



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 AM UTC

PDB ID : 9DSN / pdb_00009dsn
Title : D306A Mutant of M.tuberculosis MenD (SEPHCHC Synthase)
Authors : Johnston, J.M.; Ho, N.A.T.; Given, F.M.; Allison, T.A.; Bulloch, E.M.M.; Jiao, W.
Deposited on : 2024-09-28
Resolution : 2.30 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 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

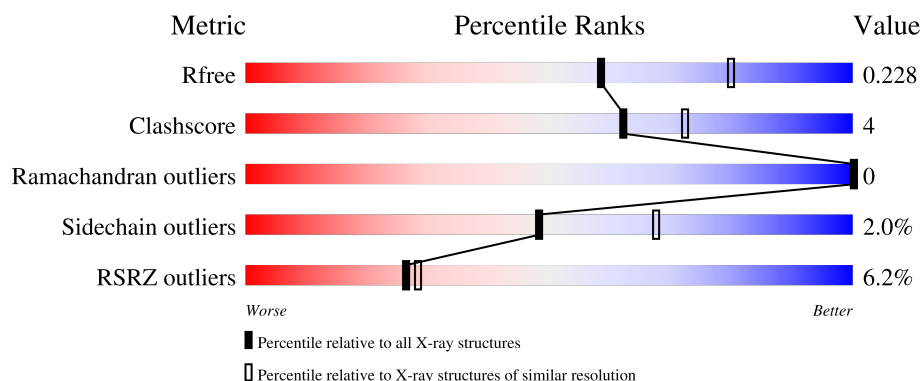
1 Overall quality at a glance

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	574	5% 84% 10% 6%
1	B	574	8% 82% 10% 8%
1	C	574	6% 81% 9% 9%
1	D	574	4% 84% 9% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16234 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	4	0
			3977	2484	737	744	12			
1	D	538	Total	C	N	O	S	0	5	0
			3978	2487	738	743	10			
1	B	530	Total	C	N	O	S	0	1	0
			3886	2425	721	729	11			
1	C	522	Total	C	N	O	S	0	2	0
			3826	2392	707	718	9			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WK11
A	-18	GLY	-	expression tag	UNP P9WK11
A	-17	SER	-	expression tag	UNP P9WK11
A	-16	SER	-	expression tag	UNP P9WK11
A	-15	HIS	-	expression tag	UNP P9WK11
A	-14	HIS	-	expression tag	UNP P9WK11
A	-13	HIS	-	expression tag	UNP P9WK11
A	-12	HIS	-	expression tag	UNP P9WK11
A	-11	HIS	-	expression tag	UNP P9WK11
A	-10	HIS	-	expression tag	UNP P9WK11
A	-9	SER	-	expression tag	UNP P9WK11
A	-8	SER	-	expression tag	UNP P9WK11
A	-7	GLY	-	expression tag	UNP P9WK11
A	-6	LEU	-	expression tag	UNP P9WK11
A	-5	VAL	-	expression tag	UNP P9WK11
A	-4	PRO	-	expression tag	UNP P9WK11
A	-3	ARG	-	expression tag	UNP P9WK11
A	-2	GLY	-	expression tag	UNP P9WK11
A	-1	SER	-	expression tag	UNP P9WK11
A	0	HIS	-	expression tag	UNP P9WK11

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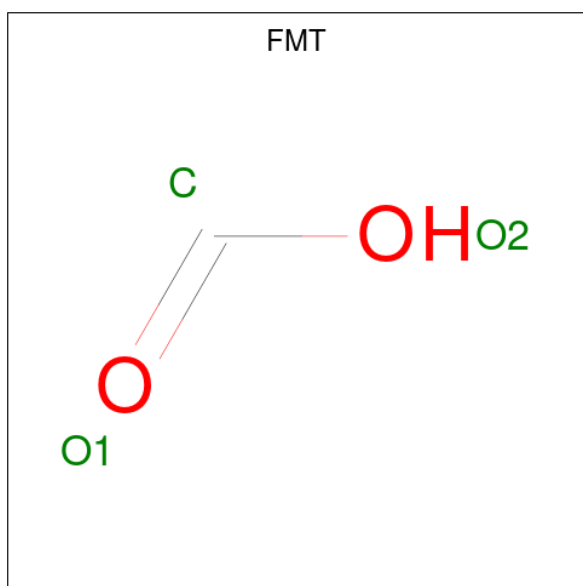
Chain	Residue	Modelled	Actual	Comment	Reference
A	306	ALA	ASP	engineered mutation	UNP P9WK11
D	-19	MET	-	initiating methionine	UNP P9WK11
D	-18	GLY	-	expression tag	UNP P9WK11
D	-17	SER	-	expression tag	UNP P9WK11
D	-16	SER	-	expression tag	UNP P9WK11
D	-15	HIS	-	expression tag	UNP P9WK11
D	-14	HIS	-	expression tag	UNP P9WK11
D	-13	HIS	-	expression tag	UNP P9WK11
D	-12	HIS	-	expression tag	UNP P9WK11
D	-11	HIS	-	expression tag	UNP P9WK11
D	-10	HIS	-	expression tag	UNP P9WK11
D	-9	SER	-	expression tag	UNP P9WK11
D	-8	SER	-	expression tag	UNP P9WK11
D	-7	GLY	-	expression tag	UNP P9WK11
D	-6	LEU	-	expression tag	UNP P9WK11
D	-5	VAL	-	expression tag	UNP P9WK11
D	-4	PRO	-	expression tag	UNP P9WK11
D	-3	ARG	-	expression tag	UNP P9WK11
D	-2	GLY	-	expression tag	UNP P9WK11
D	-1	SER	-	expression tag	UNP P9WK11
D	0	HIS	-	expression tag	UNP P9WK11
D	306	ALA	ASP	engineered mutation	UNP P9WK11
B	-19	MET	-	initiating methionine	UNP P9WK11
B	-18	GLY	-	expression tag	UNP P9WK11
B	-17	SER	-	expression tag	UNP P9WK11
B	-16	SER	-	expression tag	UNP P9WK11
B	-15	HIS	-	expression tag	UNP P9WK11
B	-14	HIS	-	expression tag	UNP P9WK11
B	-13	HIS	-	expression tag	UNP P9WK11
B	-12	HIS	-	expression tag	UNP P9WK11
B	-11	HIS	-	expression tag	UNP P9WK11
B	-10	HIS	-	expression tag	UNP P9WK11
B	-9	SER	-	expression tag	UNP P9WK11
B	-8	SER	-	expression tag	UNP P9WK11
B	-7	GLY	-	expression tag	UNP P9WK11
B	-6	LEU	-	expression tag	UNP P9WK11
B	-5	VAL	-	expression tag	UNP P9WK11
B	-4	PRO	-	expression tag	UNP P9WK11
B	-3	ARG	-	expression tag	UNP P9WK11
B	-2	GLY	-	expression tag	UNP P9WK11
B	-1	SER	-	expression tag	UNP P9WK11
B	0	HIS	-	expression tag	UNP P9WK11

