Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2025 – 06:09 AM EDT

PDB ID	:	9DTV / pdb_00009dtv
Title	:	Structure of D141A mutant of M.tuberculosis MenD (SEPHCHC Synthase)
Authors	:	Johnston, J.M.; Ho, N.A.T.; Given, F.M.; Allison, T.M.; Bulloch, E.M.M.; Jiao, W.
Deposited on	:	2024-10-02
Resolution	:	2.42 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:

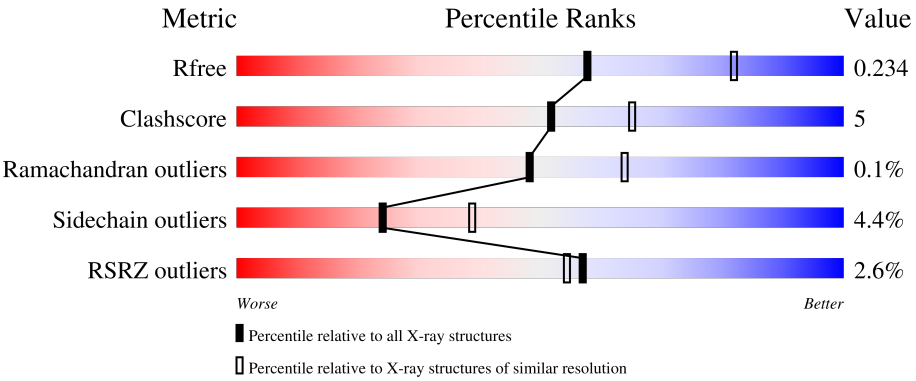
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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}	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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 <=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	2% 80% 13% • 6%
1	B	574	2% 78% 14% • 7%
1	C	574	3% 78% 14% 7%
1	D	574	3% 82% 11% 6%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16050 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	2	0
			3964	2475	732	746	11			
1	D	538	Total	C	N	O	S	0	6	0
			3999	2496	745	748	10			
1	B	533	Total	C	N	O	S	0	2	0
			3919	2445	729	734	11			
1	C	533	Total	C	N	O	S	0	2	0
			3920	2451	725	735	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	141	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	141	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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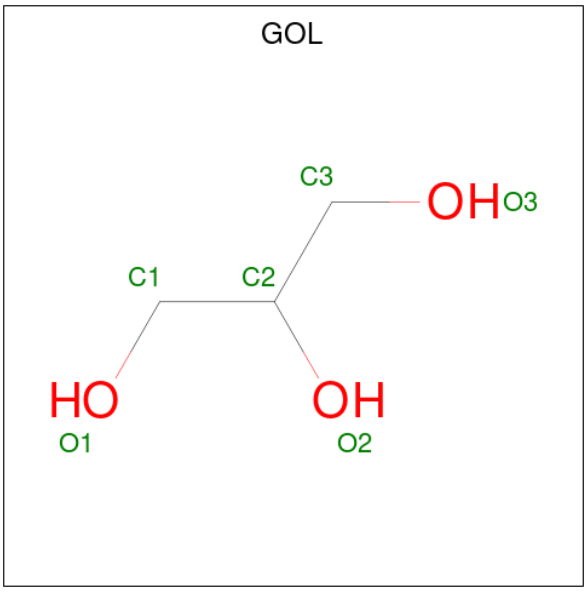
Chain	Residue	Modelled	Actual	Comment	Reference
B	141	ALA	ASP	engineered mutation	UNP P9WK11
C	-19	MET	-	initiating methionine	UNP P9WK11
C	-18	GLY	-	expression tag	UNP P9WK11
C	-17	SER	-	expression tag	UNP P9WK11
C	-16	SER	-	expression tag	UNP P9WK11
C	-15	HIS	-	expression tag	UNP P9WK11
C	-14	HIS	-	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	141	ALA	ASP	engineered mutation	UNP P9WK11

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

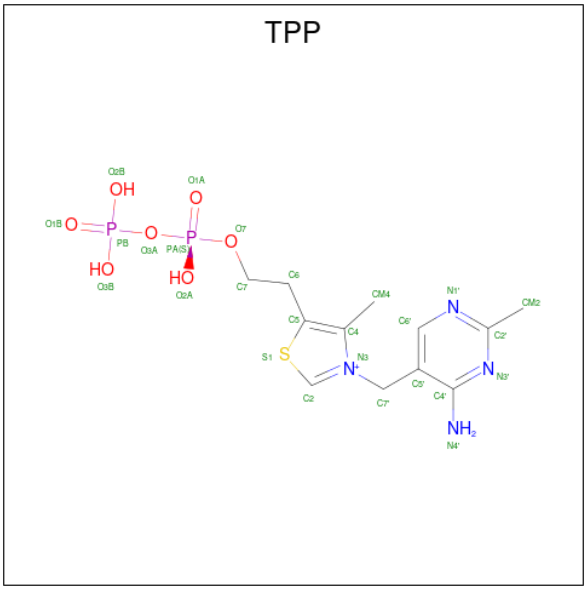


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

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

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

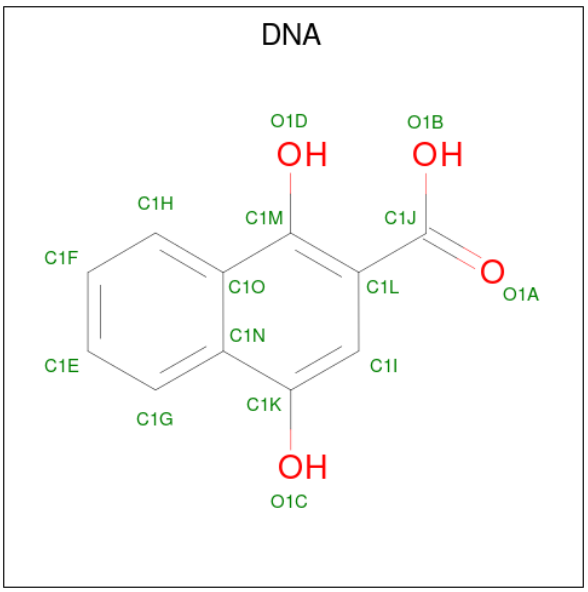
- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



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

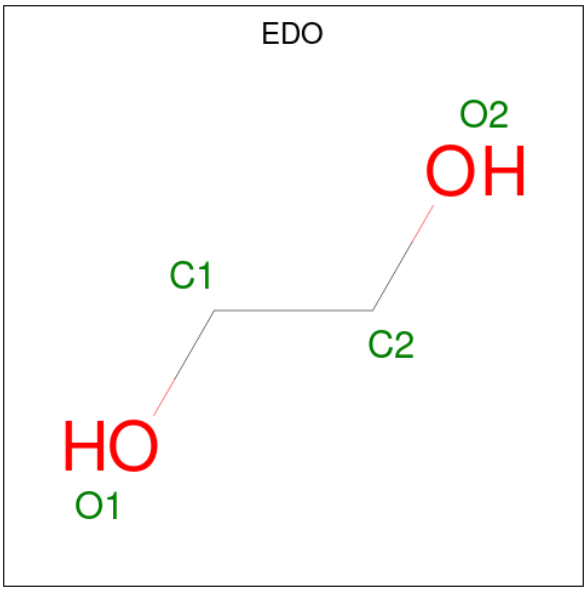
- Molecule 5 is 1,4-dihydroxy-2-naphthoic acid (CCD ID: DNA) (formula: $C_{11}H_8O_4$) (labeled

as "Ligand of Interest" by depositor).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is water.

