	0
			4	1	3	
13	h	1	Total	Al	F	0
			4	1	3	

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Mol	Chain	Residues	Atoms			AltConf
13	q	1	Total	Al	F	0
			4	1	3	
13	z	1	Total	Al	F	0
			4	1	3	

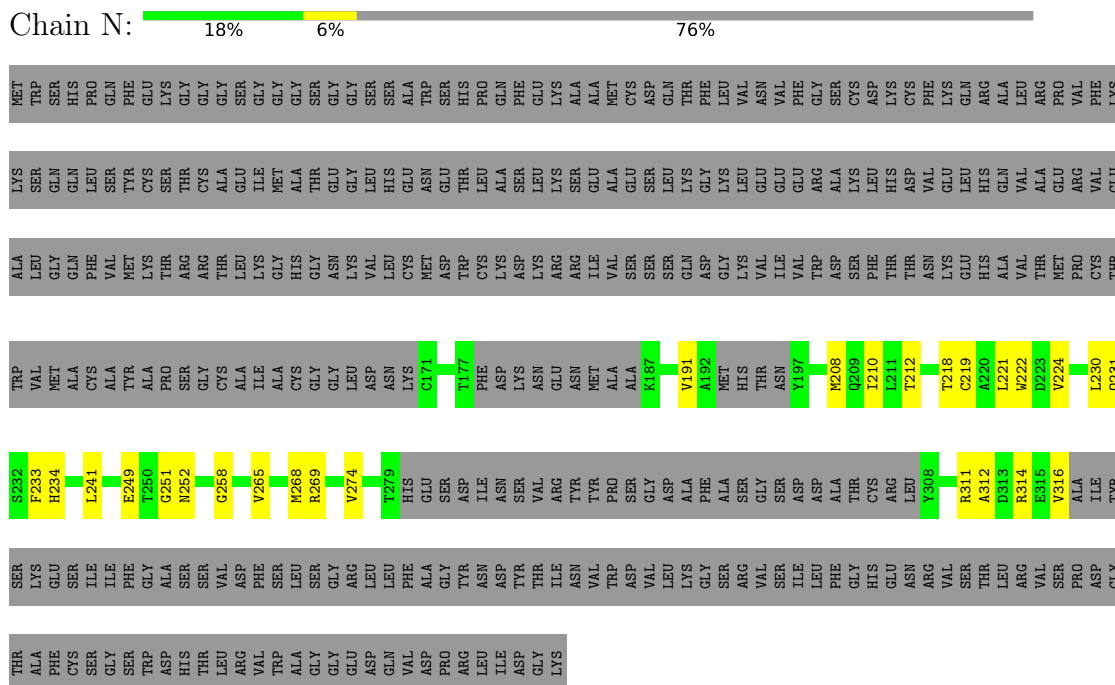
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		AltConf
14	A	2	Total	O	0
			2	2	
14	B	2	Total	O	0
			2	2	
14	D	1	Total	O	0
			1	1	
14	E	1	Total	O	0
			1	1	
14	G	1	Total	O	0
			1	1	
14	H	1	Total	O	0
			1	1	
14	Q	1	Total	O	0
			1	1	
14	Z	1	Total	O	0
			1	1	
14	a	2	Total	O	0
			2	2	
14	b	1	Total	O	0
			1	1	
14	d	1	Total	O	0
			1	1	
14	e	1	Total	O	0
			1	1	
14	g	1	Total	O	0
			1	1	
14	h	1	Total	O	0
			1	1	
14	q	1	Total	O	0
			1	1	
14	z	1	Total	O	0
			1	1	

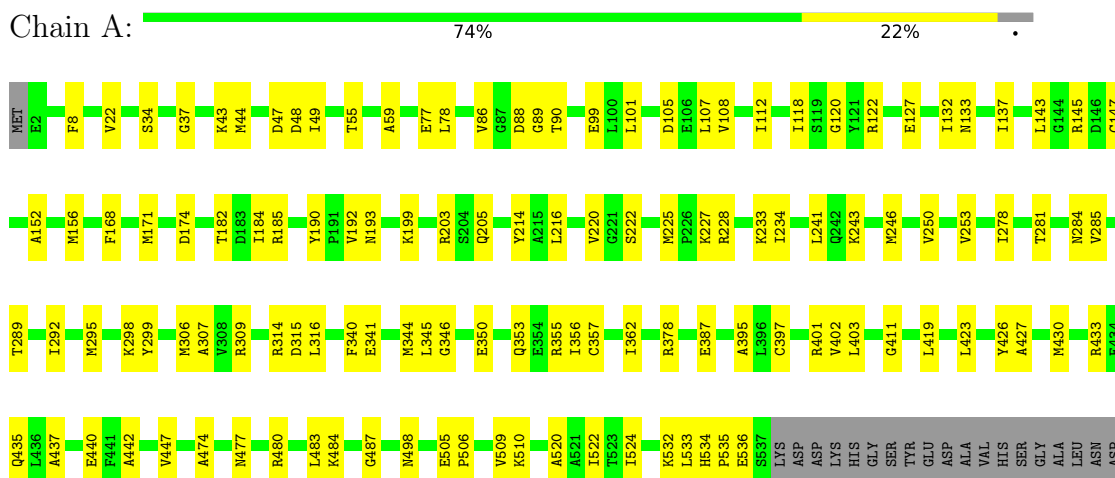
### 3 Residue-property plots

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: Guanine nucleotide-binding protein subunit beta-5

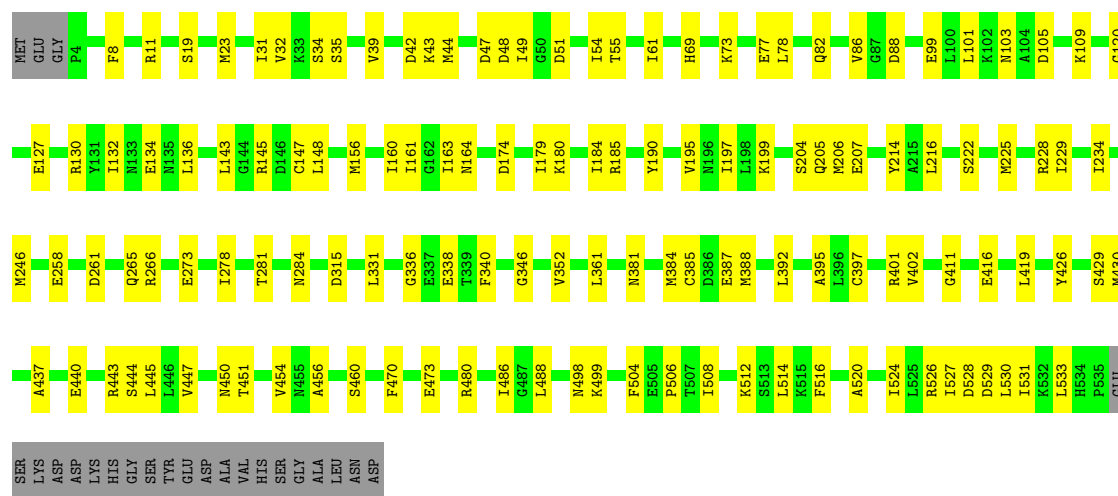


- Molecule 2: T-complex protein 1 subunit alpha




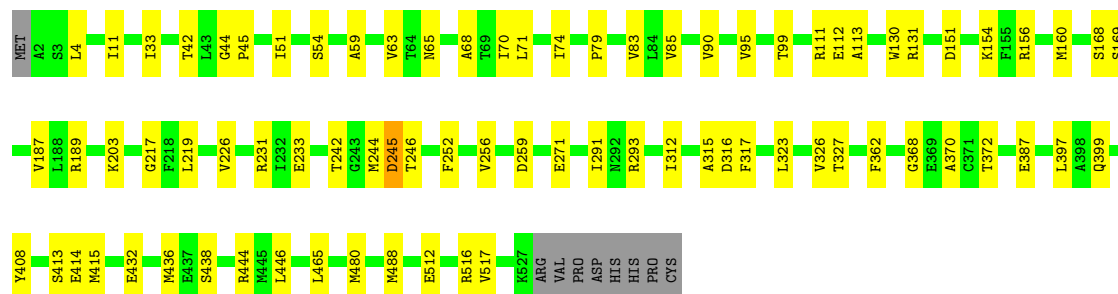
- Molecule 2: T-complex protein 1 subunit alpha

Chain a: 




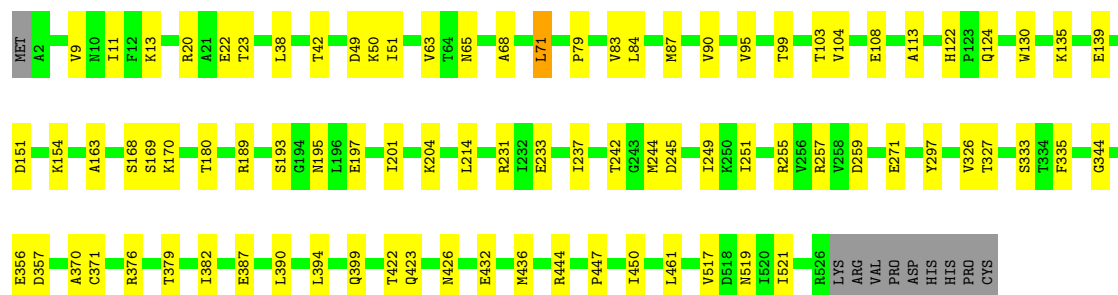
- Molecule 3: T-complex protein 1 subunit beta

Chain B: 



- Molecule 3: T-complex protein 1 subunit beta

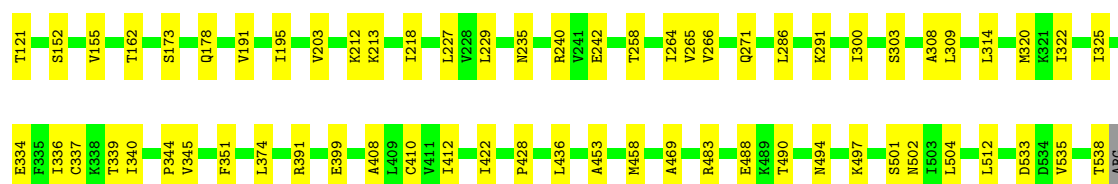
Chain b: 



- Molecule 4: T-complex protein 1 subunit delta

Chain D: 





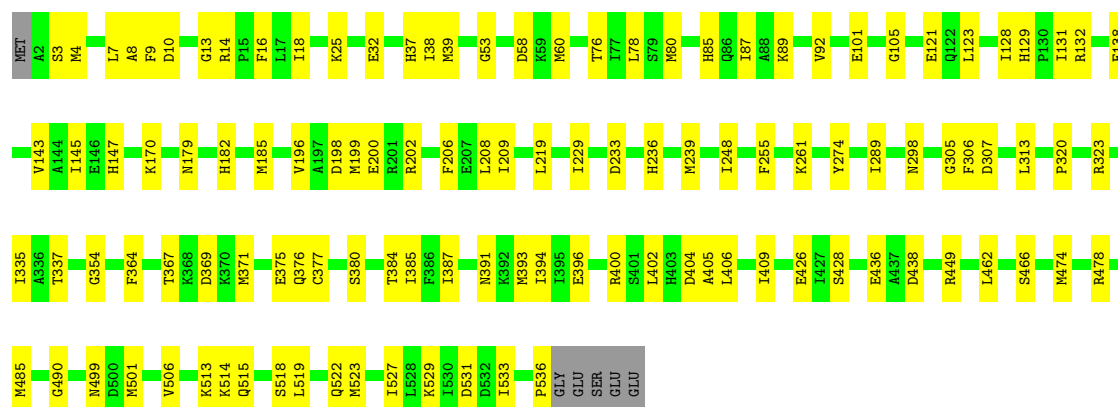
• Molecule 4: T-complex protein 1 subunit delta

Chain d: 78% 19% .



