



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:46 AM UTC

PDB ID : 5EJ5 / pdb_00005ej5
Title : EcMenD-ThDP-Mn²⁺ complex soaked with 2-ketoglutarate for 1.5 h
Authors : Song, H.G.; Dong, C.; Chen, Y.Z.; Sun, Y.R.; Guo, Z.H.
Deposited on : 2015-11-01
Resolution : 2.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

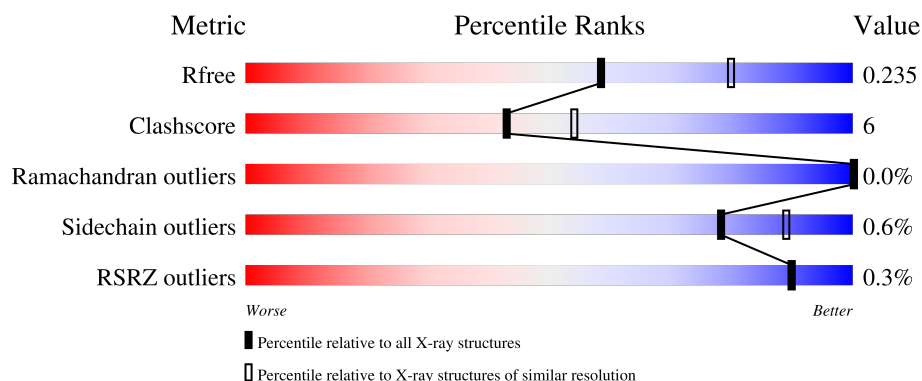
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	% 88% 12%
1	B	556	88% 12% .
1	C	556	87% 13%
1	D	556	% 85% 14% .
1	E	556	86% 14%

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Mol	Chain	Length	Quality of chain
1	F	556	 87%13%
1	G	556	 85%15%
1	H	556	 83%17%

2 Entry composition

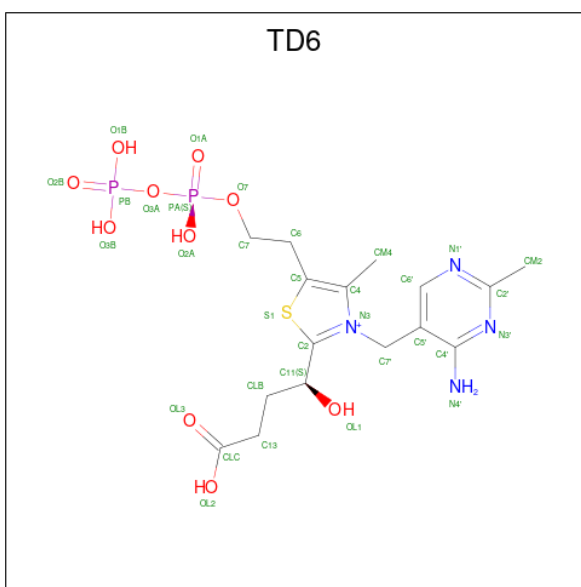
There are 5 unique types of molecules in this entry. The entry contains 36844 atoms, of which 224 are hydrogens and 0 are deuteriums.

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	4	0
			4348	2756	787	790	15			
1	B	556	Total	C	N	O	S	0	1	0
			4316	2738	776	788	14			
1	C	556	Total	C	N	O	S	0	5	0
			4355	2759	787	794	15			
1	D	556	Total	C	N	O	S	0	1	0
			4312	2738	776	783	15			
1	E	556	Total	C	N	O	S	0	5	0
			4360	2763	788	793	16			
1	F	556	Total	C	N	O	S	0	1	0
			4313	2737	776	786	14			
1	G	556	Total	C	N	O	S	0	5	0
			4350	2757	786	792	15			
1	H	556	Total	C	N	O	S	0	1	0
			4314	2738	777	784	15			

- 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 (CCD ID: TD6) (formula: C₁₆H₂₅N₄O₁₀P₂S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total 53	C 16	H 20	N 4	O 10	P 2	S 1	0	0
2	B	1	Total 53	C 16	H 20	N 4	O 10	P 2	S 1	0	0
2	C	1	Total 53	C 16	H 20	N 4	O 10	P 2	S 1	0	0
2	D	1	Total 53	C 16	H 20	N 4	O 10	P 2	S 1	0	0
2	E	1	Total 53	C 16	H 20	N 4	O 10	P 2	S 1	0	0
2	F	1	Total 53	C 16	H 20	N 4	O 10	P 2	S 1	0	0
2	G	1	Total 53	C 16	H 20	N 4	O 10	P 2	S 1	0	0
2	H	1	Total 53	C 16	H 20	N 4	O 10	P 2	S 1	0	0

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Mn 1	0	0
3	F	1	Total 1	Mn 1	0	0
3	G	1	Total 1	Mn 1	0	0
3	H	1	Total 1	Mn 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

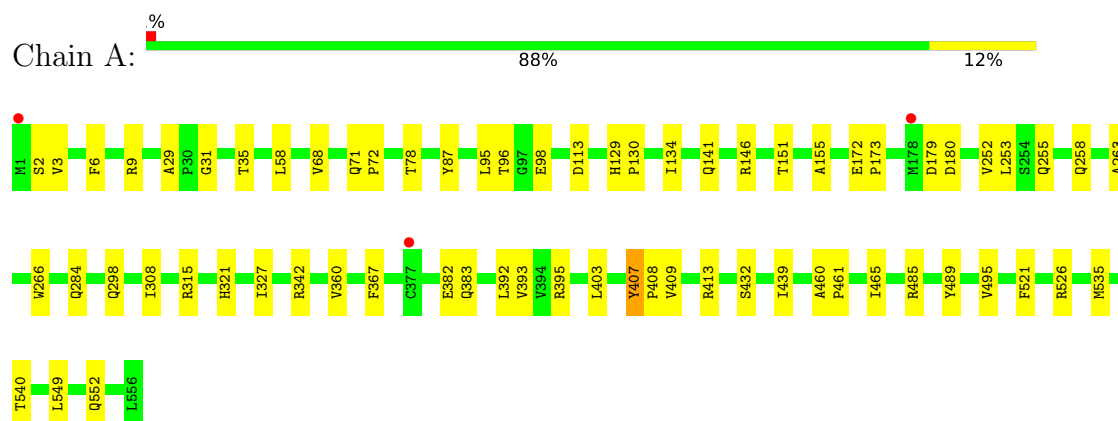
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	233	Total	O	0	0
			233	233		
5	B	216	Total	O	0	0
			216	216		
5	C	188	Total	O	0	0
			188	188		
5	D	166	Total	O	0	0
			166	166		
5	E	233	Total	O	0	0
			233	233		
5	F	207	Total	O	0	0
			207	207		
5	G	172	Total	O	0	0
			172	172		
5	H	217	Total	O	0	0
			217	217		

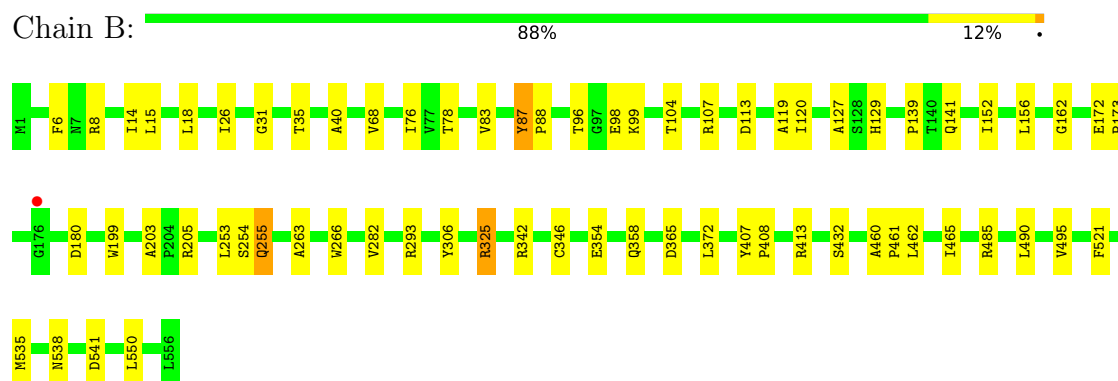
3 Residue-property plots [i](#)

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.