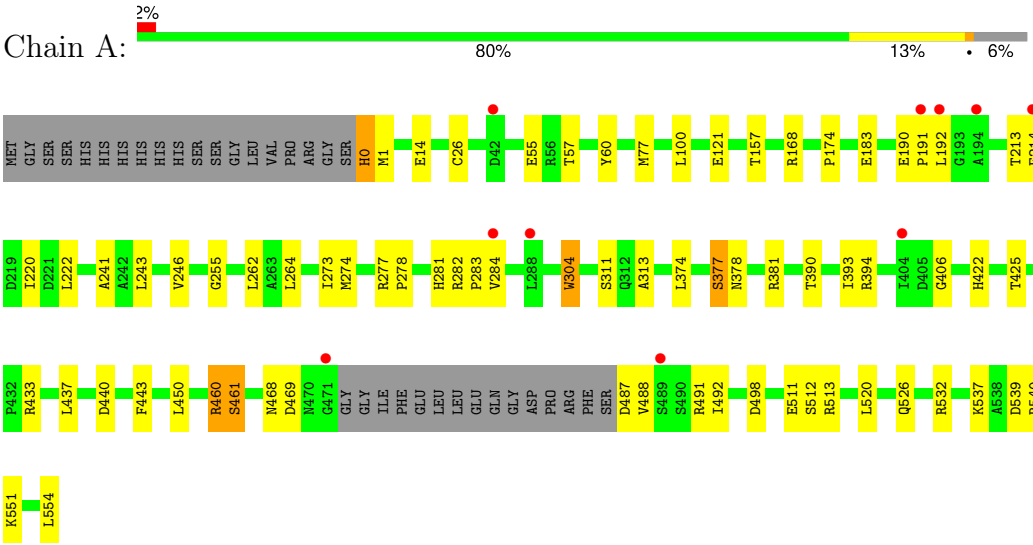
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	38	Total O 38 38	0	0
8	D	52	Total O 52 52	0	0
8	B	32	Total O 32 32	0	0
8	C	21	Total O 21 21	0	0

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.

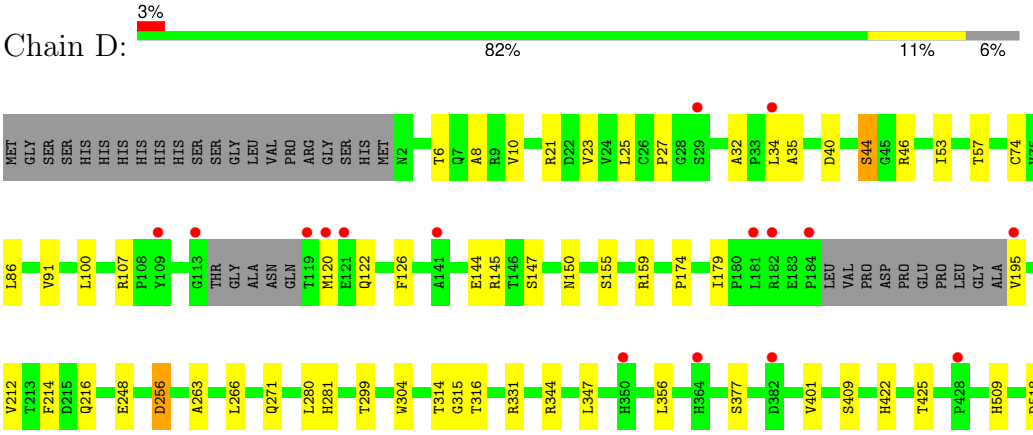
• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain A:



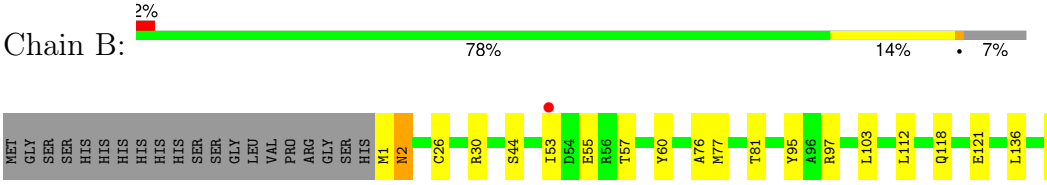
• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

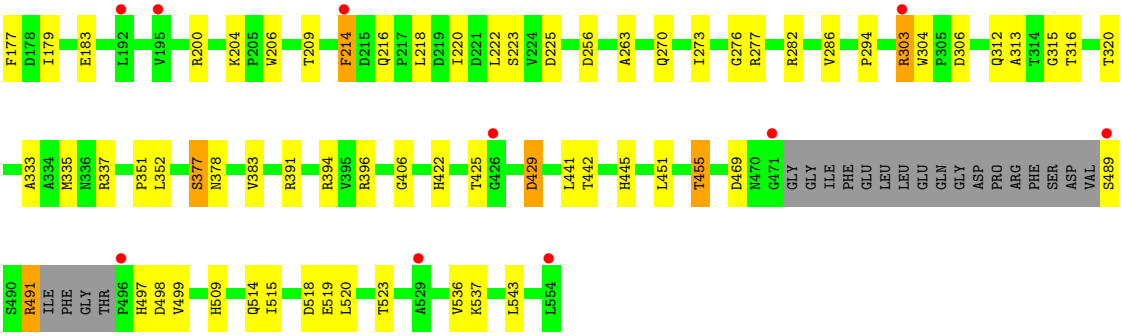
Chain D:



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

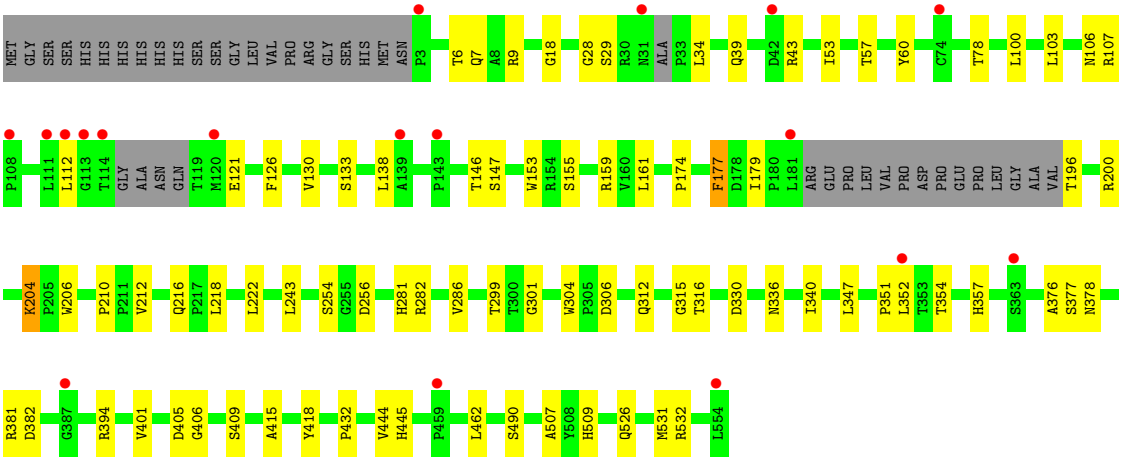
Chain B:





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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.42Å 140.44Å 184.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.42 – 2.42 44.42 – 2.42	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.42-2.42) 100.0 (44.42-2.42)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.193 , 0.234 0.193 , 0.234	Depositor DCC
R_{free} test set	5084 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16050	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: DNA, GOL, EDO, TPP, MG, 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	0.25	0/4049	0.52	0/5552
1	B	0.24	0/4005	0.52	1/5487 (0.0%)
1	C	0.25	0/4004	0.53	0/5479
1	D	0.25	0/4087	0.52	0/5595
All	All	0.25	0/16145	0.52	1/22113 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	469	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3964	0	3985	48	0
1	B	3919	0	3957	54	0
1	C	3920	0	3948	49	0
1	D	3999	0	4012	34	0
2	A	6	0	8	1	0
2	B	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	2	0	0	0	0
4	C	26	0	16	0	0
4	D	26	0	16	1	0
5	C	15	0	5	0	0
5	D	15	0	5	0	0
6	D	4	0	6	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	38	0	0	0	0
8	B	32	0	0	0	0
8	C	21	0	0	0	0
8	D	52	0	0	1	0
All	All	16050	0	15966	160	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 5.

