



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:01 PM UTC

PDB ID : 7MBU / pdb_00007mbu
EMDB ID : EMD-23747
Title : Cryo-EM structure of zebrafish TRPM5 E337A mutant in the presence of 5 mM calcium (high calcium occupancy in the transmembrane domain)
Authors : Ruan, Z.; Lu, W.; Du, J.; Haley, E.
Deposited on : 2021-04-01
Resolution : Not provided

This is a wwPDB EM Validation Summary 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

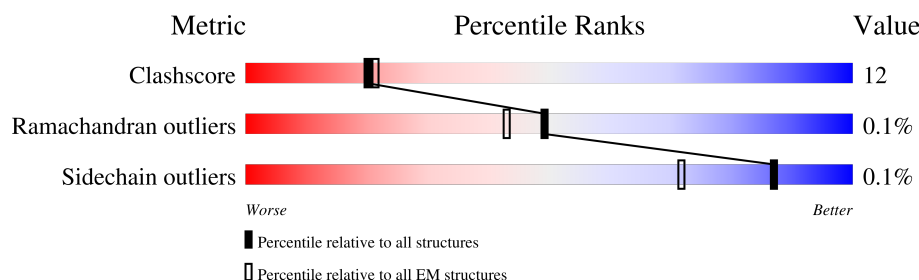
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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	A	1165	67% 18% 15%
1	B	1165	67% 19% 15%
1	C	1165	67% 19% 15%
1	D	1165	67% 19% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30780 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.

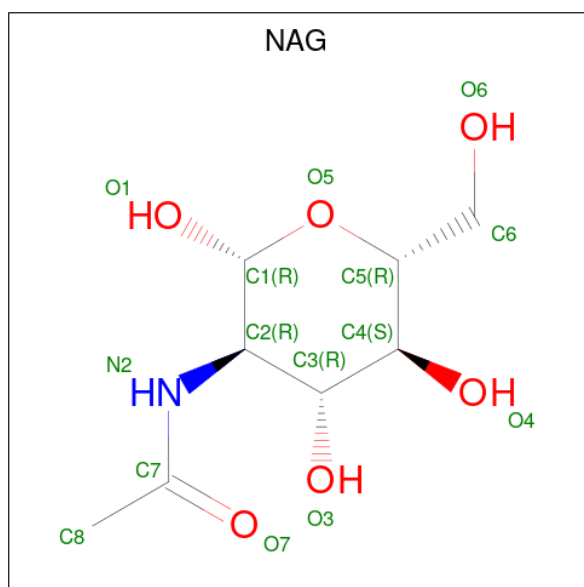
- Molecule 1 is a protein called Transient receptor potential melastatin 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	996	Total	C	N	O	S	1	0
			7591	4976	1299	1272	44		
1	B	996	Total	C	N	O	S	1	0
			7591	4976	1299	1272	44		
1	C	996	Total	C	N	O	S	1	0
			7591	4976	1299	1272	44		
1	D	996	Total	C	N	O	S	1	0
			7591	4976	1299	1272	44		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	ALA	GLU	engineered mutation	UNP S5UH55
B	337	ALA	GLU	engineered mutation	UNP S5UH55
C	337	ALA	GLU	engineered mutation	UNP S5UH55
D	337	ALA	GLU	engineered mutation	UNP S5UH55

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

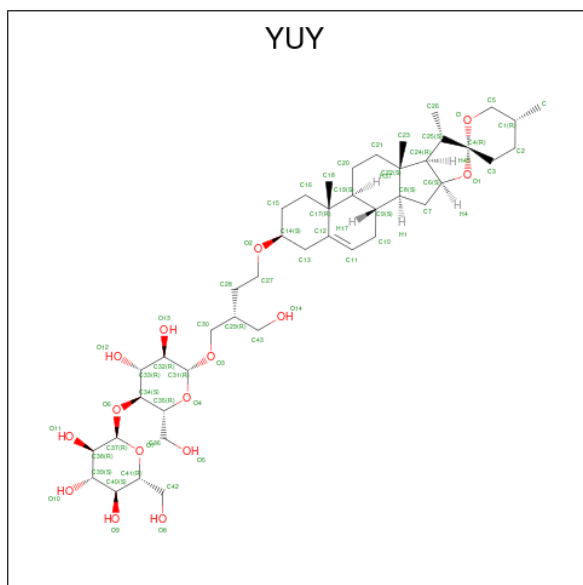


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

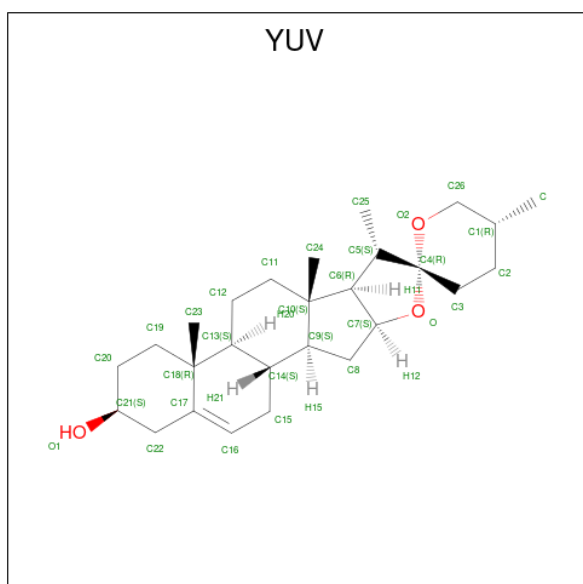
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	

- Molecule 4 is (2R)-2-(hydroxymethyl)-4-{[(25R)-10 α ,14 β ,17 β -spirost-5-en-3 β -yl]oxy}butyl 4-O- α -D-glucopyranosyl- β -D-glucopyranoside (CCD ID: YUY) (formula: C₄₄H₇₂O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			59	44	15	
4	A	1	Total	C	O	0
			59	44	15	
4	B	1	Total	C	O	0
			59	44	15	
4	C	1	Total	C	O	0
			59	44	15	

- Molecule 5 is (25R)-14beta,17beta-spirost-5-en-3beta-ol (CCD ID: YUV) (formula: $C_{27}H_{42}O_3$) (labeled as "Ligand of Interest" by depositor).

