



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 2, 2020 – 09:09 am BST

PDB ID : 5EJ7
Title : EcMenD-ThDP-Mn²⁺ complex soaked with 2-ketoglutarate for 21 s
Authors : Song, H.G.; Dong, C.; Chen, Y.Z.; Sun, Y.R.; Guo, Z.H.
Deposited on : 2015-11-01
Resolution : 1.56 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

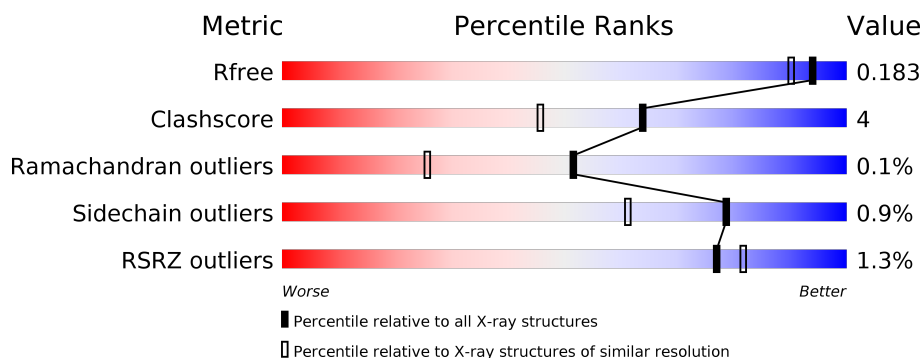
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 8%, green 90%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 92% 8% </div> </div>
1	B	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 6%, green 94%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 94% 6% </div> </div>
1	C	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 8%, green 90%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 92% 8% </div> </div>
1	D	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 10%, green 86%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 3% 90% 10% </div> </div>
1	E	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 7%, green 91%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 92% 7% </div> </div>
1	F	556	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 8%, green 90%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 92% 8% </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	556	<div><div>%</div><div><div></div><div>92%</div><div>8%</div></div></div>
1	H	556	<div><div>2%</div><div><div></div><div>92%</div><div>8%</div></div></div>

2 Entry composition

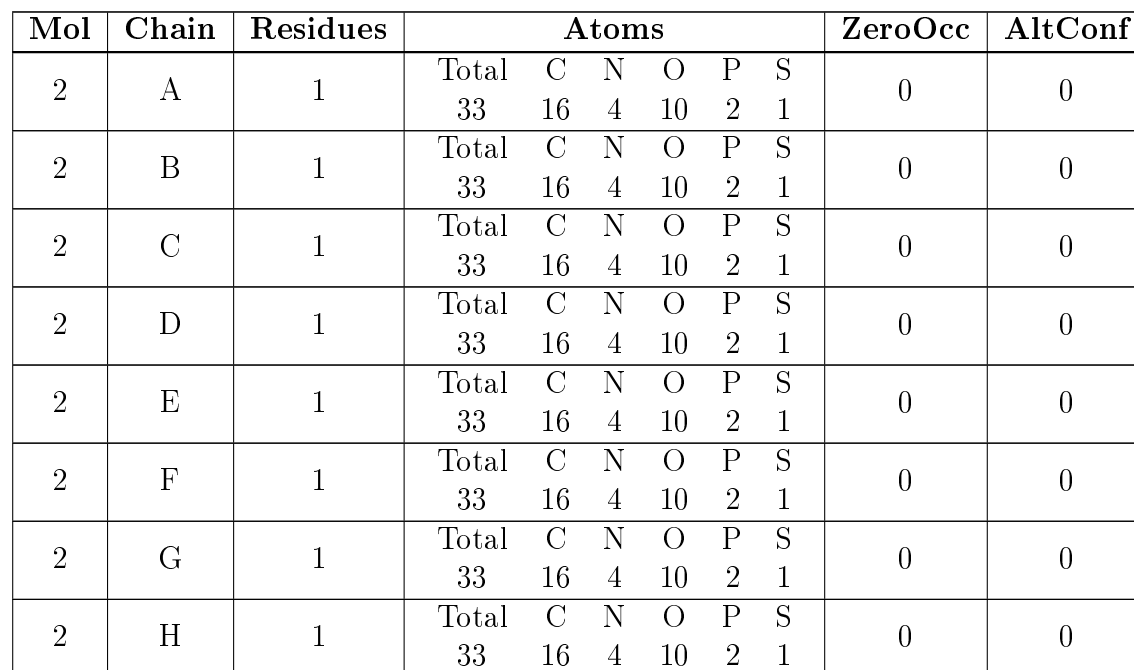
There are 5 unique types of molecules in this entry. The entry contains 42054 atoms, of which 48 are hydrogens and 0 are deuteriums.

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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	20	0
			4501	2847	820	820	14			
1	B	556	Total	C	N	O	S	0	11	0
			4424	2805	804	801	14			
1	C	556	Total	C	N	O	S	0	14	0
			4437	2810	804	809	14			
1	D	556	Total	C	N	O	S	0	11	0
			4433	2806	807	805	15			
1	E	556	Total	C	N	O	S	0	17	0
			4468	2828	815	811	14			
1	F	556	Total	C	N	O	S	0	8	0
			4387	2782	796	795	14			
1	G	556	Total	C	N	O	S	0	16	0
			4459	2827	811	807	14			
1	H	556	Total	C	N	O	S	0	12	0
			4429	2807	800	808	14			

- Molecule 2 is (4S)-4-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-(2-{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}ethyl)-4-methyl-1,3lambda 5 -thiazol-2-yl}-4-hydroxybutanoic acid (three-letter code: TD6) (formula: C₁₆H₂₅N₄O₁₀P₂S).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | G | 2 | Total Mn
2 2 | 0 | 0 |
| 3 | D | 1 | Total Mn
1 1 | 0 | 0 |
| 3 | E | 1 | Total Mn
1 1 | 0 | 0 |
| 3 | H | 1 | Total Mn
1 1 | 0 | 0 |



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			6	3	3			
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	O		0	0
			6	3	3			
4	C	1	Total	C	O		0	0
			6	3	3			
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	O		0	0
			6	3	3			
4	D	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C H O 14 3 8 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	G	1	Total C H O 14 3 8 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C H O 14 3 8 3	0	0

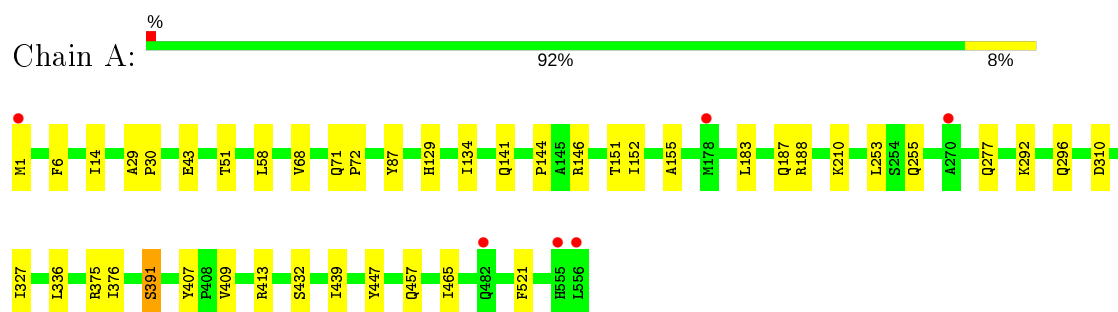
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	813	Total O 813 813	0	0
5	B	808	Total O 808 808	0	0
5	C	774	Total O 774 774	0	0
5	D	711	Total O 711 711	0	0
5	E	777	Total O 777 777	0	0
5	F	789	Total O 789 789	0	0
5	G	758	Total O 758 758	0	0
5	H	681	Total O 681 681	0	0

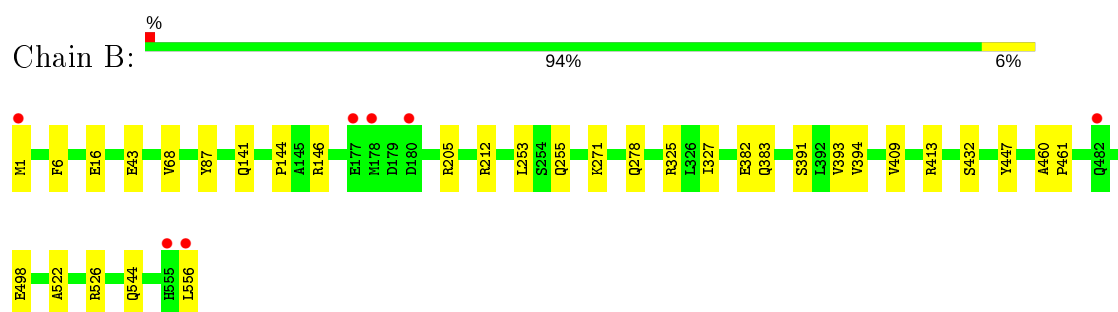
3 Residue-property plots [i](#)

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.