All (160) 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:216:GLN:HB2	1:C:316:THR:HG23	1.67	0.76
1:B:216:GLN:HB2	1:B:316:THR:HG23	1.68	0.75
1:B:509:HIS:O	1:B:509:HIS:ND1	2.20	0.74
1:B:377:SER:OG	1:B:378:ASN:N	2.23	0.71
1:D:212:VAL:HG21	1:B:214[A]:PHE:CD2	2.27	0.70
1:B:515:ILE:HD11	1:B:520:LEU:HD13	1.76	0.68
1:C:34:LEU:HD11	1:C:179:ILE:HD13	1.77	0.66
1:C:106:ASN:OD1	1:C:107:ARG:N	2.28	0.66
1:C:418:TYR:HE2	1:C:432:PRO:HB2	1.61	0.65
1:D:32:ALA:HB3	1:D:35:ALA:HB2	1.79	0.65
1:D:34:LEU:HD21	1:D:179:ILE:HD13	1.77	0.65
1:D:216:GLN:HB2	1:D:316:THR:HG23	1.81	0.63
1:A:121:GLU:N	1:A:121:GLU:OE1	2.31	0.62
1:A:498:ASP:O	1:D:509:HIS:NE2	2.25	0.62
1:B:97:ARG:HD2	1:B:303:ARG:HD2	1.82	0.61
1:A:539:ASP:OD1	1:A:541:SER:N	2.34	0.61
1:B:225:ASP:HB2	1:B:270:GLN:HG3	1.82	0.61
1:D:23:VAL:HG22	1:D:74:CYS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ASN:O	1:C:340:ILE:HG13	2.00	0.60
1:B:394:ARG:HH11	1:B:396:ARG:HH12	1.50	0.59
1:D:8:ALA:HA	1:D:34:LEU:HD22	1.85	0.59
1:A:220:ILE:HG21	1:A:273:ILE:HD11	1.86	0.58
1:B:442:THR:OG1	3:B:602:CL:CL	2.50	0.57
1:A:168:ARG:NH2	1:C:299:THR:OG1	2.34	0.57
1:B:277:ARG:HB2	2:B:601:GOL:H2	1.87	0.56
1:B:1:MET:SD	1:B:2:ASN:ND2	2.78	0.56
1:C:256:ASP:N	1:C:256:ASP:OD1	2.38	0.56
1:D:159:ARG:NH2	1:B:304:TRP:O	2.30	0.55
1:A:277:ARG:HB2	2:A:601:GOL:H2	1.87	0.55
1:A:222:LEU:HD22	1:A:243:LEU:HD11	1.87	0.54
1:D:216:GLN:HB3	1:D:315:GLY:HA2	1.88	0.54
1:D:299:THR:OG1	1:B:168:ARG:NH2	2.40	0.53
1:B:455:THR:O	1:B:455:THR:OG1	2.26	0.53
1:D:256:ASP:OD1	1:D:256:ASP:N	2.40	0.53
1:D:150:ASN:ND2	1:D:198:PRO:O	2.40	0.53
1:A:304:TRP:O	1:C:159:ARG:NH2	2.31	0.53
1:A:246:VAL:HG21	1:A:264:LEU:HD22	1.89	0.53
1:B:276:GLY:HA2	2:B:601:GOL:H31	1.90	0.52
1:D:6:THR:O	1:D:10:VAL:HG23	2.10	0.52
1:A:214[A]:PHE:CD1	1:C:212:VAL:HG21	2.44	0.52
1:C:282:ARG:O	1:C:286:VAL:HG23	2.10	0.52
1:A:216:GLN:HG2	1:C:210:PRO:HG2	1.93	0.51
1:B:333:ALA:O	1:B:337:ARG:HG3	2.10	0.51
1:B:183:GLU:H	1:B:183:GLU:CD	2.11	0.51
1:C:103:LEU:HD23	1:C:177:PHE:HB3	1.93	0.51
1:B:514:GLN:OE1	1:B:537:LYS:NZ	2.44	0.50
1:C:28:GLY:HA3	1:C:78:THR:HB	1.94	0.50
1:A:492:ILE:HD11	1:D:27:PRO:HG3	1.92	0.50
1:B:263:ALA:HB1	1:B:335:MET:HB3	1.93	0.50
1:D:44:SER:HB2	1:D:46:ARG:HG3	1.92	0.50
1:D:91:VAL:HG12	1:D:401:VAL:HG21	1.92	0.49
1:B:445:HIS:HD2	1:C:53:ILE:HG22	1.77	0.49
1:D:422:HIS:O	1:D:425:THR:HG22	2.12	0.49
1:A:26:CYS:SG	1:A:55:GLU:HG3	2.52	0.49
1:A:168:ARG:HH22	1:C:299:THR:HG1	1.59	0.49
1:B:519:GLU:O	1:B:523:THR:OG1	2.25	0.49
1:B:222:LEU:HG	1:B:320:THR:HB	1.95	0.48
1:A:304:TRP:CZ2	1:C:159:ARG:HG2	2.49	0.48
1:A:488:VAL:HG22	1:A:491:ARG:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ASP:O	1:D:44:SER:OG	2.29	0.48
1:A:431:PRO:HG3	1:A:460:ARG:HD3	1.96	0.48
1:B:256:ASP:HB3	1:B:391:ARG:NH1	2.28	0.48
1:C:18:GLY:HA3	1:C:161:LEU:HD13	1.95	0.48
1:A:513:ARG:NH2	1:A:532:ARG:HH11	2.12	0.48
1:B:81:THR:HG23	1:C:401:VAL:HG21	1.95	0.48
1:C:351:PRO:HG2	1:C:352:LEU:HD22	1.96	0.47
1:A:60:TYR:CG	1:A:406:GLY:HA3	2.48	0.47
1:A:539:ASP:OD1	1:A:540:ARG:N	2.47	0.47
1:B:112:LEU:HD21	1:B:121:GLU:HG3	1.96	0.47
1:C:130:VAL:HA	1:C:174:PRO:HG2	1.96	0.47
1:A:183:GLU:H	1:A:183:GLU:CD	2.11	0.47
1:A:183:GLU:OE1	1:A:183:GLU:N	2.26	0.47
1:A:492:ILE:HD12	1:D:53:ILE:HG13	1.96	0.47
1:D:32:ALA:HA	1:D:78:THR:HG22	1.96	0.47
1:B:26:CYS:SG	1:B:55:GLU:HG3	2.54	0.47
1:B:95:TYR:OH	1:C:121:GLU:OE1	2.28	0.47
1:C:462:LEU:HD23	1:C:531:MET:HG2	1.96	0.46
1:C:394:ARG:HD3	1:C:418:TYR:HE1	1.80	0.46
1:D:25:LEU:HD23	1:D:76:ALA:HB3	1.97	0.46
1:B:218:LEU:HD11	1:B:313:ALA:HB1	1.97	0.46
1:B:2:ASN:HD22	1:B:2:ASN:H	1.63	0.46
1:A:274:MET:HG3	1:A:278:PRO:HG2	1.98	0.46
1:D:144:GLU:HG2	1:D:145:ARG:HG3	1.97	0.46
1:B:76:ALA:HA	1:B:103:LEU:O	2.15	0.46
1:C:376:ALA:O	1:C:377:SER:OG	2.30	0.46
1:B:422:HIS:O	1:B:425:THR:HG22	2.16	0.46
1:A:377:SER:OG	1:A:378:ASN:N	2.49	0.46