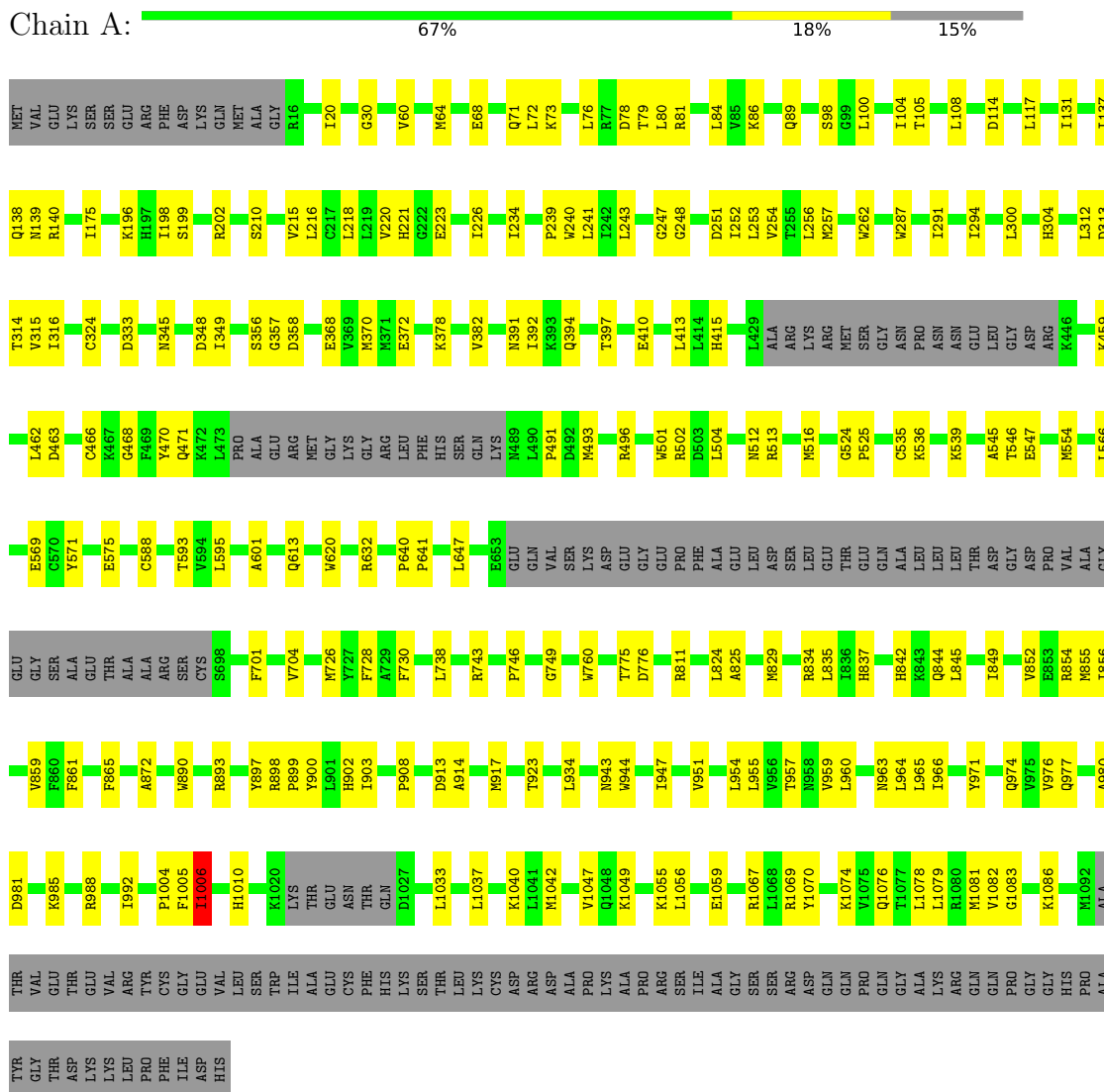


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total 30	C 27	O 3	0
5	B	1	Total 30	C 27	O 3	0
5	C	1	Total 30	C 27	O 3	0
5	D	1	Total 30	C 27	O 3	0

3 Residue-property plots

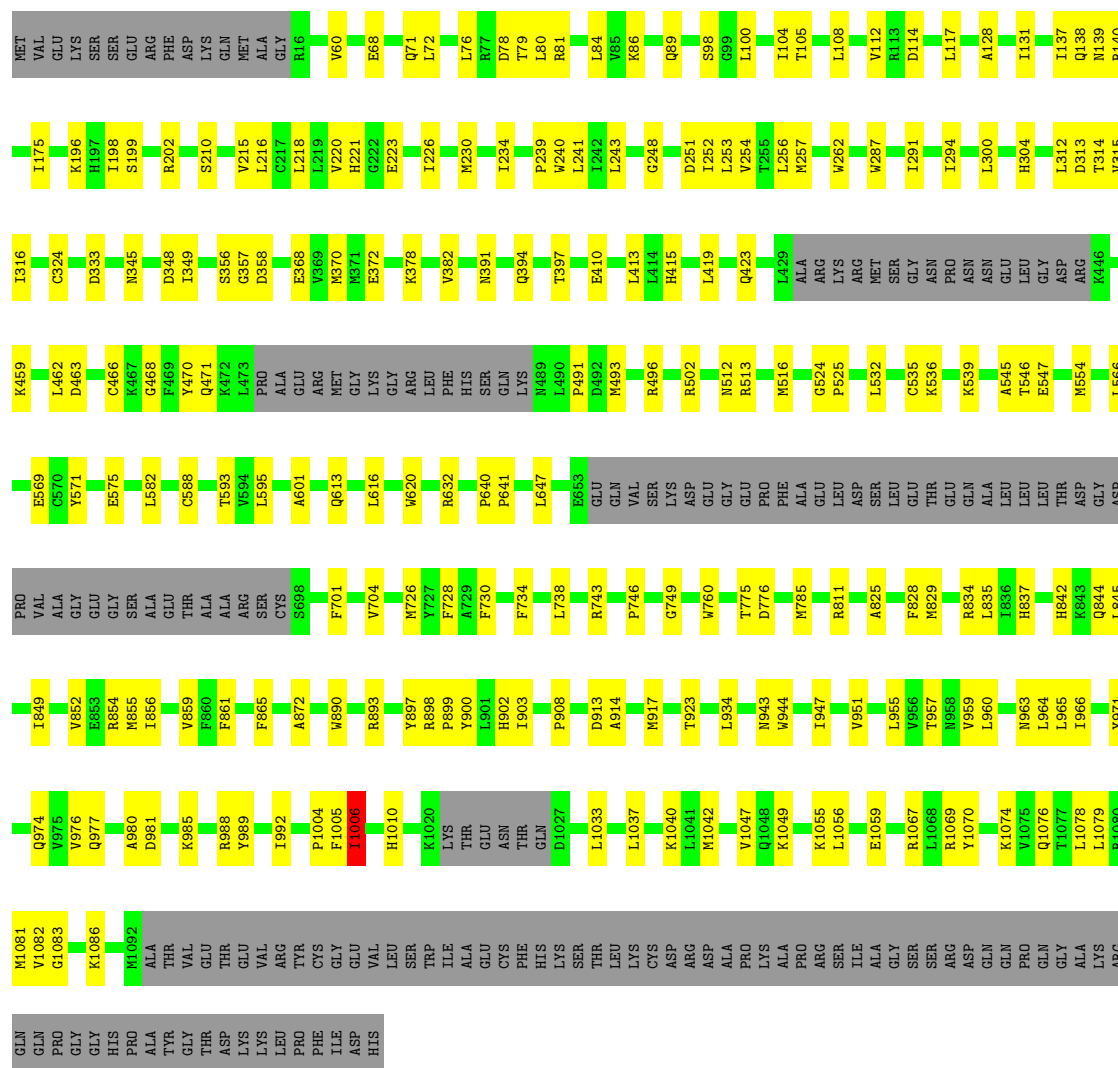
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Transient receptor potential melastatin 5



