



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2020 – 09:15 am BST

PDB ID : 5EJ8
Title : EcMenD-ThDP-Mn2+ complex structure soaked with 2-ketoglutarate for 2 min
Authors : Song, H.G.; Dong, C.; Chen, Y.Z.; Sun, Y.R.; Guo, Z.H.
Deposited on : 2015-11-01
Resolution : 1.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

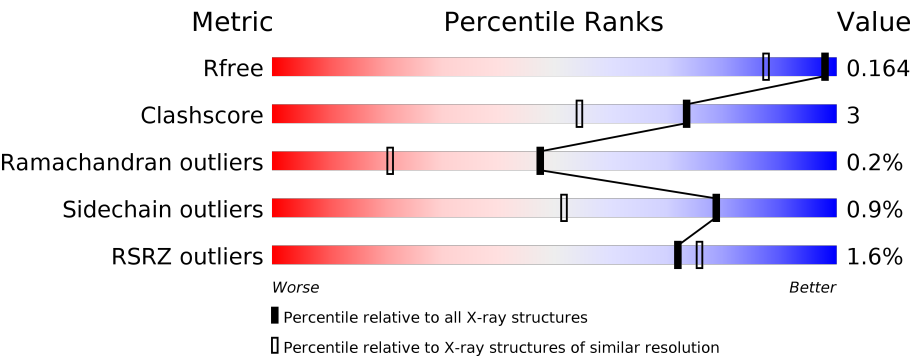
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.34 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	1385 (1.36-1.32)
Clashscore	141614	1417 (1.36-1.32)
Ramachandran outliers	138981	1397 (1.36-1.32)
Sidechain outliers	138945	1397 (1.36-1.32)
RSRZ outliers	127900	1369 (1.36-1.32)

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>%</div><div><div></div><div></div><div></div><div></div></div><div>94%6%</div></div>
1	B	556	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>95%5%</div></div>
1	C	556	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>92%8%</div></div>
1	D	556	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>94%6%</div></div>
1	E	556	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>94%6%</div></div>
1	F	556	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>92%8%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	556	
1	H	556	

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
6	EDO	A	614	-	-	X	-
6	EDO	C	601	-	-	X	-
6	EDO	D	611	-	-	X	-
6	EDO	F	610	-	-	X	-
7	FMT	A	617	-	-	X	-
7	FMT	B	613	-	-	X	-
7	FMT	D	612	-	-	X	-
7	FMT	E	609	-	-	X	-
7	FMT	E	610	-	-	X	-
7	FMT	F	611	-	-	X	-
7	FMT	G	614	-	-	X	-

2 Entry composition

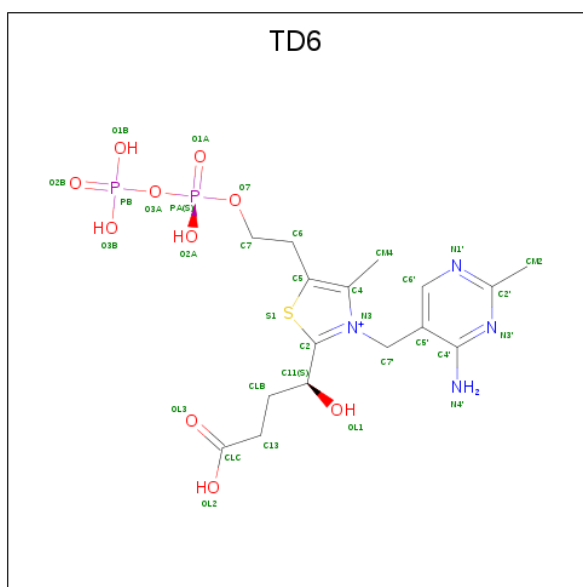
There are 9 unique types of molecules in this entry. The entry contains 77229 atoms, of which 35529 are hydrogens and 0 are deuteriums.

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	H	N	O	S	0	39	0
			8921	2834	4440	818	813	16			
1	B	556	Total	C	H	N	O	S	0	32	0
			8807	2811	4381	798	803	14			
1	C	556	Total	C	H	N	O	S	0	29	0
			8763	2800	4358	793	797	15			
1	D	556	Total	C	H	N	O	S	0	24	0
			8700	2783	4326	784	792	15			
1	E	556	Total	C	H	N	O	S	0	28	0
			8799	2801	4377	802	805	14			
1	F	556	Total	C	H	N	O	S	0	36	0
			8894	2832	4433	811	803	15			
1	G	556	Total	C	H	N	O	S	0	26	0
			8761	2798	4357	795	796	15			
1	H	556	Total	C	H	N	O	S	0	41	0
			8856	2827	4403	802	809	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 (three-letter code: 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 (three-letter code: MN) (formula: Mn).

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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

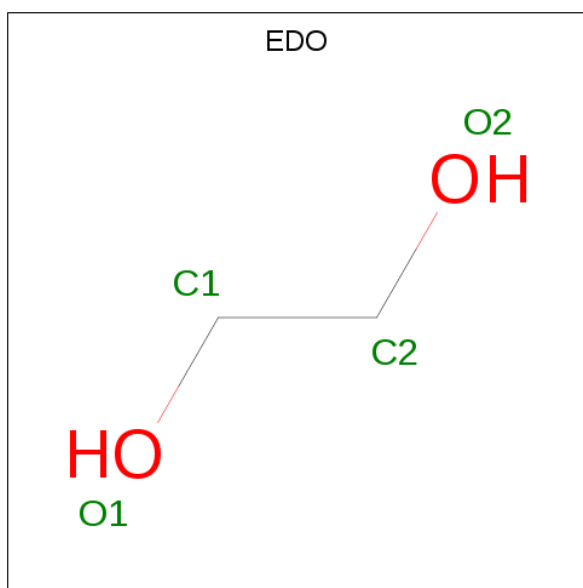
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total 2	Mg 2	0	1
4	D	2	Total 2	Mg 2	0	1
4	E	2	Total 2	Mg 2	0	1
4	H	2	Total 2	Mg 2	0	1
4	B	2	Total 2	Mg 2	0	1
4	C	2	Total 2	Mg 2	0	1
4	A	2	Total 2	Mg 2	0	1
4	F	1	Total 1	Mg 1	0	1

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		
5	G	1	Total	C	H	O	0	0
			14	3	8	3		
5	H	1	Total	C	H	O	0	0
			14	3	8	3		
5	H	1	Total	C	H	O	0	0
			13	3	7	3		
5	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



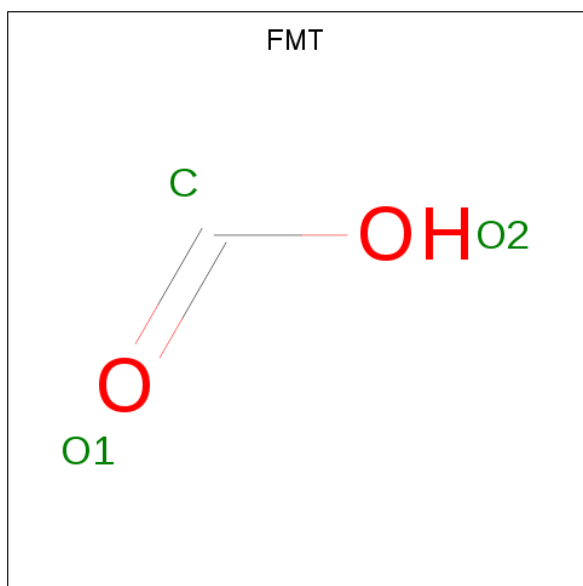
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		
6	F	1	Total	C	H	O	0	0
			10	2	6	2		
6	F	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 4	C 1	H 1	O 2	0	0
7	A	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	C	1	Total 4	C 1	H 1	O 2	0	0
7	C	1	Total 4	C 1	H 1	O 2	0	0
7	C	1	Total 4	C 1	H 1	O 2	0	0
7	C	1	Total 4	C 1	H 1	O 2	0	0
7	D	1	Total 4	C 1	H 1	O 2	0	0
7	D	1	Total 4	C 1	H 1	O 2	0	0
7	D	1	Total 4	C 1	H 1	O 2	0	0
7	D	1	Total 4	C 1	H 1	O 2	0	0
7	D	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	F	1	Total 4	C 1	H 1	O 2	0	0
7	F	1	Total 4	C 1	H 1	O 2	0	0
7	F	1	Total 4	C 1	H 1	O 2	0	0
7	F	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	H	1	Total 4	C 1	H 1	O 2	0	0
7	H	1	Total 4	C 1	H 1	O 2	0	0
7	H	1	Total 4	C 1	H 1	O 2	0	0
7	H	1	Total 4	C 1	H 1	O 2	0	0

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

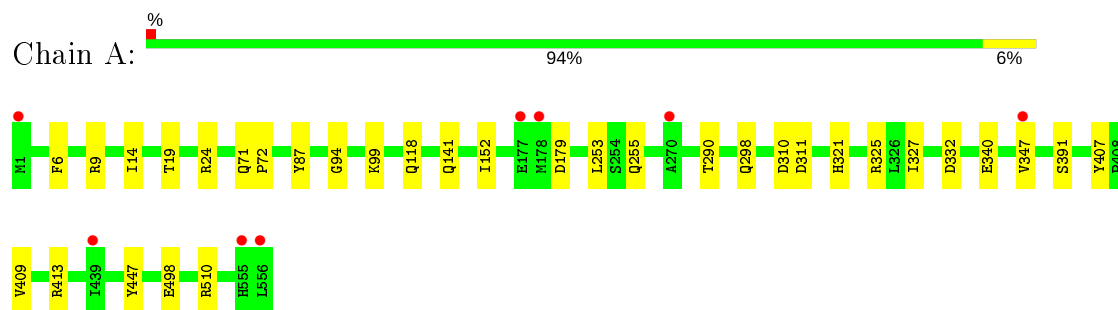
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	743	Total	O	0	0
			743	743		
9	B	757	Total	O	0	0
			757	757		
9	C	701	Total	O	0	0
			701	701		
9	D	604	Total	O	0	0
			604	604		
9	E	756	Total	O	0	0
			756	756		
9	F	735	Total	O	0	0
			735	735		
9	G	643	Total	O	0	0
			643	643		
9	H	737	Total	O	0	0
			737	737		

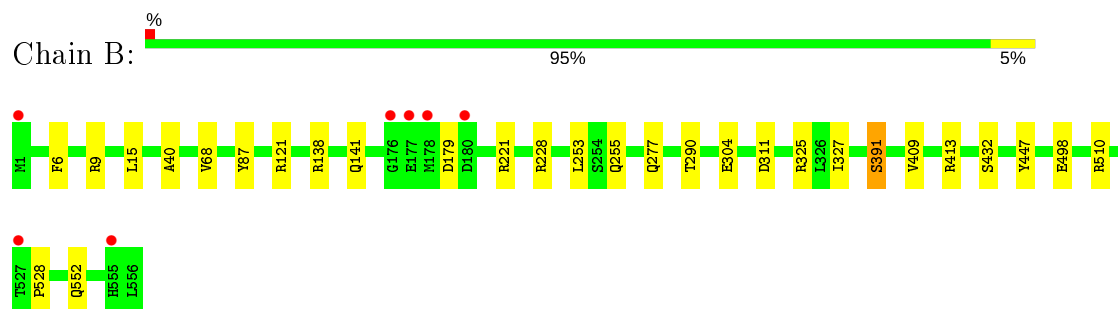
3 Residue-property plots [i](#)

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.

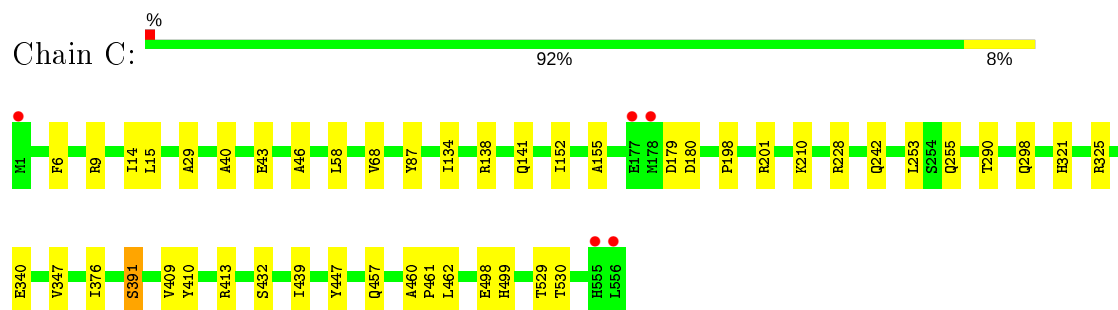
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



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

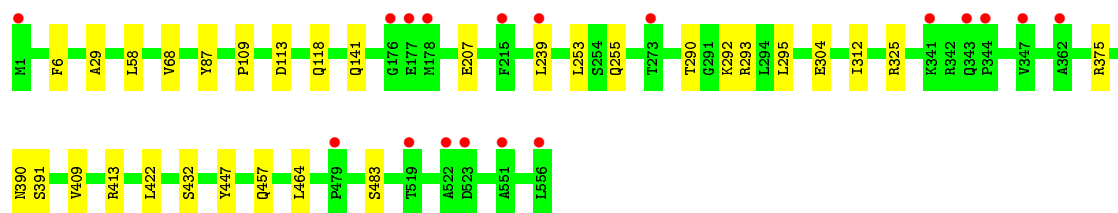


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

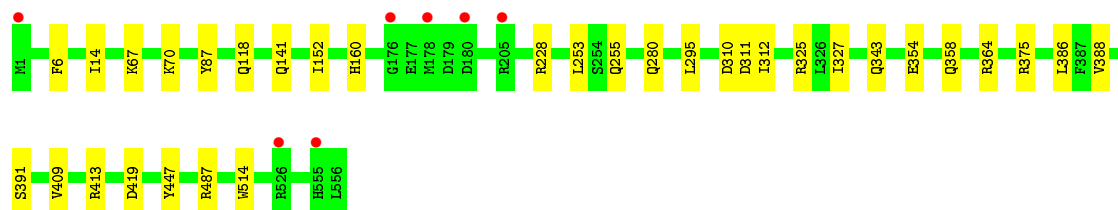
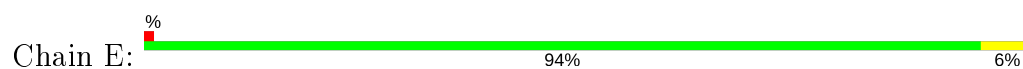


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

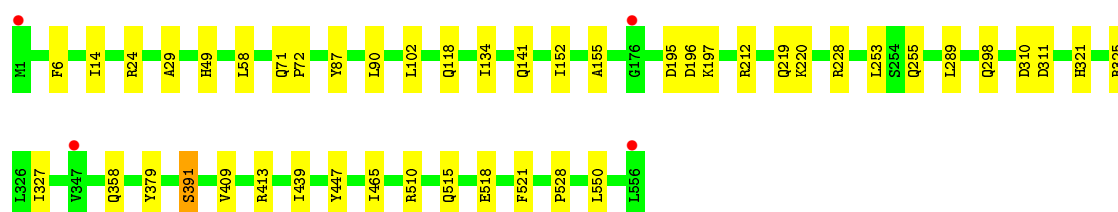




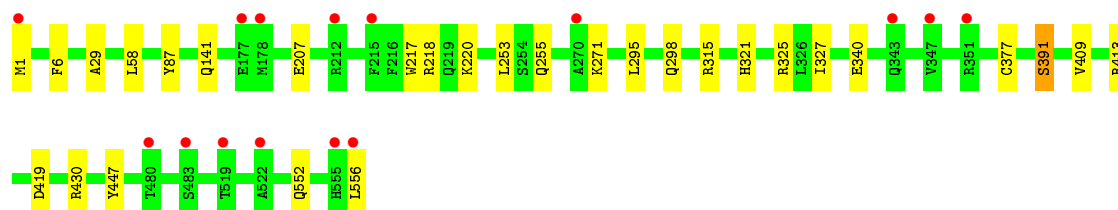
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



