



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 08:57 am BST

PDB ID : 6PXA
Title : The crystal structure of chloramphenicol acetyltransferase-like protein from *Vibrio fischeri* ES114 in complex with taurocholic acid
Authors : Tan, K.; Maltseva, N.; Jedrzejczak, R.; Kuhn, M.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2019-07-25
Resolution : 1.82 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

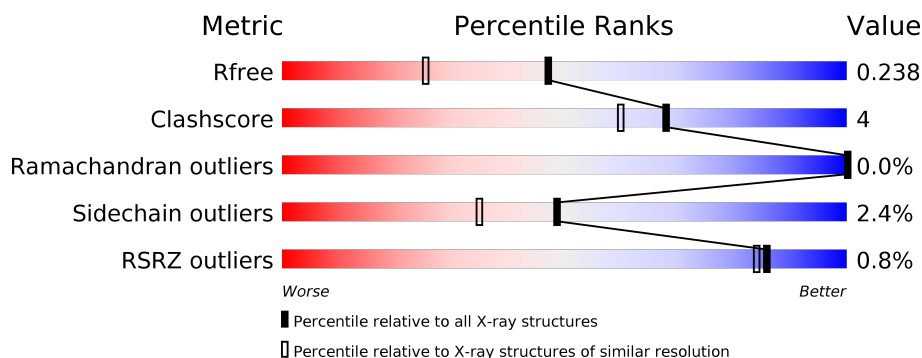
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	221	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 8%, green 90%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 90% 8% . </div> </div>
1	B	221	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 12%, green 86%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 86% 12% . </div> </div>
1	C	221	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 11%, green 88%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 88% 11% . </div> </div>
1	D	221	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 6%, green 91%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 91% 6% . </div> </div>
1	E	221	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 86%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 86% 12% . </div> </div>
1	F	221	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 8%, green 90%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 90% 8% . </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	221	 2% 89% 10%
1	H	221	 89% 8% ..
1	I	221	 2% 88% 11% .
1	J	221	 % 86% 13% .
1	K	221	 88% 11%
1	L	221	 % 87% 10% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	FMT	J	307	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22056 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Chloramphenicol acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	2	0
			1739	1114	293	324	8			
1	B	220	Total	C	N	O	S	0	4	0
			1774	1136	297	333	8			
1	C	219	Total	C	N	O	S	0	1	0
			1732	1109	290	325	8			
1	D	215	Total	C	N	O	S	0	0	0
			1702	1093	286	316	7			
1	E	221	Total	C	N	O	S	0	0	0
			1741	1115	293	325	8			
1	F	217	Total	C	N	O	S	0	1	0
			1711	1097	288	319	7			
1	G	220	Total	C	N	O	S	0	0	0
			1734	1111	292	323	8			
1	H	216	Total	C	N	O	S	0	0	0
			1702	1093	284	318	7			
1	I	221	Total	C	N	O	S	0	0	0
			1744	1116	293	327	8			
1	J	218	Total	C	N	O	S	0	0	0
			1720	1104	289	319	8			
1	K	220	Total	C	N	O	S	0	0	0
			1735	1112	292	323	8			
1	L	217	Total	C	N	O	S	0	0	0
			1715	1102	287	318	8			

There are 36 discrepancies between the modelled and reference sequences:

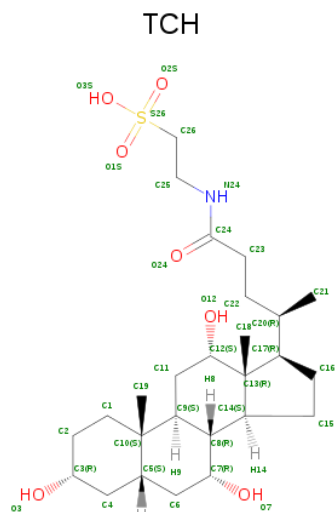
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5DZD6
A	-1	ASN	-	expression tag	UNP Q5DZD6
A	0	ALA	-	expression tag	UNP Q5DZD6
B	-2	SER	-	expression tag	UNP Q5DZD6
B	-1	ASN	-	expression tag	UNP Q5DZD6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP Q5DZD6
C	-2	SER	-	expression tag	UNP Q5DZD6
C	-1	ASN	-	expression tag	UNP Q5DZD6
C	0	ALA	-	expression tag	UNP Q5DZD6
D	-2	SER	-	expression tag	UNP Q5DZD6
D	-1	ASN	-	expression tag	UNP Q5DZD6
D	0	ALA	-	expression tag	UNP Q5DZD6
E	-2	SER	-	expression tag	UNP Q5DZD6
E	-1	ASN	-	expression tag	UNP Q5DZD6
E	0	ALA	-	expression tag	UNP Q5DZD6
F	-2	SER	-	expression tag	UNP Q5DZD6
F	-1	ASN	-	expression tag	UNP Q5DZD6
F	0	ALA	-	expression tag	UNP Q5DZD6
G	-2	SER	-	expression tag	UNP Q5DZD6
G	-1	ASN	-	expression tag	UNP Q5DZD6
G	0	ALA	-	expression tag	UNP Q5DZD6
H	-2	SER	-	expression tag	UNP Q5DZD6
H	-1	ASN	-	expression tag	UNP Q5DZD6
H	0	ALA	-	expression tag	UNP Q5DZD6
I	-2	SER	-	expression tag	UNP Q5DZD6
I	-1	ASN	-	expression tag	UNP Q5DZD6
I	0	ALA	-	expression tag	UNP Q5DZD6
J	-2	SER	-	expression tag	UNP Q5DZD6
J	-1	ASN	-	expression tag	UNP Q5DZD6
J	0	ALA	-	expression tag	UNP Q5DZD6
K	-2	SER	-	expression tag	UNP Q5DZD6
K	-1	ASN	-	expression tag	UNP Q5DZD6
K	0	ALA	-	expression tag	UNP Q5DZD6
L	-2	SER	-	expression tag	UNP Q5DZD6
L	-1	ASN	-	expression tag	UNP Q5DZD6
L	0	ALA	-	expression tag	UNP Q5DZD6

- Molecule 2 is TAUROCHOLIC ACID (three-letter code: TCH) (formula: $C_{26}H_{45}NO_7S$) (labeled as "Ligand of Interest" by author).

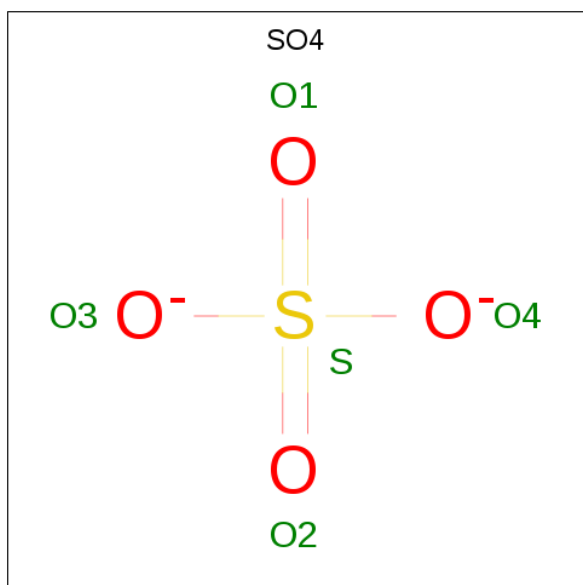


Id	Chain	Residues	Atoms					ZeroOcc	AltCon
2	A	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	B	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	C	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	D	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	E	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	F	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	G	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	H	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	I	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	J	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	K	1	Total 35	C 26	N 1	O 7	S 1	0	0
2	L	1	Total 35	C 26	N 1	O 7	S 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Cl 3 3	0	0
3	J	2	Total Cl 2 2	0	0
3	D	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	L	2	Total Cl 2 2	0	0
3	F	2	Total Cl 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



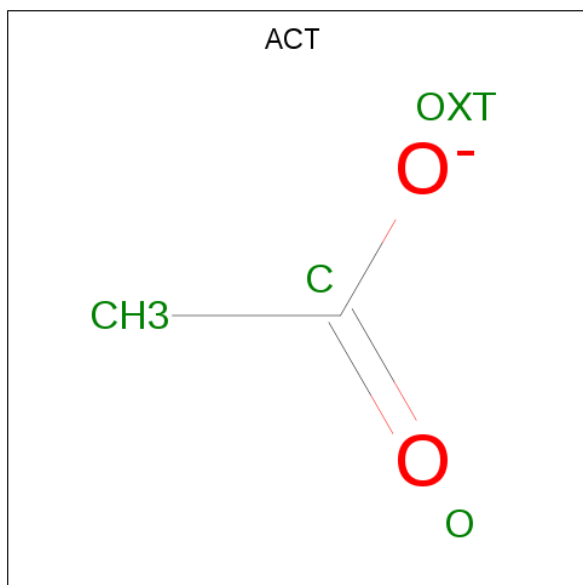
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