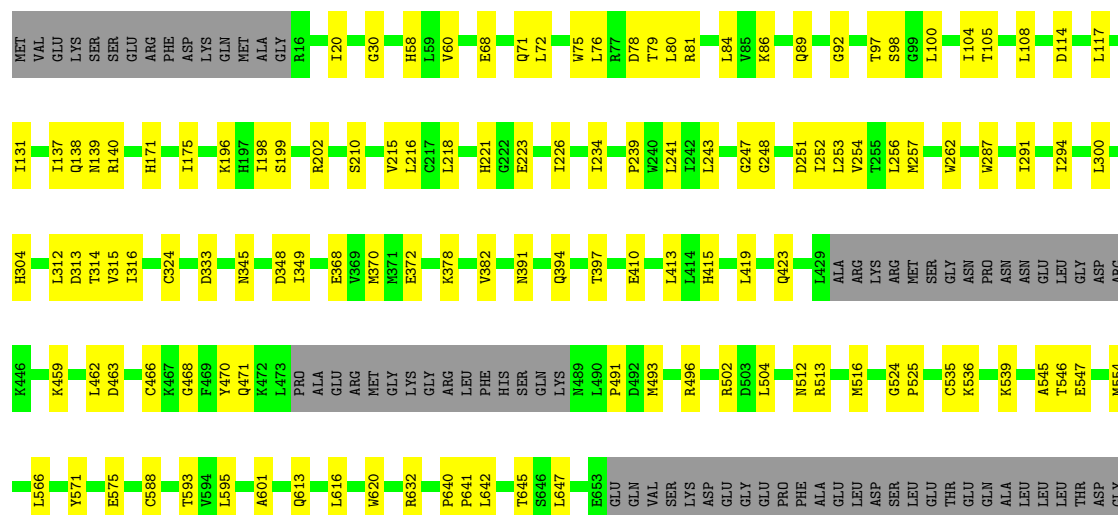
- Molecule 1: Transient receptor potential melastatin 5





• Molecule 1: Transient receptor potential melastatin 5

Chain C: 67% 19% 15%



LYS	ARG	GLN	GLN	PRO	GLY	GLY	HIS	PRO	ALA	TYR	GLY	THR	ASP	GLU	VAL	LEU	PRO	PHE	ILE	ASP	HIS
L1079	R1080	M1081	V1082	G1083	K1086	M1092	ALA	THR	VAL	GLU	THR	ASP	GLU	VAL	ARG	TYR	CYS	GLY	GLU	VAL	LEU
I966	Y971	Q974	V975	Q976	Q977	A980	D981	K985	R988	Y989	I992	P1004	F1005	I1006	H1010	K1020	LYS	THR	GLU	ASN	THR
K843	Q844	L845	I849	V852	E853	R854	M855	I856	V859	F860	F861	F865	A872	W890	R893	Y897	R898	P899	Y900	L901	H902
ASP	PRO	VAL	ALA	GLY	GLY	GLY	ALA	ALA	ALA	ARG	SER	CYS	S698	F701	V704	M726	Y727	F728	A729	F730	F734
																					L738
																					R743
																					P746
																					G749
																					W760
																					T763
																					T775
																					D776
																					M785
																					R811
																					A825
																					F828
																					M829
																					R834
																					L835
																					I836
																					H837
																					L964
																					L965

• Molecule 1: Transient receptor potential melastatin 5

Chain D:



LYS	L1079	Y971	Q844	GLY	M554	GLY	ASP	L300	L117	MET
ARG	R1080	Y971	L845	PRO	M554	ASP	ARG	L300	L117	VAL
GLN	M1081	Q974	L849	PRO	L566	ARG	ARG	H304	I131	GLU
GLN	V1082	Q975		ALA	L566					LYS
PRO	G1083	Q976		GLY	E569			L312	I137	SER
GLY		Q977	V852	GLY	E569			D313	Q138	SER
GLY	K1086	Q977	E853	GLU	C570			T314	N139	GLU
HIS		R854	R854	GLY	Y571			V315	R140	ARG
PRO	A980	M855	M855	SER	Y571			I316		PHE
ALA	D981	I856	I856	ALA	E575				I175	ASP
ALA				GLY				C324		LYS
THR	K985	V859	V859	THR	C588			D333	K196	GLN
GLY		F860	F860	ALA					H197	MET
THR	GLU	F861	F861	ALA	T593			D333		GLY
ASP	THR	R988	R988	ALA	T593			N345	S199	ALA
LYS	GLU	Y989	Y989	ARG	V594					GLY
LYS	VAL	R989	R989	SER	L595					
VAL	ARG	I992		CYS	L595			D348	R202	R16
LEU	LEU	I992	A872		A601			I349		
PRO	TYR	F1004			F701				S210	I20
PHE	CYS	F1005	W890		Q613			E368		G30
ILE	GLU	I1006	R893		L616			V369	V215	
ASP	VAL	H1010			W704			M370	L216	H58
HIS	LEU		Y897		M726			M371	C217	L59
	SER	K1020	R898		Y727			E372	L218	V60
TRP	ILE	LYS	P899		F728			K378	L219	
ALA	ALA	THR	Y900		A729			V220	H221	M64
GLU	GLU	GLU	L901		F730			V382	E223	E68
H902	ASN	ASN	H902		P640			N391	T226	Q71
PHE	THR	THR	I903		P641			I392	L227	L72
HIS	GLN	GLN	P908		L647			K393		K73
LYS	D1027	D1027						Q394		P74
SER	SER	L1033	D913		E653			LYS		W75
THR	THR	L1033	A914		R743				I234	L76
LYS	LYS	L1037			P746				P239	R77
CYS	CYS	L1037	M917		VAL			E410	W240	D78
ASP	ASP	K1040			SER			LYS	L241	T79
ARG	ARG	L1041	T923		G749			L413	I242	L80
ASP	ASP	M1042			ASP			L414	L243	R81
ALA	ALA		L934		W760			H415		
PRO	PRO	V1047			GLY				G247	L84
LYS	LYS	Q1048	N943		GLU			L419	G248	V85
ALA	ALA	K1049	W944		PRO			ARG		K86
PRO	PRO				PHE			Q423	D251	Q89
ARG	ARG	K1055	I947		ALA			L253	I252	
SER	SER	L1056			LEU			V254	L254	G92
ILE	ILE		V951		ASP			T255		
ALA	ALA	E1059			SER			ALA		S98
GLY	GLY		L955		LEU			LYS	M257	G99
SER	SER	R1067	V956		GLU			ARG		L100
SER	SER	L1068	T957		THR			MET		
ARG	ARG	R1069			GLY			SER	W262	I104
ASP	ASP	Y1070	V959		GLN			GLY		T105
GLN	GLN		L960		ALA			ASN	W287	L108
PRO	PRO	K1074	N963		LEU			ASN	I291	
GLN	GLN	V1075	L964		LEU			ASN		D114
GLY	GLY	Q1076	L965		THR			ASN	I294	
ALA	ALA	T1077	T966		ASP			LEU		
		L1078			THR			GLU		
					ASP			LEU		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139000	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (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: CA, NAG, YUV, YUY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/7784	0.37	0/10616
1	B	0.25	0/7784	0.37	0/10616
1	C	0.25	0/7784	0.37	0/10616
1	D	0.25	0/7784	0.37	0/10616
All	All	0.25	0/31136	0.37	0/42464

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	A	7591	0	7422	249	0
1	B	7591	0	7422	251	0
1	C	7591	0	7422	250	0
1	D	7591	0	7422	252	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	118	0	0	9	0
4	B	59	0	0	4	0
4	C	59	0	0	4	0
5	A	30	0	0	0	0
5	B	30	0	0	0	0
5	C	30	0	0	0	0
5	D	30	0	0	0	0
All	All	30780	0	29740	742	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 12.

