Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 03:58 PM JST

PDB ID	:	5XK9
Title	:	Crystal structure of Isosesquilavandulyl Diphosphate Synthase from Streptomyces sp. strain CNH-189 in complex with GSPP and DMAPP
Authors	:	Ko, T.P.; Guo, R.T.; Liu, W.; Chen, C.C.; Gao, J.
Deposited on	:	2017-05-05
Resolution	:	2.14 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:

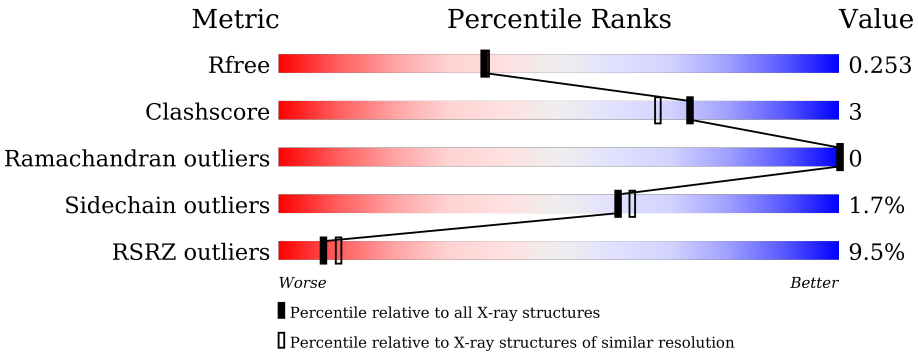
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	232	10% 83% 9% 8%
1	B	232	9% 81% 9% 10%
1	C	232	9% 84% 9% • 6%
1	D	232	6% 83% 7% 10%
1	E	232	11% 86% 6% 8%
1	F	232	7% 83% 7% 10%

