wwPDB X-ray Structure Validation Summary Report (i)

Sep 19, 2023 – 04:32 AM EDT

PDB ID	:	4ZY2
Title	:	X-ray crystal structure of PfA-M17 in complex with hydroxamic acid-based inhibitor 10o
Authors	:	Drinkwater, N.; McGowan, S.
Deposited on	:	2015-05-21
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

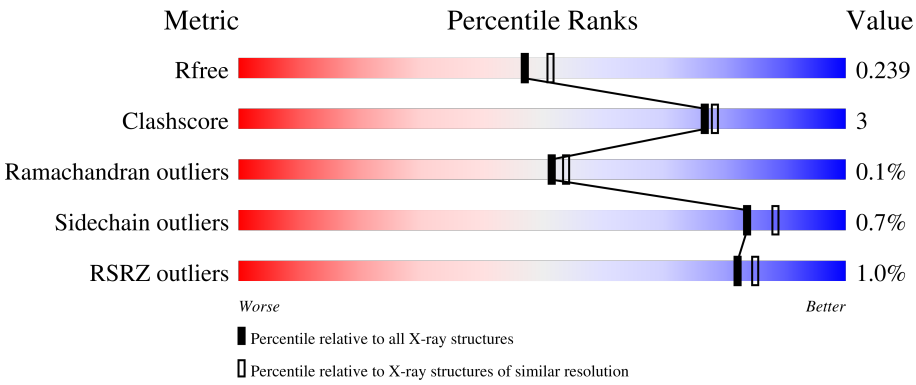
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of 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 <=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	522	% 92% 7% •
1	B	522	% 94% • •
1	C	522	% 91% 7% ••
1	D	522	92% 6% •
1	E	522	% 91% 6% •

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Mol	Chain	Length	Quality of chain
1	F	522	% 92% 6%
1	G	522	% 93% 6%
1	H	522	% 91% 9%
1	I	522	% 92% 7%
1	J	522	% 93% 6%
1	K	522	% 92% 5%
1	L	522	% 89% 9%

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
4	SO4	A	1004	-	-	X	-
5	1PE	F	1007	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 52900 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 Probable M17 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	3984	2558	641	766	19	0	0	0
1	B	517	3921	2518	635	749	19	0	0	0
1	C	518	3968	2551	641	756	20	0	0	0
1	D	513	3926	2527	632	747	20	0	0	0
1	E	513	3916	2522	630	745	19	0	0	0
1	F	512	3870	2487	625	739	19	0	0	0
1	G	518	3983	2558	641	764	20	0	0	0
1	H	518	3930	2524	636	750	20	0	0	0
1	I	518	3965	2548	639	758	20	0	0	0
1	J	514	3936	2534	635	747	20	0	0	0
1	K	512	3912	2517	629	747	19	0	0	0
1	L	513	3878	2491	625	743	19	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
A	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
A	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
B	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
B	515	GLN	ASN	engineered mutation	UNP A0A0L7M119

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
C	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
C	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
C	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
D	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
D	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
D	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
E	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
E	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
E	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
F	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
F	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
F	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
G	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
G	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
G	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
H	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
H	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
H	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
I	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
I	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
I	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
J	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
J	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
J	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
K	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
K	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
K	546	GLN	ASN	engineered mutation	UNP A0A0L7M119
L	152	GLN	ASN	engineered mutation	UNP A0A0L7M119
L	515	GLN	ASN	engineered mutation	UNP A0A0L7M119
L	546	GLN	ASN	engineered mutation	UNP A0A0L7M119

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0
			Total	Zn		
2	B	2	2	2	0	0
			Total	Zn		
2	C	2	2	2	0	0
			Total	Zn		
2	D	2	2	2	0	0

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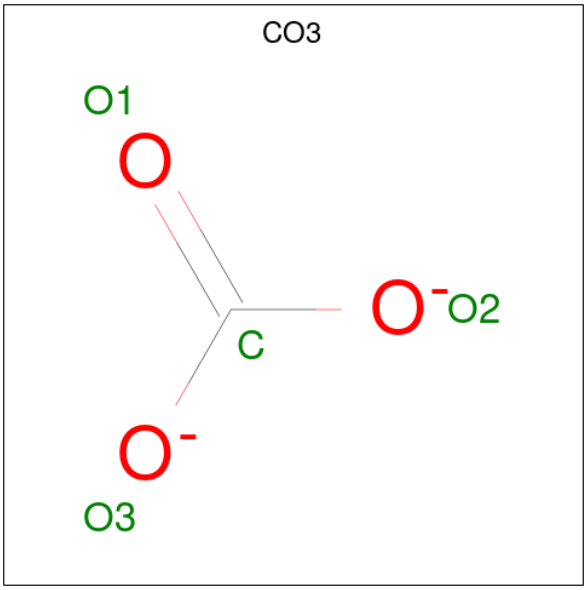
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0
2	L	2	Total Zn 2 2	0	0

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 1 3	0	0
3	B	1	Total C O 4 1 3	0	0
3	C	1	Total C O 4 1 3	0	0

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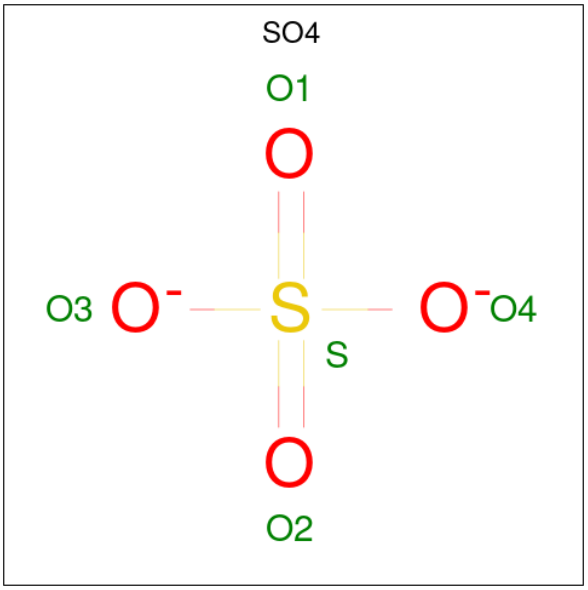
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	D	1	4	1	3	0	0
3	E	1	4	1	3	0	0
3	F	1	4	1	3	0	0
3	G	1	4	1	3	0	0
3	H	1	4	1	3	0	0
3	I	1	4	1	3	0	0
3	J	1	4	1	3	0	0
3	K	1	4	1	3	0	0
3	L	1	4	1	3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	D	1	5	4	1	0	0
			Total	O	S		
4	E	1	5	4	1	0	0
			Total	O	S		
4	E	1	5	4	1	0	0
			Total	O	S		
4	E	1	5	4	1	0	0
			Total	O	S		
4	F	1	5	4	1	0	0
			Total	O	S		
4	F	1	5	4	1	0	0
			Total	O	S		
4	G	1	5	4	1	0	0
			Total	O	S		
4	G	1	5	4	1	0	0
			Total	O	S		
4	G	1	5	4	1	0	0
			Total	O	S		
4	H	1	5	4	1	0	0
			Total	O	S		
4	H	1	5	4	1	0	0
			Total	O	S		
4	I	1	5	4	1	0	0
			Total	O	S		
4	I	1	5	4	1	0	0
			Total	O	S		
4	I	1	5	4	1	0	0
			Total	O	S		
4	I	1	5	4	1	0	0
			Total	O	S		
4	I	1	5	4	1	0	0

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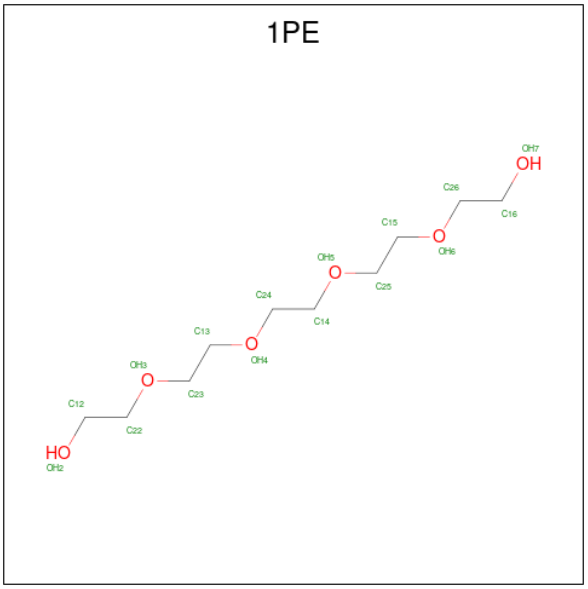
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	J	1	5	4	1	0	0
			Total	O	S		
4	J	1	5	4	1	0	0
			Total	O	S		
4	J	1	5	4	1	0	0
			Total	O	S		
4	K	1	5	4	1	0	0
			Total	O	S		
4	L	1	5	4	1	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	7	4	3	0	0
			Total	C	O		
5	A	1	10	6	4	0	0
			Total	C	O		
5	B	1	16	10	6	0	0
			Total	C	O		
5	B	1	9	6	3	0	0
			Total	C	O		
5	C	1	12	8	4	0	0
			Total	C	O		
5	C	1	10	6	4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	D	1	8	5	3	0	0
			Total	C	O		
5	D	1	8	5	3	0	0
			Total	C	O		
5	D	1	10	6	4	0	0
			Total	C	O		
5	D	1	10	6	4	0	0
			Total	C	O		
5	E	1	10	6	4	0	0
			Total	C	O		
5	E	1	10	6	4	0	0
			Total	C	O		
5	E	1	7	5	2	0	0
			Total	C	O		
5	F	1	10	6	4	0	0
			Total	C	O		
5	F	1	10	6	4	0	0
			Total	C	O		
5	F	1	10	6	4	0	0
			Total	C	O		
5	F	1	7	4	3	0	0
			Total	C	O		
5	F	1	7	4	3	0	0
			Total	C	O		
5	G	1	6	4	2	0	0
			Total	C	O		
5	G	1	6	4	2	0	0
			Total	C	O		
5	G	1	7	4	3	0	0
			Total	C	O		
5	G	1	10	6	4	0	0
			Total	C	O		
5	G	1	10	7	3	0	0
			Total	C	O		
5	H	1	11	8	3	0	0
			Total	C	O		
5	H	1	14	9	5	0	0
			Total	C	O		
5	I	1	10	6	4	0	0
			Total	C	O		
5	I	1	9	6	3	0	0

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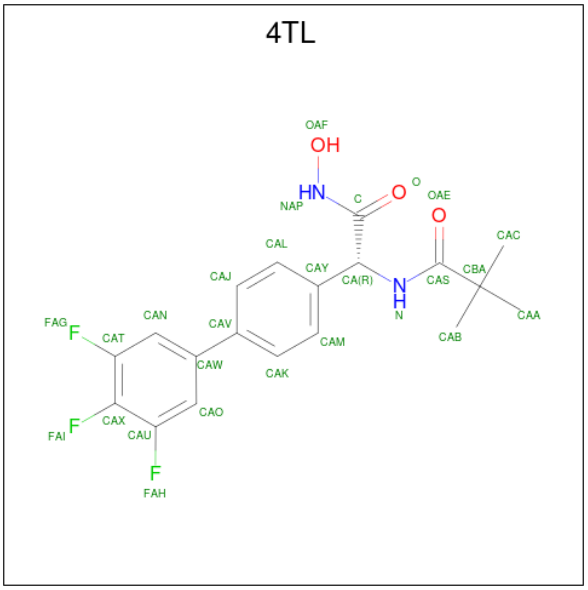
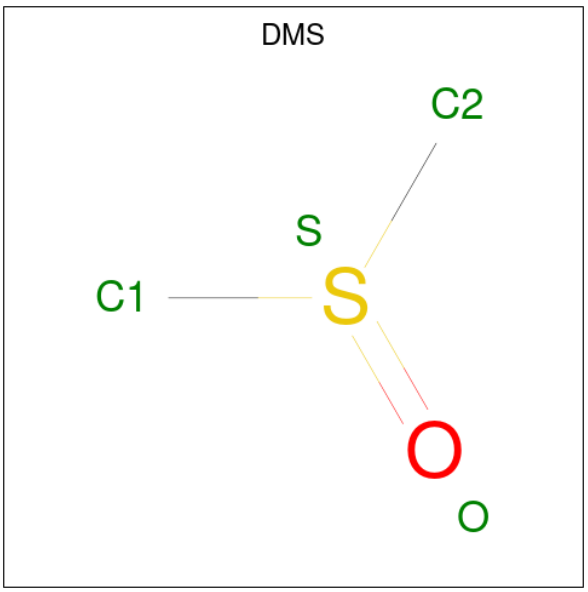
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	I	1	5	3	2		0	0
			Total	C	O			
5	J	1	11	7	4		0	0
			Total	C	O			
5	J	1	10	6	4		0	0
			Total	C	O			
5	J	1	9	6	3		0	0
			Total	C	O			
5	J	1	7	4	3		0	0
			Total	C	O			
5	K	1	10	6	4		0	0
			Total	C	O			
5	K	1	6	4	2		0	0
			Total	C	O			
5	K	1	10	6	4		0	0
			Total	C	O			
5	L	1	10	6	4		0	0
			Total	C	O			
5	L	1	10	6	4		0	0
			Total	C	O			
5	L	1	7	4	3		0	0
			Total	C	O			
5	L	1	9	6	3		0	0

- Molecule 6 is N-[(1R)-2-(hydroxyamino)-2-oxo-1-(3',4',5'-trifluorobiphenyl-4-yl)ethyl]-2,2-dimethylpropanamide (three-letter code: 4TL) (formula: $C_{19}H_{19}F_3N_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
6	A	1	27	19	3	2	3	0	0
6	B	1	27	19	3	2	3	0	0
6	C	1	27	19	3	2	3	0	0
6	D	1	27	19	3	2	3	0	0
6	E	1	27	19	3	2	3	0	0
6	F	1	27	19	3	2	3	0	0
6	G	1	27	19	3	2	3	0	0
6	H	1	27	19	3	2	3	0	0
6	I	1	27	19	3	2	3	0	0
6	J	1	27	19	3	2	3	0	0
6	K	1	27	19	3	2	3	0	0
6	L	1	27	19	3	2	3	0	0

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
7	A	1	4	2	1	1	0	0
7	H	1	4	2	1	1	0	0
7	L	1	4	2	1	1	0	0

- Molecule 8 is water.