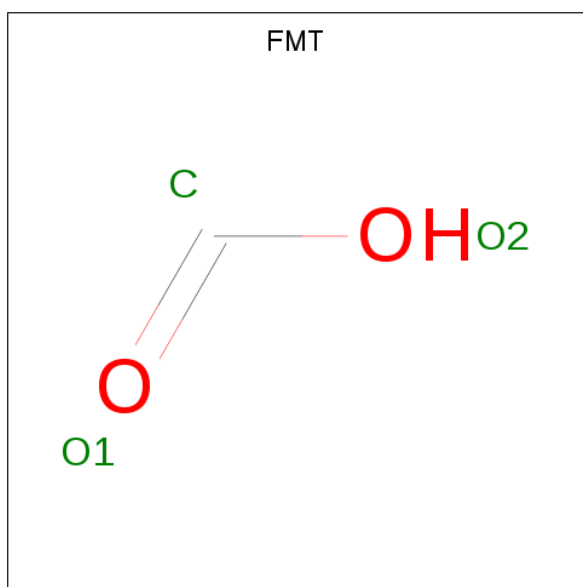
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	J	1	Total	C	O	0	0
			3	1	2		
7	J	1	Total	C	O	0	0
			3	1	2		
7	J	1	Total	C	O	0	0
			3	1	2		
7	J	1	Total	C	O	0	0
			3	1	2		
7	K	1	Total	C	O	0	0
			3	1	2		
7	K	1	Total	C	O	0	0
			3	1	2		
7	K	1	Total	C	O	0	0
			3	1	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	73	Total	O	0	0
			73	73		
8	B	67	Total	O	0	0
			67	67		
8	C	66	Total	O	0	0
			66	66		
8	D	60	Total	O	0	0
			60	60		
8	E	51	Total	O	0	0
			51	51		

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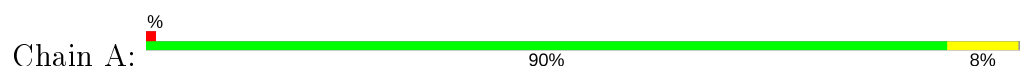
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	64	Total 64	O 64	0	0
8	G	74	Total 74	O 74	0	0
8	H	74	Total 74	O 74	0	0
8	I	54	Total 54	O 54	0	0
8	J	61	Total 61	O 61	0	0
8	K	59	Total 59	O 59	0	0
8	L	73	Total 73	O 73	0	0

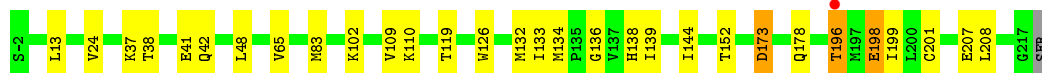
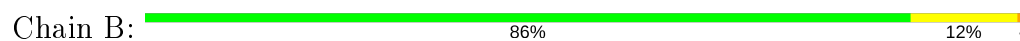
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

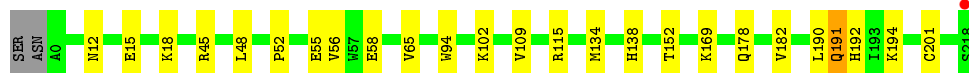
- Molecule 1: Chloramphenicol acetyltransferase



- Molecule 1: Chloramphenicol acetyltransferase



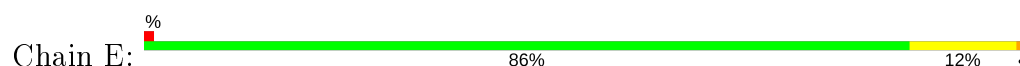
- Molecule 1: Chloramphenicol acetyltransferase




- Molecule 1: Chloramphenicol acetyltransferase

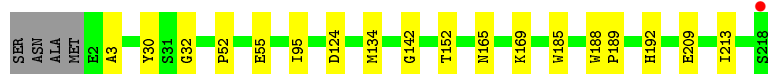


- Molecule 1: Chloramphenicol acetyltransferase

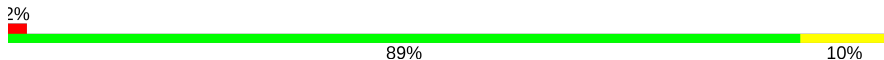


- Molecule 1: Chloramphenicol acetyltransferase

Chain F:  90% 8% .



- Molecule 1: Chloramphenicol acetyltransferase

Chain G:  89% 10% 2%




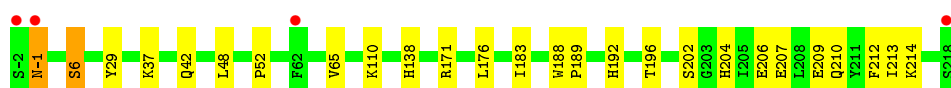
- Molecule 1: Chloramphenicol acetyltransferase

Chain H:  89% 8% ..




- Molecule 1: Chloramphenicol acetyltransferase

Chain I:  88% 11% 2%



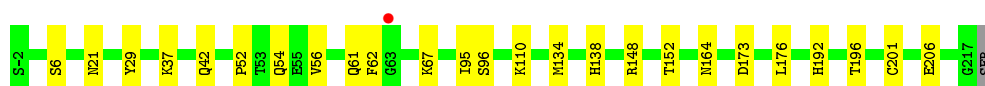
- Molecule 1: Chloramphenicol acetyltransferase

Chain J:  86% 13% .




- Molecule 1: Chloramphenicol acetyltransferase

Chain K:  88% 11%



- Molecule 1: Chloramphenicol acetyltransferase

Chain L:  87% 10% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.52Å 121.36Å 146.17Å 89.40° 89.91° 87.60°	Depositor
Resolution (Å)	46.90 – 1.82 46.90 – 1.81	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.90-1.82) 89.0 (46.90-1.81)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.197 , 0.238 0.197 , 0.238	Depositor DCC
R_{free} test set	12605 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l 0.014 for -h,k,-l 0.074 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22056	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0553e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, CL, FMT, SO4, TCH, ACT

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	0.44	0/1782	0.58	0/2410
1	B	0.45	0/1819	0.58	0/2463
1	C	0.47	0/1775	0.58	0/2402
1	D	0.45	0/1745	0.58	0/2361
1	E	0.46	0/1784	0.60	0/2413
1	F	0.47	0/1754	0.59	0/2375
1	G	0.48	0/1777	0.60	0/2404
1	H	0.47	0/1745	0.57	0/2363
1	I	0.47	0/1787	0.60	0/2417
1	J	0.47	0/1763	0.60	0/2385
1	K	0.47	0/1778	0.59	1/2405 (0.0%)
1	L	0.46	0/1758	0.59	0/2378
All	All	0.46	0/21267	0.59	1/28776 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	148	ARG	NE-CZ-NH1	-5.96	117.32	120.30

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	1739	0	1681	15	0
1	B	1774	0	1701	26	0
1	C	1732	0	1670	12	0
1	D	1702	0	1649	8	0
1	E	1741	0	1686	20	0
1	F	1711	0	1645	9	0
1	G	1734	0	1679	13	0
1	H	1702	0	1633	14	0
1	I	1744	0	1688	15	0
1	J	1720	0	1668	19	0
1	K	1735	0	1681	13	0
1	L	1715	0	1660	16	0
2	A	35	0	45	2	0
2	B	35	0	45	0	0
2	C	35	0	45	0	0
2	D	35	0	45	1	0
2	E	35	0	45	0	0
2	F	35	0	45	1	0
2	G	35	0	45	2	0
2	H	35	0	45	2	0
2	I	35	0	45	1	0
2	J	35	0	45	2	0
2	K	35	0	45	1	0
2	L	35	0	45	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	K	1	0	0	0	0
3	L	2	0	0	0	0
4	A	5	0	0	0	0
4	G	5	0	0	0	0
4	J	10	0	0	0	0
5	A	8	0	6	0	0
5	G	4	0	3	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	6	0	8	0	0
6	F	6	0	8	0	0
6	H	6	0	8	0	0
6	I	6	0	8	0	0
7	J	12	0	4	3	0
7	K	9	0	3	1	0
8	A	73	0	0	1	0
8	B	67	0	0	2	0
8	C	66	0	0	0	0
8	D	60	0	0	1	0
8	E	51	0	0	2	0
8	F	64	0	0	0	0
8	G	74	0	0	0	0
8	H	74	0	0	1	0
8	I	54	0	0	0	0
8	J	61	0	0	0	0
8	K	59	0	0	0	0
8	L	73	0	0	0	0
All	All	22056	0	20653	159	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 4.

The worst 5 of 159 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:L:196:THR:HG22	1:L:199:ILE:HD12	1.68	0.75
1:B:37:LYS:HB3	1:B:41:GLU:HG3	1.70	0.74
1:B:83:MET:HG3	1:B:134:MET:HE1	1.73	0.70
1:B:132:MET:SD	1:B:134:MET:HE1	2.32	0.69
1:C:48:LEU:HD12	1:C:65:VAL:HG11	1.75	0.69

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 X-ray entries followed by that with respect to entries of similar resolution.

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	218/221 (99%)	211 (97%)	7 (3%)	0	100	100
1	B	222/221 (100%)	214 (96%)	8 (4%)	0	100	100
1	C	218/221 (99%)	210 (96%)	8 (4%)	0	100	100
1	D	213/221 (96%)	201 (94%)	12 (6%)	0	100	100
1	E	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
1	F	216/221 (98%)	210 (97%)	5 (2%)	1 (0%)	29	15
1	G	218/221 (99%)	209 (96%)	9 (4%)	0	100	100
1	H	214/221 (97%)	207 (97%)	7 (3%)	0	100	100
1	I	219/221 (99%)	214 (98%)	5 (2%)	0	100	100
1	J	216/221 (98%)	209 (97%)	7 (3%)	0	100	100
1	K	218/221 (99%)	210 (96%)	8 (4%)	0	100	100
1	L	215/221 (97%)	207 (96%)	8 (4%)	0	100	100
All	All	2606/2652 (98%)	2514 (96%)	91 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	3	ALA

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 X-ray entries followed by that with respect to entries of similar resolution.