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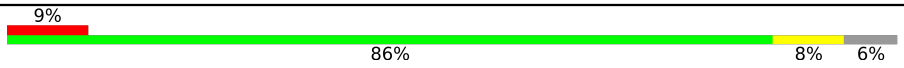
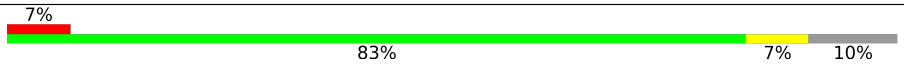
Mol	Chain	Length	Quality of chain
1	G	232	
1	H	232	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15121 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 Undecaprenyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1718	1091	288	326	13			
1	B	209	Total	C	N	O	S	0	0	0
			1672	1063	277	318	14			
1	C	218	Total	C	N	O	S	0	0	0
			1753	1115	292	332	14			
1	D	209	Total	C	N	O	S	0	0	0
			1672	1062	277	320	13			
1	E	214	Total	C	N	O	S	0	0	0
			1718	1091	288	326	13			
1	F	209	Total	C	N	O	S	0	0	0
			1672	1063	277	318	14			
1	G	217	Total	C	N	O	S	0	0	0
			1745	1110	291	330	14			
1	H	208	Total	C	N	O	S	0	0	0
			1664	1058	276	317	13			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	expression tag	UNP M4T4U9
A	-13	ALA	-	expression tag	UNP M4T4U9
A	-12	HIS	-	expression tag	UNP M4T4U9
A	-11	HIS	-	expression tag	UNP M4T4U9
A	-10	HIS	-	expression tag	UNP M4T4U9
A	-9	HIS	-	expression tag	UNP M4T4U9
A	-8	HIS	-	expression tag	UNP M4T4U9
A	-7	HIS	-	expression tag	UNP M4T4U9
A	-6	VAL	-	expression tag	UNP M4T4U9
A	-5	ASP	-	expression tag	UNP M4T4U9
A	-4	ASP	-	expression tag	UNP M4T4U9
A	-3	ASP	-	expression tag	UNP M4T4U9
A	-2	ASP	-	expression tag	UNP M4T4U9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	LYS	-	expression tag	UNP M4T4U9
A	0	MET	-	expression tag	UNP M4T4U9
B	-14	MET	-	expression tag	UNP M4T4U9
B	-13	ALA	-	expression tag	UNP M4T4U9
B	-12	HIS	-	expression tag	UNP M4T4U9
B	-11	HIS	-	expression tag	UNP M4T4U9
B	-10	HIS	-	expression tag	UNP M4T4U9
B	-9	HIS	-	expression tag	UNP M4T4U9
B	-8	HIS	-	expression tag	UNP M4T4U9
B	-7	HIS	-	expression tag	UNP M4T4U9
B	-6	VAL	-	expression tag	UNP M4T4U9
B	-5	ASP	-	expression tag	UNP M4T4U9
B	-4	ASP	-	expression tag	UNP M4T4U9
B	-3	ASP	-	expression tag	UNP M4T4U9
B	-2	ASP	-	expression tag	UNP M4T4U9
B	-1	LYS	-	expression tag	UNP M4T4U9
B	0	MET	-	expression tag	UNP M4T4U9
C	-14	MET	-	expression tag	UNP M4T4U9
C	-13	ALA	-	expression tag	UNP M4T4U9
C	-12	HIS	-	expression tag	UNP M4T4U9
C	-11	HIS	-	expression tag	UNP M4T4U9
C	-10	HIS	-	expression tag	UNP M4T4U9
C	-9	HIS	-	expression tag	UNP M4T4U9
C	-8	HIS	-	expression tag	UNP M4T4U9
C	-7	HIS	-	expression tag	UNP M4T4U9
C	-6	VAL	-	expression tag	UNP M4T4U9
C	-5	ASP	-	expression tag	UNP M4T4U9
C	-4	ASP	-	expression tag	UNP M4T4U9
C	-3	ASP	-	expression tag	UNP M4T4U9
C	-2	ASP	-	expression tag	UNP M4T4U9
C	-1	LYS	-	expression tag	UNP M4T4U9
C	0	MET	-	expression tag	UNP M4T4U9
D	-14	MET	-	expression tag	UNP M4T4U9
D	-13	ALA	-	expression tag	UNP M4T4U9
D	-12	HIS	-	expression tag	UNP M4T4U9
D	-11	HIS	-	expression tag	UNP M4T4U9
D	-10	HIS	-	expression tag	UNP M4T4U9
D	-9	HIS	-	expression tag	UNP M4T4U9
D	-8	HIS	-	expression tag	UNP M4T4U9
D	-7	HIS	-	expression tag	UNP M4T4U9
D	-6	VAL	-	expression tag	UNP M4T4U9
D	-5	ASP	-	expression tag	UNP M4T4U9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ASP	-	expression tag	UNP M4T4U9
D	-3	ASP	-	expression tag	UNP M4T4U9
D	-2	ASP	-	expression tag	UNP M4T4U9
D	-1	LYS	-	expression tag	UNP M4T4U9
D	0	MET	-	expression tag	UNP M4T4U9
E	-14	MET	-	expression tag	UNP M4T4U9
E	-13	ALA	-	expression tag	UNP M4T4U9
E	-12	HIS	-	expression tag	UNP M4T4U9
E	-11	HIS	-	expression tag	UNP M4T4U9
E	-10	HIS	-	expression tag	UNP M4T4U9
E	-9	HIS	-	expression tag	UNP M4T4U9
E	-8	HIS	-	expression tag	UNP M4T4U9
E	-7	HIS	-	expression tag	UNP M4T4U9
E	-6	VAL	-	expression tag	UNP M4T4U9
E	-5	ASP	-	expression tag	UNP M4T4U9
E	-4	ASP	-	expression tag	UNP M4T4U9
E	-3	ASP	-	expression tag	UNP M4T4U9
E	-2	ASP	-	expression tag	UNP M4T4U9
E	-1	LYS	-	expression tag	UNP M4T4U9
E	0	MET	-	expression tag	UNP M4T4U9
F	-14	MET	-	expression tag	UNP M4T4U9
F	-13	ALA	-	expression tag	UNP M4T4U9
F	-12	HIS	-	expression tag	UNP M4T4U9
F	-11	HIS	-	expression tag	UNP M4T4U9
F	-10	HIS	-	expression tag	UNP M4T4U9
F	-9	HIS	-	expression tag	UNP M4T4U9
F	-8	HIS	-	expression tag	UNP M4T4U9
F	-7	HIS	-	expression tag	UNP M4T4U9
F	-6	VAL	-	expression tag	UNP M4T4U9
F	-5	ASP	-	expression tag	UNP M4T4U9
F	-4	ASP	-	expression tag	UNP M4T4U9
F	-3	ASP	-	expression tag	UNP M4T4U9
F	-2	ASP	-	expression tag	UNP M4T4U9
F	-1	LYS	-	expression tag	UNP M4T4U9
F	0	MET	-	expression tag	UNP M4T4U9
G	-14	MET	-	expression tag	UNP M4T4U9
G	-13	ALA	-	expression tag	UNP M4T4U9
G	-12	HIS	-	expression tag	UNP M4T4U9
G	-11	HIS	-	expression tag	UNP M4T4U9
G	-10	HIS	-	expression tag	UNP M4T4U9
G	-9	HIS	-	expression tag	UNP M4T4U9
G	-8	HIS	-	expression tag	UNP M4T4U9