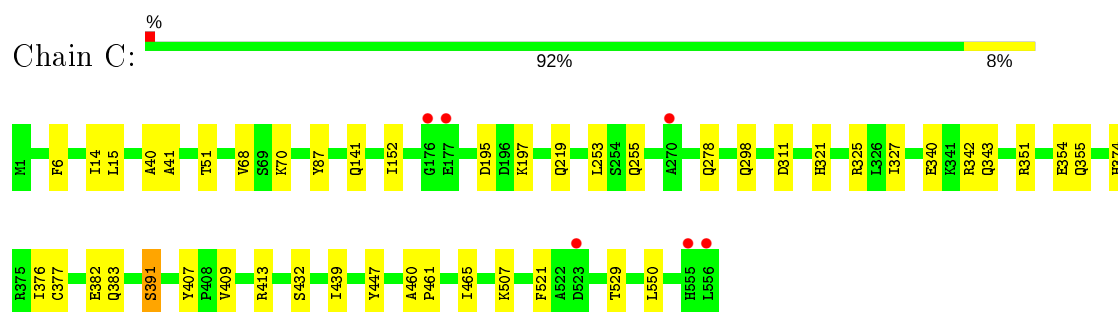
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



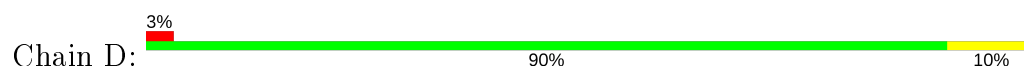
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

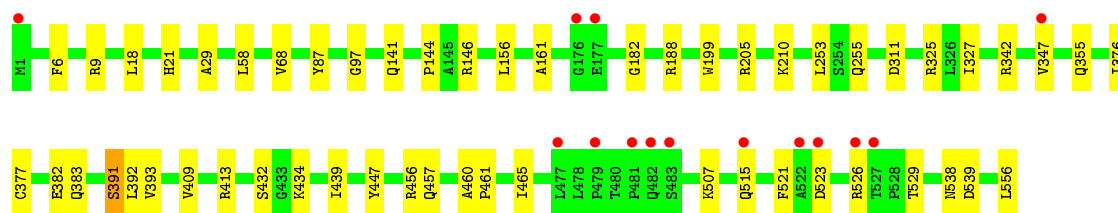


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

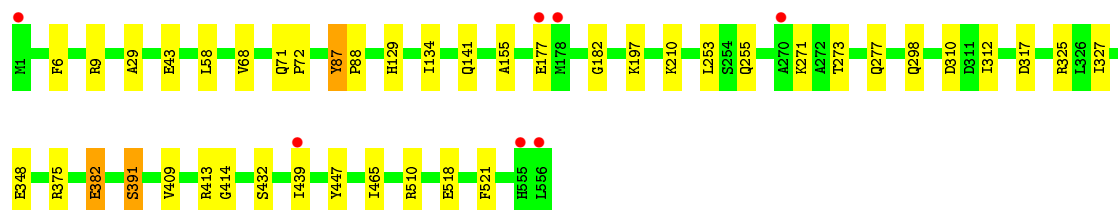


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

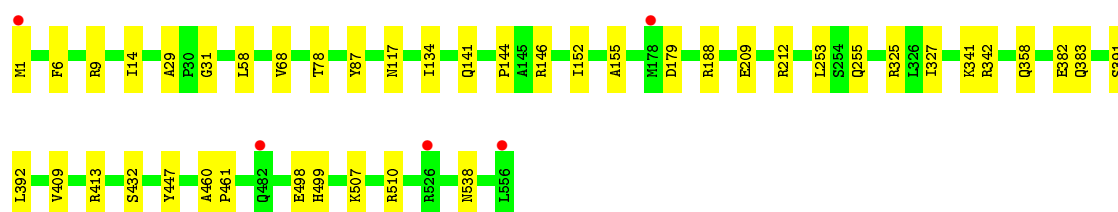
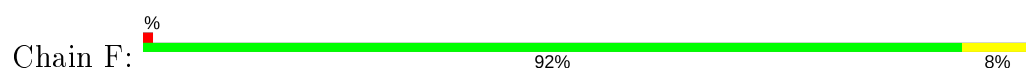




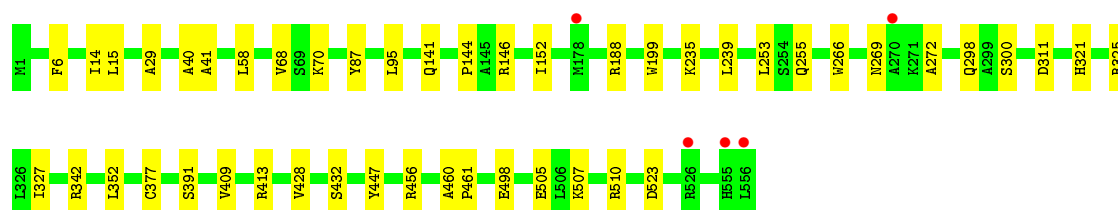
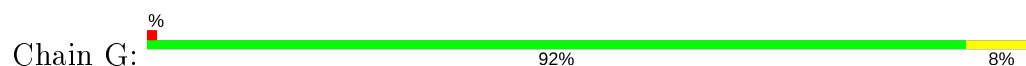
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



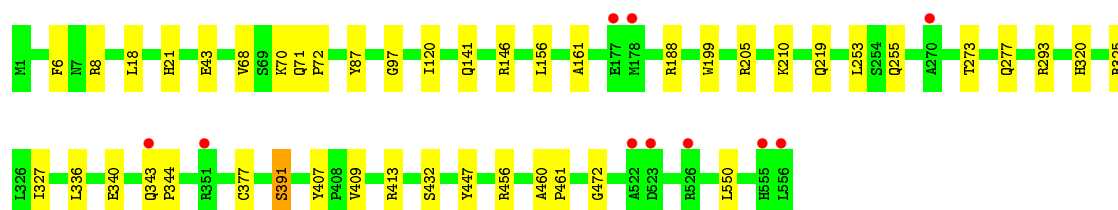
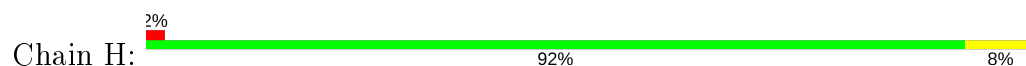
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.60Å 90.61Å 167.57Å 76.08° 83.45° 63.44°	Depositor
Resolution (Å)	32.45 – 1.56 32.45 – 1.56	Depositor EDS
% Data completeness (in resolution range)	96.0 (32.45-1.56) 95.4 (32.45-1.56)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 1.56Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.146 , 0.183 0.147 , 0.183	Depositor DCC
R_{free} test set	32112 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	42054	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, MN, TD6

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	0.36	0/4610	0.54	2/6286 (0.0%)
1	B	0.33	0/4532	0.52	0/6179
1	C	0.33	0/4546	0.51	0/6201
1	D	0.31	0/4542	0.50	0/6191
1	E	0.34	0/4578	0.53	1/6243 (0.0%)
1	F	0.32	0/4495	0.51	0/6131
1	G	0.32	0/4568	0.50	0/6230
1	H	0.36	1/4539 (0.0%)	0.50	0/6192
All	All	0.33	1/36410 (0.0%)	0.51	3/49653 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	472	GLY	C-O	-5.50	1.14	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	375	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	E	375	ARG	NE-CZ-NH1	-5.19	117.70	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	4501	0	4447	31	0
1	B	4424	0	4396	20	1
1	C	4437	0	4378	40	0
1	D	4433	0	4384	39	0
1	E	4468	0	4415	33	0
1	F	4387	0	4347	35	0
1	G	4459	0	4413	43	0
1	H	4429	0	4361	35	0
2	A	33	0	21	4	0
2	B	33	0	21	5	0
2	C	33	0	21	4	0
2	D	33	0	21	5	0
2	E	33	0	21	4	0
2	F	33	0	21	5	0
2	G	33	0	21	4	0
2	H	33	0	21	4	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	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
4	A	12	8	16	1	0
4	B	6	0	8	0	0
4	C	12	8	16	2	0
4	D	12	8	16	0	0
4	E	12	8	16	0	0
4	F	6	0	8	0	0
4	G	12	8	16	0	0
4	H	12	8	16	0	0
5	A	813	0	0	10	0
5	B	808	0	0	8	3
5	C	774	0	0	15	4
5	D	711	0	0	14	0
5	E	777	0	0	15	0
5	F	789	0	0	14	0
5	G	758	0	0	13	0
5	H	681	0	0	6	0
All	All	42006	48	35421	303	4

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 303 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)
2:B:601:TD6:H11	2:B:601:TD6:HN4A	1.22	1.03
2:G:601:TD6:HN4A	2:G:601:TD6:H11	1.19	1.02
2:E:601:TD6:H11	2:E:601:TD6:HN4A	1.24	1.01
2:F:601:TD6:H11	2:F:601:TD6:HN4A	1.26	0.97
2:H:601:TD6:H11	2:H:601:TD6:HN4A	1.32	0.94

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLU:OE2	5:C:6101:HOH:O[1_645]	2.14	0.06
5:B:1020:HOH:O	5:C:6101:HOH:O[1_645]	2.14	0.06
5:B:898:HOH:O	5:C:6101:HOH:O[1_645]	2.17	0.03
5:B:1380:HOH:O	5:C:6119:HOH:O[1_645]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	574/556 (103%)	561 (98%)	12 (2%)	1 (0%)	47	23
1	B	565/556 (102%)	551 (98%)	14 (2%)	0	100	100
1	C	568/556 (102%)	556 (98%)	11 (2%)	1 (0%)	47	23
1	D	566/556 (102%)	555 (98%)	10 (2%)	1 (0%)	47	23
1	E	571/556 (103%)	559 (98%)	11 (2%)	1 (0%)	47	23
1	F	562/556 (101%)	549 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	571/556 (103%)	557 (98%)	14 (2%)	0	100	100
1	H	567/556 (102%)	553 (98%)	13 (2%)	1 (0%)	47	23
All	All	4544/4448 (102%)	4441 (98%)	98 (2%)	5 (0%)	51	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	391	SER
1	A	391	SER
1	C	391	SER
1	D	391	SER
1	H	391	SER