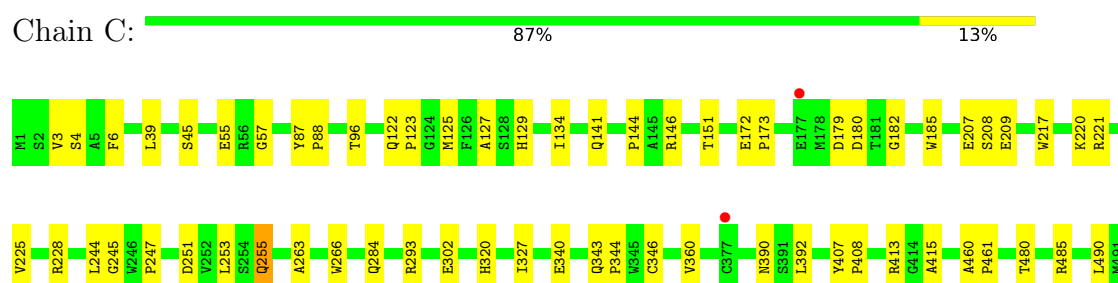
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



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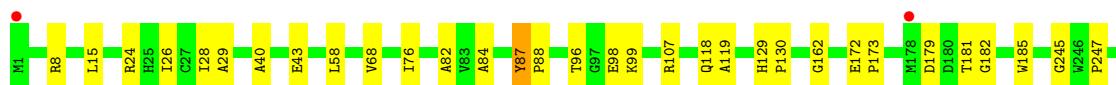
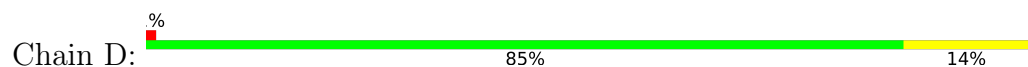


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

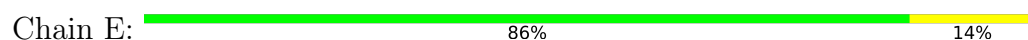




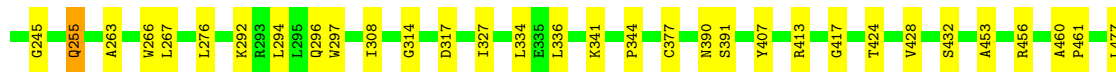
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



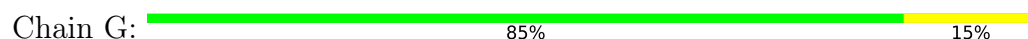
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

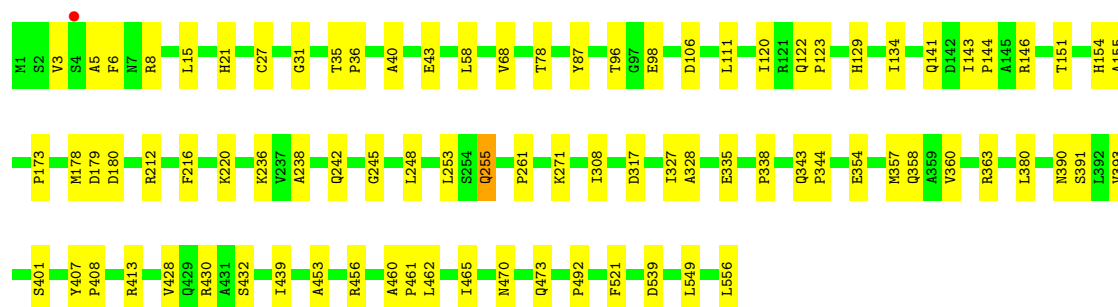


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



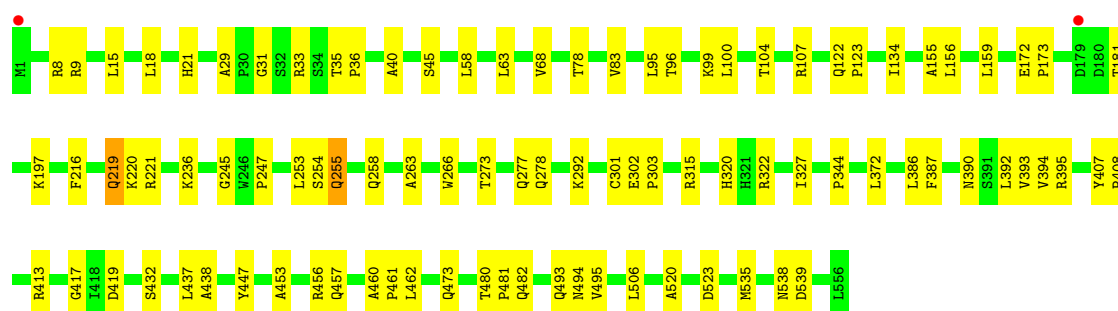
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- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain H: 83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.76Å 90.80Å 170.10Å 75.79° 83.29° 64.34°	Depositor
Resolution (Å)	33.76 – 2.30 33.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.4 (33.76-2.30) 89.8 (33.76-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.234 0.186 , 0.235	Depositor DCC
R_{free} test set	9871 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	36844	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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: MN, TD6, GOL

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	0.55	1/4457 (0.0%)	0.86	5/6082 (0.1%)
1	B	0.62	3/4425 (0.1%)	0.84	3/6041 (0.0%)
1	C	0.56	2/4464 (0.0%)	0.84	5/6092 (0.1%)
1	D	0.56	1/4421 (0.0%)	0.83	1/6034 (0.0%)
1	E	0.56	1/4469 (0.0%)	0.84	0/6096
1	F	0.60	2/4422 (0.0%)	0.85	1/6037 (0.0%)
1	G	0.50	0/4459	0.83	4/6085 (0.1%)
1	H	0.58	2/4423 (0.0%)	0.84	0/6037
All	All	0.57	12/35540 (0.0%)	0.84	19/48504 (0.0%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	325	ARG	C-O	-6.47	1.16	1.24
1	A	495	VAL	C-O	-6.21	1.16	1.23
1	C	221	ARG	C-O	-6.14	1.17	1.24
1	B	180	ASP	C-O	-6.07	1.16	1.24
1	E	495	VAL	C-O	-5.96	1.16	1.23

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	129	HIS	CA-C-N	-6.59	113.19	119.85
1	G	129	HIS	C-N-CA	-6.59	113.19	119.85
1	A	407	TYR	CA-C-N	6.21	127.18	119.98
1	A	407	TYR	C-N-CA	6.21	127.18	119.98
1	C	129	HIS	CA-C-N	-6.17	113.61	119.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4348	0	4295	42	0
1	B	4316	0	4253	43	0
1	C	4355	0	4294	50	0
1	D	4312	0	4259	57	0
1	E	4360	0	4313	62	0
1	F	4313	0	4251	47	1
1	G	4350	0	4291	57	0
1	H	4314	0	4261	65	1
2	A	33	20	21	4	0
2	B	33	20	21	2	0
2	C	33	20	21	3	0
2	D	33	20	21	3	0
2	E	33	20	21	3	0
2	F	33	20	21	3	0
2	G	33	20	21	2	0
2	H	33	20	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	1	0	0	0	0
3	H	1	0	0	0	0
4	A	6	8	8	0	0
4	B	6	8	8	0	0
4	C	6	8	8	0	0
4	D	6	8	8	0	0
4	E	6	8	8	0	0
4	F	6	8	8	0	0
4	G	6	8	8	1	0
4	H	6	8	8	0	0
5	A	233	0	0	9	0
5	B	216	0	0	9	0
5	C	188	0	0	13	0
5	D	166	0	0	8	0
5	E	233	0	0	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	207	0	0	10	0
5	G	172	0	0	10	0
5	H	217	0	0	18	0
All	All	36620	224	34449	430	1

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 6.

The worst 5 of 430 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:E:252:VAL:CG2	1:E:398:ASP:HA	1.90	1.01
1:E:252:VAL:HG23	1:E:398:ASP:HA	1.52	0.91
1:B:203:ALA:HB1	1:B:205:ARG:HH12	1.37	0.89
1:H:457:GLN:HG3	5:H:766:HOH:O	1.78	0.82
1:B:365:ASP:O	5:B:701:HOH:O	1.97	0.82

All (1) 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:F:341:LYS:NZ	1:H:45:SER:O[1_545]	2.18	0.02

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	558/556 (100%)	547 (98%)	11 (2%)	0	100	100
1	B	555/556 (100%)	544 (98%)	11 (2%)	0	100	100
1	C	559/556 (100%)	548 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	555/556 (100%)	543 (98%)	12 (2%)	0	100	100
1	E	559/556 (100%)	548 (98%)	11 (2%)	0	100	100
1	F	555/556 (100%)	544 (98%)	11 (2%)	0	100	100
1	G	559/556 (100%)	547 (98%)	11 (2%)	1 (0%)	43	55
1	H	555/556 (100%)	545 (98%)	10 (2%)	0	100	100
All	All	4455/4448 (100%)	4366 (98%)	88 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	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	451/452 (100%)	449 (100%)	2 (0%)	84	92
1	B	447/452 (99%)	443 (99%)	4 (1%)	70	84
1	C	452/452 (100%)	450 (100%)	2 (0%)	84	92
1	D	446/452 (99%)	443 (99%)	3 (1%)	76	87
1	E	454/452 (100%)	452 (100%)	2 (0%)	84	92
1	F	446/452 (99%)	441 (99%)	5 (1%)	65	81
1	G	451/452 (100%)	449 (100%)	2 (0%)	84	92
1	H	447/452 (99%)	445 (100%)	2 (0%)	84	92
All	All	3594/3616 (99%)	3572 (99%)	22 (1%)	78	89