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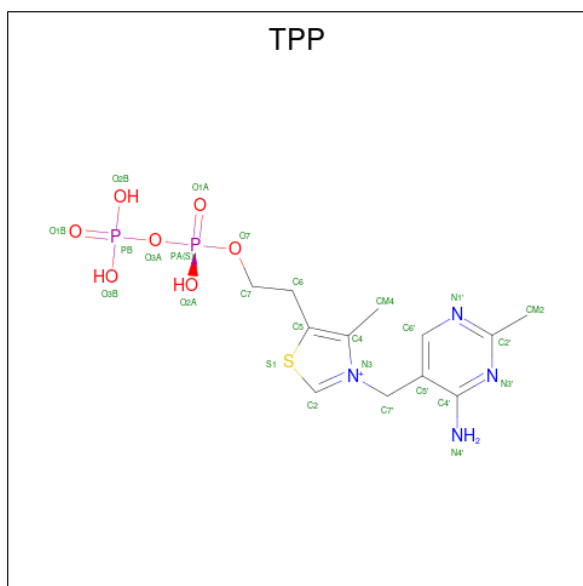
Chain	Residue	Modelled	Actual	Comment	Reference
B	306	ALA	ASP	engineered mutation	UNP P9WK11
C	-19	MET	-	initiating methionine	UNP P9WK11
C	-18	GLY	-	expression tag	UNP P9WK11
C	-17	SER	-	expression tag	UNP P9WK11
C	-16	SER	-	expression tag	UNP P9WK11
C	-15	HIS	-	expression tag	UNP P9WK11
C	-14	HIS	-	expression tag	UNP P9WK11
C	-13	HIS	-	expression tag	UNP P9WK11
C	-12	HIS	-	expression tag	UNP P9WK11
C	-11	HIS	-	expression tag	UNP P9WK11
C	-10	HIS	-	expression tag	UNP P9WK11
C	-9	SER	-	expression tag	UNP P9WK11
C	-8	SER	-	expression tag	UNP P9WK11
C	-7	GLY	-	expression tag	UNP P9WK11
C	-6	LEU	-	expression tag	UNP P9WK11
C	-5	VAL	-	expression tag	UNP P9WK11
C	-4	PRO	-	expression tag	UNP P9WK11
C	-3	ARG	-	expression tag	UNP P9WK11
C	-2	GLY	-	expression tag	UNP P9WK11
C	-1	SER	-	expression tag	UNP P9WK11
C	0	HIS	-	expression tag	UNP P9WK11
C	306	ALA	ASP	engineered mutation	UNP P9WK11

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



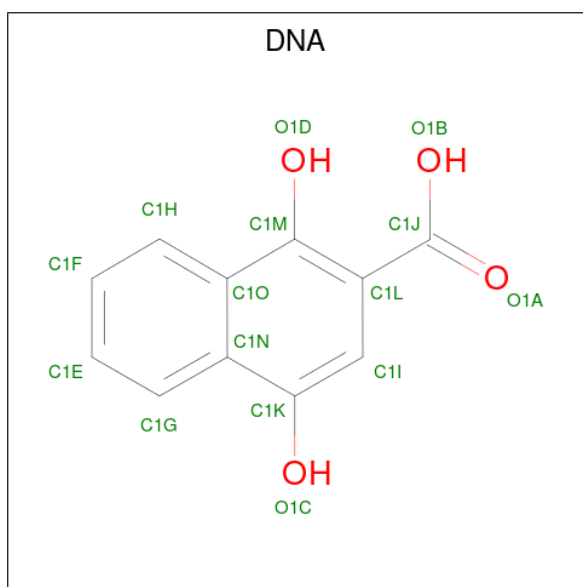
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		
2	D	1	Total	C	O	0	0
			3	1	2		
2	D	1	Total	C	O	0	0
			3	1	2		
2	D	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		
2	C	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is 1,4-dihydroxy-2-naphthoic acid (CCD ID: DNA) (formula: $C_{11}H_8O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			15	11	4		
4	C	1	Total	C	O	0	0
			15	11	4		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

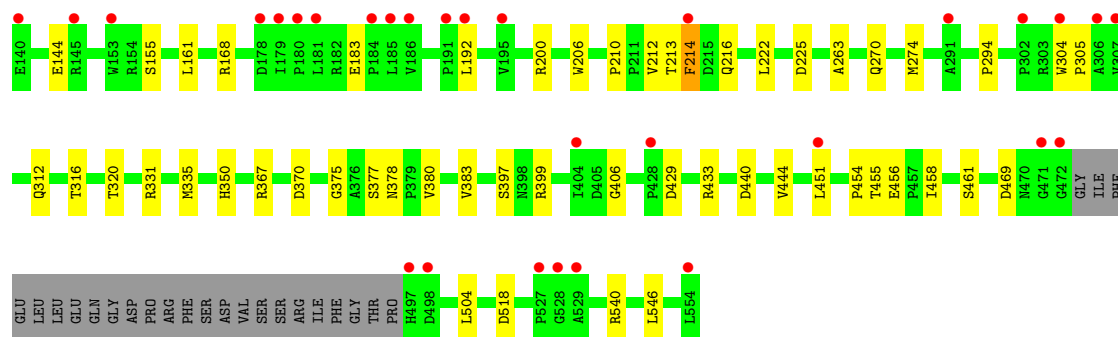
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	138	Total	O	0	0
			138	138		
7	D	170	Total	O	0	0
			170	170		

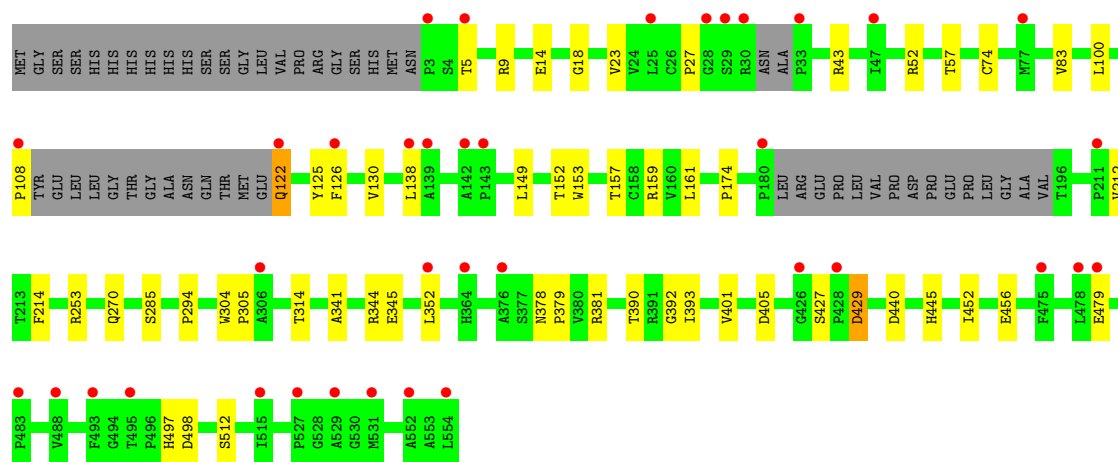
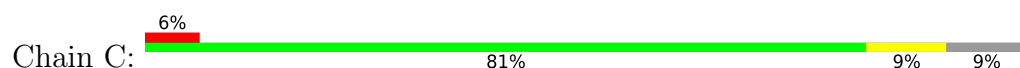
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	103	Total 103	O 103	0	0
7	C	50	Total 50	O 50	0	0



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.22Å 139.26Å 181.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.30 48.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.75-2.30) 99.7 (48.75-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.192 , 0.228 0.192 , 0.228	Depositor DCC
R_{free} test set	5794 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16234	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: FMT, DNA, MG, CL, TPP

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	0.17	0/4069	0.35	0/5578
1	B	0.16	0/3968	0.35	0/5439
1	C	0.15	0/3909	0.33	0/5351
1	D	0.18	0/4069	0.35	0/5573
All	All	0.17	0/16015	0.34	0/21941

