



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:23 AM UTC

PDB ID : 9DQI / pdb_00009dqi
Title : D306N Mutant of M.tuberculosis MenD (SEPHCHC Synthase)
Authors : Johnston, J.M.; Ho, N.A.T.; Given, F.M.; Bulloch, E.M.M.; Allison, T.M.; Jiao, W.
Deposited on : 2024-09-24
Resolution : 2.39 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

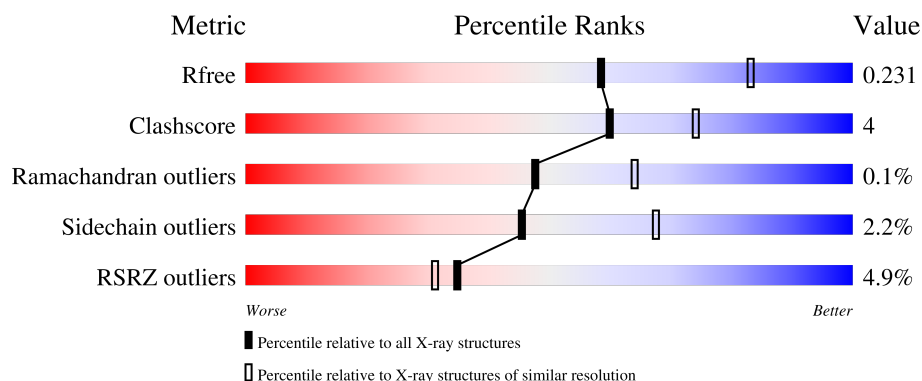
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	4% 83% 10% 6%
1	B	574	6% 80% 12% 7%
1	C	574	5% 82% 10% 9%
1	D	574	3% 86% 7% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15965 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	538	Total	C	N	O	S	0	3	0
			3960	2474	736	739	11			
1	D	535	Total	C	N	O	S	0	6	0
			3955	2470	736	739	10			
1	B	532	Total	C	N	O	S	0	2	0
			3913	2439	731	732	11			
1	C	525	Total	C	N	O	S	0	3	0
			3845	2404	710	722	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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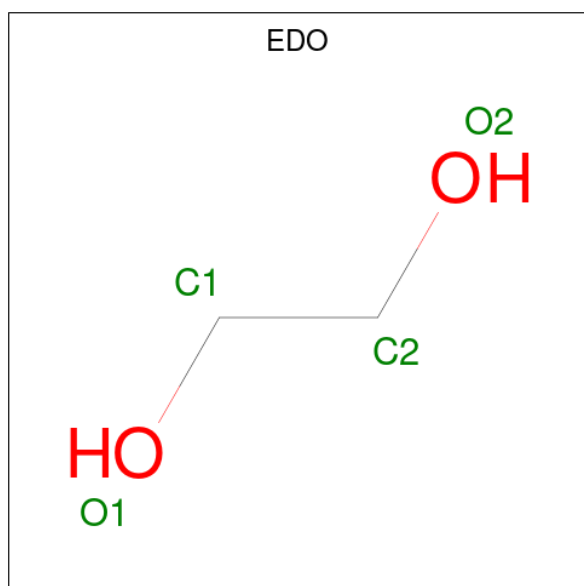
Chain	Residue	Modelled	Actual	Comment	Reference
A	306	ASN	ASP	engineered mutation	UNP P9WK11
D	-19	MET	-	initiating methionine	UNP P9WK11
D	-18	GLY	-	expression tag	UNP P9WK11
D	-17	SER	-	expression tag	UNP P9WK11
D	-16	SER	-	expression tag	UNP P9WK11
D	-15	HIS	-	expression tag	UNP P9WK11
D	-14	HIS	-	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	ASN	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	ASN	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	ASN	ASP	engineered mutation	UNP P9WK11

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

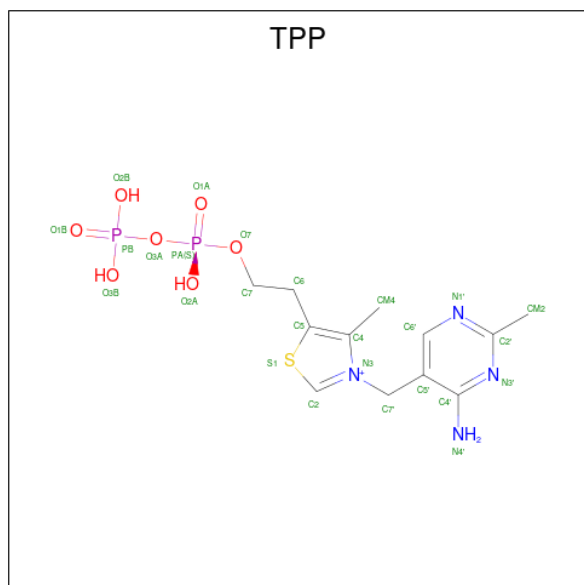


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

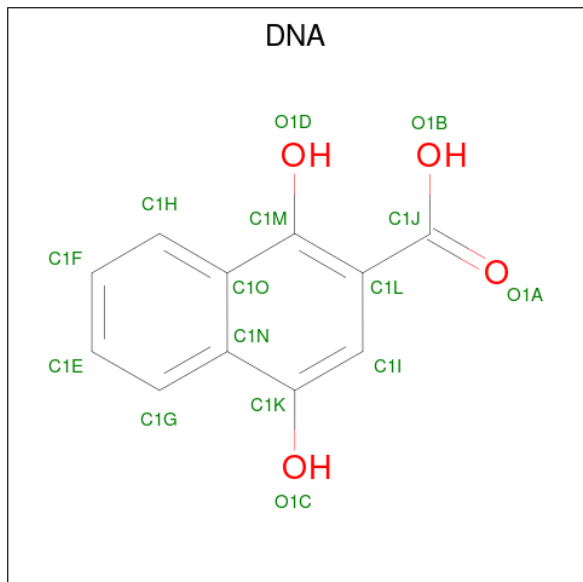
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S) (labeled as "Ligand of Interest" by depositor).



- Molecule 5 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
5	D	1	Total	C	O	0	0
			15	11	4		
5	C	1	Total	C	O	0	0
			15	11	4		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

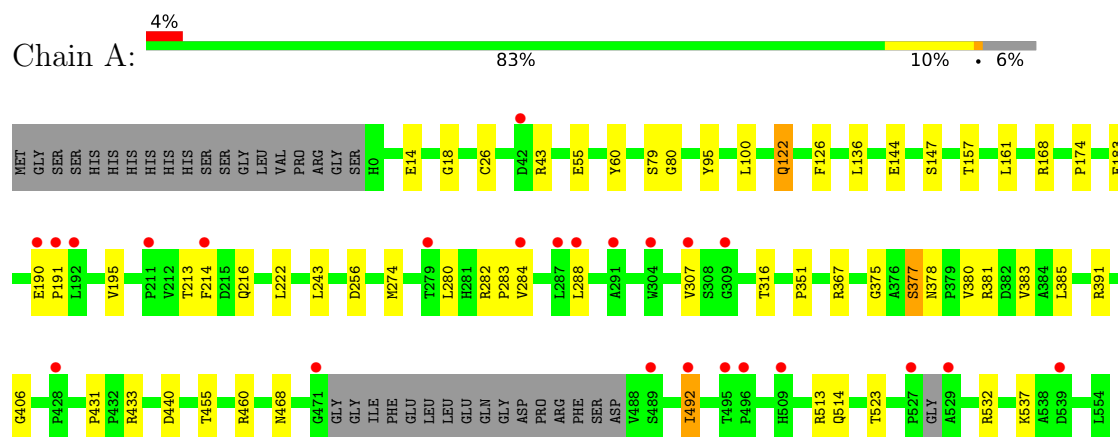
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	53	Total	O	0	0
			53	53		
7	D	91	Total	O	0	0
			91	91		
7	B	25	Total	O	0	0
			25	25		
7	C	18	Total	O	0	0
			18	18		