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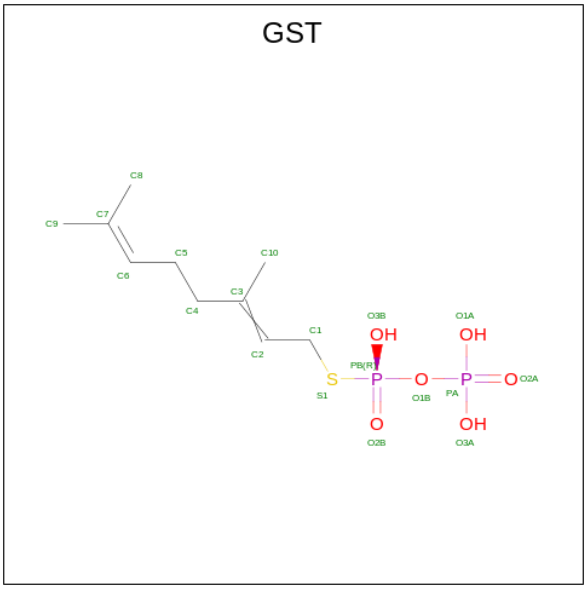
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	HIS	-	expression tag	UNP M4T4U9
G	-6	VAL	-	expression tag	UNP M4T4U9
G	-5	ASP	-	expression tag	UNP M4T4U9
G	-4	ASP	-	expression tag	UNP M4T4U9
G	-3	ASP	-	expression tag	UNP M4T4U9
G	-2	ASP	-	expression tag	UNP M4T4U9
G	-1	LYS	-	expression tag	UNP M4T4U9
G	0	MET	-	expression tag	UNP M4T4U9
H	-14	MET	-	expression tag	UNP M4T4U9
H	-13	ALA	-	expression tag	UNP M4T4U9
H	-12	HIS	-	expression tag	UNP M4T4U9
H	-11	HIS	-	expression tag	UNP M4T4U9
H	-10	HIS	-	expression tag	UNP M4T4U9
H	-9	HIS	-	expression tag	UNP M4T4U9
H	-8	HIS	-	expression tag	UNP M4T4U9
H	-7	HIS	-	expression tag	UNP M4T4U9
H	-6	VAL	-	expression tag	UNP M4T4U9
H	-5	ASP	-	expression tag	UNP M4T4U9
H	-4	ASP	-	expression tag	UNP M4T4U9
H	-3	ASP	-	expression tag	UNP M4T4U9
H	-2	ASP	-	expression tag	UNP M4T4U9
H	-1	LYS	-	expression tag	UNP M4T4U9
H	0	MET	-	expression tag	UNP M4T4U9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

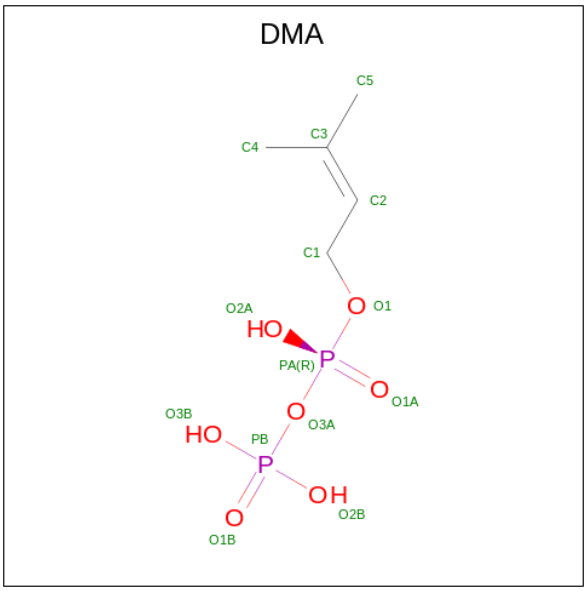
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is GERANYL S-THIOLODIPHOSPHATE (three-letter code: GST) (formula: $C_{10}H_{20}O_6P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
3	B	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
3	C	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
3	D	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
3	E	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
3	F	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
3	G	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
3	H	1	Total	C	O	P	S	0	0
			19	10	6	2	1		

- Molecule 4 is DIMETHYLALLYL DIPHOSPHATE (three-letter code: DMA) (formula: $C_5H_{12}O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 22 5 13 4	0	1
4	B	1	Total C O P 14 5 7 2	0	0
4	C	1	Total C O P 22 5 13 4	0	1
4	D	1	Total C O P 14 5 7 2	0	0
4	E	1	Total C O P 22 5 13 4	0	1
4	F	1	Total C O P 14 5 7 2	0	0
4	G	1	Total C O P 22 5 13 4	0	1
4	H	1	Total C O P 14 5 7 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	143	Total O 143 143	0	0
5	B	152	Total O 152 152	0	0
5	C	171	Total O 171 171	0	0
5	D	139	Total O 139 139	0	0