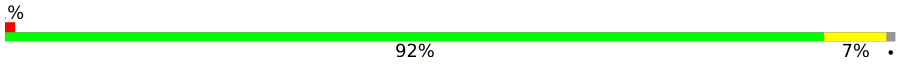
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	441	441	441	0	0
8	B	330	330	330	0	0
8	C	433	433	433	0	0
8	D	412	412	412	0	0
8	E	457	457	457	0	0
8	F	360	360	360	0	0
8	G	430	430	430	0	0
8	H	351	351	351	0	0
8	I	396	396	396	0	0
8	J	398	398	398	0	0
8	K	414	414	414	0	0
8	L	383	383	383	0	0

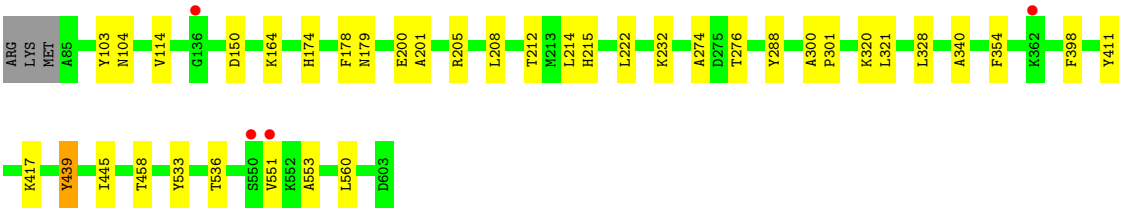
3 Residue-property plots (i)

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 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: Probable M17 family aminopeptidase

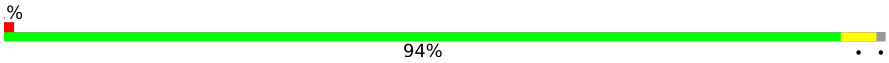
Chain A:

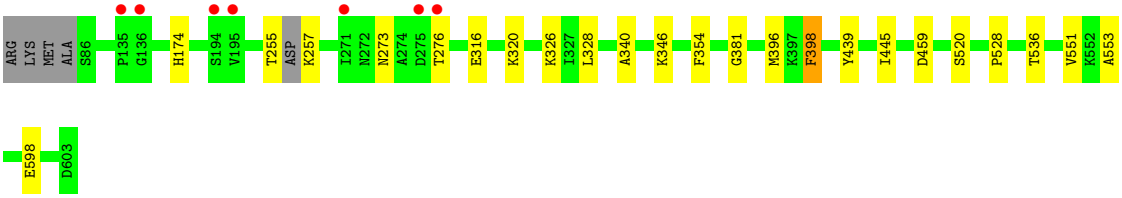




• Molecule 1: Probable M17 family aminopeptidase

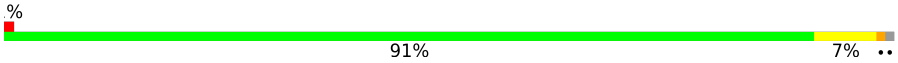
Chain B:





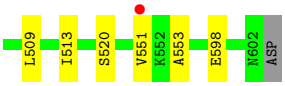
• Molecule 1: Probable M17 family aminopeptidase

Chain C:



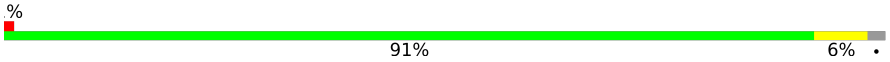
• Molecule 1: Probable M17 family aminopeptidase

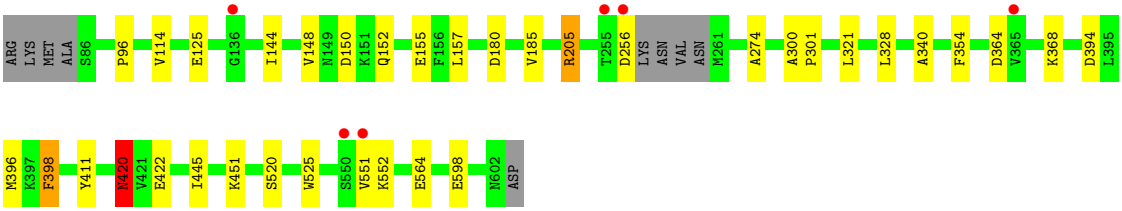
Chain D:



• Molecule 1: Probable M17 family aminopeptidase

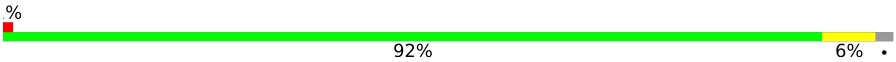
Chain E:

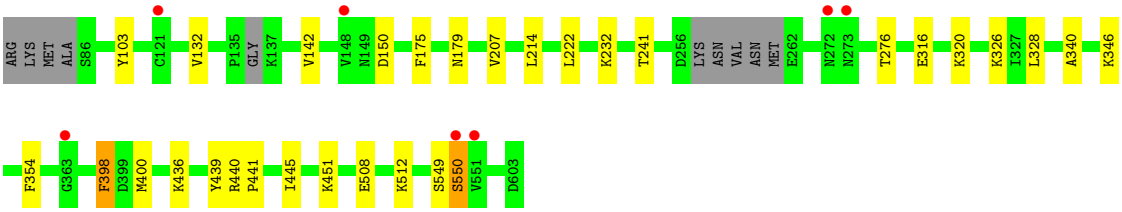




• Molecule 1: Probable M17 family aminopeptidase

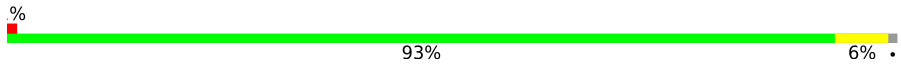
Chain F:

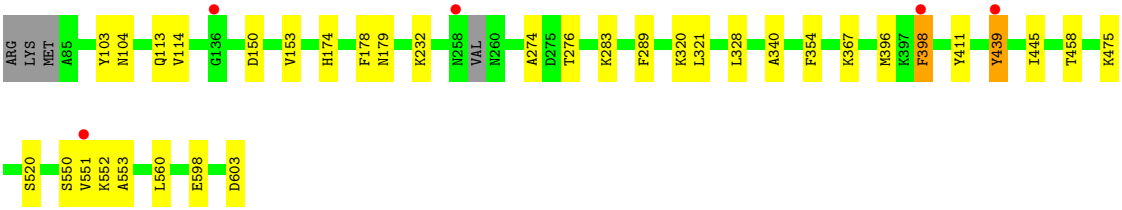




• Molecule 1: Probable M17 family aminopeptidase

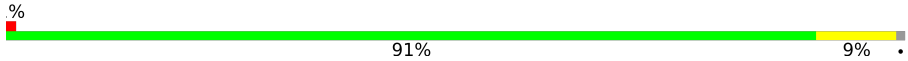
Chain G:

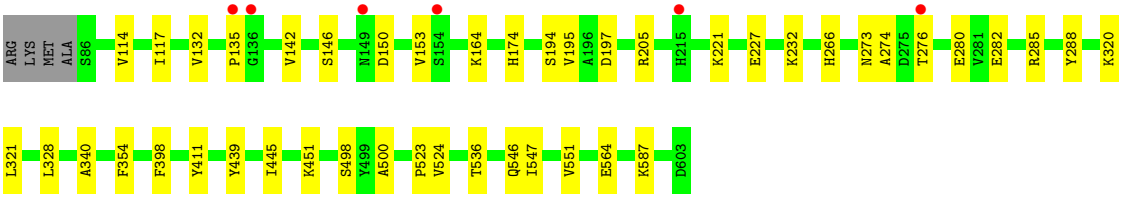




• Molecule 1: Probable M17 family aminopeptidase

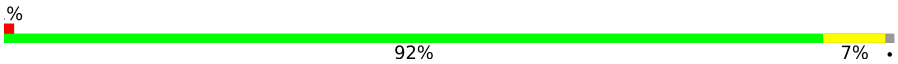
Chain H:

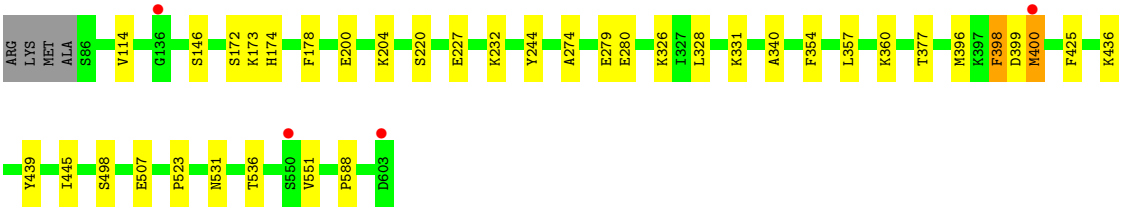




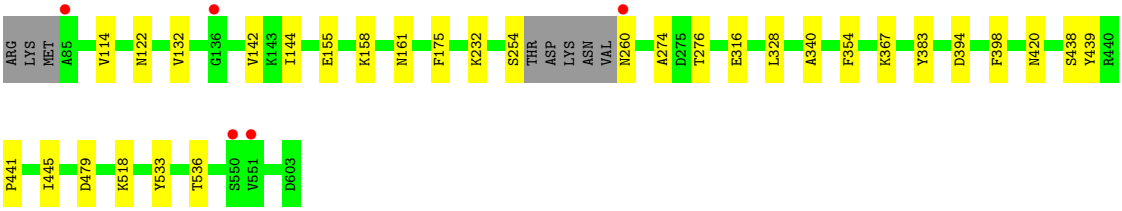
• Molecule 1: Probable M17 family aminopeptidase

Chain I:

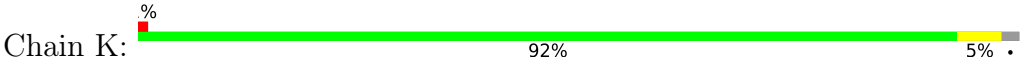


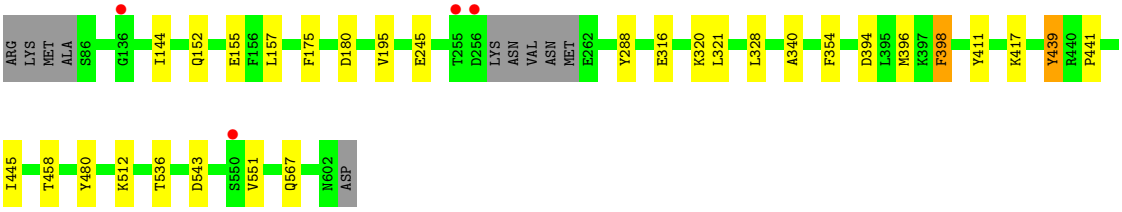


• Molecule 1: Probable M17 family aminopeptidase

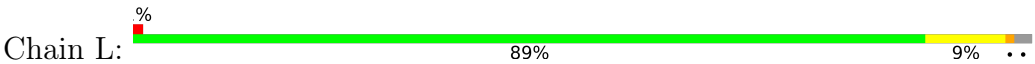


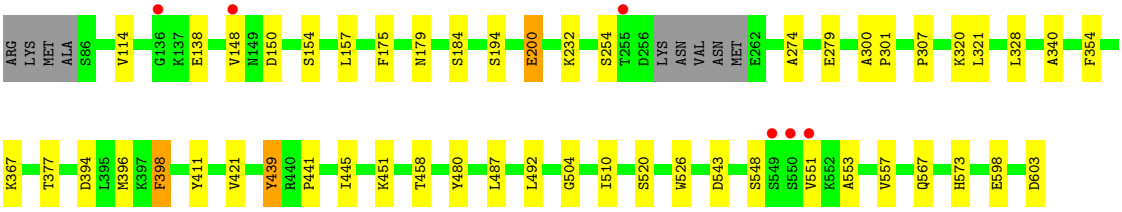
• Molecule 1: Probable M17 family aminopeptidase





• Molecule 1: Probable M17 family aminopeptidase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	174.06Å 177.25Å 230.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 2.10 48.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.54-2.10) 86.8 (48.54-2.10)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.194 , 0.239 0.195 , 0.239	Depositor DCC
R_{free} test set	20661 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	52900	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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 45.83 % 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 1.2488e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 4TL, DMS, CO3, 1PE, ZN

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	0.23	0/4062	0.40	0/5510
1	B	0.23	0/3998	0.39	0/5432
1	C	0.24	0/4046	0.42	0/5488
1	D	0.23	0/4003	0.40	0/5429
1	E	0.32	1/3993 (0.0%)	0.42	1/5416 (0.0%)
1	F	0.23	0/3946	0.40	0/5363
1	G	0.23	0/4060	0.40	0/5503
1	H	0.24	0/4008	0.40	0/5445
1	I	0.23	0/4043	0.40	0/5486
1	J	0.23	0/4013	0.40	0/5440
1	K	0.23	0/3989	0.39	0/5414
1	L	0.23	0/3955	0.39	0/5377
All	All	0.24	1/48116 (0.0%)	0.40	1/65303 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	205	ARG	NE-CZ	13.02	1.50	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	205	ARG	CD-NE-CZ	-8.05	112.33	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	547	ILE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3984	0	3909	23	0
1	B	3921	0	3806	15	0
1	C	3968	0	3904	29	0
1	D	3926	0	3860	21	0
1	E	3916	0	3837	21	0
1	F	3870	0	3748	29	0
1	G	3983	0	3923	25	0
1	H	3930	0	3824	28	0
1	I	3965	0	3897	26	0
1	J	3936	0	3874	22	0
1	K	3912	0	3825	19	0
1	L	3878	0	3748	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	1	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	A	10	0	0	2	0
4	C	25	0	0	1	0
4	D	5	0	0	0	0
4	E	15	0	0	1	0
4	F	10	0	0	0	0
4	G	15	0	0	1	0
4	H	10	0	0	0	0
4	I	25	0	0	1	0
4	J	15	0	0	0	0
4	K	5	0	0	0	0
4	L	5	0	0	0	0
5	A	17	0	20	1	0
5	B	25	0	30	2	0
5	C	22	0	26	3	0
5	D	36	0	41	1	0
5	E	27	0	30	1	0
5	F	44	0	56	12	0
5	G	39	0	43	5	0
5	H	25	0	29	4	0
5	I	24	0	26	3	0
5	J	37	0	44	2	0
5	K	26	0	28	3	0
5	L	36	0	44	12	0
6	A	27	0	0	0	0
6	B	27	0	0	0	0
6	C	27	0	0	0	0
6	D	27	0	0	0	0
6	E	27	0	0	0	0
6	F	27	0	0	0	0
6	G	27	0	0	1	0
6	H	27	0	0	0	0
6	I	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	27	0	0	0	0
6	K	27	0	0	0	0
6	L	27	0	0	0	0
7	A	4	0	6	0	0
7	H	4	0	6	1	0
7	L	4	0	6	0	0
8	A	441	0	0	4	0
8	B	330	0	0	0	0
8	C	433	0	0	2	0
8	D	412	0	0	3	0
8	E	457	0	0	3	0
8	F	360	0	0	3	0
8	G	430	0	0	3	0
8	H	351	0	0	1	0
8	I	396	0	0	5	0
8	J	398	0	0	4	0
8	K	414	0	0	2	0
8	L	383	0	0	2	0
All	All	52900	0	46590	281	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 3.