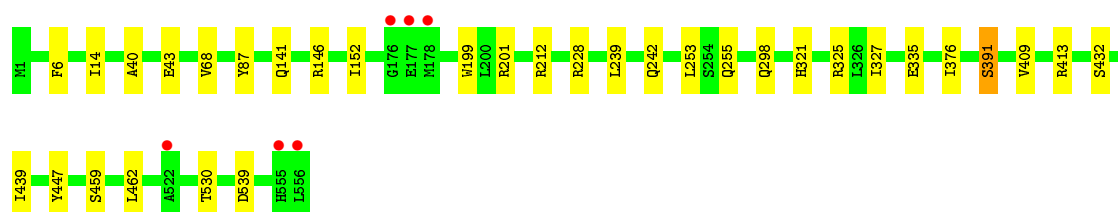
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- 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	90.66Å 90.76Å 169.34Å 83.25° 76.03° 64.32°	Depositor
Resolution (Å)	27.65 – 1.34 27.65 – 1.34	Depositor EDS
% Data completeness (in resolution range)	94.5 (27.65-1.34) 91.7 (27.65-1.34)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.34Å)	Xtriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, R_{free}	0.133 , 0.164 0.134 , 0.164	Depositor DCC
R_{free} test set	50289 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	77229	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 2.94% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, FMT, MN, EDO, TRS, 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	0.42	0/4745	0.67	0/6475
1	B	0.40	0/4652	0.65	1/6350 (0.0%)
1	C	0.39	0/4625	0.65	1/6315 (0.0%)
1	D	0.38	0/4586	0.64	0/6262
1	E	0.38	0/4639	0.66	3/6329 (0.0%)
1	F	0.39	0/4702	0.65	1/6416 (0.0%)
1	G	0.37	0/4614	0.64	1/6296 (0.0%)
1	H	0.39	0/4715	0.65	1/6436 (0.0%)
All	All	0.39	0/37278	0.65	8/50879 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	228	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	H	228	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	B	228	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	C	228	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	F	228	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	E	419	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	228	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	G	419	ASP	CB-CG-OD1	5.08	122.87	118.30

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	4481	4440	4285	22	1
1	B	4426	4381	4268	25	0
1	C	4405	4358	4245	34	0
1	D	4374	4326	4222	24	0
1	E	4422	4377	4268	21	1
1	F	4461	4433	4292	35	1
1	G	4404	4357	4255	20	0
1	H	4453	4403	4241	20	0
2	A	33	20	21	2	0
2	B	33	20	21	2	0
2	C	33	20	21	3	0
2	D	33	20	21	2	0
2	E	33	20	21	3	0
2	F	33	20	21	3	0
2	G	33	20	21	3	0
2	H	33	20	21	3	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	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
5	A	12	16	16	0	0
5	B	6	8	8	0	0
5	C	12	16	16	0	0
5	D	12	16	16	0	0
5	E	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	12	16	16	0	0
5	G	6	8	8	0	0
5	H	18	23	23	1	0
6	A	28	42	42	12	0
6	C	24	36	35	13	0
6	D	4	6	6	5	0
6	E	4	6	6	0	0
6	F	8	12	12	5	0
6	G	8	12	12	0	0
6	H	8	12	12	0	0
7	A	15	5	5	2	0
7	B	24	8	8	3	0
7	C	12	4	4	1	0
7	D	15	5	5	2	0
7	E	21	7	7	4	0
7	F	12	4	4	4	0
7	G	24	8	8	5	0
7	H	12	4	4	0	0
8	C	8	12	12	1	0
9	A	743	0	0	10	0
9	B	757	0	0	11	3
9	C	701	0	0	15	3
9	D	604	0	0	8	2
9	E	756	0	0	9	2
9	F	735	0	0	18	0
9	G	643	0	0	10	2
9	H	737	0	0	6	3
All	All	41700	35529	34537	239	9

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.

All (239) 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)
7:E:610:FMT:O1	9:E:701:HOH:O	1.89	0.90
1:G:1:MET:N	9:G:701:HOH:O	2.03	0.89
1:B:179:ASP:O	9:B:701:HOH:O	1.93	0.86
1:F:379:TYR:OH	9:F:701:HOH:O	1.93	0.85
1:C:347:VAL:O	9:C:702:HOH:O	1.96	0.84
1:A:298[A]:GLN:NE2	9:A:705:HOH:O	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43[A]:GLU:OE1	9:C:701:HOH:O	1.96	0.83
1:H:335:GLU:OE1	9:H:701:HOH:O	1.96	0.83
1:A:347:VAL:O	9:A:701:HOH:O	1.96	0.82
1:C:180:ASP:OD2	9:C:703:HOH:O	1.98	0.81
1:A:332:ASP:HB3	6:A:615:EDO:H11	1.63	0.79
6:C:601:EDO:O2	9:C:704:HOH:O	1.99	0.79
1:H:298[A]:GLN:OE1	9:H:702:HOH:O	2.00	0.79
6:A:606:EDO:O1	9:A:704:HOH:O	2.02	0.78
1:B:311[A]:ASP:OD2	9:B:702:HOH:O	2.01	0.78
7:G:609:FMT:O1	9:G:702:HOH:O	2.03	0.77
1:F:196:ASP:OD2	9:F:703:HOH:O	2.03	0.76
6:A:611:EDO:O1	9:A:702:HOH:O	1.96	0.76
1:F:310:ASP:OD1	9:F:702:HOH:O	2.02	0.76
1:B:255:GLN:HE21	1:B:409:VAL:H	1.33	0.75
1:E:310:ASP:OD1	9:E:702:HOH:O	2.04	0.75
1:E:255:GLN:HE21	1:E:409:VAL:H	1.36	0.74
1:F:255:GLN:HE21	1:F:409:VAL:H	1.34	0.74
1:H:255:GLN:HE21	1:H:409:VAL:H	1.36	0.73
1:A:255:GLN:HE21	1:A:409:VAL:H	1.35	0.72
1:C:179:ASP:O	9:C:705:HOH:O	2.07	0.72
1:D:255:GLN:HE21	1:D:409:VAL:H	1.37	0.72
1:C:201[B]:ARG:HG3	1:C:201[B]:ARG:HH21	1.54	0.72
1:A:310[A]:ASP:OD1	9:A:707:HOH:O	2.08	0.71
1:C:255:GLN:HE21	1:C:409:VAL:H	1.37	0.71
2:F:602:TD6:HN4A	2:F:602:TD6:H11	1.56	0.71
7:G:614:FMT:O2	9:G:703:HOH:O	2.10	0.69
2:C:602:TD6:HN4A	2:C:602:TD6:H11	1.58	0.69
1:G:255:GLN:HE21	1:G:409:VAL:H	1.41	0.68
2:B:602:TD6:HN4A	2:B:602:TD6:H11	1.59	0.67
1:D:304:GLU:OE1	9:D:701:HOH:O	2.12	0.67
1:G:298[A]:GLN:OE1	9:G:704:HOH:O	2.13	0.66
2:H:602:TD6:H11	2:H:602:TD6:HN4A	1.60	0.66
1:F:528:PRO:O	9:F:706:HOH:O	2.14	0.66
1:H:146[B]:ARG:HG2	1:H:199:TRP:CZ2	2.30	0.66
2:D:602:TD6:HN4A	2:D:602:TD6:H11	1.61	0.66
1:G:340[B]:GLU:N	1:G:340[B]:GLU:OE2	2.28	0.65
2:G:601:TD6:HN4A	2:G:601:TD6:H11	1.62	0.65
1:B:221:ARG:NH1	9:B:704:HOH:O	2.21	0.65
1:F:220:LYS:O	9:F:704:HOH:O	2.12	0.65
7:F:611:FMT:O1	9:F:705:HOH:O	2.14	0.65
2:E:601:TD6:H11	2:E:601:TD6:HN4A	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:609:FMT:O2	9:E:703:HOH:O	2.15	0.64
1:D:113:ASP:OD2	9:D:702:HOH:O	2.14	0.64
2:A:601:TD6:H11	2:A:601:TD6:HN4A	1.63	0.64
1:A:99:LYS:NZ	9:A:706:HOH:O	2.07	0.63
1:G:295:LEU:HD21	7:G:614:FMT:H	1.81	0.63
1:B:290:THR:HA	7:B:613:FMT:H	1.81	0.62
1:E:364:ARG:O	1:E:375[B]:ARG:NH1	2.32	0.62
1:C:46:ALA:HB2	8:C:606:TRS:H22	1.82	0.62
1:D:207:GLU:OE2	9:D:703:HOH:O	2.15	0.61
1:H:239:LEU:HD12	1:H:242[B]:GLN:OE1	2.00	0.61
1:F:24[A]:ARG:NH2	9:F:712:HOH:O	2.34	0.60
1:A:498[A]:GLU:OE1	1:A:510[A]:ARG:NH2	2.34	0.60
1:C:15[A]:LEU:HD12	1:C:40:ALA:HB3	1.83	0.60
1:H:43:GLU:OE2	9:H:704:HOH:O	2.17	0.59
2:B:602:TD6:HN4A	2:B:602:TD6:C11	2.17	0.58
1:A:311[A]:ASP:OD1	9:A:708:HOH:O	2.17	0.57
1:E:358:GLN:NE2	9:E:708:HOH:O	2.34	0.57
2:H:602:TD6:C11	2:H:602:TD6:HN4A	2.17	0.57
1:F:219:GLN:NE2	9:F:713:HOH:O	2.37	0.56
1:D:6:PHE:CE1	1:D:141:GLN:HG2	2.39	0.56
1:E:295:LEU:HD21	7:E:610:FMT:H	1.88	0.56
1:D:295:LEU:HD21	7:D:612:FMT:H	1.88	0.56
1:A:94:GLY:HA3	6:A:611:EDO:H21	1.87	0.55
1:B:552:GLN:NE2	9:B:710:HOH:O	2.39	0.55
1:F:358:GLN:HG3	9:F:1403:HOH:O	2.06	0.55
1:B:528:PRO:O	9:B:703:HOH:O	2.18	0.55
2:C:602:TD6:C11	2:C:602:TD6:HN4A	2.20	0.55
2:E:601:TD6:C11	2:E:601:TD6:HN4A	2.19	0.55
1:B:498:GLU:OE2	1:B:510[A]:ARG:NH2	2.39	0.55
1:C:198:PRO:O	1:C:201[B]:ARG:NH2	2.39	0.55
2:G:601:TD6:HN4A	2:G:601:TD6:C11	2.19	0.55
1:B:304:GLU:CG	9:B:1430:HOH:O	2.55	0.54
1:G:552:GLN:NE2	9:G:712:HOH:O	2.41	0.54
1:B:9:ARG:NH2	9:B:701:HOH:O	2.30	0.54
2:E:601:TD6:H11	1:F:118[B]:GLN:HE22	1.73	0.54
1:A:19:THR:O	1:A:24[A]:ARG:NH1	2.41	0.54
1:F:311:ASP:HB3	9:F:1196:HOH:O	2.07	0.54
2:D:602:TD6:HN4A	2:D:602:TD6:C11	2.20	0.53
1:E:343:GLN:NE2	9:E:706:HOH:O	2.30	0.53
1:F:358:GLN:HG3	9:F:1295:HOH:O	2.09	0.53
1:B:277:GLN:HG2	9:B:1301:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:LEU:HD12	9:D:712:HOH:O	2.08	0.53
2:A:601:TD6:C11	2:A:601:TD6:HN4A	2.21	0.52
2:F:602:TD6:HN4A	2:F:602:TD6:C11	2.20	0.52
1:G:315:ARG:NE	9:G:706:HOH:O	2.21	0.52
1:D:413:ARG:NH1	6:D:611:EDO:H12	2.25	0.52
1:F:311:ASP:OD2	9:F:707:HOH:O	2.19	0.52
7:E:609:FMT:C	9:E:703:HOH:O	2.57	0.51
7:G:614:FMT:C	9:G:703:HOH:O	2.56	0.51
1:A:6:PHE:CE1	1:A:141:GLN:HG2	2.45	0.51
1:E:280:GLN:NE2	9:E:707:HOH:O	2.44	0.51
1:F:6:PHE:CE1	1:F:141:GLN:HG2	2.45	0.51
1:H:201[B]:ARG:HG3	1:H:201[B]:ARG:HH11	1.75	0.51
1:F:49:HIS:ND1	6:F:610:EDO:H11	2.26	0.51
1:C:290:THR:O	6:C:615:EDO:H12	2.11	0.51
1:E:118[B]:GLN:HE22	2:F:602:TD6:H11	1.76	0.50
1:C:6:PHE:CE1	1:C:141:GLN:HG2	2.47	0.50
1:C:40:ALA:HB2	9:C:803:HOH:O	2.12	0.50
1:G:6:PHE:CE1	1:G:141:GLN:HG2	2.46	0.50
1:A:71[B]:GLN:HB3	1:A:72:PRO:HD2	1.94	0.50
1:D:483:SER:OG	9:D:704:HOH:O	2.19	0.50
6:A:611:EDO:C2	1:B:121:ARG:HH22	2.25	0.49
1:F:71[A]:GLN:HB3	1:F:72:PRO:HD2	1.93	0.49
1:G:207:GLU:OE1	9:G:705:HOH:O	2.20	0.49
1:G:298[B]:GLN:O	1:G:321:HIS:HE1	1.95	0.49
1:B:15[A]:LEU:HD12	1:B:40:ALA:HB3	1.93	0.49
1:E:364:ARG:HB2	1:E:375[B]:ARG:HH12	1.77	0.49
6:C:607:EDO:H11	9:C:995:HOH:O	2.12	0.49
1:D:413:ARG:HH11	6:D:611:EDO:H12	1.77	0.49
1:G:377:CYS:HB2	9:G:707:HOH:O	2.12	0.49
1:A:9[B]:ARG:NH1	1:A:179:ASP:O	2.34	0.49
1:F:195:ASP:OD1	1:F:197:LYS:HE3	2.13	0.49
1:H:298[B]:GLN:O	1:H:321:HIS:HE1	1.95	0.49
1:C:43[A]:GLU:HG3	9:C:1021:HOH:O	2.12	0.49
1:D:422[A]:LEU:HD11	1:D:464:LEU:HD21	1.95	0.49
1:C:290:THR:HA	6:C:615:EDO:H12	1.93	0.48
1:A:290:THR:O	6:A:614:EDO:H11	2.12	0.48
1:F:550[A]:LEU:HD22	9:F:1289:HOH:O	2.12	0.48
1:E:487:ARG:HH22	6:F:610:EDO:H12	1.77	0.48
1:C:15[A]:LEU:HD12	1:C:40:ALA:CB	2.42	0.48
1:C:9:ARG:NH2	9:C:705:HOH:O	2.42	0.48
1:D:290:THR:O	6:D:611:EDO:H11	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:ASP:HB2	9:E:1289:HOH:O	2.12	0.48
1:C:14:ILE:HA	1:C:152[A]:ILE:HD13	1.95	0.48
1:D:422[A]:LEU:HD11	1:D:464:LEU:CD2	2.43	0.48
7:D:612:FMT:C	9:D:706:HOH:O	2.61	0.48
1:G:430:ARG:NE	7:G:608:FMT:H	2.29	0.48
1:F:298[B]:GLN:O	1:F:321:HIS:HE1	1.97	0.48
1:E:386:LEU:HG	1:E:388[B]:VAL:HG13	1.96	0.47
1:E:6:PHE:CE1	1:E:141:GLN:HG2	2.49	0.47
1:A:298[B]:GLN:O	1:A:321:HIS:HE1	1.98	0.47
1:H:212:ARG:NE	9:H:724:HOH:O	2.48	0.47
1:E:160[B]:HIS:HD2	9:E:725:HOH:O	1.98	0.47
1:E:67:LYS:O	1:E:70:LYS:HE2	2.14	0.47
1:B:6:PHE:CE1	1:B:141:GLN:HG2	2.50	0.47
1:A:253:LEU:HD11	1:A:413:ARG:HG3	1.97	0.47
1:C:410:TYR:CE1	6:C:611:EDO:H22	2.50	0.47
6:C:616:EDO:H21	9:C:748:HOH:O	2.15	0.47
1:C:9:ARG:NE	9:C:705:HOH:O	2.22	0.47
7:F:611:FMT:C	9:F:705:HOH:O	2.62	0.46
1:F:49:HIS:ND1	6:F:610:EDO:C1	2.78	0.46
7:A:617:FMT:C	9:A:710:HOH:O	2.63	0.46
1:G:217:TRP:CZ3	1:G:220[B]:LYS:HD2	2.51	0.46
1:G:315:ARG:NH2	9:G:706:HOH:O	2.45	0.46
1:E:327:ILE:N	1:E:327:ILE:HD12	2.31	0.46
1:F:327:ILE:N	1:F:327:ILE:HD12	2.30	0.46
1:C:376:ILE:HD11	1:C:439[A]:ILE:HD11	1.97	0.46
1:B:40:ALA:HB2	9:B:989:HOH:O	2.16	0.46
1:C:68:VAL:HG11	1:C:432:SER:HB3	1.98	0.46
1:G:253:LEU:HD11	1:G:413:ARG:HG3	1.98	0.46
1:H:43:GLU:HG3	9:H:1073:HOH:O	2.15	0.46
1:B:290:THR:O	7:B:613:FMT:H	2.16	0.45
1:E:375[B]:ARG:HD2	1:E:514:TRP:CZ3	2.51	0.45
1:H:253:LEU:HD11	1:H:413:ARG:HG3	1.97	0.45
7:A:617:FMT:O1	9:A:710:HOH:O	2.21	0.45
1:H:327:ILE:HD12	1:H:327:ILE:N	2.32	0.45
6:C:615:EDO:O1	6:C:616:EDO:H12	2.16	0.45
1:D:390:ASN:OD1	1:D:413:ARG:HD2	2.17	0.45
2:C:602:TD6:H11	1:D:118[A]:GLN:HE22	1.82	0.45
1:H:40:ALA:HB2	9:H:1065:HOH:O	2.17	0.45
1:G:327:ILE:HD12	1:G:327:ILE:N	2.32	0.45
1:B:413:ARG:HH11	7:B:613:FMT:C	2.29	0.45
1:C:253:LEU:HD11	1:C:413:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:515:GLN:NE2	9:F:721:HOH:O	2.44	0.45
2:H:602:TD6:C2	2:H:602:TD6:HN4A	2.30	0.45
1:H:6:PHE:CE1	1:H:141:GLN:HG2	2.51	0.45
1:E:253:LEU:HD11	1:E:413:ARG:HG3	1.99	0.44
1:B:138:ARG:H	6:C:601:EDO:C1	2.31	0.44
1:H:459:SER:HB2	5:H:611:GOL:H12	1.99	0.44
1:F:253:LEU:HD11	1:F:413:ARG:HG3	1.98	0.44
1:B:253:LEU:HD11	1:B:413:ARG:HG3	1.99	0.44
1:A:14:ILE:HG12	1:A:152[A]:ILE:HD11	2.00	0.44
1:A:407:TYR:HA	6:A:612:EDO:H11	1.98	0.44
1:F:518:GLU:HG3	9:F:701:HOH:O	2.17	0.44
1:B:138:ARG:H	6:C:601:EDO:H12	1.82	0.43
1:D:253:LEU:HD11	1:D:413:ARG:HG3	2.00	0.43
1:H:298[B]:GLN:O	1:H:321:HIS:CE1	2.71	0.43
1:D:290:THR:HA	6:D:611:EDO:H11	1.99	0.43
1:E:487:ARG:HH22	6:F:610:EDO:C1	2.30	0.43
1:F:439[B]:ILE:HD13	9:F:1253:HOH:O	2.19	0.43
1:F:49:HIS:H	6:F:610:EDO:C1	2.32	0.43
2:G:601:TD6:HN4A	2:G:601:TD6:C2	2.32	0.43
1:A:413:ARG:HH11	6:A:614:EDO:H12	1.84	0.43
1:D:292:LYS:HE2	1:D:293:ARG:NH1	2.33	0.43
1:C:462:LEU:O	1:C:530:THR:HA	2.19	0.42
1:C:498:GLU:HG2	1:C:499:HIS:N	2.35	0.42
1:C:460:ALA:HB1	1:C:461:PRO:HD2	2.02	0.42
1:D:29:ALA:HB2	1:D:58:LEU:HD22	2.02	0.42
1:D:457:GLN:OE1	9:D:705:HOH:O	2.22	0.42
1:D:375:ARG:HD3	9:D:860:HOH:O	2.19	0.42
1:F:14:ILE:HG12	1:F:152[B]:ILE:HD11	2.01	0.42
1:D:68:VAL:HG11	1:D:432:SER:HB3	2.02	0.41
1:A:327:ILE:HD12	1:A:327:ILE:N	2.34	0.41
1:B:68:VAL:HG11	1:B:432:SER:HB3	2.00	0.41
1:D:413:ARG:HH11	6:D:611:EDO:C1	2.33	0.41
1:F:298[B]:GLN:O	1:F:321:HIS:CE1	2.73	0.41
1:H:376:ILE:HD11	1:H:439[A]:ILE:HD11	2.02	0.41
1:B:9:ARG:NE	9:B:701:HOH:O	2.29	0.41
1:F:90[B]:LEU:HD12	1:F:102:LEU:CD1	2.51	0.41
1:C:134:ILE:HD11	1:C:155:ALA:HB2	2.02	0.41
1:F:510[B]:ARG:NH2	9:F:734:HOH:O	2.53	0.41
1:G:29:ALA:HB2	1:G:58:LEU:HD22	2.03	0.41
1:C:29:ALA:HB2	1:C:58:LEU:HD22	2.03	0.41
6:C:610:EDO:H11	9:C:1080:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:ILE:HD11	1:F:155:ALA:HB2	2.02	0.41
1:F:289:LEU:O	7:F:611:FMT:H	2.20	0.41
1:G:218:ARG:HG3	1:G:340[B]:GLU:OE1	2.20	0.41
1:G:271:LYS:HE3	1:G:556:LEU:O	2.21	0.41
6:A:613:EDO:H12	6:A:614:EDO:O1	2.21	0.41
6:A:613:EDO:H21	9:A:784:HOH:O	2.21	0.41
1:C:529:THR:HB	7:C:612:FMT:C	2.51	0.41
1:F:289:LEU:O	7:F:611:FMT:C	2.68	0.41
1:H:462:LEU:O	1:H:530:THR:HA	2.21	0.41
1:A:413:ARG:HH11	6:A:614:EDO:C1	2.33	0.41
1:C:242:GLN:HB2	6:C:610:EDO:C2	2.51	0.41
1:C:340:GLU:CG	9:C:1218:HOH:O	2.69	0.40
1:C:457:GLN:HG3	9:C:733:HOH:O	2.20	0.40
1:C:138:ARG:H	6:C:601:EDO:H21	1.86	0.40
1:C:210:LYS:NZ	9:C:706:HOH:O	2.20	0.40
1:F:465:ILE:HD11	1:F:521:PHE:HZ	1.86	0.40
1:H:14:ILE:HG12	1:H:152[A]:ILE:HD11	2.03	0.40
1:B:304:GLU:CG	9:B:1434:HOH:O	2.68	0.40
1:G:298[B]:GLN:O	1:G:321:HIS:CE1	2.73	0.40
1:H:68:VAL:HG11	1:H:432:SER:HB3	2.03	0.40
1:A:413:ARG:NH1	6:A:614:EDO:H12	2.37	0.40
1:E:14:ILE:HG12	1:E:152[A]:ILE:HD11	2.03	0.40
1:F:29:ALA:HB2	1:F:58:LEU:HD22	2.03	0.40
1:B:138:ARG:CB	6:C:601:EDO:H12	2.52	0.40
1:B:327:ILE:N	1:B:327:ILE:HD12	2.36	0.40
1:C:298[B]:GLN:O	1:C:321:HIS:HE1	2.04	0.40