The worst 5 of 742 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1083:GLY:CA	1:C:1081:MET:HE1	1.43	1.47
1:A:1083:GLY:CA	1:B:1081:MET:HE1	1.41	1.45
1:C:1083:GLY:CA	1:D:1081:MET:HE1	1.43	1.45
1:A:1081:MET:HE1	1:D:1083:GLY:CA	1.43	1.44
1:A:1078:LEU:HD11	1:D:1078:LEU:CD2	1.58	1.34

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	987/1165 (85%)	948 (96%)	38 (4%)	1 (0%)	48	48
1	B	987/1165 (85%)	949 (96%)	37 (4%)	1 (0%)	48	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	987/1165 (85%)	948 (96%)	38 (4%)	1 (0%)	48	48
1	D	987/1165 (85%)	948 (96%)	38 (4%)	1 (0%)	48	48
All	All	3948/4660 (85%)	3793 (96%)	151 (4%)	4 (0%)	49	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1006	ILE
1	B	1006	ILE
1	C	1006	ILE
1	D	1006	ILE

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	747/1017 (74%)	746 (100%)	1 (0%)	88	88
1	B	747/1017 (74%)	746 (100%)	1 (0%)	88	88
1	C	747/1017 (74%)	746 (100%)	1 (0%)	88	88
1	D	747/1017 (74%)	746 (100%)	1 (0%)	88	88
All	All	2988/4068 (74%)	2984 (100%)	4 (0%)	87	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1006	ILE
1	B	1006	ILE
1	C	1006	ILE
1	D	1006	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	723	ASN
1	D	71	GLN
1	C	842	HIS
1	C	990	ASN
1	D	391	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](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
4	YUY	A	1505	-	66,66,66	0.12	0	98,102,102	0.19	0
5	YUV	B	1503	-	35,35,35	0.11	0	58,58,58	0.18	0
5	YUV	C	1503	-	35,35,35	0.12	0	58,58,58	0.18	0
4	YUY	A	1503	-	66,66,66	0.12	0	98,102,102	0.19	0
4	YUY	C	1504	-	66,66,66	0.12	0	98,102,102	0.19	0
2	NAG	A	1501	1	14,14,15	0.29	0	17,19,21	0.59	0
5	YUV	D	1503	-	35,35,35	0.11	0	58,58,58	0.18	0
2	NAG	B	1501	1	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	C	1501	1	14,14,15	0.28	0	17,19,21	0.59	0
4	YUY	B	1504	-	66,66,66	0.12	0	98,102,102	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	YUV	A	1504	-	35,35,35	0.11	0	58,58,58	0.18	0
2	NAG	D	1501	1	14,14,15	0.29	0	17,19,21	0.59	0

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
4	YUY	A	1505	-	-	11/21/149/149	0/8/8/8
5	YUV	B	1503	-	-	-	0/6/6/6
5	YUV	C	1503	-	-	-	0/6/6/6
4	YUY	A	1503	-	-	11/21/149/149	0/8/8/8
4	YUY	C	1504	-	-	11/21/149/149	0/8/8/8
2	NAG	A	1501	1	-	3/6/23/26	0/1/1/1
5	YUV	D	1503	-	-	-	0/6/6/6
2	NAG	B	1501	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1501	1	-	3/6/23/26	0/1/1/1
4	YUY	B	1504	-	-	11/21/149/149	0/8/8/8
5	YUV	A	1504	-	-	-	0/6/6/6
2	NAG	D	1501	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	NAG	O7-C7-N2-C2
2	B	1501	NAG	O7-C7-N2-C2
2	C	1501	NAG	O7-C7-N2-C2
2	D	1501	NAG	O7-C7-N2-C2
4	A	1503	YUY	C43-C29-C30-O3

There are no ring outliers.

4 monomers are involved in 17 short contacts:

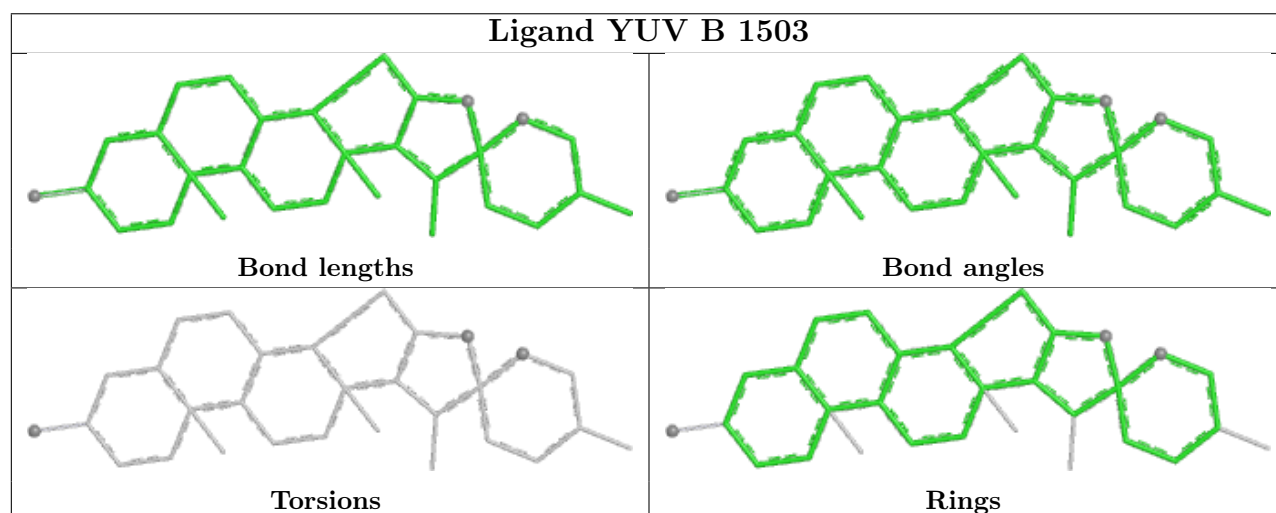
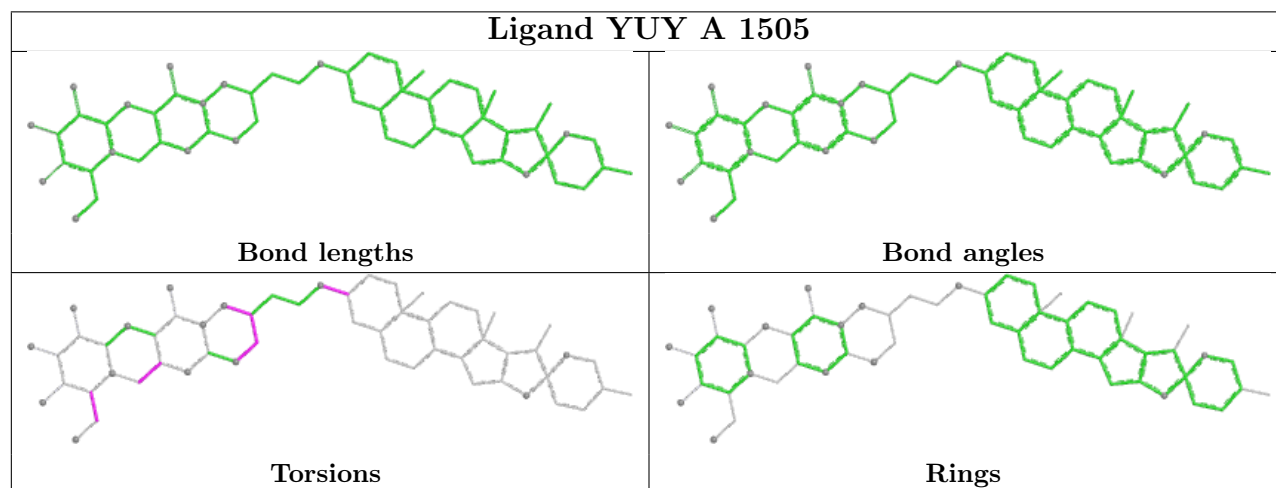
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1505	YUY	5	0