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	182/184 (99%)	177 (97%)	5 (3%)	44	30
1	B	186/184 (101%)	181 (97%)	5 (3%)	44	30
1	C	182/184 (99%)	175 (96%)	7 (4%)	33	18
1	D	179/184 (97%)	175 (98%)	4 (2%)	52	39
1	E	183/184 (100%)	177 (97%)	6 (3%)	38	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	179/184 (97%)	176 (98%)	3 (2%)	60	50
1	G	182/184 (99%)	179 (98%)	3 (2%)	62	53
1	H	177/184 (96%)	172 (97%)	5 (3%)	43	29
1	I	184/184 (100%)	179 (97%)	5 (3%)	44	30
1	J	180/184 (98%)	180 (100%)	0	100	100
1	K	182/184 (99%)	177 (97%)	5 (3%)	44	30
1	L	179/184 (97%)	175 (98%)	4 (2%)	52	39
All	All	2175/2208 (98%)	2123 (98%)	52 (2%)	49	35

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	173	ASP
1	F	169	LYS
1	L	38	THR
1	E	175	ASN
1	E	205	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 16 are monoatomic - leaving 33 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	$\# Z > 2$
7	FMT	K	305	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TCH	H	301	-	38,38,38	3.58	19 (50%)	59,60,60	1.76	10 (16%)
4	SO4	J	305	-	4,4,4	0.13	0	6,6,6	0.09	0
7	FMT	K	304	-	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	F	304	-	5,5,5	0.95	0	5,5,5	0.97	0
5	ACT	G	306	-	1,3,3	6.39	1 (100%)	0,3,3	0.00	-
2	TCH	B	301	-	38,38,38	3.54	19 (50%)	59,60,60	1.77	17 (28%)
6	GOL	H	302	-	5,5,5	0.99	0	5,5,5	0.87	0
4	SO4	J	304	-	4,4,4	0.14	0	6,6,6	0.09	0
5	ACT	A	304	-	1,3,3	6.41	1 (100%)	0,3,3	0.00	-
2	TCH	C	301	-	38,38,38	3.62	18 (47%)	59,60,60	1.79	13 (22%)
2	TCH	E	301	-	38,38,38	3.56	19 (50%)	59,60,60	1.93	11 (18%)
2	TCH	J	301	-	38,38,38	3.55	18 (47%)	59,60,60	1.78	14 (23%)
7	FMT	J	308	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TCH	D	301	-	38,38,38	3.59	18 (47%)	59,60,60	1.85	12 (20%)
6	GOL	B	303	-	5,5,5	0.78	0	5,5,5	1.15	0
6	GOL	C	303	-	5,5,5	0.89	0	5,5,5	1.00	0
7	FMT	J	306	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TCH	L	301	-	38,38,38	3.52	19 (50%)	59,60,60	1.82	14 (23%)
6	GOL	I	303	-	5,5,5	0.99	0	5,5,5	0.96	0
7	FMT	J	307	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TCH	I	301	-	38,38,38	3.55	18 (47%)	59,60,60	1.96	14 (23%)
6	GOL	D	303	-	5,5,5	0.74	0	5,5,5	1.09	0
2	TCH	G	301	-	38,38,38	3.65	19 (50%)	59,60,60	1.78	15 (25%)
2	TCH	A	301	-	38,38,38	3.55	16 (42%)	59,60,60	1.89	13 (22%)
2	TCH	F	301	-	38,38,38	3.65	19 (50%)	59,60,60	1.86	11 (18%)
4	SO4	A	303	-	4,4,4	0.15	0	6,6,6	0.06	0
6	GOL	E	303	-	5,5,5	1.07	0	5,5,5	0.71	0
7	FMT	K	303	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	J	309	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TCH	K	301	-	38,38,38	3.59	17 (44%)	59,60,60	1.88	14 (23%)
4	SO4	G	305	-	4,4,4	0.15	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	305	-	1,3,3	6.32	1 (100%)	0,3,3	0.00	-

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
2	TCH	A	301	-	-	0/16/81/81	0/4/4/4
2	TCH	C	301	-	-	2/16/81/81	0/4/4/4
2	TCH	L	301	-	-	0/16/81/81	0/4/4/4
6	GOL	I	303	-	-	2/4/4/4	-
2	TCH	H	301	-	-	2/16/81/81	0/4/4/4
2	TCH	E	301	-	-	1/16/81/81	0/4/4/4
2	TCH	J	301	-	-	0/16/81/81	0/4/4/4
2	TCH	D	301	-	-	2/16/81/81	0/4/4/4
6	GOL	D	303	-	-	2/4/4/4	-
6	GOL	F	304	-	-	2/4/4/4	-
2	TCH	F	301	-	-	3/16/81/81	0/4/4/4
6	GOL	B	303	-	-	4/4/4/4	-
2	TCH	B	301	-	-	0/16/81/81	0/4/4/4
2	TCH	I	301	-	-	2/16/81/81	0/4/4/4
6	GOL	H	302	-	-	2/4/4/4	-
2	TCH	K	301	-	-	2/16/81/81	1/4/4/4
6	GOL	C	303	-	-	2/4/4/4	-
6	GOL	E	303	-	-	3/4/4/4	-
2	TCH	G	301	-	-	1/16/81/81	0/4/4/4

The worst 5 of 222 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	TCH	C13-C14	-11.84	1.35	1.55
2	F	301	TCH	C13-C14	-11.80	1.35	1.55
2	E	301	TCH	C13-C14	-11.67	1.35	1.55
2	D	301	TCH	C13-C14	-11.64	1.35	1.55
2	C	301	TCH	C13-C14	-11.60	1.35	1.55

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	TCH	C17-C13-C12	6.67	123.75	117.67
2	C	301	TCH	C17-C13-C12	6.53	123.62	117.67
2	E	301	TCH	C15-C14-C8	-6.37	109.43	118.33
2	D	301	TCH	C15-C14-C8	-6.22	109.64	118.33
2	L	301	TCH	C15-C14-C8	-6.12	109.78	118.33

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	303	GOL	O1-C1-C2-C3
6	F	304	GOL	O1-C1-C2-C3
6	B	303	GOL	C1-C2-C3-O3
6	C	303	GOL	O1-C1-C2-C3
6	D	303	GOL	O1-C1-C2-O2

All (1) ring outliers are listed below:

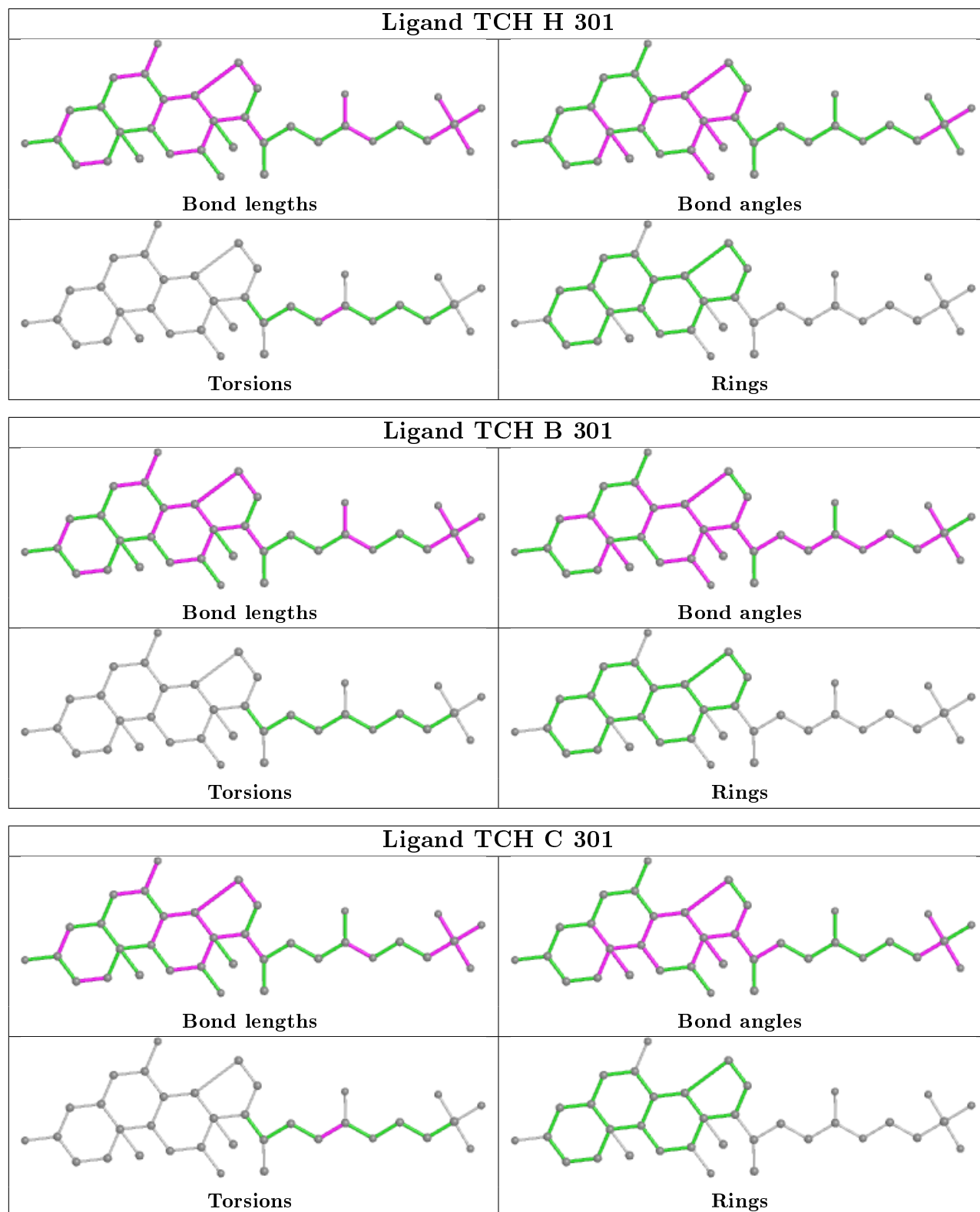
Mol	Chain	Res	Type	Atoms
2	K	301	TCH	C1-C10-C2-C3-C4-C5