• Molecule 5: T-complex protein 1 subunit epsilon

Chain E: 77% 21% .



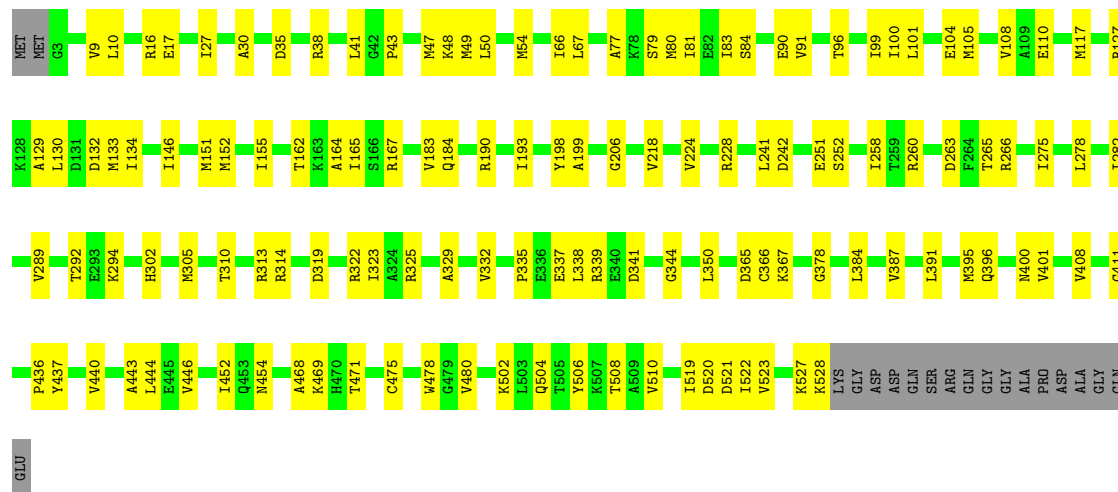
• Molecule 5: T-complex protein 1 subunit epsilon

Chain e: 78% 21%



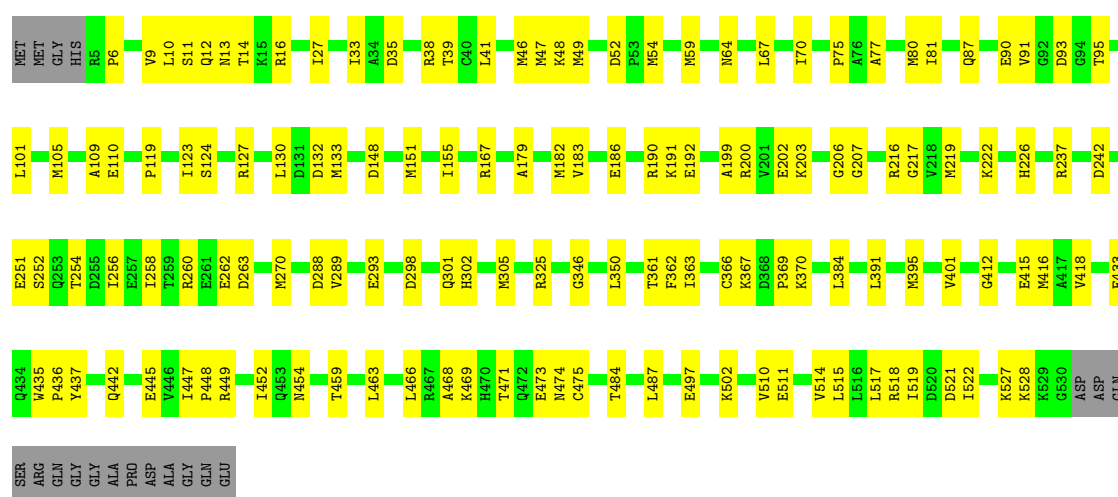
- Molecule 6: T-complex protein 1 subunit gamma

Chain G:  73% 24% .

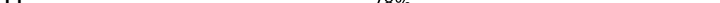


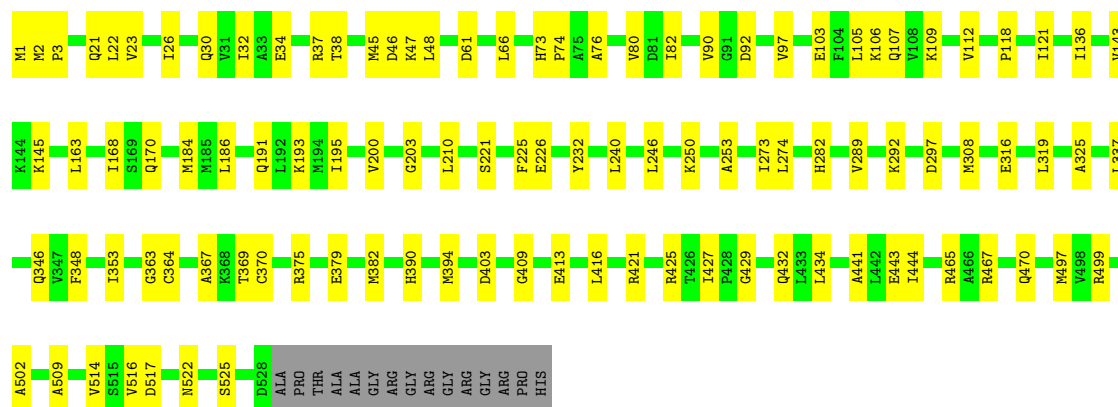
- Molecule 6: T-complex protein 1 subunit gamma

Chain g:  71% 25% .



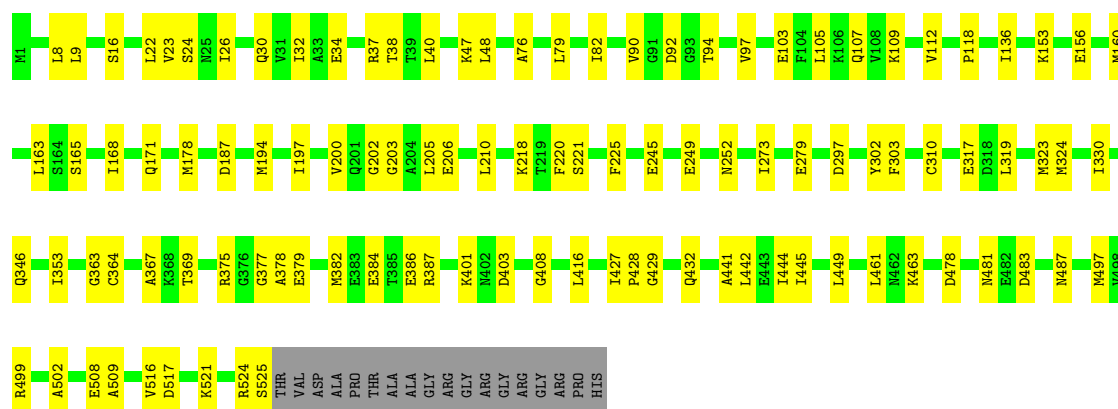
- Molecule 7: T-complex protein 1 subunit eta

Chain H:  78% 19%



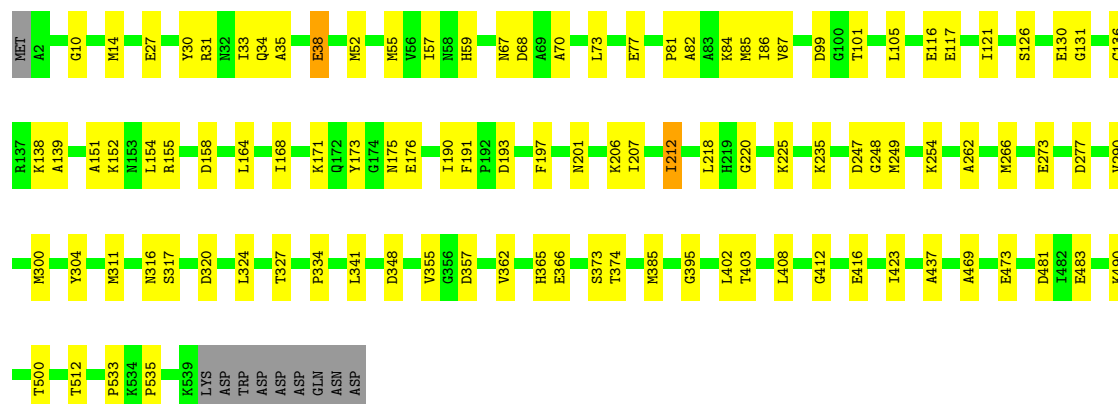
• Molecule 7: T-complex protein 1 subunit eta

Chain h: 77% 20% .



• Molecule 8: T-complex protein 1 subunit theta

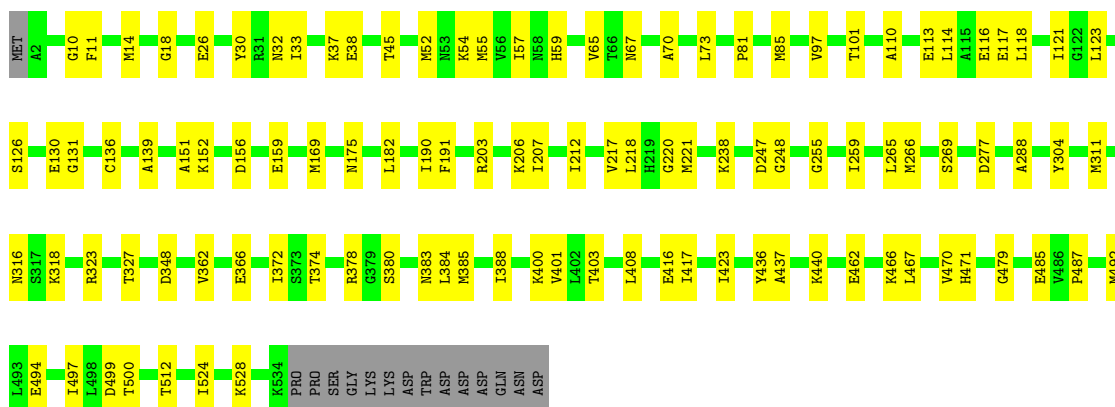
Chain Q: 79% 19% .