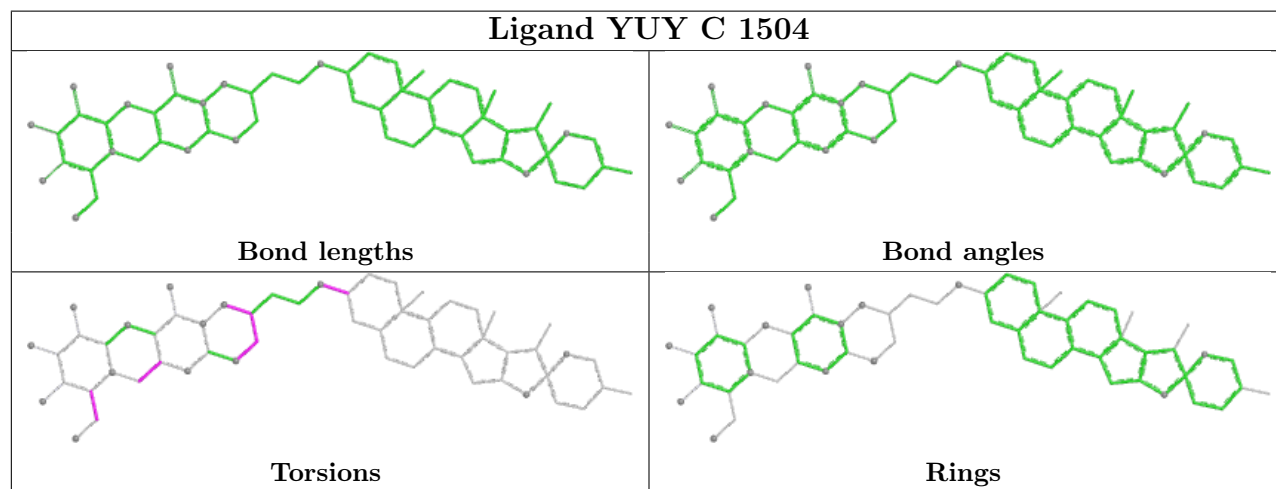
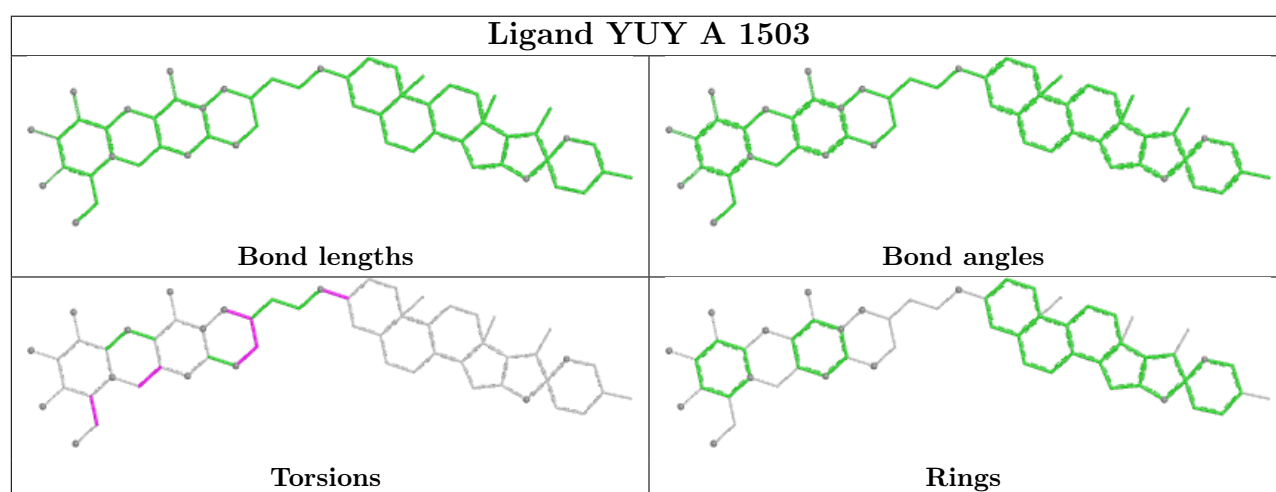
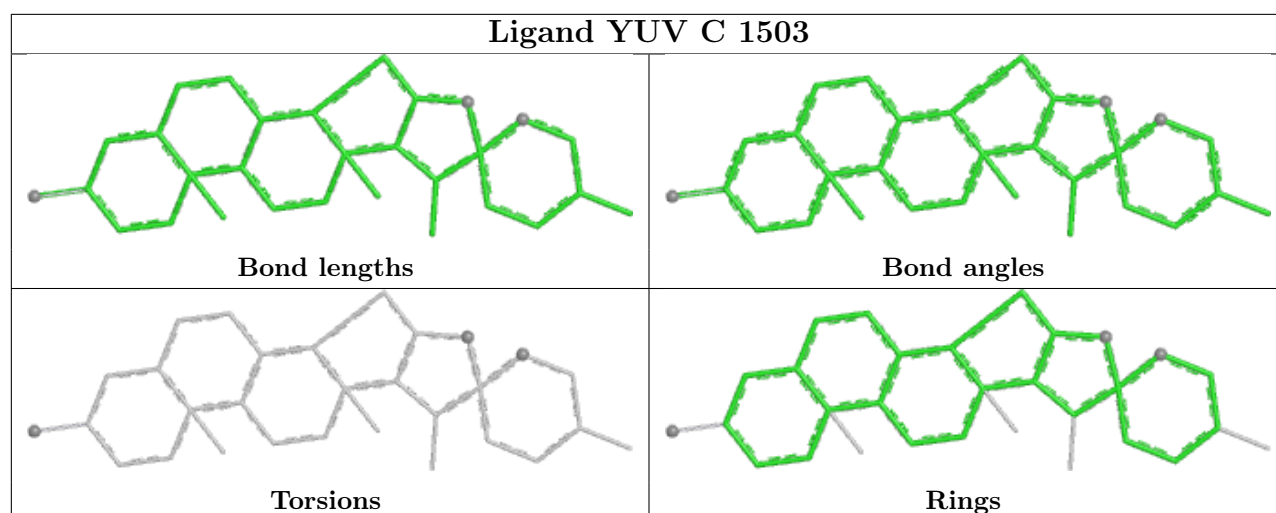
Continued on next page...