11 monomers are involved in 16 short contacts:

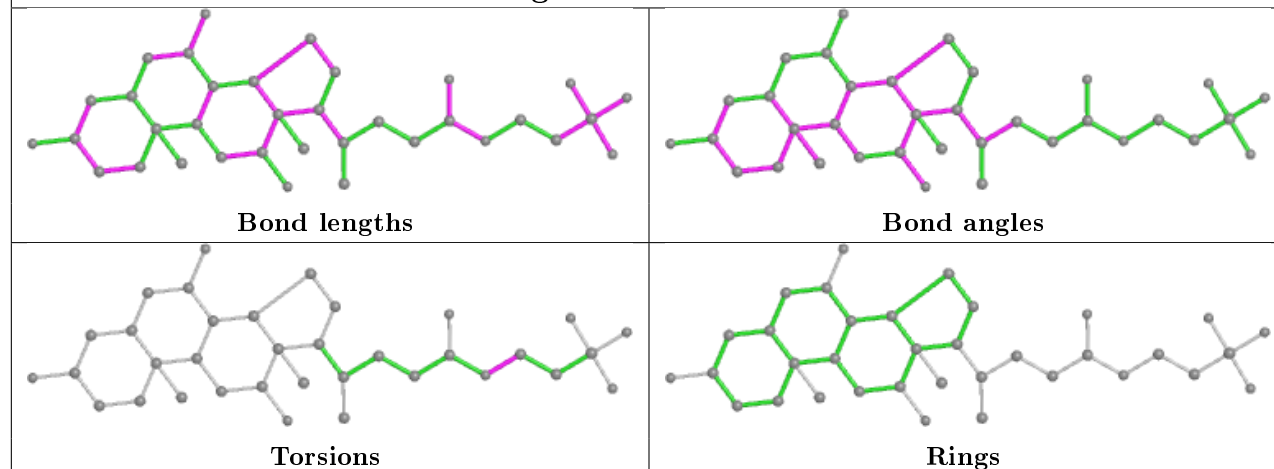
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	305	FMT	1	0
2	H	301	TCH	2	0
2	J	301	TCH	2	0
7	J	308	FMT	1	0
2	D	301	TCH	1	0
7	J	307	FMT	2	0
2	I	301	TCH	1	0
2	G	301	TCH	2	0
2	A	301	TCH	2	0
2	F	301	TCH	1	0
2	K	301	TCH	1	0

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

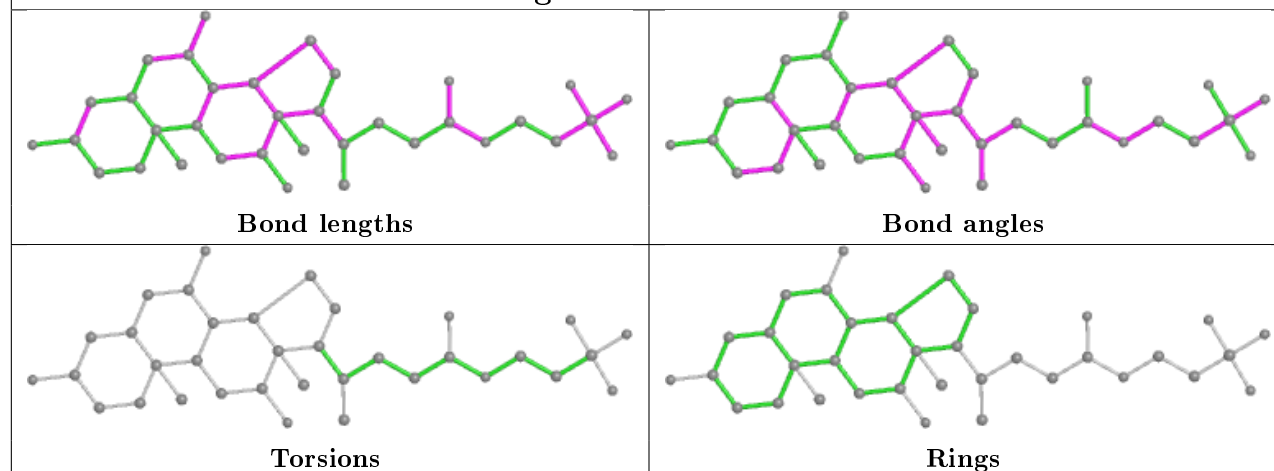
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