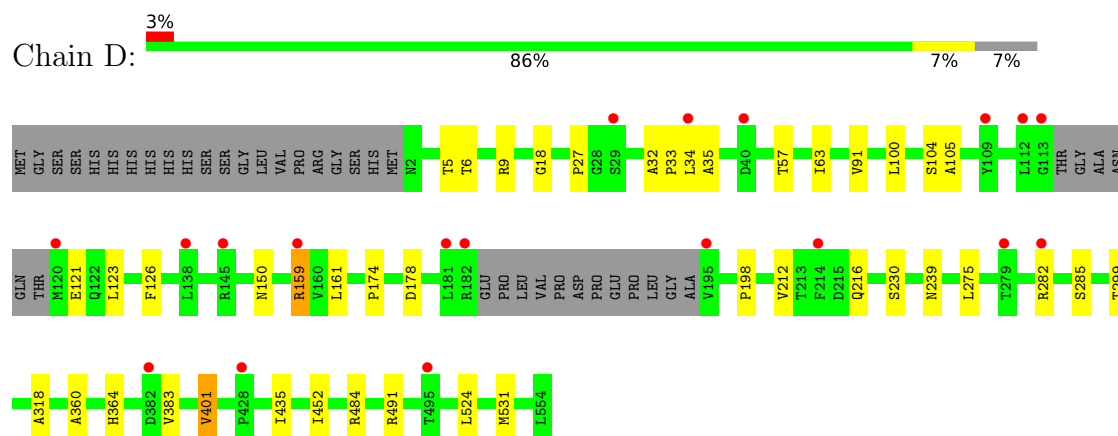
3 Residue-property plots [i](#)

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

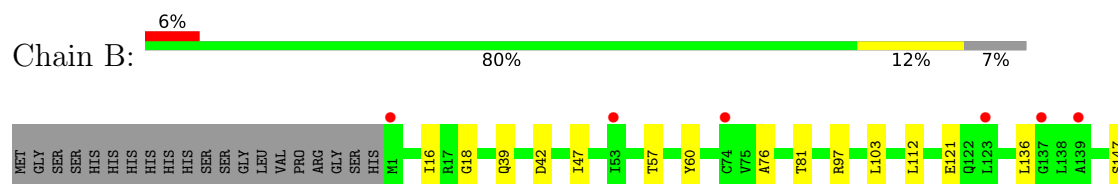
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

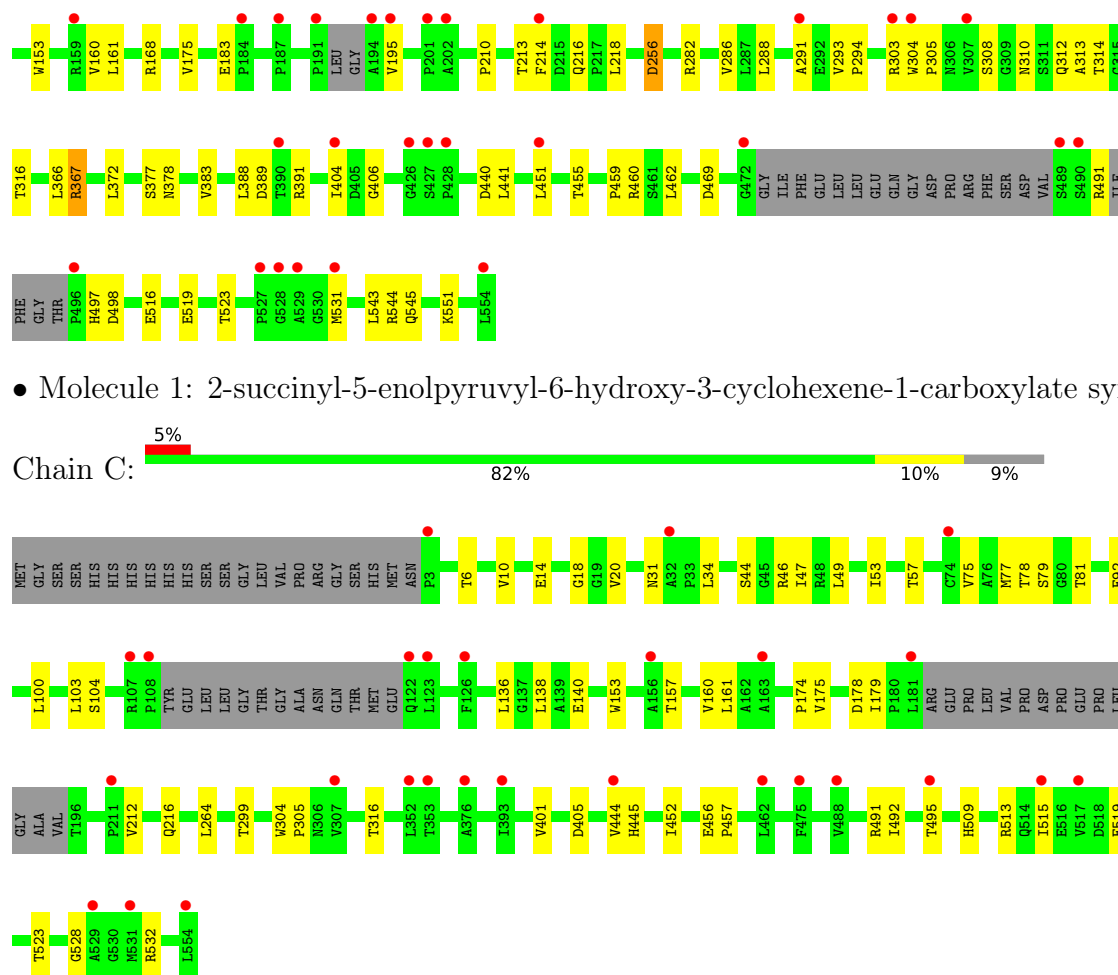


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.56Å 139.98Å 183.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 2.39 49.13 – 2.39	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.13-2.39) 100.0 (49.13-2.39)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.195 , 0.231 0.195 , 0.231	Depositor DCC
R_{free} test set	5247 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15965	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: MG, EDO, TPP, CL, DNA

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	0.15	0/4045	0.33	0/5545
1	B	0.17	0/3994	0.33	0/5470
1	C	0.15	0/3932	0.31	0/5387
1	D	0.17	0/4043	0.34	0/5536
All	All	0.16	0/16014	0.33	0/21938