• Molecule 8: T-complex protein 1 subunit theta

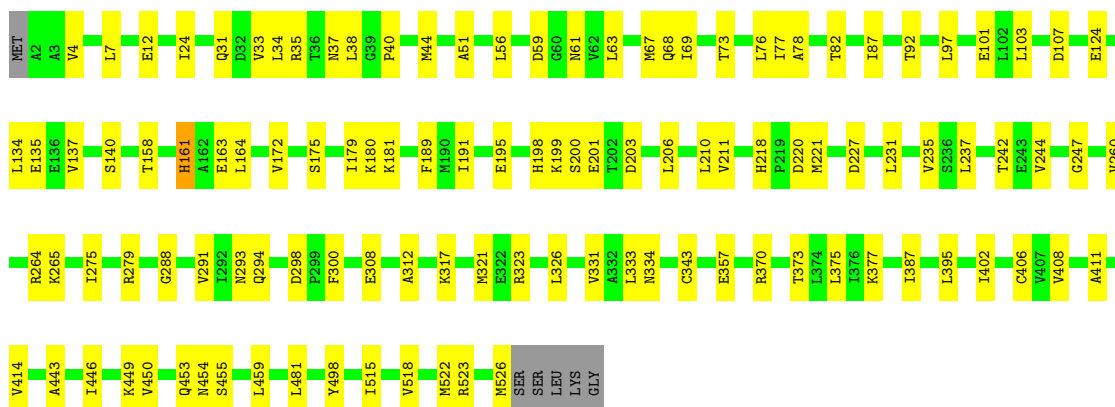
Chain q: 78% 20% .





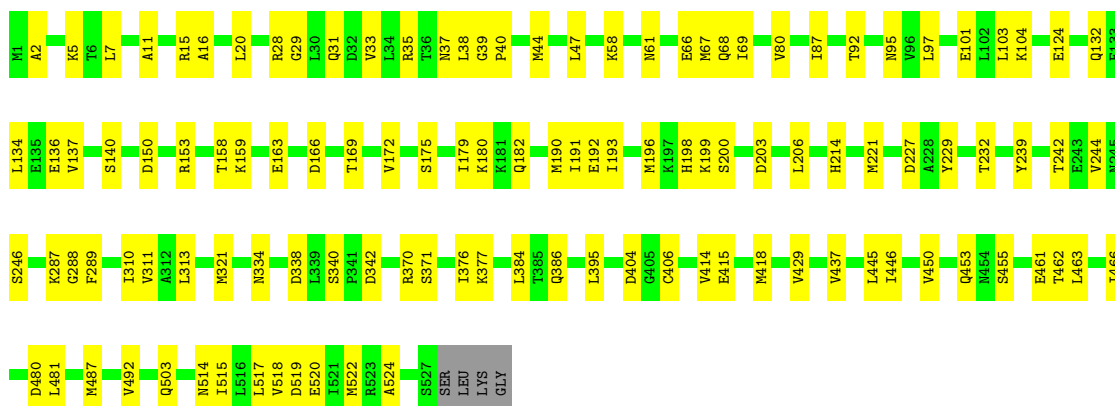
• Molecule 9: T-complex protein 1 subunit zeta

Chain Z: 77% 21% .



• Molecule 9: T-complex protein 1 subunit zeta

Chain z: 77% 22% .



• Molecule 10: Phosducin-like protein

Chain P: 41% 23% 36%

S226	R230	L233	L237	I238	Y239	K240	E243	L244	D253	V262	D263	L264	L274	P275	S288	A289	T290	C291	H292	I300	D301	ALA	LEU	GLU	GLY	PRO	ARG	PHE	GLU	GLN	LYS	ILE	SER	GLU	GLU	ASP	LEU	ASN	MET	HIS	HIS	HIS	HIS	HIS										
GLU	PHE	LEU	GLN	TYR	ARG	K142	Q143	E146	R149	L152	H153	K154	G155	P156	Q160	E163	L171	K176	E177	Q178	K179	V182	I183	M184	V185	H186	I187	Y188	E189	T195	E196	A197	M198	N199	G200	C201	M202	V212	K213	F214	C215	K216	S219	I222										
Q71	L72	E73	Q76	R77	E78	C81	R82	E85	R86	L87	I88	K89	K90	L91	S92	M93	THR	CYS	ARG	SER	HIS	LEU	ASP	GLU	GLU	GLU	GLU	GLN	GLN	LYS	ILE	SER	GLY	LYS	MET	THR	LEU	LYS	GLU	PHE	ALA	ILE	MET	ASN	GLU	ASP	GLN	ASP						
MET	THR	LEU	ASP	ASP	LYS	LEU	GLY	LYS	GLN	TYR	TYR	SER	SER	SER	S20	D24	SER	ASP	HIS	GLU	LYS	ASP	LYS	ASP	ARG	GLY	ARG	CYS	ALA	PRO	ALA	SER	SER	SER	VAL	PRO	ALA	GLU	GLU	ALA	LEU	LEU	ALA	G50	P59	K60	G61	V62	I63	N64	D65	W66	R67	K70

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76653	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, MG, 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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	N	0.13	0/805	0.39	0/1084
2	A	0.15	0/4109	0.32	0/5548
2	a	0.15	0/4081	0.31	0/5510
3	B	0.15	0/3995	0.29	0/5386
3	b	0.15	0/3986	0.27	0/5375
4	D	0.15	0/3955	0.29	0/5338
4	d	0.15	0/3949	0.29	0/5331
5	E	0.16	0/4183	0.32	0/5635
5	e	0.16	0/4220	0.32	0/5684
6	G	0.15	0/4136	0.31	0/5579
6	g	0.15	0/4134	0.30	0/5575
7	H	0.15	0/4111	0.29	0/5550
7	h	0.15	0/4089	0.31	0/5519
8	Q	0.14	0/4147	0.29	0/5606
8	q	0.14	0/4112	0.28	0/5558
9	Z	0.14	0/4069	0.29	0/5486
9	z	0.15	0/4080	0.29	0/5501
10	P	0.19	0/1672	0.49	0/2240
All	All	0.15	0/67833	0.31	0/91505

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 [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	N	794	0	752	23	0
2	A	4069	0	4224	98	0
2	a	4041	0	4205	98	0
3	B	3952	0	4070	58	0
3	b	3943	0	4057	63	0
4	D	3923	0	4131	59	0
4	d	3917	0	4120	72	0
5	E	4132	0	4246	89	0
5	e	4169	0	4272	94	0
6	G	4089	0	4224	83	0
6	g	4088	0	4230	102	0
7	H	4054	0	4160	70	0
7	h	4032	0	4140	86	0
8	Q	4086	0	4160	72	0
8	q	4053	0	4125	69	0
9	Z	4022	0	4161	77	0
9	z	4033	0	4171	82	0
10	P	1650	0	1628	68	0
11	A	27	0	12	3	0
11	B	27	0	12	4	0
11	D	27	0	12	2	0
11	E	27	0	12	4	0
11	G	27	0	12	4	0
11	H	27	0	12	2	0
11	Q	27	0	12	2	0
11	Z	27	0	12	2	0
11	a	27	0	12	1	0
11	b	27	0	12	2	0
11	d	27	0	12	1	0
11	e	27	0	12	0	0
11	g	27	0	12	2	0
11	h	27	0	12	2	0
11	q	27	0	12	3	0
11	z	27	0	12	2	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
12	E	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
12	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1	0	0	0	0
12	a	1	0	0	0	0
12	b	1	0	0	0	0
12	d	1	0	0	0	0
12	e	1	0	0	0	0
12	g	1	0	0	0	0
12	h	1	0	0	0	0
12	q	1	0	0	0	0
12	z	1	0	0	0	0
13	A	4	0	0	1	0
13	B	4	0	0	1	0
13	D	4	0	0	2	0
13	E	4	0	0	1	0
13	G	4	0	0	2	0
13	H	4	0	0	2	0
13	Q	4	0	0	2	0
13	Z	4	0	0	2	0
13	a	4	0	0	1	0
13	b	4	0	0	1	0
13	d	4	0	0	1	0
13	e	4	0	0	0	0
13	g	4	0	0	2	0
13	h	4	0	0	3	0
13	q	4	0	0	1	0
13	z	4	0	0	2	0
14	A	2	0	0	0	0
14	B	2	0	0	0	0
14	D	1	0	0	0	0
14	E	1	0	0	1	0
14	G	1	0	0	0	0
14	H	1	0	0	0	0
14	Q	1	0	0	0	0
14	Z	1	0	0	0	0
14	a	2	0	0	0	0
14	b	1	0	0	0	0
14	d	1	0	0	0	0
14	e	1	0	0	0	0
14	g	1	0	0	0	0
14	h	1	0	0	0	0
14	q	1	0	0	0	0
14	z	1	0	0	0	0
All	All	67578	0	69268	1228	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 9.

The worst 5 of 1228 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)
3:B:4:LEU:HD22	3:B:11:ILE:HD11	1.54	0.86
10:P:189:GLU:HB2	10:P:233:LEU:HD21	1.57	0.85
2:A:534:HIS:HE1	10:P:71:GLN:HG2	1.42	0.82
2:A:44:MET:HE3	6:G:519:ILE:HG21	1.63	0.81
6:G:206:GLY:HA3	9:Z:87:ILE:HG13	1.65	0.78

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	N	97/441 (22%)	86 (89%)	11 (11%)	0	100	100
2	A	534/556 (96%)	517 (97%)	17 (3%)	0	100	100
2	a	530/556 (95%)	510 (96%)	20 (4%)	0	100	100
3	B	524/535 (98%)	511 (98%)	13 (2%)	0	100	100
3	b	523/535 (98%)	507 (97%)	16 (3%)	0	100	100
4	D	518/539 (96%)	511 (99%)	7 (1%)	0	100	100
4	d	518/539 (96%)	497 (96%)	21 (4%)	0	100	100
5	E	534/541 (99%)	516 (97%)	18 (3%)	0	100	100
5	e	539/541 (100%)	529 (98%)	10 (2%)	0	100	100
6	G	524/545 (96%)	510 (97%)	14 (3%)	0	100	100
6	g	524/545 (96%)	509 (97%)	15 (3%)	0	100	100
7	H	526/543 (97%)	504 (96%)	22 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	h	523/543 (96%)	504 (96%)	19 (4%)	0	100	100
8	Q	536/548 (98%)	523 (98%)	13 (2%)	0	100	100
8	q	531/548 (97%)	517 (97%)	14 (3%)	0	100	100
9	Z	523/531 (98%)	509 (97%)	14 (3%)	0	100	100
9	z	525/531 (99%)	509 (97%)	16 (3%)	0	100	100
10	P	203/326 (62%)	186 (92%)	17 (8%)	0	100	100
All	All	8732/9443 (92%)	8455 (97%)	277 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	N	88/367 (24%)	88 (100%)	0	100	100
2	A	447/463 (96%)	447 (100%)	0	100	100
2	a	444/463 (96%)	443 (100%)	1 (0%)	87	89
3	B	418/427 (98%)	417 (100%)	1 (0%)	87	89
3	b	417/427 (98%)	416 (100%)	1 (0%)	87	89
4	D	442/452 (98%)	442 (100%)	0	100	100
4	d	441/452 (98%)	441 (100%)	0	100	100
5	E	452/456 (99%)	451 (100%)	1 (0%)	87	89
5	e	456/456 (100%)	455 (100%)	1 (0%)	87	89
6	G	456/469 (97%)	456 (100%)	0	100	100
6	g	456/469 (97%)	455 (100%)	1 (0%)	87	89
7	H	435/443 (98%)	435 (100%)	0	100	100
7	h	432/443 (98%)	432 (100%)	0	100	100
8	Q	442/452 (98%)	440 (100%)	2 (0%)	81	85
8	q	438/452 (97%)	436 (100%)	2 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Z	437/442 (99%)	436 (100%)	1 (0%)	87	89
9	z	438/442 (99%)	438 (100%)	0	100	100
10	P	183/289 (63%)	183 (100%)	0	100	100
All	All	7322/7864 (93%)	7311 (100%)	11 (0%)	85	89