All (9) 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)
9:B:1405:HOH:O	9:C:714:HOH:O[1_655]	1.84	0.36
9:E:1410:HOH:O	9:H:728:HOH:O[1_565]	1.87	0.33
9:E:1357:HOH:O	9:H:1046:HOH:O[1_565]	1.88	0.32
9:C:1320:HOH:O	9:G:809:HOH:O[1_554]	1.96	0.24
9:B:1207:HOH:O	9:C:1366:HOH:O[1_655]	2.08	0.12
1:A:340:GLU:OE1	9:B:920:HOH:O[1_455]	2.10	0.10
9:D:1226:HOH:O	9:G:1026:HOH:O[1_654]	2.13	0.07
1:E:354:GLU:OE2	1:F:212:ARG:NH2[1_565]	2.15	0.05
9:D:907:HOH:O	9:H:1295:HOH:O[1_554]	2.15	0.05

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	593/556 (107%)	580 (98%)	12 (2%)	1 (0%)	47	21
1	B	586/556 (105%)	574 (98%)	11 (2%)	1 (0%)	47	21
1	C	583/556 (105%)	570 (98%)	12 (2%)	1 (0%)	47	21
1	D	578/556 (104%)	566 (98%)	11 (2%)	1 (0%)	47	21
1	E	582/556 (105%)	568 (98%)	13 (2%)	1 (0%)	47	21
1	F	590/556 (106%)	578 (98%)	11 (2%)	1 (0%)	47	21
1	G	580/556 (104%)	566 (98%)	13 (2%)	1 (0%)	47	21
1	H	595/556 (107%)	582 (98%)	10 (2%)	3 (0%)	29	8
All	All	4687/4448 (105%)	4584 (98%)	93 (2%)	10 (0%)	47	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	391	SER
1	B	391	SER
1	C	391	SER
1	D	391	SER
1	E	391	SER
1	F	391	SER
1	G	391	SER
1	H	391	SER
1	H	539[A]	ASP
1	H	539[B]	ASP

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	477/452 (106%)	472 (99%)	5 (1%)	76	47
1	B	464/452 (103%)	460 (99%)	4 (1%)	78	52
1	C	462/452 (102%)	458 (99%)	4 (1%)	78	52
1	D	458/452 (101%)	454 (99%)	4 (1%)	78	52
1	E	466/452 (103%)	463 (99%)	3 (1%)	86	67
1	F	470/452 (104%)	466 (99%)	4 (1%)	78	52
1	G	459/452 (102%)	455 (99%)	4 (1%)	78	52
1	H	471/452 (104%)	467 (99%)	4 (1%)	81	57
All	All	3727/3616 (103%)	3695 (99%)	32 (1%)	78	52

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	TYR
1	A	118[A]	GLN
1	A	118[B]	GLN
1	A	325	ARG
1	A	447	TYR
1	B	87	TYR
1	B	325	ARG
1	B	391	SER
1	B	447	TYR
1	C	87	TYR
1	C	325	ARG
1	C	391	SER
1	C	447	TYR
1	D	87	TYR
1	D	109	PRO
1	D	325	ARG
1	D	447	TYR
1	E	87	TYR
1	E	325	ARG
1	E	447	TYR
1	F	87	TYR
1	F	325	ARG
1	F	391	SER
1	F	447	TYR

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Mol	Chain	Res	Type
1	G	87	TYR
1	G	325	ARG
1	G	391	SER
1	G	447	TYR
1	H	87	TYR
1	H	325	ARG
1	H	391	SER
1	H	447	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN
1	B	255	GLN
1	C	255	GLN
1	D	141	GLN
1	D	255	GLN
1	E	255	GLN
1	F	219	GLN
1	F	255	GLN
1	G	255	GLN
1	G	358	GLN
1	H	255	GLN
1	H	296	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 ⓘ

