WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Apr 9, 2025 – 06:09 AM EDT

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)

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

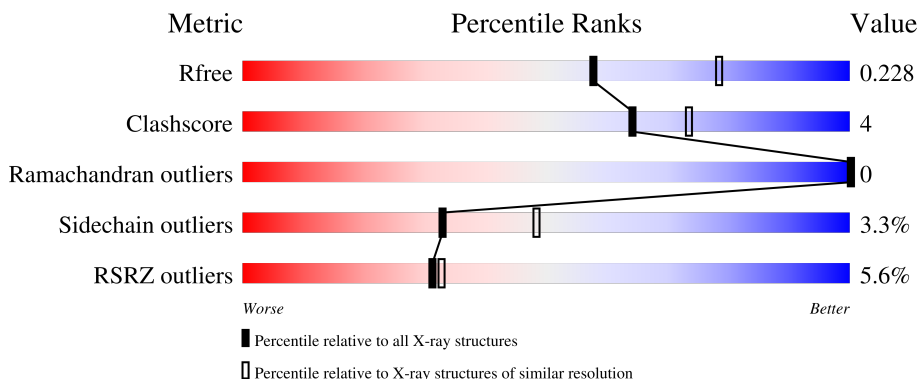|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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	Percentile Ranks	Value
Rfree		0.228
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		3.3%
RSRZ outliers		5.6%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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 <=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	4% / 84% / 10% · 6%
1	B	574	7% / 82% / 10% 8%
1	C	574	6% / 80% / 10% 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).
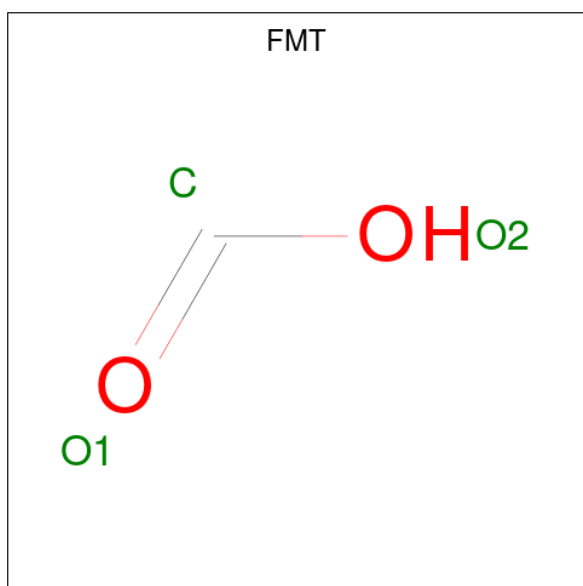
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 3	C 1	O 2	0	0
2	D	1	Total 3	C 1	O 2	0	0
2	D	1	Total 3	C 1	O 2	0	0
2	D	1	Total 3	C 1	O 2	0	0
2	B	1	Total 3	C 1	O 2	0	0
2	B	1	Total 3	C 1	O 2	0	0
2	C	1	Total 3	C 1	O 2	0	0

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

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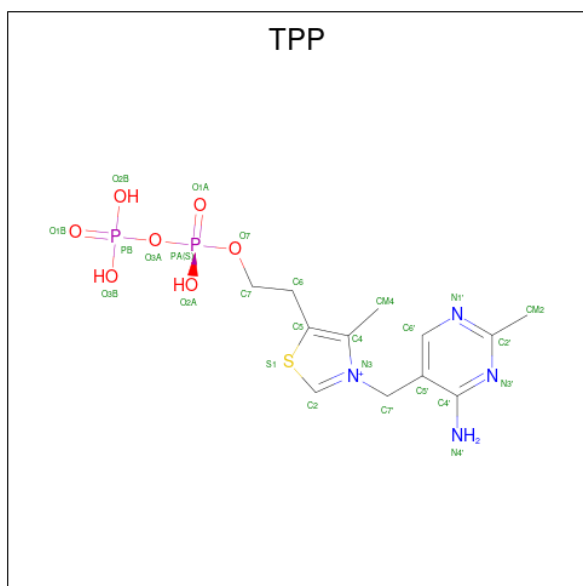
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- 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).

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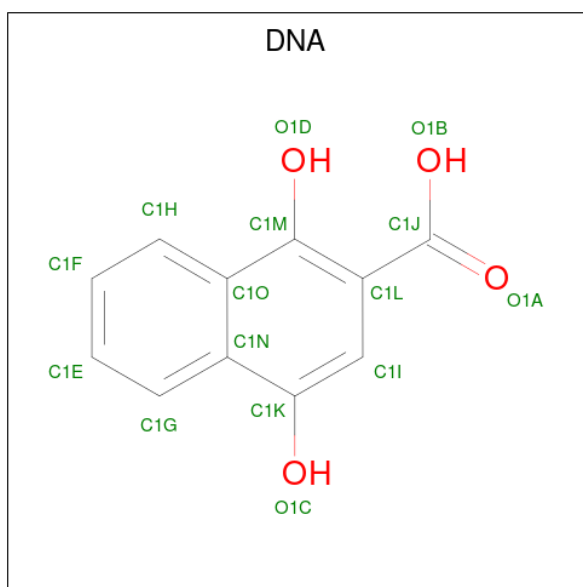
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 15	C 11	O 4	0	0
4	C	1	Total 15	C 11	O 4	0	0

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

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

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

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

• Molecule 7 is water.