1:C:39:GLN:HG2	1:C:43:ARG:NH1	2.31	0.45
1:C:222:LEU:HD22	1:C:243:LEU:HD11	1.97	0.45
1:D:122:GLN:H	1:D:122:GLN:CD	2.20	0.45
1:B:497:HIS:CE1	1:B:499:VAL:H	2.34	0.45
1:D:314:THR:HB	1:B:168:ARG:NH1	2.32	0.45
1:A:190:GLU:N	1:A:191:PRO:HD2	2.30	0.45
1:D:100:LEU:O	1:D:174:PRO:HA	2.17	0.45
1:A:241:ALA:HB1	1:A:255:GLY:HA3	1.99	0.44
1:B:282:ARG:O	1:B:286:VAL:HG13	2.17	0.44
1:C:200:ARG:HG3	1:C:206:TRP:HA	1.98	0.44
1:A:422:HIS:O	1:A:425:THR:HG22	2.18	0.44
1:B:429:ASP:N	1:B:429:ASP:OD1	2.51	0.44
1:A:281:HIS:HB2	1:A:284:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:PRO:HA	1:D:211:PRO:HD2	1.91	0.44
1:A:168:ARG:NH2	1:C:301:GLY:O	2.51	0.44
1:D:347:LEU:HD21	1:D:356:LEU:HD23	1.99	0.44
1:B:294:PRO:HB3	1:B:312:GLN:HG3	2.00	0.44
1:B:543:LEU:HD23	1:B:543:LEU:HA	1.83	0.44
1:A:374:LEU:HD23	1:A:437:LEU:HB3	2.00	0.43
1:A:168:ARG:NH1	1:C:216:GLN:OE1	2.51	0.43
1:A:100:LEU:O	1:A:174:PRO:HA	2.19	0.43
1:B:441:LEU:HD21	1:C:53:ILE:HD13	2.00	0.43
1:C:9:ARG:NH1	1:C:196:THR:OG1	2.51	0.43
1:D:77:MET:SD	1:D:86:LEU:HD12	2.58	0.43
1:D:271:GLN:NE2	8:D:703:HOH:O	2.52	0.43
1:B:520:LEU:HD22	1:B:536:VAL:HG21	1.99	0.43
1:C:204:LYS:H	1:C:204:LYS:HG2	1.59	0.43
1:A:304:TRP:CH2	1:C:159:ARG:HG2	2.54	0.43
1:D:248:GLU:HG2	1:D:280:LEU:HD12	2.00	0.42
1:C:100:LEU:O	1:C:174:PRO:HA	2.19	0.42
1:C:216:GLN:HB3	1:C:315:GLY:HA2	2.00	0.42
1:C:415:ALA:HB2	1:C:462:LEU:HD13	2.00	0.42
1:A:537:LYS:HB3	1:A:537:LYS:HE3	1.70	0.42
1:B:204:LYS:HE3	1:B:204:LYS:HB3	1.76	0.42
1:B:53:ILE:HD12	1:B:53:ILE:N	2.35	0.42
1:A:440:ASP:HB3	1:A:468:ASN:HA	2.02	0.42
1:D:263:ALA:HA	1:D:266:LEU:HD12	2.02	0.42
1:D:543:LEU:HD23	1:D:543:LEU:HA	1.90	0.42
1:B:491:ARG:H	1:B:491:ARG:HG3	1.51	0.42
1:C:218:LEU:HD23	1:C:218:LEU:HA	1.81	0.42
1:C:381:ARG:NH1	3:C:604:CL:CL	2.63	0.42
1:A:433:ARG:HA	1:A:461:SER:OG	2.20	0.41
1:D:216:GLN:HE22	1:B:209:THR:HG23	1.85	0.41
1:B:451:LEU:HD12	1:C:444:VAL:HG11	2.01	0.41
1:B:499:VAL:HG13	1:C:507:ALA:O	2.20	0.41
1:B:351:PRO:HG2	1:B:352:LEU:HD22	2.03	0.41
1:C:222:LEU:HD13	1:C:243:LEU:HD21	2.02	0.41
1:A:214[A]:PHE:CE1	1:C:212:VAL:HG21	2.56	0.41
4:D:601:TPP:HN42	4:D:601:TPP:C2	2.34	0.41
1:C:378:ASN:HB3	1:C:382:ASP:OD2	2.21	0.41
1:A:543:LEU:HD23	1:A:543:LEU:HA	1.91	0.41
1:A:390:THR:HA	1:A:393:ILE:HD11	2.03	0.41
1:A:0:HIS:HB3	1:A:1:MET:H	1.47	0.41
1:A:218:LEU:HD11	1:A:313:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ARG:HG3	1:B:206:TRP:HA	2.02	0.41
1:B:216:GLN:HB3	1:B:315:GLY:HA2	2.03	0.41
1:B:220:ILE:HG21	1:B:273:ILE:HD11	2.01	0.41
1:B:498:ASP:O	1:C:509:HIS:NE2	2.48	0.41
1:C:138:LEU:HD23	1:C:138:LEU:HA	1.83	0.41
1:A:443:PHE:CZ	1:A:450:LEU:HD11	2.56	0.40
1:C:347:LEU:HD22	1:C:357:HIS:NE2	2.35	0.40
1:A:14:GLU:HB3	1:A:157:THR:HG21	2.03	0.40
1:A:262:LEU:HD13	1:A:554:LEU:HD11	2.02	0.40
1:D:159:ARG:HG2	1:B:304:TRP:CH2	2.56	0.40
1:C:405:ASP:HB3	1:C:445:HIS:CE1	2.56	0.40
1:B:306:ASP:OD1	1:B:306:ASP:N	2.42	0.40
1:C:7:GLN:HG3	1:C:153:TRP:CE2	2.55	0.40
1:A:282:ARG:N	1:A:283:PRO:HD2	2.36	0.40
1:A:520:LEU:HD12	1:A:520:LEU:HA	1.88	0.40
1:B:60:TYR:CG	1:B:406:GLY:HA3	2.56	0.40
1:B:136:LEU:HD12	1:B:179:ILE:HD12	2.03	0.40
1:A:511:GLU:OE2	1:A:513:ARG:NH2	2.54	0.40
1:C:60:TYR:CG	1:C:406:GLY:HA3	2.57	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	538/574 (94%)	518 (96%)	19 (4%)	1 (0%)	44	58
1	B	529/574 (92%)	515 (97%)	14 (3%)	0	100	100
1	C	527/574 (92%)	507 (96%)	19 (4%)	1 (0%)	44	58
1	D	538/574 (94%)	523 (97%)	14 (3%)	1 (0%)	44	58
All	All	2132/2296 (93%)	2063 (97%)	66 (3%)	3 (0%)	48	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	281	HIS
1	A	377	SER
1	C	281	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/444 (94%)	398 (96%)	17 (4%)	26	42
1	B	411/444 (93%)	392 (95%)	19 (5%)	23	37
1	C	410/444 (92%)	389 (95%)	21 (5%)	20	33
1	D	418/444 (94%)	400 (96%)	18 (4%)	25	40
All	All	1654/1776 (93%)	1579 (96%)	75 (4%)	24	38