Of 112 ligands modelled in this entry, 23 are monoatomic - leaving 89 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	GOL	C	613	-	5,5,5	0.40	0	5,5,5	0.49	0
7	FMT	D	612	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	A	615	-	3,3,3	0.47	0	2,2,2	0.70	0
7	FMT	C	612	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	A	610	-	3,3,3	0.48	0	2,2,2	0.12	0
7	FMT	E	610	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	F	607	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	609	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	A	612	-	3,3,3	0.49	0	2,2,2	0.14	0
7	FMT	B	608	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	F	608	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	G	604	-	5,5,5	0.43	0	5,5,5	0.69	0
7	FMT	G	612	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	D	607	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	F	606	-	5,5,5	0.41	0	5,5,5	0.42	0
7	FMT	C	609	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	605	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	C	605	-	5,5,5	0.28	0	5,5,5	1.01	0
6	EDO	F	609	-	3,3,3	0.52	0	2,2,2	0.25	0
2	TD6	E	601	3,4	26,34,34	2.10	5 (19%)	32,50,50	1.73	7 (21%)
7	FMT	B	611	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	H	610	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	F	605	-	5,5,5	0.39	0	5,5,5	1.06	0
2	TD6	D	602	3,4	26,34,34	2.35	4 (15%)	32,50,50	1.82	7 (21%)
6	EDO	G	610	-	3,3,3	0.44	0	2,2,2	0.33	0
5	GOL	A	605	-	5,5,5	0.35	0	5,5,5	0.31	0
7	FMT	G	611	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	H	607	4	5,5,5	0.42	0	5,5,5	0.24	0
2	TD6	B	602	3,4	26,34,34	2.53	4 (15%)	32,50,50	1.74	9 (28%)
2	TD6	H	602	3,4	26,34,34	1.53	4 (15%)	32,50,50	1.67	7 (21%)
7	FMT	H	606	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FMT	B	612	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	610	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	D	611	-	3,3,3	0.46	0	2,2,2	0.29	0
7	FMT	G	614	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	G	613	-	3,3,3	0.49	0	2,2,2	0.21	0
6	EDO	E	612	-	3,3,3	0.49	0	2,2,2	0.29	0
7	FMT	B	601	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	C	615	-	3,3,3	0.43	0	2,2,2	0.58	0
7	FMT	G	609	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	C	617	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	H	609	-	3,3,3	0.60	0	2,2,2	0.60	0
7	FMT	D	609	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	H	612	-	3,3,3	0.52	0	2,2,2	0.16	0
6	EDO	C	616	-	3,3,3	0.72	0	2,2,2	0.92	0
7	FMT	G	615	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	H	613	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	609	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TD6	C	602	3,4	26,34,34	2.00	5 (19%)	32,50,50	1.89	8 (25%)
7	FMT	G	607	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	A	614	-	3,3,3	0.44	0	2,2,2	0.26	0
7	FMT	A	617	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	H	605	-	5,5,5	0.32	0	5,5,5	1.06	0
6	EDO	A	606	-	3,3,3	0.49	0	2,2,2	0.41	0
7	FMT	E	609	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	C	607	4	3,3,3	0.48	0	2,2,2	0.21	0
7	FMT	A	618	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	613	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	E	604	-	5,5,5	0.39	0	5,5,5	1.09	0
5	GOL	D	606	-	5,5,5	0.40	0	5,5,5	0.35	0
7	FMT	F	611	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	616	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	D	610	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	C	610	-	3,3,3	0.23	0	2,2,2	0.60	0
5	GOL	A	604	-	5,5,5	0.45	0	5,5,5	0.88	0
7	FMT	H	601	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	B	605	-	5,5,5	0.31	0	5,5,5	0.98	0
5	GOL	H	611	-	5,5,5	0.45	0	5,5,5	0.33	0
2	TD6	F	602	3,4	26,34,34	2.28	5 (19%)	32,50,50	1.91	9 (28%)
7	FMT	C	614	-	0,2,2	0.00	-	0,1,1	0.00	-
8	TRS	C	606	-	7,7,7	0.52	0	9,9,9	1.07	0
6	EDO	F	610	-	3,3,3	0.29	0	2,2,2	1.23	0
7	FMT	E	606	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FMT	E	611	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	606	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TD6	G	601	3,4	26,34,34	1.97	5 (19%)	32,50,50	1.93	8 (25%)
6	EDO	C	601	-	3,3,3	0.33	0	2,2,2	0.07	0
6	EDO	A	613	-	3,3,3	0.57	0	2,2,2	0.58	0
7	FMT	G	606	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	D	601	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TD6	A	601	3,4	26,34,34	1.95	5 (19%)	32,50,50	1.71	8 (25%)
7	FMT	F	601	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	A	611	-	3,3,3	0.57	0	2,2,2	0.12	0
7	FMT	G	608	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	608	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	613	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	608	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	D	605	-	5,5,5	0.40	0	5,5,5	0.58	0
6	EDO	C	611	-	3,3,3	0.39	0	2,2,2	0.43	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	GOL	C	613	-	-	4/4/4/4	-
2	TD6	F	602	3,4	-	3/19/26/26	0/2/2/2
6	EDO	H	609	-	-	1/1/1/1	-
6	EDO	H	612	-	-	0/1/1/1	-
6	EDO	C	616	-	-	1/1/1/1	-
2	TD6	H	602	3,4	-	3/19/26/26	0/2/2/2
5	GOL	F	605	-	-	2/4/4/4	-
6	EDO	A	615	-	-	1/1/1/1	-
8	TRS	C	606	-	-	1/9/9/9	-
2	TD6	C	602	3,4	-	2/19/26/26	0/2/2/2
6	EDO	A	610	-	-	1/1/1/1	-
6	EDO	G	610	-	-	0/1/1/1	-
5	GOL	H	605	-	-	2/4/4/4	-
5	GOL	A	605	-	-	0/4/4/4	-
6	EDO	A	606	-	-	1/1/1/1	-
6	EDO	A	612	-	-	1/1/1/1	-
2	TD6	G	601	3,4	-	3/19/26/26	0/2/2/2
5	GOL	H	607	4	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TD6	D	602	3,4	-	3/19/26/26	0/2/2/2
6	EDO	C	607	4	-	0/1/1/1	-
2	TD6	B	602	3,4	-	3/19/26/26	0/2/2/2
6	EDO	C	601	-	-	0/1/1/1	-
6	EDO	A	613	-	-	1/1/1/1	-
5	GOL	G	604	-	-	1/4/4/4	-
5	GOL	D	606	-	-	2/4/4/4	-
6	EDO	F	610	-	-	1/1/1/1	-
2	TD6	A	601	3,4	-	2/19/26/26	0/2/2/2
6	EDO	A	614	-	-	1/1/1/1	-
6	EDO	A	611	-	-	1/1/1/1	-
6	EDO	D	611	-	-	1/1/1/1	-
6	EDO	C	610	-	-	1/1/1/1	-
5	GOL	A	604	-	-	1/4/4/4	-
6	EDO	G	613	-	-	0/1/1/1	-
5	GOL	E	604	-	-	2/4/4/4	-
5	GOL	F	606	-	-	0/4/4/4	-
5	GOL	B	605	-	-	2/4/4/4	-
6	EDO	E	612	-	-	1/1/1/1	-
5	GOL	D	605	-	-	1/4/4/4	-
5	GOL	C	605	-	-	2/4/4/4	-
6	EDO	F	609	-	-	0/1/1/1	-
6	EDO	C	615	-	-	0/1/1/1	-
6	EDO	C	611	-	-	0/1/1/1	-
5	GOL	H	611	-	-	2/4/4/4	-
2	TD6	E	601	3,4	-	3/19/26/26	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	TD6	C6-C5	11.52	1.56	1.50
2	D	602	TD6	C6-C5	10.28	1.55	1.50
2	F	602	TD6	C6-C5	9.89	1.55	1.50
2	E	601	TD6	C6-C5	8.59	1.54	1.50
2	G	601	TD6	C6-C5	8.06	1.54	1.50
2	C	602	TD6	C6-C5	7.87	1.54	1.50
2	A	601	TD6	C6-C5	7.73	1.54	1.50
2	H	602	TD6	C6-C5	5.35	1.53	1.50
2	C	602	TD6	CM4-C4	3.29	1.56	1.49
2	C	602	TD6	C7'-C5'	2.75	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	TD6	CM2-C2'	2.73	1.57	1.49
2	D	602	TD6	CM4-C4	2.71	1.55	1.49
2	A	601	TD6	C4-N3	-2.71	1.34	1.39
2	G	601	TD6	CM4-C4	2.64	1.55	1.49
2	E	601	TD6	CM2-C2'	2.57	1.57	1.49
2	A	601	TD6	CM4-C4	2.53	1.55	1.49
2	A	601	TD6	C7'-C5'	2.51	1.56	1.51
2	H	602	TD6	CM4-C4	2.48	1.54	1.49
2	E	601	TD6	C7'-C5'	2.47	1.56	1.51
2	B	602	TD6	CM4-C4	2.39	1.54	1.49
2	G	601	TD6	CM2-C2'	2.39	1.56	1.49
2	H	602	TD6	C4-N3	-2.39	1.34	1.39
2	E	601	TD6	CM4-C4	2.36	1.54	1.49
2	G	601	TD6	C4-N3	-2.36	1.34	1.39
2	F	602	TD6	C4-N3	-2.34	1.34	1.39
2	F	602	TD6	C7'-C5'	2.31	1.56	1.51
2	B	602	TD6	CM2-C2'	2.31	1.56	1.49
2	D	602	TD6	C4-N3	-2.30	1.34	1.39
2	C	602	TD6	CM2-C2'	2.29	1.56	1.49
2	F	602	TD6	CM4-C4	2.29	1.54	1.49
2	E	601	TD6	C4-N3	-2.28	1.34	1.39
2	G	601	TD6	C7'-C5'	2.18	1.55	1.51
2	A	601	TD6	CM2-C2'	2.16	1.55	1.49
2	F	602	TD6	CM2-C2'	2.15	1.55	1.49
2	H	602	TD6	CM2-C2'	2.07	1.55	1.49
2	C	602	TD6	C4-N3	-2.04	1.35	1.39
2	B	602	TD6	C4'-N3'	2.03	1.37	1.35

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	TD6	C13-CLB-C11	-5.40	106.47	114.44
2	G	601	TD6	C13-CLB-C11	-5.13	106.88	114.44
2	F	602	TD6	C13-CLB-C11	-4.75	107.44	114.44
2	F	602	TD6	C5-C4-N3	4.10	116.24	107.66
2	A	601	TD6	C5-C4-N3	4.01	116.04	107.66
2	D	602	TD6	C6'-N1'-C2'	3.91	122.62	115.96
2	F	602	TD6	C6'-N1'-C2'	3.87	122.55	115.96
2	D	602	TD6	C5-C4-N3	3.86	115.72	107.66
2	E	601	TD6	C6'-N1'-C2'	3.77	122.37	115.96
2	E	601	TD6	C5-C4-N3	3.71	115.41	107.66
2	G	601	TD6	C5'-C6'-N1'	-3.67	117.71	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	TD6	C6'-N1'-C2'	3.66	122.19	115.96
2	D	602	TD6	CLB-C13-CLC	-3.64	105.76	113.59
2	H	602	TD6	C13-CLB-C11	-3.62	109.09	114.44
2	B	602	TD6	C5-C4-N3	3.58	115.15	107.66
2	G	601	TD6	C5-C4-N3	3.54	115.06	107.66
2	B	602	TD6	C6'-N1'-C2'	3.50	121.92	115.96
2	C	602	TD6	C6'-N1'-C2'	3.49	121.90	115.96
2	D	602	TD6	C5'-C6'-N1'	-3.46	118.05	123.82
2	H	602	TD6	C6'-N1'-C2'	3.45	121.83	115.96
2	E	601	TD6	N1'-C2'-N3'	-3.37	119.73	125.54
2	H	602	TD6	C5'-C6'-N1'	-3.36	118.22	123.82
2	H	602	TD6	C5-C4-N3	3.28	114.52	107.66
2	A	601	TD6	C13-CLB-C11	-3.17	109.76	114.44
2	B	602	TD6	CLB-C13-CLC	-3.14	106.83	113.59
2	D	602	TD6	C13-CLB-C11	-3.12	109.84	114.44
2	F	602	TD6	C5'-C6'-N1'	-3.11	118.64	123.82
2	A	601	TD6	C6'-N1'-C2'	2.95	120.98	115.96
2	B	602	TD6	OL1-C11-CLB	-2.88	98.42	109.55
2	C	602	TD6	C5'-C6'-N1'	-2.86	119.06	123.82
2	G	601	TD6	CM2-C2'-N1'	2.86	120.28	117.14
2	E	601	TD6	C13-CLB-C11	-2.84	110.25	114.44
2	B	602	TD6	CM4-C4-C5	-2.83	121.42	127.60
2	F	602	TD6	OL1-C11-CLB	-2.78	98.81	109.55
2	C	602	TD6	C5-C4-N3	2.77	113.46	107.66
2	C	602	TD6	OL1-C11-CLB	-2.71	99.09	109.55
2	B	602	TD6	N1'-C2'-N3'	-2.69	120.92	125.54
2	C	602	TD6	N1'-C2'-N3'	-2.68	120.93	125.54
2	A	601	TD6	OL1-C11-CLB	-2.64	99.36	109.55
2	C	602	TD6	C6-C5-C4	-2.62	125.33	127.43
2	E	601	TD6	CM2-C2'-N3'	2.62	121.23	117.15
2	F	602	TD6	N1'-C2'-N3'	-2.59	121.08	125.54
2	G	601	TD6	CLB-C13-CLC	-2.59	108.03	113.59
2	G	601	TD6	N1'-C2'-N3'	-2.55	121.14	125.54
2	C	602	TD6	CM2-C2'-N1'	2.55	119.94	117.14
2	H	602	TD6	CLB-C13-CLC	-2.54	108.12	113.59
2	F	602	TD6	CM4-C4-C5	-2.50	122.13	127.60
2	B	602	TD6	C5'-C6'-N1'	-2.47	119.70	123.82
2	E	601	TD6	OL1-C11-CLB	-2.47	100.01	109.55
2	D	602	TD6	N1'-C2'-N3'	-2.44	121.34	125.54
2	E	601	TD6	C5'-C6'-N1'	-2.43	119.76	123.82
2	F	602	TD6	CLB-C13-CLC	-2.41	108.41	113.59
2	A	601	TD6	C5'-C6'-N1'	-2.37	119.88	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	602	TD6	OL1-C11-CLB	-2.33	100.56	109.55
2	A	601	TD6	C5'-C7'-N3	-2.31	109.44	113.26
2	B	602	TD6	C5'-C7'-N3	-2.29	109.48	113.26
2	H	602	TD6	N1'-C2'-N3'	-2.28	121.62	125.54
2	A	601	TD6	CM2-C2'-N1'	2.28	119.64	117.14
2	D	602	TD6	CM4-C4-C5	-2.21	122.76	127.60
2	A	601	TD6	CLB-C13-CLC	-2.18	108.91	113.59
2	G	601	TD6	C6'-C5'-C4'	2.16	118.67	115.72
2	F	602	TD6	N4'-C4'-N3'	-2.08	114.09	117.03
2	B	602	TD6	CM2-C2'-N3'	2.07	120.38	117.15

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	613	GOL	O1-C1-C2-C3
5	C	613	GOL	C1-C2-C3-O3
2	E	601	TD6	C2-C11-CLB-C13
2	E	601	TD6	C4'-C5'-C7'-N3
2	D	602	TD6	C2-C11-CLB-C13
2	D	602	TD6	OL1-C11-CLB-C13
2	D	602	TD6	C4'-C5'-C7'-N3
2	B	602	TD6	C2-C11-CLB-C13
2	B	602	TD6	OL1-C11-CLB-C13
2	B	602	TD6	C4'-C5'-C7'-N3
2	H	602	TD6	C2-C11-CLB-C13
2	H	602	TD6	OL1-C11-CLB-C13
2	H	602	TD6	C4'-C5'-C7'-N3
2	C	602	TD6	C2-C11-CLB-C13
2	C	602	TD6	C4'-C5'-C7'-N3
5	D	606	GOL	O1-C1-C2-C3
5	H	611	GOL	C1-C2-C3-O3
2	F	602	TD6	C2-C11-CLB-C13
2	F	602	TD6	OL1-C11-CLB-C13
2	G	601	TD6	C2-C11-CLB-C13
2	G	601	TD6	OL1-C11-CLB-C13
2	G	601	TD6	C4'-C5'-C7'-N3
2	A	601	TD6	C2-C11-CLB-C13
2	A	601	TD6	C4'-C5'-C7'-N3
5	C	613	GOL	O1-C1-C2-O2
6	C	616	EDO	O1-C1-C2-O2
6	H	609	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	C	605	GOL	C1-C2-C3-O3
5	F	605	GOL	C1-C2-C3-O3
5	H	605	GOL	C1-C2-C3-O3
5	E	604	GOL	C1-C2-C3-O3
5	A	604	GOL	C1-C2-C3-O3
5	B	605	GOL	C1-C2-C3-O3
5	C	613	GOL	O2-C2-C3-O3
5	D	606	GOL	O1-C1-C2-O2
5	H	611	GOL	O2-C2-C3-O3
6	A	615	EDO	O1-C1-C2-O2
6	A	612	EDO	O1-C1-C2-O2
6	A	606	EDO	O1-C1-C2-O2
6	C	610	EDO	O1-C1-C2-O2
6	A	613	EDO	O1-C1-C2-O2
6	E	612	EDO	O1-C1-C2-O2
5	H	605	GOL	O2-C2-C3-O3
6	A	614	EDO	O1-C1-C2-O2
5	C	605	GOL	O2-C2-C3-O3
5	F	605	GOL	O2-C2-C3-O3
5	E	604	GOL	O2-C2-C3-O3
5	B	605	GOL	O2-C2-C3-O3
2	E	601	TD6	C4-C5-C6-C7
6	A	610	EDO	O1-C1-C2-O2
6	F	610	EDO	O1-C1-C2-O2
5	G	604	GOL	C1-C2-C3-O3
6	A	611	EDO	O1-C1-C2-O2
5	D	605	GOL	C1-C2-C3-O3
2	F	602	TD6	C4'-C5'-C7'-N3
6	D	611	EDO	O1-C1-C2-O2
8	C	606	TRS	N-C-C1-O1

There are no ring outliers.