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	35	THR
1	F	495	VAL

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Mol	Chain	Res	Type
1	F	255	GLN
1	G	87	TYR
1	C	179	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	320	HIS
1	H	343	GLN
1	H	544	GLN
1	G	298	GLN
1	C	194	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	H	601	3	31,34,34	1.65	7 (22%)	38,50,50	1.77	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	E	603	-	5,5,5	0.35	0	5,5,5	0.32	0
2	TD6	E	601	3	31,34,34	1.68	8 (25%)	38,50,50	1.65	9 (23%)
2	TD6	B	601	3	31,34,34	1.73	8 (25%)	38,50,50	1.82	9 (23%)
4	GOL	A	603	-	5,5,5	0.31	0	5,5,5	0.25	0
2	TD6	G	601	3	31,34,34	1.74	9 (29%)	38,50,50	1.75	8 (21%)
4	GOL	C	603	-	5,5,5	0.38	0	5,5,5	0.20	0
4	GOL	F	603	-	5,5,5	0.31	0	5,5,5	0.35	0
2	TD6	D	601	3	31,34,34	1.63	7 (22%)	38,50,50	1.78	9 (23%)
2	TD6	F	601	3	31,34,34	1.67	8 (25%)	38,50,50	1.75	8 (21%)
4	GOL	G	603	-	5,5,5	0.34	0	5,5,5	0.38	0
4	GOL	H	603	-	5,5,5	0.36	0	5,5,5	0.28	0
4	GOL	D	603	-	5,5,5	0.41	0	5,5,5	0.46	0
2	TD6	A	601	3	31,34,34	1.72	9 (29%)	38,50,50	1.82	9 (23%)
2	TD6	C	601	3	31,34,34	1.65	8 (25%)	38,50,50	1.84	10 (26%)
4	GOL	B	603	-	5,5,5	0.35	0	5,5,5	0.37	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
2	TD6	H	601	3	-	3/25/26/26	0/2/2/2
4	GOL	E	603	-	-	2/4/4/4	-
2	TD6	E	601	3	-	5/25/26/26	0/2/2/2
2	TD6	B	601	3	-	4/25/26/26	0/2/2/2
4	GOL	A	603	-	-	2/4/4/4	-
2	TD6	G	601	3	-	4/25/26/26	0/2/2/2
4	GOL	C	603	-	-	2/4/4/4	-
4	GOL	F	603	-	-	2/4/4/4	-
2	TD6	D	601	3	-	5/25/26/26	0/2/2/2
2	TD6	F	601	3	-	5/25/26/26	0/2/2/2
4	GOL	G	603	-	-	2/4/4/4	-
4	GOL	H	603	-	-	2/4/4/4	-
4	GOL	D	603	-	-	2/4/4/4	-
2	TD6	A	601	3	-	4/25/26/26	0/2/2/2
2	TD6	C	601	3	-	8/25/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	603	-	-	2/4/4/4	-

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	TD6	C4-N3	-3.99	1.35	1.40
2	A	601	TD6	CM4-C4	3.59	1.57	1.49
2	H	601	TD6	CM4-C4	3.56	1.57	1.49
2	D	601	TD6	C4-N3	-3.47	1.35	1.40
2	F	601	TD6	C4-N3	-3.45	1.35	1.40

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	TD6	C4-C5-S1	-5.41	104.96	110.56
2	G	601	TD6	C4-C5-S1	-5.17	105.21	110.56
2	H	601	TD6	C4-C5-S1	-4.98	105.40	110.56
2	B	601	TD6	C4-C5-S1	-4.81	105.58	110.56
2	A	601	TD6	C4-C5-S1	-4.62	105.77	110.56

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TD6	CLB-C11-C2-S1
2	A	601	TD6	OL1-C11-C2-N3
2	B	601	TD6	CLB-C11-C2-S1
2	B	601	TD6	OL1-C11-C2-N3
2	C	601	TD6	OL1-C11-C2-N3

There are no ring outliers.

9 monomers are involved in 25 short contacts:

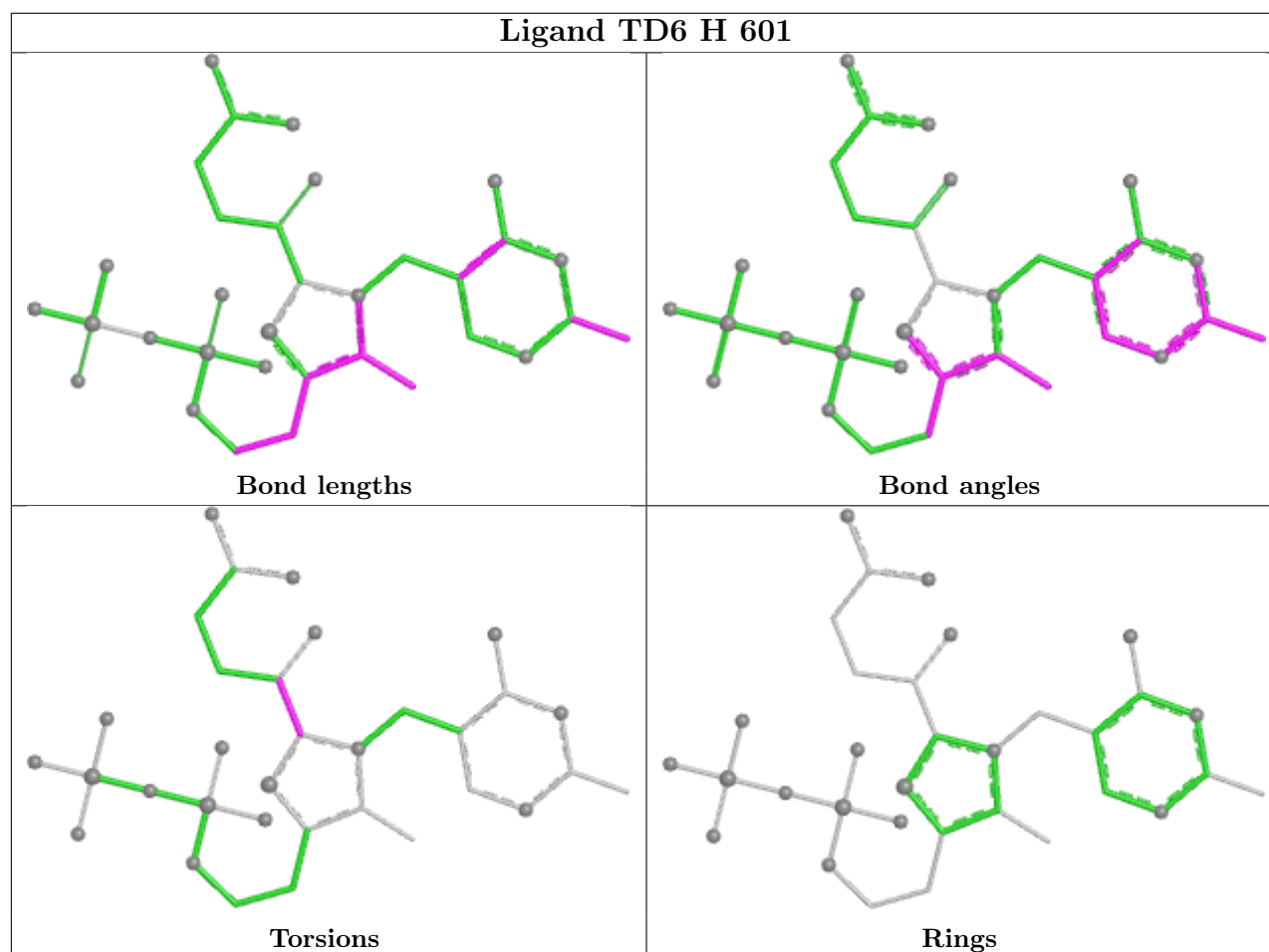
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	601	TD6	4	0
2	E	601	TD6	3	0
2	B	601	TD6	2	0
2	G	601	TD6	2	0
2	D	601	TD6	3	0
2	F	601	TD6	3	0
4	G	603	GOL	1	0