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	57	THR
1	A	77	MET
1	A	192	LEU
1	A	213	THR
1	A	304	TRP
1	A	311	SER
1	A	381	ARG
1	A	394	ARG
1	A	430	SER
1	A	460	ARG
1	A	461	SER
1	A	469	ASP
1	A	487	ASP
1	A	512	SER
1	A	526	GLN
1	A	551	LYS

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Mol	Chain	Res	Type
1	D	21	ARG
1	D	44	SER
1	D	57	THR
1	D	107	ARG
1	D	120	MET
1	D	126	PHE
1	D	147	SER
1	D	155	SER
1	D	195	VAL
1	D	214[A]	PHE
1	D	214[B]	PHE
1	D	256	ASP
1	D	304	TRP
1	D	331	ARG
1	D	344	ARG
1	D	377	SER
1	D	409	SER
1	D	518	ASP
1	B	2	ASN
1	B	30	ARG
1	B	44	SER
1	B	57	THR
1	B	77	MET
1	B	118	GLN
1	B	147	SER
1	B	177	PHE
1	B	214[A]	PHE
1	B	214[B]	PHE
1	B	223	SER
1	B	303	ARG
1	B	377	SER
1	B	383	VAL
1	B	429	ASP
1	B	455	THR
1	B	489	SER
1	B	491	ARG
1	B	518	ASP
1	C	6	THR
1	C	29	SER
1	C	57	THR
1	C	112	LEU
1	C	126	PHE

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Mol	Chain	Res	Type
1	C	133	SER
1	C	146	THR
1	C	147	SER
1	C	155	SER
1	C	177	PHE
1	C	204	LYS
1	C	254	SER
1	C	304	TRP
1	C	306	ASP
1	C	312	GLN
1	C	330	ASP
1	C	354	THR
1	C	409	SER
1	C	490	SER
1	C	526	GLN
1	C	532	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	HIS
1	D	545	GLN
1	B	2	ASN
1	B	281	HIS
1	C	338	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 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DNA	C	602	-	16,16,16	2.16	4 (25%)	23,23,23	1.06	0
2	GOL	B	601	-	5,5,5	0.11	0	5,5,5	0.29	0
4	TPP	C	601	7	23,27,27	0.51	0	30,40,40	0.58	1 (3%)
6	EDO	D	603	-	3,3,3	0.43	0	2,2,2	0.33	0
4	TPP	D	601	7	23,27,27	0.50	0	30,40,40	0.58	1 (3%)
2	GOL	A	601	-	5,5,5	0.09	0	5,5,5	0.29	0
5	DNA	D	602	-	16,16,16	2.18	4 (25%)	23,23,23	1.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DNA	C	602	-	-	0/4/4/4	0/2/2/2
2	GOL	B	601	-	-	2/4/4/4	-
4	TPP	C	601	7	-	2/16/17/17	0/2/2/2
6	EDO	D	603	-	-	1/1/1/1	-
4	TPP	D	601	7	-	4/16/17/17	0/2/2/2
2	GOL	A	601	-	-	3/4/4/4	-
5	DNA	D	602	-	-	0/4/4/4	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	602	DNA	C1L-C1M	6.16	1.48	1.39
5	C	602	DNA	C1L-C1M	6.13	1.48	1.39
5	C	602	DNA	C1K-C1N	3.28	1.49	1.42
5	D	602	DNA	C1K-C1N	3.26	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	602	DNA	C1M-C1O	2.62	1.48	1.43
5	C	602	DNA	C1M-C1O	2.60	1.48	1.43
5	D	602	DNA	C1O-C1N	2.49	1.48	1.43
5	C	602	DNA	C1O-C1N	2.38	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	601	TPP	C5-C4-N3	2.06	111.70	107.57
4	C	601	TPP	C5-C4-N3	2.06	111.69	107.57

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O2-C2-C3-O3
2	B	601	GOL	C1-C2-C3-O3
4	C	601	TPP	PA-O3A-PB-O2B
4	C	601	TPP	PA-O3A-PB-O3B
2	A	601	GOL	C1-C2-C3-O3
2	B	601	GOL	O2-C2-C3-O3
2	A	601	GOL	O1-C1-C2-O2
6	D	603	EDO	O1-C1-C2-O2
4	D	601	TPP	PA-O3A-PB-O1B
4	D	601	TPP	C4'-C5'-C7'-N3
4	D	601	TPP	PA-O3A-PB-O2B
4	D	601	TPP	PA-O3A-PB-O3B

There are no ring outliers.

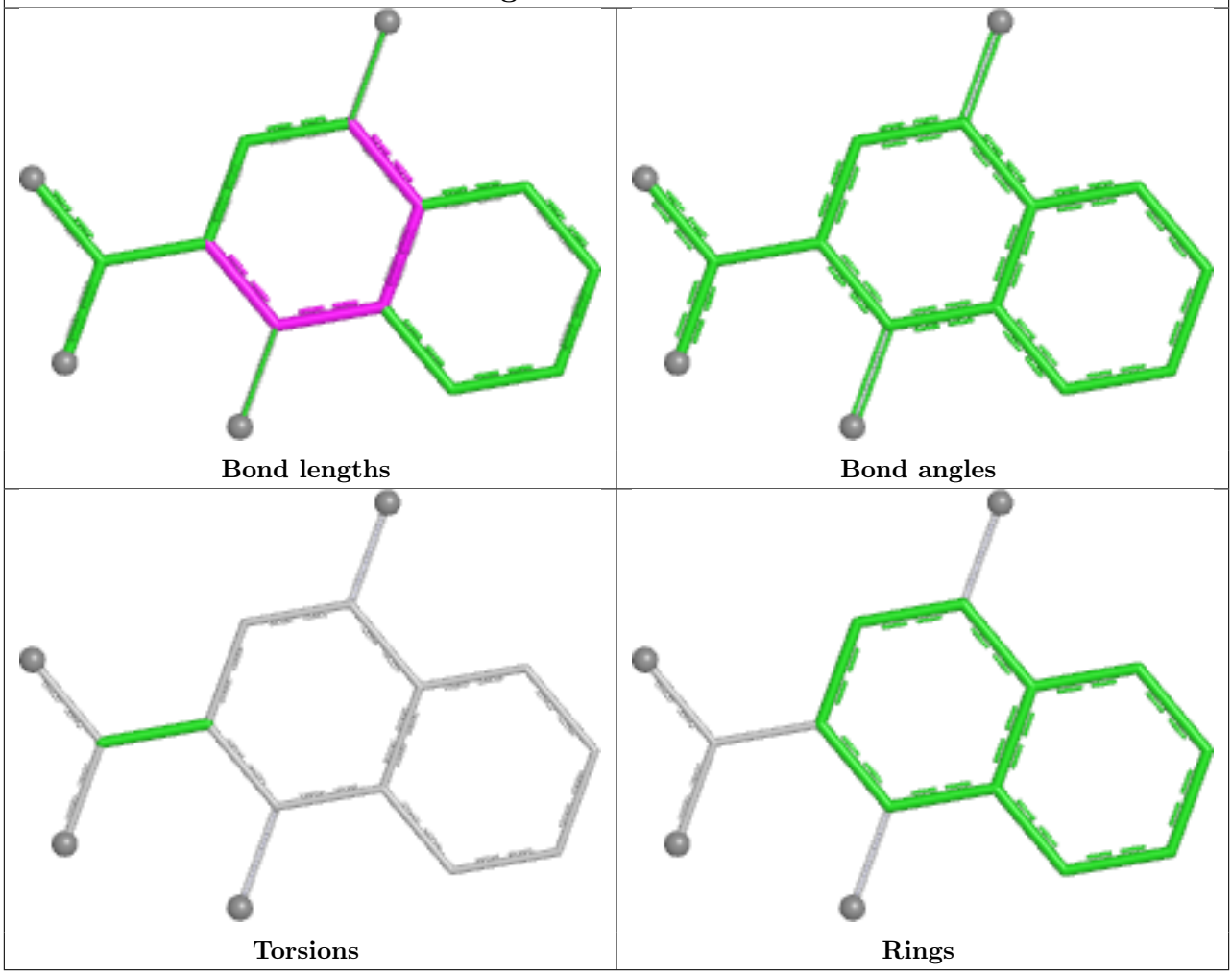
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GOL	2	0
4	D	601	TPP	1	0
2	A	601	GOL	1	0