The worst 5 of 281 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:551:VAL:HG11	1:L:557:VAL:HG21	1.52	0.92
1:L:320:LYS:HZ1	5:L:1010:1PE:H231	1.41	0.85
1:H:164:LYS:NZ	1:L:184:SER:OG	2.13	0.82
1:I:436:LYS:NZ	8:I:1101:HOH:O	2.10	0.81
1:L:451:LYS:HG2	5:L:1006:1PE:H131	1.68	0.75

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	517/522 (99%)	504 (98%)	13 (2%)	0	100	100
1	B	513/522 (98%)	500 (98%)	13 (2%)	0	100	100
1	C	516/522 (99%)	501 (97%)	14 (3%)	1 (0%)	47	49
1	D	509/522 (98%)	495 (97%)	14 (3%)	0	100	100
1	E	509/522 (98%)	492 (97%)	15 (3%)	2 (0%)	34	32
1	F	506/522 (97%)	493 (97%)	12 (2%)	1 (0%)	47	49
1	G	514/522 (98%)	496 (96%)	17 (3%)	1 (0%)	47	49
1	H	516/522 (99%)	499 (97%)	17 (3%)	0	100	100
1	I	516/522 (99%)	507 (98%)	9 (2%)	0	100	100
1	J	510/522 (98%)	499 (98%)	11 (2%)	0	100	100
1	K	508/522 (97%)	494 (97%)	14 (3%)	0	100	100
1	L	509/522 (98%)	493 (97%)	16 (3%)	0	100	100
All	All	6143/6264 (98%)	5973 (97%)	165 (3%)	5 (0%)	51	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	550	SER
1	C	549	SER
1	E	420	ASN
1	G	550	SER
1	E	551	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	425/450 (94%)	421 (99%)	4 (1%)	78	84
1	B	412/450 (92%)	410 (100%)	2 (0%)	88	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	423/450 (94%)	419 (99%)	4 (1%)	78	84
1	D	417/450 (93%)	415 (100%)	2 (0%)	88	92
1	E	414/450 (92%)	412 (100%)	2 (0%)	88	92
1	F	406/450 (90%)	404 (100%)	2 (0%)	88	92
1	G	427/450 (95%)	424 (99%)	3 (1%)	84	88
1	H	414/450 (92%)	411 (99%)	3 (1%)	84	88
1	I	424/450 (94%)	420 (99%)	4 (1%)	78	84
1	J	417/450 (93%)	415 (100%)	2 (0%)	88	92
1	K	414/450 (92%)	409 (99%)	5 (1%)	71	77
1	L	406/450 (90%)	402 (99%)	4 (1%)	76	82
All	All	4999/5400 (93%)	4962 (99%)	37 (1%)	84	88

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	195	VAL
1	L	421	VAL
1	K	288	TYR
1	K	567	GLN
1	E	398	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	229	ASN
1	H	215	HIS
1	J	161	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 118 ligands modelled in this entry, 24 are monoatomic - leaving 94 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	$\#\|Z\| > 2$
5	1PE	J	1009	-	8,8,15	0.72	0	7,7,14	0.22	0
4	SO4	H	1005	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	A	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
5	1PE	L	1007	-	6,6,15	0.63	0	5,5,14	0.31	0
3	CO3	D	1002	-	2,3,3	0.44	0	2,3,3	0.23	0
6	4TL	J	1011	2	28,28,28	2.61	5 (17%)	40,41,41	1.00	2 (5%)
6	4TL	A	1008	2	28,28,28	2.58	5 (17%)	40,41,41	1.01	1 (2%)
3	CO3	L	1002	-	2,3,3	0.45	0	2,3,3	0.25	0
5	1PE	L	1005	-	9,9,15	0.62	0	8,8,14	0.21	0
6	4TL	D	1009	2	28,28,28	2.62	5 (17%)	40,41,41	0.89	1 (2%)
4	SO4	J	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
5	1PE	F	1006	-	9,9,15	0.62	0	8,8,14	0.25	0
5	1PE	L	1010	-	8,8,15	0.64	0	7,7,14	0.23	0
4	SO4	C	1006	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	K	1004	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	E	1004	-	4,4,4	0.14	0	6,6,6	0.04	0
3	CO3	E	1002	-	2,3,3	0.41	0	2,3,3	0.17	0
5	1PE	C	1010	-	9,9,15	0.69	0	8,8,14	0.31	0
6	4TL	L	1008	2	28,28,28	2.59	5 (17%)	40,41,41	1.00	1 (2%)
3	CO3	I	1002	-	2,3,3	0.41	0	2,3,3	0.20	0
4	SO4	G	1005	-	4,4,4	0.13	0	6,6,6	0.09	0
5	1PE	F	1010	-	6,6,15	0.55	0	5,5,14	0.33	0
4	SO4	C	1004	-	4,4,4	0.13	0	6,6,6	0.09	0
4	SO4	J	1006	-	4,4,4	0.13	0	6,6,6	0.08	0
4	SO4	I	1008	-	4,4,4	0.12	0	6,6,6	0.10	0
4	SO4	F	1004	-	4,4,4	0.16	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	1PE	F	1007	-	9,9,15	0.63	0	8,8,14	0.26	0
6	4TL	B	1004	2	28,28,28	2.58	5 (17%)	40,41,41	1.00	1 (2%)
5	1PE	I	1009	-	9,9,15	0.67	0	8,8,14	0.20	0
4	SO4	G	1006	-	4,4,4	0.14	0	6,6,6	0.07	0
5	1PE	F	1011	-	6,6,15	0.62	0	5,5,14	0.26	0
6	4TL	C	1011	2	28,28,28	2.61	5 (17%)	40,41,41	0.95	1 (2%)
5	1PE	D	1005	-	7,7,15	0.66	0	6,6,14	0.19	0
5	1PE	K	1006	-	5,5,15	0.61	0	4,4,14	0.19	0
5	1PE	K	1005	-	9,9,15	0.68	0	8,8,14	0.26	0
7	DMS	A	1009	-	3,3,3	0.60	0	3,3,3	0.54	0
4	SO4	C	1007	-	4,4,4	0.15	0	6,6,6	0.04	0
4	SO4	I	1007	-	4,4,4	0.17	0	6,6,6	0.07	0
3	CO3	H	1002	-	2,3,3	0.39	0	2,3,3	0.06	0
5	1PE	D	1006	-	7,7,15	0.63	0	6,6,14	0.21	0
5	1PE	B	1005	-	15,15,15	0.64	0	14,14,14	0.22	0
5	1PE	B	1006	-	8,8,15	0.64	0	7,7,14	0.18	0
4	SO4	H	1004	-	4,4,4	0.13	0	6,6,6	0.04	0
5	1PE	L	1006	-	9,9,15	0.68	0	8,8,14	0.23	0
5	1PE	H	1009	-	13,13,15	0.65	0	12,12,14	0.18	0
4	SO4	I	1004	-	4,4,4	0.14	0	6,6,6	0.08	0
3	CO3	C	1002	-	2,3,3	0.41	0	2,3,3	0.18	0
4	SO4	A	1004	-	4,4,4	0.14	0	6,6,6	0.06	0
6	4TL	E	1009	2	28,28,28	2.57	5 (17%)	40,41,41	0.98	0
6	4TL	F	1009	2	28,28,28	2.57	5 (17%)	40,41,41	1.01	1 (2%)
5	1PE	J	1010	-	6,6,15	0.68	0	5,5,14	0.30	0
5	1PE	G	1007	-	5,5,15	0.61	0	4,4,14	0.37	0
3	CO3	J	1002	-	2,3,3	0.43	0	2,3,3	0.28	0
5	1PE	C	1009	-	11,11,15	0.69	0	10,10,14	0.24	0
5	1PE	G	1009	-	6,6,15	0.64	0	5,5,14	0.24	0
6	4TL	G	1010	2	28,28,28	2.59	5 (17%)	40,41,41	0.99	0
3	CO3	F	1002	-	2,3,3	0.40	0	2,3,3	0.18	0
5	1PE	A	1006	-	6,6,15	0.63	0	5,5,14	0.23	0
4	SO4	G	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
3	CO3	G	1002	-	2,3,3	0.41	0	2,3,3	0.23	0
5	1PE	J	1008	-	9,9,15	0.63	0	8,8,14	0.22	0
5	1PE	G	1012	-	9,9,15	0.68	0	8,8,14	0.20	0
4	SO4	F	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
5	1PE	F	1008	-	9,9,15	0.63	0	8,8,14	0.24	0
4	SO4	C	1008	-	4,4,4	0.16	0	6,6,6	0.07	0
5	1PE	G	1008	-	5,5,15	0.63	0	4,4,14	0.29	0
7	DMS	H	1007	-	3,3,3	0.63	0	3,3,3	0.49	0
7	DMS	L	1009	-	3,3,3	0.67	0	3,3,3	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	1PE	J	1007	-	10,10,15	0.64	0	9,9,14	0.23	0
5	1PE	A	1007	-	9,9,15	0.67	0	8,8,14	0.25	0
5	1PE	H	1008	-	10,10,15	0.71	0	9,9,14	0.26	0
4	SO4	D	1004	-	4,4,4	0.13	0	6,6,6	0.06	0
5	1PE	D	1007	-	9,9,15	0.63	0	8,8,14	0.24	0
4	SO4	E	1005	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	J	1004	-	4,4,4	0.17	0	6,6,6	0.08	0
4	SO4	I	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
6	4TL	K	1008	2	28,28,28	2.58	5 (17%)	40,41,41	1.02	1 (2%)
3	CO3	B	1002	-	2,3,3	0.40	0	2,3,3	0.17	0
5	1PE	K	1007	-	9,9,15	0.68	0	8,8,14	0.23	0
5	1PE	I	1011	-	4,4,15	0.60	0	3,3,14	0.24	0
3	CO3	K	1002	-	2,3,3	0.39	0	2,3,3	0.21	0
6	4TL	I	1012	2	28,28,28	2.57	5 (17%)	40,41,41	0.94	1 (2%)
4	SO4	E	1006	-	4,4,4	0.14	0	6,6,6	0.06	0
5	1PE	E	1007	-	9,9,15	0.69	0	8,8,14	0.20	0
3	CO3	A	1002	-	2,3,3	0.42	0	2,3,3	0.26	0
4	SO4	I	1006	-	4,4,4	0.14	0	6,6,6	0.06	0
5	1PE	E	1010	-	6,6,15	0.62	0	5,5,14	0.26	0
4	SO4	C	1005	-	4,4,4	0.13	0	6,6,6	0.05	0
4	SO4	L	1004	-	4,4,4	0.15	0	6,6,6	0.07	0
6	4TL	H	1006	2	28,28,28	2.57	5 (17%)	40,41,41	0.99	1 (2%)
5	1PE	I	1010	-	8,8,15	0.72	0	7,7,14	0.26	0
5	1PE	G	1011	-	9,9,15	0.60	0	8,8,14	0.25	0
5	1PE	D	1008	-	9,9,15	0.69	0	8,8,14	0.22	0
5	1PE	E	1008	-	9,9,15	0.67	0	8,8,14	0.22	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
5	1PE	F	1011	-	-	4/4/4/13	-
5	1PE	J	1009	-	-	4/6/6/13	-
6	4TL	C	1011	2	-	2/24/24/24	0/2/2/2
5	1PE	J	1010	-	-	2/4/4/13	-
5	1PE	G	1007	-	-	0/3/3/13	-
5	1PE	D	1005	-	-	5/5/5/13	-
5	1PE	C	1009	-	-	4/9/9/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	G	1009	-	-	2/4/4/13	-
5	1PE	K	1006	-	-	2/3/3/13	-
6	4TL	K	1008	2	-	2/24/24/24	0/2/2/2
5	1PE	L	1007	-	-	3/4/4/13	-
5	1PE	K	1007	-	-	5/7/7/13	-
6	4TL	J	1011	2	-	2/24/24/24	0/2/2/2
5	1PE	K	1005	-	-	2/7/7/13	-
5	1PE	I	1011	-	-	1/2/2/13	-
6	4TL	G	1010	2	-	1/24/24/24	0/2/2/2
5	1PE	A	1006	-	-	2/4/4/13	-
6	4TL	A	1008	2	-	2/24/24/24	0/2/2/2
5	1PE	J	1008	-	-	4/7/7/13	-
6	4TL	I	1012	2	-	1/24/24/24	0/2/2/2
5	1PE	L	1005	-	-	1/7/7/13	-
5	1PE	E	1007	-	-	0/7/7/13	-
6	4TL	D	1009	2	-	1/24/24/24	0/2/2/2
5	1PE	F	1006	-	-	3/7/7/13	-
5	1PE	L	1010	-	-	4/6/6/13	-
5	1PE	G	1012	-	-	7/7/7/13	-
5	1PE	D	1006	-	-	2/5/5/13	-
5	1PE	B	1005	-	-	6/13/13/13	-
5	1PE	F	1008	-	-	2/7/7/13	-
5	1PE	B	1006	-	-	4/6/6/13	-
5	1PE	E	1010	-	-	1/4/4/13	-
5	1PE	G	1008	-	-	0/3/3/13	-
5	1PE	L	1006	-	-	5/7/7/13	-
6	4TL	H	1006	2	-	2/24/24/24	0/2/2/2
5	1PE	C	1010	-	-	4/7/7/13	-
6	4TL	L	1008	2	-	2/24/24/24	0/2/2/2
5	1PE	H	1009	-	-	4/11/11/13	-
5	1PE	I	1010	-	-	0/6/6/13	-
5	1PE	G	1011	-	-	5/7/7/13	-
5	1PE	F	1010	-	-	3/4/4/13	-
5	1PE	I	1009	-	-	3/7/7/13	-
5	1PE	J	1007	-	-	1/8/8/13	-
5	1PE	A	1007	-	-	5/7/7/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	H	1008	-	-	1/8/8/13	-
6	4TL	E	1009	2	-	2/24/24/24	0/2/2/2
5	1PE	D	1007	-	-	3/7/7/13	-
5	1PE	F	1007	-	-	6/7/7/13	-
5	1PE	D	1008	-	-	3/7/7/13	-
6	4TL	B	1004	2	-	4/24/24/24	0/2/2/2
5	1PE	E	1008	-	-	0/7/7/13	-
6	4TL	F	1009	2	-	2/24/24/24	0/2/2/2

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1009	4TL	CAN-CAT	8.20	1.51	1.37
6	J	1011	4TL	CAN-CAT	8.19	1.51	1.37
6	C	1011	4TL	CAN-CAT	8.14	1.51	1.37
6	L	1008	4TL	CAN-CAT	8.09	1.51	1.37
6	I	1012	4TL	CAN-CAT	8.08	1.51	1.37

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1008	4TL	O-C-NAP	-2.76	119.69	123.27
6	A	1008	4TL	O-C-NAP	-2.50	120.03	123.27
6	F	1009	4TL	O-C-NAP	-2.48	120.05	123.27
6	J	1011	4TL	O-C-NAP	-2.25	120.36	123.27
6	C	1011	4TL	O-C-NAP	-2.25	120.36	123.27