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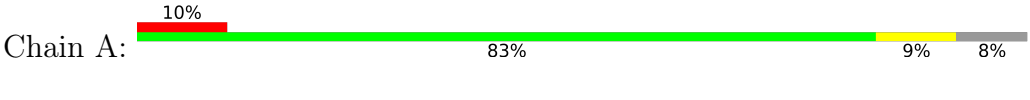
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	137	Total O 137 137	0	0
5	F	162	Total O 162 162	0	0
5	G	160	Total O 160 160	0	0
5	H	139	Total O 139 139	0	0

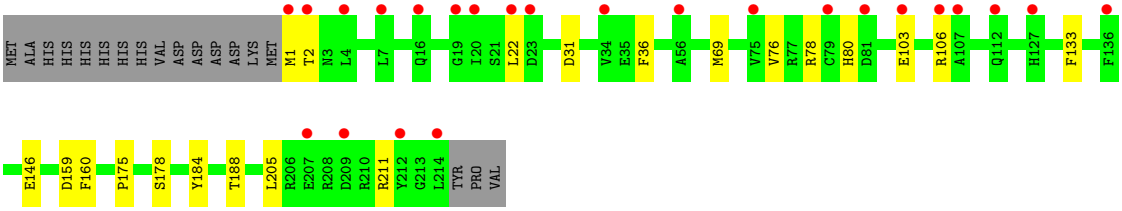
3 Residue-property plots (i)

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: Undecaprenyl diphosphate synthase

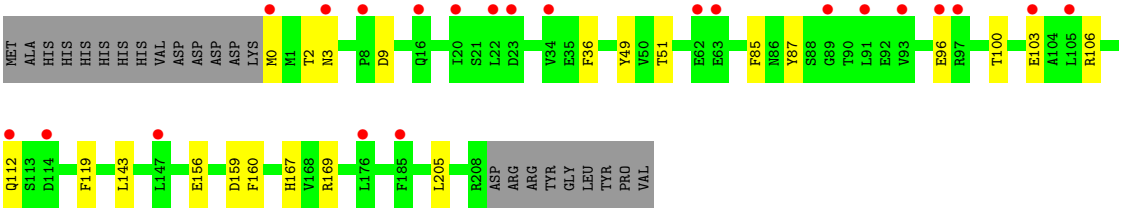
Chain A:





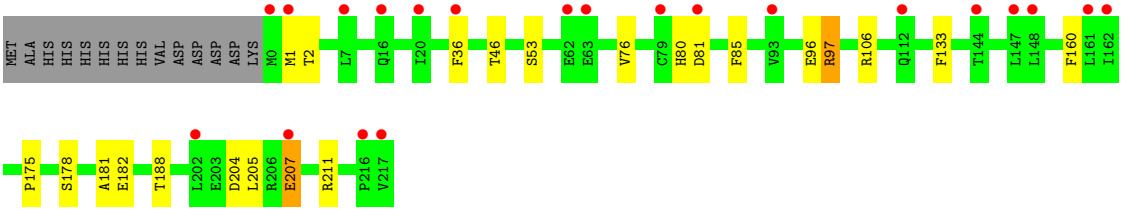
• Molecule 1: Undecaprenyl diphosphate synthase

Chain B:



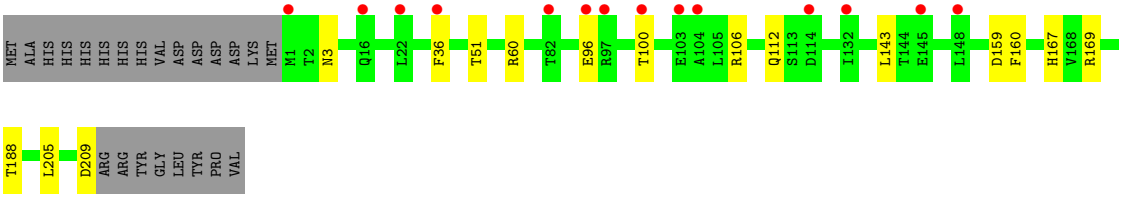
• Molecule 1: Undecaprenyl diphosphate synthase

Chain C:

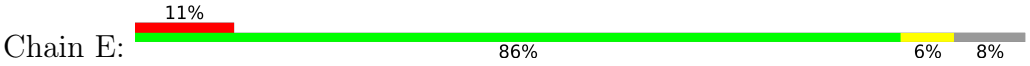


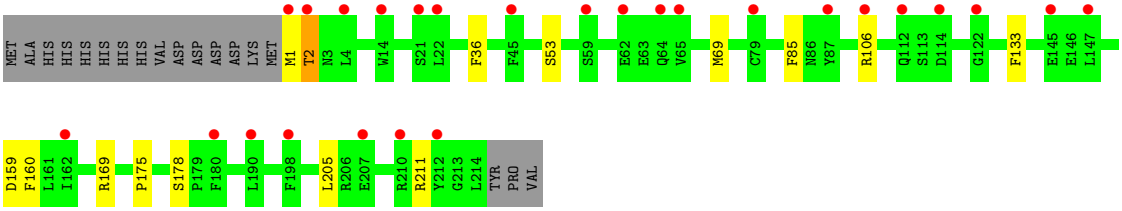
• Molecule 1: Undecaprenyl diphosphate synthase

Chain D:

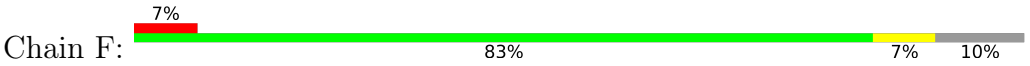


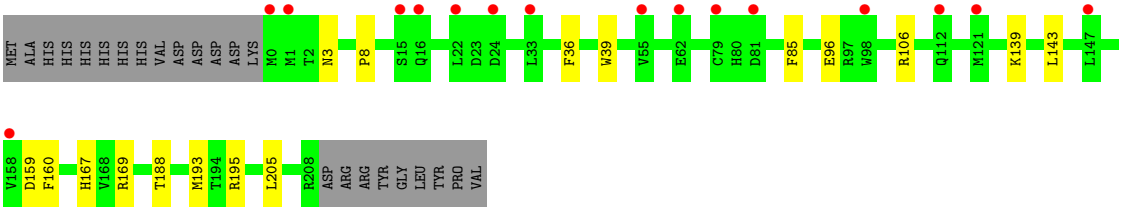
• Molecule 1: Undecaprenyl diphosphate synthase



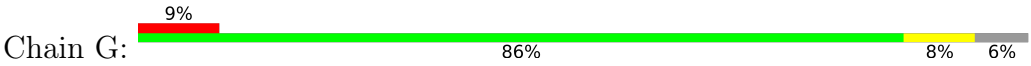


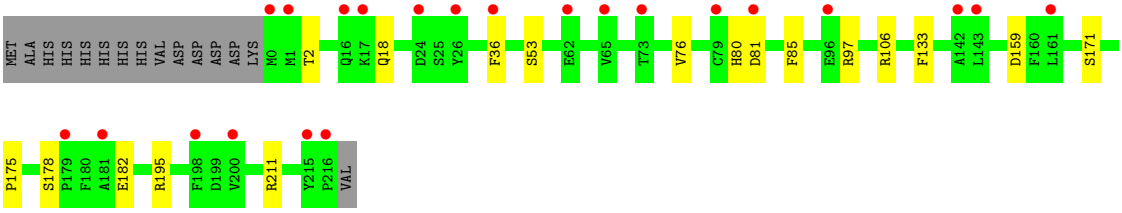
• Molecule 1: Undecaprenyl diphosphate synthase



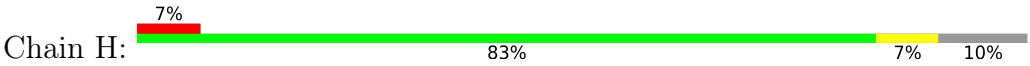


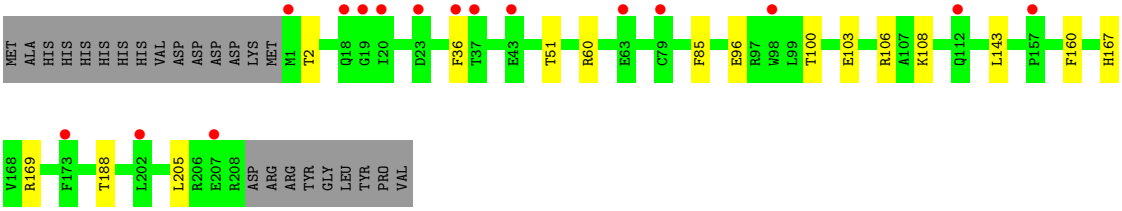
• Molecule 1: Undecaprenyl diphosphate synthase