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3977	0	4006	36	0
1	B	3886	0	3923	37	0
1	C	3826	0	3849	37	0
1	D	3978	0	3997	37	0
2	A	3	0	1	1	0
2	B	6	0	2	0	0
2	C	3	0	1	1	0
2	D	9	0	3	0	0
3	C	26	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	26	0	16	0	0
4	C	15	0	6	2	0
4	D	15	0	5	1	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	1	0	0	0	0
7	A	138	0	0	2	0
7	B	103	0	0	1	0
7	C	50	0	0	0	0
7	D	170	0	0	2	0
All	All	16234	0	15825	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (128) 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:D:34:LEU:HD21	1:D:179:ILE:HD13	1.65	0.77
1:D:32:ALA:HB3	1:D:35:ALA:HB2	1.71	0.71
1:B:81:THR:HG23	1:C:401:VAL:HG11	1.73	0.70
1:A:274:MET:HE3	1:A:305:PRO:HG2	1.74	0.69
1:B:183:GLU:H	1:B:183:GLU:CD	2.02	0.68
1:B:144:GLU:N	1:B:144:GLU:OE2	2.27	0.66
1:D:212:VAL:HG21	1:B:214[A]:PHE:HD1	1.60	0.65
1:A:144:GLU:OE1	1:A:144:GLU:N	2.20	0.65
1:B:294:PRO:HB3	1:B:312:GLN:HG3	1.80	0.64
1:C:341:ALA:O	1:C:345:GLU:HG2	1.97	0.64
1:D:216:GLN:HB3	1:D:316:THR:HG23	1.81	0.63
1:A:222:LEU:HD22	1:A:243:LEU:HD11	1.83	0.61
1:A:225:ASP:HB2	1:A:270[B]:GLN:HG3	1.82	0.61
1:D:212:VAL:HG21	1:B:214[A]:PHE:CD1	2.36	0.59
1:D:18:GLY:HA3	1:D:161:LEU:HD13	1.85	0.58
1:D:388:LEU:HD22	1:D:390:THR:HG22	1.85	0.58
1:C:429:ASP:OD1	1:C:429:ASP:N	2.34	0.57
1:A:280:LEU:HD11	1:A:381:ARG:HG2	1.85	0.57
1:A:305:PRO:HB2	1:A:307:VAL:HG22	1.86	0.57
1:C:5:THR:O	1:C:9:ARG:HG2	2.05	0.56
1:B:440:ASP:O	1:B:444:VAL:HG23	2.06	0.56
1:A:506:ARG:NH1	1:D:506:ARG:HH21	2.02	0.56
1:A:469:ASP:HB2	1:A:540:ARG:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:ASP:HB3	1:C:445:HIS:CE1	2.41	0.55
1:A:217:PRO:HB3	1:A:317:ARG:NH1	2.22	0.55
1:D:23:VAL:HG22	1:D:74:CYS:HB2	1.88	0.54
1:D:216:GLN:HG2	1:B:210:PRO:HG2	1.89	0.54
1:C:122:GLN:HE21	1:C:122:GLN:N	2.04	0.54
1:A:304:TRP:CZ2	1:C:159:ARG:HG2	2.43	0.53
1:B:274:MET:HE1	1:B:305:PRO:HB2	1.90	0.53
1:B:397:SER:HB3	1:B:399:ARG:HG2	1.91	0.53
1:D:44:SER:HB2	1:D:46:ARG:HG3	1.91	0.53
1:D:216:GLN:OE1	1:B:168:ARG:NH1	2.42	0.53
1:B:76:ALA:HA	1:B:103:LEU:O	2.10	0.52
1:B:433:ARG:HA	1:B:461:SER:OG	2.10	0.51
1:C:18:GLY:HA3	1:C:161:LEU:HD13	1.92	0.51
1:D:151:ALA:O	1:D:155:SER:OG	2.24	0.51
1:A:212:VAL:HG21	1:C:214[B]:PHE:CD1	2.46	0.51
1:C:378:ASN:N	1:C:379:PRO:HD2	2.25	0.51
1:A:216:GLN:HB3	1:A:316:THR:HG23	1.94	0.50
1:C:479:GLU:OE1	1:C:479:GLU:N	2.36	0.50
1:D:100:LEU:O	1:D:174:PRO:HA	2.12	0.50
1:A:470:ASN:CG	1:A:496:PRO:HB3	2.36	0.50
1:A:507:ALA:HA	1:D:500:ASP:HB3	1.92	0.50
1:C:83:VAL:HG22	1:C:126:PHE:HE2	1.77	0.50
1:B:107:ARG:HD3	1:B:119:THR:OG1	2.11	0.50
1:A:100:LEU:O	1:A:174:PRO:HA	2.12	0.49
1:A:218:LEU:HD12	1:A:219:ASP:H	1.78	0.49
1:A:304:TRP:O	1:C:159:ARG:NH2	2.28	0.49
1:A:431:PRO:HG3	1:A:460:ARG:NH1	2.27	0.49
1:D:216:GLN:HB2	1:B:212:VAL:HG23	1.95	0.49
1:B:216:GLN:HB3	1:B:316:THR:HG23	1.95	0.49
1:A:514:GLN:NE2	1:A:537:LYS:HD3	2.28	0.49
1:C:452:ILE:HG22	1:C:456:GLU:HB2	1.93	0.49
1:D:91:VAL:HG12	1:D:401:VAL:HG21	1.94	0.48
1:B:367:ARG:HG3	1:B:433:ARG:NH2	2.28	0.48
1:D:210:PRO:HG2	1:B:216:GLN:HG3	1.94	0.48
1:B:18:GLY:HA3	1:B:161:LEU:HD13	1.96	0.48
1:B:60:TYR:CG	1:B:406:GLY:HA3	2.49	0.48
1:D:5:THR:HG22	1:D:9:ARG:HD2	1.94	0.47
1:C:126:PHE:O	1:C:130:VAL:HG22	2.14	0.47
1:D:304:TRP:C	4:D:602:DNA:H1H	2.39	0.47
1:C:23:VAL:HG22	1:C:74:CYS:HB2	1.96	0.47
1:A:18:GLY:HA3	1:A:161:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:SER:H	2:A:601:FMT:C	2.27	0.47
1:B:461:SER:OG	1:B:461:SER:O	2.33	0.46
1:A:216:GLN:HB2	1:C:212:VAL:HG12	1.98	0.46
1:D:256:ASP:N	1:D:256:ASP:OD1	2.49	0.46
1:A:144:GLU:H	1:A:144:GLU:CD	2.16	0.46
1:A:246:VAL:HG21	1:A:264:LEU:HD22	1.98	0.46
1:C:381:ARG:HH12	2:C:603:FMT:C	2.27	0.46
1:B:375:GLY:O	1:B:380:VAL:HG23	2.16	0.46
1:A:304:TRP:N	7:A:702:HOH:O	2.40	0.46
1:B:225:ASP:HB2	1:B:270:GLN:HG3	1.98	0.45
1:D:214[B]:PHE:CE1	1:B:212:VAL:HG21	2.51	0.45
1:B:377:SER:OG	1:B:378:ASN:N	2.49	0.45
1:C:427:SER:HB3	1:C:429:ASP:OD1	2.17	0.45
7:A:808:HOH:O	1:D:81:THR:HG23	2.17	0.45
1:D:8:ALA:HA	1:D:34:LEU:HD22	1.99	0.45
1:D:145:ARG:HH11	1:D:145:ARG:HG3	1.81	0.44
1:A:140:GLU:CD	1:A:145:ARG:HH21	2.23	0.44
1:A:498:ASP:O	1:D:509:HIS:NE2	2.48	0.44
1:A:190:GLU:N	1:A:191:PRO:HD2	2.32	0.44
1:D:388:LEU:HD23	1:D:389:ASP:C	2.42	0.44
1:D:522:PRO:O	1:D:526:GLN:HG2	2.18	0.44
1:A:341:ALA:O	1:A:345:GLU:HG3	2.17	0.44
1:A:438:ILE:HD11	1:A:443:PHE:HD1	1.83	0.44
1:C:14:GLU:HB3	1:C:157:THR:HG21	1.98	0.44
1:D:360:ALA:O	1:D:364[A]:HIS:ND1	2.45	0.43
1:B:370:ASP:OD1	1:B:433:ARG:HB2	2.18	0.43
1:D:253:ARG:NH2	7:D:709:HOH:O	2.46	0.43
1:C:138:LEU:HD23	1:C:138:LEU:HA	1.80	0.43
1:C:253:ARG:HD2	1:C:390:THR:OG1	2.18	0.43
1:B:454:PRO:HG3	1:C:498:ASP:OD2	2.19	0.43
1:A:159:ARG:HG2	1:C:304:TRP:CZ2	2.54	0.43
1:B:263:ALA:HB1	1:B:335:MET:HB3	2.01	0.43
1:B:331:ARG:NH2	7:B:710:HOH:O	2.49	0.43
1:B:451:LEU:HD11	1:C:497:HIS:HB2	2.00	0.43
1:A:260:HIS:HE1	1:A:385:LEU:HD12	1.84	0.43
1:A:94:ASN:O	1:A:303:ARG:NH2	2.51	0.43
1:B:350:HIS:CE1	1:B:546:LEU:HB2	2.54	0.42
1:C:344:ARG:HG3	1:C:345:GLU:N	2.34	0.42
1:C:405:ASP:OD1	1:C:405:ASP:N	2.36	0.42
1:C:100:LEU:O	1:C:174:PRO:HA	2.19	0.42
1:C:305:PRO:HD3	4:C:602:DNA:O1D	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:GLY:C	1:C:393:ILE:HD13	2.45	0.42
1:D:299:THR:OG1	1:B:168:ARG:NH2	2.50	0.42
1:D:108:PRO:HG2	1:D:138:LEU:HG	2.02	0.42
1:B:200:ARG:HG3	1:B:206:TRP:HA	2.00	0.42
1:B:444:VAL:HG13	1:B:504:LEU:HD11	2.02	0.42
1:A:218:LEU:HD12	1:A:219:ASP:N	2.34	0.42
1:D:136:LEU:HA	1:D:136:LEU:HD23	1.77	0.42
1:D:25:LEU:HG	1:D:76:ALA:HB3	2.02	0.42
1:C:108:PRO:HG2	1:C:138:LEU:HG	2.02	0.42
1:C:270:GLN:O	1:C:294:PRO:HD2	2.20	0.41
1:B:456:GLU:O	1:B:458:ILE:HD12	2.19	0.41
1:B:469:ASP:HB2	1:B:540:ARG:HB3	2.01	0.41
1:C:149:LEU:HD12	1:C:153:TRP:CZ2	2.55	0.41
1:A:60:TYR:CG	1:A:406:GLY:HA3	2.55	0.41
1:A:76:ALA:HA	1:A:103:LEU:O	2.21	0.41
1:C:125:TYR:CD1	1:C:125:TYR:C	2.99	0.41
1:D:25:LEU:CD1	1:D:49:LEU:HD22	2.51	0.40
1:C:304:TRP:C	4:C:602:DNA:H1H	2.46	0.40
1:D:14:GLU:HB3	1:D:157:THR:HG21	2.03	0.40
1:D:551:LYS:NZ	7:D:720:HOH:O	2.54	0.40
1:C:27:PRO:HD2	1:C:52:ARG:O	2.21	0.40
1:B:222:LEU:HG	1:B:320:THR:HB	2.04	0.40
1:C:440:ASP:OD2	1:C:440:ASP:N	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	540/574 (94%)	526 (97%)	14 (3%)	0	100	100
1	B	527/574 (92%)	516 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	516/574 (90%)	499 (97%)	17 (3%)	0	100	100
1	D	537/574 (94%)	523 (97%)	14 (3%)	0	100	100
All	All	2120/2296 (92%)	2064 (97%)	56 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	417/444 (94%)	410 (98%)	7 (2%)	53	72
1	B	406/444 (91%)	394 (97%)	12 (3%)	36	53
1	C	400/444 (90%)	391 (98%)	9 (2%)	44	63
1	D	416/444 (94%)	409 (98%)	7 (2%)	53	72
All	All	1639/1776 (92%)	1604 (98%)	35 (2%)	48	66