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1010	1PE	C15-C25-OH5-C14
5	B	1005	1PE	OH6-C15-C25-OH5
5	D	1007	1PE	OH6-C15-C25-OH5
5	J	1009	1PE	OH5-C14-C24-OH4
5	D	1005	1PE	OH5-C14-C24-OH4

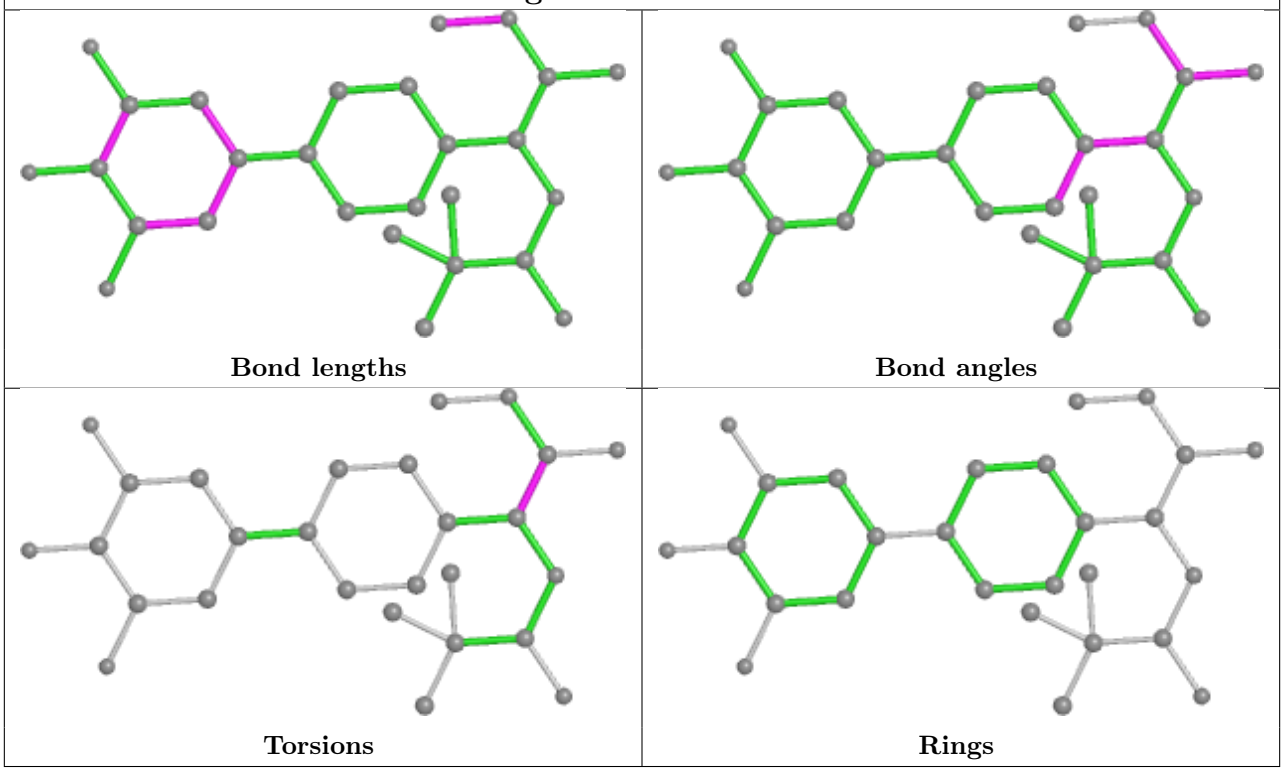
There are no ring outliers.

30 monomers are involved in 57 short contacts:

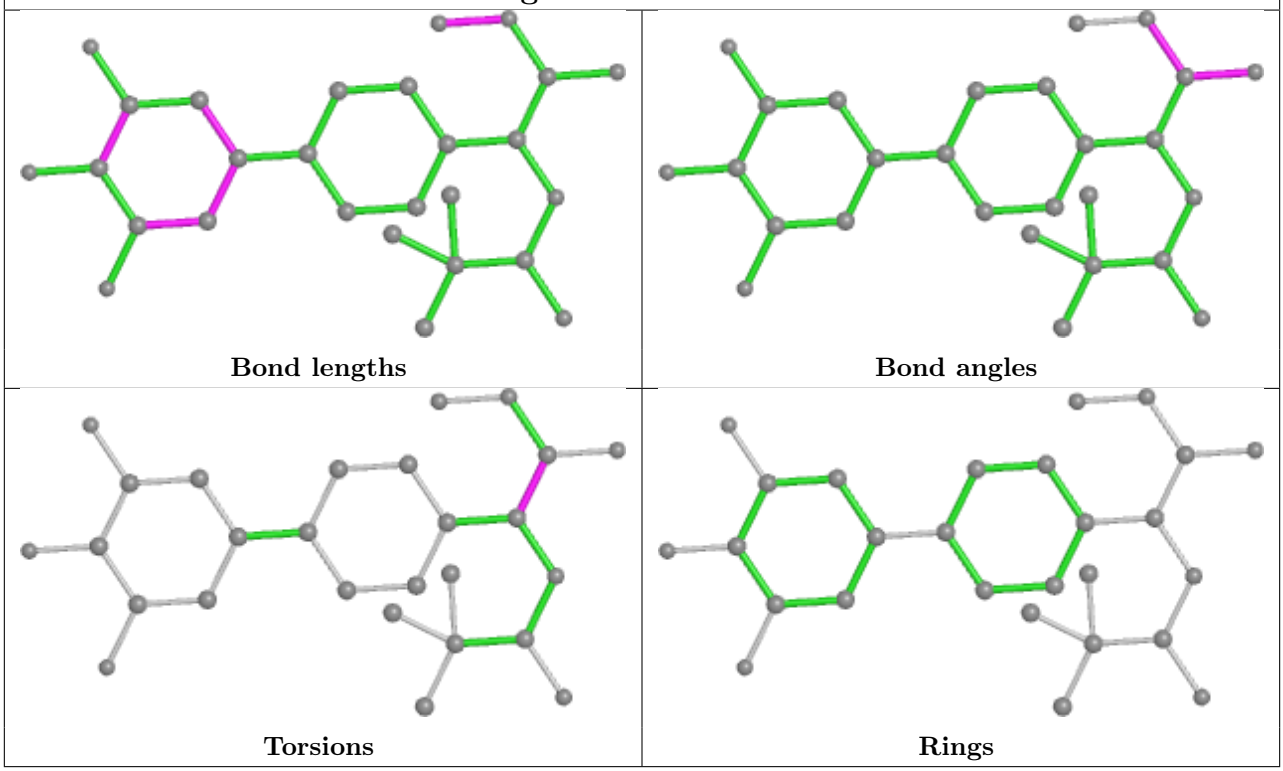
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1009	1PE	1	0
5	L	1007	1PE	2	0
5	F	1006	1PE	1	0
5	L	1010	1PE	6	0
4	E	1004	SO4	1	0
5	C	1010	1PE	3	0
5	F	1007	1PE	7	0
5	I	1009	1PE	1	0
5	K	1005	1PE	1	0
5	B	1005	1PE	2	0
5	L	1006	1PE	4	0
5	H	1009	1PE	3	0
4	A	1004	SO4	2	0
5	G	1009	1PE	2	0
6	G	1010	4TL	1	0
4	G	1004	SO4	1	0
3	G	1002	CO3	1	0
5	J	1008	1PE	1	0
5	G	1012	1PE	1	0
5	F	1008	1PE	4	0
4	C	1008	SO4	1	0
7	H	1007	DMS	1	0
5	A	1007	1PE	1	0
5	H	1008	1PE	1	0
4	I	1005	SO4	1	0
5	K	1007	1PE	2	0
5	I	1011	1PE	2	0
5	E	1010	1PE	1	0
5	G	1011	1PE	2	0
5	D	1008	1PE	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 then 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.