34 monomers are involved in 79 short contacts:

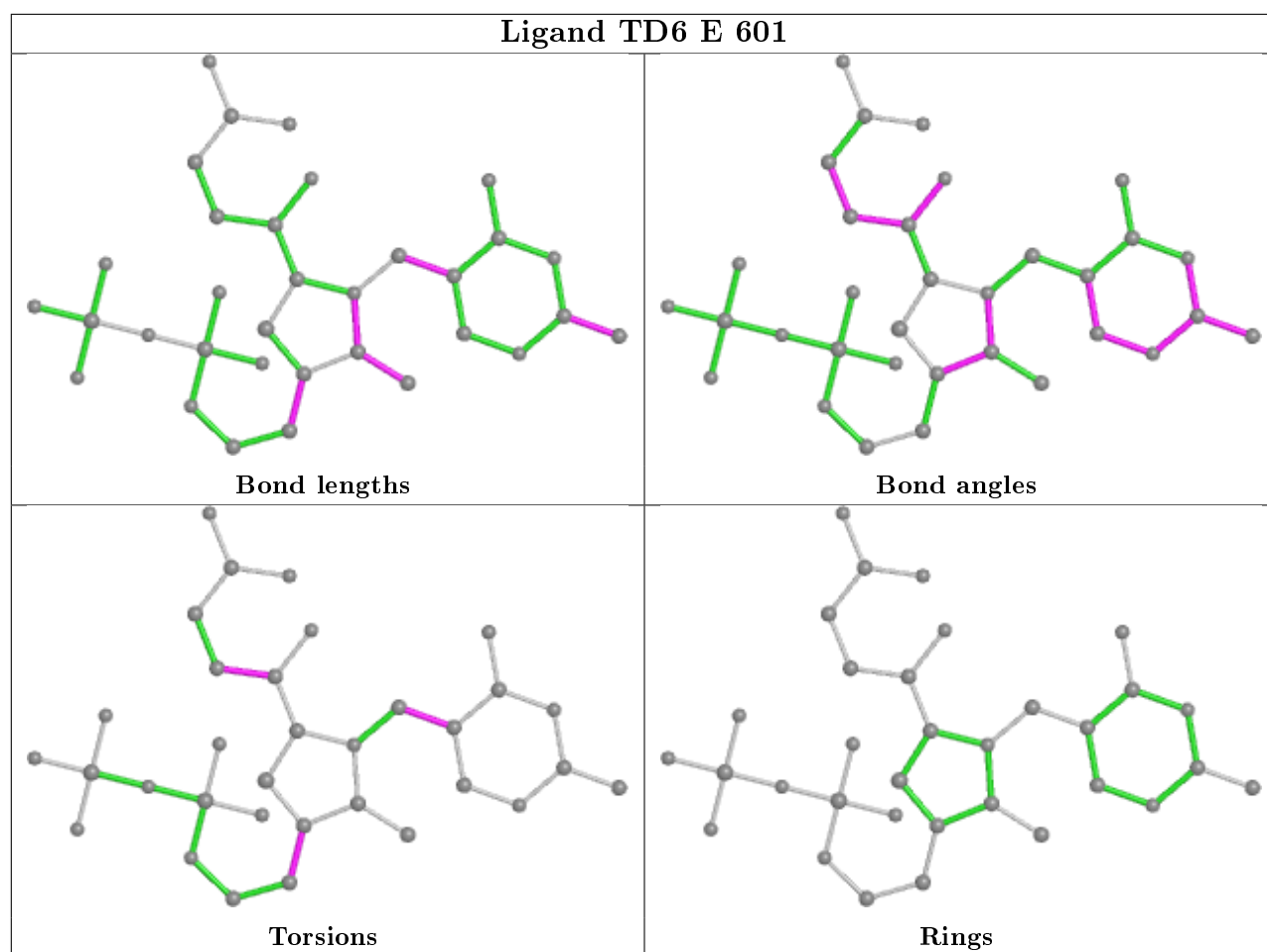
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	612	FMT	2	0
6	A	615	EDO	1	0
7	C	612	FMT	1	0
7	E	610	FMT	2	0
6	A	612	EDO	1	0
2	E	601	TD6	3	0
2	D	602	TD6	2	0

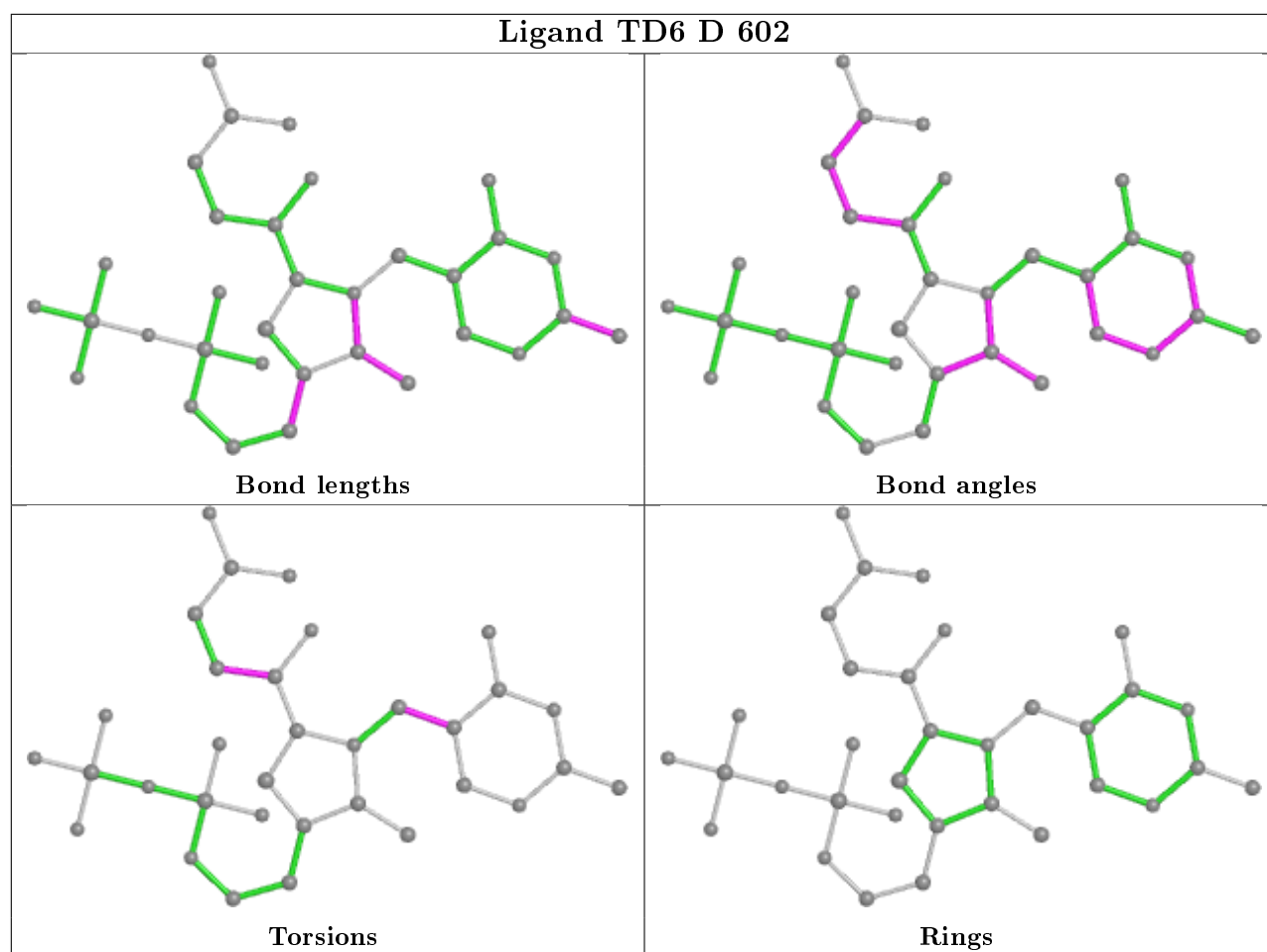
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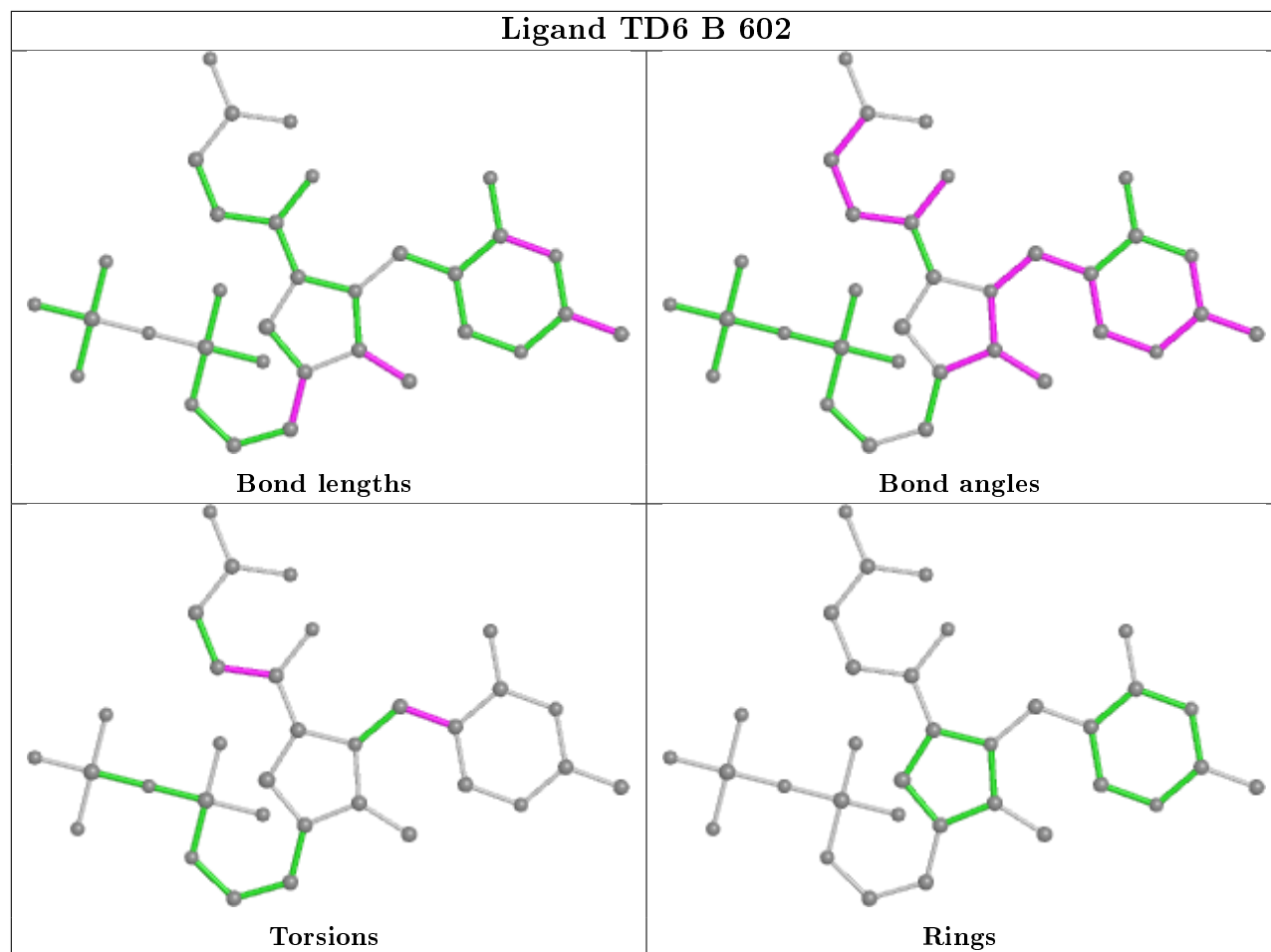
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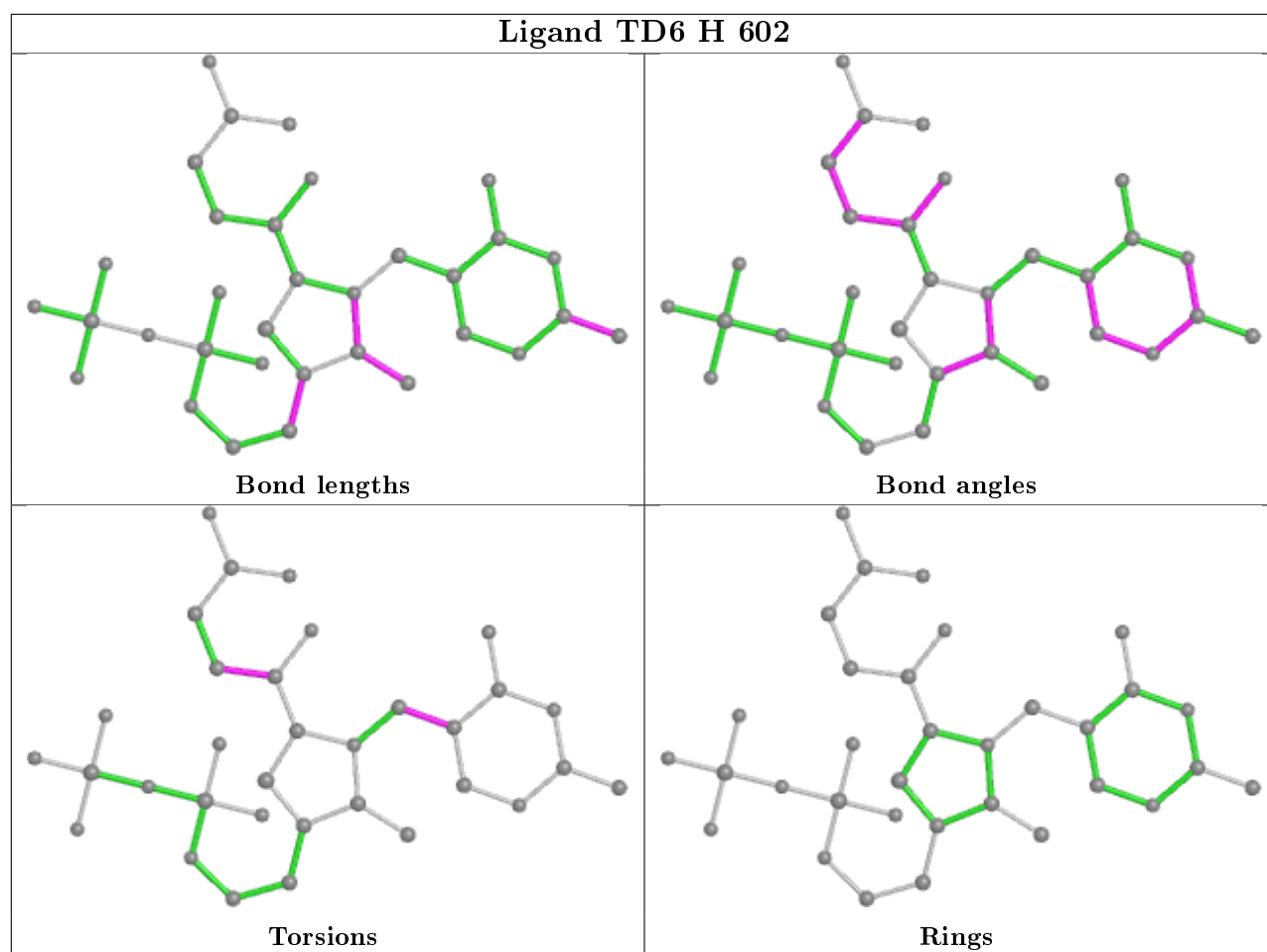
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	TD6	2	0
2	H	602	TD6	3	0
6	D	611	EDO	5	0
7	G	614	FMT	3	0
6	C	615	EDO	3	0
7	G	609	FMT	1	0
6	C	616	EDO	2	0
2	C	602	TD6	3	0
6	A	614	EDO	5	0
7	A	617	FMT	2	0
6	A	606	EDO	1	0
7	E	609	FMT	2	0
6	C	607	EDO	1	0
7	F	611	FMT	4	0
6	C	610	EDO	2	0
5	H	611	GOL	1	0
2	F	602	TD6	3	0
8	C	606	TRS	1	0
6	F	610	EDO	5	0
2	G	601	TD6	3	0
6	C	601	EDO	5	0
6	A	613	EDO	2	0
2	A	601	TD6	2	0
6	A	611	EDO	3	0
7	G	608	FMT	1	0
7	B	613	FMT	3	0
6	C	611	EDO	1	0