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	288	MET
6	g	484	THR
8	q	316	ASN
8	q	73	LEU
9	Z	161	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
8	q	93	GLN
9	z	198	HIS
6	G	420	HIS
6	G	400	ASN
9	z	380	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 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
13	AF3	d	603	11	0,3,3	-	-	-		
13	AF3	q	603	8,11	0,3,3	-	-	-		
11	ADP	E	601	12,13	28,29,29	1.39	5 (17%)	43,45,45	1.81	10 (23%)
13	AF3	h	603	11	0,3,3	-	-	-		
11	ADP	Z	601	12,13	28,29,29	1.38	4 (14%)	43,45,45	1.83	9 (20%)
11	ADP	z	601	12	28,29,29	1.39	4 (14%)	43,45,45	1.86	8 (18%)
11	ADP	B	601	12	28,29,29	1.37	4 (14%)	43,45,45	1.82	10 (23%)
11	ADP	G	601	12,13	28,29,29	1.38	5 (17%)	43,45,45	1.83	10 (23%)
13	AF3	b	603	11	0,3,3	-	-	-		
13	AF3	G	603	11	0,3,3	-	-	-		
11	ADP	e	601	12,13	28,29,29	1.39	4 (14%)	43,45,45	1.82	10 (23%)
11	ADP	q	601	12,13	28,29,29	1.38	4 (14%)	43,45,45	1.85	10 (23%)
13	AF3	a	603	11	0,3,3	-	-	-		
11	ADP	d	601	12,13	28,29,29	1.40	4 (14%)	43,45,45	1.81	8 (18%)
11	ADP	h	601	12,13	28,29,29	1.38	4 (14%)	43,45,45	1.82	9 (20%)
13	AF3	H	603	11	0,3,3	-	-	-		
11	ADP	a	601	12,13	28,29,29	1.39	4 (14%)	43,45,45	1.86	11 (25%)
11	ADP	b	601	12,13	28,29,29	1.40	4 (14%)	43,45,45	1.85	10 (23%)
11	ADP	H	601	12,13	28,29,29	1.36	4 (14%)	43,45,45	1.84	9 (20%)
11	ADP	Q	601	12,13	28,29,29	1.38	5 (17%)	43,45,45	1.83	10 (23%)
11	ADP	A	601	12,13	28,29,29	1.39	4 (14%)	43,45,45	1.81	10 (23%)
13	AF3	g	603	6,11	0,3,3	-	-	-		
11	ADP	D	601	12,13	28,29,29	1.39	4 (14%)	43,45,45	1.81	10 (23%)
13	AF3	Q	603	11	0,3,3	-	-	-		
13	AF3	A	603	11	0,3,3	-	-	-		
13	AF3	z	603	-	0,3,3	-	-	-		
11	ADP	g	601	12,13	28,29,29	1.38	5 (17%)	43,45,45	1.82	9 (20%)
13	AF3	D	603	11	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	AF3	E	603	11	0,3,3	-	-	-		
13	AF3	B	603	-	0,3,3	-	-	-		
13	AF3	Z	603	11	0,3,3	-	-	-		
13	AF3	e	603	11	0,3,3	-	-	-		

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	ADP	e	601	12,13	-	0/16/32/32	0/3/3/3
11	ADP	E	601	12,13	-	7/16/32/32	0/3/3/3
11	ADP	g	601	12,13	-	2/16/32/32	0/3/3/3
11	ADP	Z	601	12,13	-	6/16/32/32	0/3/3/3
11	ADP	d	601	12,13	-	4/16/32/32	0/3/3/3
11	ADP	h	601	12,13	-	1/16/32/32	0/3/3/3
11	ADP	q	601	12,13	-	6/16/32/32	0/3/3/3
11	ADP	z	601	12	-	5/16/32/32	0/3/3/3
11	ADP	D	601	12,13	-	6/16/32/32	0/3/3/3
11	ADP	a	601	12,13	-	3/16/32/32	0/3/3/3
11	ADP	B	601	12	-	4/16/32/32	0/3/3/3
11	ADP	b	601	12,13	-	3/16/32/32	0/3/3/3
11	ADP	G	601	12,13	-	0/16/32/32	0/3/3/3
11	ADP	H	601	12,13	-	2/16/32/32	0/3/3/3
11	ADP	Q	601	12,13	-	5/16/32/32	0/3/3/3
11	ADP	A	601	12,13	-	4/16/32/32	0/3/3/3

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	z	601	ADP	C5-C4	4.58	1.47	1.39
11	a	601	ADP	C5-C4	4.57	1.47	1.39
11	D	601	ADP	C5-C4	4.55	1.47	1.39
11	Q	601	ADP	C5-C4	4.54	1.47	1.39
11	G	601	ADP	C5-C4	4.53	1.47	1.39

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	601	ADP	C5-C4-N3	-5.94	118.54	126.72
11	z	601	ADP	C5-C4-N3	-5.91	118.58	126.72
11	q	601	ADP	C5-C4-N3	-5.83	118.69	126.72
11	e	601	ADP	C5-C4-N3	-5.83	118.69	126.72
11	d	601	ADP	C5-C4-N3	-5.82	118.71	126.72

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	601	ADP	C5'-O5'-PA-O1A
11	A	601	ADP	C5'-O5'-PA-O2A
11	A	601	ADP	C5'-O5'-PA-O3A
11	B	601	ADP	C5'-O5'-PA-O1A
11	D	601	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

30 monomers are involved in 44 short contacts:

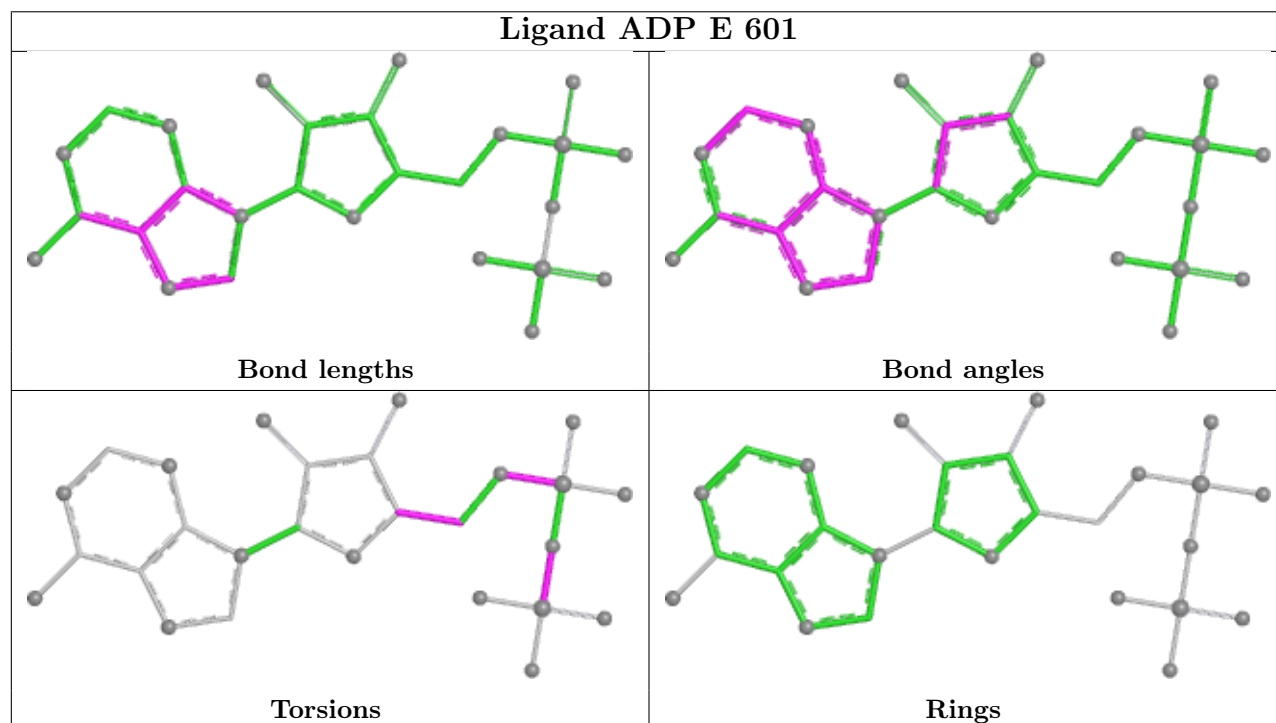
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	d	603	AF3	1	0
13	q	603	AF3	1	0
11	E	601	ADP	4	0
13	h	603	AF3	3	0
11	Z	601	ADP	2	0
11	z	601	ADP	2	0
11	B	601	ADP	4	0
11	G	601	ADP	4	0
13	b	603	AF3	1	0
13	G	603	AF3	2	0
11	q	601	ADP	3	0
13	a	603	AF3	1	0
11	d	601	ADP	1	0
11	h	601	ADP	2	0
13	H	603	AF3	2	0
11	a	601	ADP	1	0
11	b	601	ADP	2	0
11	H	601	ADP	2	0
11	Q	601	ADP	2	0
11	A	601	ADP	3	0
13	g	603	AF3	2	0
11	D	601	ADP	2	0