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	57	THR
1	A	190	GLU
1	A	230	SER
1	A	307	VAL
1	A	311	SER
1	A	517	VAL
1	D	44	SER
1	D	47	ILE
1	D	57	THR
1	D	213	THR
1	D	350[A]	HIS
1	D	350[B]	HIS
1	D	401	VAL

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Mol	Chain	Res	Type
1	B	4	SER
1	B	57	THR
1	B	155	SER
1	B	192	LEU
1	B	213	THR
1	B	214[A]	PHE
1	B	214[B]	PHE
1	B	304	TRP
1	B	383	VAL
1	B	429	ASP
1	B	455	THR
1	B	518	ASP
1	C	43	ARG
1	C	57	THR
1	C	122	GLN
1	C	152	THR
1	C	285	SER
1	C	314	THR
1	C	352	LEU
1	C	429	ASP
1	C	512	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	HIS
1	D	281	HIS
1	C	270	GLN
1	C	281	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	FMT	D	603	-	2,2,2	0.78	0	1,1,1	0.30	0
4	DNA	D	602	-	16,16,16	2.36	4 (25%)	23,23,23	1.11	1 (4%)
2	FMT	B	601	-	2,2,2	0.73	0	1,1,1	0.23	0
3	TPP	C	601	5	26,27,27	0.49	1 (3%)	38,40,40	0.27	0
2	FMT	D	605	-	2,2,2	0.73	0	1,1,1	0.25	0
2	FMT	D	604	-	2,2,2	0.74	0	1,1,1	0.20	0
2	FMT	A	601	-	2,2,2	0.73	0	1,1,1	0.23	0
4	DNA	C	602	-	16,16,16	2.38	4 (25%)	23,23,23	1.30	4 (17%)
2	FMT	C	603	-	2,2,2	0.74	0	1,1,1	0.25	0
3	TPP	D	601	5	26,27,27	0.29	0	38,40,40	0.32	0
2	FMT	B	602	-	2,2,2	0.73	0	1,1,1	0.23	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
3	TPP	C	601	5	-	3/17/17/17	0/2/2/2
3	TPP	D	601	5	-	2/17/17/17	0/2/2/2
4	DNA	C	602	-	-	0/4/4/4	0/2/2/2
4	DNA	D	602	-	-	0/4/4/4	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	DNA	C1L-C1M	6.98	1.49	1.39
4	C	602	DNA	C1L-C1M	6.80	1.49	1.39
4	C	602	DNA	C1K-C1N	3.68	1.49	1.42
4	D	602	DNA	C1K-C1N	3.16	1.48	1.42
4	C	602	DNA	C1M-C1O	2.96	1.49	1.43
4	C	602	DNA	C1O-C1N	2.92	1.49	1.43
4	D	602	DNA	C1M-C1O	2.78	1.48	1.43
4	D	602	DNA	C1O-C1N	2.74	1.48	1.43
3	C	601	TPP	PA-O3A	2.08	1.61	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	DNA	C1I-C1L-C1M	2.70	121.19	119.05
4	C	602	DNA	O1D-C1M-C1O	2.34	121.37	116.62
4	D	602	DNA	C1I-C1L-C1M	2.30	120.88	119.05
4	C	602	DNA	O1C-C1K-C1N	2.27	120.31	116.42
4	C	602	DNA	O1D-C1M-C1L	-2.09	120.08	122.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	TPP	PA-O3A-PB-O3B
3	C	601	TPP	PA-O3A-PB-O2B
3	C	601	TPP	PA-O3A-PB-O3B
3	D	601	TPP	PA-O3A-PB-O1B
3	C	601	TPP	PA-O3A-PB-O1B