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	3960	0	3983	34	0
1	B	3913	0	3944	57	0
1	C	3845	0	3863	41	0
1	D	3955	0	3969	25	0
2	A	8	0	12	0	0
2	B	4	0	6	1	0
2	D	4	0	6	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	C	26	0	16	0	0
4	D	26	0	16	0	0
5	C	15	0	5	1	0
5	D	15	0	6	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	53	0	0	0	0
7	B	25	0	0	0	0
7	C	18	0	0	0	0
7	D	91	0	0	1	0
All	All	15965	0	15826	136	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 (136) 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:C:515:ILE:HB	1:C:519:GLU:HG3	1.64	0.78
1:D:32:ALA:HB3	1:D:35:ALA:HB2	1.70	0.73
1:B:491:ARG:NH2	1:C:456:GLU:HA	2.07	0.70
1:D:159[A]:ARG:NH1	7:D:701:HOH:O	2.22	0.69
1:C:452:ILE:HG22	1:C:456:GLU:HB2	1.73	0.69
1:A:431:PRO:HG3	1:A:460:ARG:HE	1.58	0.67
1:A:216:GLN:HB3	1:A:316:THR:HG23	1.80	0.64
1:C:103:LEU:HD22	1:C:179:ILE:HD11	1.78	0.63
1:A:455:THR:HG21	1:D:491:ARG:HG2	1.81	0.62
1:B:460:ARG:HH11	1:B:460:ARG:HG2	1.64	0.62
1:C:216:GLN:HB3	1:C:316:THR:HG23	1.82	0.61
1:C:31:ASN:HB2	1:C:78:THR:HG22	1.82	0.61
1:A:168:ARG:NH1	1:C:216:GLN:OE1	2.34	0.60
1:D:212:VAL:HG21	1:B:214[A]:PHE:CD1	2.36	0.60
1:A:222:LEU:HD22	1:A:243:LEU:HD11	1.82	0.60
1:A:513:ARG:NH2	1:A:532:ARG:HH11	1.99	0.59
1:B:491:ARG:HH22	1:C:456:GLU:HA	1.66	0.59
1:B:440:ASP:HB2	1:B:497:HIS:HE1	1.67	0.59
1:B:256:ASP:OD2	1:B:391:ARG:NH1	2.35	0.59
1:D:33:PRO:HB3	1:D:105:ALA:HB2	1.86	0.58
1:B:404:ILE:CD1	1:B:441:LEU:HD12	2.33	0.58
1:D:91:VAL:HG12	1:D:401:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HD11	1:A:381:ARG:HG2	1.85	0.58
1:B:441:LEU:HD21	1:C:53:ILE:HD13	1.84	0.58
1:D:216:GLN:HG2	1:B:210:PRO:HG2	1.85	0.57
1:A:214[A]:PHE:CE1	1:C:212:VAL:HG21	2.40	0.57
1:C:136:LEU:HD12	1:C:179:ILE:HG23	1.86	0.57
1:B:42:ASP:OD2	1:C:491:ARG:NH1	2.38	0.56
1:A:377:SER:OG	1:A:378:ASN:N	2.38	0.56
1:C:34:LEU:HD21	1:C:103:LEU:HD13	1.87	0.56
1:A:440:ASP:HB3	1:A:468:ASN:HA	1.86	0.56
1:B:183:GLU:H	1:B:183:GLU:CD	2.13	0.56
1:A:183:GLU:H	1:A:183:GLU:CD	2.14	0.55
1:B:404:ILE:HD12	1:B:441:LEU:HD12	1.88	0.55
1:A:492:ILE:HD11	1:D:27:PRO:HG3	1.88	0.54
1:D:104:SER:OG	1:D:178:ASP:OD1	2.26	0.54
1:B:440:ASP:HB2	1:B:497:HIS:CE1	2.43	0.52
1:B:282:ARG:O	1:B:286:VAL:HG23	2.09	0.52
1:B:377:SER:OG	1:B:378:ASN:N	2.43	0.52
1:A:274:MET:HE2	1:A:288:LEU:HD13	1.92	0.52
1:B:544:ARG:HG2	1:B:544:ARG:HH11	1.75	0.52
1:B:81:THR:HG23	1:C:401:VAL:HG11	1.91	0.51
1:B:404:ILE:HD11	1:B:441:LEU:CD1	2.41	0.51
1:B:76:ALA:HA	1:B:103:LEU:O	2.11	0.51
1:D:452:ILE:HD12	1:D:531:MET:HE1	1.93	0.51
1:C:18:GLY:HA3	1:C:161:LEU:HD13	1.93	0.51
1:B:498:ASP:OD2	1:C:509:HIS:NE2	2.44	0.51
1:D:299:THR:HG1	1:B:168:ARG:NH2	2.09	0.50
1:B:305:PRO:HD3	2:B:601:EDO:H22	1.93	0.50
1:A:126:PHE:HA	1:D:123:LEU:HD23	1.92	0.50
1:B:97:ARG:HD2	1:B:303:ARG:HD2	1.93	0.50
1:C:10:VAL:HG11	1:C:153:TRP:CE3	2.47	0.50
1:B:519:GLU:O	1:B:523:THR:OG1	2.23	0.50
1:B:516:GLU:N	1:B:519:GLU:OE2	2.45	0.50
1:C:495:THR:O	1:C:495:THR:OG1	2.26	0.50
1:D:18:GLY:HA3	1:D:161:LEU:HD13	1.94	0.50
1:B:497:HIS:H	1:B:497:HIS:CD2	2.29	0.50
1:B:291:ALA:O	1:B:310:ASN:ND2	2.44	0.49
1:A:144:GLU:OE1	1:A:144:GLU:N	2.28	0.49
1:D:5:THR:HG22	1:D:9:ARG:HE	1.77	0.49
1:A:168:ARG:NH2	1:C:299:THR:OG1	2.45	0.49
1:A:80:GLY:H	1:A:122:GLN:NE2	2.11	0.49
1:D:216:GLN:OE1	1:B:168:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:TRP:C	5:C:602:DNA:H1H	2.38	0.48
1:A:513:ARG:HH22	1:A:532:ARG:HH11	1.61	0.48
1:B:469:ASP:OD1	1:B:469:ASP:N	2.46	0.48
1:C:513:ARG:HH21	1:C:523:THR:HG23	1.78	0.48
1:B:218:LEU:HD11	1:B:313:ALA:HB1	1.96	0.47
1:C:6:THR:O	1:C:10:VAL:HG12	2.14	0.47
1:A:14:GLU:HB3	1:A:157:THR:HG21	1.96	0.47
1:D:100:LEU:O	1:D:174:PRO:HA	2.15	0.47
1:A:256:ASP:OD1	1:A:391:ARG:NH1	2.48	0.47
1:B:294:PRO:HB3	1:B:312:GLN:HG3	1.97	0.47
1:C:31:ASN:ND2	1:C:77:MET:O	2.47	0.47
1:C:104:SER:OG	1:C:178:ASP:OD1	2.32	0.47
1:D:150:ASN:ND2	1:D:198:PRO:O	2.45	0.47
1:C:100:LEU:O	1:C:174:PRO:HA	2.15	0.47
1:B:388:LEU:HD12	1:B:389:ASP:N	2.30	0.47
1:D:239:ASN:ND2	1:D:318:ALA:O	2.45	0.46
1:C:160:VAL:HG13	1:C:175:VAL:HG11	1.96	0.46
1:A:514:GLN:OE1	1:A:537:LYS:HD2	2.14	0.46
1:C:20:VAL:HG12	1:C:47:ILE:HD11	1.98	0.46
1:B:451:LEU:HD12	1:C:444:VAL:HG21	1.97	0.46
1:A:214[A]:PHE:CD1	1:C:212:VAL:HG21	2.51	0.46
1:C:10:VAL:HG11	1:C:153:TRP:HE3	1.79	0.46
1:B:491:ARG:HH22	1:C:457:PRO:HD3	1.81	0.45
1:B:459:PRO:HD2	1:B:531:MET:HE2	1.98	0.45
1:C:405:ASP:HB3	1:C:445:HIS:CE1	2.52	0.45
1:B:160:VAL:HG13	1:B:175:VAL:HG11	1.98	0.45
1:A:375:GLY:O	1:A:380:VAL:HG23	2.17	0.45
1:D:6:THR:HA	1:D:9:ARG:HD2	1.99	0.45
1:B:404:ILE:CD1	1:B:441:LEU:CD1	2.95	0.44
1:B:136:LEU:HD22	1:B:153:TRP:HD1	1.82	0.44
1:B:441:LEU:C	1:B:441:LEU:HD13	2.42	0.44
1:B:440:ASP:OD1	1:B:440:ASP:N	2.50	0.44
1:D:282[B]:ARG:HE	1:D:282[B]:ARG:HB3	1.53	0.44
1:B:366:LEU:HD11	1:B:372:LEU:HD22	2.00	0.44
1:A:26:CYS:SG	1:A:55:GLU:HG3	2.58	0.43
1:A:190:GLU:N	1:A:191:PRO:HD2	2.33	0.43
1:B:18:GLY:HA3	1:B:161:LEU:HD13	2.00	0.43
1:B:112:LEU:HD21	1:B:121:GLU:HG3	2.00	0.43
1:A:60:TYR:CG	1:A:406:GLY:HA3	2.53	0.43
1:A:367:ARG:HG3	1:A:433:ARG:NH2	2.33	0.43
1:A:18:GLY:HA3	1:A:161:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:VAL:O	1:A:288:LEU:HG	2.18	0.43
1:C:138:LEU:HD13	1:C:138:LEU:HA	1.88	0.43
1:A:282:ARG:N	1:A:283:PRO:HD2	2.33	0.43
1:B:288:LEU:O	1:B:308:SER:OG	2.31	0.43
1:B:543:LEU:HA	1:B:543:LEU:HD23	1.81	0.43
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.88	0.43
1:B:497:HIS:CD2	1:B:498:ASP:H	2.37	0.43
1:B:60:TYR:CG	1:B:406:GLY:HA3	2.54	0.42
1:B:216:GLN:HB3	1:B:316:THR:HG23	2.01	0.42
1:C:14:GLU:HB3	1:C:157:THR:HG21	2.00	0.42
1:A:95:TYR:OH	1:D:121:GLU:OE1	2.32	0.42
1:C:44:SER:HB2	1:C:46:ARG:HG3	2.02	0.42
1:A:79:SER:HB2	1:A:122:GLN:HE22	1.85	0.42
1:B:367:ARG:HE	1:B:367:ARG:HB2	1.54	0.42
1:C:49:LEU:HD12	1:C:49:LEU:HA	1.91	0.42
1:C:528:GLY:HA3	1:C:532:ARG:NH1	2.35	0.41
1:A:100:LEU:O	1:A:174:PRO:HA	2.19	0.41
1:C:264:LEU:HD12	1:C:264:LEU:HA	1.92	0.41
1:D:33:PRO:O	1:D:34:LEU:HB2	2.20	0.41
1:B:291:ALA:C	1:B:310:ASN:HD22	2.28	0.41
1:B:441:LEU:HD13	1:B:441:LEU:O	2.20	0.41
1:A:136:LEU:HD23	1:A:136:LEU:HA	1.92	0.41
1:D:360:ALA:O	1:D:364:HIS:CD2	2.74	0.41
1:B:16:ILE:HG12	1:B:47:ILE:HG23	2.03	0.41
1:B:462:LEU:HD23	1:B:531:MET:HG3	2.03	0.41
1:B:498:ASP:O	1:B:498:ASP:CG	2.64	0.41
1:C:92:GLU:OE1	1:C:401:VAL:HG12	2.21	0.41
1:D:230:SER:HB3	1:D:275:LEU:HD12	2.03	0.40
1:B:441:LEU:HD22	1:B:441:LEU:HA	1.95	0.40
1:B:39:GLN:HG3	1:C:492:ILE:HD13	2.02	0.40
1:C:304:TRP:HA	1:C:305:PRO:HD3	1.91	0.40
1:D:435:ILE:HD13	1:D:524:LEU:HD22	2.03	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	535/574 (93%)	520 (97%)	13 (2%)	2 (0%)	30	43
1	B	526/574 (92%)	517 (98%)	9 (2%)	0	100	100
1	C	522/574 (91%)	507 (97%)	15 (3%)	0	100	100
1	D	535/574 (93%)	521 (97%)	14 (3%)	0	100	100
All	All	2118/2296 (92%)	2065 (98%)	51 (2%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	SER
1	A	351	PRO