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	469/452 (104%)	466 (99%)	3 (1%)	86	73
1	B	460/452 (102%)	456 (99%)	4 (1%)	78	61
1	C	461/452 (102%)	457 (99%)	4 (1%)	78	61
1	D	461/452 (102%)	457 (99%)	4 (1%)	78	61
1	E	465/452 (103%)	460 (99%)	5 (1%)	73	53
1	F	454/452 (100%)	450 (99%)	4 (1%)	78	61
1	G	463/452 (102%)	459 (99%)	4 (1%)	78	61
1	H	459/452 (102%)	455 (99%)	4 (1%)	78	61
All	All	3692/3616 (102%)	3660 (99%)	32 (1%)	78	61

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	447	TYR
1	E	382	GLU

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Mol	Chain	Res	Type
1	H	325	ARG
1	E	325	ARG
1	E	391	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	141	GLN
1	E	129	HIS
1	H	255	GLN
1	D	255	GLN
1	D	544	GLN

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 31 ligands modelled in this entry, 9 are monoatomic - leaving 22 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	$\# Z > 2$
2	TD6	A	601	3	26,34,34	2.30	7 (26%)	32,50,50	1.82	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	604	-	5,5,5	0.33	0	5,5,5	0.22	0
2	TD6	D	601	3	26,34,34	2.92	6 (23%)	32,50,50	1.74	9 (28%)
2	TD6	C	601	3	26,34,34	2.72	7 (26%)	32,50,50	1.75	8 (25%)
4	GOL	G	604	-	5,5,5	0.34	0	5,5,5	0.31	0
4	GOL	E	603	-	5,5,5	0.32	0	5,5,5	0.49	0
4	GOL	D	603	-	5,5,5	0.35	0	5,5,5	0.39	0
4	GOL	C	603	-	5,5,5	0.29	0	5,5,5	0.35	0
4	GOL	B	603	-	5,5,5	0.41	0	5,5,5	0.45	0
2	TD6	F	601	3	26,34,34	2.61	5 (19%)	32,50,50	1.74	8 (25%)
4	GOL	H	603	-	5,5,5	0.39	0	5,5,5	0.26	0
4	GOL	E	604	-	5,5,5	0.38	0	5,5,5	0.27	0
4	GOL	G	603	-	5,5,5	0.32	0	5,5,5	0.31	0
4	GOL	A	603	-	5,5,5	0.34	0	5,5,5	0.50	0
4	GOL	F	603	-	5,5,5	0.31	0	5,5,5	0.40	0
4	GOL	A	604	-	5,5,5	0.39	0	5,5,5	0.31	0
4	GOL	H	604	-	5,5,5	0.35	0	5,5,5	0.20	0
4	GOL	C	604	-	5,5,5	0.42	0	5,5,5	0.58	0
2	TD6	G	601	3	26,34,34	2.88	5 (19%)	32,50,50	1.81	9 (28%)
2	TD6	H	601	3	26,34,34	2.18	9 (34%)	32,50,50	2.12	10 (31%)
2	TD6	E	601	3	26,34,34	2.61	4 (15%)	32,50,50	1.89	9 (28%)
2	TD6	B	601	3	26,34,34	2.74	5 (19%)	32,50,50	1.83	9 (28%)

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	TD6	A	601	3	-	3/19/26/26	0/2/2/2
4	GOL	D	604	-	-	2/4/4/4	-
2	TD6	D	601	3	-	3/19/26/26	0/2/2/2
2	TD6	C	601	3	-	2/19/26/26	0/2/2/2
4	GOL	G	604	-	-	0/4/4/4	-
4	GOL	E	603	-	-	2/4/4/4	-
4	GOL	D	603	-	-	0/4/4/4	-
4	GOL	C	603	-	-	1/4/4/4	-
4	GOL	B	603	-	-	0/4/4/4	-
2	TD6	F	601	3	-	2/19/26/26	0/2/2/2
4	GOL	H	603	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	604	-	-	3/4/4/4	-
4	GOL	G	603	-	-	0/4/4/4	-
4	GOL	A	603	-	-	1/4/4/4	-
4	GOL	F	603	-	-	0/4/4/4	-
4	GOL	A	604	-	-	0/4/4/4	-
4	GOL	H	604	-	-	4/4/4/4	-
4	GOL	C	604	-	-	4/4/4/4	-
2	TD6	G	601	3	-	3/19/26/26	0/2/2/2
2	TD6	H	601	3	-	3/19/26/26	0/2/2/2
2	TD6	E	601	3	-	3/19/26/26	0/2/2/2
2	TD6	B	601	3	-	3/19/26/26	0/2/2/2

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	TD6	C6-C5	13.32	1.56	1.50
2	G	601	TD6	C6-C5	13.10	1.56	1.50
2	B	601	TD6	C6-C5	12.19	1.56	1.50
2	C	601	TD6	C6-C5	12.09	1.56	1.50
2	F	601	TD6	C6-C5	11.59	1.56	1.50

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	TD6	C5-C4-N3	5.24	118.61	107.66
2	B	601	TD6	C13-CLB-C11	-5.16	106.82	114.44
2	H	601	TD6	C13-CLB-C11	-5.09	106.93	114.44
2	E	601	TD6	C13-CLB-C11	-4.71	107.49	114.44
2	G	601	TD6	C13-CLB-C11	-3.99	108.55	114.44

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

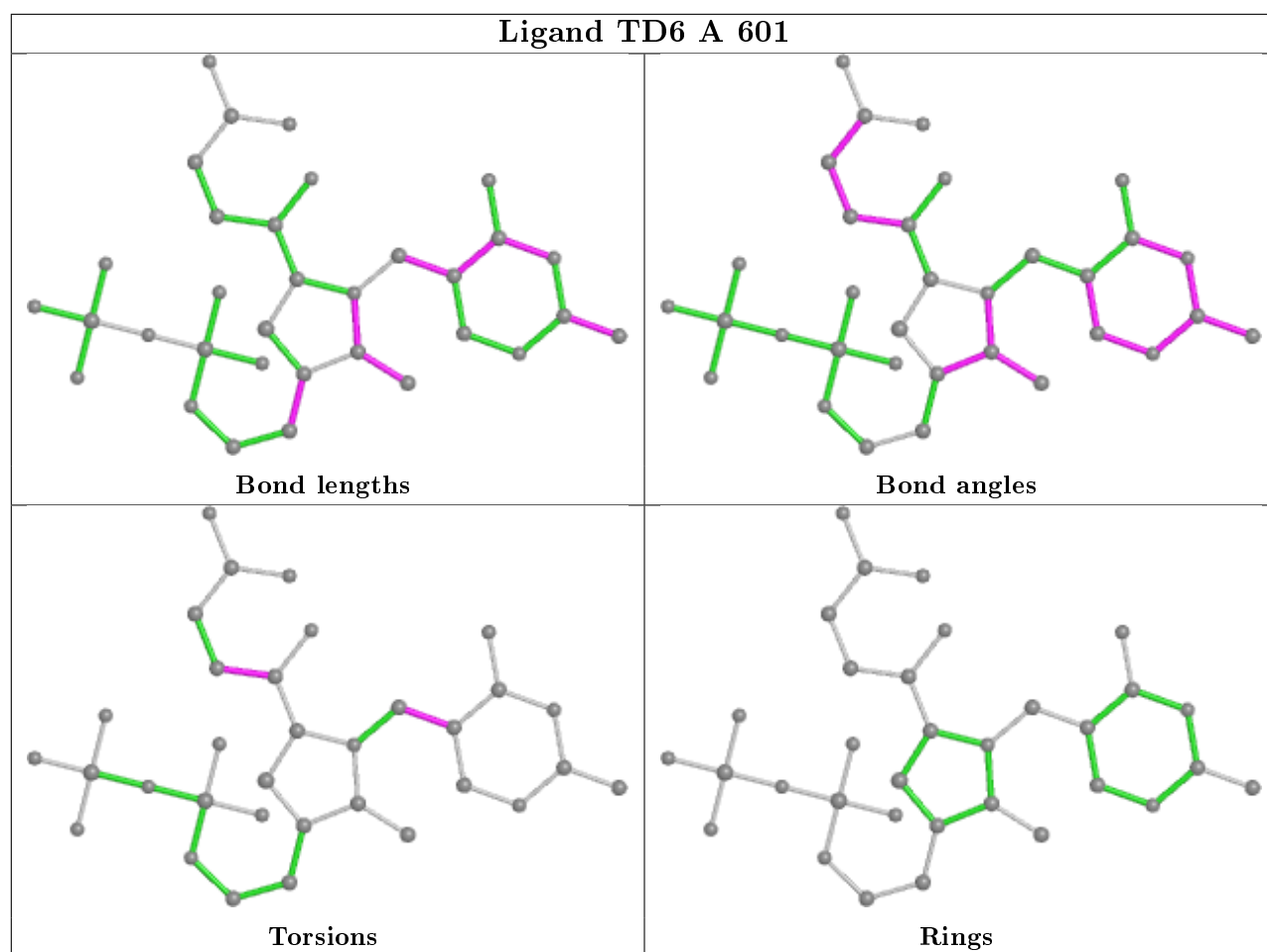
Mol	Chain	Res	Type	Atoms
2	A	601	TD6	C2-C11-CLB-C13
2	A	601	TD6	OL1-C11-CLB-C13
2	A	601	TD6	C4'-C5'-C7'-N3
4	H	604	GOL	C1-C2-C3-O3
2	D	601	TD6	C2-C11-CLB-C13