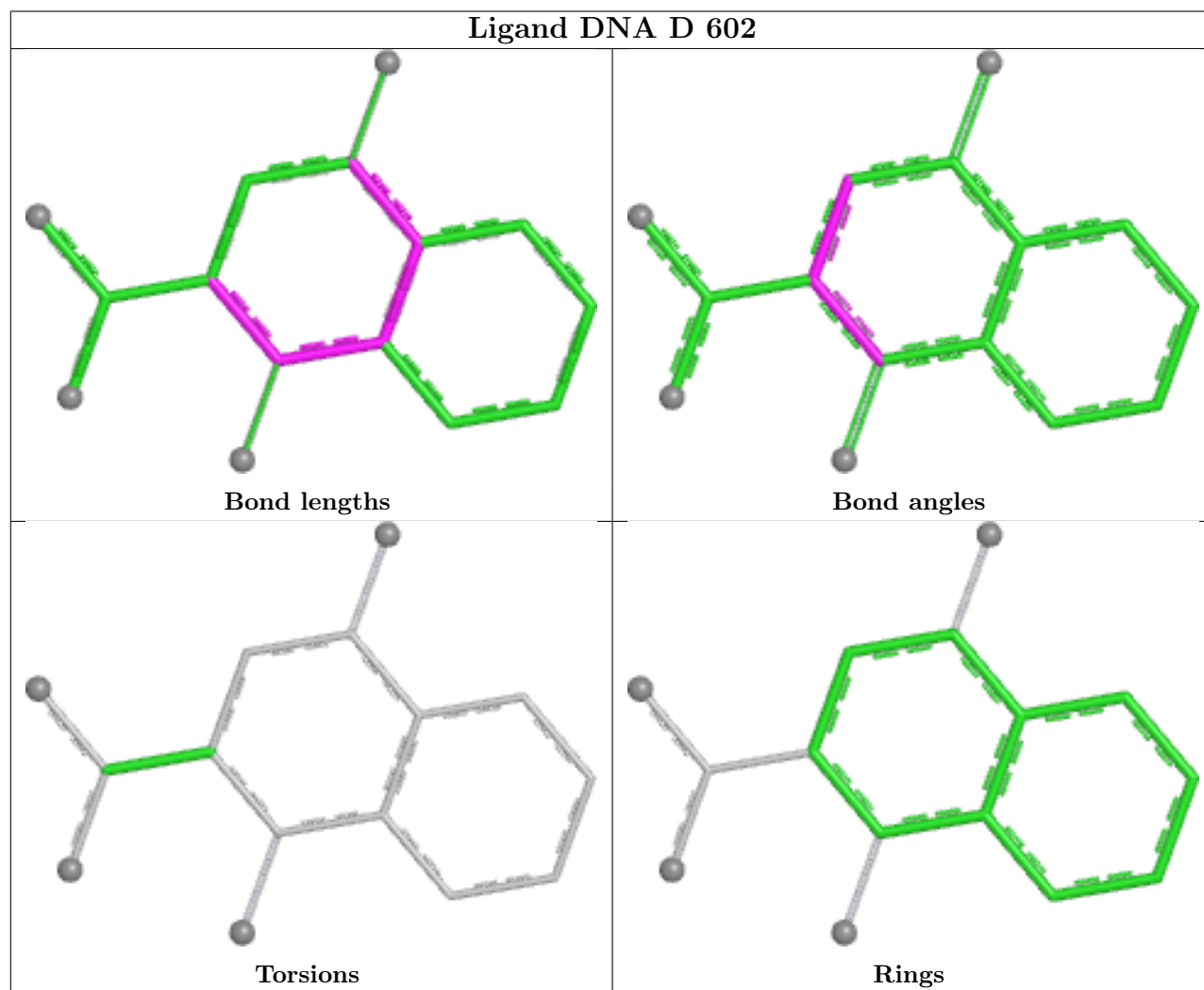
There are no ring outliers.