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	414/445 (93%)	404 (98%)	10 (2%)	43	65
1	B	409/445 (92%)	396 (97%)	13 (3%)	34	56
1	C	402/445 (90%)	397 (99%)	5 (1%)	63	81
1	D	412/445 (93%)	403 (98%)	9 (2%)	45	67
All	All	1637/1780 (92%)	1600 (98%)	37 (2%)	45	66

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	122	GLN
1	A	147	SER
1	A	195	VAL

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Mol	Chain	Res	Type
1	A	213	THR
1	A	307	VAL
1	A	383	VAL
1	A	385	LEU
1	A	492	ILE
1	A	523	THR
1	D	57	THR
1	D	63	ILE
1	D	126	PHE
1	D	159[A]	ARG
1	D	159[B]	ARG
1	D	285	SER
1	D	383	VAL
1	D	401	VAL
1	D	484	ARG
1	B	57	THR
1	B	147	SER
1	B	195	VAL
1	B	213	THR
1	B	256	ASP
1	B	293	VAL
1	B	304	TRP
1	B	314	THR
1	B	367	ARG
1	B	383	VAL
1	B	455	THR
1	B	545	GLN
1	B	551	LYS
1	C	57	THR
1	C	75	VAL
1	C	79	SER
1	C	81	THR
1	C	140	GLU