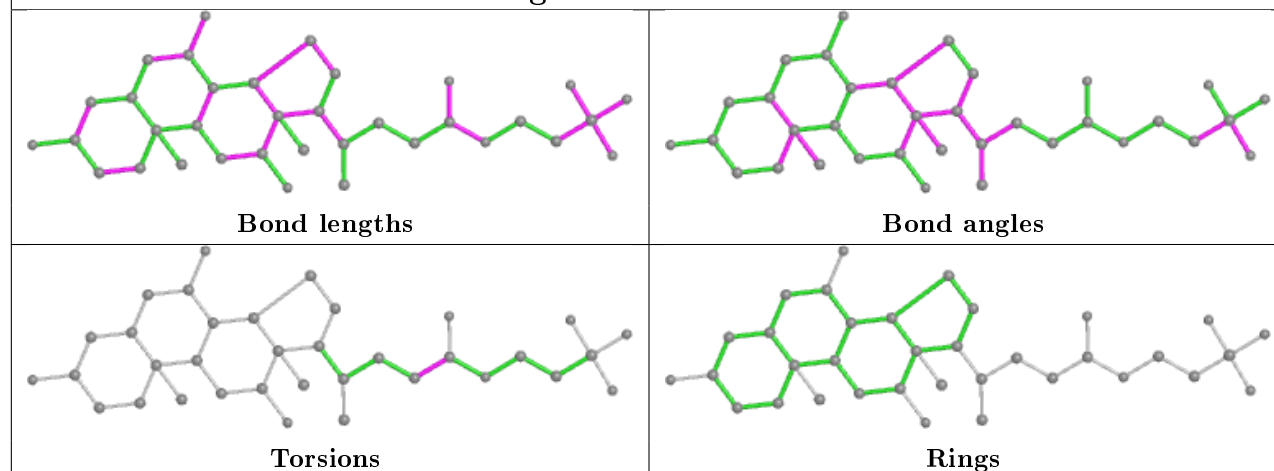
Ligand TCH E 301



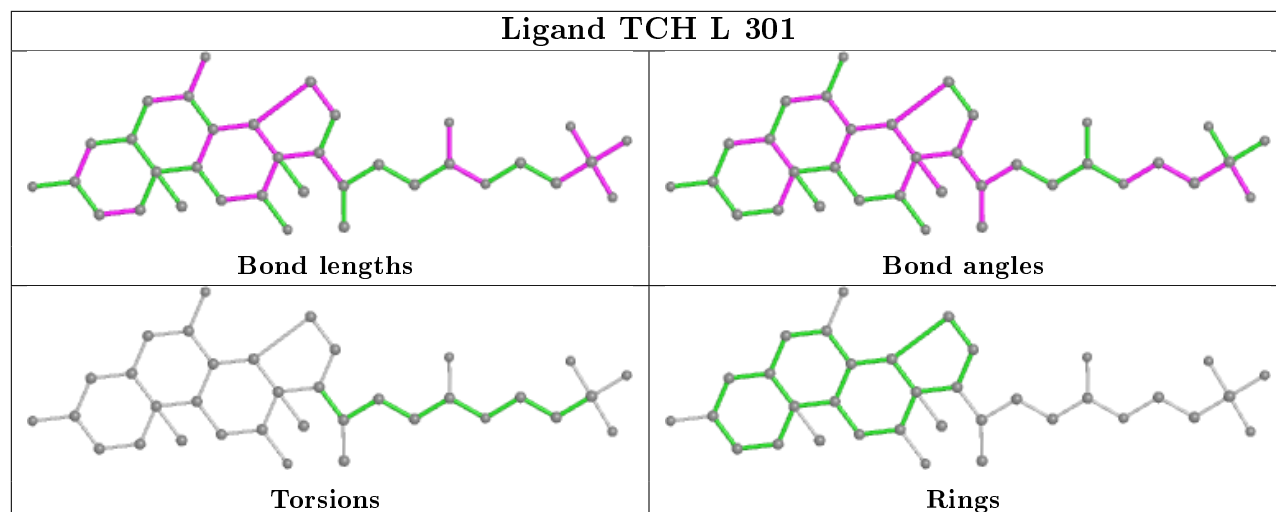
Ligand TCH J 301



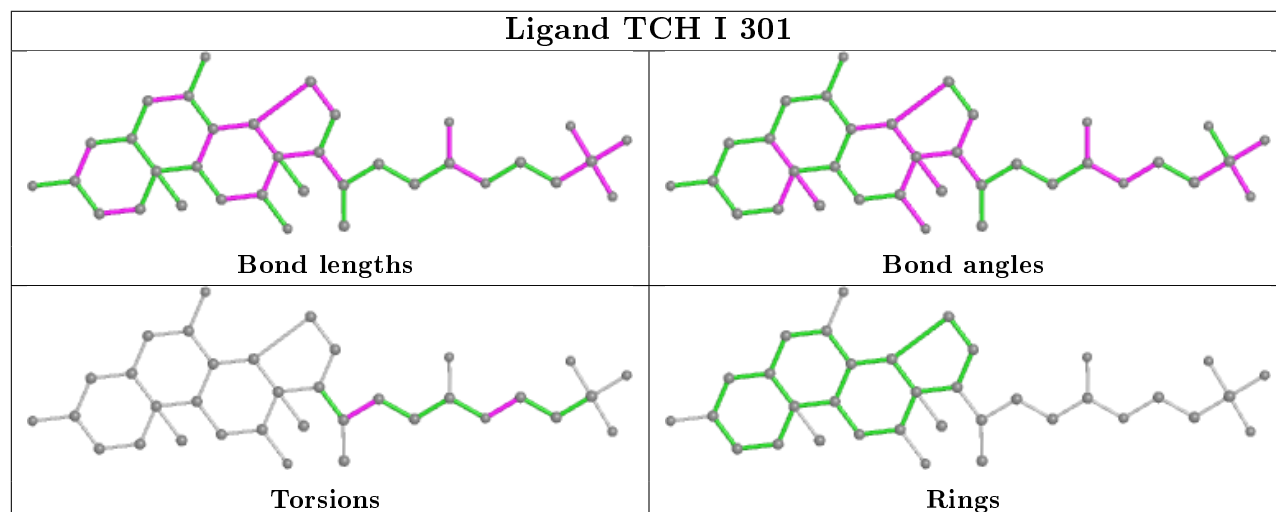
Ligand TCH D 301



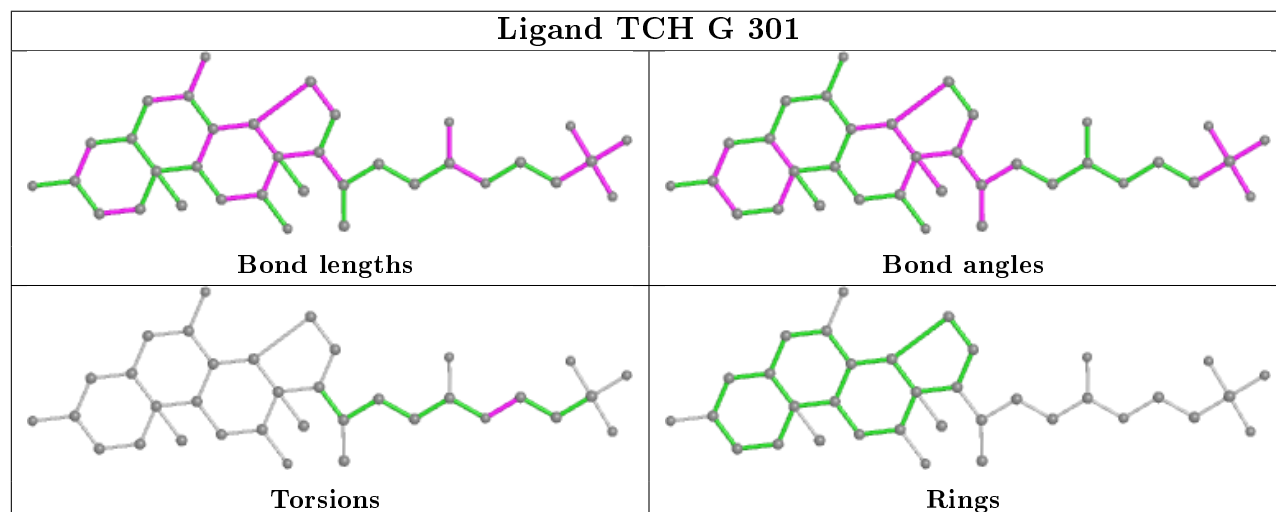
Ligand TCH L 301

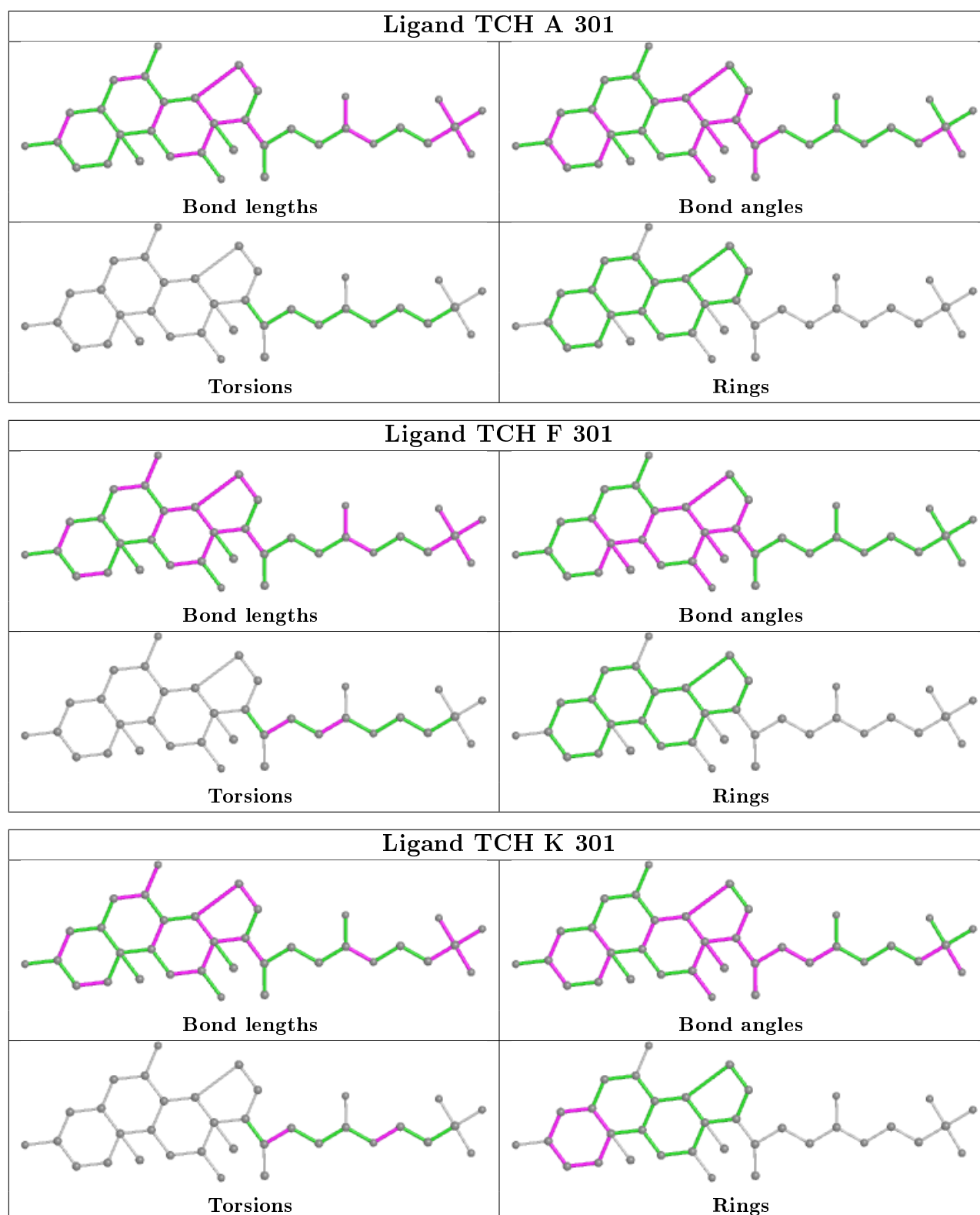


Ligand TCH I 301



Ligand TCH G 301





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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/221 (98%)	-0.28	3 (1%) 75 72	33, 46, 89, 132	0
1	B	220/221 (99%)	-0.31	1 (0%) 91 89	33, 46, 76, 98	0
1	C	219/221 (99%)	-0.36	1 (0%) 91 89	32, 45, 76, 104	0
1	D	215/221 (97%)	-0.33	1 (0%) 91 89	34, 47, 78, 111	0
1	E	221/221 (100%)	-0.21	2 (0%) 84 82	35, 50, 81, 127	0
1	F	217/221 (98%)	-0.37	1 (0%) 91 89	32, 45, 78, 128	0
1	G	220/221 (99%)	-0.30	4 (1%) 68 64	33, 44, 81, 119	0
1	H	216/221 (97%)	-0.31	0 100 100	34, 46, 71, 117	0
1	I	221/221 (100%)	-0.26	4 (1%) 68 64	33, 47, 86, 121	0
1	J	218/221 (98%)	-0.34	2 (0%) 84 82	29, 42, 77, 115	0
1	K	220/221 (99%)	-0.30	1 (0%) 91 89	32, 48, 79, 106	0
1	L	217/221 (98%)	-0.24	2 (0%) 84 82	33, 50, 84, 141	0
All	All	2622/2652 (98%)	-0.30	22 (0%) 86 84	29, 46, 81, 141	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	10.3
1	I	-2	SER	7.5
1	J	0	ALA	6.8
1	A	0	ALA	5.9
1	L	1	MET	5.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