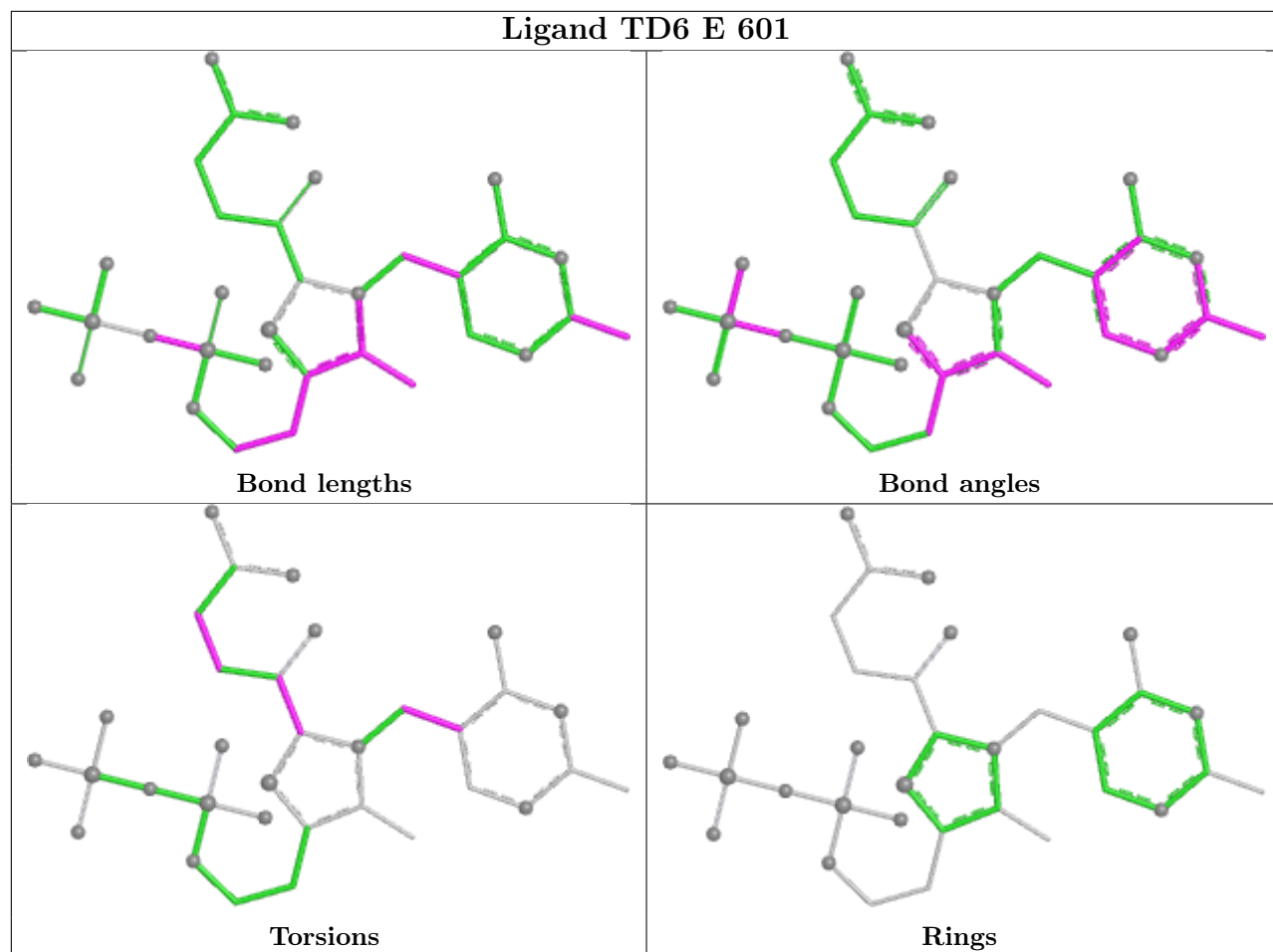
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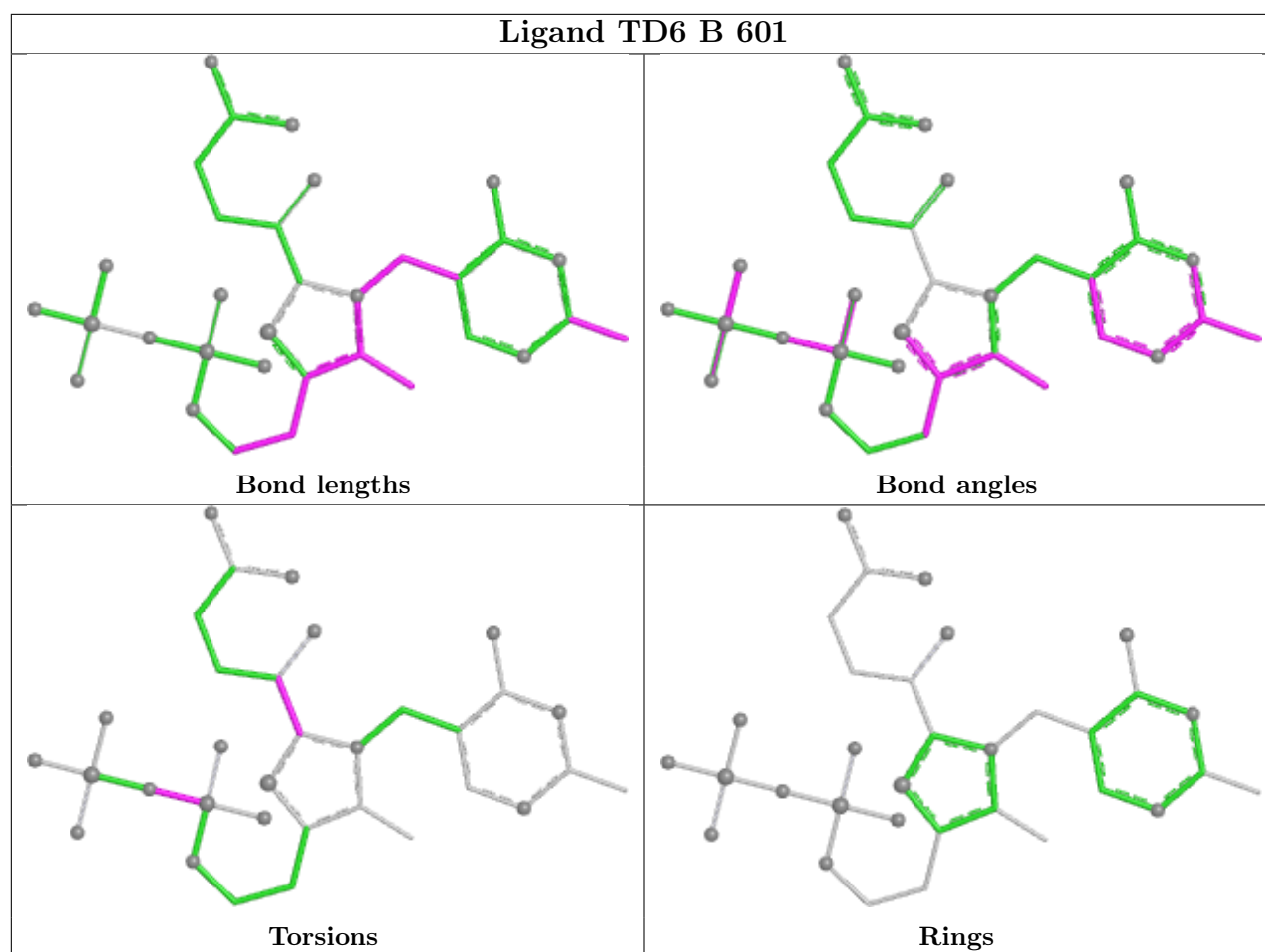
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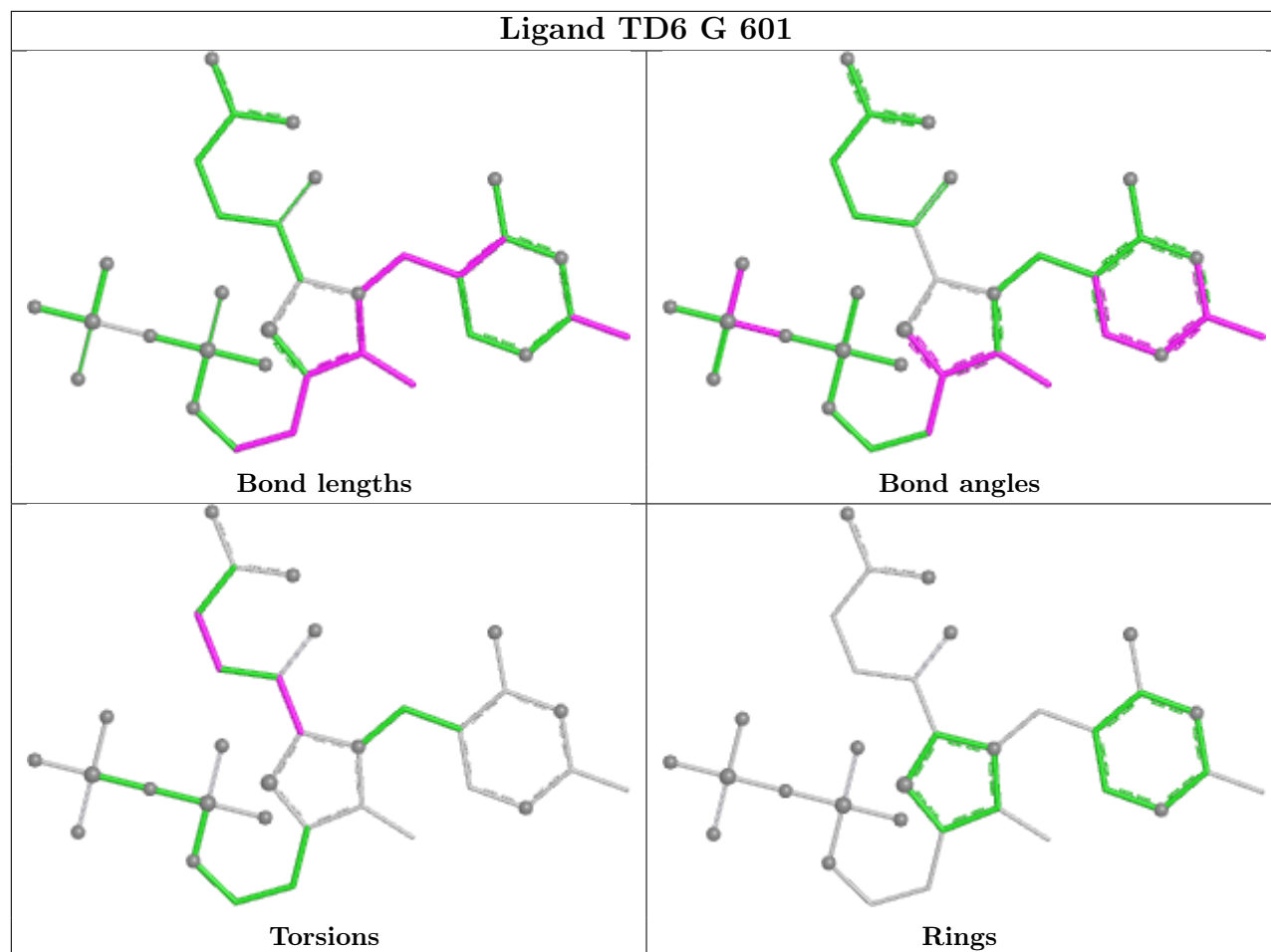
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TD6	4	0
2	C	601	TD6	3	0