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

Mol	Chain	Res	Type
1	A	122	GLN
1	A	237	HIS
1	A	346	GLN
1	A	378	ASN
1	D	31	ASN

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Mol	Chain	Res	Type
1	D	281	HIS
1	D	364	HIS
1	B	117	ASN
1	B	497	HIS
1	B	509	HIS
1	C	7	GLN
1	C	364	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	$\# Z > 2$
4	TPP	C	601	6	26,27,27	0.33	0	38,40,40	0.36	0
2	EDO	B	601	-	3,3,3	0.47	0	2,2,2	0.45	0
4	TPP	D	601	6	26,27,27	0.28	0	38,40,40	0.30	0
2	EDO	A	601	-	3,3,3	0.29	0	2,2,2	1.14	0
5	DNA	D	602	-	16,16,16	2.25	4 (25%)	23,23,23	1.28	2 (8%)
5	DNA	C	602	-	16,16,16	2.36	4 (25%)	23,23,23	1.28	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	602	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	D	603	-	3,3,3	0.44	0	2,2,2	0.40	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	TPP	C	601	6	-	1/17/17/17	0/2/2/2
2	EDO	B	601	-	-	1/1/1/1	-
4	TPP	D	601	6	-	1/17/17/17	0/2/2/2
2	EDO	A	601	-	-	1/1/1/1	-
5	DNA	D	602	-	-	0/4/4/4	0/2/2/2
5	DNA	C	602	-	-	0/4/4/4	0/2/2/2
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	D	603	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	602	DNA	C1L-C1M	6.72	1.49	1.39
5	D	602	DNA	C1L-C1M	6.52	1.48	1.39
5	C	602	DNA	C1K-C1N	3.58	1.49	1.42
5	D	602	DNA	C1K-C1N	3.25	1.49	1.42
5	C	602	DNA	C1O-C1N	2.95	1.49	1.43
5	C	602	DNA	C1M-C1O	2.95	1.49	1.43
5	D	602	DNA	C1M-C1O	2.72	1.48	1.43
5	D	602	DNA	C1O-C1N	2.59	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	602	DNA	C1I-C1L-C1M	2.84	121.31	119.05
5	D	602	DNA	C1I-C1L-C1M	2.81	121.28	119.05
5	C	602	DNA	O1D-C1M-C1O	2.25	121.18	116.62
5	D	602	DNA	O1D-C1M-C1O	2.21	121.10	116.62
5	C	602	DNA	O1C-C1K-C1N	2.09	120.01	116.42

There are no chirality outliers.

All (5) torsion outliers are listed below:

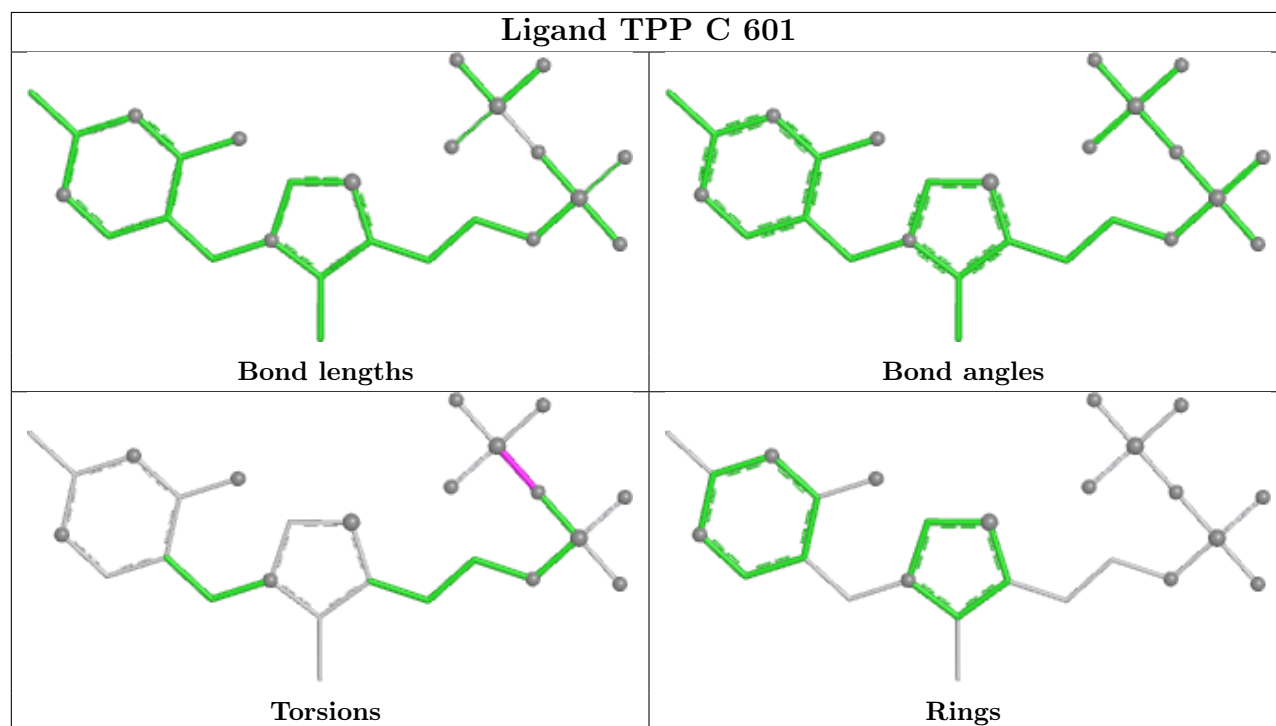
Mol	Chain	Res	Type	Atoms
4	D	601	TPP	PA-O3A-PB-O2B
4	C	601	TPP	PA-O3A-PB-O2B
2	A	602	EDO	O1-C1-C2-O2
2	A	601	EDO	O1-C1-C2-O2
2	B	601	EDO	O1-C1-C2-O2