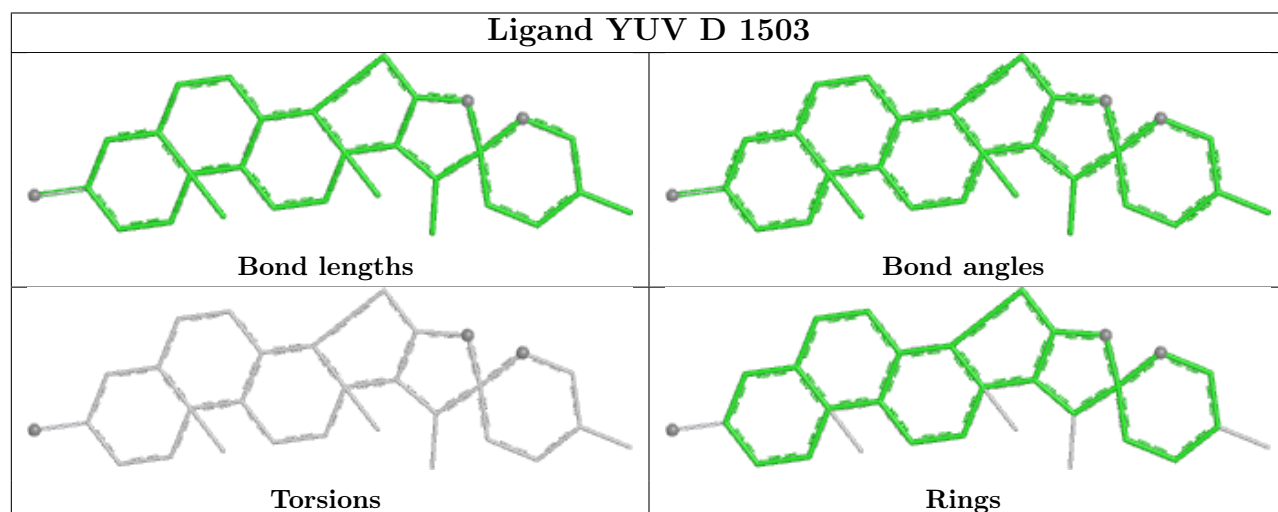
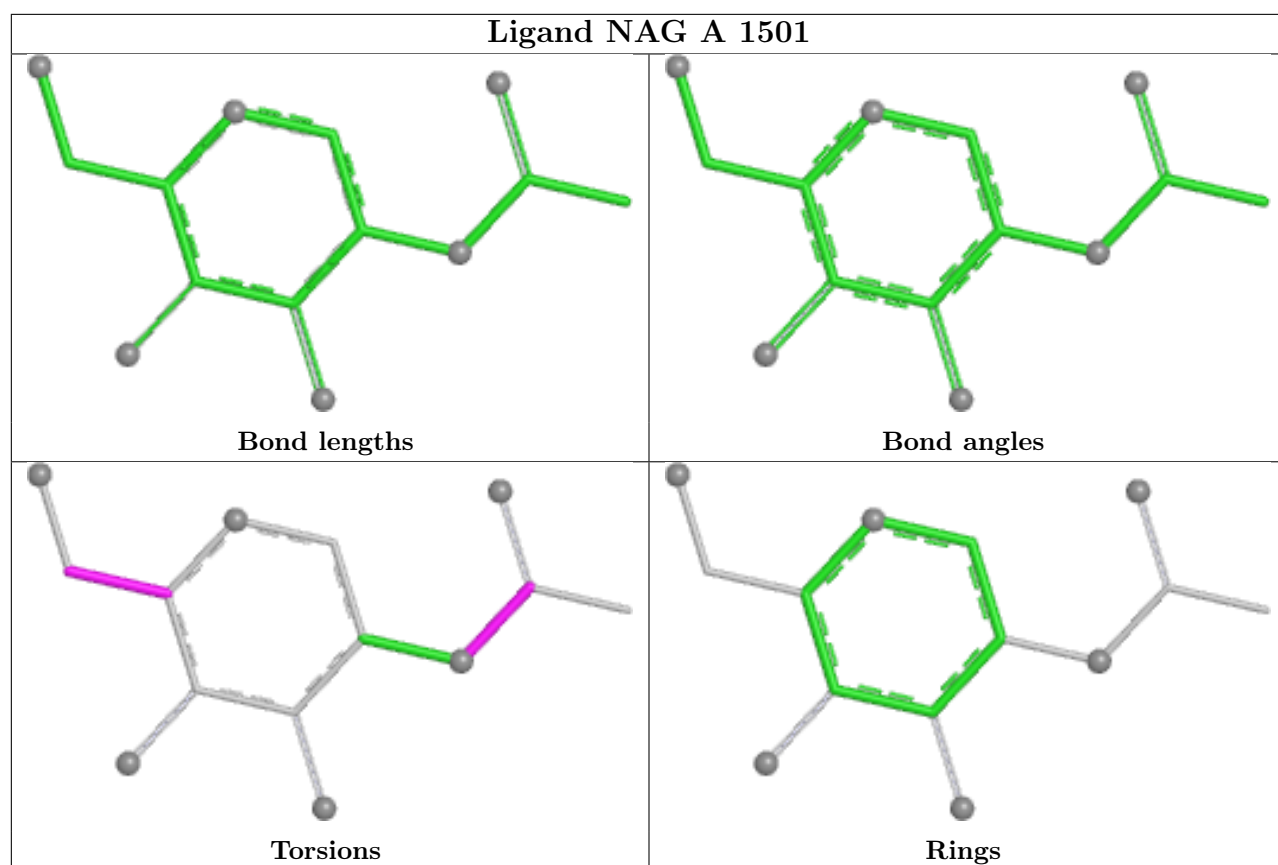
Continued from previous page...