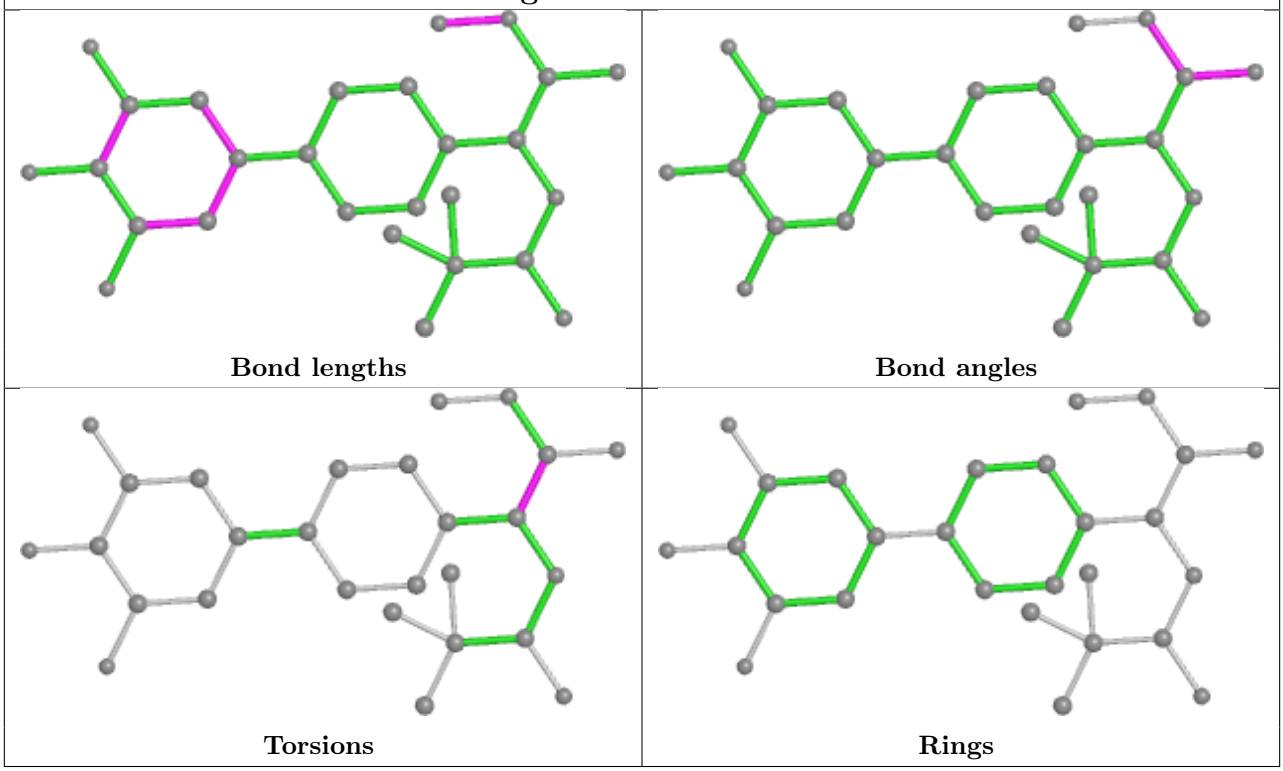
Ligand 4TL J 1011



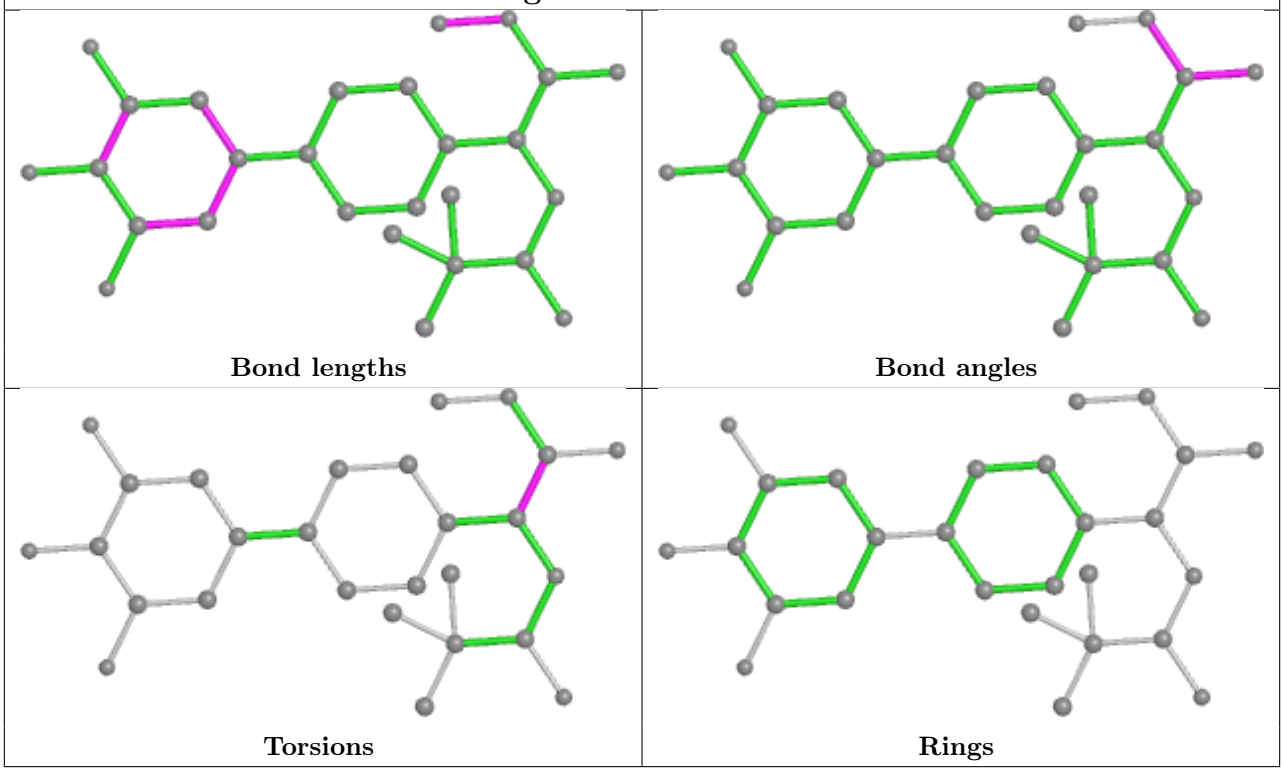
Ligand 4TL A 1008



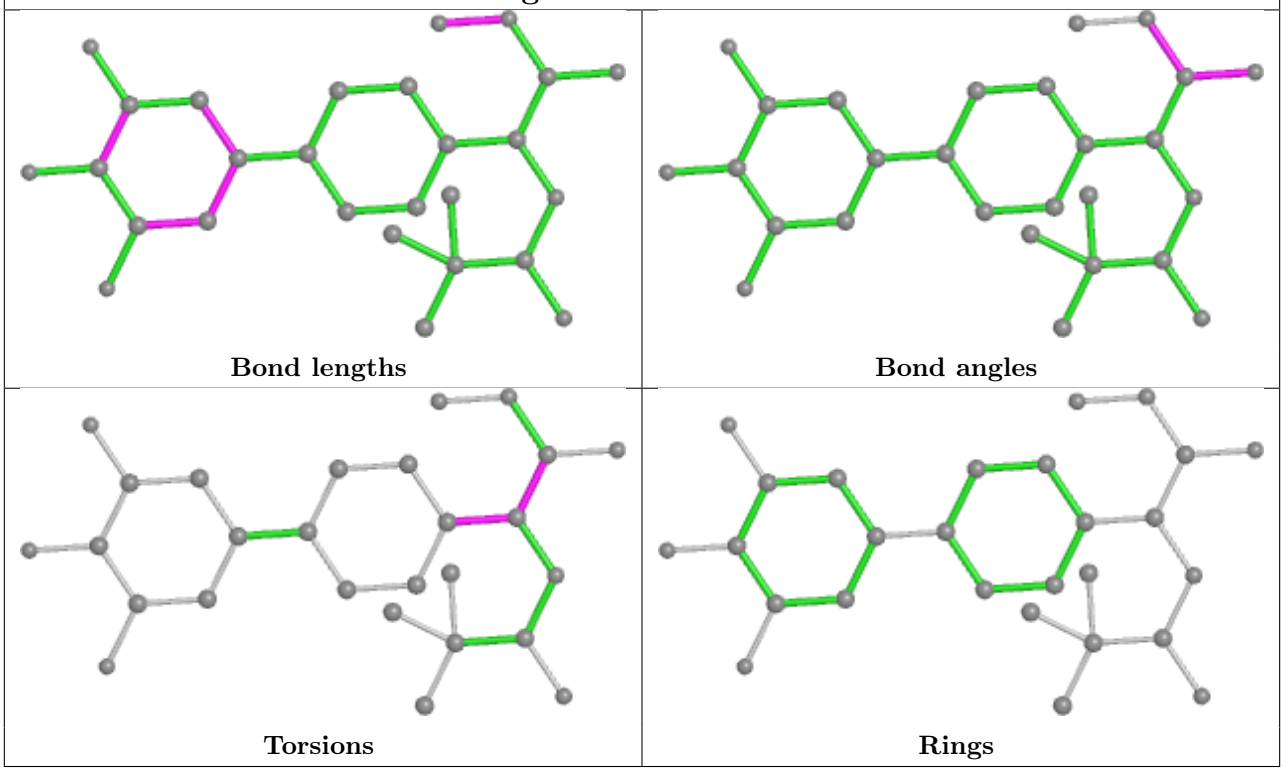
Ligand 4TL D 1009



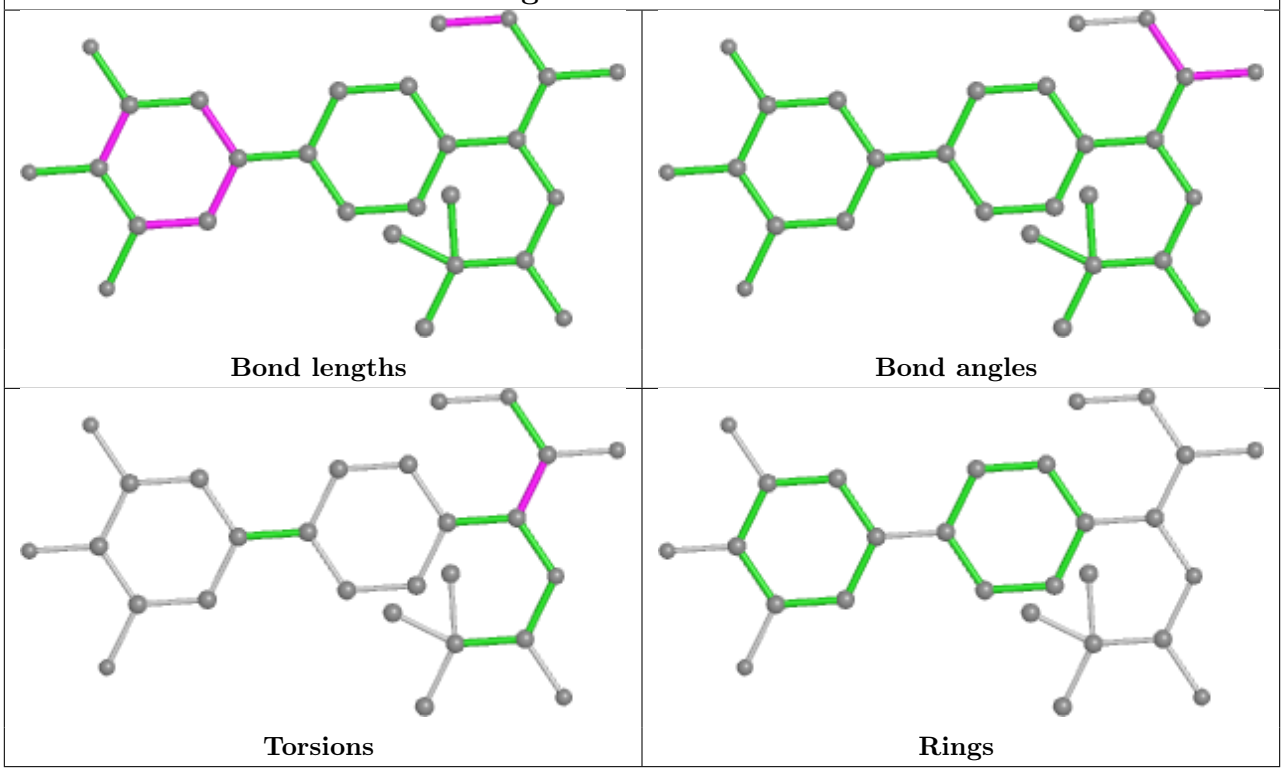
Ligand 4TL L 1008



Ligand 4TL B 1004



Ligand 4TL C 1011



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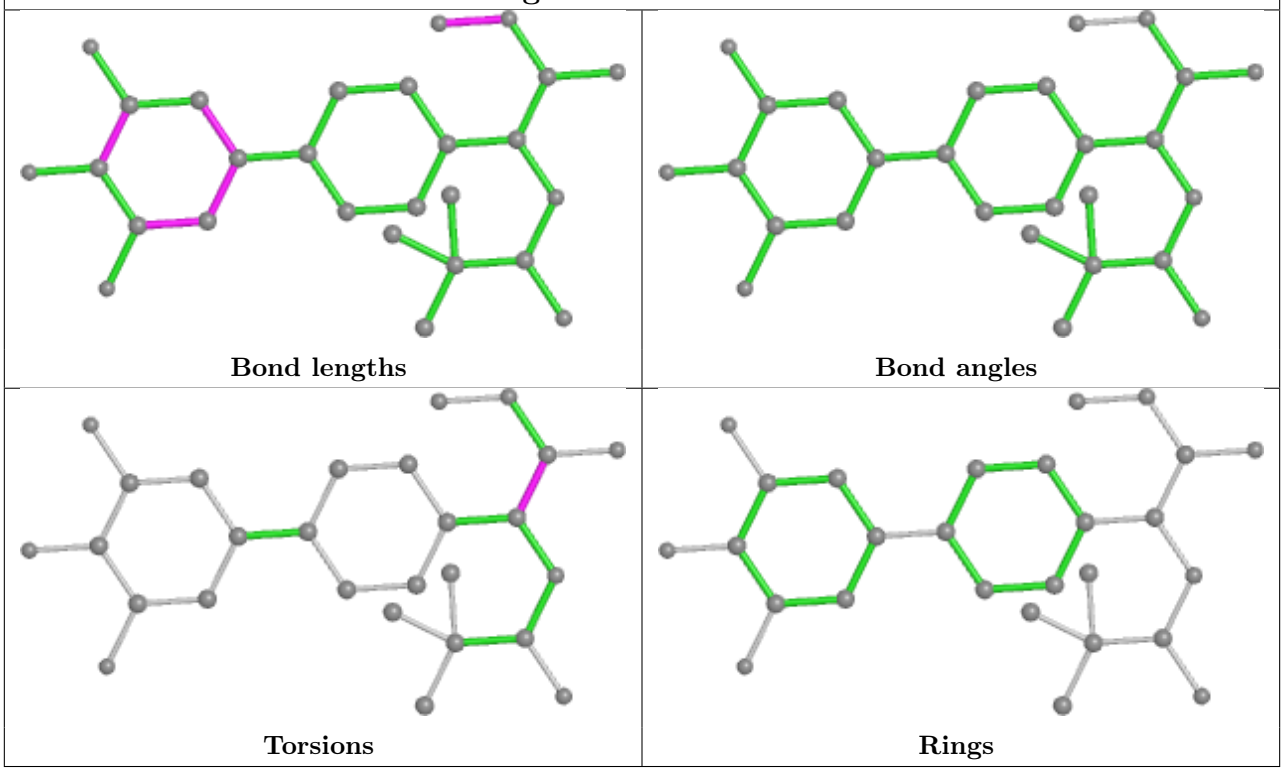
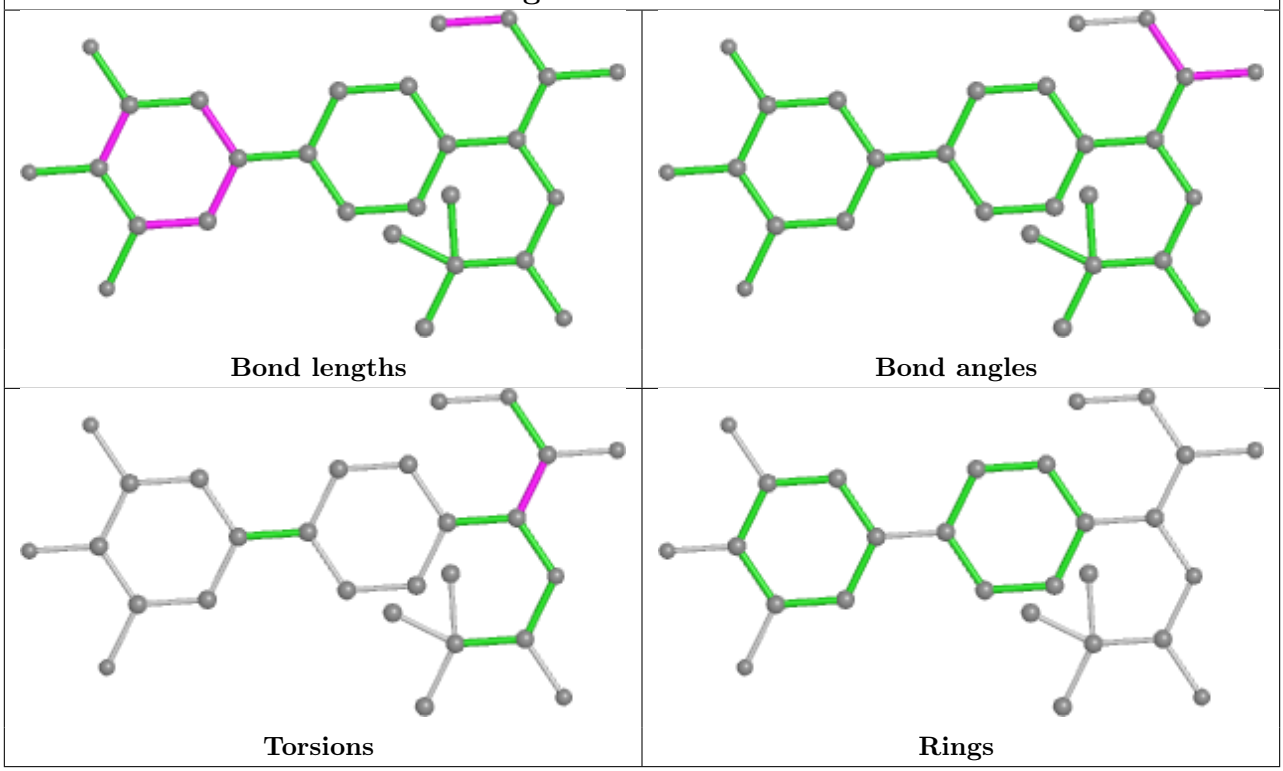
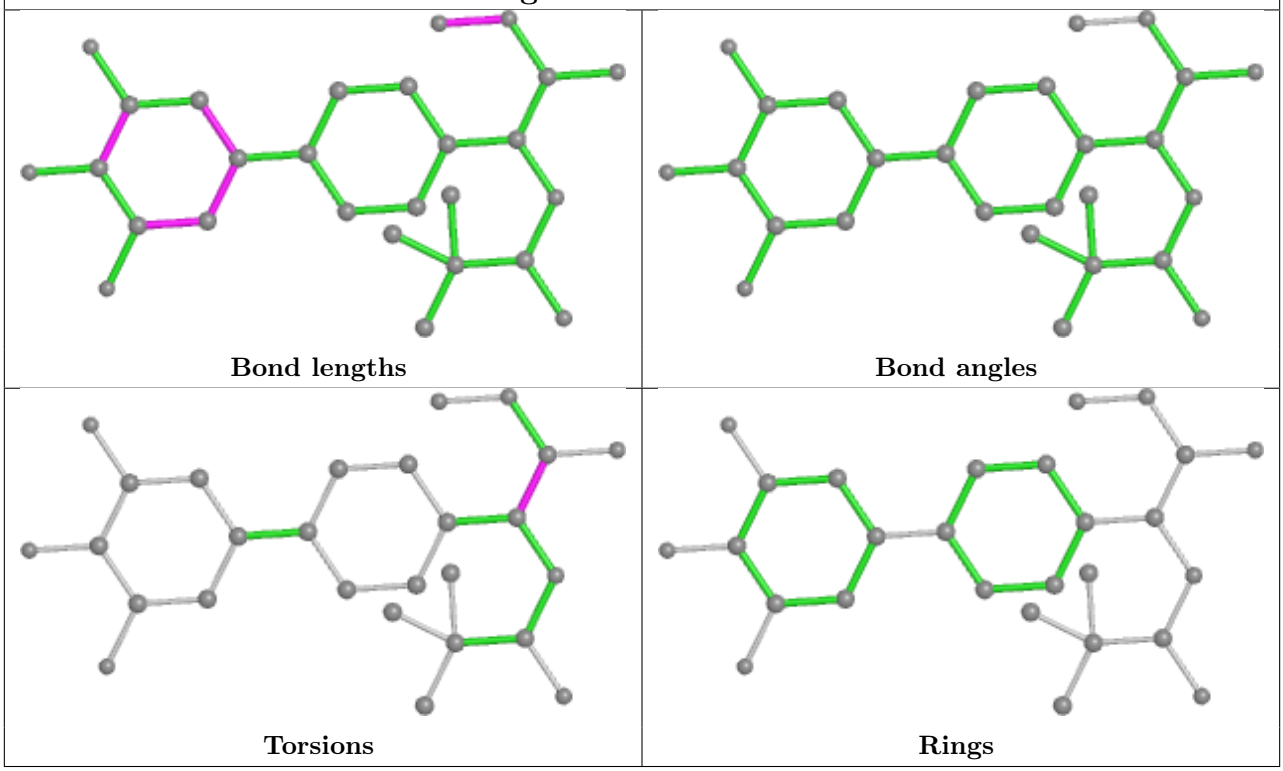