• Molecule 1: Undecaprenyl diphosphate synthase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.95Å 68.77Å 129.47Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	24.78 – 2.14 24.78 – 2.14	Depositor EDS
% Data completeness (in resolution range)	97.4 (24.78-2.14) 78.1 (24.78-2.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 2.13Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.233 , 0.253 0.233 , 0.253	Depositor DCC
R_{free} test set	2003 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 100.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.339 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15121	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.21% 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: GST, MG, DMA

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	0/1758	0.46	0/2382
1	B	0.30	0/1711	0.47	0/2319
1	C	0.29	0/1795	0.46	0/2432
1	D	0.28	0/1711	0.46	0/2320
1	E	0.27	0/1758	0.45	0/2382
1	F	0.28	0/1711	0.45	0/2319
1	G	0.29	0/1787	0.46	0/2422
1	H	0.28	0/1703	0.46	0/2309
All	All	0.28	0/13934	0.46	0/18885

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	1718	0	1664	13	0
1	B	1672	0	1620	14	0
1	C	1753	0	1698	12	0
1	D	1672	0	1615	12	0
1	E	1718	0	1664	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1672	0	1620	12	0
1	G	1745	0	1689	11	0
1	H	1664	0	1611	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	19	0	17	1	0
3	B	19	0	17	2	0
3	C	19	0	17	2	0
3	D	19	0	17	2	0
3	E	19	0	17	4	0
3	F	19	0	17	0	0
3	G	19	0	17	3	0
3	H	19	0	17	1	0
4	A	22	0	0	0	0
4	B	14	0	9	2	0
4	C	22	0	0	0	0
4	D	14	0	9	2	0
4	E	22	0	0	1	0
4	F	14	0	9	2	0
4	G	22	0	0	1	0
4	H	14	0	9	1	0
5	A	143	0	0	2	0
5	B	152	0	0	0	0
5	C	171	0	0	0	0
5	D	139	0	0	2	0
5	E	137	0	0	2	0
5	F	162	0	0	1	0
5	G	160	0	0	2	0
5	H	139	0	0	1	0
All	All	15121	0	13353	89	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 3.