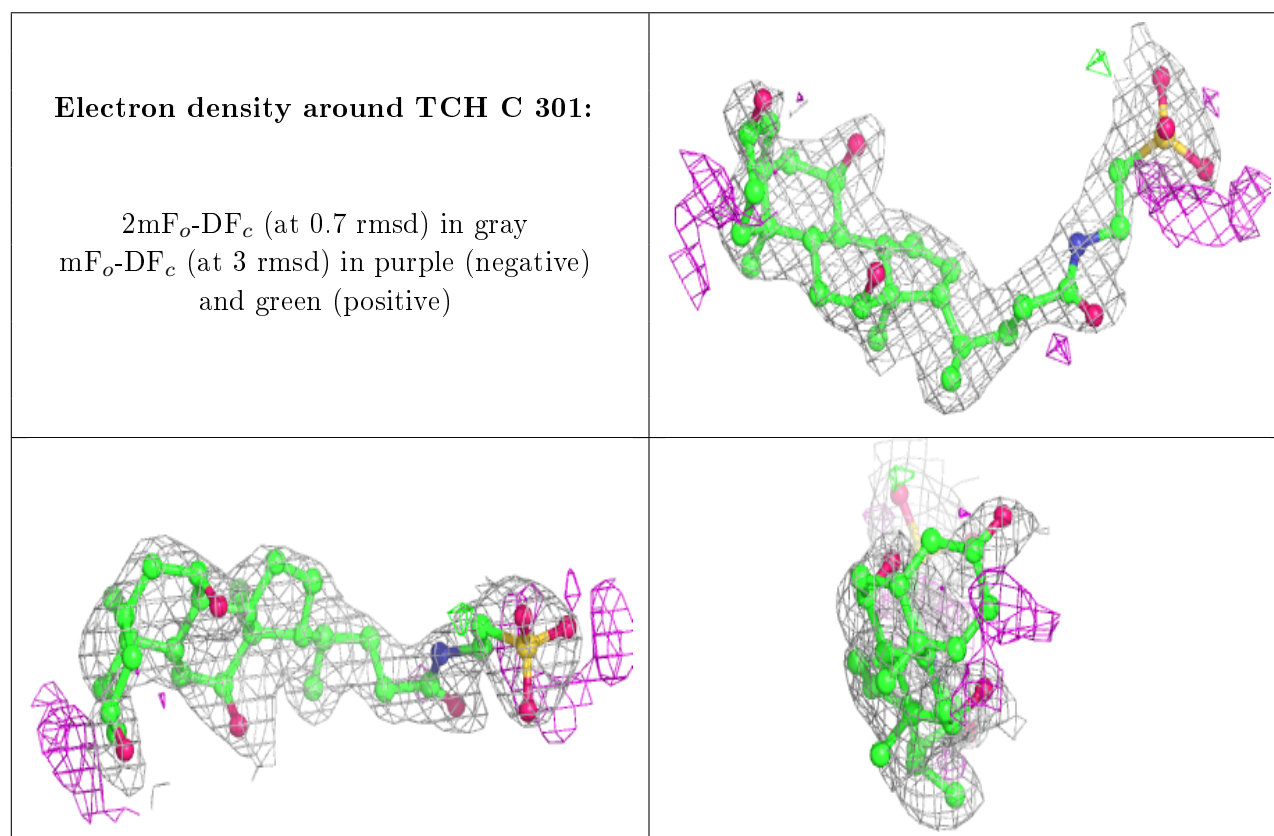
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	FMT	K	305	3/3	0.59	0.22	93,93,93,95	0
5	ACT	G	306	4/4	0.69	0.16	96,97,97,98	0
6	GOL	D	303	6/6	0.73	0.24	90,94,96,98	0
3	CL	F	303	1/1	0.74	0.16	115,115,115,115	0
7	FMT	J	309	3/3	0.77	0.11	78,78,80,81	0
6	GOL	C	303	6/6	0.79	0.24	66,77,79,79	0
6	GOL	F	304	6/6	0.80	0.20	72,76,80,81	0
6	GOL	B	303	6/6	0.81	0.13	58,65,72,74	0
5	ACT	A	305	4/4	0.81	0.22	97,98,100,103	0
7	FMT	J	307	3/3	0.82	0.38	83,83,87,87	0
7	FMT	J	308	3/3	0.83	0.21	66,66,69,69	0
6	GOL	I	303	6/6	0.84	0.18	52,62,66,66	0
5	ACT	A	304	4/4	0.87	0.10	74,75,78,79	0
6	GOL	E	303	6/6	0.87	0.12	67,71,71,72	0
7	FMT	K	304	3/3	0.88	0.09	70,70,71,71	0
4	SO4	A	303	5/5	0.89	0.26	139,140,142,143	0
4	SO4	J	304	5/5	0.89	0.21	133,134,135,136	0
2	TCH	C	301	35/35	0.90	0.20	55,74,84,86	0
2	TCH	G	301	35/35	0.92	0.19	58,70,77,78	0
2	TCH	A	301	35/35	0.92	0.10	47,59,66,72	0
4	SO4	J	305	5/5	0.92	0.20	140,141,141,143	0
2	TCH	F	301	35/35	0.93	0.18	58,67,73,73	0
2	TCH	D	301	35/35	0.93	0.12	48,58,67,72	0
6	GOL	H	302	6/6	0.93	0.08	66,75,78,82	0
4	SO4	G	305	5/5	0.93	0.18	132,132,133,135	0
7	FMT	J	306	3/3	0.93	0.07	69,69,70,71	0
3	CL	A	302	1/1	0.94	0.05	56,56,56,56	0
7	FMT	K	303	3/3	0.94	0.06	58,58,59,62	0
3	CL	G	304	1/1	0.94	0.08	76,76,76,76	0
2	TCH	J	301	35/35	0.95	0.14	51,56,65,70	0
2	TCH	K	301	35/35	0.95	0.11	42,52,67,77	0
2	TCH	H	301	35/35	0.95	0.12	43,56,64,68	0

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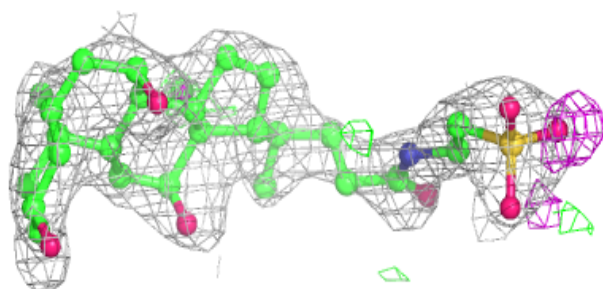
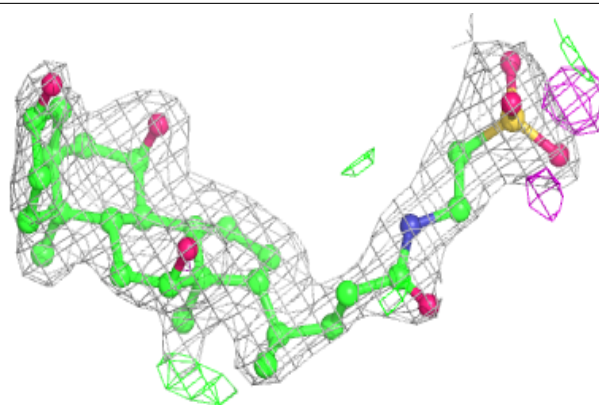
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TCH	B	301	35/35	0.95	0.12	41,51,57,60	0
3	CL	L	302	1/1	0.96	0.07	49,49,49,49	0
2	TCH	I	301	35/35	0.96	0.11	41,53,62,63	0
2	TCH	E	301	35/35	0.96	0.12	37,50,61,64	0
2	TCH	L	301	35/35	0.96	0.09	38,45,58,61	0
3	CL	J	303	1/1	0.97	0.10	79,79,79,79	0
3	CL	C	302	1/1	0.98	0.09	45,45,45,45	0
3	CL	G	302	1/1	0.98	0.08	44,44,44,44	0
3	CL	I	302	1/1	0.98	0.04	53,53,53,53	0
3	CL	E	302	1/1	0.99	0.08	61,61,61,61	0
3	CL	K	302	1/1	0.99	0.07	51,51,51,51	0
3	CL	B	302	1/1	0.99	0.04	52,52,52,52	0
3	CL	G	303	1/1	0.99	0.06	52,52,52,52	0
3	CL	L	303	1/1	0.99	0.05	54,54,54,54	0
3	CL	D	302	1/1	0.99	0.05	54,54,54,54	0
3	CL	F	302	1/1	0.99	0.08	45,45,45,45	0
3	CL	J	302	1/1	0.99	0.06	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