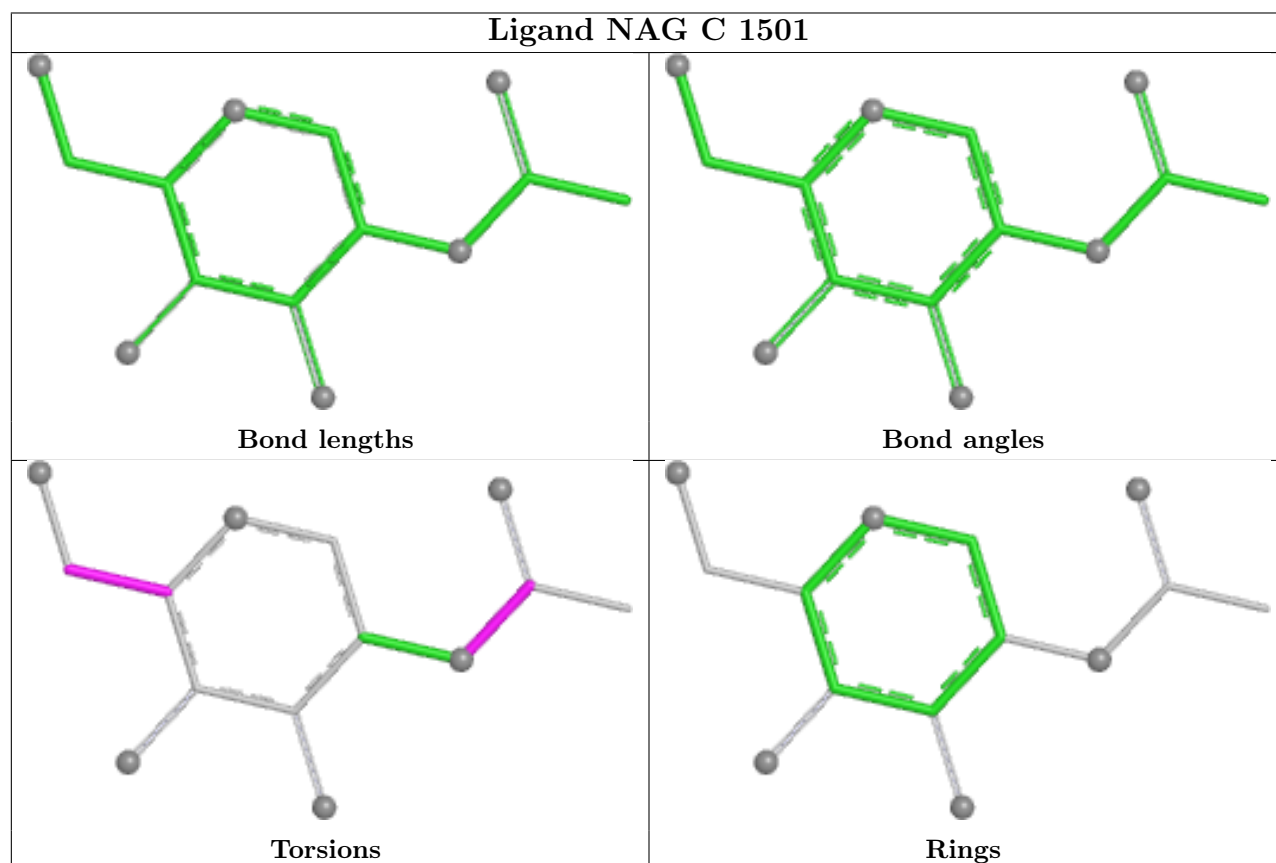
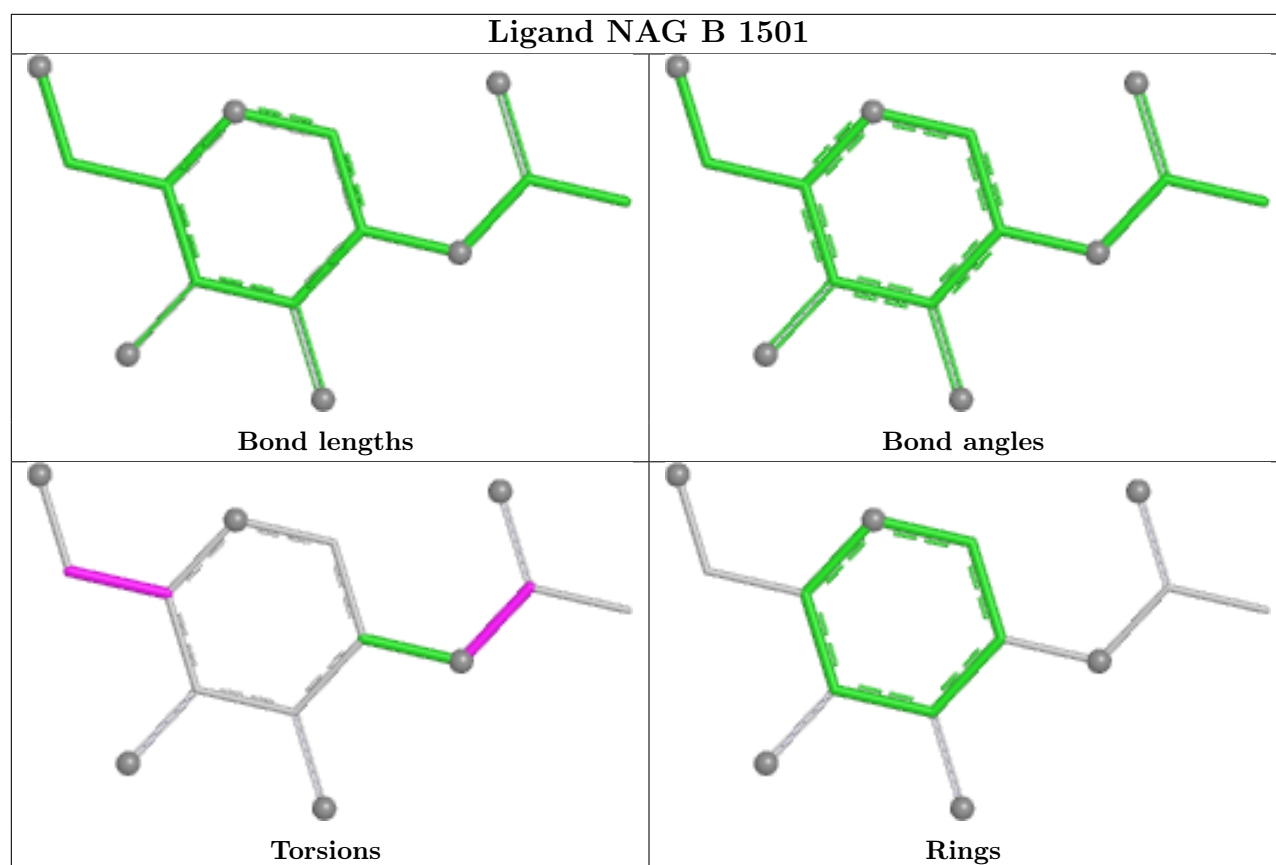
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1503	YUY	4	0
4	C	1504	YUY	4	0
4	B	1504	YUY	4	0