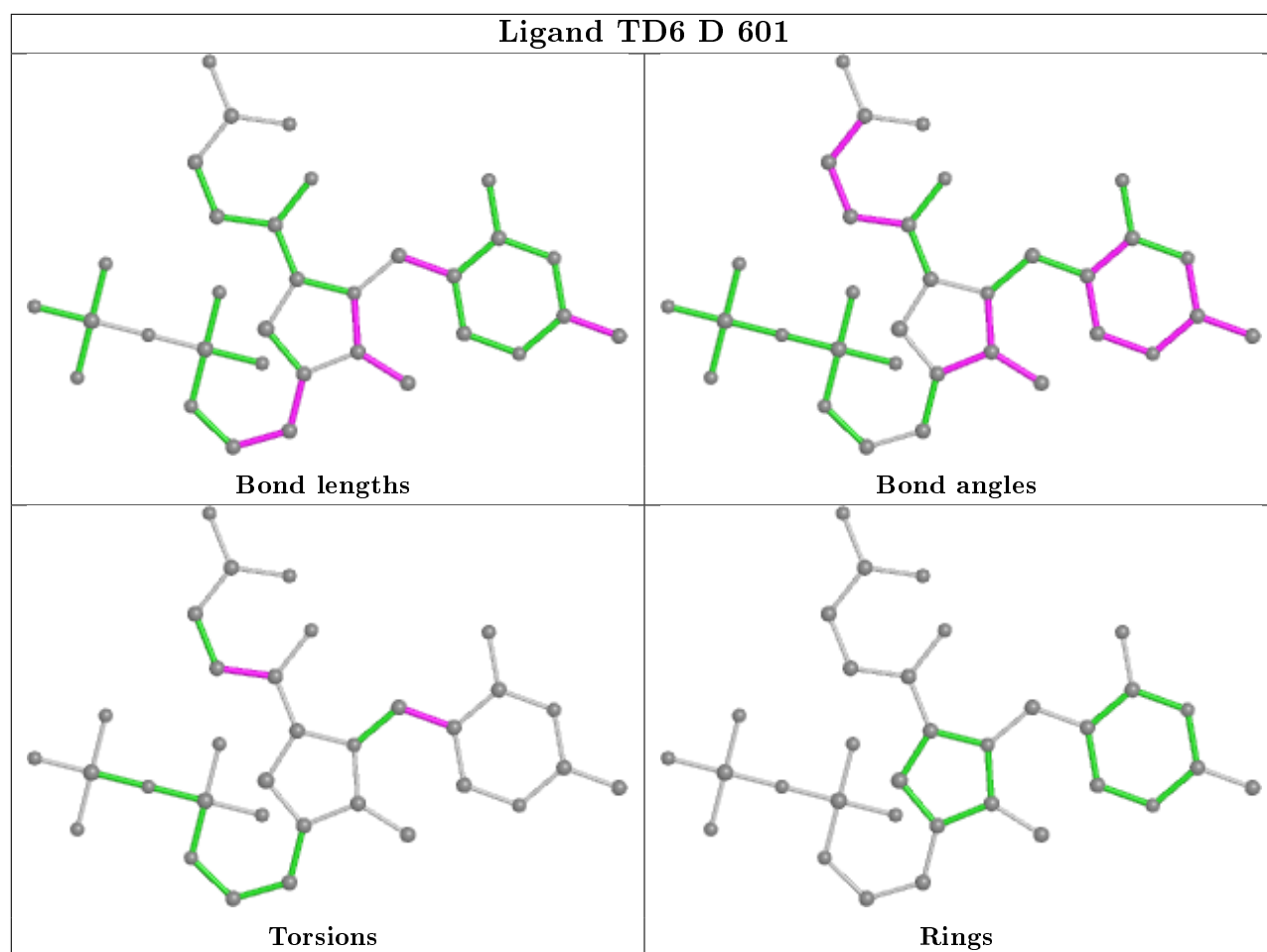
There are no ring outliers.

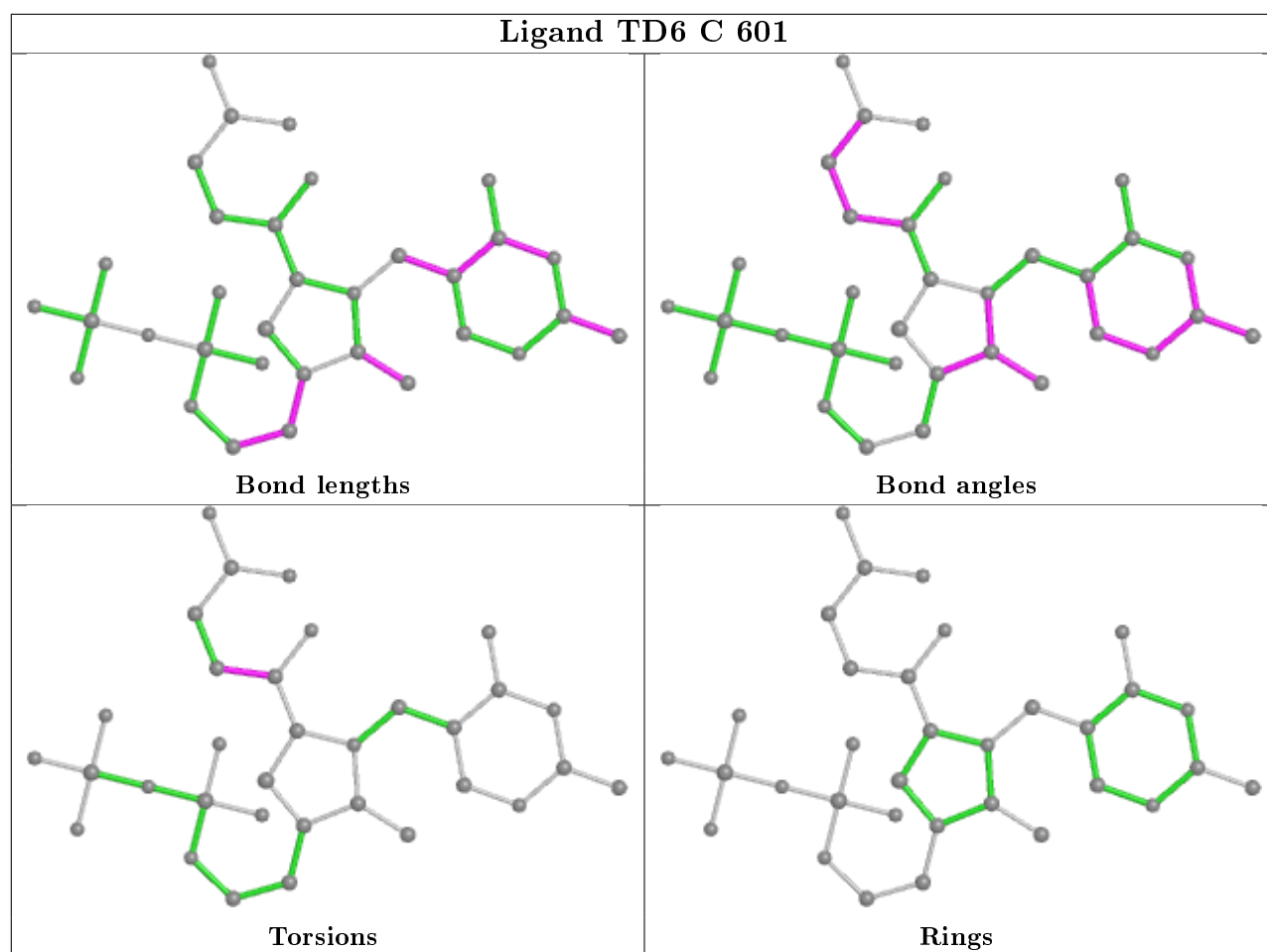
11 monomers are involved in 38 short contacts:

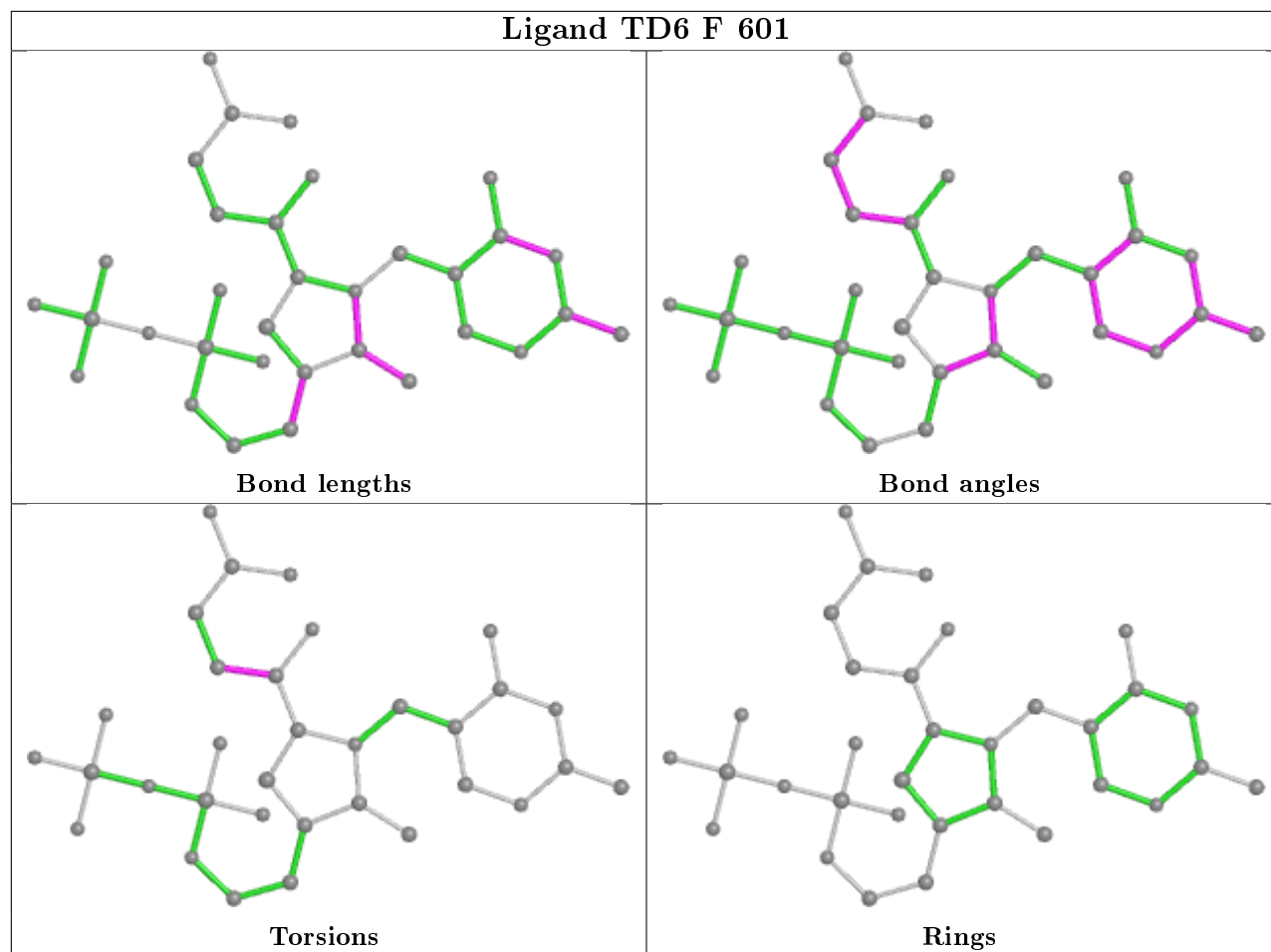
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TD6	4	0
2	D	601	TD6	5	0
2	C	601	TD6	4	0
4	C	603	GOL	1	0
2	F	601	TD6	5	0
4	A	603	GOL	1	0
4	C	604	GOL	1	0
2	G	601	TD6	4	0
2	H	601	TD6	4	0
2	E	601	TD6	4	0
2	B	601	TD6	5	0

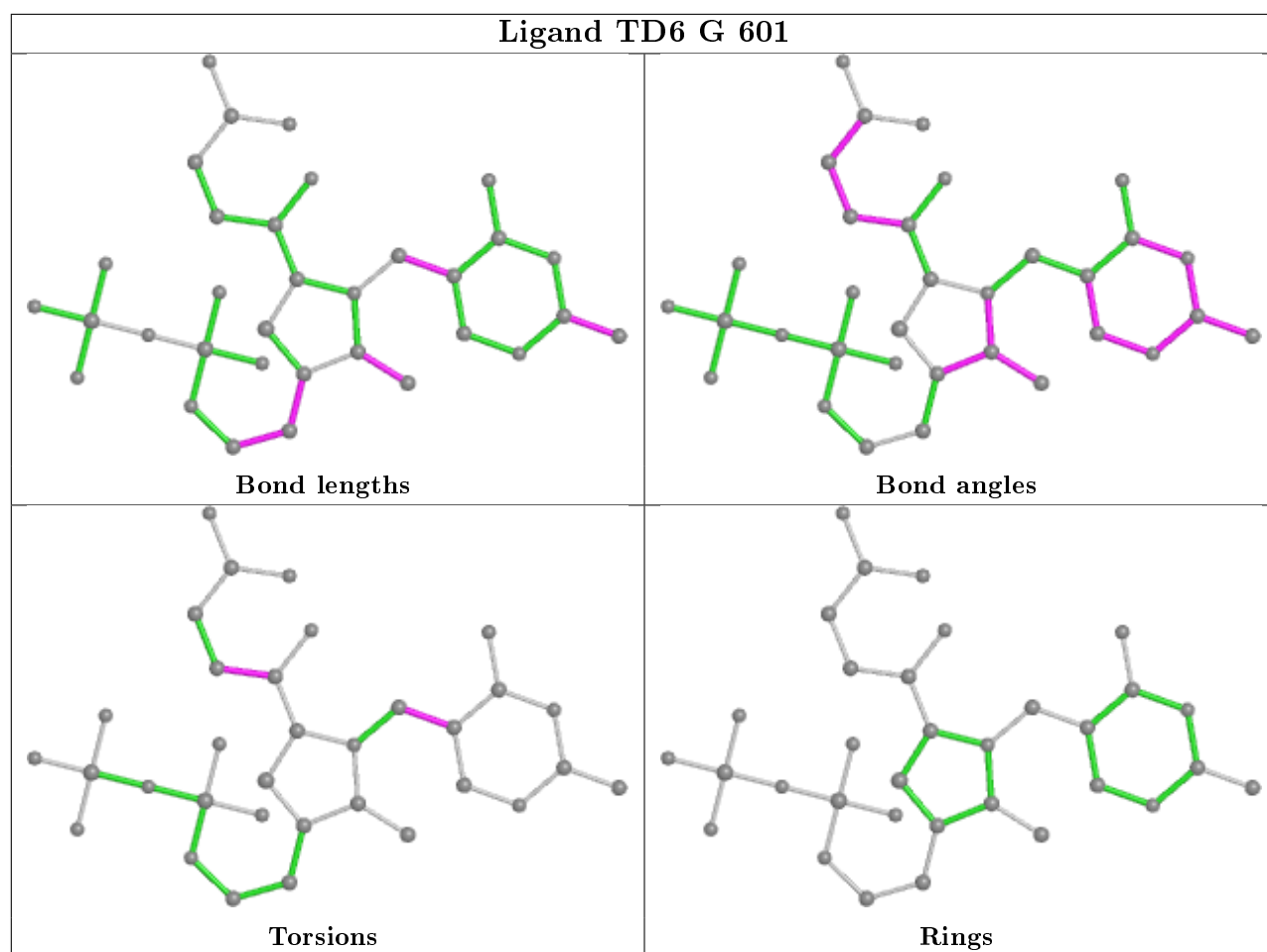
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