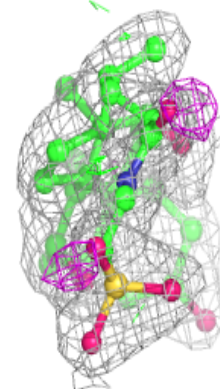
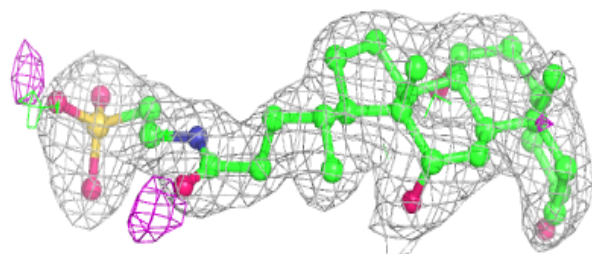
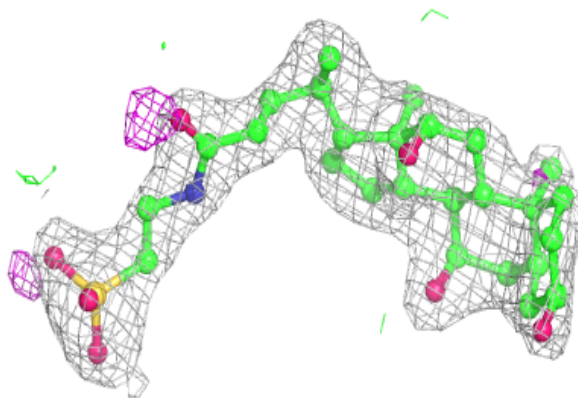


Electron density around TCH G 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

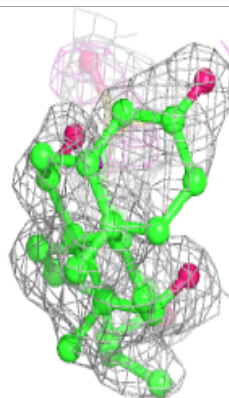
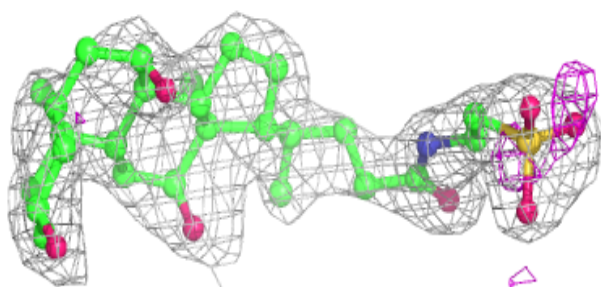
**Electron density around TCH A 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

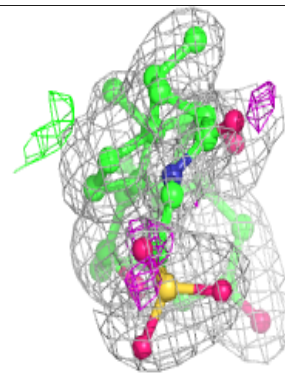
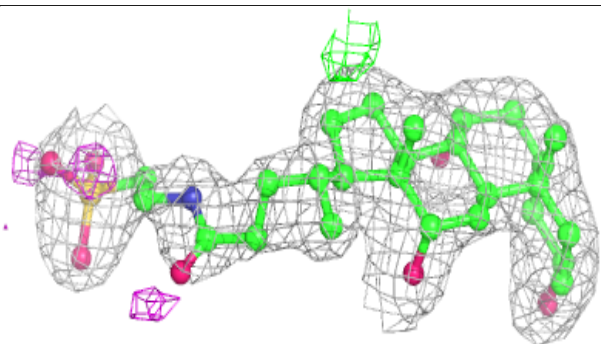
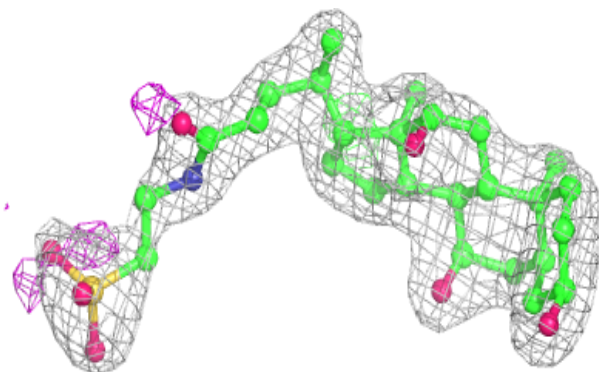


Electron density around TCH F 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

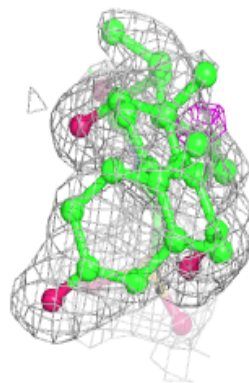
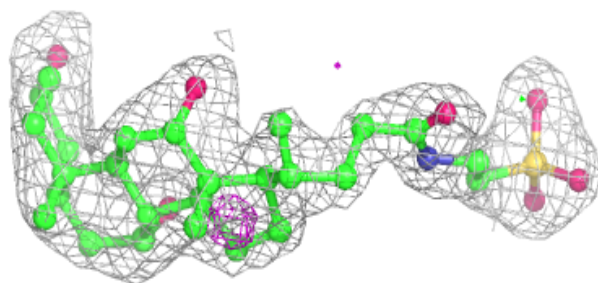
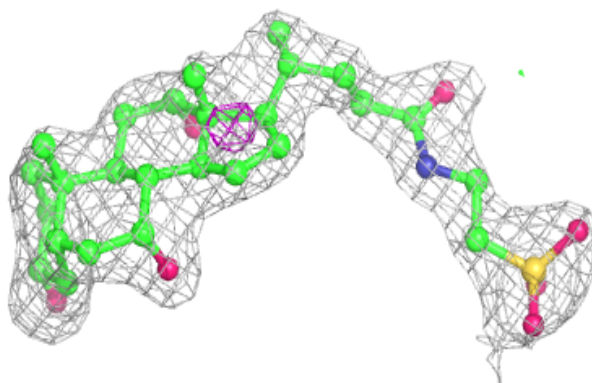
**Electron density around TCH D 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

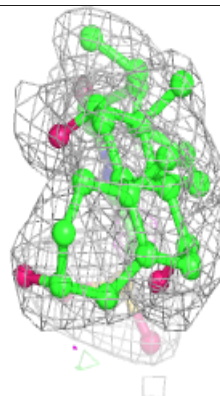
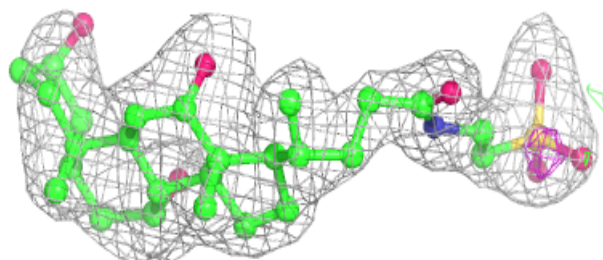
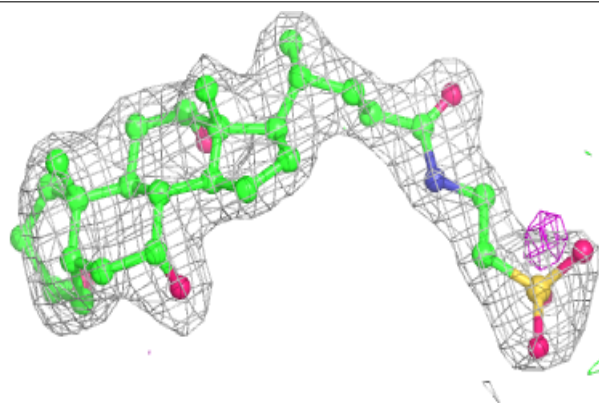


Electron density around TCH J 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

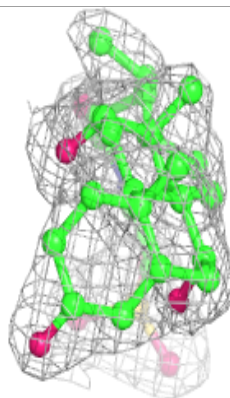
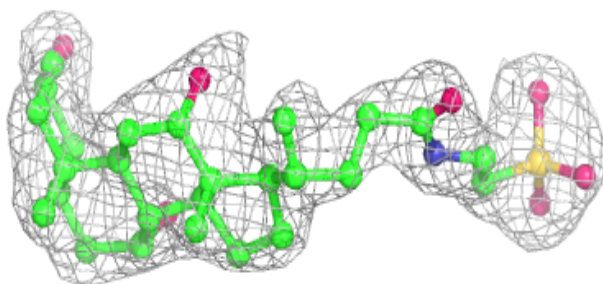
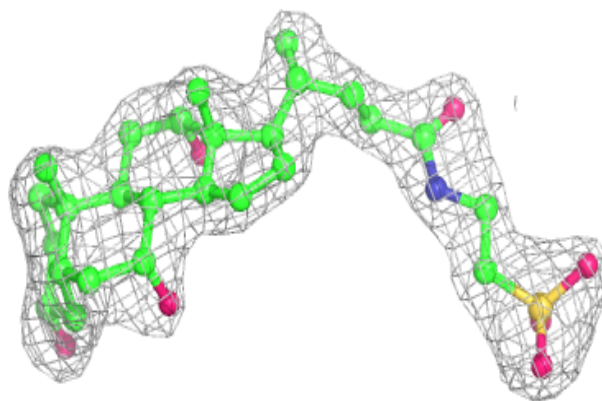
**Electron density around TCH K 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