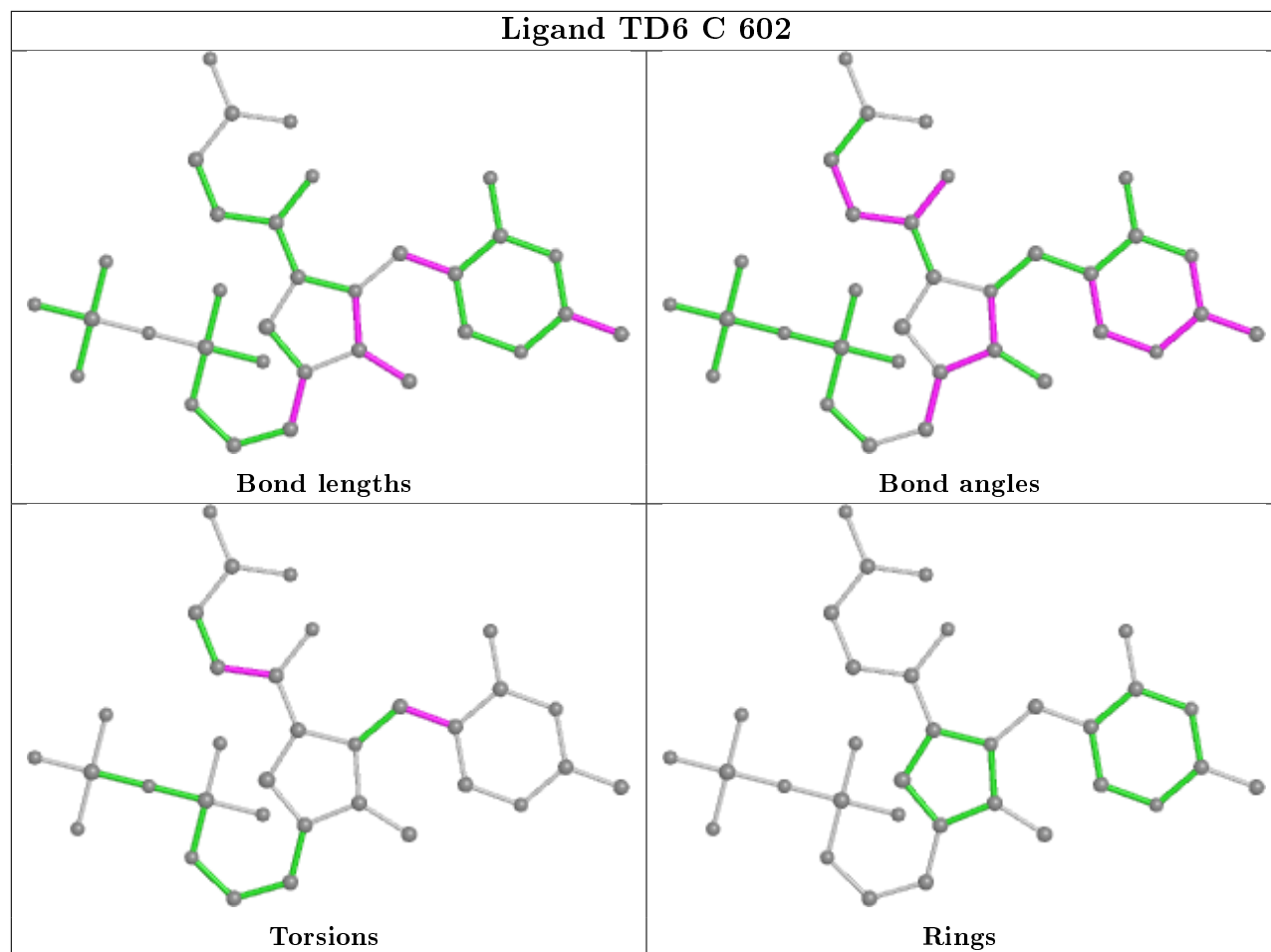
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