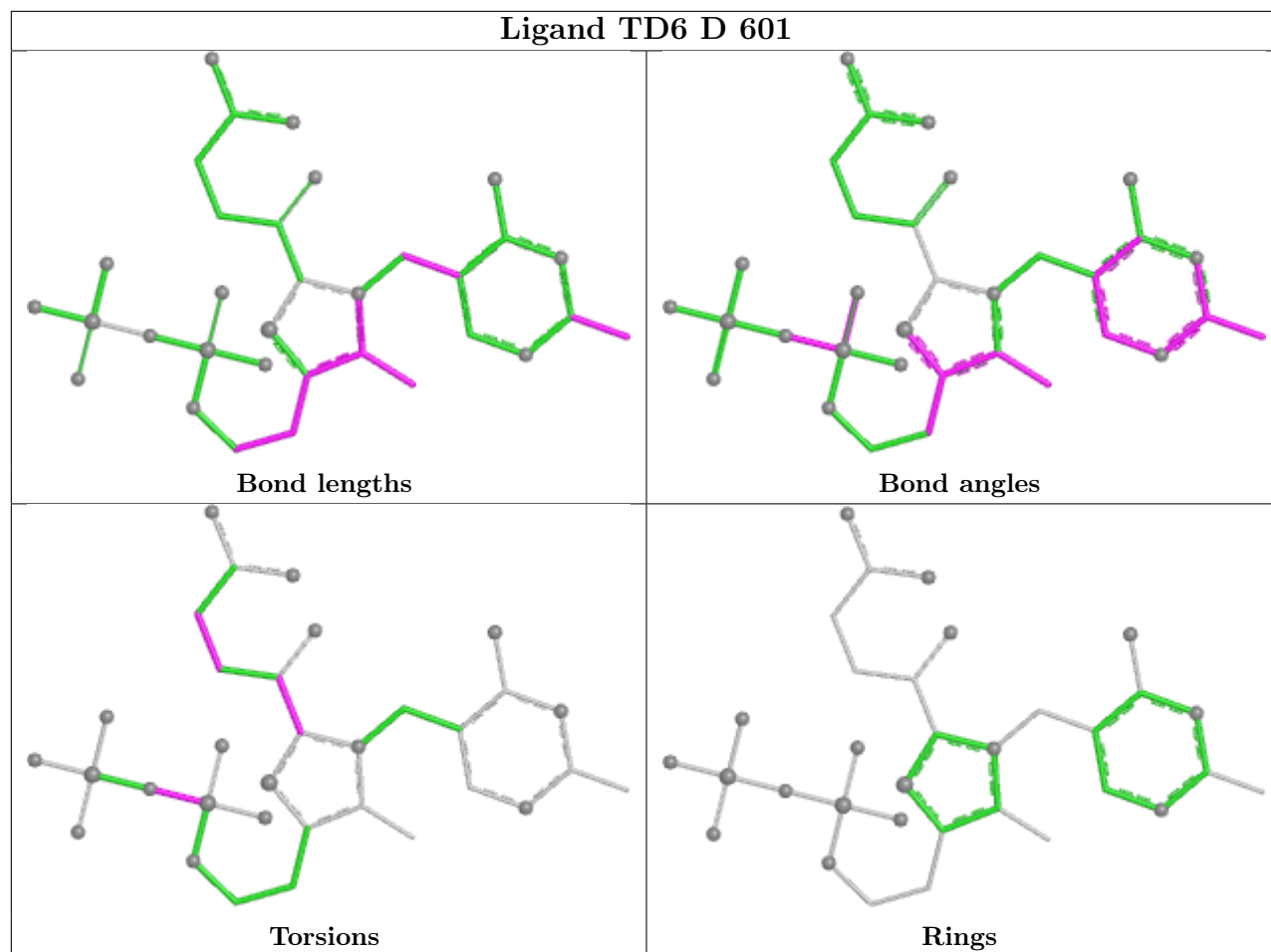
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