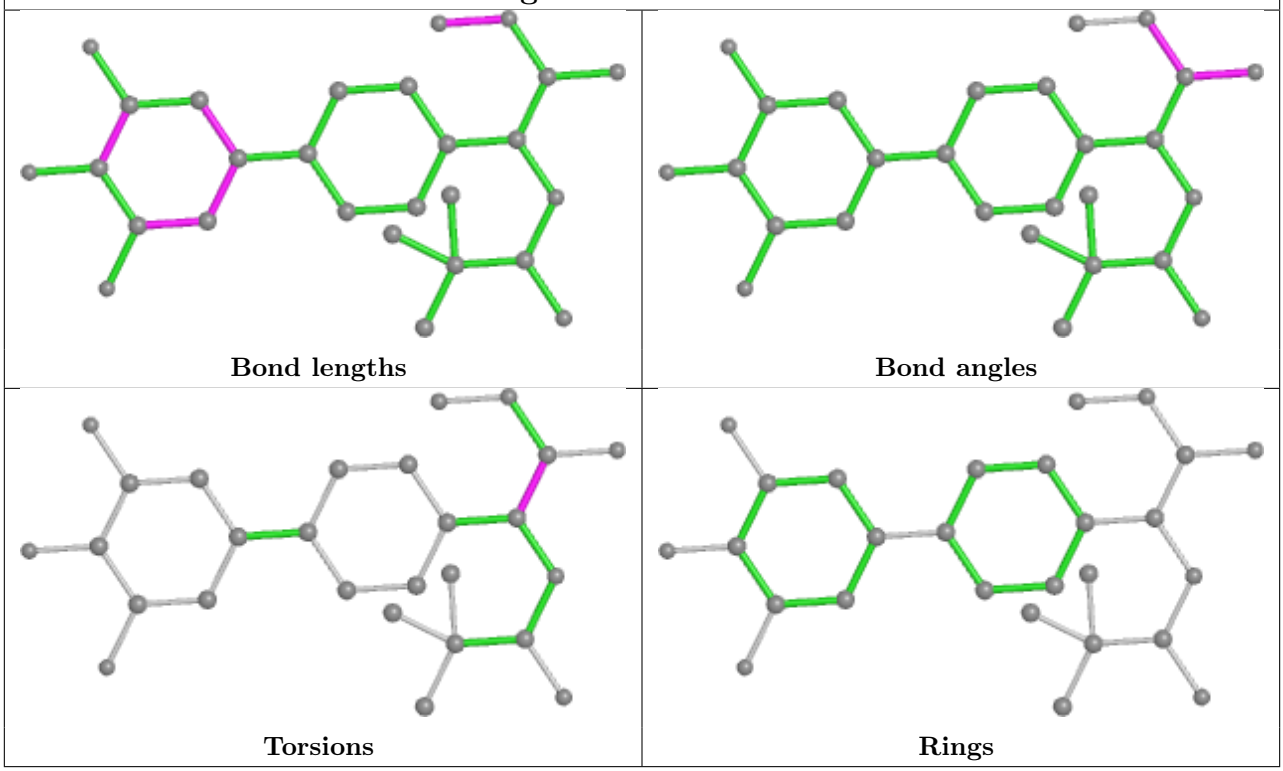
Ligand 4TL F 1009



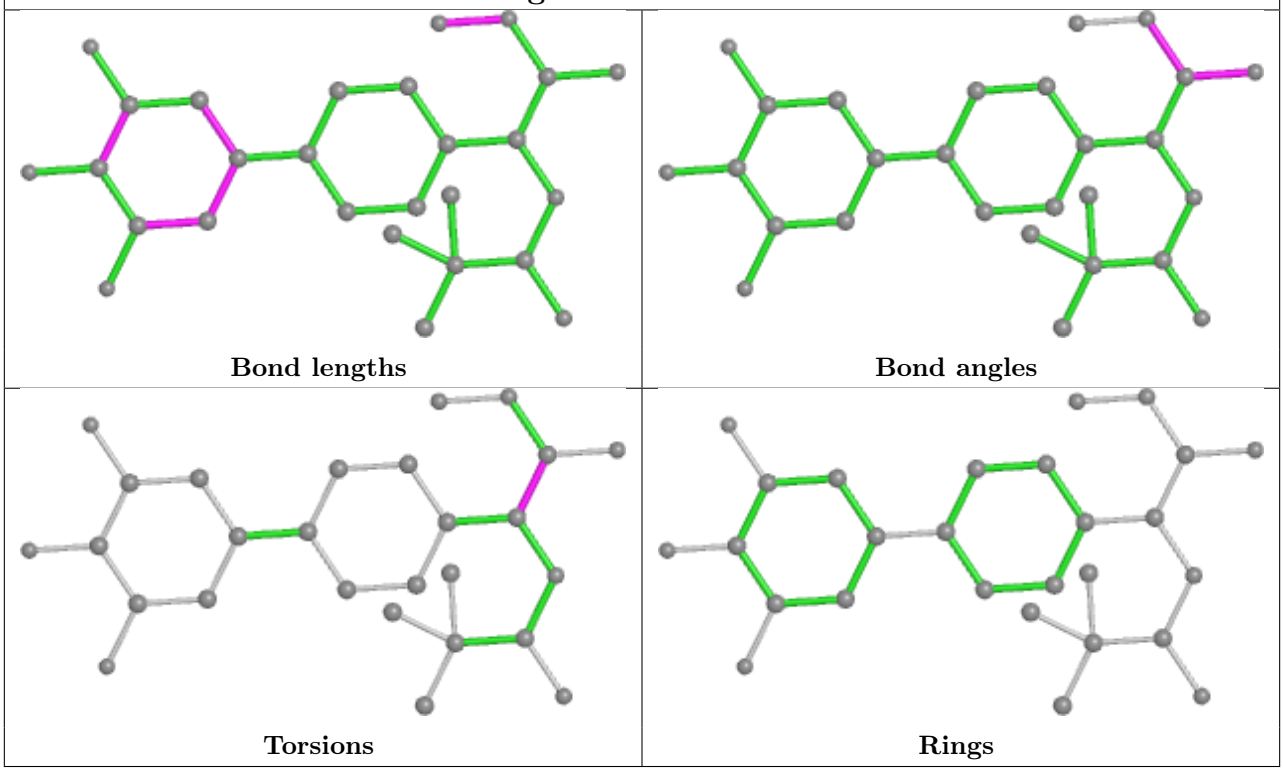
Ligand 4TL G 1010



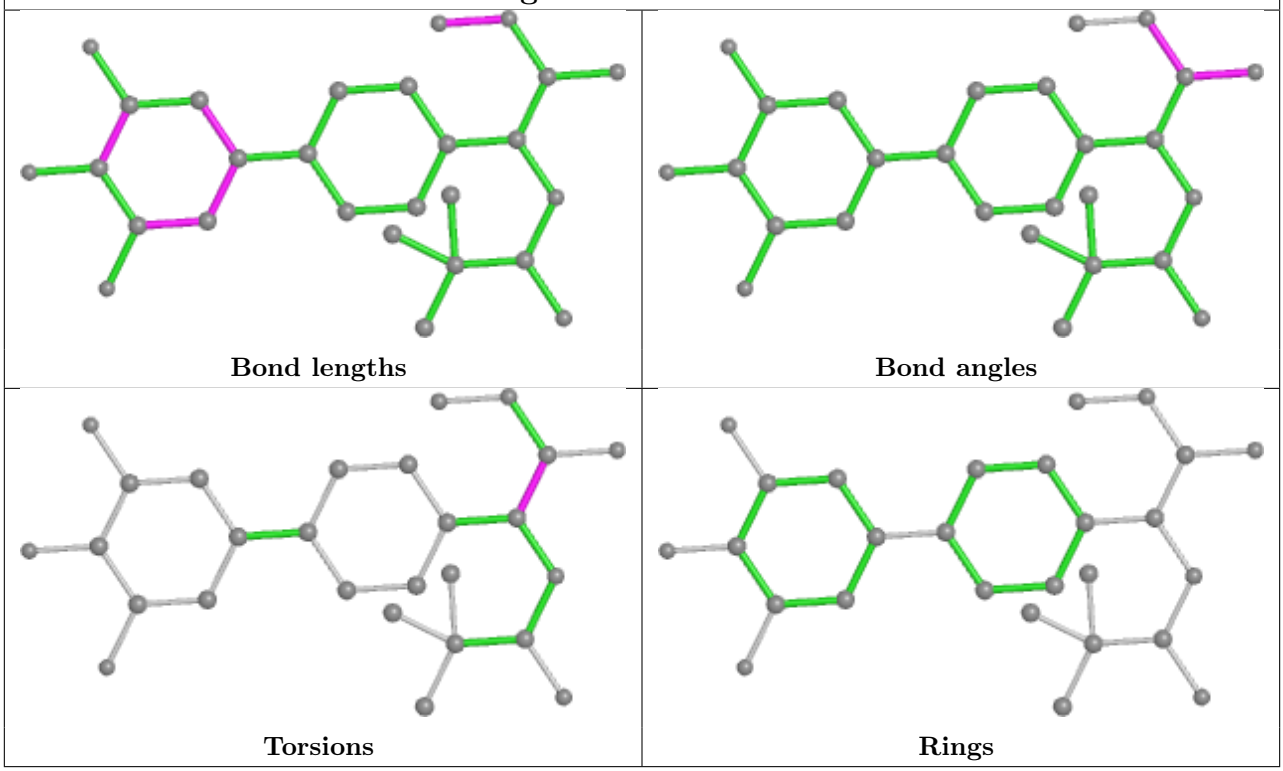
Ligand 4TL K 1008



Ligand 4TL I 1012



Ligand 4TL H 1006



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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	519/522 (99%)	-0.43	4 (0%)	86	88	10, 21, 43, 74	0
1	B	517/522 (99%)	-0.27	7 (1%)	75	78	11, 24, 57, 82	1 (0%)
1	C	518/522 (99%)	-0.37	7 (1%)	75	78	11, 22, 49, 87	0
1	D	513/522 (98%)	-0.58	1 (0%)	95	95	9, 20, 42, 76	0
1	E	513/522 (98%)	-0.54	6 (1%)	79	82	12, 20, 38, 82	0
1	F	512/522 (98%)	-0.32	7 (1%)	75	78	12, 25, 50, 77	0
1	G	518/522 (99%)	-0.42	5 (0%)	82	85	10, 20, 41, 73	0
1	H	518/522 (99%)	-0.22	6 (1%)	79	82	12, 25, 60, 84	1 (0%)
1	I	518/522 (99%)	-0.39	4 (0%)	86	88	10, 23, 49, 98	0
1	J	514/522 (98%)	-0.55	5 (0%)	82	85	12, 21, 43, 85	0
1	K	512/522 (98%)	-0.53	4 (0%)	86	88	12, 21, 39, 79	0
1	L	513/522 (98%)	-0.40	6 (1%)	79	82	13, 23, 49, 104	0
All	All	6185/6264 (98%)	-0.42	62 (1%)	82	85	9, 22, 49, 104	2 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	256	ASP	6.2
1	C	603	ASP	5.9
1	L	136	GLY	5.0
1	F	551	VAL	4.7
1	K	256	ASP	4.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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
5	1PE	J	1009	9/16	0.65	0.20	52,62,63,64	0
5	1PE	D	1007	10/16	0.72	0.20	54,56,65,66	0
5	1PE	B	1005	16/16	0.72	0.21	55,58,64,67	0
5	1PE	H	1009	14/16	0.74	0.20	43,55,69,69	0
5	1PE	L	1010	9/16	0.74	0.18	46,50,58,58	0
5	1PE	D	1008	10/16	0.76	0.17	45,48,60,60	0
5	1PE	K	1007	10/16	0.78	0.16	38,60,64,65	0
4	SO4	I	1008	5/5	0.78	0.23	94,95,98,98	0
4	SO4	E	1004	5/5	0.79	0.24	123,124,124,124	0
5	1PE	F	1008	10/16	0.80	0.16	41,54,61,63	0
4	SO4	C	1006	5/5	0.80	0.29	102,102,104,106	0
5	1PE	J	1008	10/16	0.80	0.16	45,49,59,60	0
5	1PE	D	1006	8/16	0.83	0.15	53,57,62,63	0
5	1PE	G	1012	10/16	0.83	0.15	50,52,59,61	0
5	1PE	E	1007	10/16	0.83	0.14	39,43,46,48	0
5	1PE	I	1009	10/16	0.83	0.12	38,41,45,46	0
5	1PE	F	1007	10/16	0.84	0.15	52,55,58,61	0
5	1PE	L	1006	10/16	0.84	0.16	42,55,62,63	0
5	1PE	I	1011	5/16	0.84	0.15	28,31,33,33	0
5	1PE	E	1010	7/16	0.85	0.12	39,41,43,44	0
4	SO4	A	1005	5/5	0.85	0.22	75,78,80,82	0
5	1PE	D	1005	8/16	0.86	0.13	31,35,44,44	0
4	SO4	I	1005	5/5	0.86	0.12	89,91,92,92	0
5	1PE	F	1011	7/16	0.86	0.17	39,41,45,46	0
5	1PE	L	1007	7/16	0.86	0.16	46,47,47,50	0
5	1PE	B	1006	9/16	0.86	0.18	41,44,55,56	0
7	DMS	L	1009	4/4	0.86	0.20	30,36,50,55	0
5	1PE	K	1006	6/16	0.87	0.11	38,40,42,43	0
5	1PE	H	1008	11/16	0.88	0.18	30,37,50,50	0
4	SO4	C	1005	5/5	0.88	0.20	108,109,110,111	0
5	1PE	F	1010	7/16	0.88	0.16	43,44,45,48	0
5	1PE	F	1006	10/16	0.89	0.11	38,41,46,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	1PE	G	1008	6/16	0.89	0.12	31,34,37,42	0
4	SO4	G	1006	5/5	0.89	0.31	64,68,70,72	0
4	SO4	E	1006	5/5	0.90	0.20	57,61,63,64	0
4	SO4	F	1005	5/5	0.90	0.27	74,75,77,81	0
5	1PE	C	1010	10/16	0.90	0.10	42,46,53,53	0
4	SO4	G	1005	5/5	0.90	0.15	54,59,63,69	0
5	1PE	G	1007	6/16	0.91	0.18	34,37,40,48	0
5	1PE	A	1006	7/16	0.91	0.12	47,49,51,52	0
5	1PE	C	1009	12/16	0.91	0.14	32,37,46,48	0
5	1PE	I	1010	9/16	0.92	0.11	23,29,41,45	0
5	1PE	J	1010	7/16	0.92	0.12	36,41,45,45	0
4	SO4	D	1004	5/5	0.92	0.21	78,78,80,81	0
5	1PE	G	1011	10/16	0.92	0.15	29,33,46,51	0
4	SO4	C	1007	5/5	0.93	0.19	64,70,74,75	0
4	SO4	C	1008	5/5	0.93	0.19	58,60,63,66	0
5	1PE	K	1005	10/16	0.93	0.11	21,32,53,55	0
4	SO4	J	1005	5/5	0.93	0.24	88,90,91,93	0
4	SO4	J	1006	5/5	0.93	0.19	56,57,60,66	0
4	SO4	K	1004	5/5	0.93	0.21	63,66,70,70	0
4	SO4	H	1005	5/5	0.93	0.25	78,79,80,83	0
5	1PE	A	1007	10/16	0.93	0.16	30,34,39,43	0
7	DMS	A	1009	4/4	0.93	0.14	16,29,47,49	0
7	DMS	H	1007	4/4	0.93	0.16	19,57,68,69	0
4	SO4	I	1004	5/5	0.93	0.22	72,73,76,78	0
4	SO4	I	1007	5/5	0.94	0.21	67,68,69,74	0