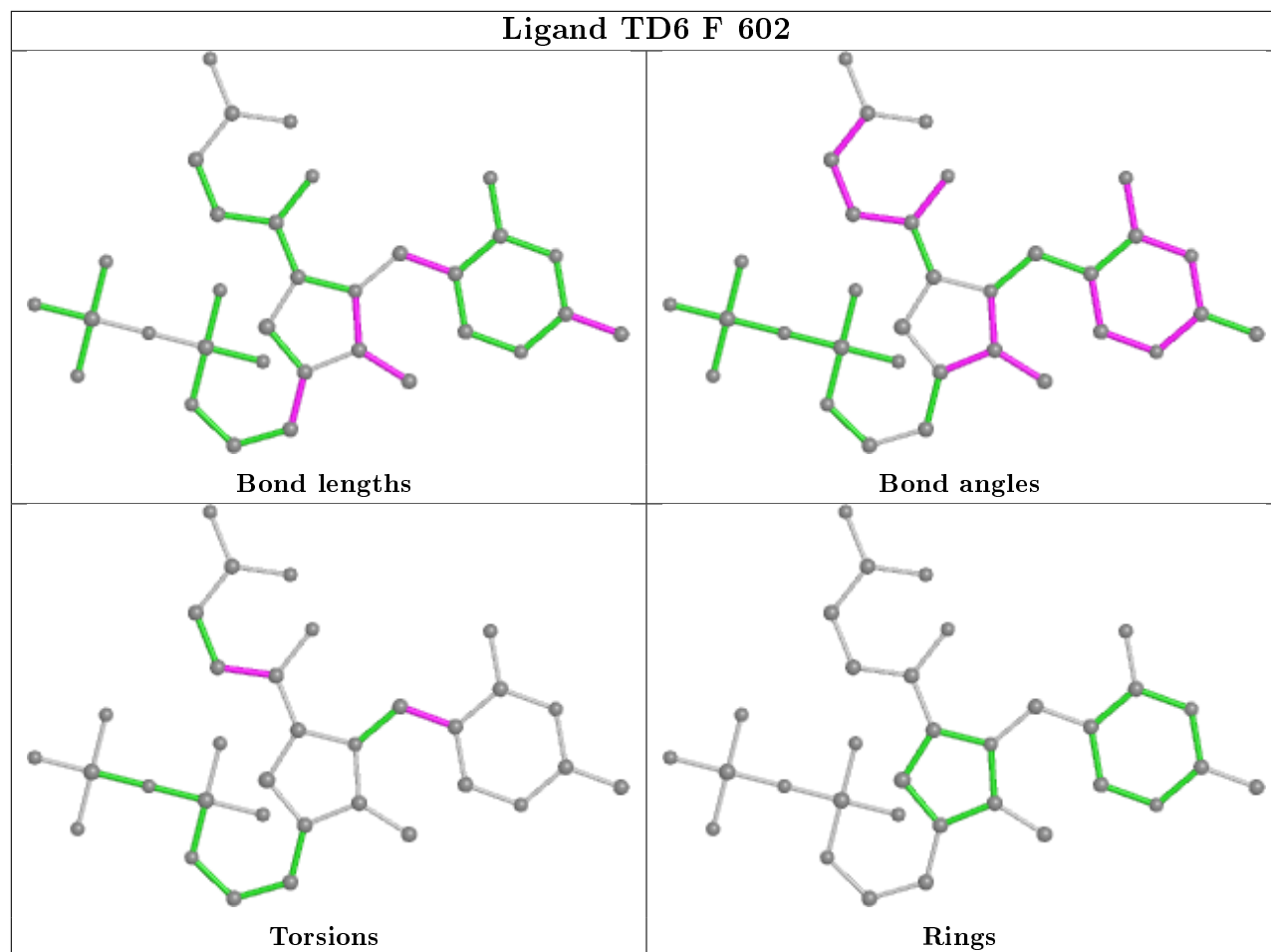


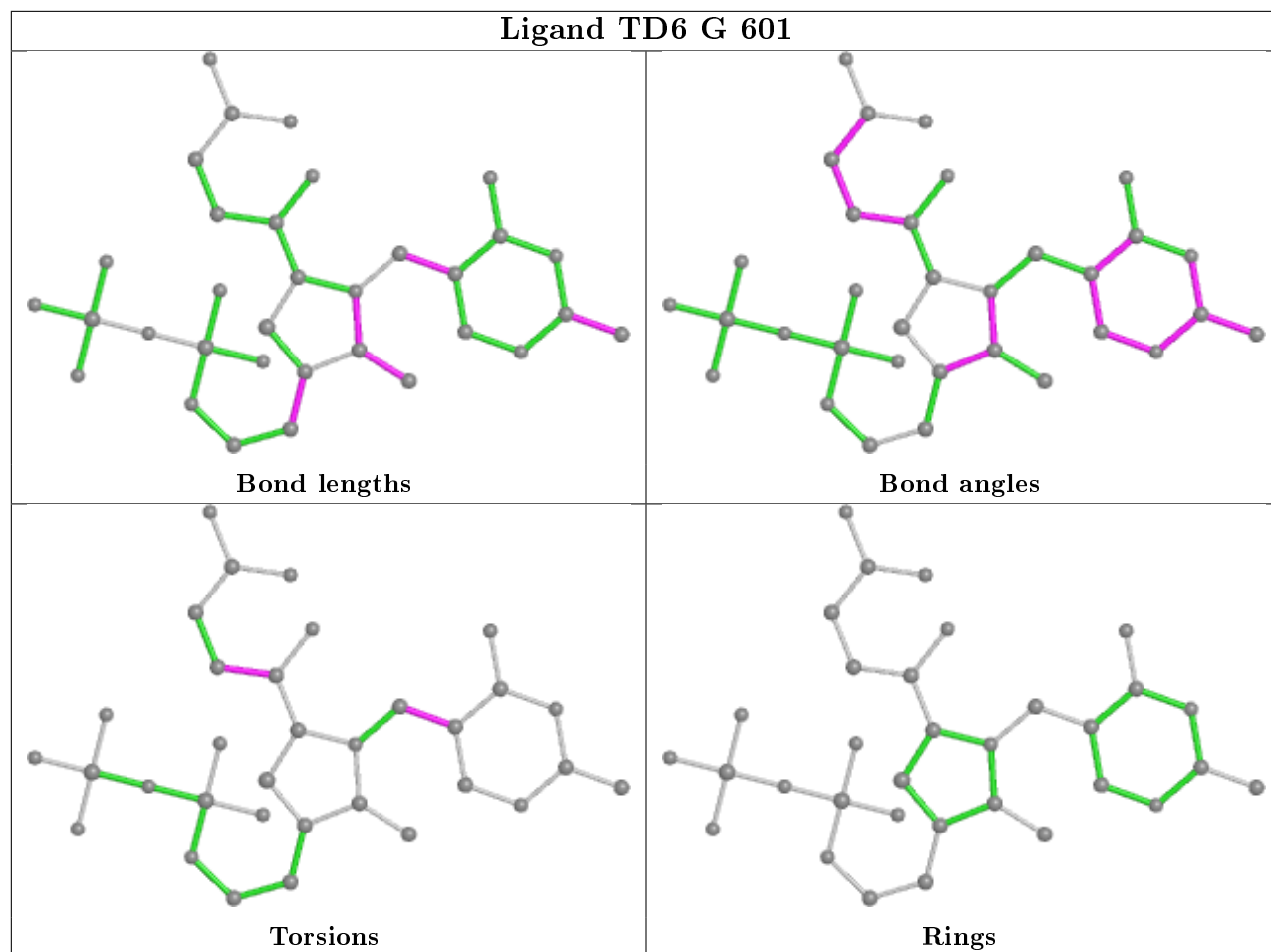


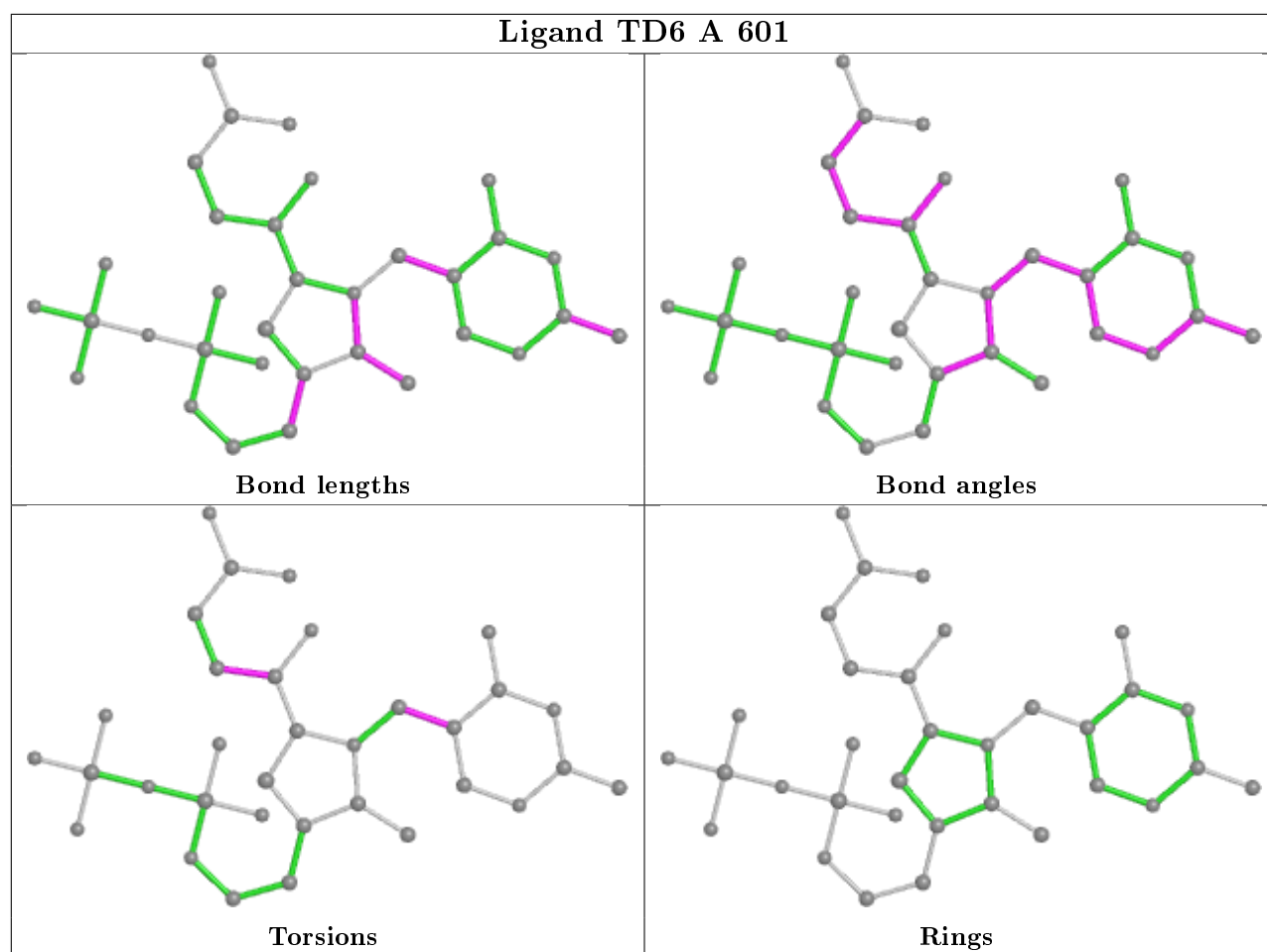












5.7 Other polymers [i](#)

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%)	-0.15	8 (1%) 75 79	8, 12, 28, 43	0
1	B	556/556 (100%)	-0.16	7 (1%) 77 80	8, 13, 24, 43	0
1	C	556/556 (100%)	-0.16	5 (0%) 84 87	8, 13, 28, 48	0
1	D	556/556 (100%)	-0.01	18 (3%) 47 54	9, 16, 33, 50	0
1	E	556/556 (100%)	-0.16	7 (1%) 77 80	8, 13, 27, 41	0
1	F	556/556 (100%)	-0.16	4 (0%) 87 89	7, 12, 27, 43	0
1	G	556/556 (100%)	-0.07	15 (2%) 54 61	9, 14, 31, 46	0
1	H	556/556 (100%)	-0.15	6 (1%) 80 83	8, 13, 26, 41	0
All	All	4448/4448 (100%)	-0.13	70 (1%) 72 76	7, 13, 28, 50	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	VAL	6.2
1	C	1	MET	5.5
1	B	1	MET	4.4
1	E	176	GLY	3.9
1	D	347	VAL	3.9
1	F	347	VAL	3.9
1	G	347	VAL	3.8
1	D	215	PHE	3.7
1	A	556	LEU	3.7
1	D	556	LEU	3.6
1	G	555	HIS	3.6
1	D	1	MET	3.5
1	E	1	MET	3.5
1	F	556	LEU	3.4
1	D	176	GLY	3.4
1	H	176	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	177	GLU	3.2
1	A	178	MET	3.0
1	H	556	LEU	3.0
1	D	343	GLN	2.9
1	H	178	MET	2.9
1	B	176	GLY	2.9
1	G	556	LEU	2.9
1	D	178	MET	2.8
1	A	1	MET	2.7
1	D	519	THR	2.7
1	D	239	LEU	2.7
1	G	270	ALA	2.7
1	D	177	GLU	2.7
1	D	479	PRO	2.6
1	C	555	HIS	2.6
1	H	522	ALA	2.6
1	C	177	GLU	2.6
1	B	177	GLU	2.6
1	C	178	MET	2.6
1	F	1	MET	2.5
1	E	178	MET	2.5
1	C	556	LEU	2.5
1	B	178	MET	2.5
1	D	341	LYS	2.5
1	E	205	ARG	2.4
1	D	273	THR	2.4
1	G	519	THR	2.4
1	D	344	PRO	2.4
1	F	176	GLY	2.3
1	G	1	MET	2.3
1	G	343	GLN	2.3
1	A	270	ALA	2.3
1	B	555	HIS	2.3
1	H	555	HIS	2.3
1	G	480	THR	2.2
1	D	362	ALA	2.2
1	E	180	ASP	2.2
1	D	523	ASP	2.2
1	G	522	ALA	2.1
1	G	483	SER	2.1
1	B	527	THR	2.1
1	D	551	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	177	GLU	2.1
1	G	178	MET	2.1
1	G	215	PHE	2.1
1	A	555	HIS	2.1
1	G	212	ARG	2.1
1	G	351	ARG	2.1
1	H	177	GLU	2.0
1	E	555	HIS	2.0
1	D	522	ALA	2.0
1	E	526	ARG	2.0
1	A	439[A]	ILE	2.0
1	B	180	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	FMT	G	608	3/3	0.59	0.23	34,36,36,44	0
7	FMT	G	611	3/3	0.60	0.25	35,37,38,45	0
7	FMT	B	609	3/3	0.62	0.16	43,46,47,56	0
7	FMT	H	613	3/3	0.68	0.15	42,43,43,52	0
6	EDO	G	613	4/4	0.68	0.14	42,50,51,54	0
7	FMT	C	609	3/3	0.70	0.18	29,31,31,37	0
7	FMT	E	608	3/3	0.70	0.17	34,35,36,43	0
6	EDO	A	615	4/4	0.71	0.21	40,48,49,49	0
7	FMT	B	608	3/3	0.73	0.17	28,30,30,37	0
6	EDO	F	610	4/4	0.73	0.22	29,34,37,41	0
7	FMT	B	606	3/3	0.74	0.19	33,38,38,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	FMT	A	608	3/3	0.74	0.18	23,24,24,29	0
7	FMT	B	610	3/3	0.76	0.24	26,26,30,32	0
7	FMT	F	608	3/3	0.76	0.19	21,23,24,27	0
6	EDO	A	614	4/4	0.77	0.31	31,37,41,42	0
7	FMT	E	609	3/3	0.77	0.25	22,23,23,28	0
6	EDO	E	612	4/4	0.79	0.12	41,49,50,51	0
5	GOL	D	606	6/6	0.79	0.23	28,35,43,45	0
7	FMT	E	611	3/3	0.80	0.23	42,44,45,53	0
7	FMT	A	609	3/3	0.80	0.19	17,26,28,31	0
7	FMT	A	617	3/3	0.80	0.25	21,21,26,26	0
5	GOL	C	613	6/6	0.80	0.19	37,45,50,50	0
6	EDO	F	609	4/4	0.80	0.12	39,47,50,50	0
7	FMT	G	614	3/3	0.80	0.23	30,31,33,37	0
6	EDO	A	606	4/4	0.82	0.20	33,42,47,51	0
7	FMT	D	601	3/3	0.82	0.12	26,28,29,35	0
6	EDO	A	610	4/4	0.83	0.29	41,49,51,53	0
6	EDO	A	613	4/4	0.83	0.24	19,23,26,27	0
6	EDO	C	616	4/4	0.83	0.21	17,20,23,26	0
7	FMT	B	612	3/3	0.83	0.26	37,38,39,46	0
8	TRS	C	606	8/8	0.83	0.25	25,35,41,45	0
7	FMT	E	610	3/3	0.83	0.17	31,32,33,37	0
7	FMT	D	612	3/3	0.83	0.20	30,32,34,36	0
7	FMT	H	610	3/3	0.84	0.13	34,34,35,41	0
6	EDO	H	609	4/4	0.84	0.18	17,21,26,27	0
6	EDO	C	601	4/4	0.84	0.14	30,37,38,40	0
6	EDO	A	612	4/4	0.85	0.22	37,44,46,48	0
7	FMT	B	613	3/3	0.87	0.14	29,31,34,37	0
6	EDO	A	611	4/4	0.87	0.18	27,35,37,42	0
7	FMT	F	611	3/3	0.88	0.19	25,26,28,30	0
5	GOL	F	606	6/6	0.88	0.18	24,31,36,41	0
7	FMT	C	612	3/3	0.89	0.17	24,26,26,31	0
7	FMT	G	606	3/3	0.89	0.24	29,29,29,35	0
7	FMT	D	609	3/3	0.89	0.16	28,30,32,36	0
7	FMT	G	609	3/3	0.90	0.07	43,44,44,52	0
7	FMT	C	614	3/3	0.90	0.11	21,26,31,32	0
6	EDO	D	611	4/4	0.90	0.17	25,30,34,38	0
7	FMT	G	612	3/3	0.90	0.25	33,34,34,41	0
7	FMT	A	618	3/3	0.91	0.17	18,19,21,23	0
5	GOL	A	605	6/6	0.91	0.16	22,32,38,40	0
6	EDO	C	610	4/4	0.92	0.23	21,27,32,32	0
6	EDO	C	615	4/4	0.92	0.17	26,31,35,35	0
5	GOL	H	611	6/6	0.93	0.22	30,36,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	FMT	F	607	3/3	0.93	0.14	42,43,44,51	0
7	FMT	E	605	3/3	0.93	0.19	27,31,34,38	0
6	EDO	H	612	4/4	0.93	0.12	20,28,32,33	0
7	FMT	B	611	3/3	0.94	0.12	20,21,21,25	0
5	GOL	H	607	6/6	0.94	0.14	15,20,25,30	0
5	GOL	D	605	6/6	0.94	0.10	16,24,29,29	0
7	FMT	D	607	3/3	0.95	0.11	23,26,27,32	0
6	EDO	G	610	4/4	0.95	0.10	23,28,31,32	0
7	FMT	G	607	3/3	0.95	0.13	23,26,28,31	0
7	FMT	A	616	3/3	0.95	0.09	20,20,20,25	0
7	FMT	E	606	3/3	0.95	0.14	24,25,26,31	0
6	EDO	C	607	4/4	0.95	0.10	16,20,25,25	0
5	GOL	E	604	6/6	0.96	0.06	14,19,23,23	0
5	GOL	B	605	6/6	0.96	0.07	13,17,24,24	0
5	GOL	G	604	6/6	0.96	0.09	15,22,26,27	0
7	FMT	H	606	3/3	0.96	0.07	23,28,31,33	0
5	GOL	C	605	6/6	0.96	0.09	16,24,28,28	0
6	EDO	C	611	4/4	0.96	0.12	16,20,25,25	0
5	GOL	H	605	6/6	0.97	0.07	15,22,25,26	0
7	FMT	B	601	3/3	0.97	0.07	20,22,22,26	0
5	GOL	F	605	6/6	0.97	0.11	12,20,24,24	0
4	MG	G	605	1/1	0.98	0.15	24,24,24,24	0
5	GOL	A	604	6/6	0.98	0.07	12,18,23,23	0
7	FMT	H	601	3/3	0.98	0.07	21,21,22,26	0
2	TD6	B	602	33/33	0.98	0.07	8,12,22,30	0
7	FMT	E	613	3/3	0.98	0.06	22,22,22,27	0
7	FMT	F	601	3/3	0.98	0.07	21,21,22,27	0
4	MG	B	607	1/1	0.98	0.24	26,26,26,26	0
4	MG	A	607	1/1	0.98	0.24	29,29,29,29	0
7	FMT	G	615	3/3	0.98	0.06	19,20,21,24	0
7	FMT	C	617	3/3	0.98	0.06	21,21,22,25	0
2	TD6	D	602	33/33	0.98	0.06	10,14,23,27	0
7	FMT	D	610	3/3	0.98	0.05	21,21,22,26	0
3	MN	F	603[A]	1/1	0.99	0.08	11,11,11,11	1
4	MG	F	604[B]	1/1	0.99	0.08	10,10,10,10	1
2	TD6	F	602	33/33	0.99	0.06	8,12,25,30	0
2	TD6	H	602	33/33	0.99	0.06	9,12,22,27	0
3	MN	B	603[A]	1/1	0.99	0.06	16,16,16,16	1
2	TD6	A	601	33/33	0.99	0.07	8,12,22,26	0
4	MG	B	604[B]	1/1	0.99	0.06	2,2,2,2	1
2	TD6	E	601	33/33	0.99	0.07	8,12,22,26	0
4	MG	C	608	1/1	0.99	0.10	15,15,15,15	0

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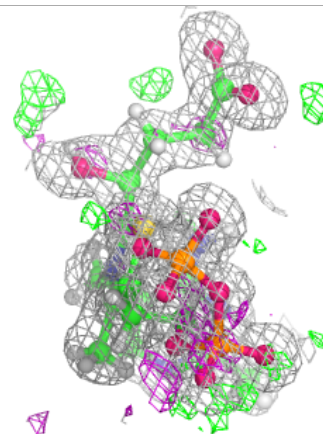
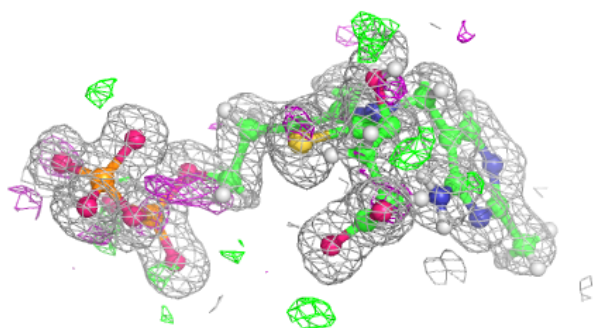
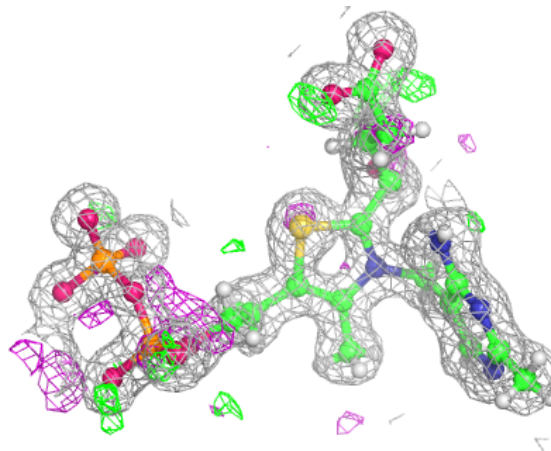
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	E	607	1/1	0.99	0.21	29,29,29,29	0
2	TD6	C	602	33/33	0.99	0.06	9,12,22,29	0
4	MG	D	608	1/1	0.99	0.10	23,23,23,23	0
2	TD6	G	601	33/33	0.99	0.06	9,13,22,27	0
3	MN	C	603[A]	1/1	0.99	0.08	15,15,15,15	1
4	MG	E	603[B]	1/1	1.00	0.07	8,8,8,8	1
3	MN	G	602[A]	1/1	1.00	0.07	14,14,14,14	1
4	MG	A	603[B]	1/1	1.00	0.04	6,6,6,6	1
3	MN	D	603[A]	1/1	1.00	0.05	16,16,16,16	1
4	MG	H	608	1/1	1.00	0.07	15,15,15,15	0
4	MG	D	604[B]	1/1	1.00	0.05	7,7,7,7	1
4	MG	G	603[B]	1/1	1.00	0.07	6,6,6,6	1
4	MG	C	604[B]	1/1	1.00	0.07	5,5,5,5	1
4	MG	H	604[B]	1/1	1.00	0.04	6,6,6,6	1
3	MN	H	603[A]	1/1	1.00	0.04	13,13,13,13	1
3	MN	A	602[A]	1/1	1.00	0.04	11,11,11,11	1
3	MN	E	602[A]	1/1	1.00	0.07	11,11,11,11	1

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.