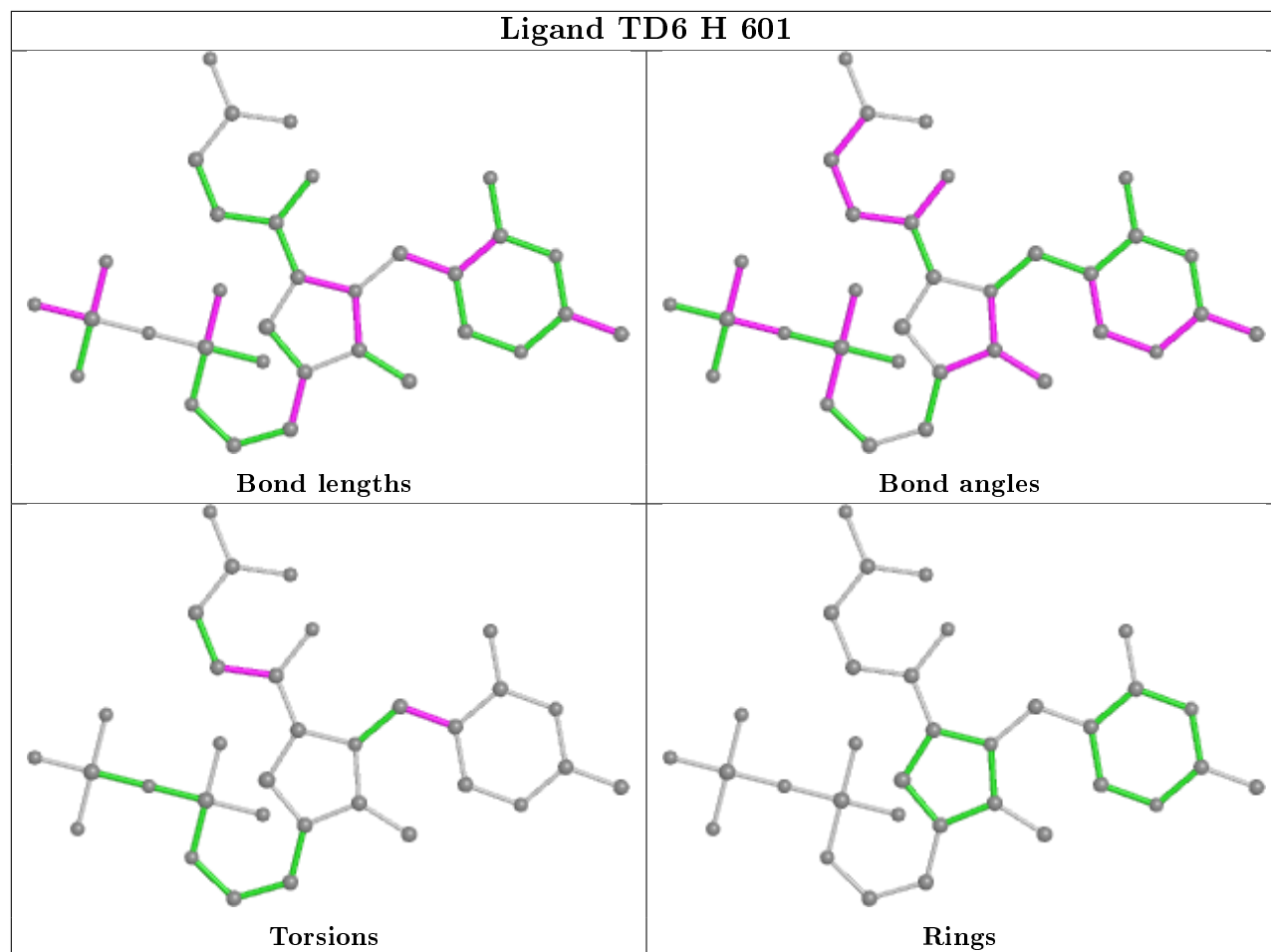


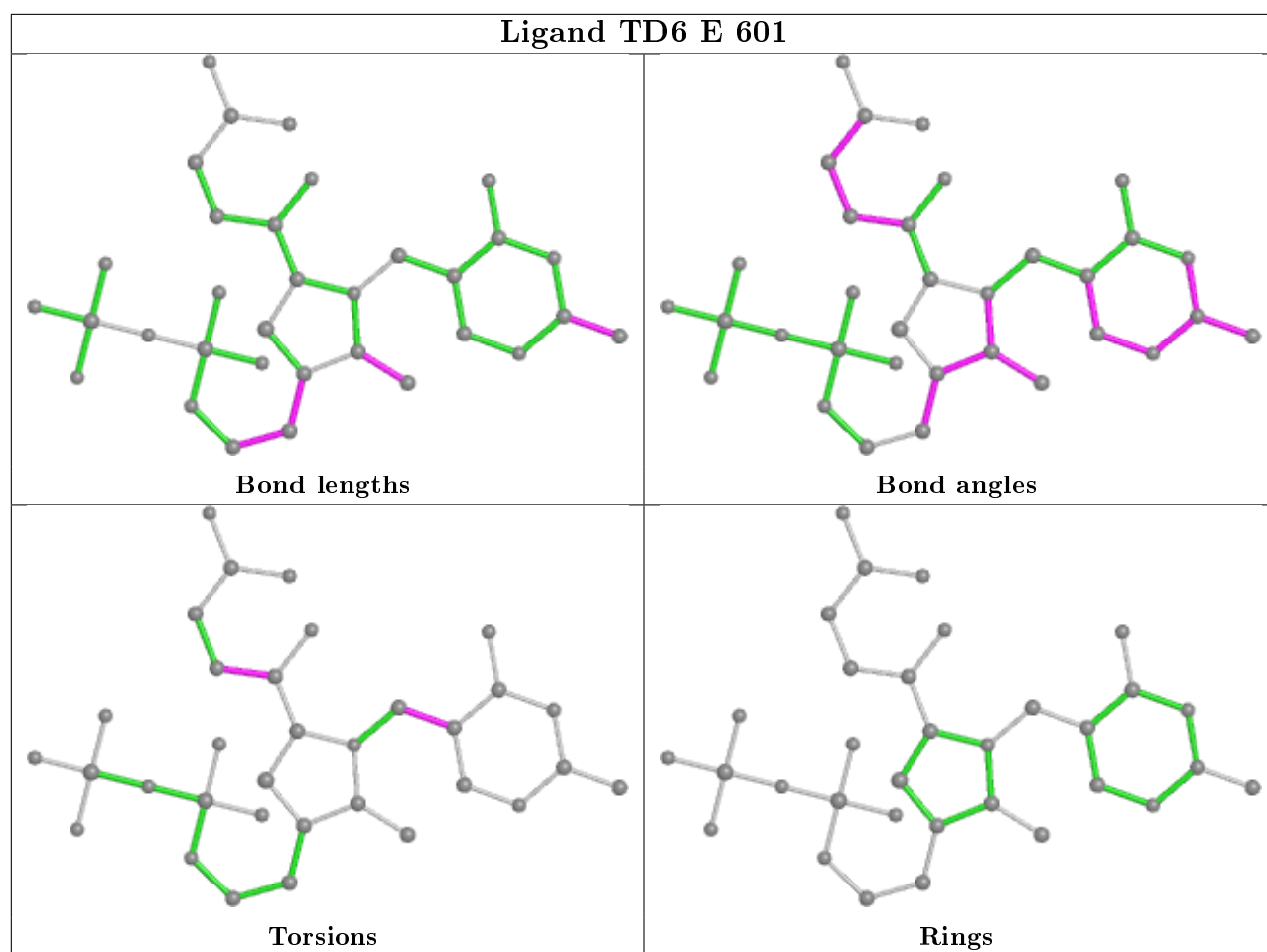


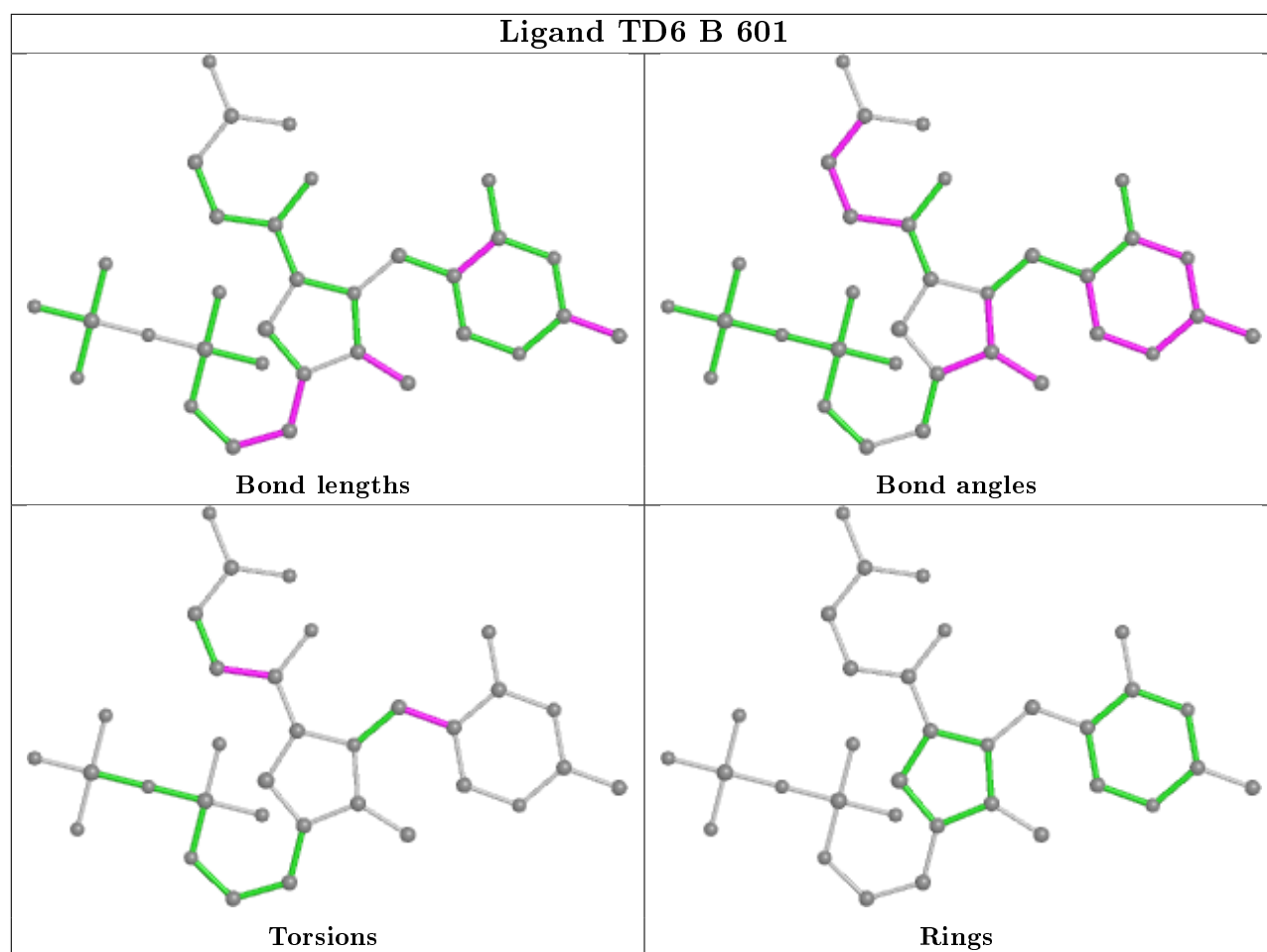












5.7 Other polymers [i](#)

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 ⓘ

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	556/556 (100%)	-0.27	6 (1%) 80 84	5, 11, 28, 48	0
1	B	556/556 (100%)	-0.34	7 (1%) 77 82	5, 11, 28, 46	0
1	C	556/556 (100%)	-0.29	6 (1%) 80 84	6, 12, 28, 54	0
1	D	556/556 (100%)	-0.10	14 (2%) 57 64	6, 15, 36, 56	0
1	E	556/556 (100%)	-0.27	7 (1%) 77 82	6, 11, 30, 48	0
1	F	556/556 (100%)	-0.31	5 (0%) 84 87	6, 12, 27, 50	0
1	G	556/556 (100%)	-0.29	5 (0%) 84 87	6, 12, 29, 45	0
1	H	556/556 (100%)	-0.14	10 (1%) 68 74	7, 14, 34, 62	0
All	All	4448/4448 (100%)	-0.25	60 (1%) 77 82	5, 12, 31, 62	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	347	VAL	4.4
1	E	178	MET	4.0
1	H	555	HIS	3.7
1	B	1	MET	3.7
1	A	556	LEU	3.6