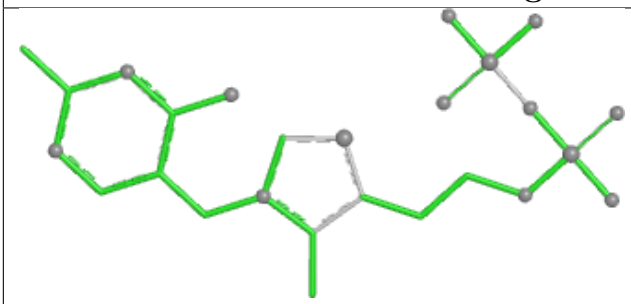
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

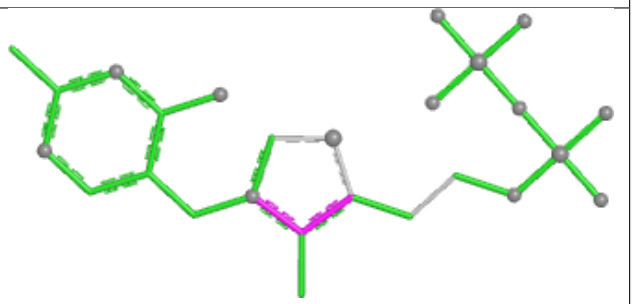
Ligand DNA C 602



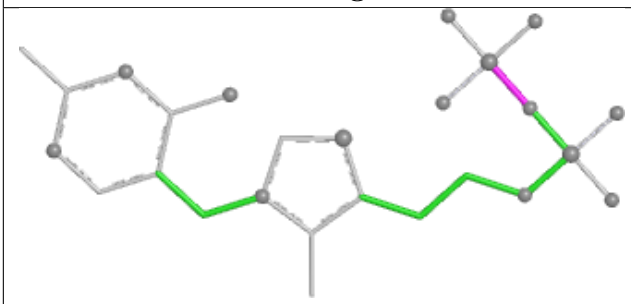
Ligand TPP C 601



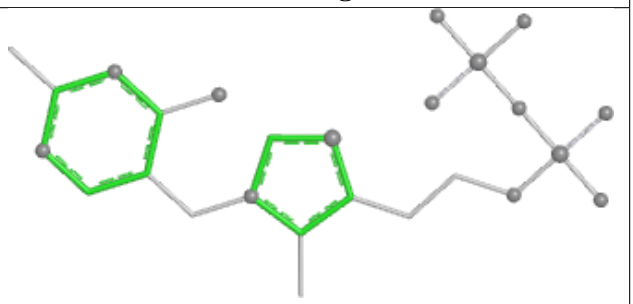
Bond lengths



Bond angles

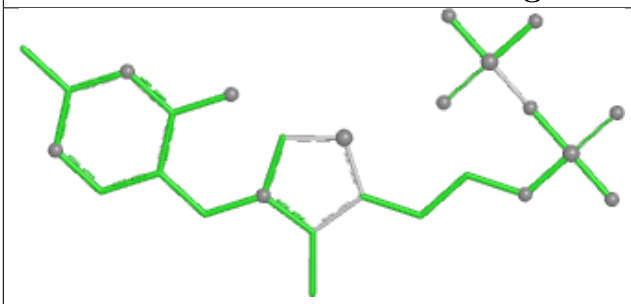


Torsions

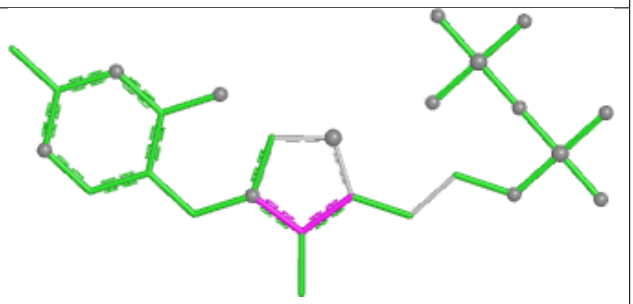


Rings

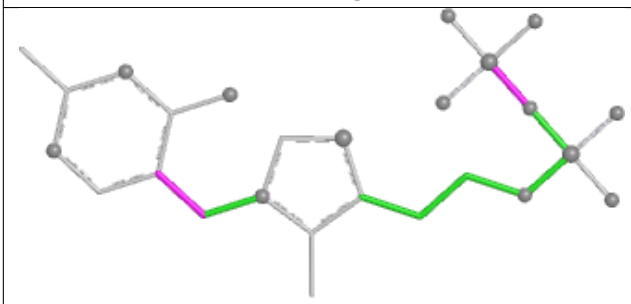
Ligand TPP D 601



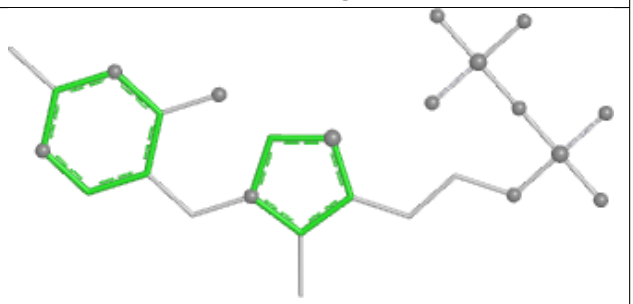
Bond lengths



Bond angles

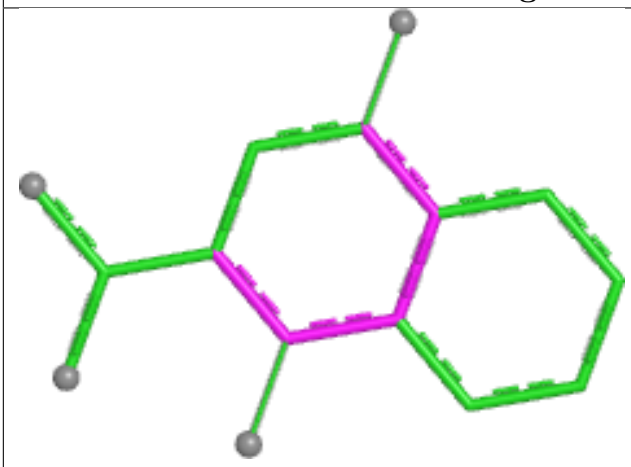


Torsions

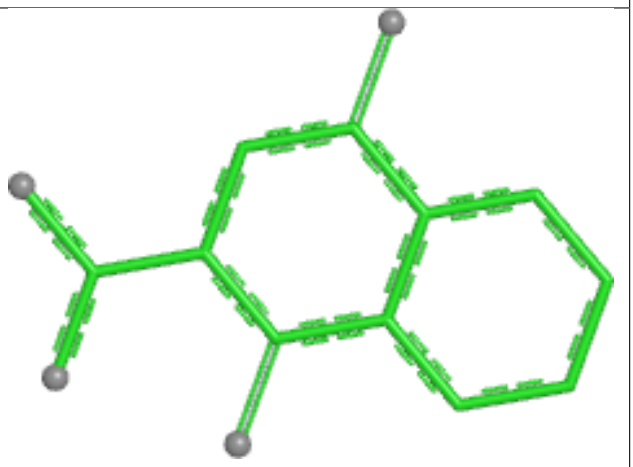


Rings

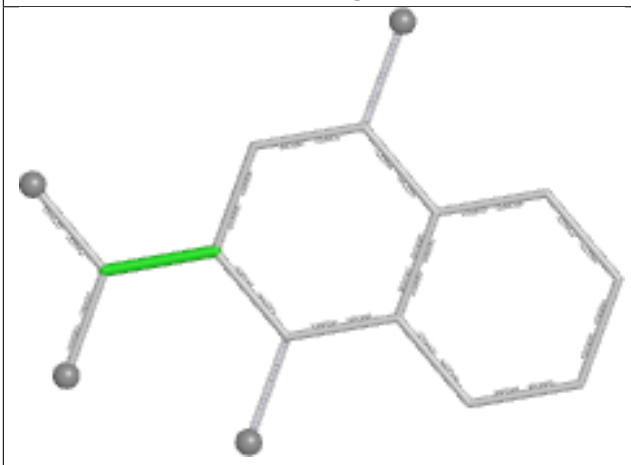
Ligand DNA D 602



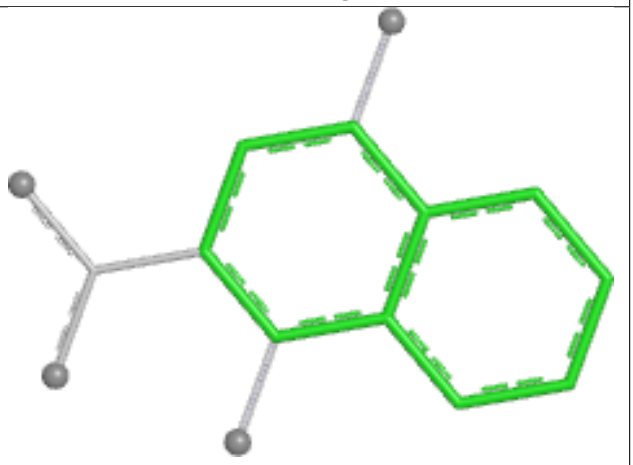
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	-0.02	11 (2%)	64	62	30, 60, 107, 141	2 (0%)
1	B	533/574 (92%)	0.02	11 (2%)	63	61	32, 63, 105, 126	2 (0%)
1	C	533/574 (92%)	0.26	18 (3%)	48	46	31, 72, 114, 148	2 (0%)
1	D	538/574 (93%)	-0.04	16 (2%)	52	50	28, 59, 105, 155	6 (1%)
All	All	2144/2296 (93%)	0.06	56 (2%)	57	54	28, 64, 108, 155	12 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	GLY	5.2