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

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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

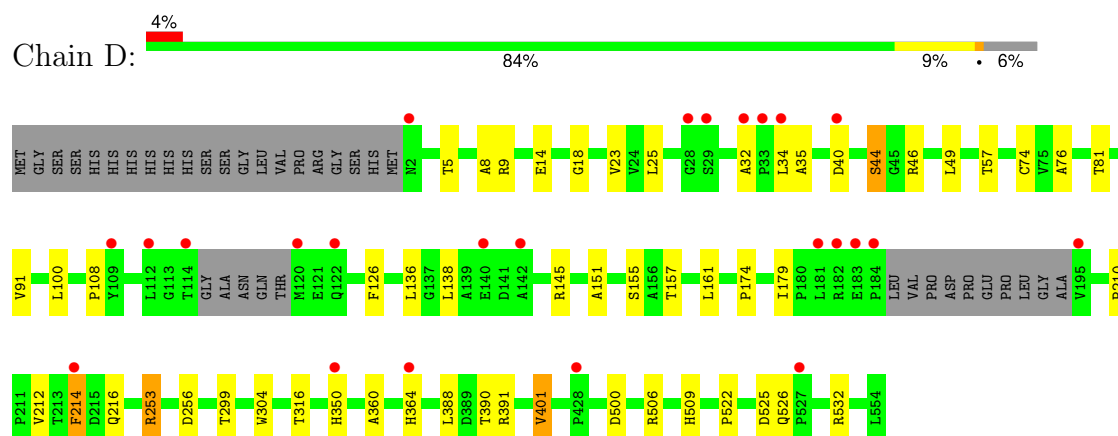# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
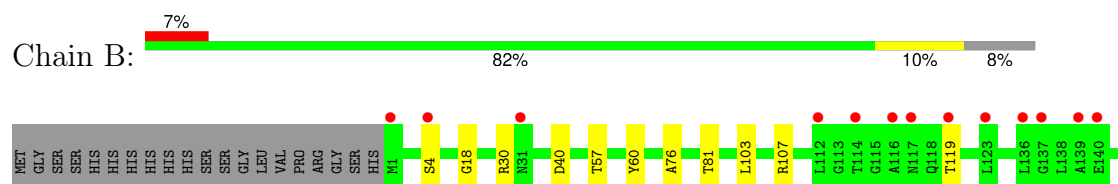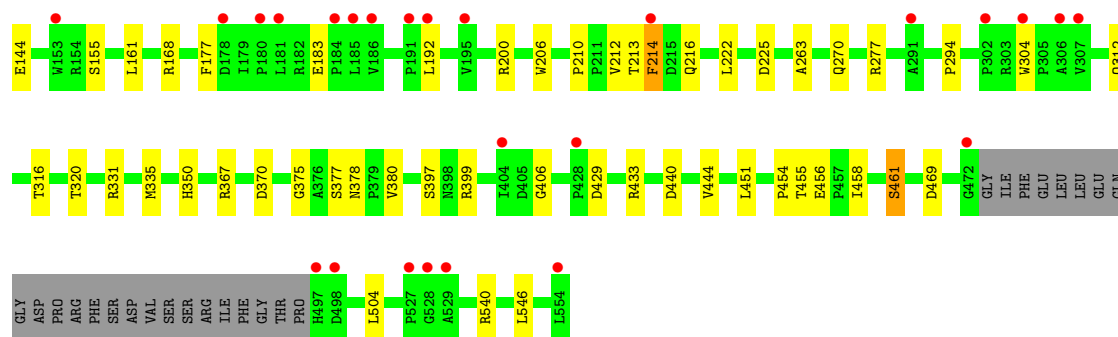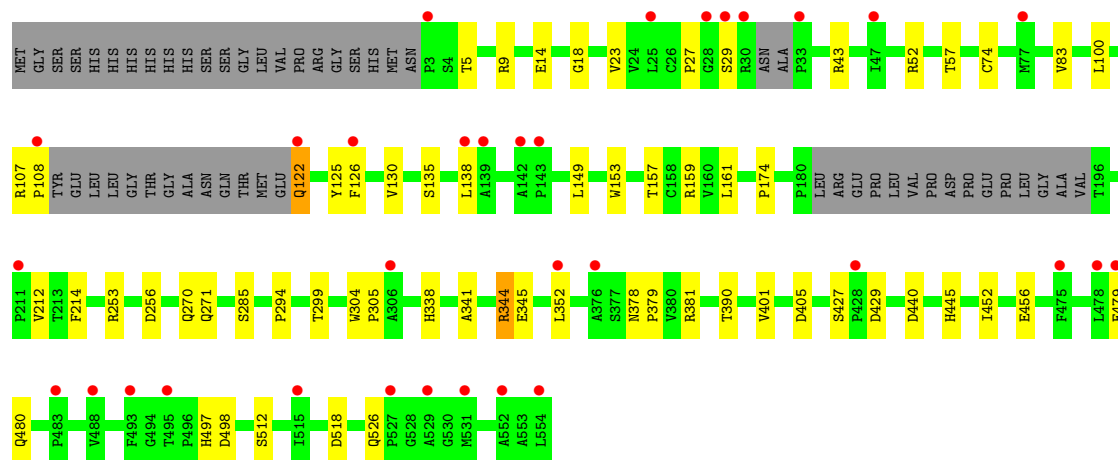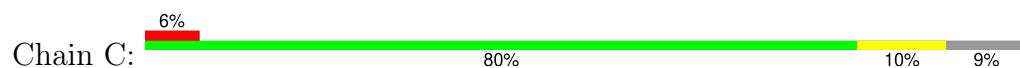
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

- 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

E144 W153 R154 S155 L161 R168 F177 D178 I179 P180 L181 R182 E183 P184 L185 V186 P191 L192 V195 R200 W206 P210 P211 V212 T213 F214 D215 Q216 L222 D225 A263 Q270 R277 A291 P294 P302 R303 W304 P305 A306 V307 Q312

T316 T320 R331 M335 H350 R367 D370 G375 A376 S377 N378 P379 V380 S397 N398 R399 I404 D405 G406 P428 D429 R433 D440 V444 L451 P454 T455 E456 P457 I458 S461 D469 G472 GLY ILE PHE GLU LEU LEU GLU GLN

GLY ASP PRO ARG PHE SER ASP VAL SER SER ARG SER ARG ILE PHE GLY THR PRO H497 D498 L504 P527 G528 A529 R540 L546 L554

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

Chain C:

6%
80%
10%
9%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ASN P3 S4 T5 R9 E14 G18 V23 V24 L25 C26 P27 G28 S29 R30 ASN ALA P33 R43 I47 R52 T57 C74 M77 V83 L100

R107 P108 TYR GLU LEU LEU GLY THR GLY ALA ASN GLN THR MET GLU Q122 Y125 F126 V130 S135 L138 A139 A142 P143 L149 W153 T157 C158 R159 V160 L161 P174 P180 LEU ARG GLU PRO LEU VAL PRO ASP PRO GLU PRO LEU GLY ALA VAL T196

P211 V212 T213 F214 R253 D256 Q270 Q271 S285 P294 T299 W304 P305 A306 H338 A341 R344 E345 L352 A376 S377 N378 P379 V380 R381 T390 V401 D405 S427 P428 D429 D440 H445 I452 E456 F475 L478 E479

Q480 P483 V488 F493 G494 T495 P496 H497 D498 S512 I515 D518 Q526 P527 G528 A529 G530 M531 A552 A553 L554

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	5812 reflections (5.08%)	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]	$< |L| > = 0.50, < L^2 > = 0.33$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FMT, DNA, TPP, CL

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	0.27	0/4069	0.54	0/5578
1	B	0.27	0/3968	0.54	0/5439
1	C	0.27	0/3909	0.53	0/5351
1	D	0.27	0/4069	0.55	0/5573
All	All	0.27	0/16015	0.54	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 ⓘ

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	35	0
1	B	3886	0	3923	36	0
1	C	3826	0	3849	35	0
1	D	3978	0	3997	35	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	1	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	1	0
All	All	16234	0	15825	121	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 (121) 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: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:B:183:GLU:H	1:B:183:GLU:CD	2.02	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
1:C:405:ASP:HB3	1:C:445:HIS:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:470:ASN:CG	1:A:496:PRO:HB3	2.36	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: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: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:D:304:TRP:C	4:D:602:DNA:H1H	2.39	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
1:A:168:ARG:HH22	1:C:299:THR:HG1	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:144:GLU:H	1:A:144:GLU:CD	2.16	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:D:25:LEU:CD1	1:D:49:LEU:HD22	2.51	0.40
1:D:14:GLU:HB3	1:D:157:THR:HG21	2.03	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	540/574 (94%)	526 (97%)	14 (3%)	0	100	100
1	B	527/574 (92%)	516 (98%)	11 (2%)	0	100	100
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%)	405 (97%)	12 (3%)	37	54
1	B	406/444 (91%)	391 (96%)	15 (4%)	29	43
1	C	400/444 (90%)	383 (96%)	17 (4%)	25	36
1	D	416/444 (94%)	403 (97%)	13 (3%)	35	51
All	All	1639/1776 (92%)	1582 (96%)	57 (4%)	33	46

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	47	ILE
1	A	57	THR
1	A	77	MET
1	A	147	SER
1	A	155	SER
1	A	230	SER
1	A	304	TRP
1	A	307	VAL
1	A	311	SER
1	A	317	ARG
1	A	517	VAL
1	D	40	ASP
1	D	44	SER
1	D	57	THR
1	D	126	PHE
1	D	214[A]	PHE
1	D	214[B]	PHE
1	D	253	ARG
1	D	350[A]	HIS
1	D	350[B]	HIS
1	D	391	ARG
1	D	401	VAL
1	D	525	ASP

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Mol	Chain	Res	Type
1	D	532	ARG
1	B	4	SER
1	B	30	ARG
1	B	40	ASP
1	B	57	THR
1	B	155	SER
1	B	177	PHE
1	B	192	LEU
1	B	213	THR
1	B	214[A]	PHE
1	B	214[B]	PHE
1	B	277	ARG
1	B	304	TRP
1	B	429	ASP
1	B	455	THR
1	B	461	SER
1	C	29	SER
1	C	43	ARG
1	C	57	THR
1	C	107	ARG
1	C	122	GLN
1	C	125	TYR
1	C	135	SER
1	C	256	ASP
1	C	271	GLN
1	C	285	SER
1	C	338	HIS
1	C	344	ARG
1	C	352	LEU
1	C	480	GLN
1	C	512	SER
1	C	518	ASP
1	C	526	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	HIS
1	C	7	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	604	-	2,2,2	0.74	0	1,1,1	0.20	0
2	FMT	B	601	-	2,2,2	0.73	0	1,1,1	0.23	0
2	FMT	B	602	-	2,2,2	0.73	0	1,1,1	0.23	0
2	FMT	D	603	-	2,2,2	0.78	0	1,1,1	0.30	0
3	TPP	D	601	5	23,27,27	0.49	0	30,40,40	0.59	1 (3%)
2	FMT	C	603	-	2,2,2	0.74	0	1,1,1	0.25	0
3	TPP	C	601	5	23,27,27	0.62	1 (4%)	30,40,40	0.57	1 (3%)
4	DNA	C	602	-	16,16,16	2.38	4 (25%)	23,23,23	1.30	4 (17%)
2	FMT	A	601	-	2,2,2	0.73	0	1,1,1	0.23	0
4	DNA	D	602	-	16,16,16	2.36	4 (25%)	23,23,23	1.11	1 (4%)
2	FMT	D	605	-	2,2,2	0.73	0	1,1,1	0.25	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
4	DNA	D	602	-	-	0/4/4/4	0/2/2/2
3	TPP	C	601	5	-	<mark>3/16/17/17</mark>	0/2/2/2
3	TPP	D	601	5	-	<mark>2/16/17/17</mark>	0/2/2/2
4	DNA	C	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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
3	D	601	TPP	C5-C4-N3	2.09	111.75	107.57
3	C	601	TPP	C5-C4-N3	2.04	111.65	107.57