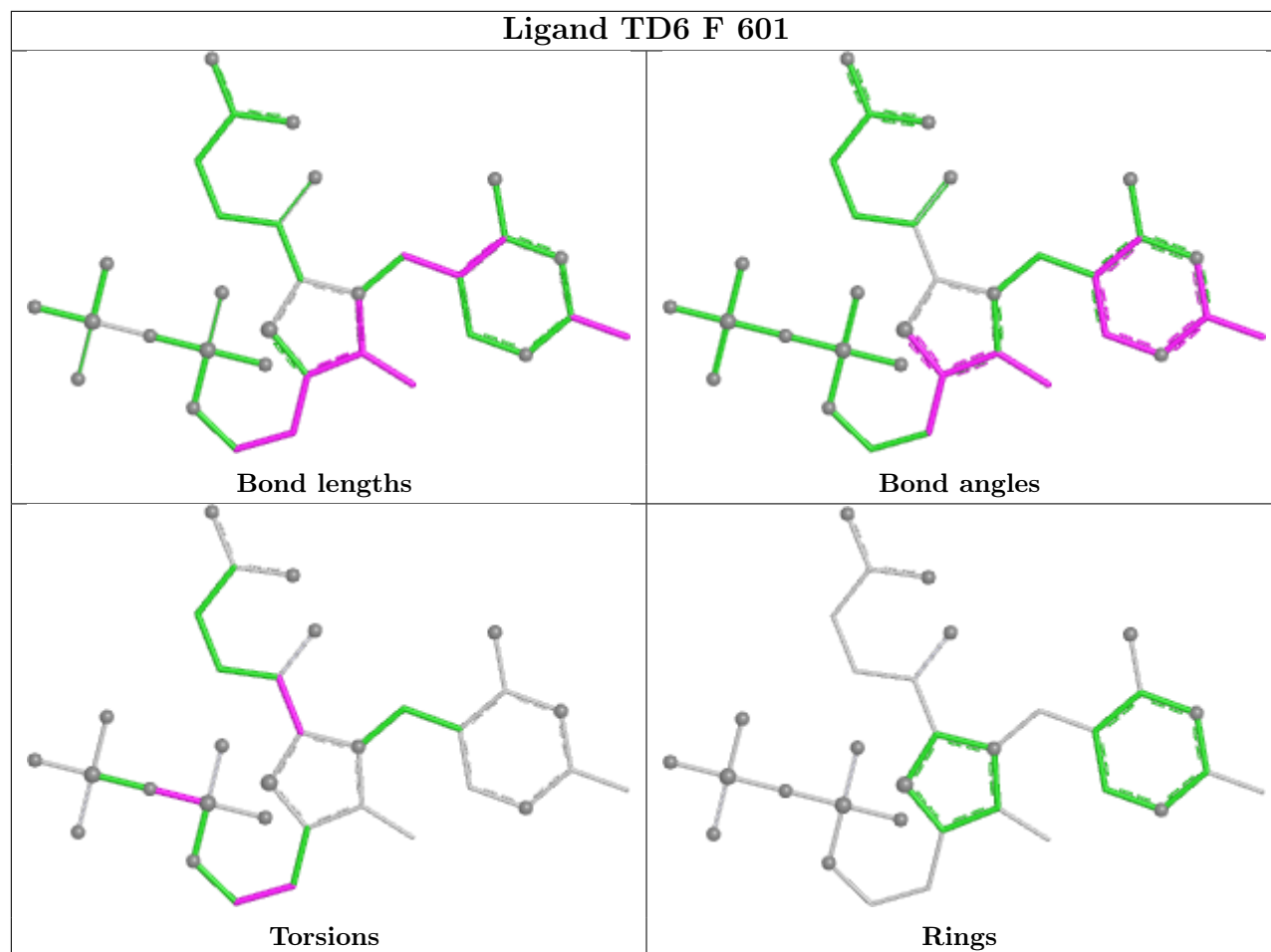


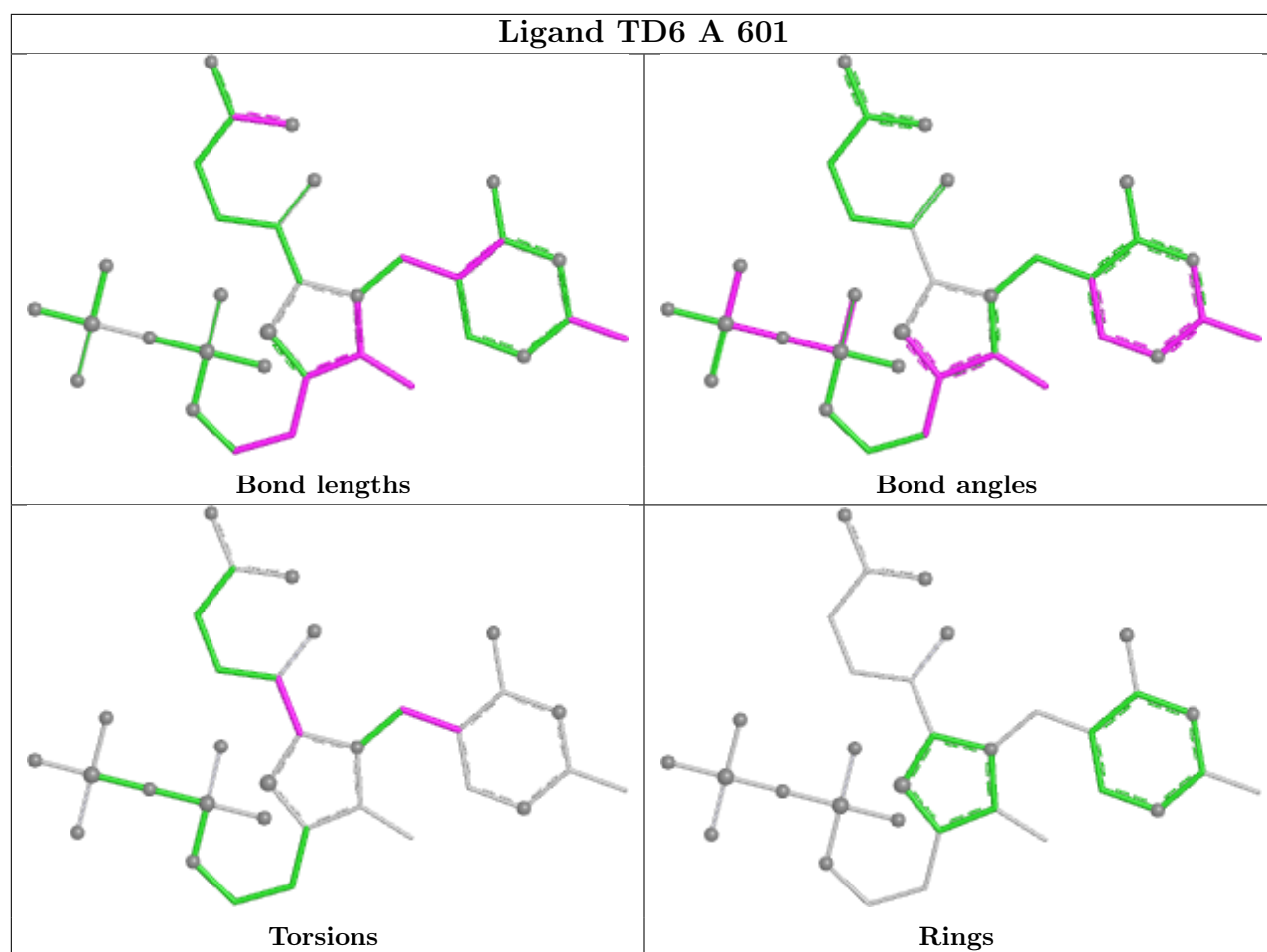


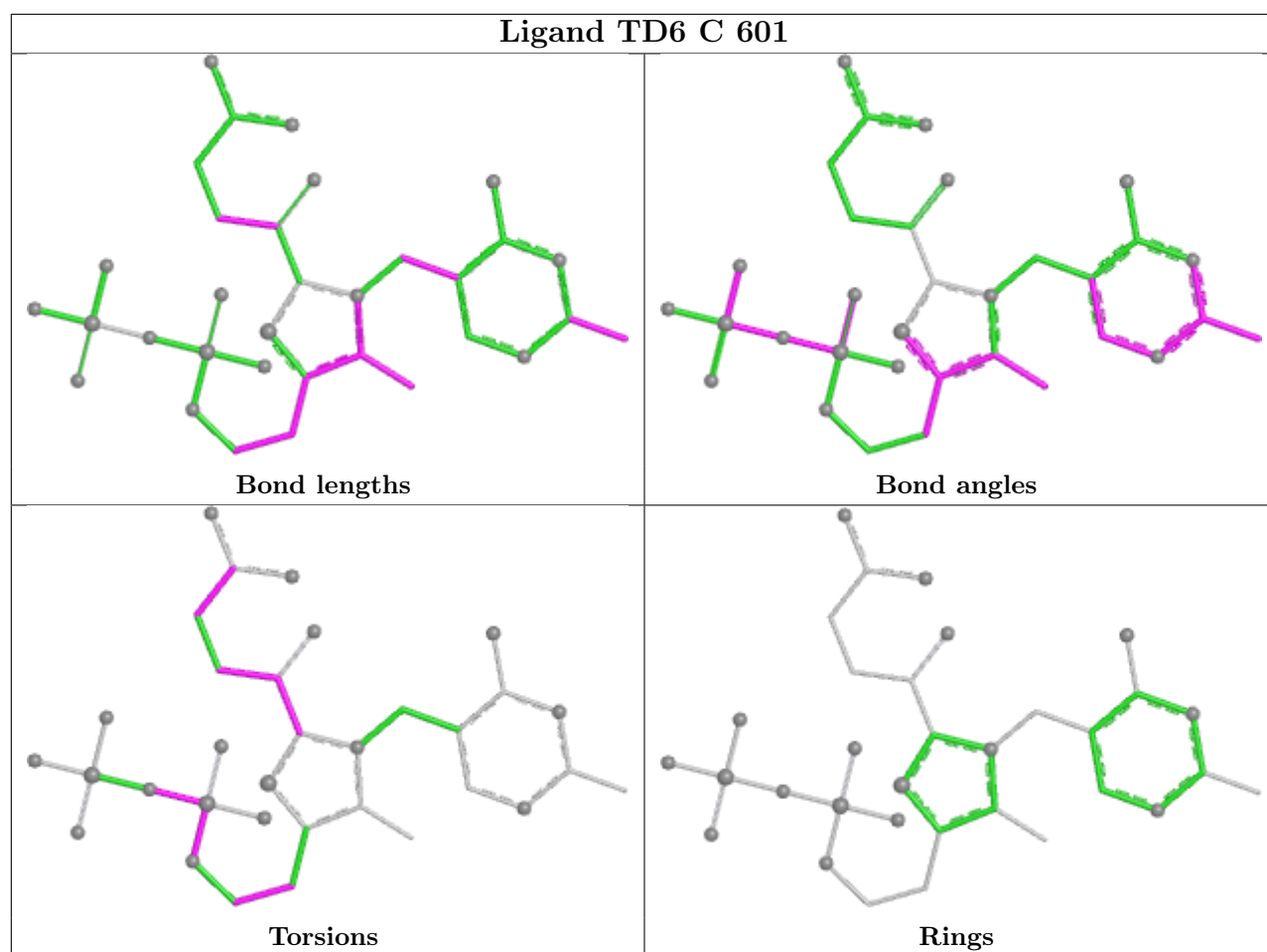












5.7 Other polymers [i](#)

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 [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	556/556 (100%)	-0.19	3 (0%) 87 87	9, 22, 38, 61	4 (0%)
1	B	556/556 (100%)	-0.16	1 (0%) 91 91	13, 22, 35, 55	3 (0%)
1	C	556/556 (100%)	-0.13	2 (0%) 88 89	9, 23, 38, 57	6 (1%)
1	D	556/556 (100%)	0.04	3 (0%) 87 87	12, 27, 46, 63	3 (0%)
1	E	556/556 (100%)	-0.19	2 (0%) 88 89	10, 22, 36, 72	7 (1%)
1	F	556/556 (100%)	-0.15	1 (0%) 91 91	14, 23, 35, 65	2 (0%)
1	G	556/556 (100%)	0.02	1 (0%) 91 91	11, 28, 45, 74	7 (1%)
1	H	556/556 (100%)	-0.12	2 (0%) 88 89	14, 23, 38, 63	1 (0%)
All	All	4448/4448 (100%)	-0.11	15 (0%) 90 90	9, 24, 40, 74	33 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	4[A]	SER	6.1
1	C	377[A]	CYS	4.2
1	D	1	MET	3.0
1	D	178	MET	2.9
1	A	178	MET	2.9