1	D	120	MET	4.6
1	D	34	LEU	4.1
1	B	496	PRO	3.9
1	C	114	THR	3.8
1	B	529	ALA	3.7
1	A	192	LEU	3.6
1	D	195	VAL	3.6
1	A	214[A]	PHE	3.5
1	C	112	LEU	3.4
1	C	74	CYS	3.2
1	D	364[A]	HIS	3.2
1	A	42	ASP	3.1
1	B	471	GLY	3.1
1	C	139	ALA	3.1
1	C	3	PRO	2.8
1	C	111	LEU	2.8
1	D	350[A]	HIS	2.7
1	C	554	LEU	2.7
1	A	428	PRO	2.7
1	D	29	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	113	GLY	2.6
1	C	120	MET	2.6
1	D	141	ALA	2.6
1	B	192	LEU	2.5
1	B	554	LEU	2.5
1	D	428	PRO	2.5
1	D	181	LEU	2.5
1	C	363[A]	SER	2.5
1	C	181	LEU	2.4
1	C	31	ASN	2.4
1	A	489	SER	2.4
1	C	387	GLY	2.4
1	C	459	PRO	2.4
1	D	121	GLU	2.4
1	B	489	SER	2.4
1	C	143	PRO	2.3
1	A	404	ILE	2.3
1	B	53	ILE	2.3
1	D	184	PRO	2.3
1	C	108	PRO	2.3
1	B	195	VAL	2.3
1	B	214[A]	PHE	2.3
1	B	303	ARG	2.2
1	D	109	TYR	2.2
1	A	194	ALA	2.2
1	D	119	THR	2.2
1	D	182	ARG	2.2
1	A	288	LEU	2.1
1	B	426	GLY	2.1
1	D	113	GLY	2.1
1	D	382	ASP	2.1
1	C	42	ASP	2.1
1	C	352	LEU	2.1
1	A	284	VAL	2.0
1	A	191	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

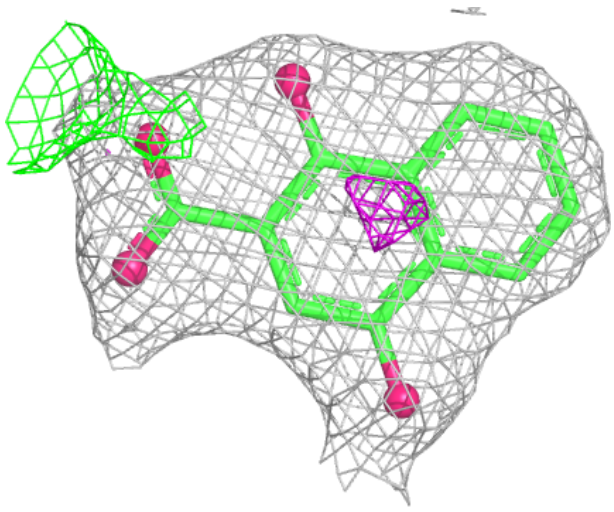
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