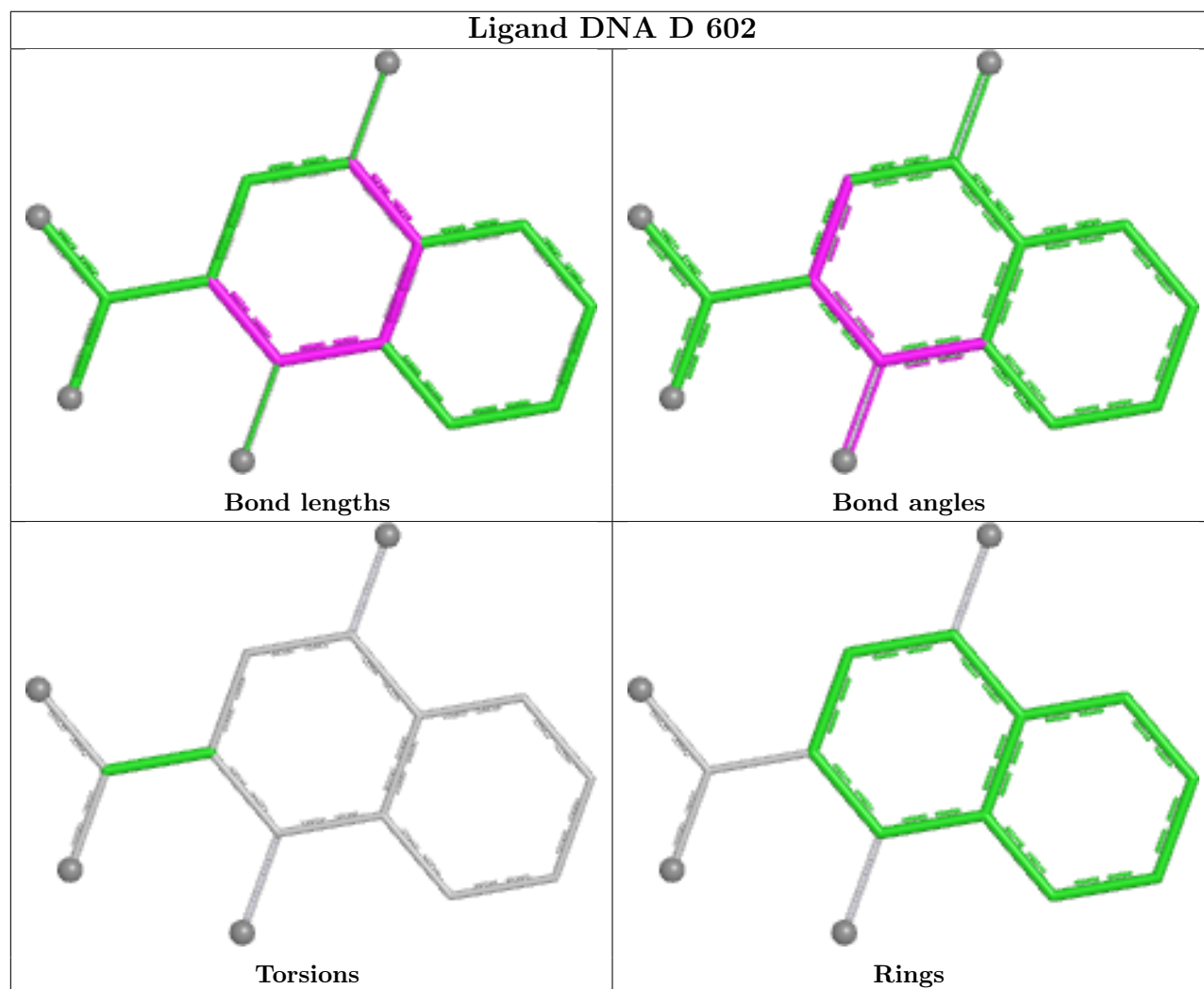
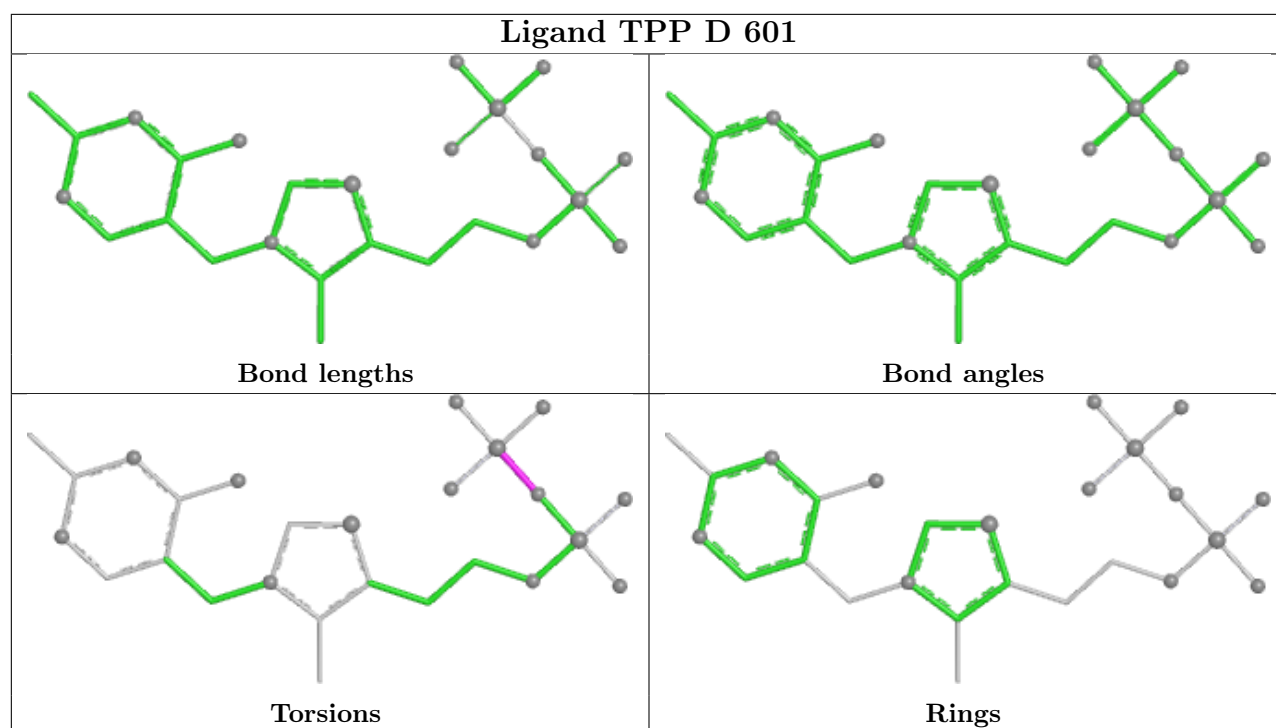
There are no ring outliers.