4	SO4	I	1006	5/5	0.94	0.14	55,59,63,65	0
5	1PE	J	1007	11/16	0.94	0.09	27,34,48,51	0
5	1PE	G	1009	7/16	0.94	0.09	41,44,48,52	0
5	1PE	E	1008	10/16	0.94	0.10	23,27,44,45	0
6	4TL	G	1010	27/27	0.95	0.11	11,19,27,28	0
6	4TL	I	1012	27/27	0.95	0.11	17,20,26,31	0
6	4TL	L	1008	27/27	0.95	0.10	11,19,26,27	0
5	1PE	L	1005	10/16	0.95	0.11	23,36,46,51	0
6	4TL	E	1009	27/27	0.95	0.10	10,20,26,31	0
6	4TL	F	1009	27/27	0.95	0.10	12,19,28,30	0
6	4TL	D	1009	27/27	0.96	0.09	12,20,29,30	0
6	4TL	J	1011	27/27	0.96	0.08	9,21,27,29	0
6	4TL	K	1008	27/27	0.96	0.10	13,19,27,29	0
4	SO4	L	1004	5/5	0.96	0.15	58,62,62,64	0
4	SO4	G	1004	5/5	0.96	0.17	64,65,66,67	0
6	4TL	B	1004	27/27	0.96	0.10	13,18,27,31	0
6	4TL	H	1006	27/27	0.96	0.10	11,18,28,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	4TL	A	1008	27/27	0.97	0.10	9,18,25,29	0
4	SO4	A	1004	5/5	0.97	0.14	58,59,60,62	0
6	4TL	C	1011	27/27	0.97	0.09	12,17,26,28	0
3	CO3	A	1002	4/4	0.97	0.09	14,15,16,17	0
4	SO4	E	1005	5/5	0.97	0.13	61,64,67,67	0
3	CO3	J	1002	4/4	0.98	0.07	12,15,16,18	0
3	CO3	L	1002	4/4	0.98	0.11	12,14,15,17	0
3	CO3	B	1002	4/4	0.98	0.07	12,14,16,18	0
3	CO3	D	1002	4/4	0.98	0.09	11,14,14,17	0
3	CO3	G	1002	4/4	0.98	0.08	18,18,20,23	0
3	CO3	I	1002	4/4	0.99	0.06	15,16,20,22	0
4	SO4	J	1004	5/5	0.99	0.05	10,15,19,20	0
2	ZN	L	1001	1/1	0.99	0.07	17,17,17,17	0
3	CO3	K	1002	4/4	0.99	0.05	15,17,17,19	0
4	SO4	F	1004	5/5	0.99	0.07	16,16,18,19	0
2	ZN	B	1003	1/1	0.99	0.06	15,15,15,15	0
2	ZN	D	1001	1/1	0.99	0.06	17,17,17,17	0
3	CO3	C	1002	4/4	0.99	0.05	13,15,19,19	0
4	SO4	C	1004	5/5	0.99	0.07	14,16,20,20	0
4	SO4	H	1004	5/5	0.99	0.07	16,16,20,21	0
2	ZN	F	1001	1/1	0.99	0.08	20,20,20,20	0
3	CO3	E	1002	4/4	0.99	0.10	16,19,22,24	0
3	CO3	F	1002	4/4	0.99	0.10	18,19,19,20	0
2	ZN	I	1003	1/1	0.99	0.07	18,18,18,18	0
3	CO3	H	1002	4/4	0.99	0.06	14,15,16,16	0
2	ZN	L	1003	1/1	1.00	0.07	17,17,17,17	0
2	ZN	C	1003	1/1	1.00	0.06	14,14,14,14	0
2	ZN	A	1003	1/1	1.00	0.09	15,15,15,15	0
2	ZN	D	1003	1/1	1.00	0.07	16,16,16,16	0
2	ZN	E	1001	1/1	1.00	0.07	17,17,17,17	0
2	ZN	E	1003	1/1	1.00	0.08	18,18,18,18	0
2	ZN	B	1001	1/1	1.00	0.05	17,17,17,17	0
2	ZN	F	1003	1/1	1.00	0.09	19,19,19,19	0
2	ZN	G	1001	1/1	1.00	0.09	15,15,15,15	0
2	ZN	G	1003	1/1	1.00	0.09	16,16,16,16	0
2	ZN	H	1001	1/1	1.00	0.05	18,18,18,18	0
2	ZN	H	1003	1/1	1.00	0.06	17,17,17,17	0
2	ZN	I	1001	1/1	1.00	0.09	16,16,16,16	0
2	ZN	A	1001	1/1	1.00	0.08	18,18,18,18	0
2	ZN	J	1001	1/1	1.00	0.07	17,17,17,17	0
2	ZN	J	1003	1/1	1.00	0.07	17,17,17,17	0
2	ZN	K	1001	1/1	1.00	0.08	19,19,19,19	0

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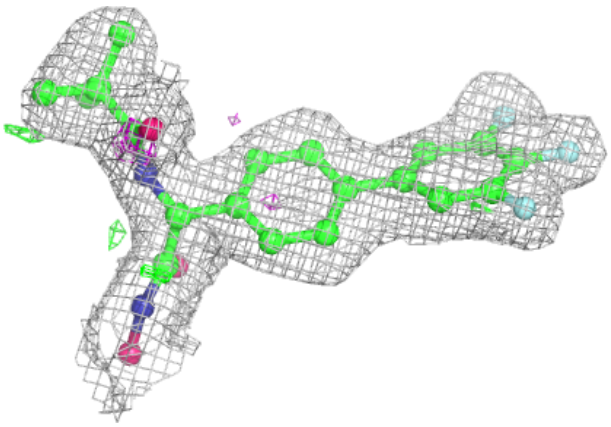
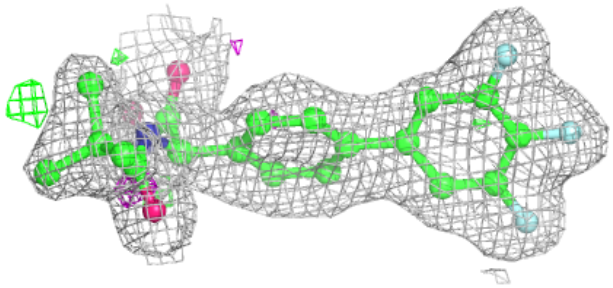
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	K	1003	1/1	1.00	0.07	16,16,16,16	0
2	ZN	C	1001	1/1	1.00	0.08	16,16,16,16	0

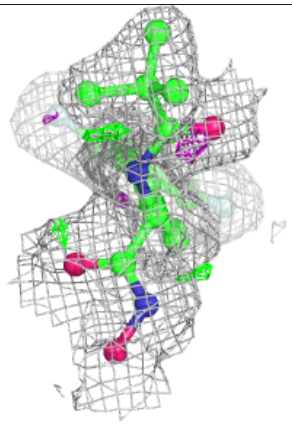
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4TL G 1010:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

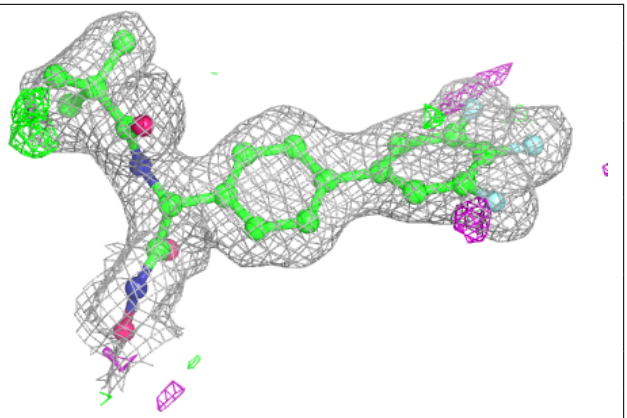


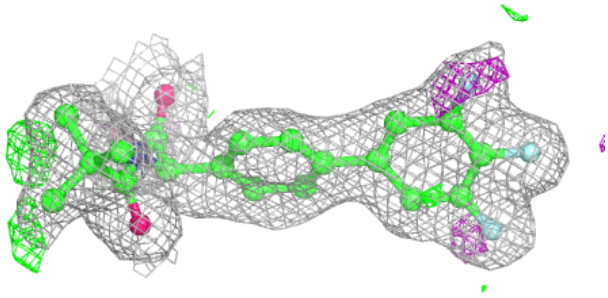


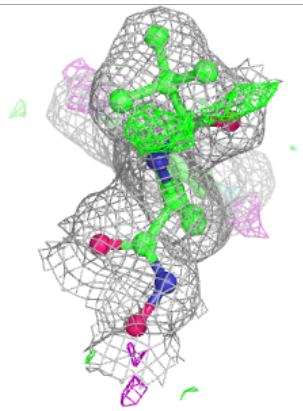


Electron density around 4TL I 1012:

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

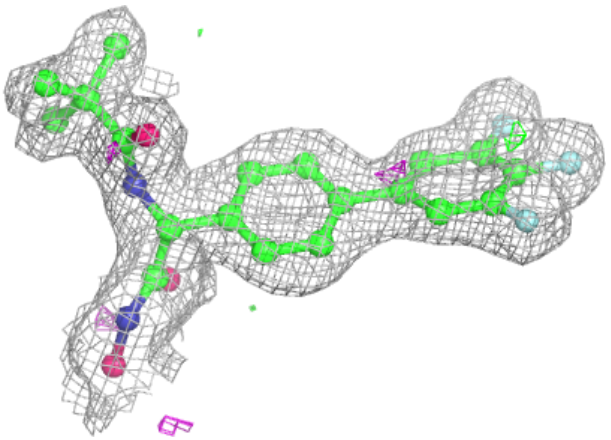


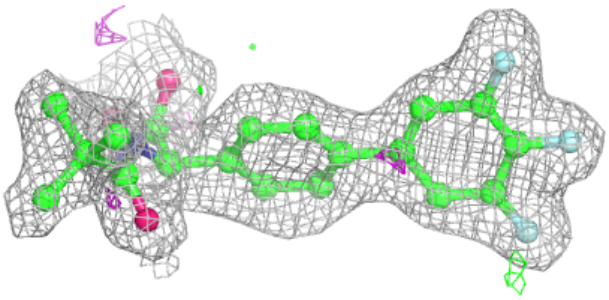


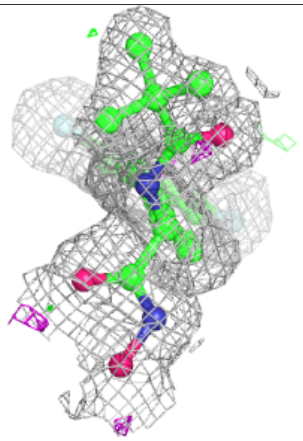


Electron density around 4TL L 1008:

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

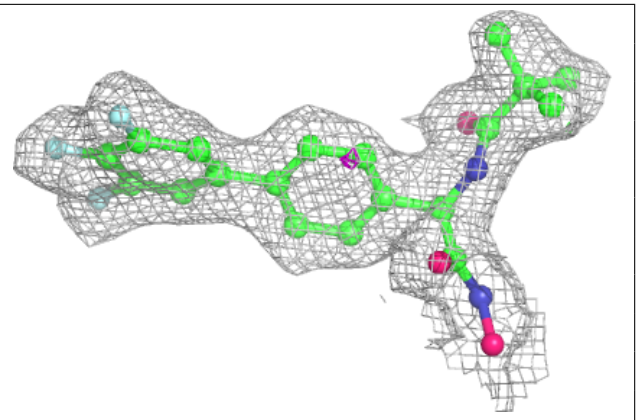


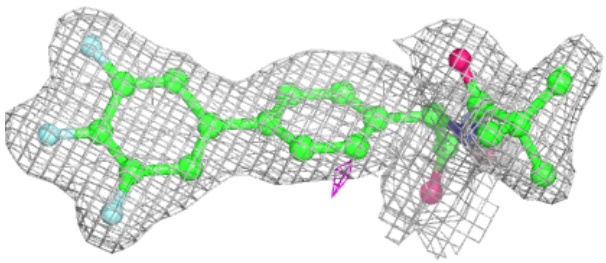


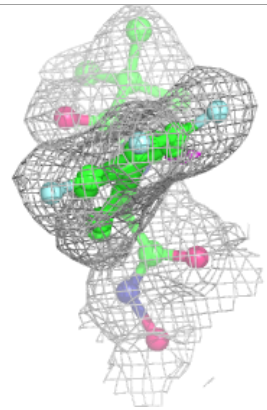


Electron density around 4TL E 1009:

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

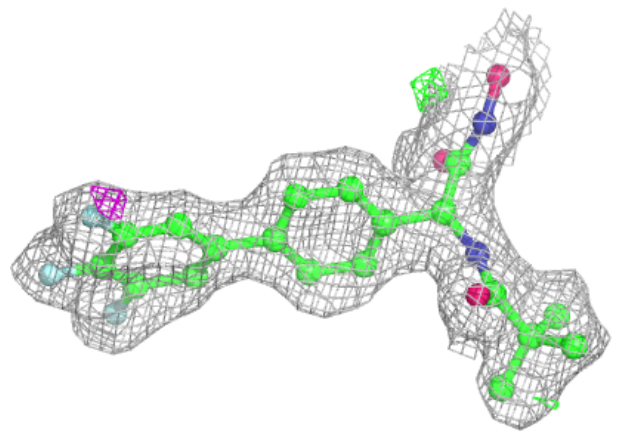


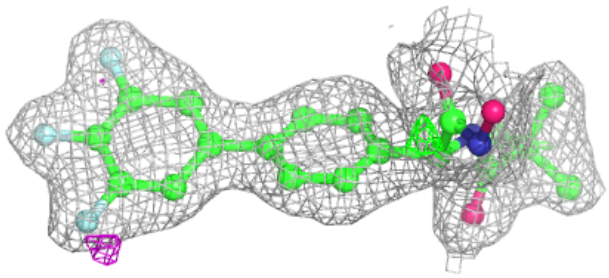


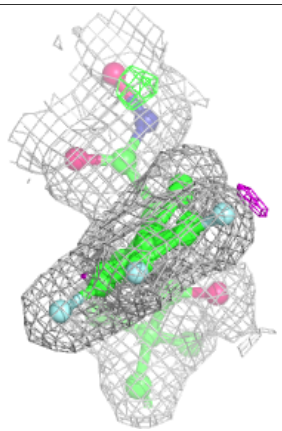


Electron density around 4TL F 1009:

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

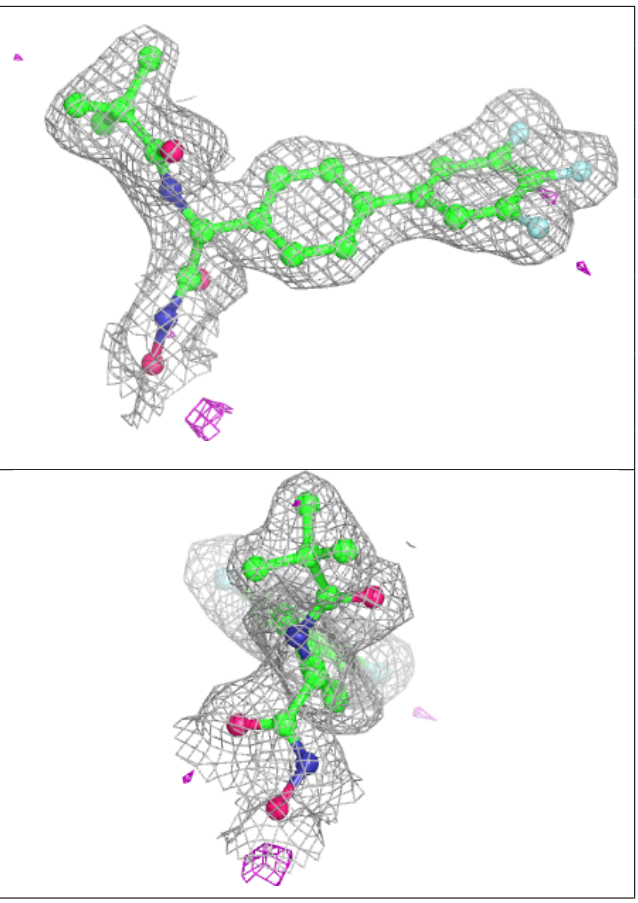


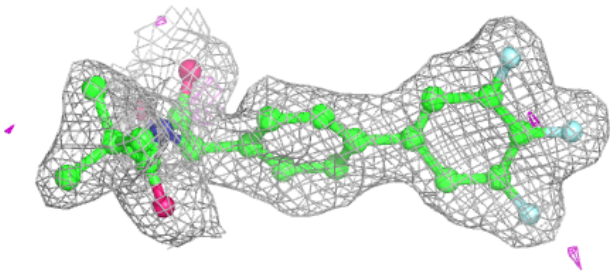




Electron density around 4TL D 1009:

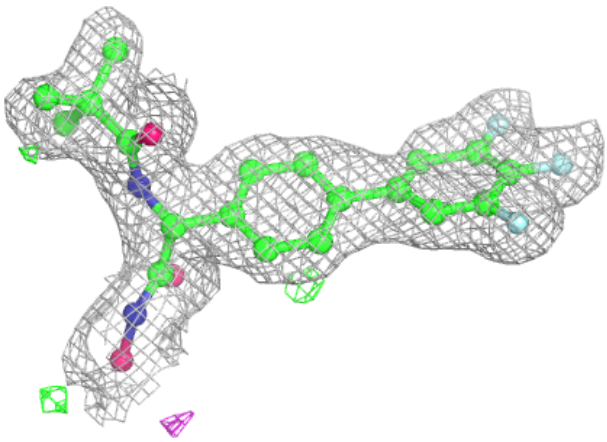
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

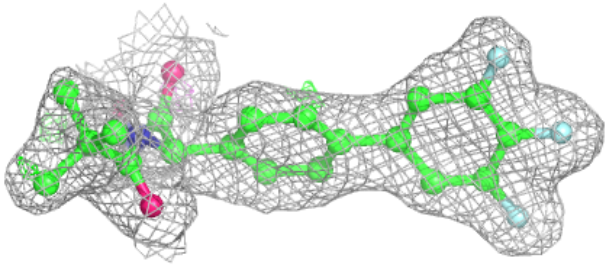


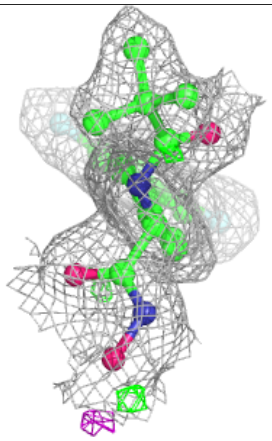


Electron density around 4TL J 1011:

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

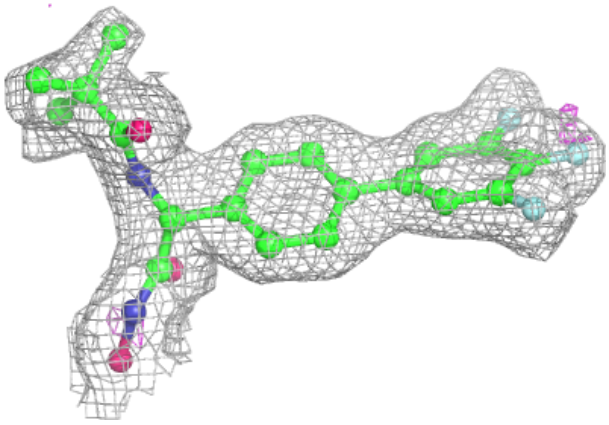


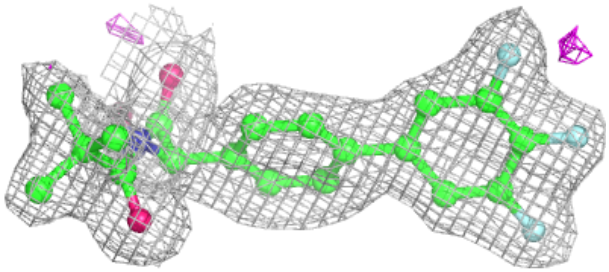


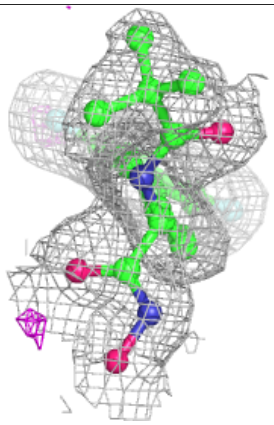


Electron density around 4TL K 1008:

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

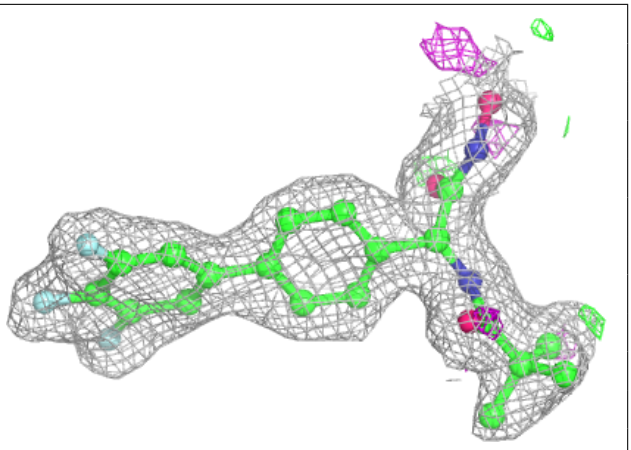


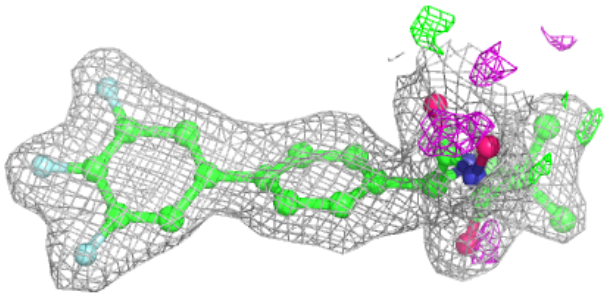


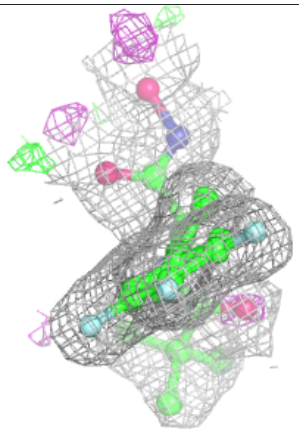


Electron density around 4TL B 1004:

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

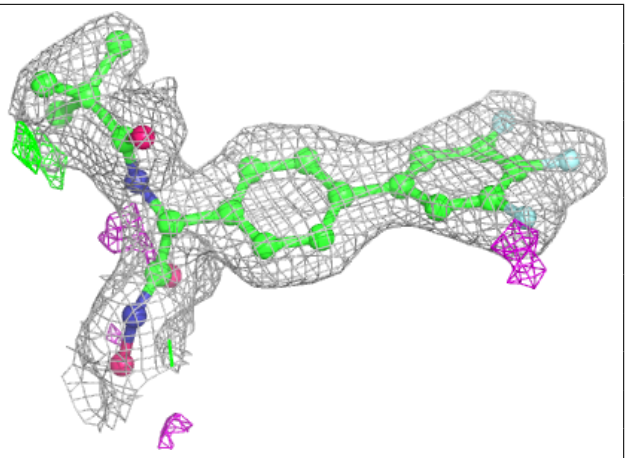


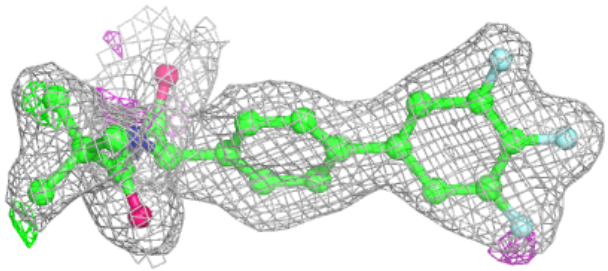


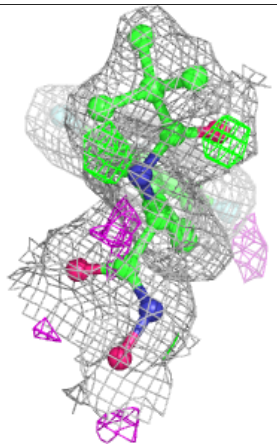


Electron density around 4TL H 1006:

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

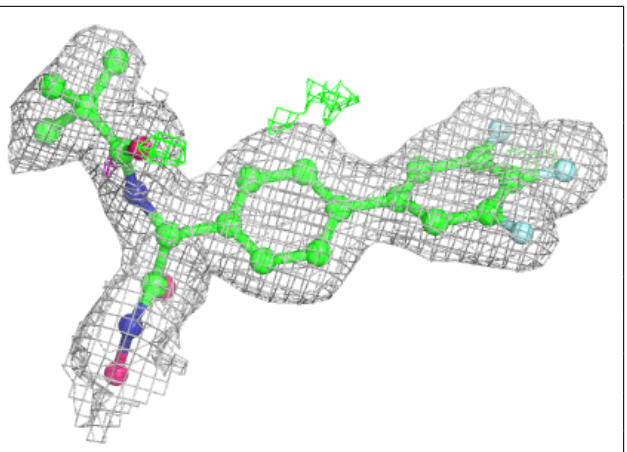


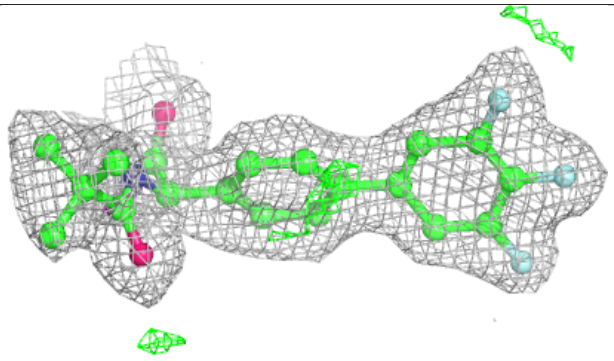


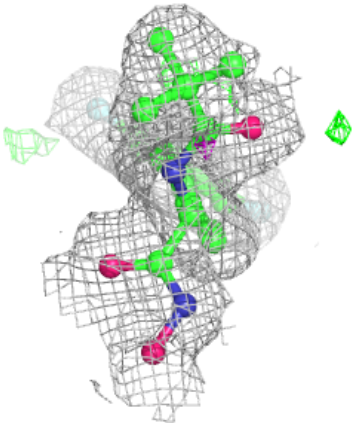


Electron density around 4TL A 1008:

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

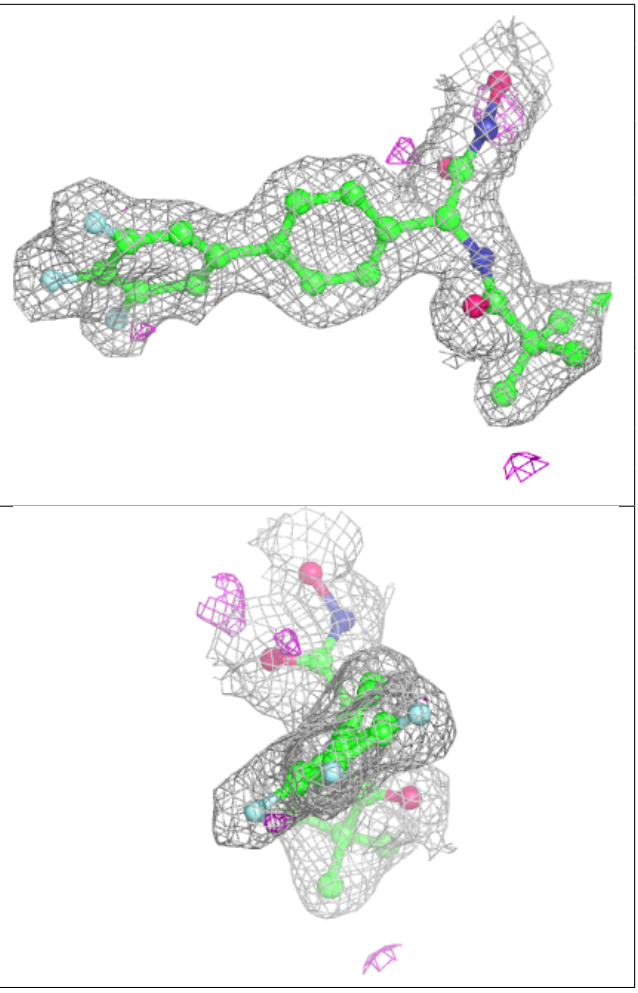






Electron density around 4TL C 1011:

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.