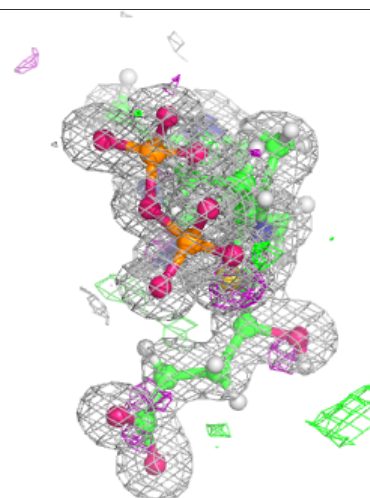
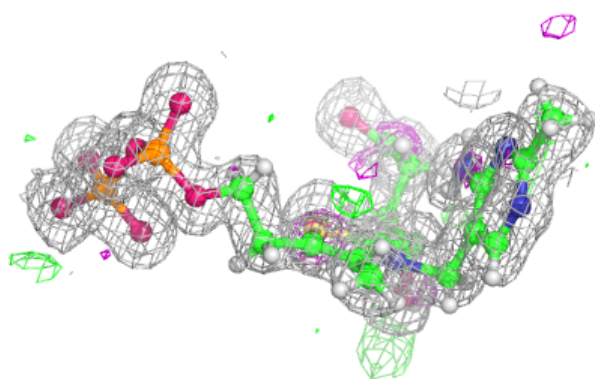
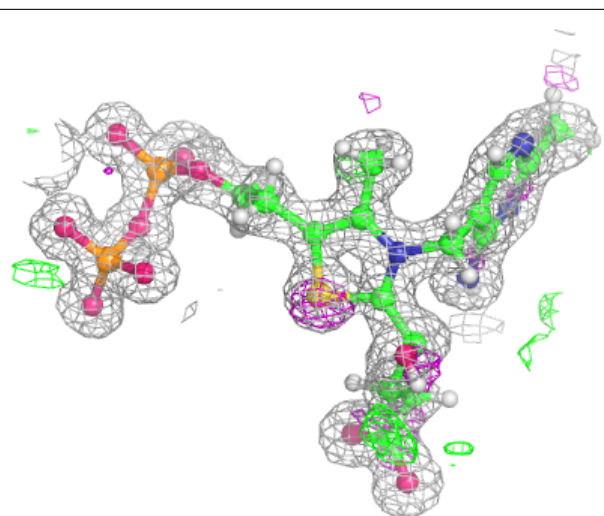
Electron density around TD6 B 602:

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



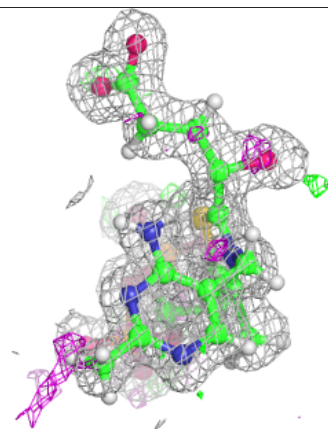
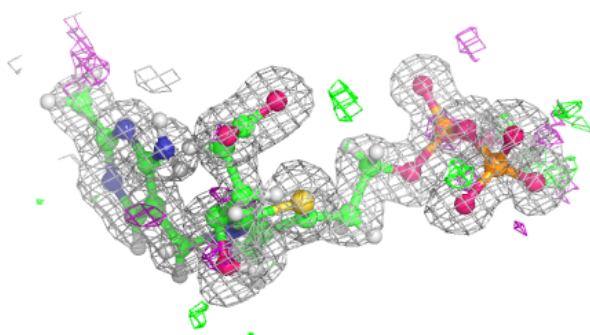
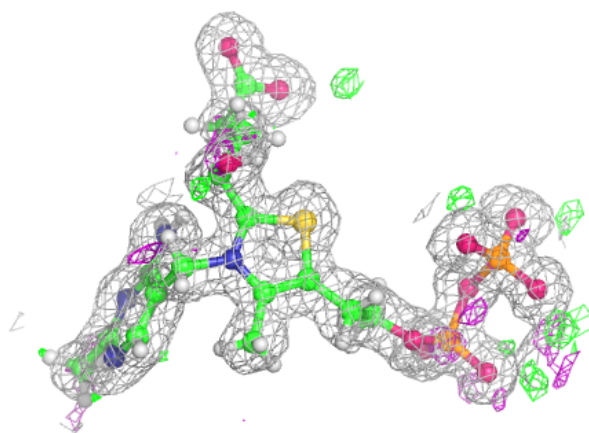
Electron density around TD6 D 602:

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



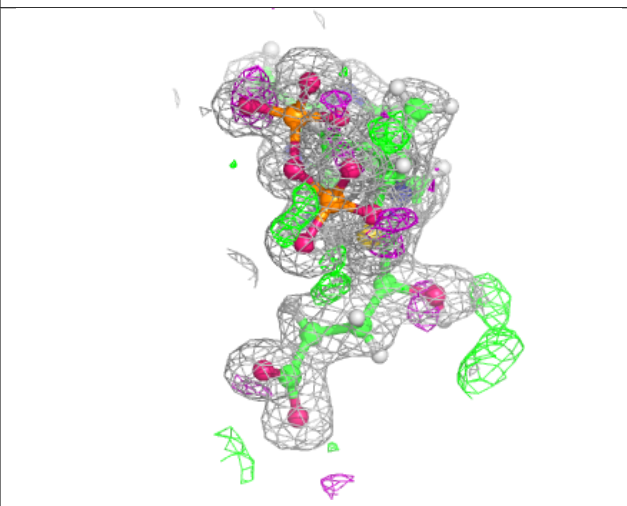
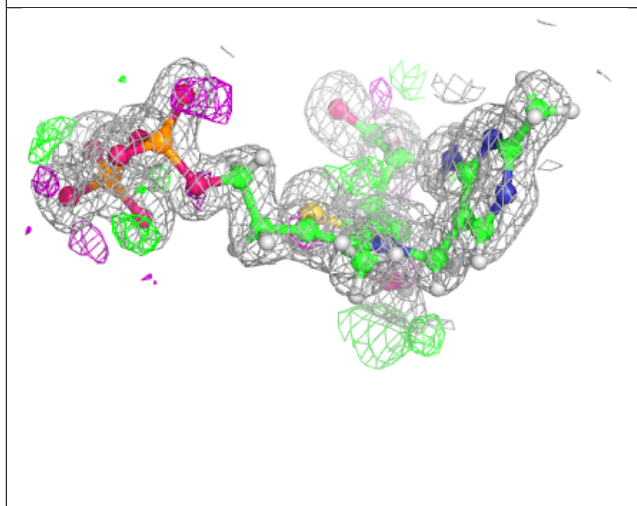
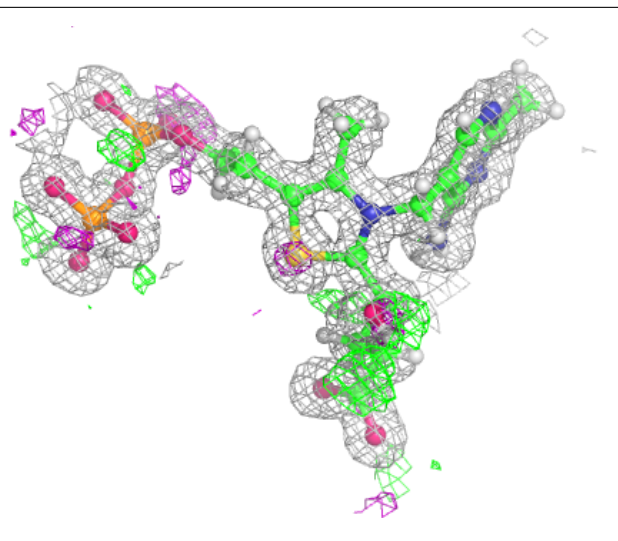
Electron density around TD6 F 602:

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



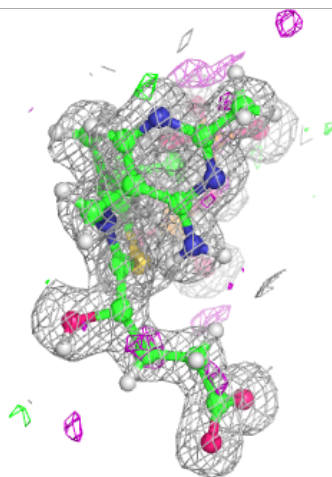
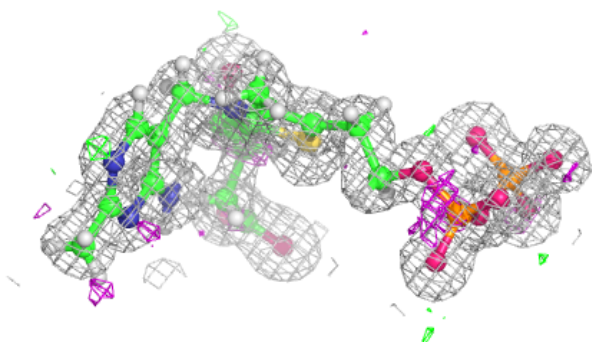
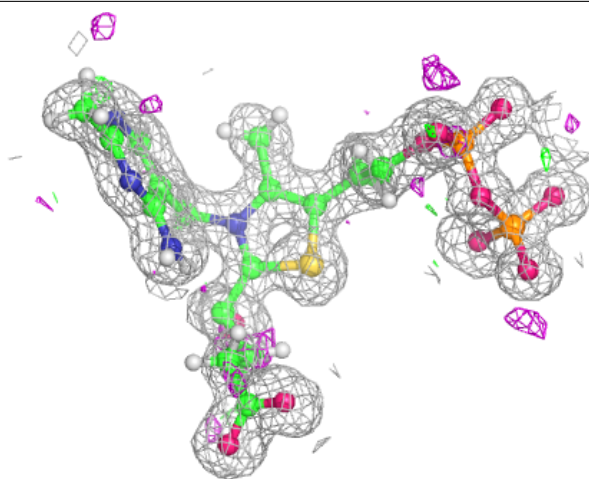
Electron density around TD6 H 602:

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



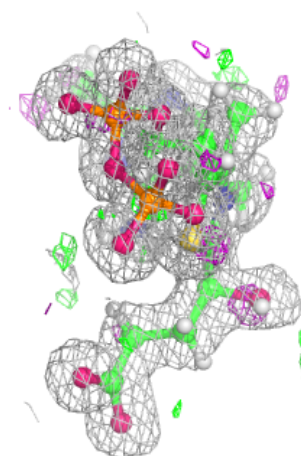
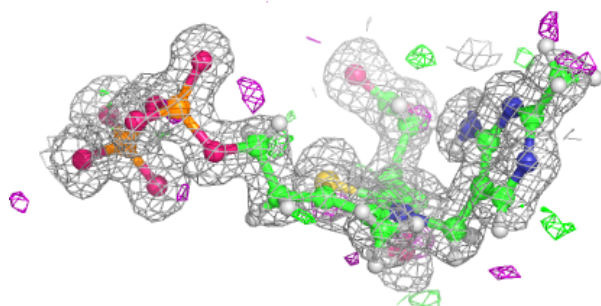
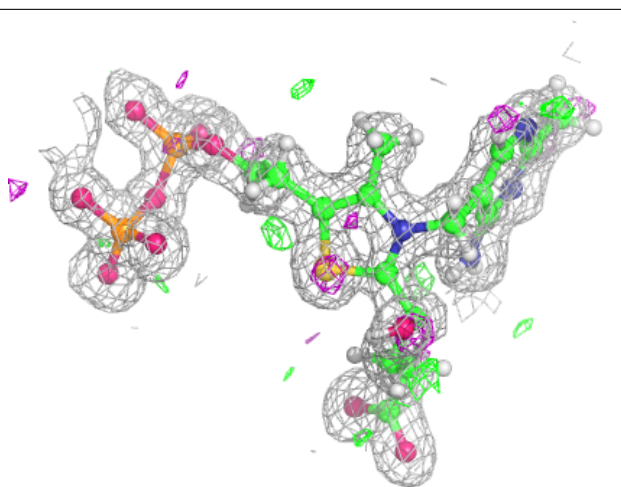
Electron density around TD6 A 601:

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



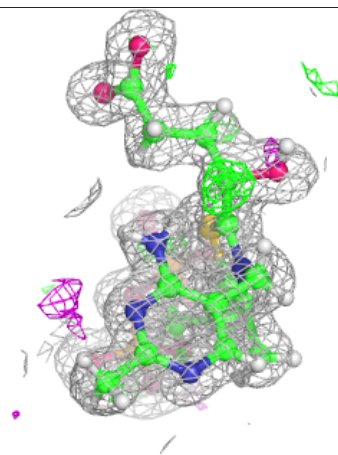
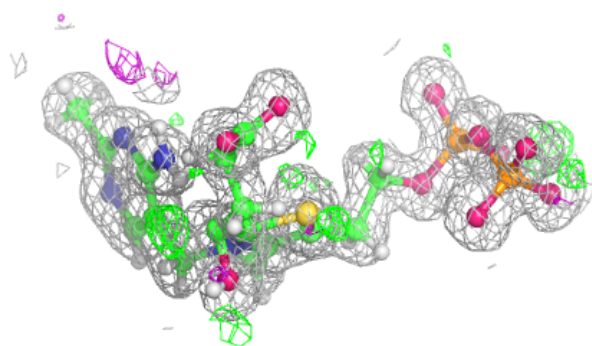
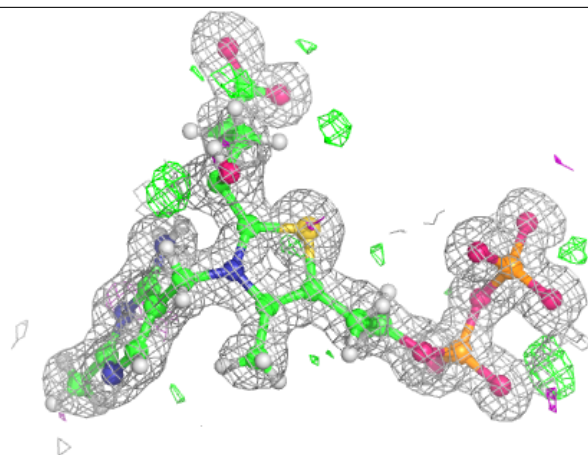
Electron density around TD6 E 601:

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



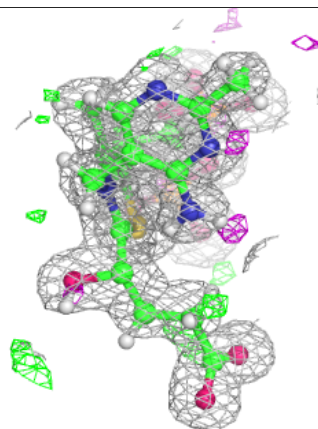
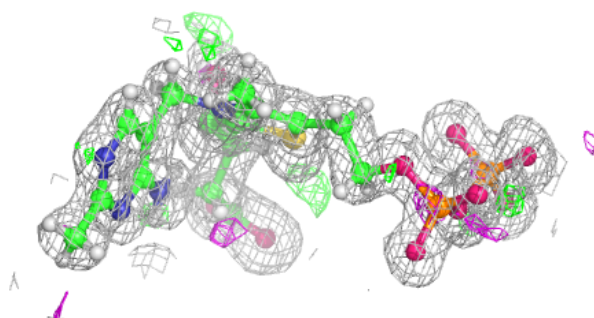
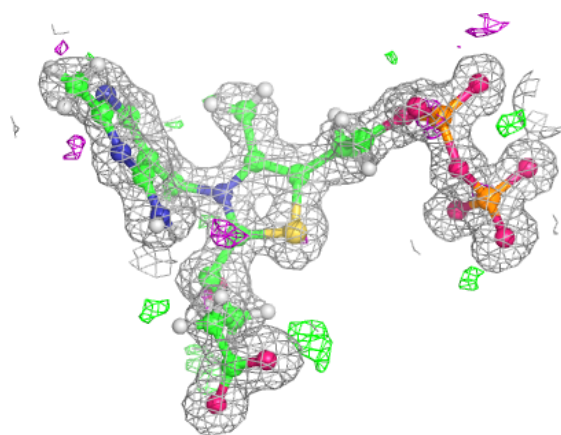
Electron density around TD6 C 602:

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



Electron density around TD6 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.