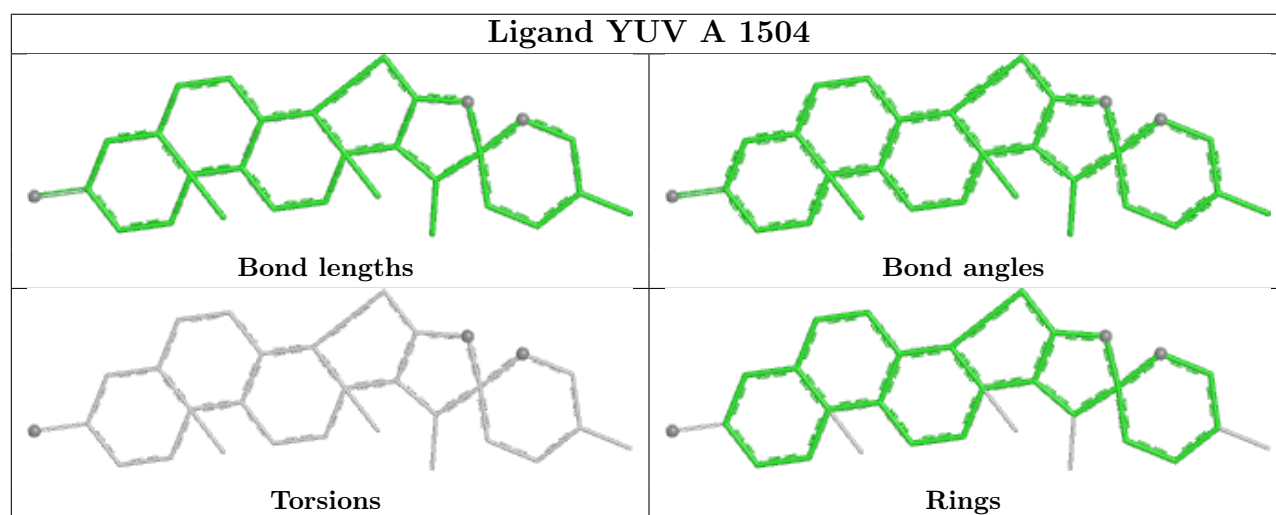
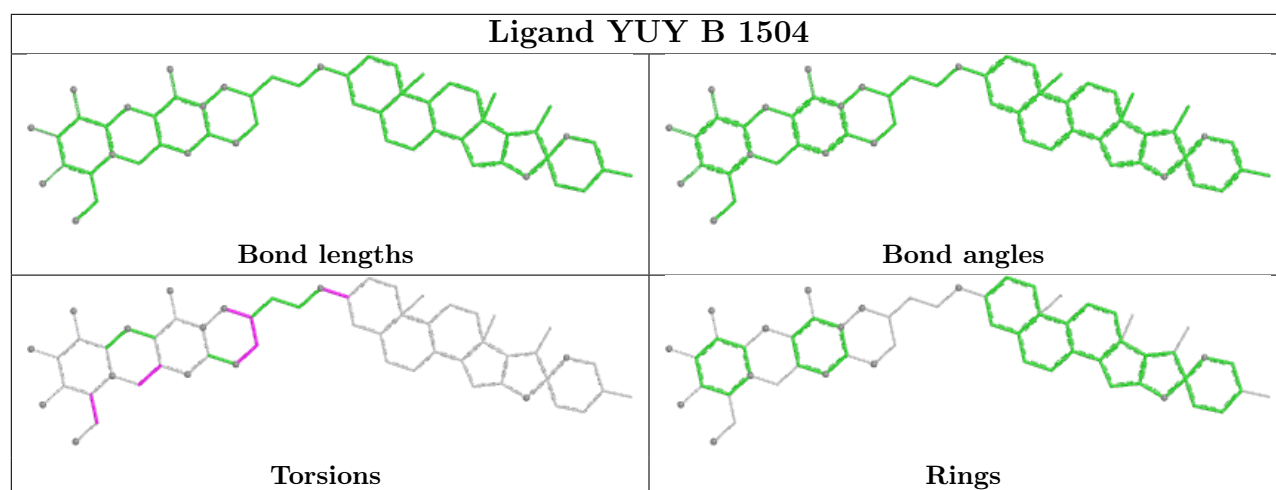
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

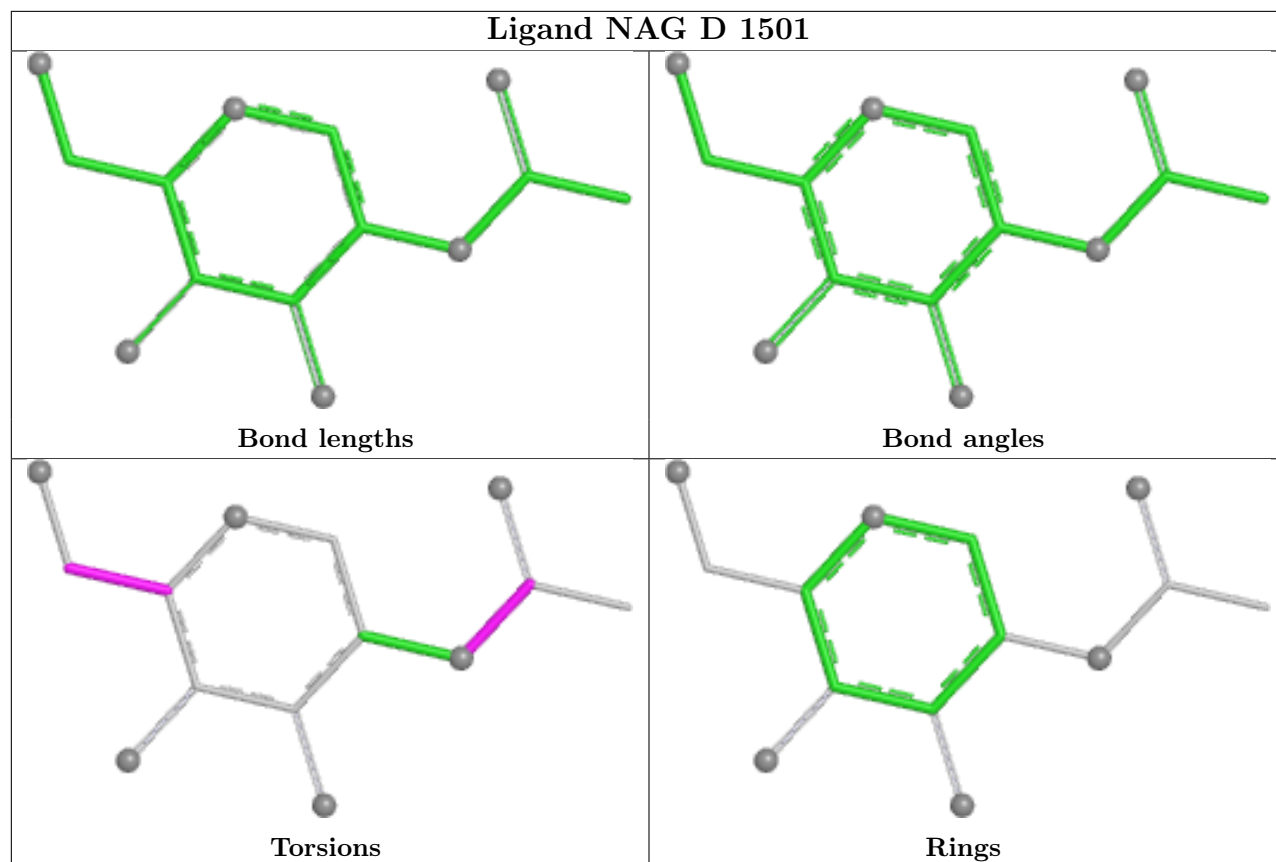












5.7 Other polymers [i](#)

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-23747. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal 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.