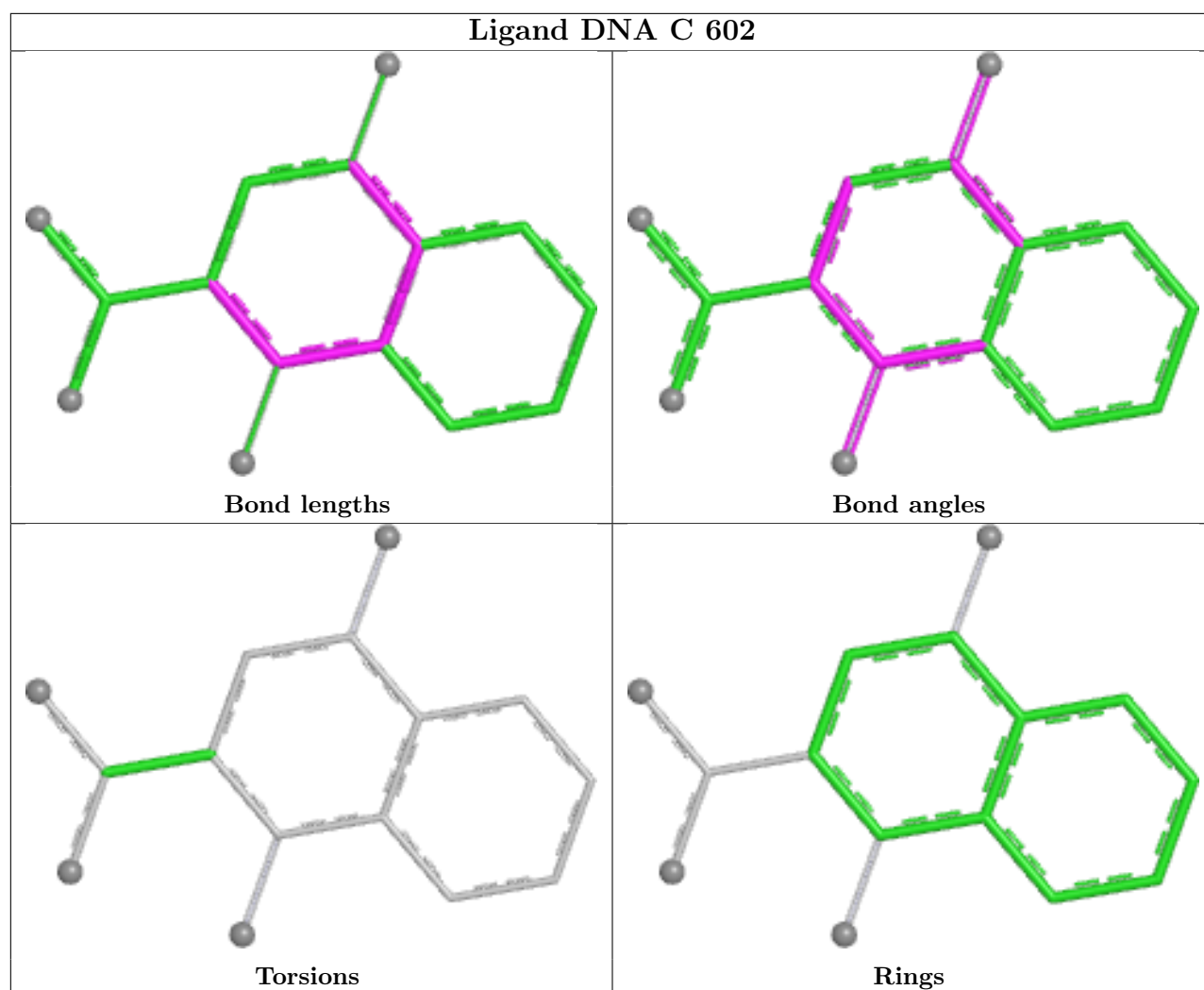
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	EDO	1	0
5	C	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	538/574 (93%)	0.30	24 (4%)	38	34	30, 61, 102, 142	3 (0%)
1	B	532/574 (92%)	0.50	34 (6%)	25	22	29, 66, 107, 150	2 (0%)
1	C	525/574 (91%)	0.58	27 (5%)	33	30	31, 75, 113, 169	3 (0%)
1	D	535/574 (93%)	0.22	19 (3%)	46	42	27, 59, 103, 135	6 (1%)
All	All	2130/2296 (92%)	0.40	104 (4%)	35	31	27, 66, 108, 169	14 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	GLY	6.2
1	B	496	PRO	6.0
1	B	472	GLY	5.8
1	B	214[A]	PHE	5.2
1	B	489	SER	5.0
1	D	34	LEU	4.7
1	D	195	VAL	4.6
1	C	32	ALA	4.5
1	C	108	PRO	4.3
1	A	539	ASP	4.0
1	C	126	PHE	3.8
1	B	195	VAL	3.8
1	A	42	ASP	3.7
1	D	112	LEU	3.7
1	C	3	PRO	3.7
1	D	120	MET	3.6
1	A	192	LEU	3.6
1	C	554	LEU	3.6
1	B	191	PRO	3.5
1	B	307	VAL	3.4
1	A	529	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	194	ALA	3.4
1	A	288	LEU	3.4
1	B	554	LEU	3.3
1	A	307	VAL	3.2
1	B	74	CYS	3.2
1	D	279	THR	3.2
1	C	74	CYS	3.1
1	B	490	SER	3.1
1	B	426	GLY	3.1
1	B	529	ALA	3.1
1	D	181	LEU	3.0
1	B	184	PRO	3.0
1	B	404	ILE	3.0
1	B	159[A]	ARG	2.9
1	A	190	GLU	2.9
1	B	1	MET	2.9
1	D	182	ARG	2.9
1	A	428	PRO	2.9
1	D	428	PRO	2.8
1	C	122	GLN	2.8
1	C	181	LEU	2.7
1	C	352	LEU	2.7
1	D	109	TYR	2.7
1	C	444	VAL	2.6
1	B	390	THR	2.6
1	D	29	SER	2.6
1	A	304	TRP	2.6
1	B	304	TRP	2.6
1	A	527	PRO	2.6
1	B	527	PRO	2.6
1	C	488	VAL	2.6
1	B	53	ILE	2.6
1	D	138	LEU	2.5
1	D	159[A]	ARG	2.5
1	C	163	ALA	2.5
1	B	187	PRO	2.5
1	A	495	THR	2.5
1	C	531	MET	2.5
1	B	291	ALA	2.5
1	D	113	GLY	2.4
1	D	382	ASP	2.4
1	A	489	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	287	LEU	2.3
1	C	495	THR	2.3
1	C	107	ARG	2.3
1	C	123	LEU	2.3
1	A	279	THR	2.3
1	B	451	LEU	2.3
1	B	428	PRO	2.3
1	D	145	ARG	2.3
1	C	393	ILE	2.3
1	C	211	PRO	2.2
1	C	529	ALA	2.2
1	B	427	SER	2.2
1	D	214[A]	PHE	2.2
1	D	282[A]	ARG	2.2
1	C	156	ALA	2.2
1	C	515	ILE	2.2
1	B	123	LEU	2.2
1	A	214[A]	PHE	2.2
1	A	291	ALA	2.2
1	C	376	ALA	2.2
1	A	492	ILE	2.2
1	C	462	LEU	2.2
1	B	202	ALA	2.2
1	B	531	MET	2.1
1	A	191	PRO	2.1
1	A	211	PRO	2.1
1	A	496	PRO	2.1
1	C	475	PHE	2.1
1	B	137	GLY	2.1
1	B	139	ALA	2.1
1	B	303	ARG	2.1
1	B	201	PRO	2.1
1	C	517	VAL	2.1
1	A	309	GLY	2.1
1	D	495	THR	2.1
1	A	509[A]	HIS	2.1
1	D	40	ASP	2.1
1	A	284	VAL	2.1
1	B	528	GLY	2.1
1	C	307	VAL	2.0
1	C	353	THR	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](#)

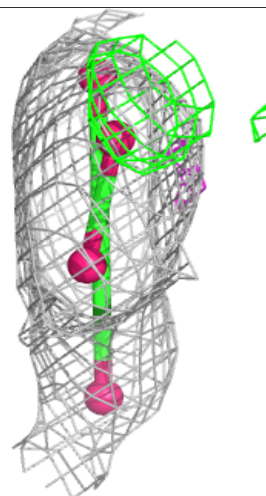
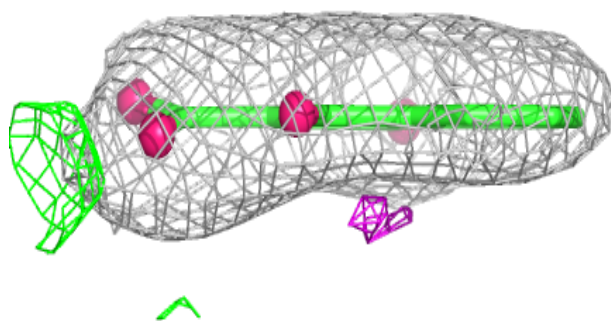
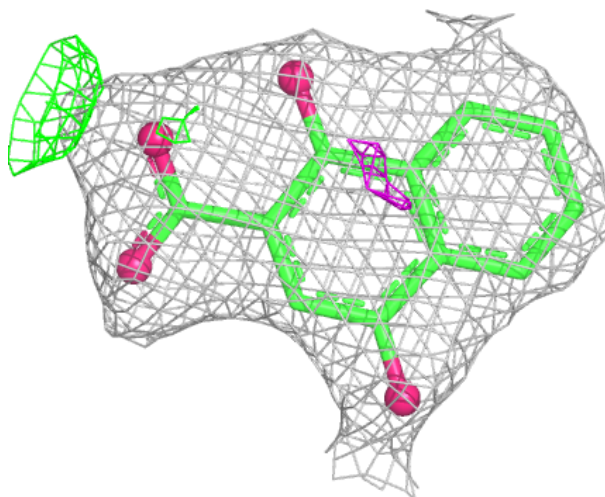
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	D	603	4/4	0.71	0.20	81,84,85,91	0
2	EDO	B	601	4/4	0.85	0.30	48,48,86,91	0
2	EDO	A	601	4/4	0.88	0.23	35,41,66,74	0
2	EDO	A	602	4/4	0.89	0.16	69,72,77,82	0
5	DNA	C	602	15/15	0.90	0.11	58,68,73,75	0
4	TPP	C	601	26/26	0.91	0.12	75,85,96,98	0
3	CL	A	603	1/1	0.94	0.08	68,68,68,68	0
3	CL	D	605	1/1	0.95	0.09	71,71,71,71	0
3	CL	A	604	1/1	0.96	0.09	73,73,73,73	0
3	CL	B	603	1/1	0.96	0.09	70,70,70,70	0
5	DNA	D	602	15/15	0.97	0.06	43,45,49,54	0
3	CL	B	602	1/1	0.97	0.06	54,54,54,54	0
4	TPP	D	601	26/26	0.98	0.05	38,52,56,62	0
6	MG	C	603	1/1	0.98	0.08	80,80,80,80	0
6	MG	D	604	1/1	0.99	0.02	46,46,46,46	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.