All (89) 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:175:PRO:HG2	1:C:178:SER:HB2	1.74	0.70
1:G:175:PRO:HG2	1:G:178:SER:HB2	1.76	0.66
1:F:159:ASP:OD1	5:F:601:HOH:O	2.15	0.64
1:A:146:GLU:OE2	5:A:601:HOH:O	2.15	0.63
1:H:108:LYS:NZ	5:H:602:HOH:O	2.31	0.63
1:G:171:SER:OG	4:G:502[B]:DMA:O1B	2.19	0.59
1:A:175:PRO:HG2	1:A:178:SER:HB2	1.87	0.57
1:G:195:ARG:NH2	5:G:606:HOH:O	2.39	0.55
1:B:160:PHE:HB3	1:B:205:LEU:HD13	1.88	0.54
1:G:2:THR:HA	1:G:159:ASP:OD2	2.07	0.54
1:F:169:ARG:NH2	4:F:502:DMA:O1B	2.35	0.54
1:D:159:ASP:OD1	1:F:139:LYS:NZ	2.35	0.54
1:A:69:MET:SD	3:A:501:GST:H91	2.48	0.53
1:E:169:ARG:NH2	5:E:605:HOH:O	2.40	0.53
1:B:96:GLU:OE2	1:B:100:THR:OG1	2.27	0.52
1:B:9:ASP:HA	3:B:501:GST:H11	1.91	0.52
1:C:160:PHE:HB3	1:C:205:LEU:HD13	1.92	0.51
1:G:18:GLN:NE2	5:G:603:HOH:O	2.36	0.51
1:D:96:GLU:OE2	1:D:100:THR:OG1	2.29	0.51
1:E:211:ARG:HH12	1:F:167:HIS:HE1	1.59	0.51
1:C:85:PHE:O	1:C:106:ARG:HG3	2.10	0.51
1:A:2:THR:HA	1:A:159:ASP:OD2	2.12	0.50
1:H:96:GLU:OE1	1:H:100:THR:OG1	2.29	0.50
1:G:53:SER:HB3	3:G:501:GST:H92	1.94	0.49
1:B:169:ARG:NH2	4:B:502:DMA:O1B	2.37	0.49
1:F:96:GLU:H	1:F:96:GLU:CD	2.15	0.49
1:C:76:VAL:O	1:C:80:HIS:HB3	2.12	0.49
1:D:160:PHE:HB3	1:D:205:LEU:HD13	1.94	0.49
1:C:53:SER:HB3	3:C:501:GST:H82	1.95	0.49
1:H:103:GLU:OE2	1:H:106:ARG:NH1	2.47	0.48
1:G:85:PHE:O	1:G:106:ARG:HG3	2.13	0.47
1:D:112:GLN:NE2	5:D:614:HOH:O	2.46	0.47
1:F:188:THR:OG1	1:F:193:MET:SD	2.73	0.47
1:E:85:PHE:O	1:E:106:ARG:HG3	2.14	0.47
1:B:3:ASN:O	1:B:159:ASP:HB2	2.14	0.47
1:G:133:PHE:CD1	1:H:143:LEU:HB2	2.48	0.47
4:E:502[A]:DMA:O1B	5:E:601:HOH:O	2.20	0.46
1:B:49:TYR:OH	1:B:156:GLU:HG2	2.14	0.46
1:E:2:THR:HA	1:E:159:ASP:OD2	2.15	0.46
1:B:85:PHE:O	1:B:106:ARG:HG3	2.16	0.46
1:G:211:ARG:HH12	1:H:167:HIS:HE1	1.64	0.46
1:E:175:PRO:HG2	1:E:178:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:PHE:O	1:H:106:ARG:HG3	2.15	0.46
1:C:182:GLU:OE2	1:D:169:ARG:NH1	2.45	0.46
1:A:160:PHE:HB3	1:A:205:LEU:HD13	1.98	0.45
1:B:103:GLU:OE2	1:B:106:ARG:NH1	2.51	0.44
1:E:69:MET:SD	3:E:501:GST:H91	2.56	0.44
1:C:133:PHE:CD1	1:D:143:LEU:HB2	2.52	0.44
1:D:3:ASN:OD1	1:D:159:ASP:N	2.28	0.44
1:F:160:PHE:HB3	1:F:205:LEU:HD13	1.99	0.44
1:H:51:THR:O	4:H:502:DMA:H41	2.18	0.44
1:D:106:ARG:NH1	5:D:610:HOH:O	2.41	0.44
1:E:53:SER:HB3	3:E:501:GST:H92	2.00	0.44
1:H:160:PHE:HB3	1:H:205:LEU:HD13	1.99	0.43
1:B:9:ASP:HA	3:B:501:GST:C1	2.48	0.43
1:B:51:THR:O	4:B:502:DMA:H41	2.18	0.43
1:F:8:PRO:O	4:F:502:DMA:H53	2.19	0.43
1:A:76:VAL:O	1:A:80:HIS:HB3	2.18	0.43
1:D:3:ASN:O	1:D:159:ASP:HB2	2.18	0.43
1:F:3:ASN:O	1:F:159:ASP:HB2	2.18	0.43
1:F:39:TRP:CD1	1:F:195:ARG:HD3	2.54	0.43
1:C:97:ARG:H	1:C:97:ARG:HG3	1.53	0.43
1:D:51:THR:O	4:D:502:DMA:H41	2.19	0.43
1:A:103:GLU:OE1	1:A:106:ARG:NH2	2.52	0.42
1:B:2:THR:HA	1:B:159:ASP:OD2	2.19	0.42
1:C:178:SER:HB3	1:C:181:ALA:HB2	2.01	0.42
1:A:211:ARG:HH12	1:B:167:HIS:HE1	1.67	0.42
1:E:133:PHE:CD1	1:F:143:LEU:HB2	2.53	0.42
1:H:60:ARG:HD2	3:H:501:GST:H93	2.00	0.42
1:E:160:PHE:HB3	1:E:205:LEU:HD13	2.02	0.42
1:A:133:PHE:CD1	1:B:143:LEU:HB2	2.54	0.42
1:A:31:ASP:OD1	1:A:78:ARG:NH1	2.36	0.42
1:C:211:ARG:HH12	1:D:167:HIS:HE1	1.68	0.42
1:G:76:VAL:O	1:G:80:HIS:HB3	2.19	0.42
1:A:211:ARG:NH1	5:A:613:HOH:O	2.51	0.42
1:A:184:TYR:HB2	1:A:205:LEU:HD21	2.02	0.42
1:B:87:TYR:HA	1:B:119:PHE:O	2.20	0.41
1:C:204:ASP:O	1:C:207:GLU:HG3	2.20	0.41
1:G:182:GLU:OE2	1:H:169:ARG:NH1	2.48	0.41
1:C:1:MET:HG3	1:C:46:THR:OG1	2.19	0.41
1:F:85:PHE:O	1:F:106:ARG:HG3	2.19	0.41
1:A:22:LEU:HD12	1:A:22:LEU:HA	1.95	0.41
3:D:501:GST:C10	4:D:502:DMA:H42	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ARG:HD2	3:D:501:GST:H93	2.03	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	212/232 (91%)	209 (99%)	3 (1%)	0	100	100
1	B	207/232 (89%)	204 (99%)	3 (1%)	0	100	100
1	C	216/232 (93%)	213 (99%)	3 (1%)	0	100	100
1	D	207/232 (89%)	203 (98%)	4 (2%)	0	100	100
1	E	212/232 (91%)	209 (99%)	3 (1%)	0	100	100
1	F	207/232 (89%)	205 (99%)	2 (1%)	0	100	100
1	G	215/232 (93%)	212 (99%)	3 (1%)	0	100	100
1	H	206/232 (89%)	202 (98%)	4 (2%)	0	100	100
All	All	1682/1856 (91%)	1657 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	187/204 (92%)	184 (98%)	3 (2%)	62	65
1	B	183/204 (90%)	180 (98%)	3 (2%)	62	65
1	C	191/204 (94%)	184 (96%)	7 (4%)	34	31
1	D	183/204 (90%)	180 (98%)	3 (2%)	62	65
1	E	187/204 (92%)	184 (98%)	3 (2%)	62	65
1	F	183/204 (90%)	182 (100%)	1 (0%)	88	91
1	G	190/204 (93%)	187 (98%)	3 (2%)	62	65
1	H	182/204 (89%)	179 (98%)	3 (2%)	62	65
All	All	1486/1632 (91%)	1460 (98%)	26 (2%)	60	63