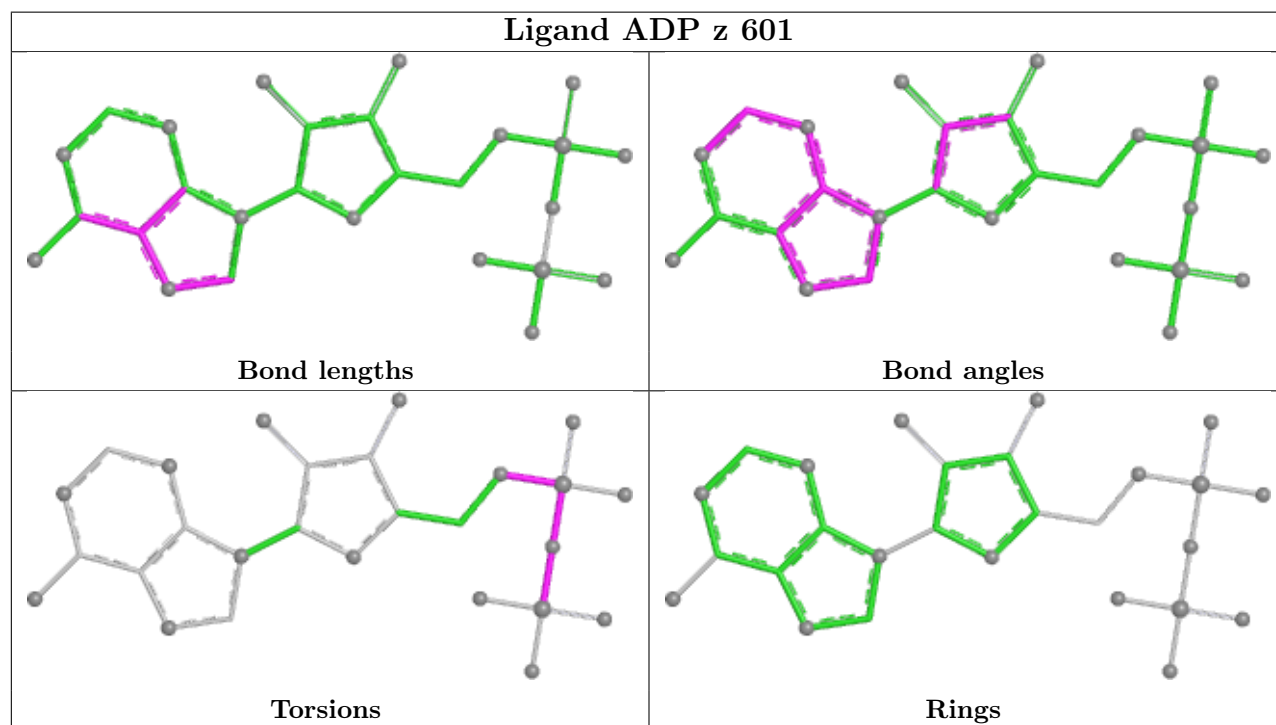
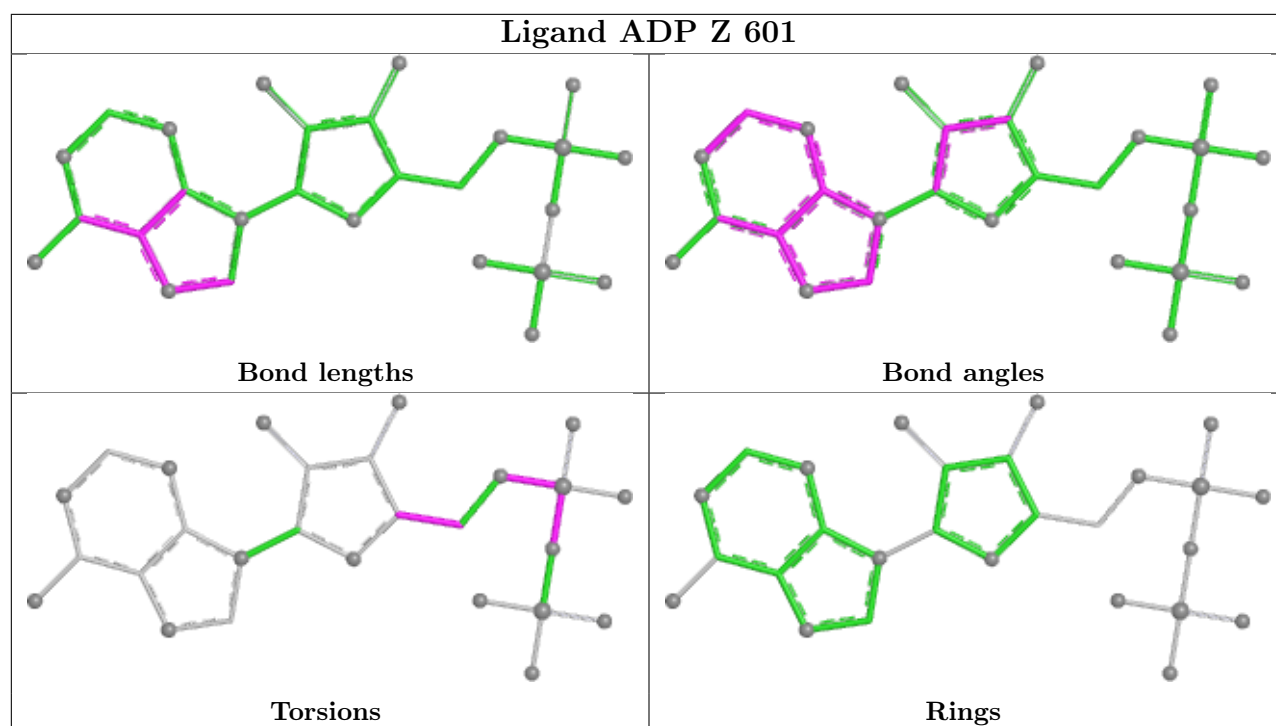
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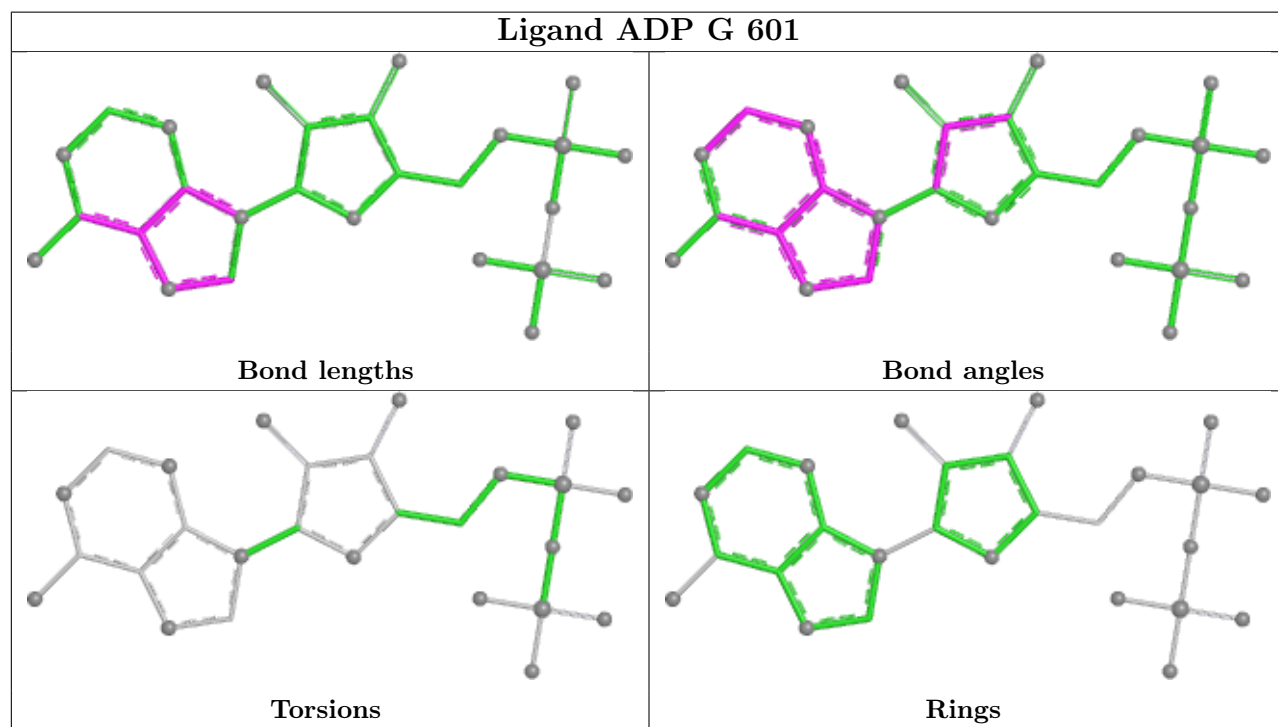
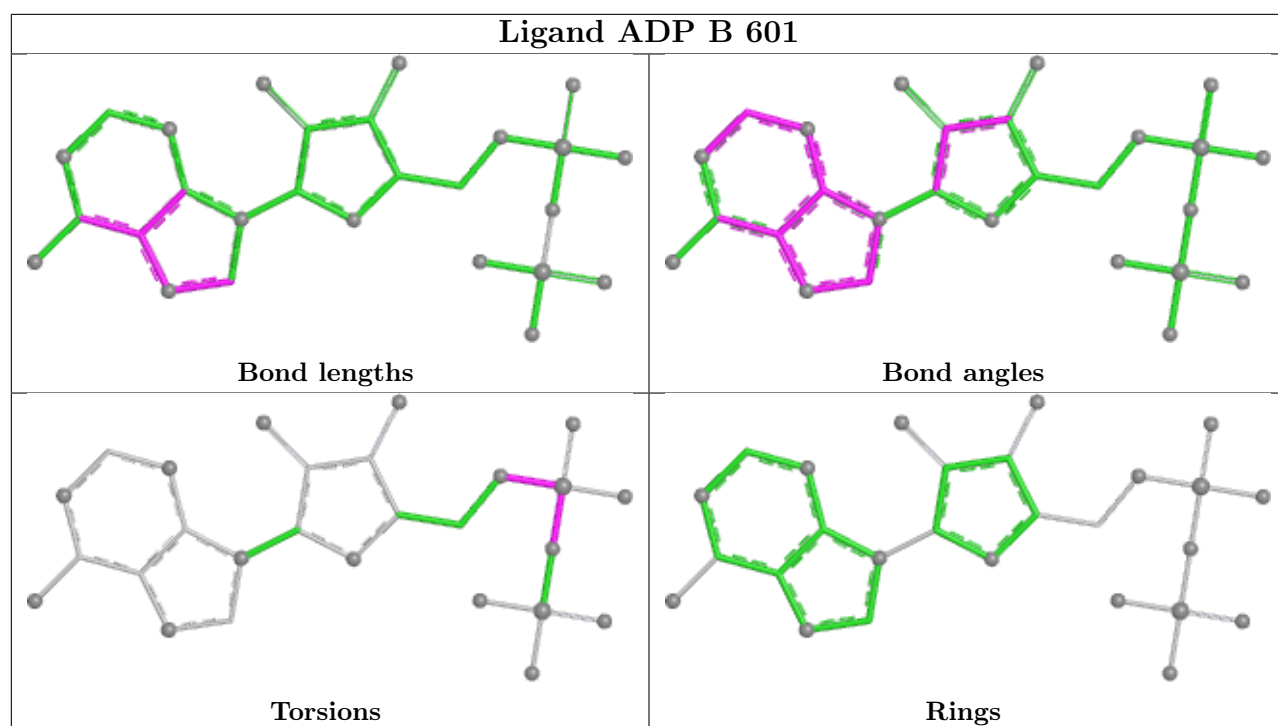
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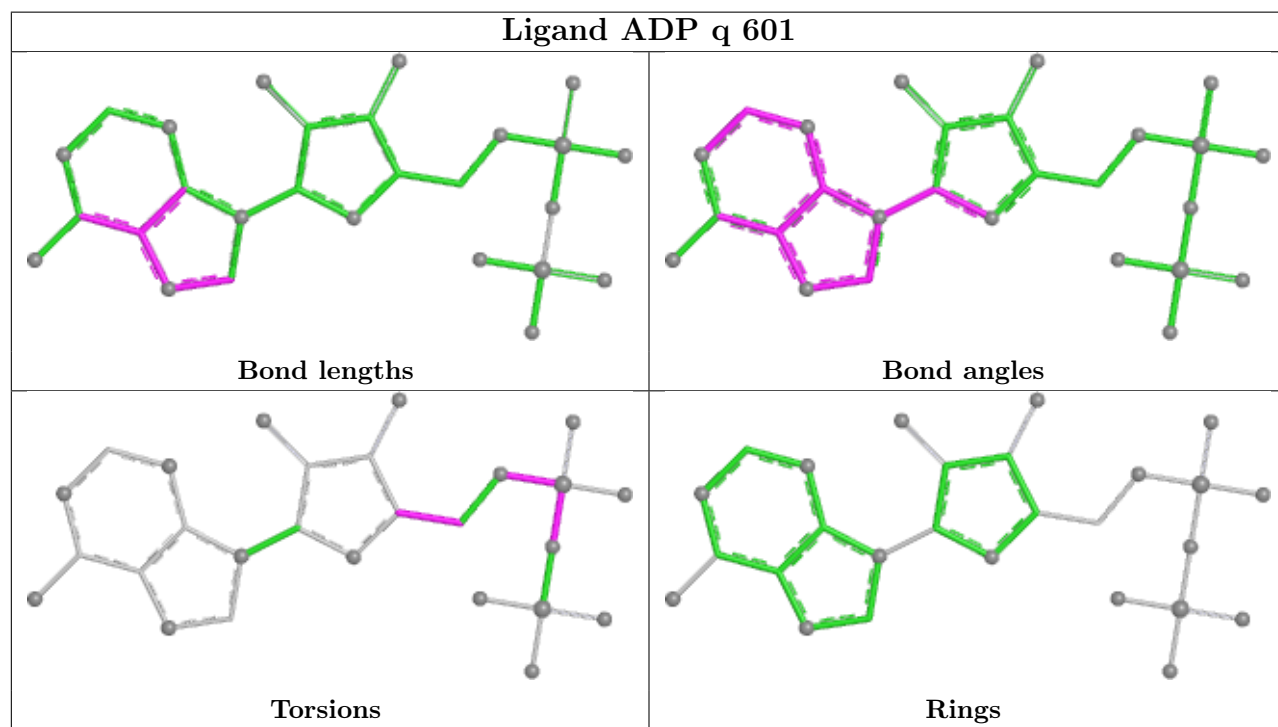
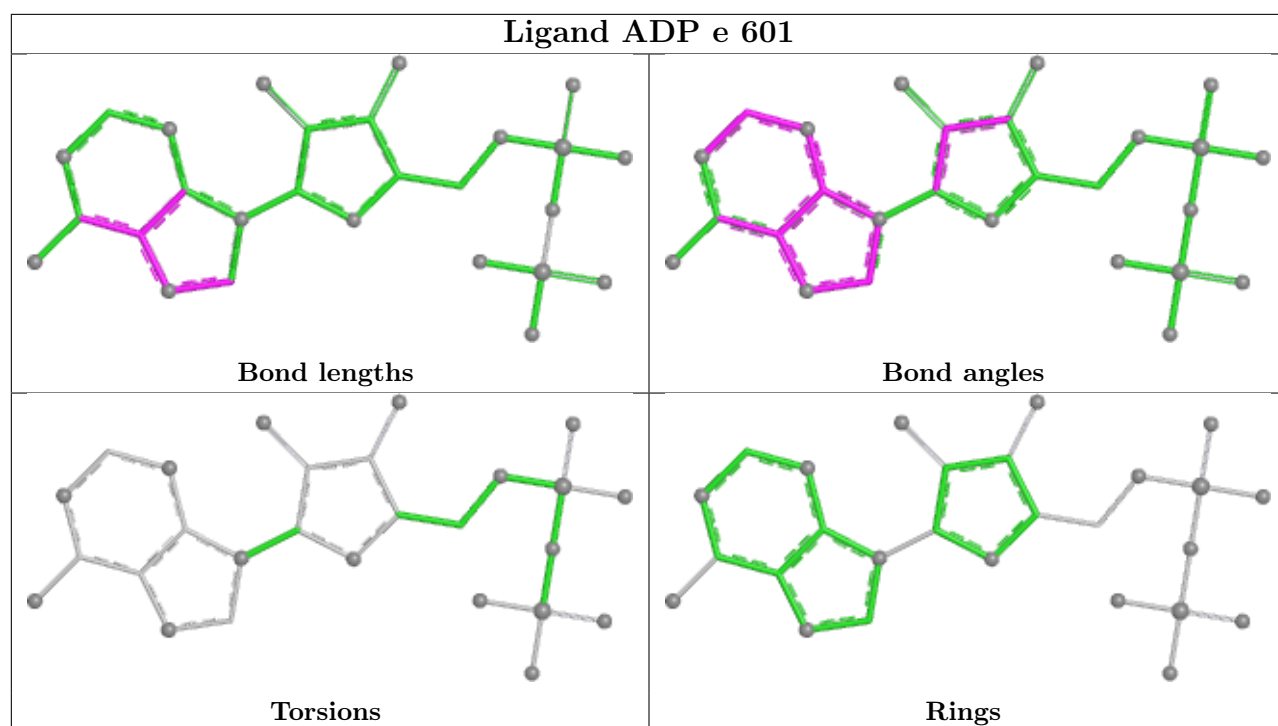
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Q	603	AF3	2	0
13	A	603	AF3	1	0
13	z	603	AF3	2	0
11	g	601	ADP	2	0
13	D	603	AF3	2	0
13	E	603	AF3	1	0
13	B	603	AF3	1	0
13	Z	603	AF3	2	0