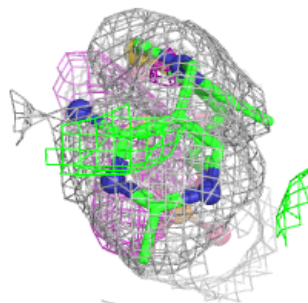
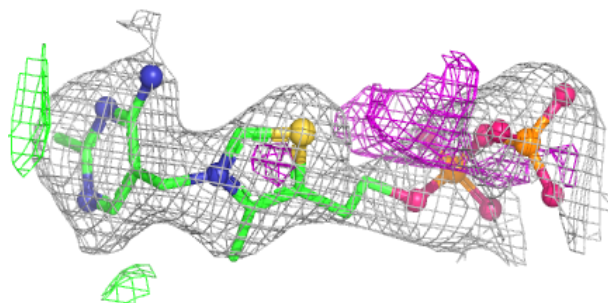
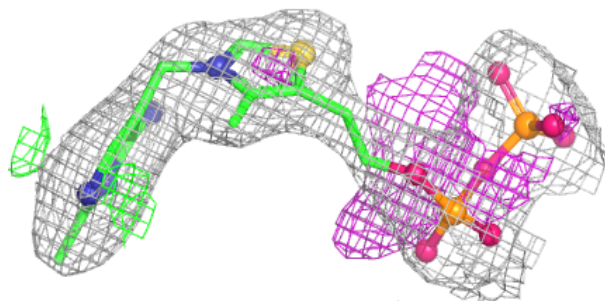
Electron density around DNA C 602:

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



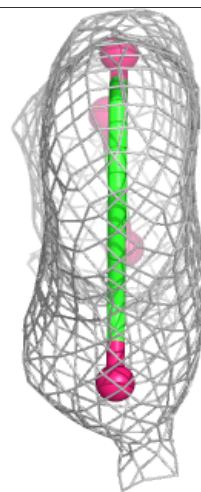
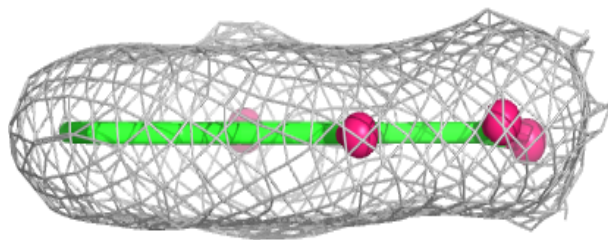
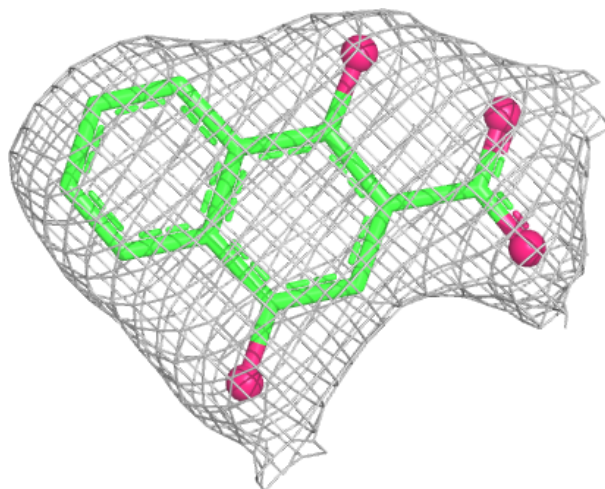
Electron density around TPP C 601:

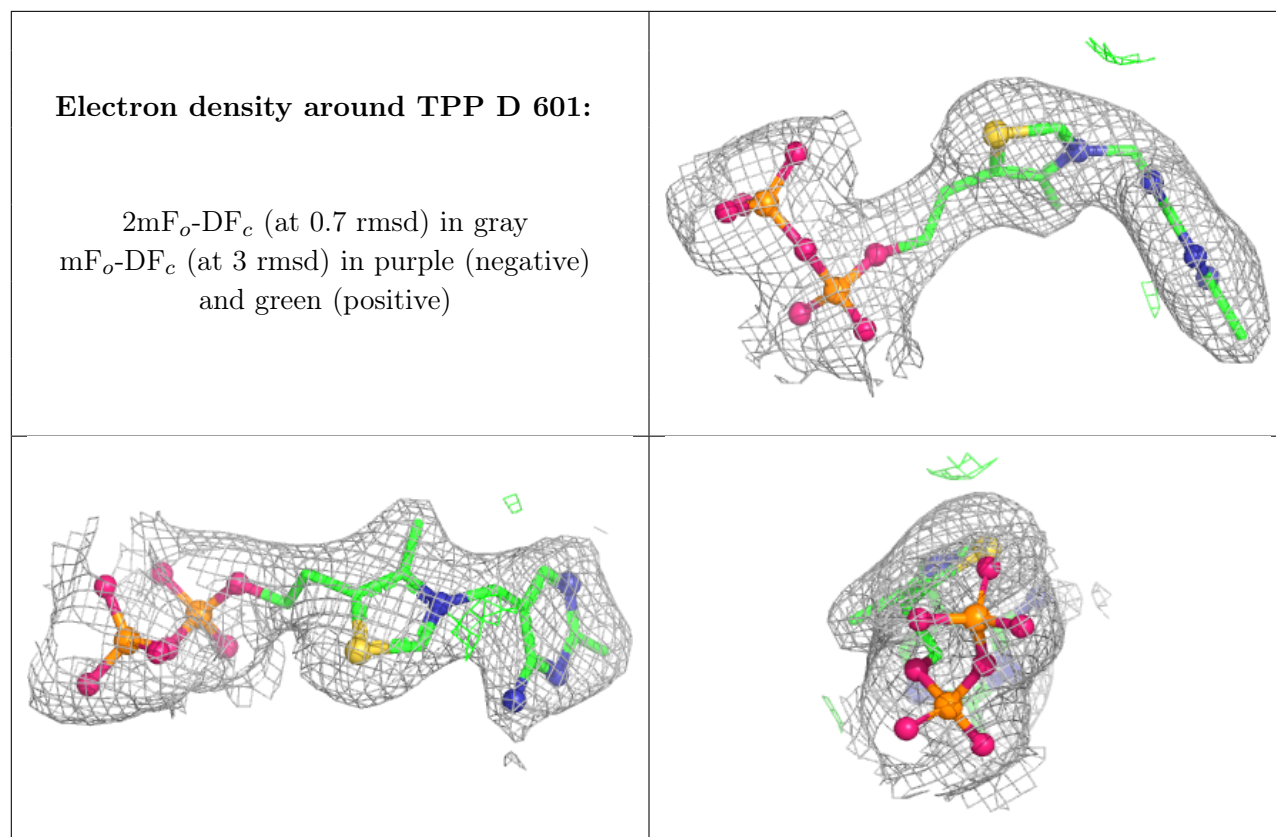
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.