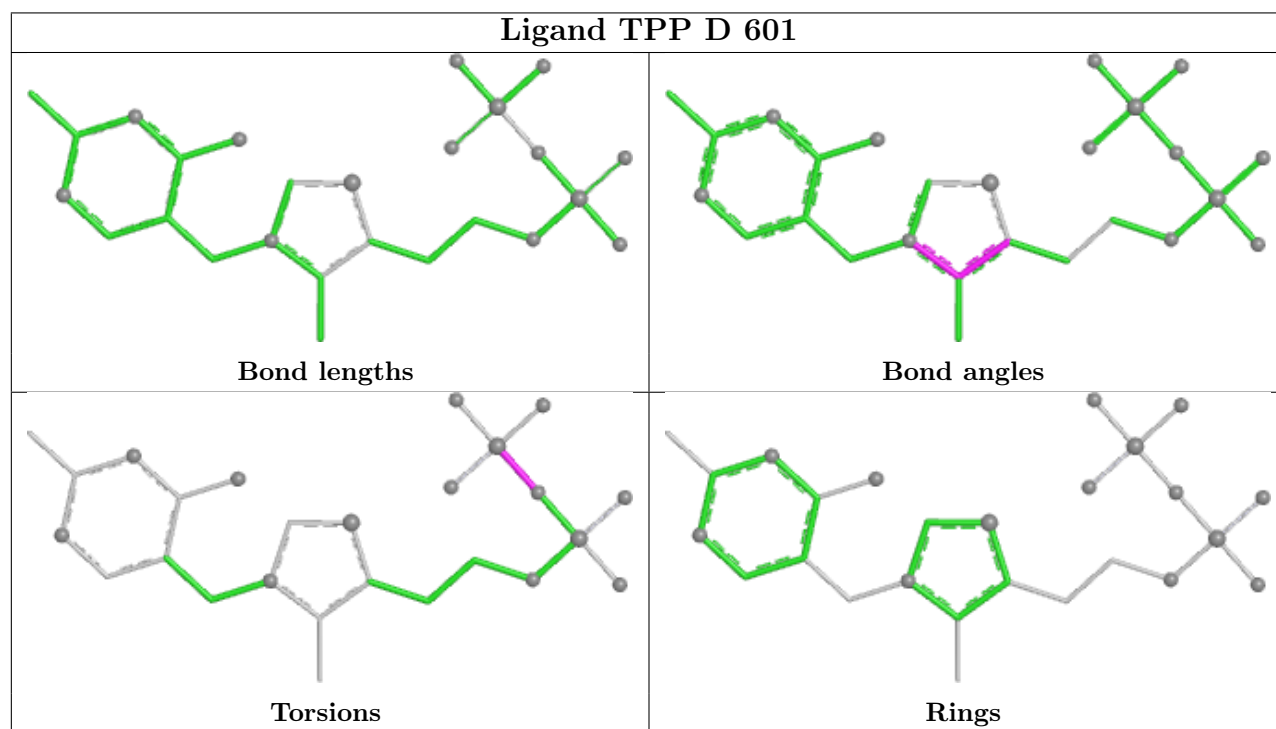There are no chirality outliers.

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 4 short contacts:

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

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

Ligand TPP D 601

Ligand TPP C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand DNA C 602

Bond lengths

Bond angles

Torsions

Rings

Ligand DNA D 602
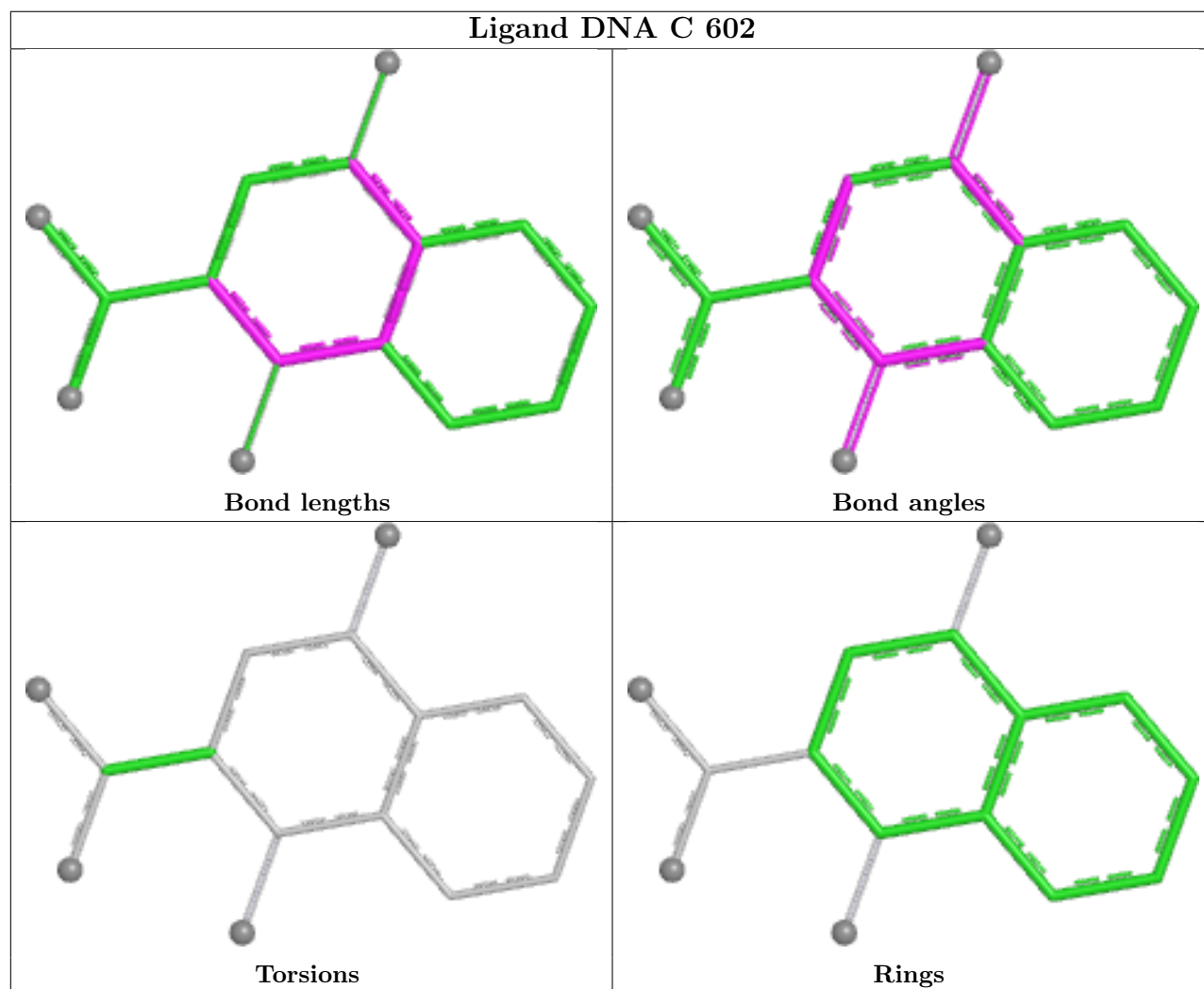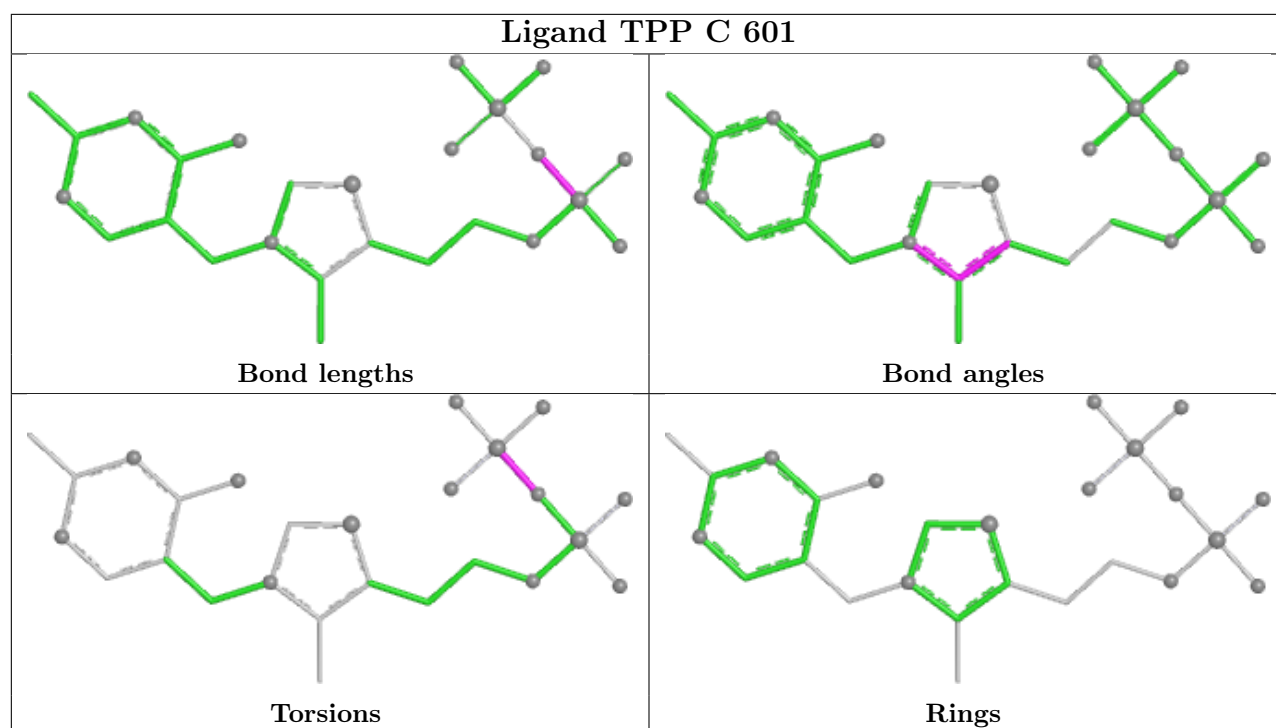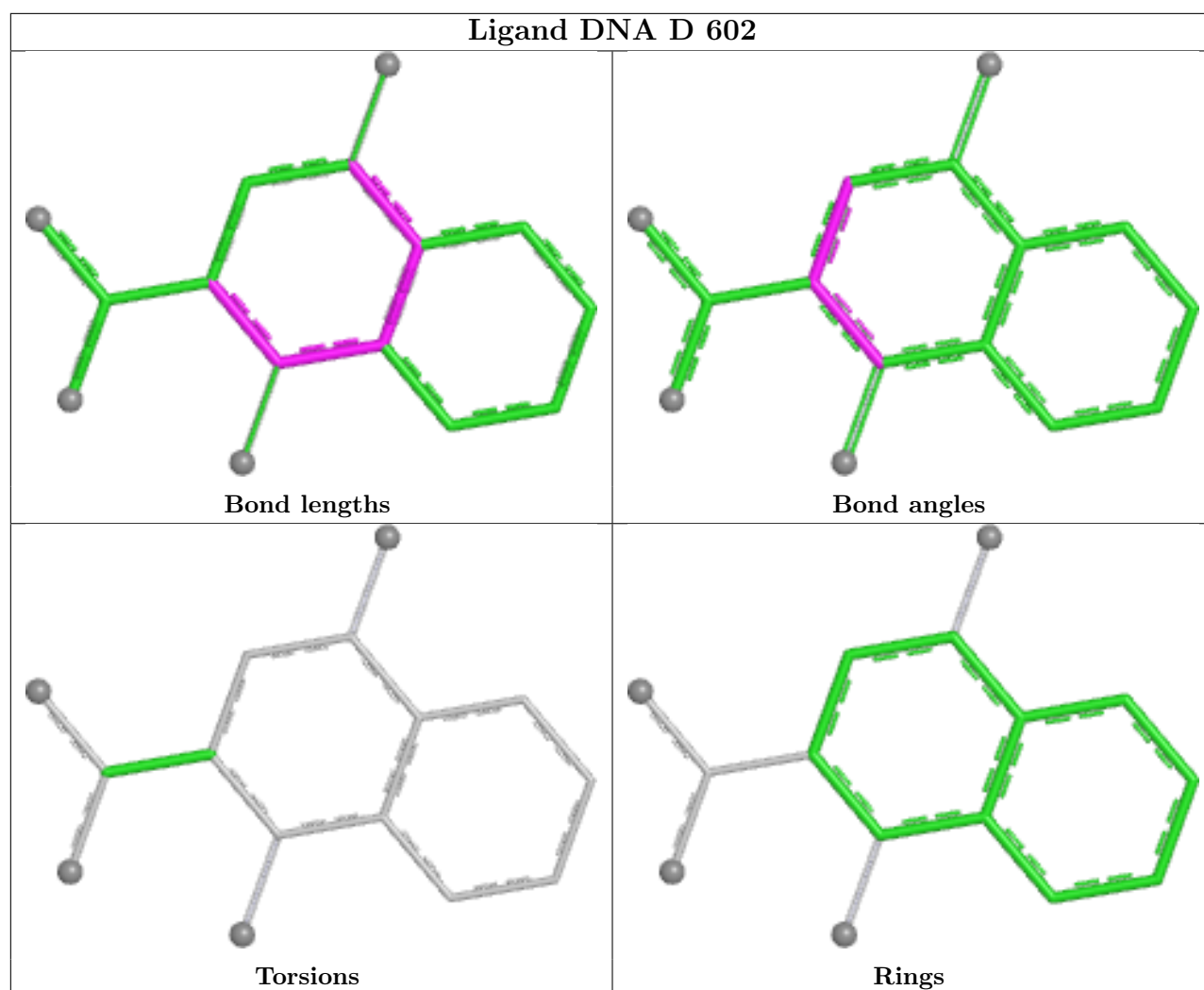
5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	540/574 (94%)	0.08	25 (4%)	38	39	20, 49, 90, 122	4 (0%)
1	B	530/574 (92%)	0.39	38 (7%)	23	24	25, 55, 92, 129	1 (0%)
1	C	522/574 (90%)	0.51	33 (6%)	27	29	26, 64, 101, 130	2 (0%)
1	D	538/574 (93%)	0.07	24 (4%)	39	40	24, 47, 89, 129	5 (0%)
All	All	2130/2296 (92%)	0.26	120 (5%)	31	33	20, 54, 95, 130	12 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214[A]	PHE	4.7
1	C	108	PRO	4.6
1	C	211	PRO	4.4
1	B	307	VAL	4.3
1	A	192	LEU	4.3
1	D	195	VAL	4.3
1	D	34	LEU	4.2
1	B	529	ALA	4.2
1	D	184	PRO	3.9
1	B	472	GLY	3.9
1	D	29	SER	3.9
1	A	487	ASP	3.9
1	A	471	GLY	3.8
1	C	3	PRO	3.7
1	B	304	TRP	3.6
1	A	529	ALA	3.6