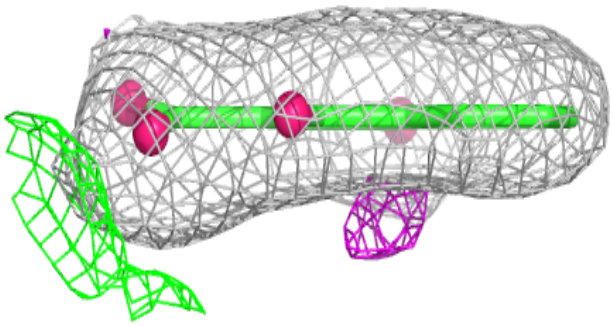
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	D	603	4/4	0.88	0.13	57,62,68,76	0
2	GOL	A	601	6/6	0.90	0.14	57,74,85,86	0
2	GOL	B	601	6/6	0.91	0.16	45,74,83,84	0
5	DNA	C	602	15/15	0.93	0.10	46,55,64,67	0
3	CL	A	602	1/1	0.94	0.07	72,72,72,72	0
5	DNA	D	602	15/15	0.94	0.08	39,45,55,58	0
3	CL	C	604	1/1	0.95	0.09	81,81,81,81	0
3	CL	B	602	1/1	0.96	0.08	82,82,82,82	0
4	TPP	C	601	26/26	0.97	0.07	49,68,81,83	0
3	CL	D	606	1/1	0.98	0.06	75,75,75,75	0
4	TPP	D	601	26/26	0.98	0.05	37,51,60,62	0
3	CL	D	605	1/1	0.99	0.05	60,60,60,60	0
7	MG	D	604	1/1	0.99	0.03	42,42,42,42	0
7	MG	C	603	1/1	0.99	0.03	61,61,61,61	0

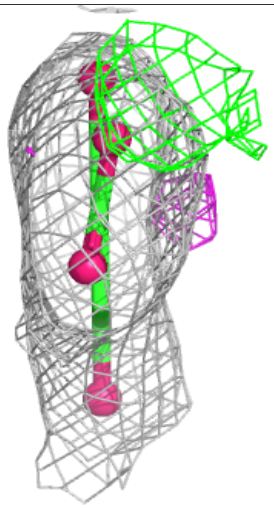
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

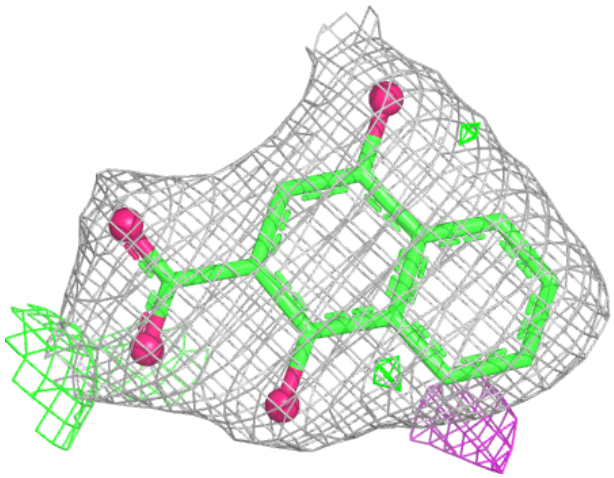


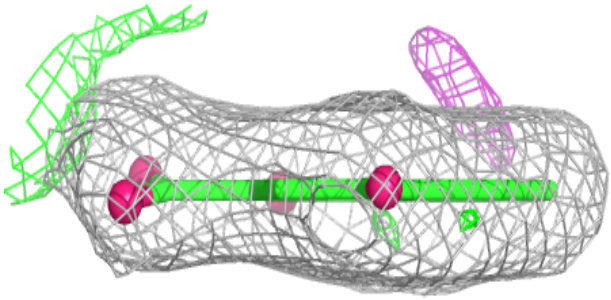


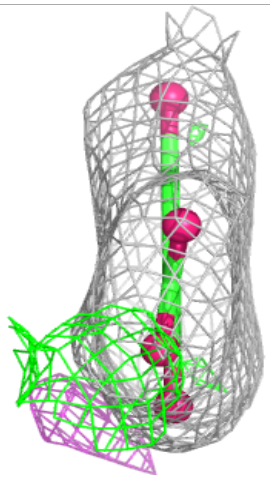


Electron density around DNA D 602:

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

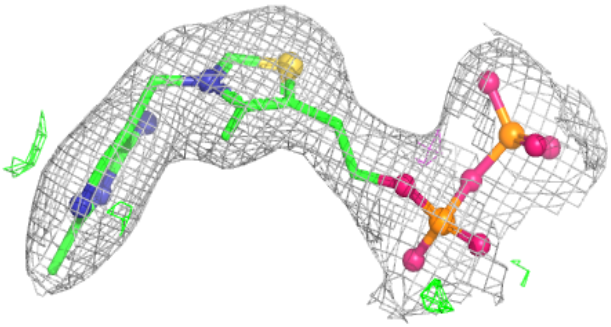


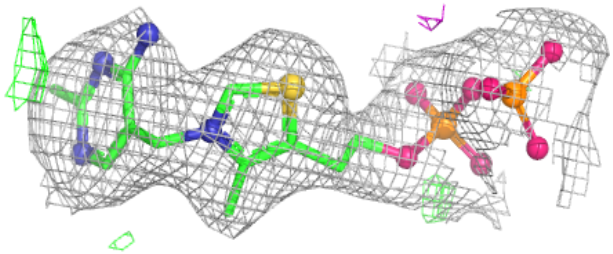


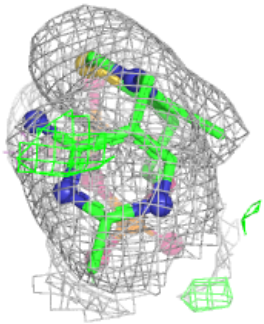


Electron density around TPP C 601:

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

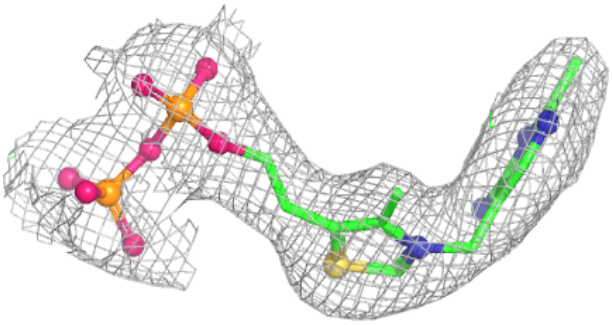


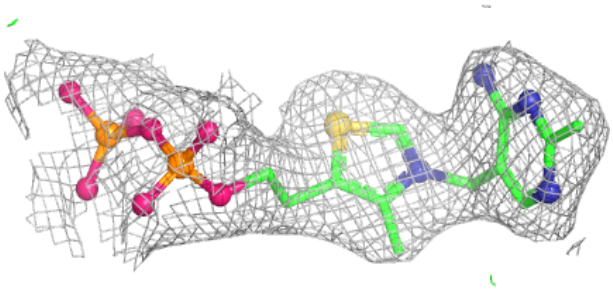


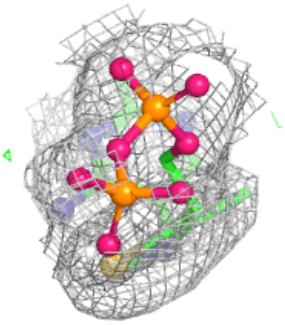


Electron density around TPP D 601:

$2mF_o$-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 (i)

There are no such residues in this entry.