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.

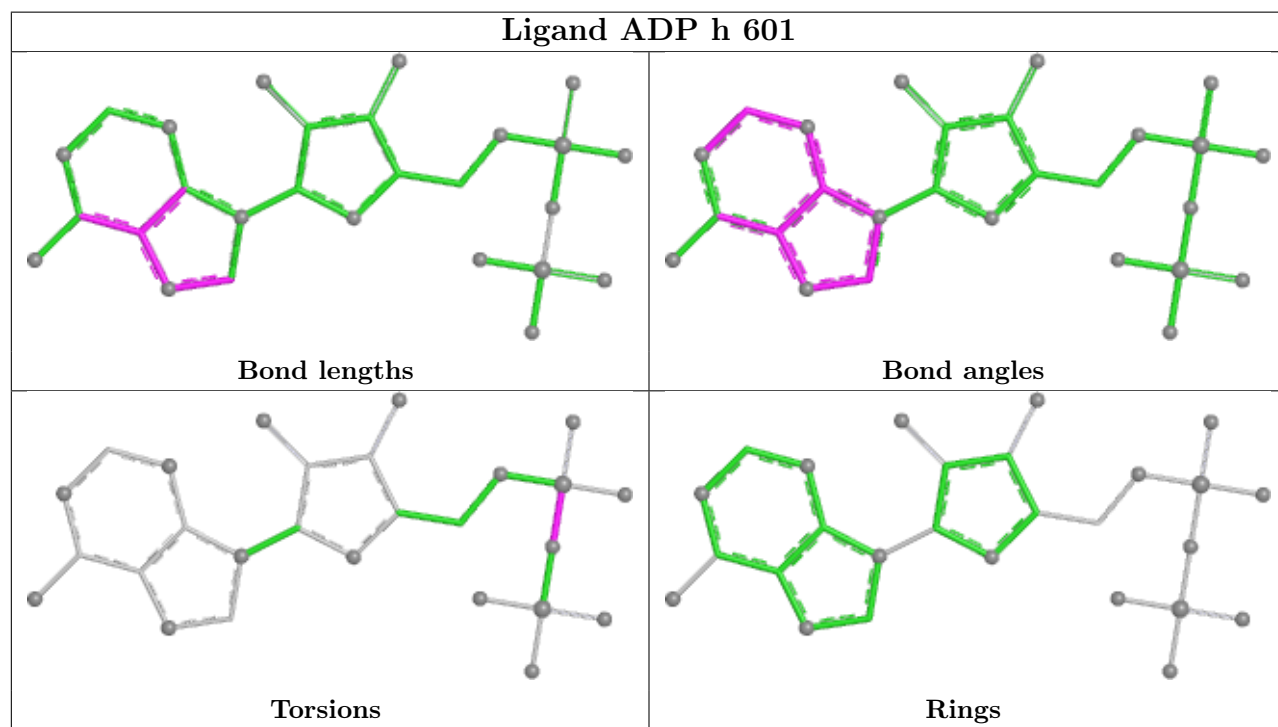
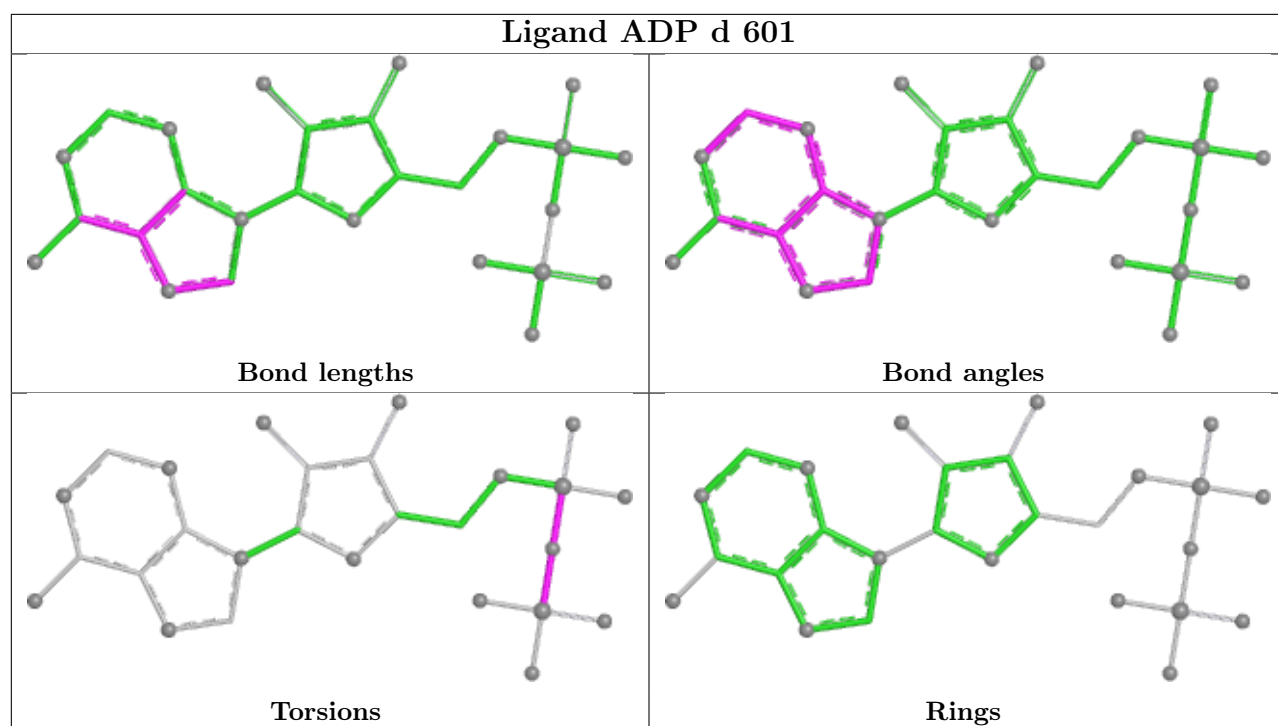