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

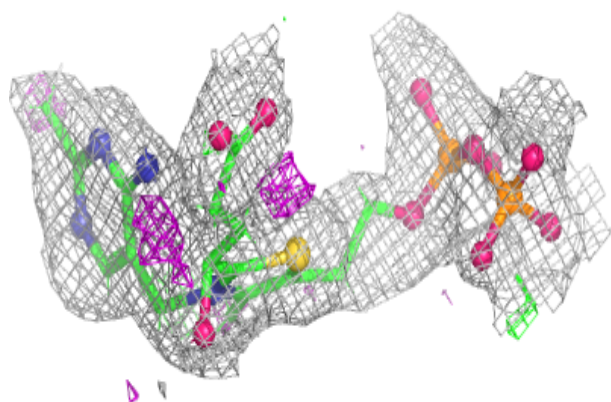
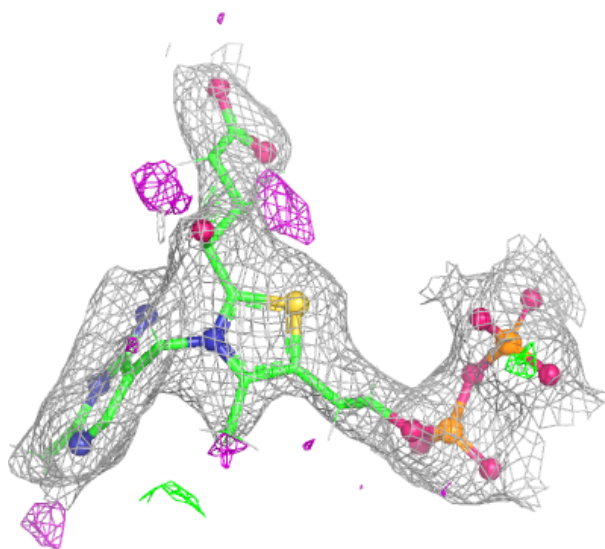
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	G	603	6/6	0.81	0.17	37,46,55,55	0
4	GOL	A	603	6/6	0.88	0.12	23,31,38,38	0
4	GOL	D	603	6/6	0.90	0.13	31,38,44,46	0
4	GOL	C	603	6/6	0.92	0.14	31,47,61,61	0
4	GOL	H	603	6/6	0.92	0.12	26,39,47,48	0
4	GOL	B	603	6/6	0.94	0.09	23,33,39,43	0
4	GOL	E	603	6/6	0.94	0.09	23,29,34,40	0
2	TD6	E	601	33/33	0.96	0.08	12,23,42,46	0
2	TD6	F	601	33/33	0.96	0.07	15,28,45,49	0
2	TD6	G	601	33/33	0.96	0.07	15,29,46,50	0
4	GOL	F	603	6/6	0.96	0.06	17,29,33,35	0
2	TD6	B	601	33/33	0.96	0.07	17,26,39,58	0
2	TD6	D	601	33/33	0.96	0.07	18,27,45,56	0
2	TD6	H	601	33/33	0.97	0.07	16,26,40,48	0
2	TD6	A	601	33/33	0.97	0.08	16,28,42,50	0
2	TD6	C	601	33/33	0.97	0.07	13,28,37,42	0
3	MN	E	602	1/1	0.98	0.05	30,30,30,30	0
3	MN	F	602	1/1	0.98	0.04	34,34,34,34	0
3	MN	G	602	1/1	0.99	0.03	34,34,34,34	0
3	MN	H	602	1/1	0.99	0.08	30,30,30,30	0
3	MN	D	602	1/1	0.99	0.04	34,34,34,34	0
3	MN	B	602	1/1	0.99	0.04	31,31,31,31	0
3	MN	C	602	1/1	0.99	0.09	39,39,39,39	0
3	MN	A	602	1/1	1.00	0.02	34,34,34,34	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.

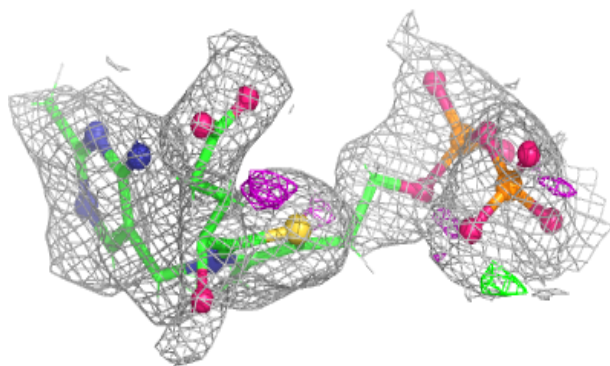
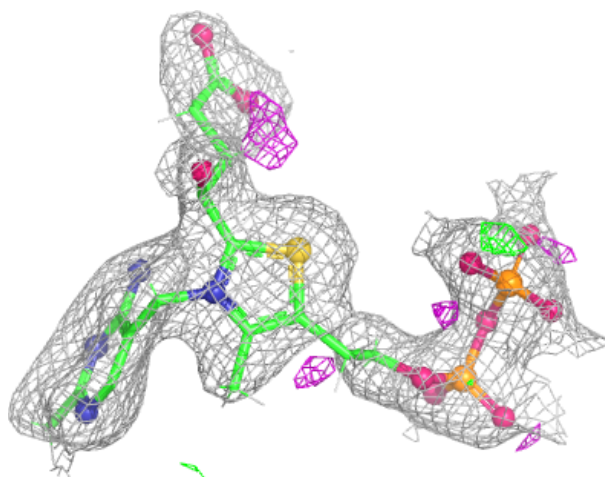
Electron density around TD6 E 601:

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



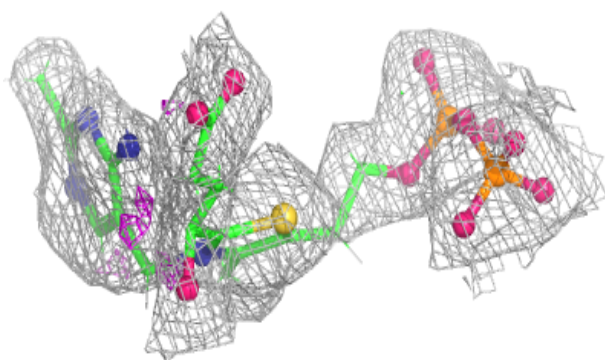
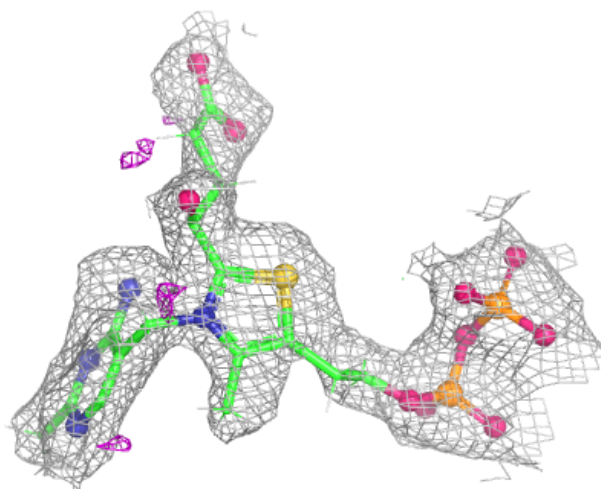
Electron density around TD6 F 601:

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



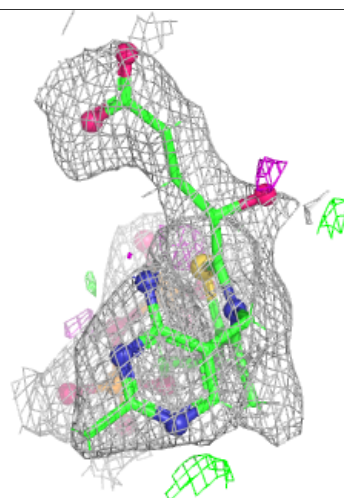
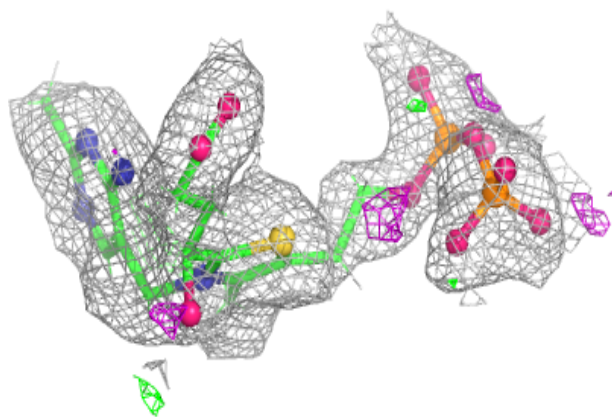
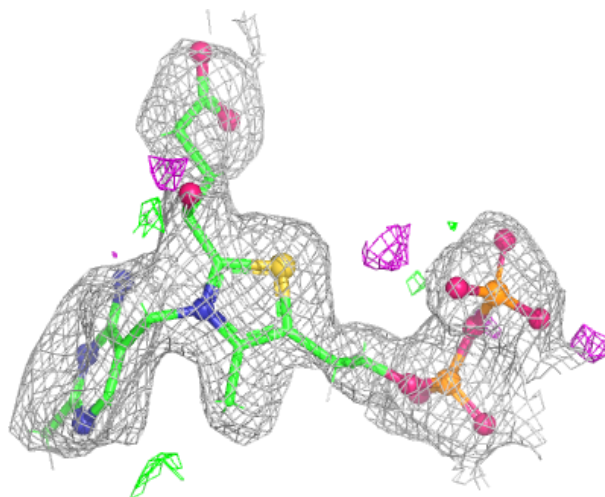
Electron density around TD6 G 601:

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



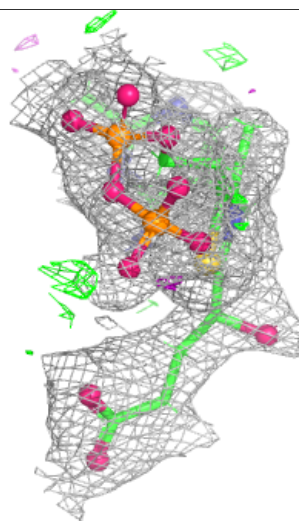
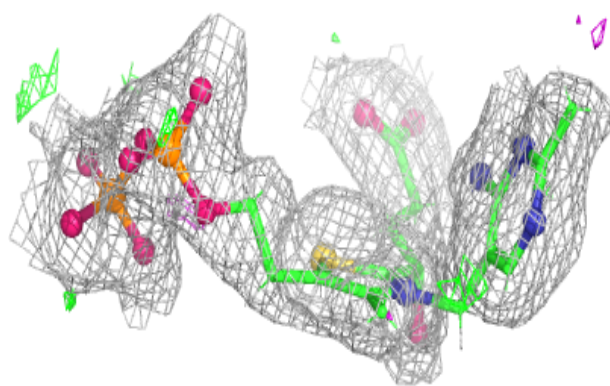
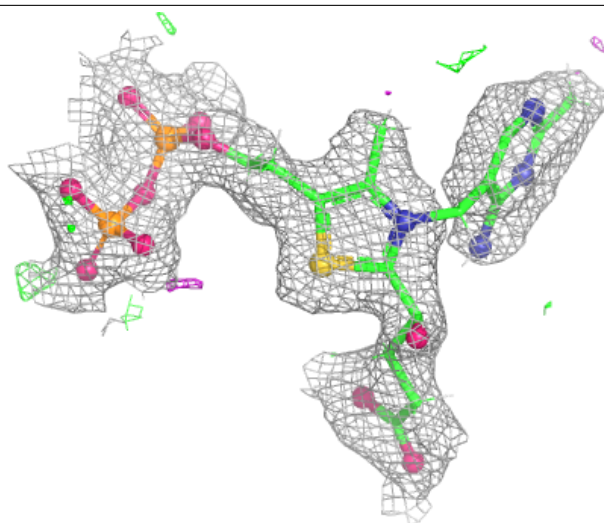
Electron density around TD6 B 601:

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



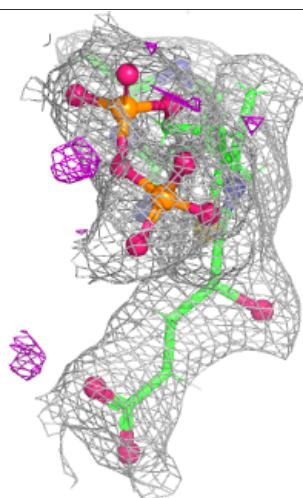
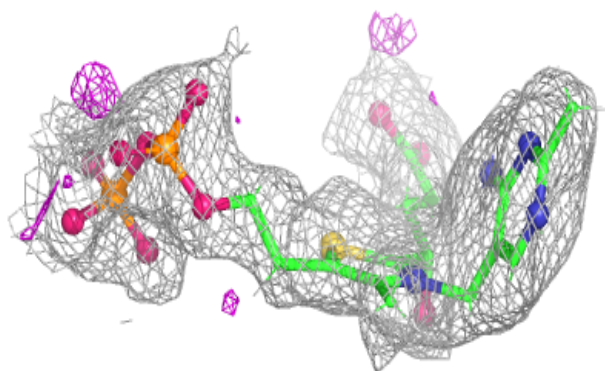
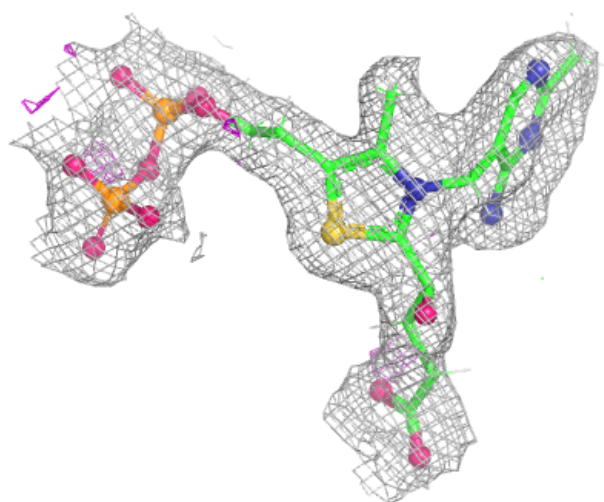
Electron density around TD6 D 601:

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



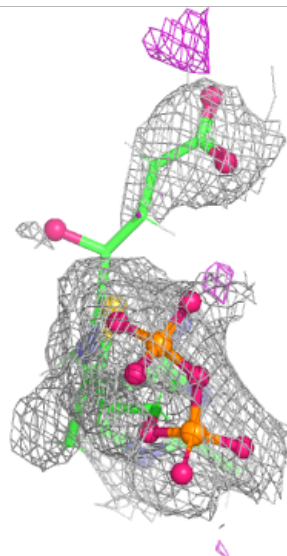
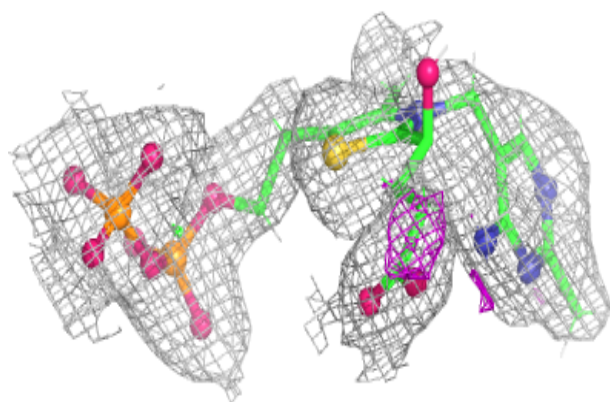
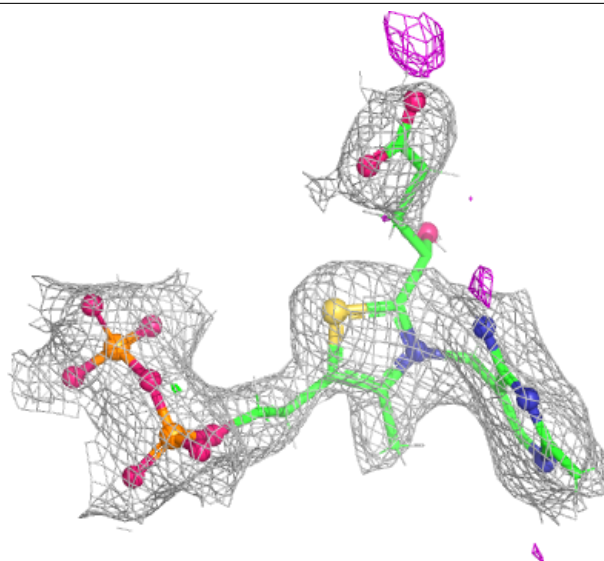
Electron density around TD6 H 601:

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and green (positive)



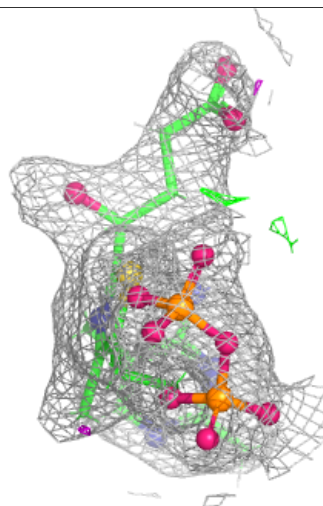
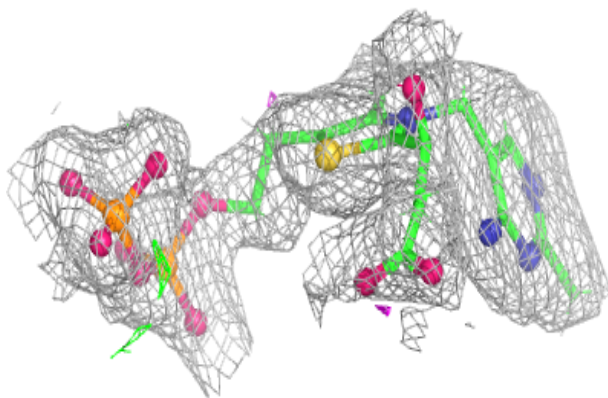
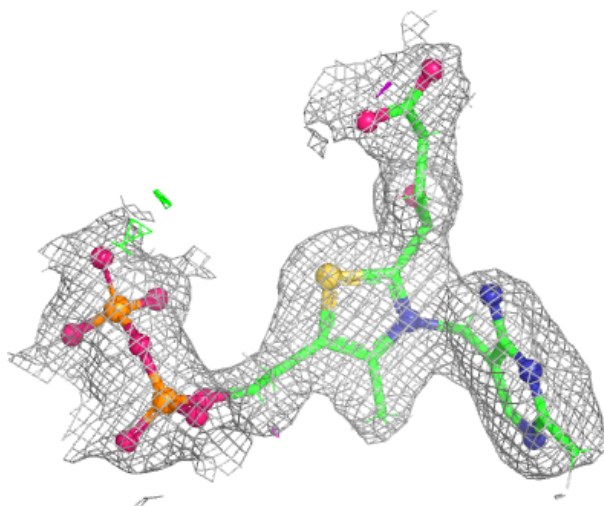
Electron density around TD6 A 601:

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



Electron density around TD6 C 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.