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 ⓘ

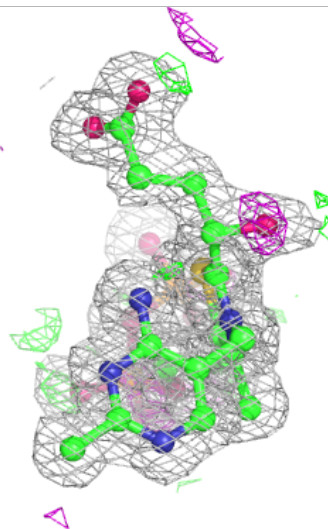
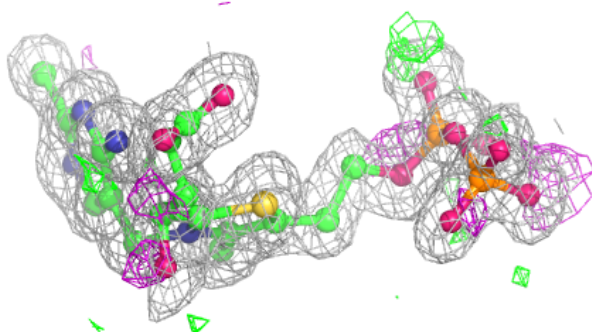
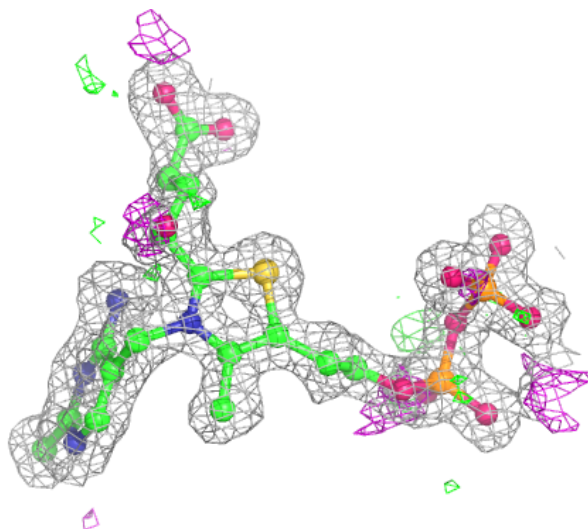
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	H	604	6/6	0.73	0.17	33,39,43,44	0
4	GOL	D	604	6/6	0.81	0.16	31,37,40,42	0
4	GOL	E	604	6/6	0.82	0.16	33,40,41,43	0
4	GOL	A	604	6/6	0.88	0.15	28,33,37,38	0
4	GOL	C	604	6/6	0.89	0.17	23,30,34,36	0
4	GOL	G	604	6/6	0.89	0.17	24,29,33,35	0
4	GOL	G	603	6/6	0.92	0.13	18,21,22,24	0
4	GOL	C	603	6/6	0.93	0.10	15,20,22,22	0
4	GOL	H	603	6/6	0.94	0.09	17,19,20,22	0
4	GOL	D	603	6/6	0.94	0.10	19,21,23,24	0
4	GOL	B	603	6/6	0.95	0.09	15,19,20,20	0
4	GOL	E	603	6/6	0.96	0.07	12,15,15,16	0
4	GOL	A	603	6/6	0.96	0.08	12,15,16,16	0
4	GOL	F	603	6/6	0.96	0.09	15,18,19,19	0
2	TD6	H	601	33/33	0.97	0.08	8,12,21,26	0
2	TD6	D	601	33/33	0.97	0.07	9,11,21,27	0
2	TD6	C	601	33/33	0.98	0.07	7,10,16,21	0
2	TD6	B	601	33/33	0.98	0.07	7,10,17,22	0
2	TD6	G	601	33/33	0.98	0.07	8,10,21,27	0
2	TD6	F	601	33/33	0.98	0.07	7,10,20,24	0
2	TD6	E	601	33/33	0.98	0.07	6,9,20,26	0
2	TD6	A	601	33/33	0.98	0.07	5,8,17,22	0
3	MN	G	602	1/1	1.00	0.06	15,15,15,15	0
3	MN	G	605	1/1	1.00	0.08	36,36,36,36	0
3	MN	A	602	1/1	1.00	0.06	12,12,12,12	0
3	MN	H	602	1/1	1.00	0.08	16,16,16,16	0
3	MN	F	602	1/1	1.00	0.04	13,13,13,13	0
3	MN	C	602	1/1	1.00	0.06	15,15,15,15	0
3	MN	E	602	1/1	1.00	0.05	13,13,13,13	0
3	MN	D	602	1/1	1.00	0.06	18,18,18,18	0
3	MN	B	602	1/1	1.00	0.06	13,13,13,13	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.

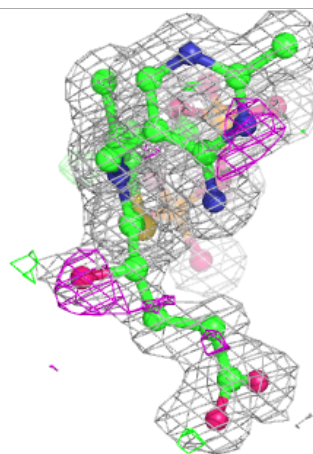
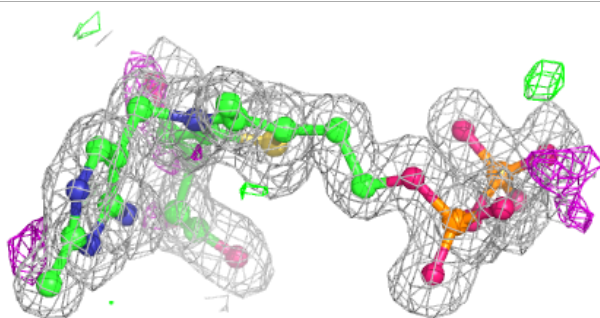
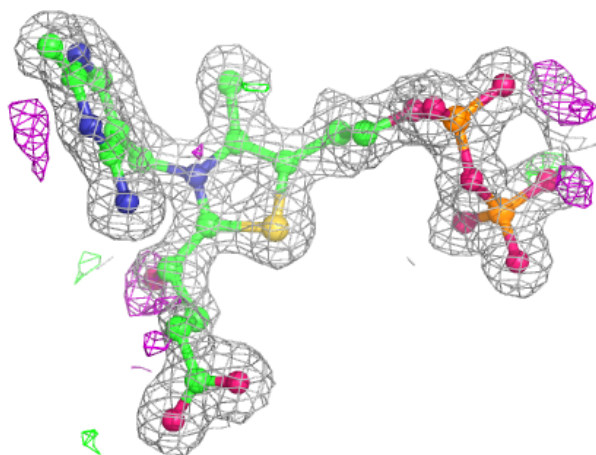
Electron density around TD6 H 601:

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



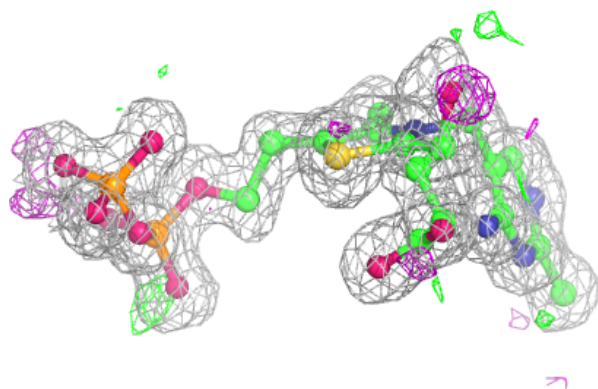
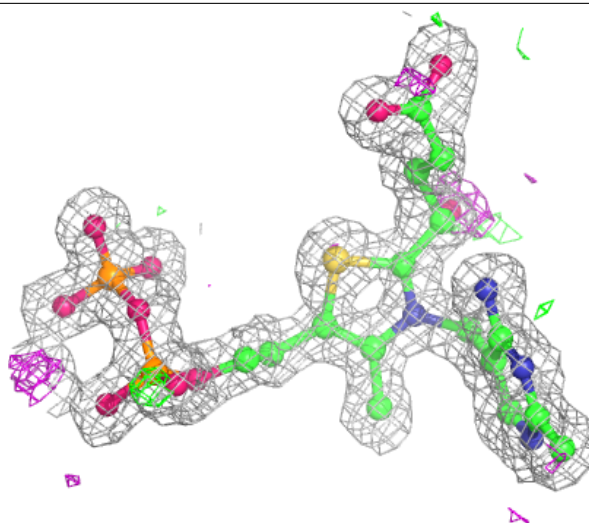
Electron density around TD6 D 601:

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



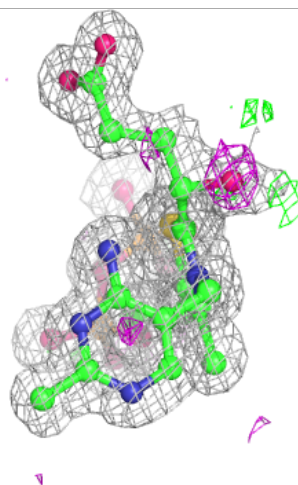
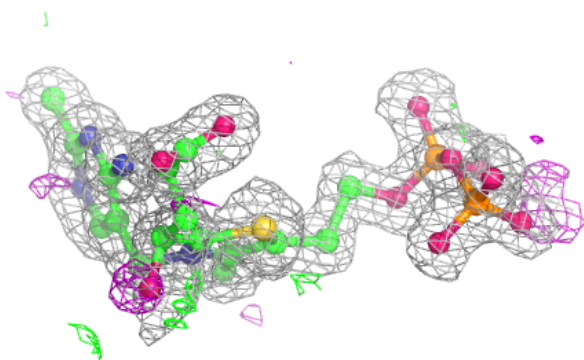
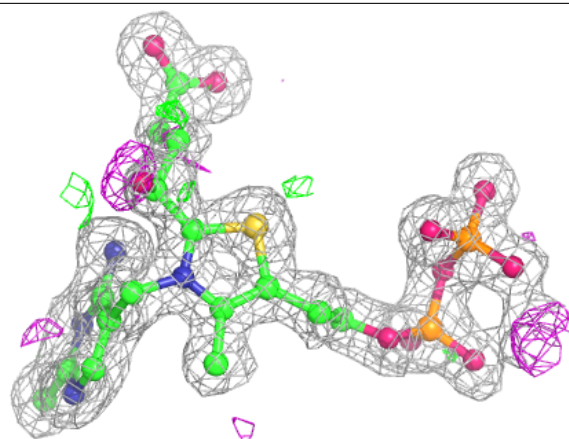
Electron density around TD6 C 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



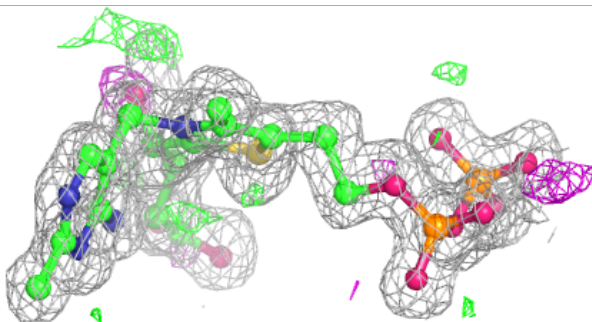
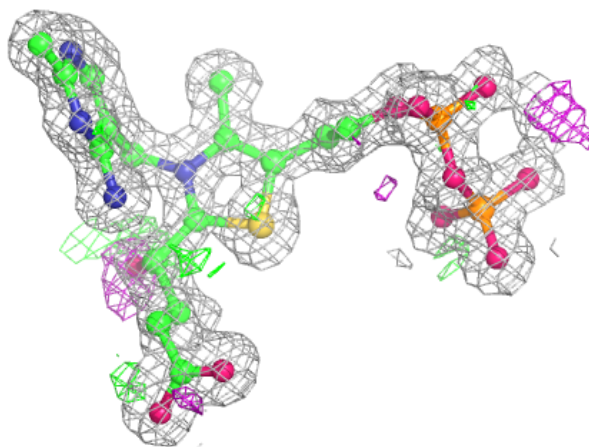
Electron density around TD6 B 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



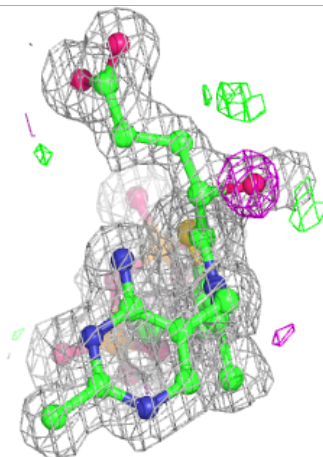
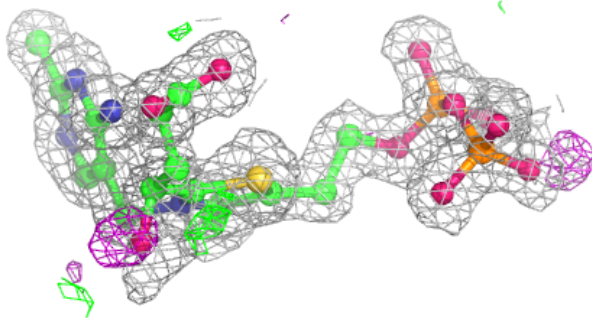
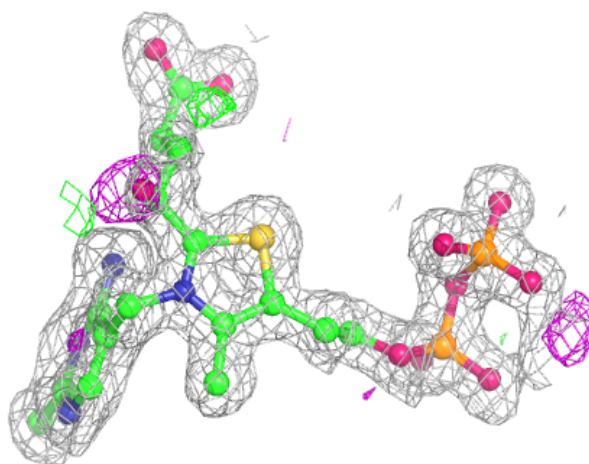
Electron density around TD6 G 601:

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



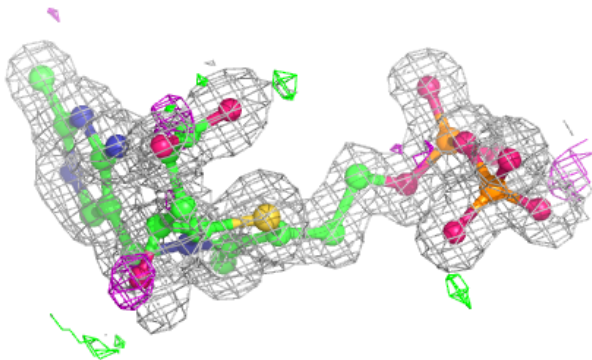
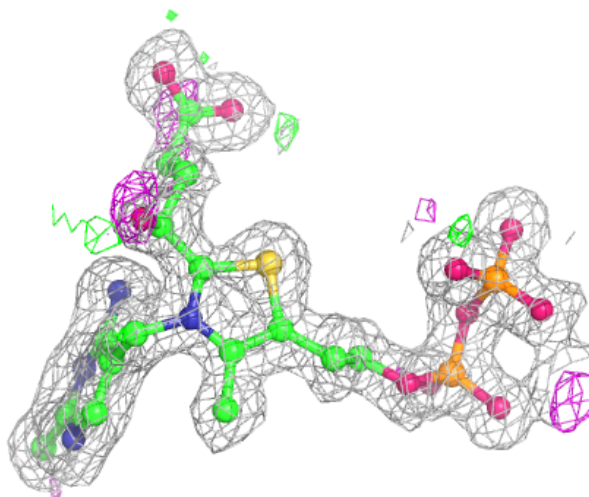
Electron density around TD6 F 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



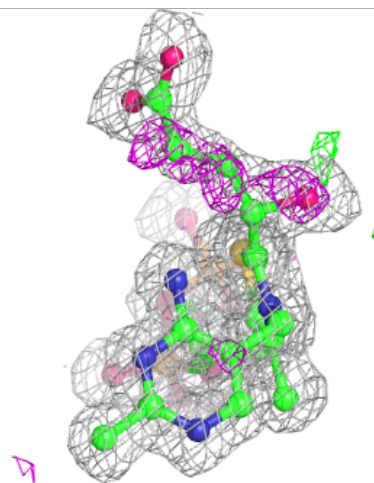
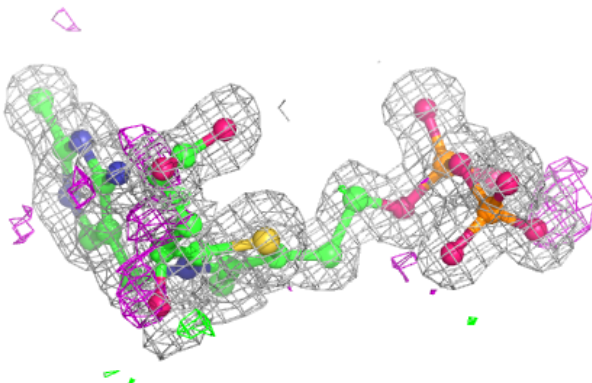
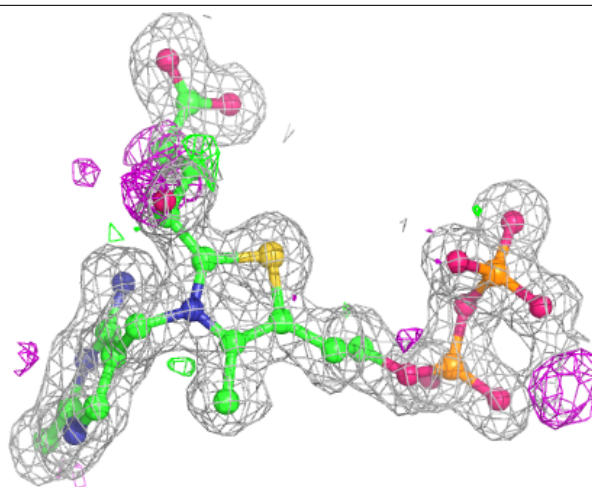
Electron density around TD6 E 601:

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



Electron density around TD6 A 601:

$2mF_o-DF_c$ (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.