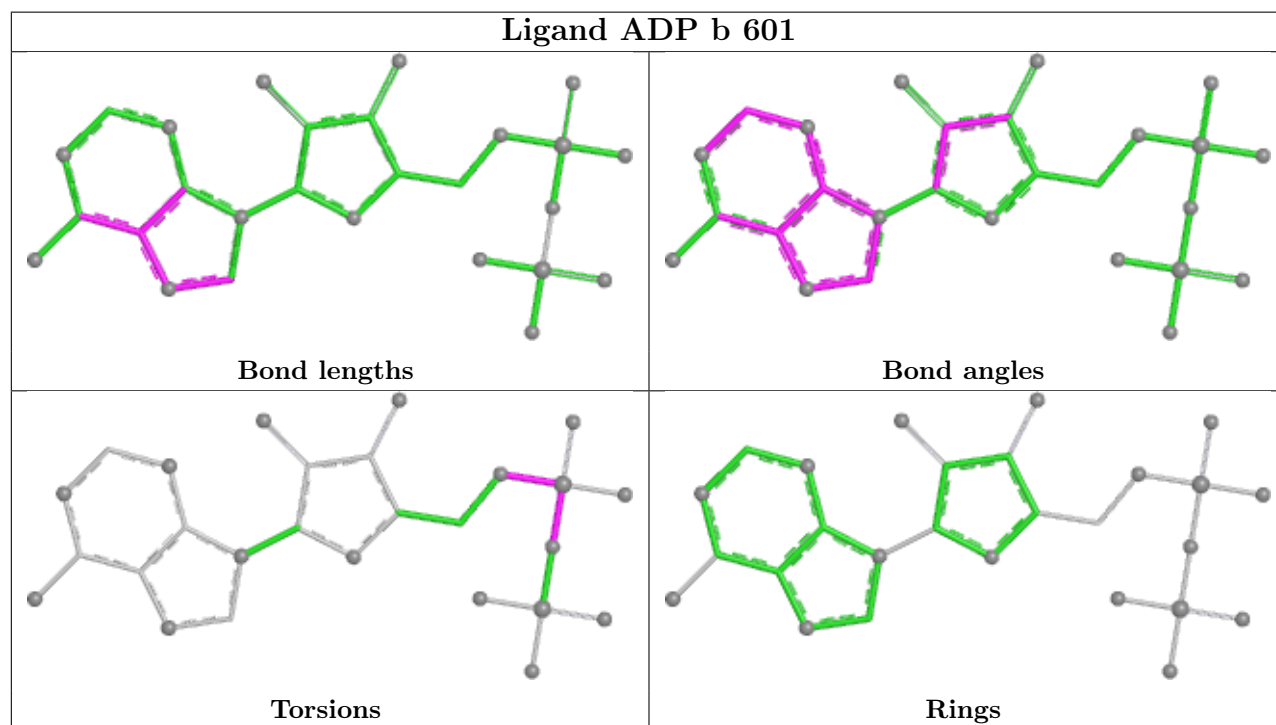
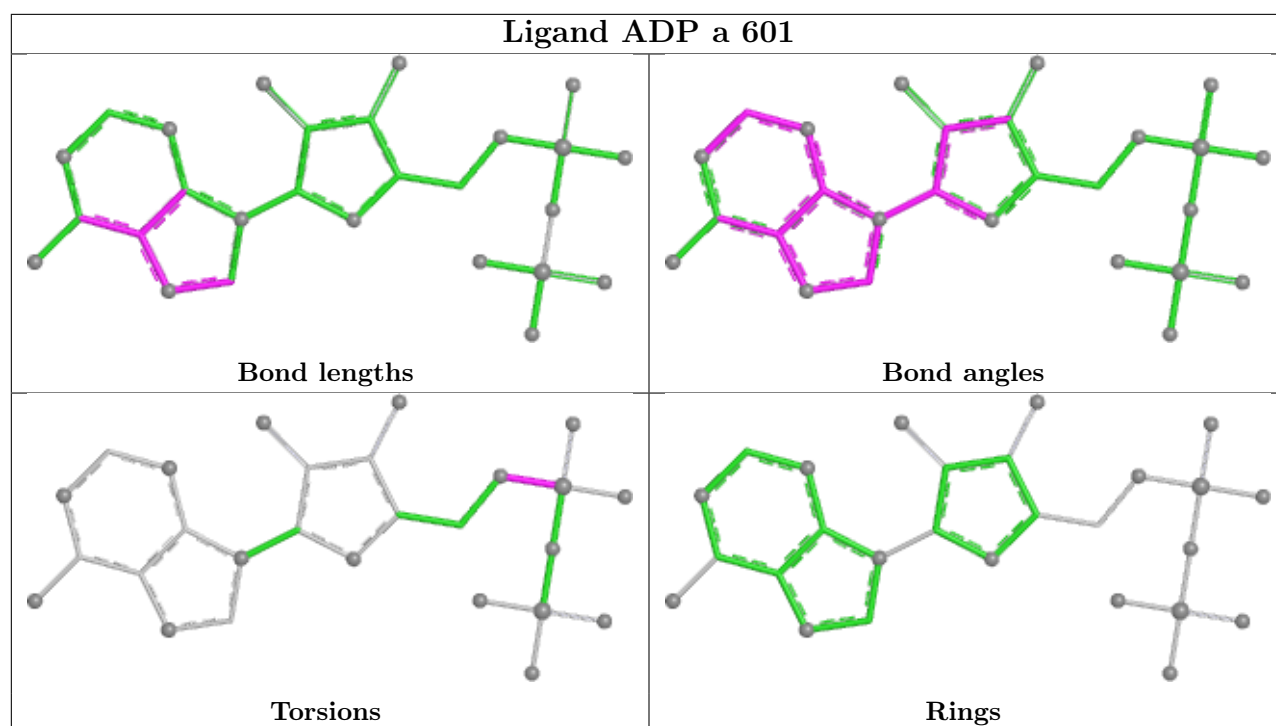


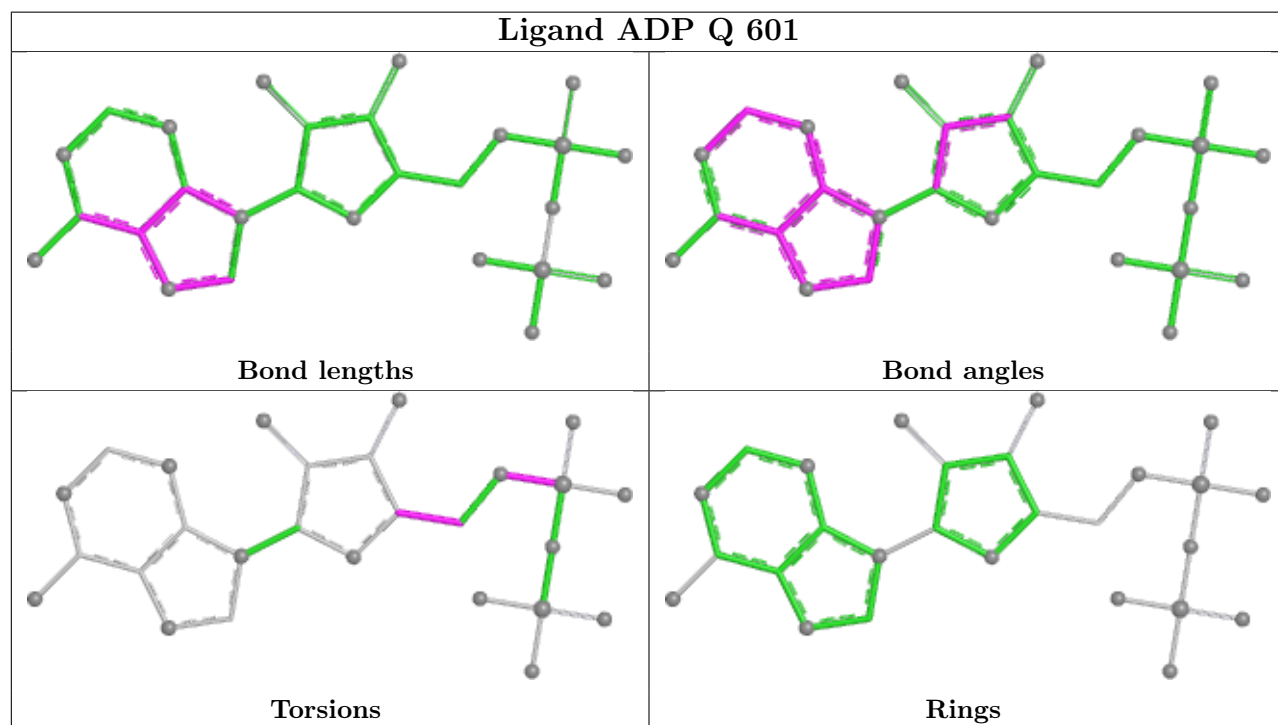
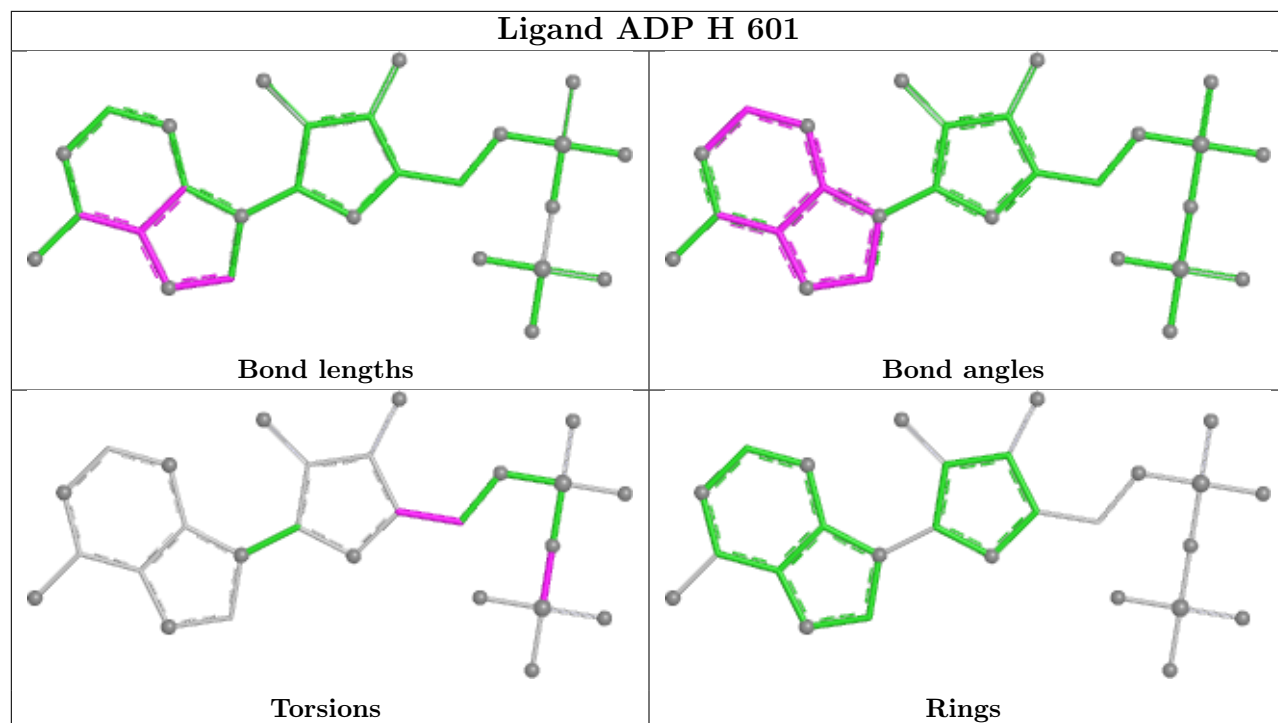