1	B	192	LEU	3.5
1	A	494	GLY	3.5
1	C	495	THR	3.4
1	C	527	PRO	3.4
1	A	404	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	4	SER	3.3
1	D	120	MET	3.3
1	B	527	PRO	3.3
1	B	195	VAL	3.2
1	A	291	ALA	3.2
1	D	142	ALA	3.2
1	D	428	PRO	3.2
1	B	181	LEU	3.2
1	D	33	PRO	3.2
1	D	32	ALA	3.1
1	B	123	LEU	3.1
1	A	42	ASP	3.1
1	C	529	ALA	3.0
1	A	495	THR	3.0
1	B	116	ALA	3.0
1	D	112	LEU	3.0
1	A	191	PRO	3.0
1	B	306	ALA	3.0
1	C	306	ALA	3.0
1	C	475	PHE	2.9
1	B	31	ASN	2.9
1	C	30	ARG	2.9
1	B	117	ASN	2.9
1	C	488	VAL	2.9
1	B	185	LEU	2.9
1	C	47	ILE	2.9
1	D	140	GLU	2.8
1	C	478	LEU	2.8
1	A	364[A]	HIS	2.8
1	C	122	GLN	2.8
1	B	497	HIS	2.8
1	A	493	PHE	2.8
1	A	528	GLY	2.7
1	D	182	ARG	2.7
1	C	143	PRO	2.7
1	D	114	THR	2.7
1	A	428	PRO	2.7
1	C	376	ALA	2.7
1	C	515	ILE	2.6
1	B	180	PRO	2.6
1	D	40	ASP	2.6
1	B	191	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	126	PHE	2.6
1	A	214[A]	PHE	2.5
1	D	109	TYR	2.5
1	C	483	PRO	2.5
1	A	492	ILE	2.5
1	B	140	GLU	2.5
1	C	77	MET	2.5
1	B	528	GLY	2.5
1	B	291	ALA	2.5
1	B	112	LEU	2.5
1	B	428	PRO	2.5
1	C	29	SER	2.4
1	A	0	HIS	2.4
1	A	195	VAL	2.4