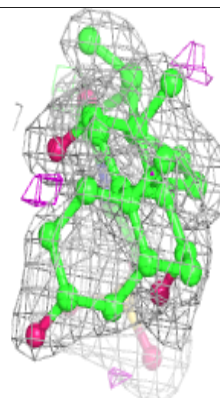
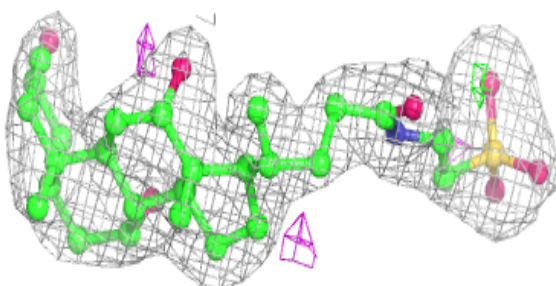
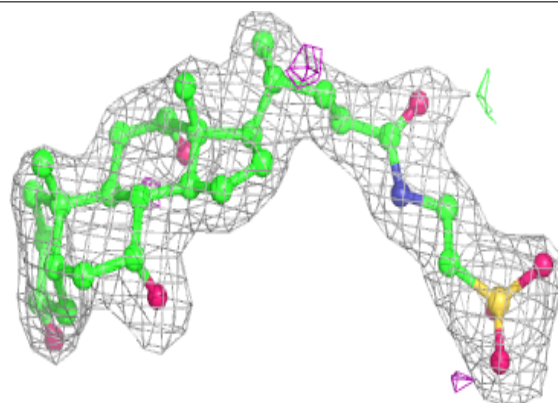


Electron density around TCH H 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

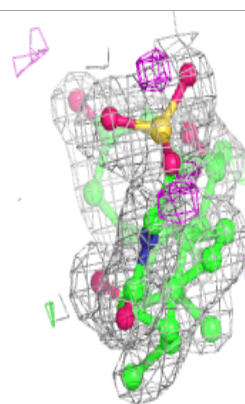
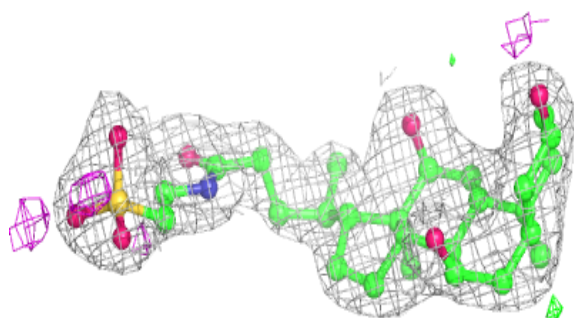
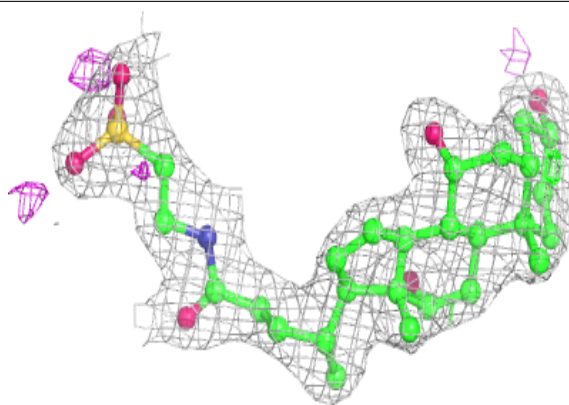
**Electron density around TCH B 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

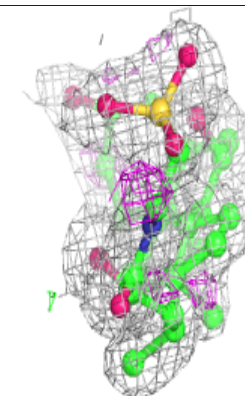
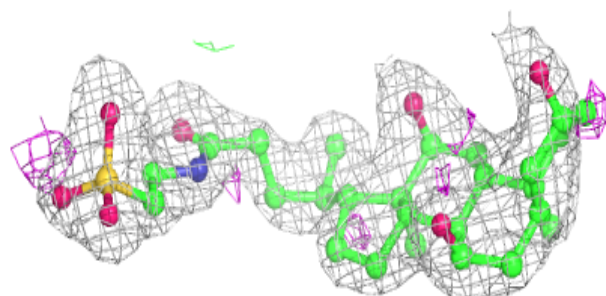
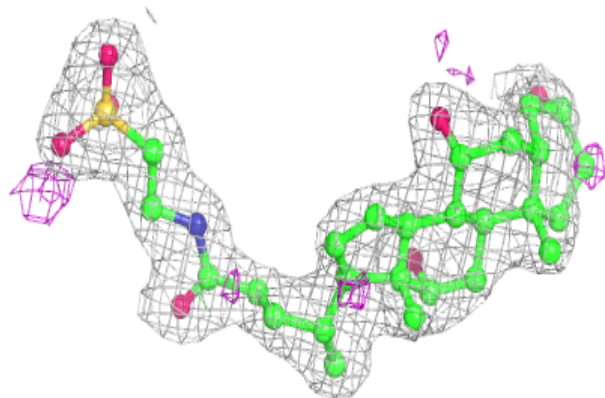


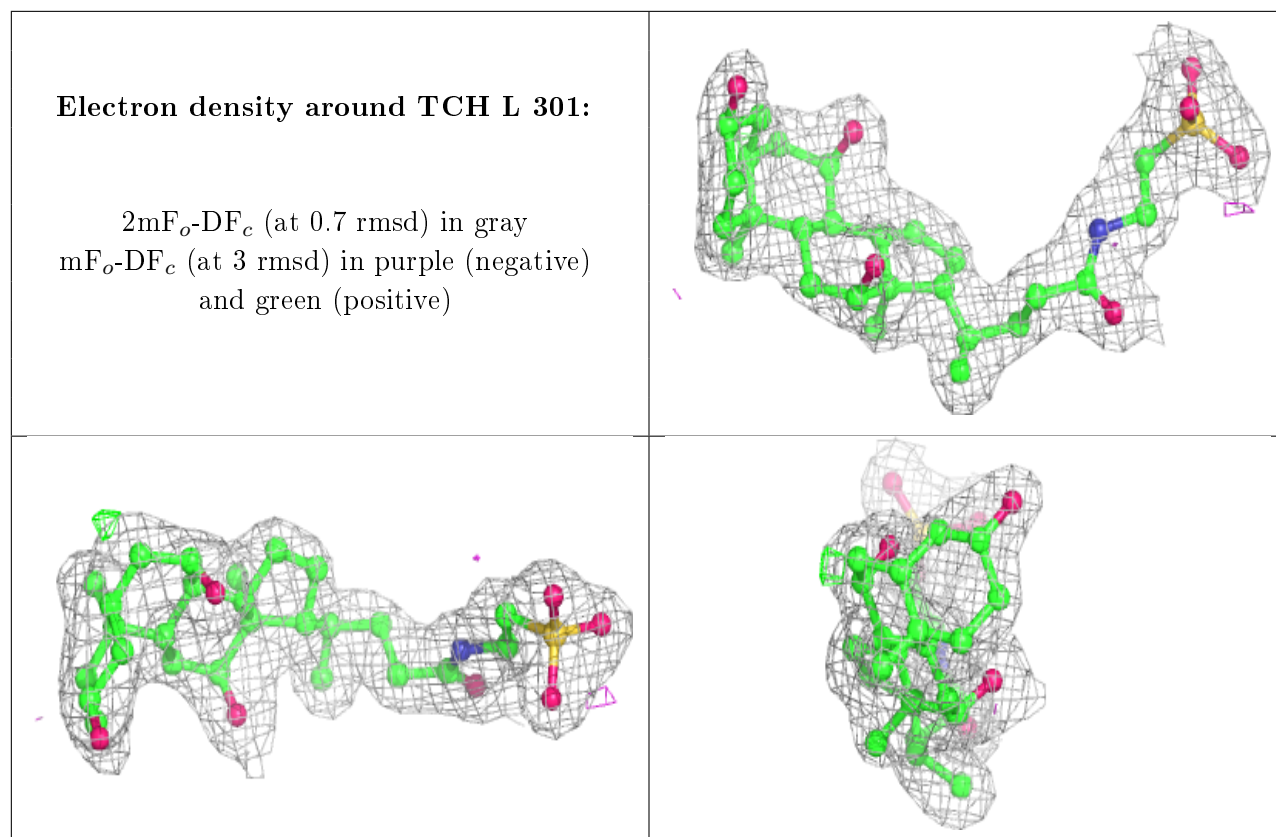
Electron density around TCH I 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TCH E 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.