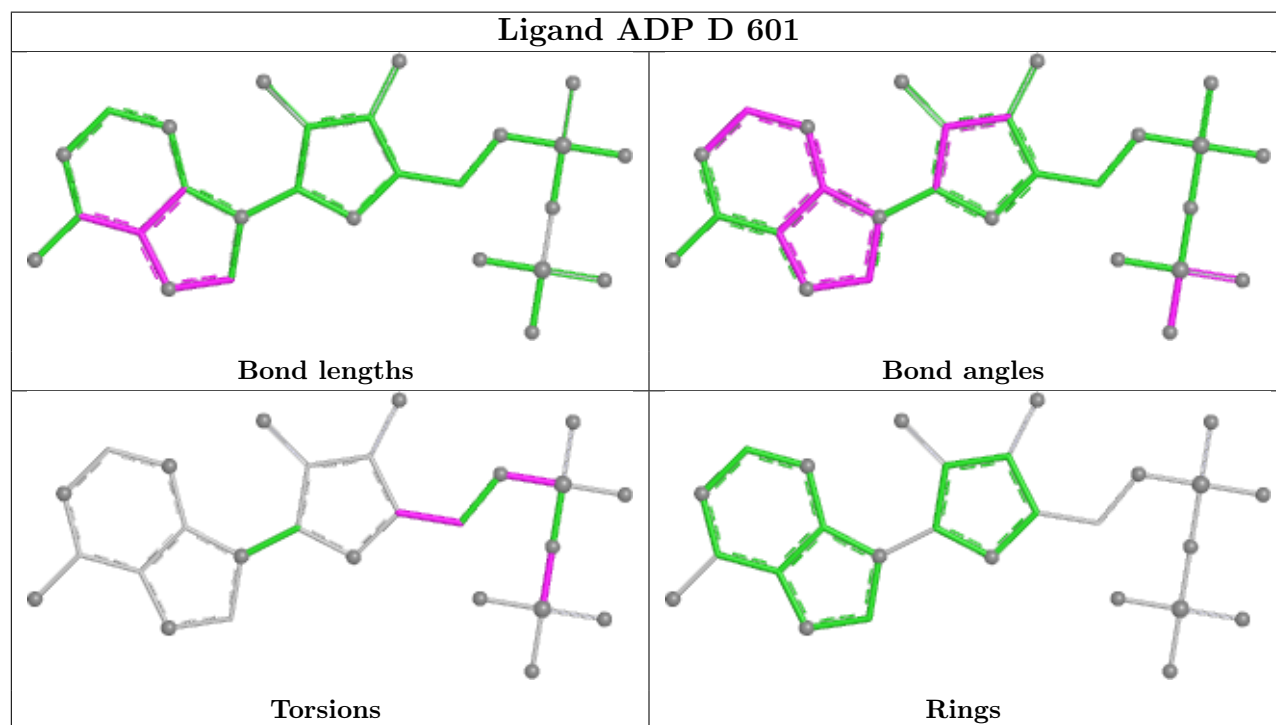
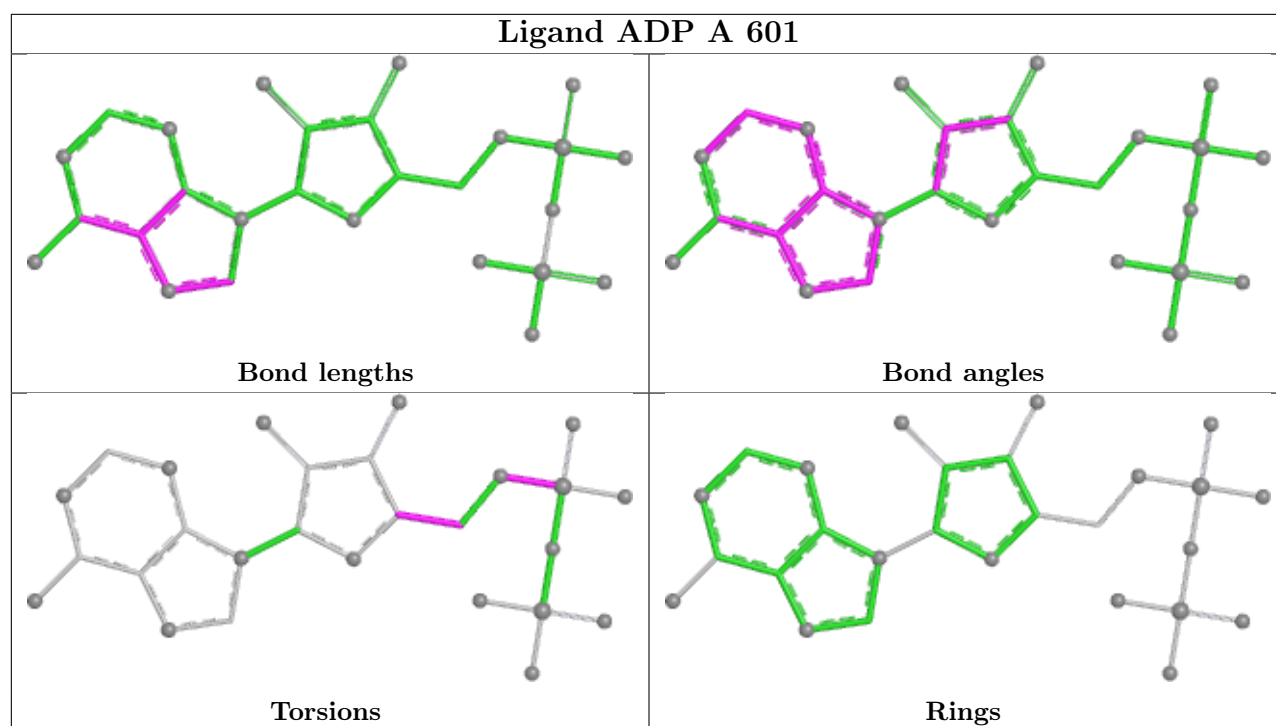


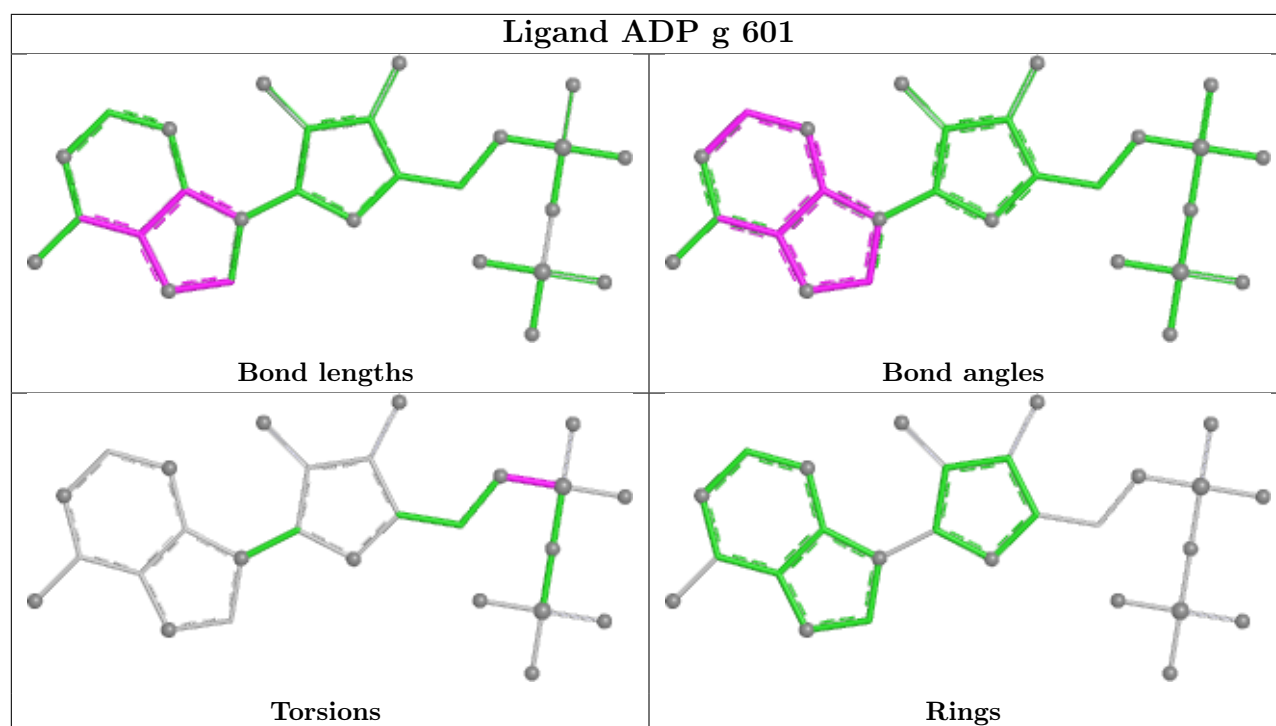












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49731. 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.