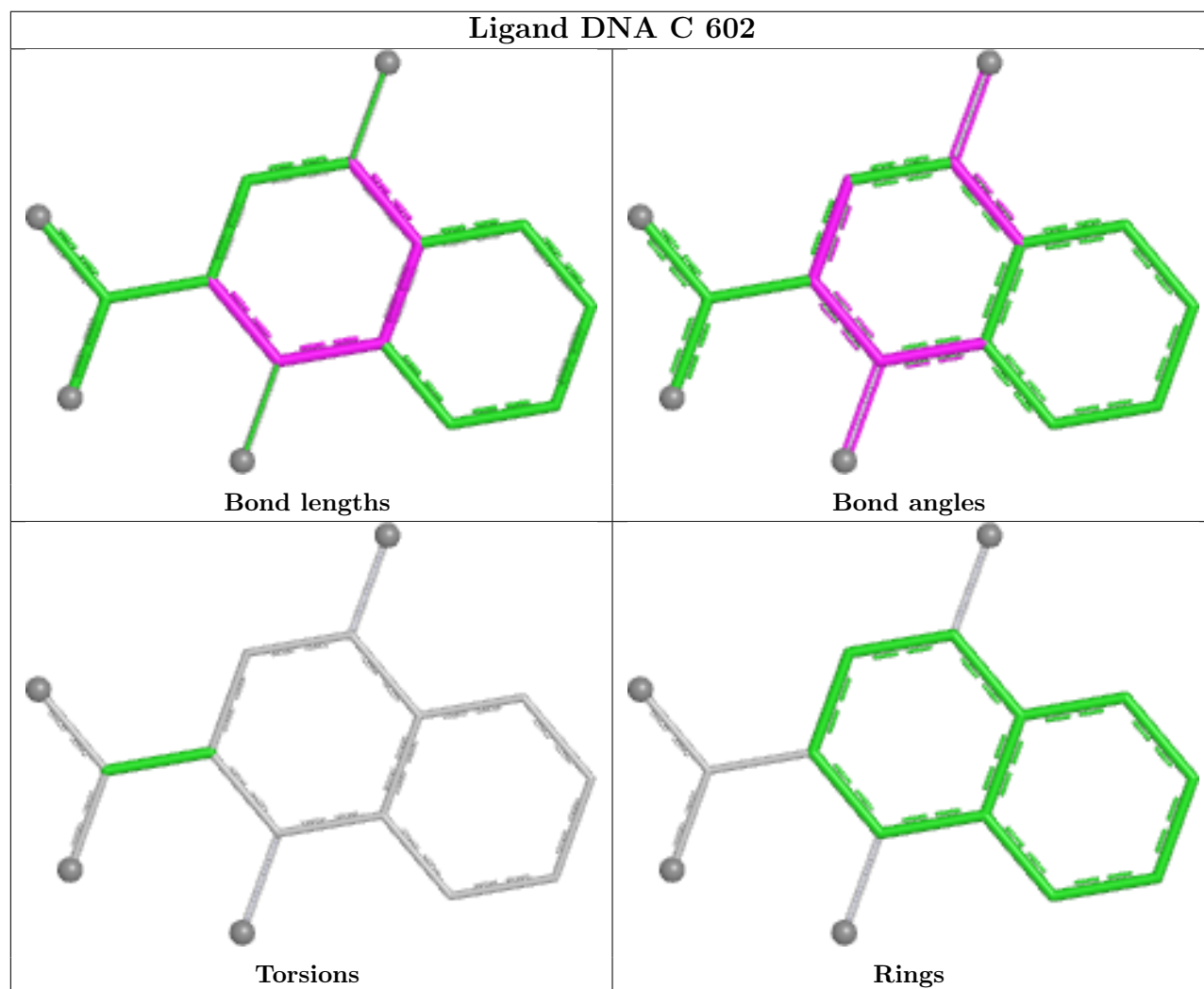
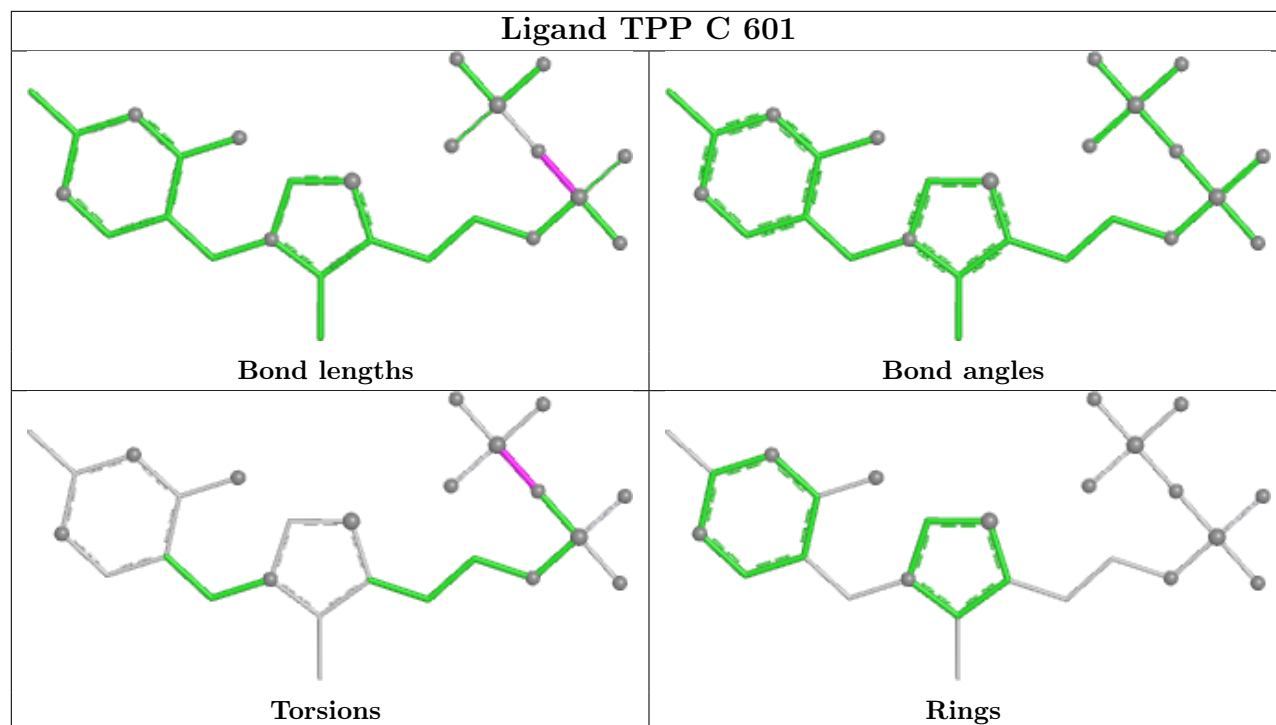
4 monomers are involved in 5 short contacts:

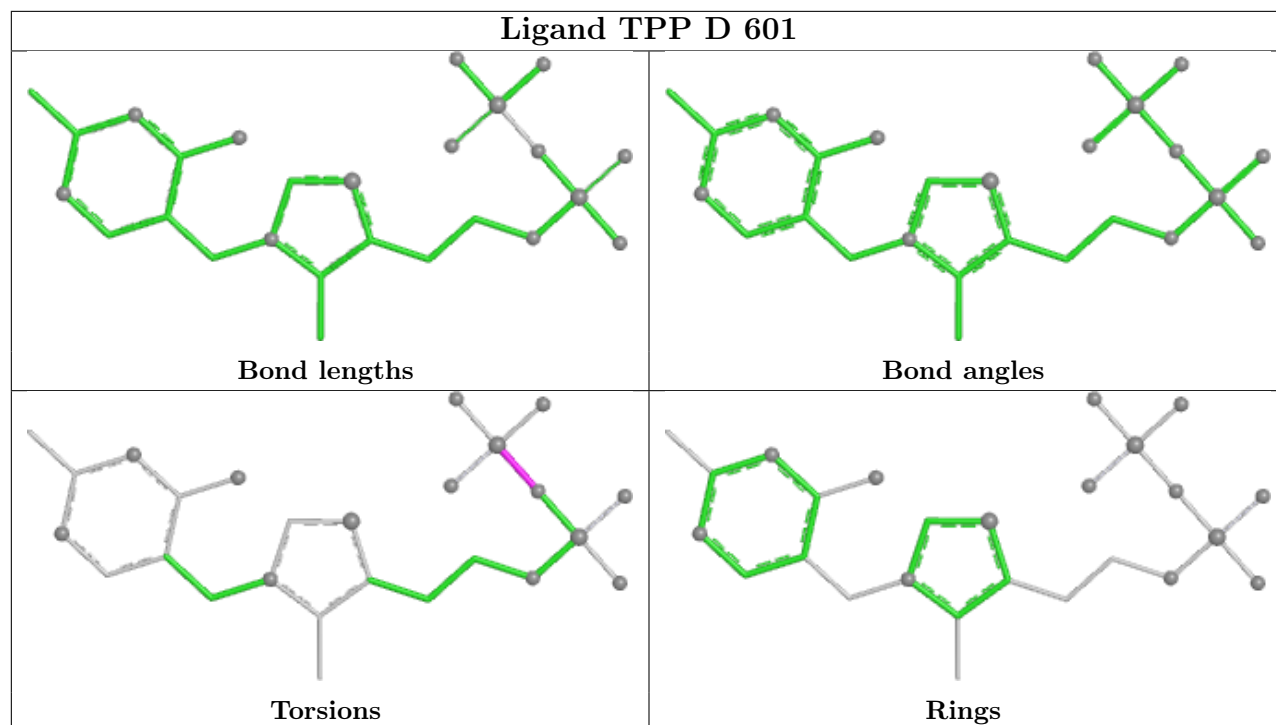
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	DNA	1	0
2	A	601	FMT	1	0
4	C	602	DNA	2	0
2	C	603	FMT	1	0