1	D	364[A]	HIS	2.4
1	D	122	GLN	2.4
1	D	181	LEU	2.4
1	D	28	GLY	2.4
1	B	137	GLY	2.3
1	B	136	LEU	2.3
1	B	186	VAL	2.3
1	A	527	PRO	2.3
1	B	184	PRO	2.3
1	C	142	ALA	2.3
1	B	302	PRO	2.3
1	C	493	PHE	2.3
1	B	498	ASP	2.3
1	C	33	PRO	2.3
1	B	1	MET	2.2
1	A	304	TRP	2.2
1	A	309	GLY	2.2
1	D	183	GLU	2.2
1	A	211	PRO	2.2
1	A	488	VAL	2.2
1	C	531	MET	2.2
1	D	214[A]	PHE	2.2
1	B	178	ASP	2.2
1	B	153	TRP	2.1
1	C	139	ALA	2.1
1	C	479	GLU	2.1
1	B	554	LEU	2.1
1	D	527	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	428	PRO	2.1
1	A	307	VAL	2.1
1	B	139	ALA	2.1
1	D	2	ASN	2.1
1	C	25	LEU	2.1
1	A	376	ALA	2.1
1	B	114	THR	2.1
1	B	119	THR	2.1
1	C	28	GLY	2.0
1	D	350[A]	HIS	2.0
1	B	404	ILE	2.0
1	C	138	LEU	2.0
1	C	554	LEU	2.0
1	C	552	ALA	2.0
1	C	352	LEU	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 monosaccharides 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($\mathring{A}^2$)	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.
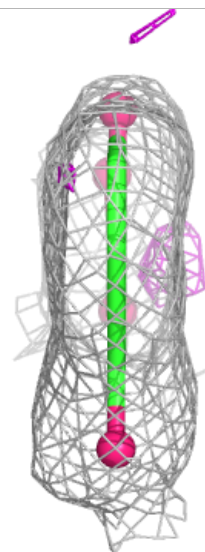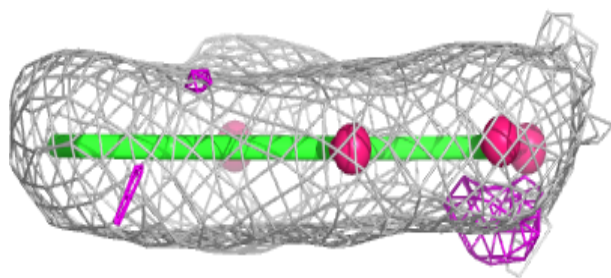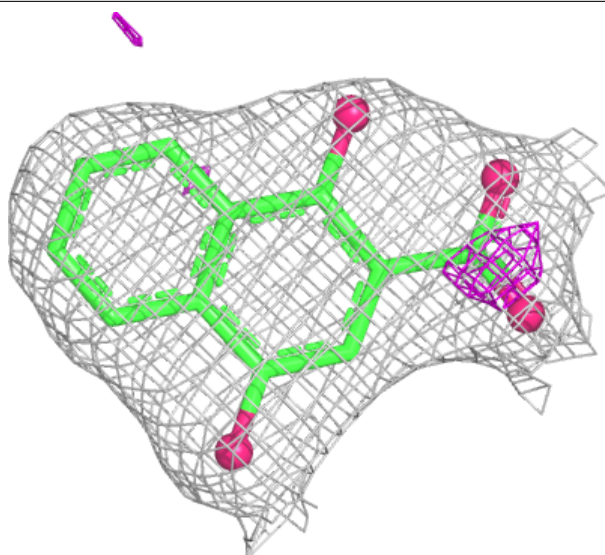