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	540/574 (94%)	0.19	27 (5%)	34	35	20, 49, 90, 122	4 (0%)
1	B	530/574 (92%)	0.49	45 (8%)	16	18	25, 55, 92, 129	1 (0%)
1	C	522/574 (90%)	0.61	37 (7%)	22	24	26, 64, 101, 130	2 (0%)
1	D	538/574 (93%)	0.17	24 (4%)	38	40	24, 47, 89, 129	5 (0%)
All	All	2130/2296 (92%)	0.36	133 (6%)	26	28	20, 54, 95, 130	12 (0%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214[A]	PHE	4.9
1	C	108	PRO	4.7
1	C	211	PRO	4.5
1	B	307	VAL	4.4
1	A	192	LEU	4.4
1	D	195	VAL	4.4
1	B	529	ALA	4.3
1	D	34	LEU	4.3
1	B	472	GLY	4.0
1	D	184	PRO	4.0
1	D	29	SER	4.0
1	A	471	GLY	3.9
1	A	487	ASP	3.9
1	C	3	PRO	3.8
1	B	304	TRP	3.8
1	A	529	ALA	3.7
1	B	192	LEU	3.6
1	A	494	GLY	3.6
1	C	495	THR	3.5
1	C	527	PRO	3.5
1	A	404	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	120	MET	3.4
1	B	527	PRO	3.4
1	B	4	SER	3.4
1	B	195	VAL	3.4
1	A	291	ALA	3.4
1	D	142	ALA	3.4
1	B	181	LEU	3.3
1	D	428	PRO	3.3
1	D	33	PRO	3.3
1	D	32	ALA	3.3
1	B	123	LEU	3.2
1	C	529	ALA	3.2
1	A	42	ASP	3.1
1	B	116	ALA	3.1
1	A	495	THR	3.1
1	B	306	ALA	3.1
1	C	306	ALA	3.1
1	D	112	LEU	3.1
1	C	475	PHE	3.1
1	A	191	PRO	3.1
1	C	488	VAL	3.0
1	B	31	ASN	3.0
1	B	185	LEU	3.0
1	C	47	ILE	3.0
1	B	117	ASN	3.0
1	C	30	ARG	2.9
1	C	478	LEU	2.9
1	A	364[A]	HIS	2.9
1	A	493	PHE	2.9
1	B	497	HIS	2.9
1	C	122	GLN	2.9
1	D	140	GLU	2.9
1	A	528	GLY	2.8
1	C	143	PRO	2.8
1	D	114	THR	2.8
1	A	428	PRO	2.8
1	C	376	ALA	2.8
1	D	182	ARG	2.8
1	C	515	ILE	2.7
1	B	180	PRO	2.7
1	C	126	PHE	2.7
1	B	191	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	109	TYR	2.7
1	A	214[A]	PHE	2.7
1	D	40	ASP	2.7
1	A	492	ILE	2.6
1	C	483	PRO	2.6
1	B	291	ALA	2.6
1	B	528	GLY	2.6
1	C	77	MET	2.6
1	B	112	LEU	2.6
1	A	195	VAL	2.6
1	B	428	PRO	2.6
1	A	0	HIS	2.5
1	C	29	SER	2.5
1	B	140	GLU	2.5
1	D	181	LEU	2.5
1	D	28	GLY	2.5
1	D	364[A]	HIS	2.5
1	D	122	GLN	2.5
1	B	137	GLY	2.5
1	B	186	VAL	2.4
1	B	136	LEU	2.4
1	A	527	PRO	2.4
1	B	184	PRO	2.4
1	C	142	ALA	2.4
1	C	493	PHE	2.4
1	B	302	PRO	2.4
1	A	304	TRP	2.4
1	C	33	PRO	2.4
1	B	498	ASP	2.3
1	A	309	GLY	2.3
1	B	1	MET	2.3
1	A	488	VAL	2.3
1	A	211	PRO	2.3
1	B	153	TRP	2.3
1	D	214[A]	PHE	2.3
1	C	531	MET	2.3
1	C	139	ALA	2.3
1	D	183	GLU	2.3
1	A	307	VAL	2.2
1	B	554	LEU	2.2
1	B	178	ASP	2.2
1	D	527	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	428	PRO	2.2
1	B	139	ALA	2.2
1	A	376	ALA	2.2
1	C	25	LEU	2.2
1	C	479	GLU	2.2
1	C	28	GLY	2.2
1	B	114	THR	2.2
1	B	119	THR	2.2
1	C	552	ALA	2.2
1	B	404	ILE	2.1
1	C	138	LEU	2.1
1	C	554	LEU	2.1
1	D	2	ASN	2.1
1	D	350[A]	HIS	2.1
1	B	109	TYR	2.1
1	C	352	LEU	2.1
1	A	194	ALA	2.1
1	B	32	ALA	2.1
1	B	179	ILE	2.1
1	C	364	HIS	2.1
1	B	471	GLY	2.1
1	C	426	GLY	2.1
1	B	451	LEU	2.0
1	C	180	PRO	2.0
1	A	303	ARG	2.0
1	C	5	THR	2.0
1	B	105	ALA	2.0
1	B	145	ARG	2.0

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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

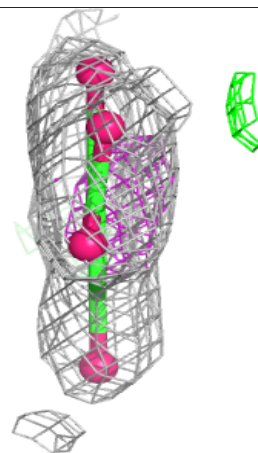
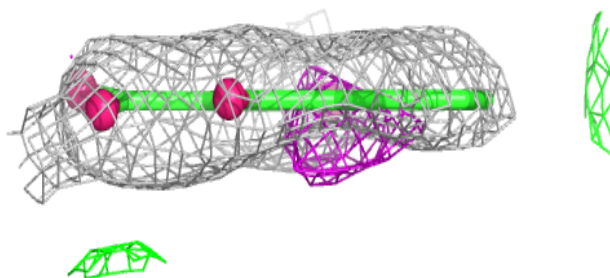
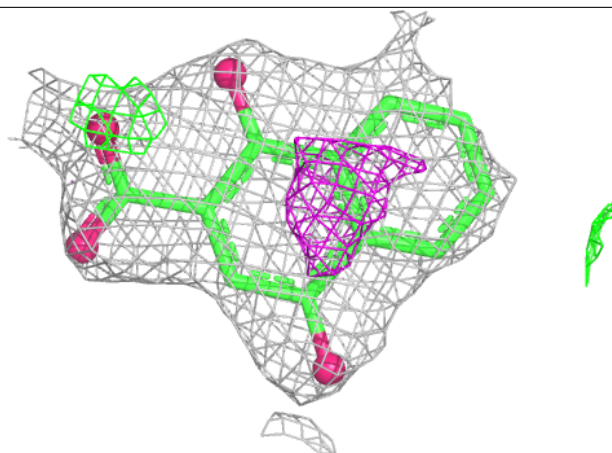
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMT	D	605	3/3	0.68	0.20	73,73,77,82	0
2	FMT	B	602	3/3	0.74	0.15	73,73,74,79	0
2	FMT	D	604	3/3	0.78	0.16	63,63,64,66	0
2	FMT	B	601	3/3	0.81	0.20	65,65,72,75	0
2	FMT	C	603	3/3	0.81	0.17	77,77,77,84	0
4	DNA	C	602	15/15	0.83	0.15	63,70,76,77	0
3	TPP	C	601	26/26	0.88	0.13	69,81,96,99	0
2	FMT	D	603	3/3	0.89	0.13	43,43,51,66	0
4	DNA	D	602	15/15	0.93	0.08	38,43,47,47	0
5	MG	C	604	1/1	0.95	0.10	84,84,84,84	0
2	FMT	A	601	3/3	0.96	0.10	38,38,46,59	0
3	TPP	D	601	26/26	0.98	0.05	31,37,40,45	0
6	CL	B	603	1/1	0.99	0.03	44,44,44,44	0
5	MG	D	606	1/1	1.00	0.02	34,34,34,34	0