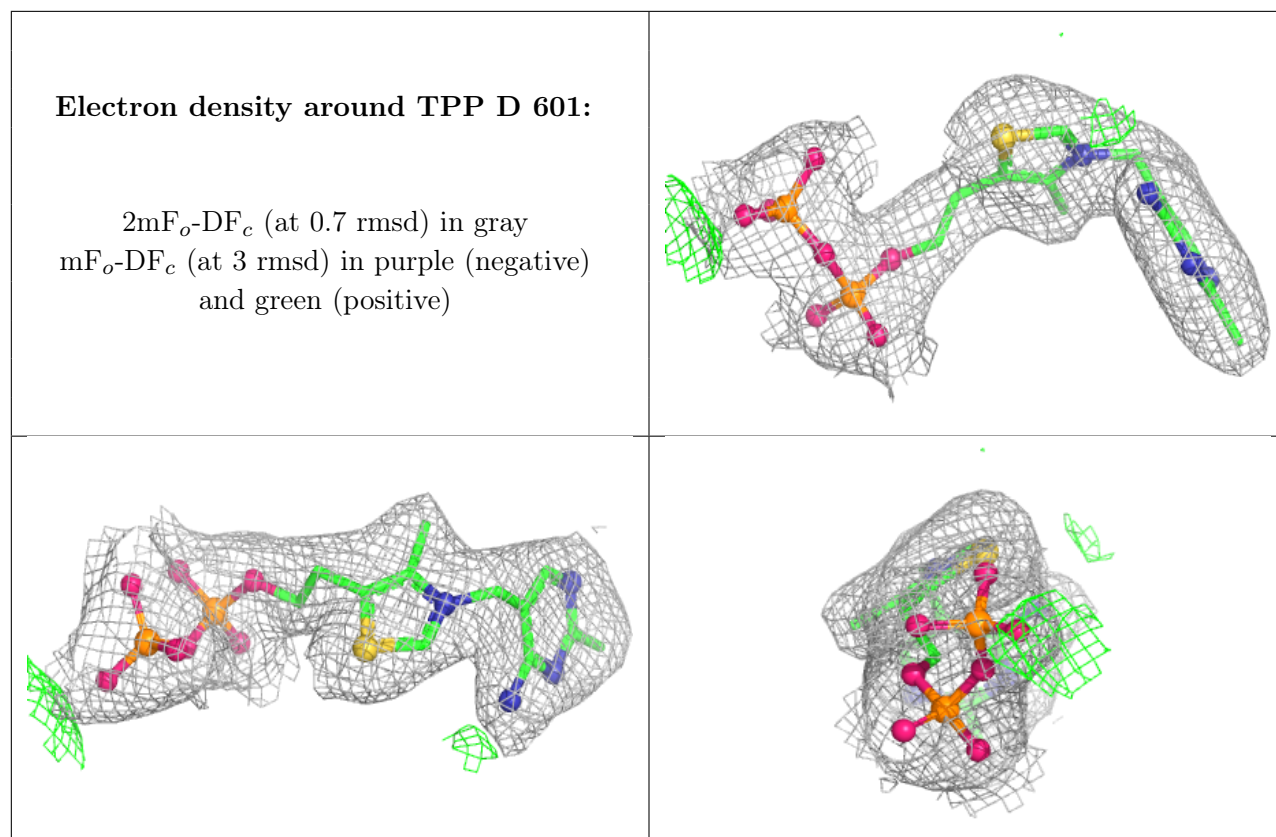**Electron density around DNA C 602:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
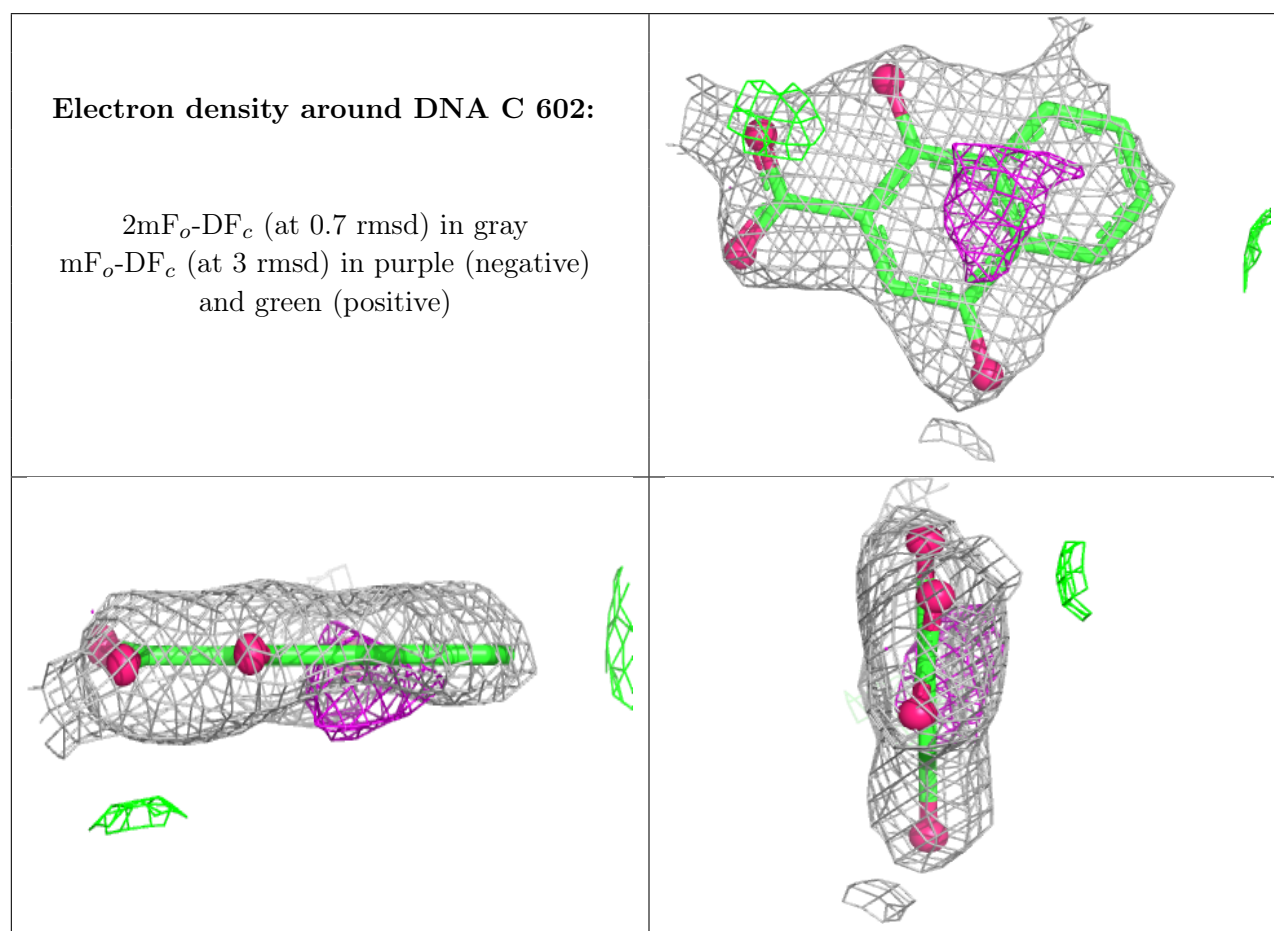
Electron density around TPP C 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
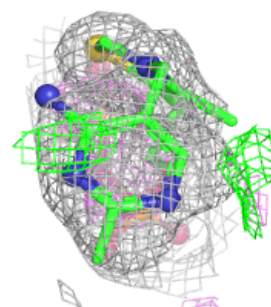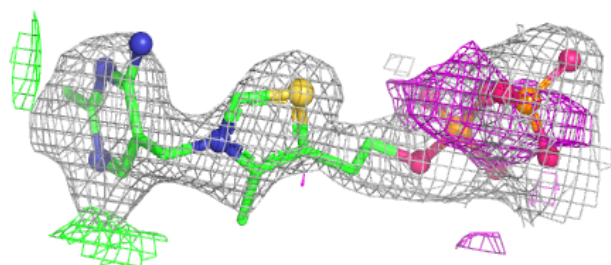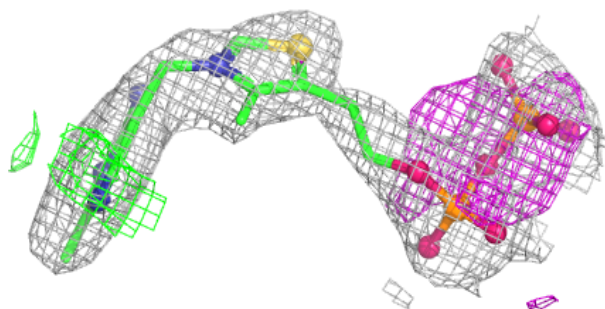
Electron density around DNA D 602:

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

Electron density around TPP D 601:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.