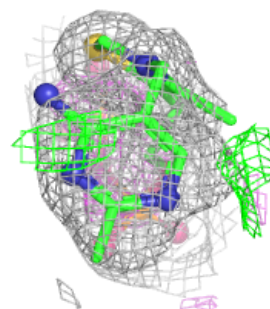
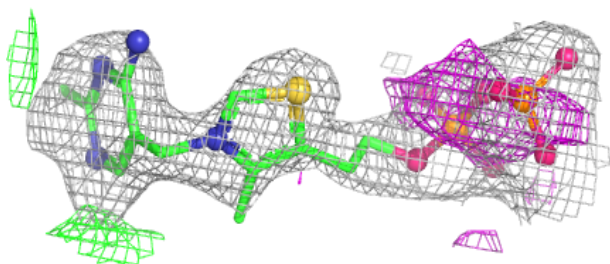
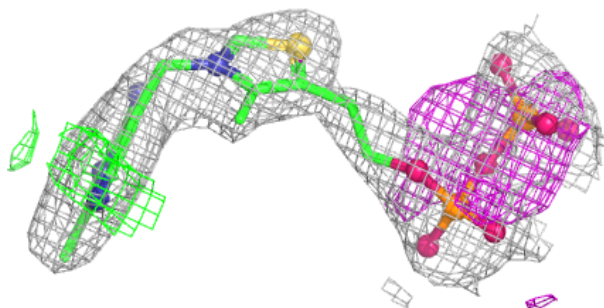
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DNA 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)

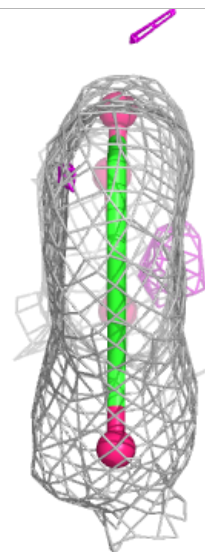
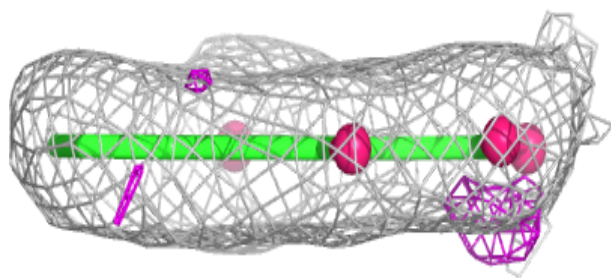
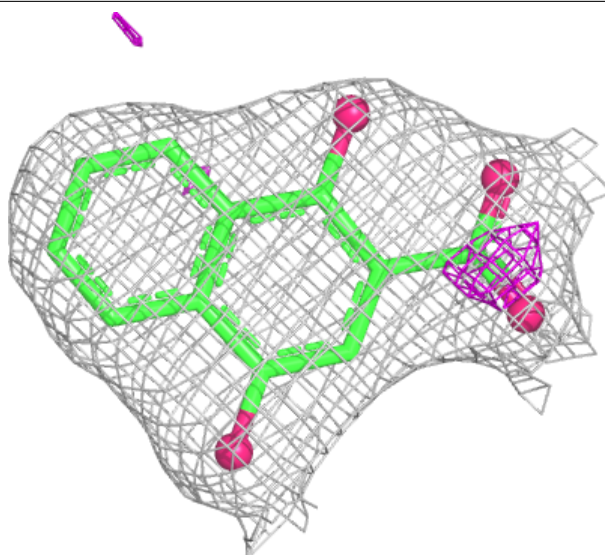
**Electron density around TPP C 601:**

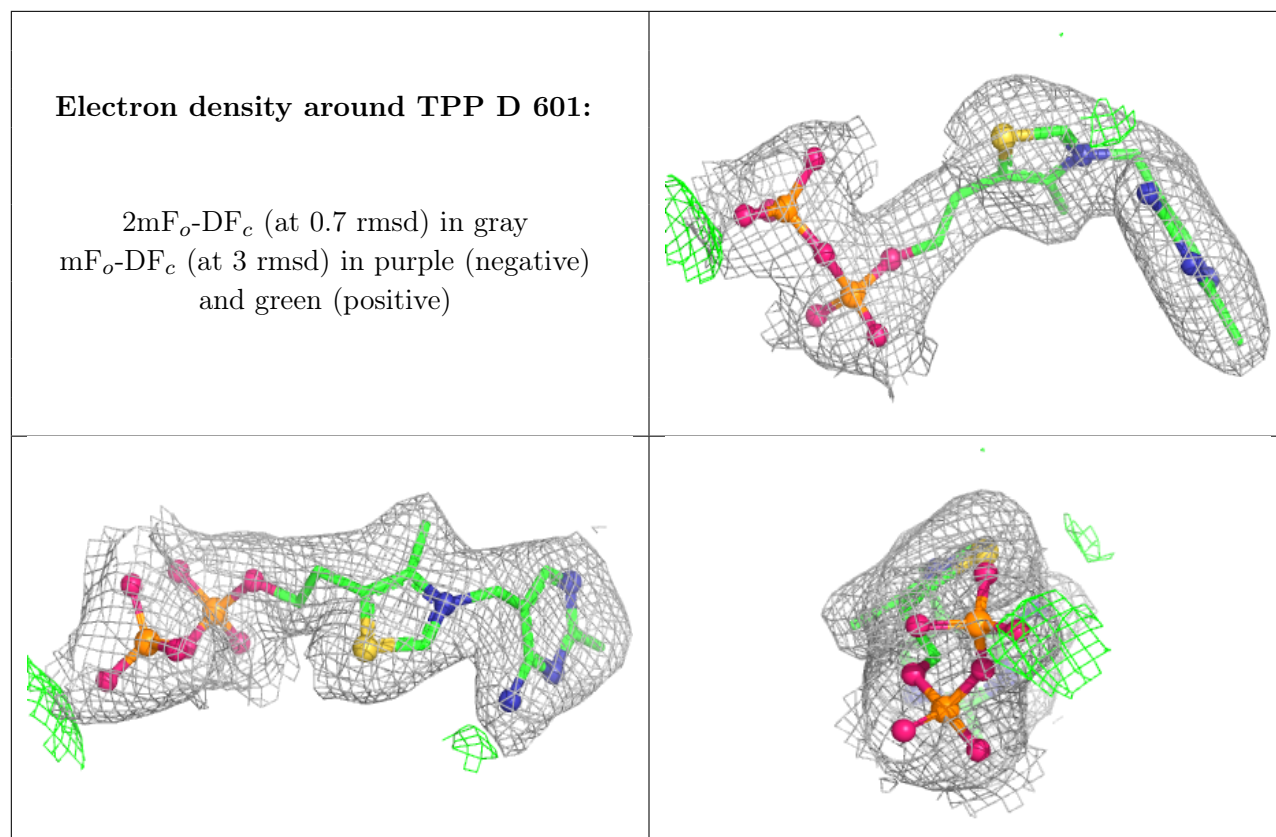
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DNA D 602:

$2mF_o-DF_c$ (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.