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	36	PHE
1	A	188	THR
1	B	0	MET
1	B	36	PHE
1	B	112	GLN
1	C	2	THR
1	C	36	PHE
1	C	81	ASP
1	C	96	GLU
1	C	97	ARG
1	C	188	THR
1	C	207	GLU
1	D	36	PHE
1	D	188	THR
1	D	209	ASP
1	E	1	MET
1	E	2	THR
1	E	36	PHE
1	F	36	PHE
1	G	36	PHE
1	G	81	ASP
1	G	97	ARG
1	H	2	THR
1	H	36	PHE
1	H	188	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	B	167	HIS
1	C	18	GLN
1	D	112	GLN
1	D	167	HIS
1	E	18	GLN
1	F	167	HIS
1	G	18	GLN
1	H	167	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	DMA	C	502[B]	2	11,13,13	1.11	1 (9%)	15,19,19	1.50	3 (20%)
4	DMA	A	502[B]	2	11,13,13	1.10	1 (9%)	15,19,19	1.45	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DMA	C	502[A]	-	11,13,13	1.10	1 (9%)	15,19,19	1.42	2 (13%)
4	DMA	A	502[A]	2	11,13,13	1.06	1 (9%)	15,19,19	1.38	3 (20%)
3	GST	D	501	2	14,18,18	1.02	1 (7%)	17,25,25	1.39	3 (17%)
4	DMA	B	502	2	11,13,13	1.16	1 (9%)	15,19,19	1.36	3 (20%)
3	GST	G	501	2	14,18,18	1.04	0	17,25,25	1.26	2 (11%)
3	GST	H	501	2	14,18,18	1.09	2 (14%)	17,25,25	1.32	3 (17%)
4	DMA	H	502	2	11,13,13	1.17	1 (9%)	15,19,19	1.36	3 (20%)
3	GST	F	501	2	14,18,18	1.08	2 (14%)	17,25,25	1.29	3 (17%)
4	DMA	D	502	2	11,13,13	1.19	1 (9%)	15,19,19	1.27	2 (13%)
3	GST	C	501	2	14,18,18	1.12	2 (14%)	17,25,25	1.31	2 (11%)
3	GST	A	501	2	14,18,18	1.08	2 (14%)	17,25,25	1.53	3 (17%)
4	DMA	G	502[B]	2	11,13,13	1.11	1 (9%)	15,19,19	1.46	3 (20%)
4	DMA	E	502[B]	2	11,13,13	1.13	1 (9%)	15,19,19	1.47	3 (20%)
4	DMA	G	502[A]	-	11,13,13	1.09	1 (9%)	15,19,19	1.42	2 (13%)
3	GST	E	501	2	14,18,18	1.11	2 (14%)	17,25,25	1.47	3 (17%)
4	DMA	F	502	2	11,13,13	1.15	1 (9%)	15,19,19	1.47	3 (20%)
4	DMA	E	502[A]	2	11,13,13	1.12	1 (9%)	15,19,19	1.42	3 (20%)
3	GST	B	501	2	14,18,18	1.12	2 (14%)	17,25,25	1.42	3 (17%)

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	DMA	C	502[B]	2	-	3/13/13/13	-
4	DMA	A	502[B]	2	-	7/13/13/13	-
4	DMA	C	502[A]	-	-	7/13/13/13	-
4	DMA	A	502[A]	2	-	7/13/13/13	-
3	GST	D	501	2	-	1/13/19/19	-
4	DMA	B	502	2	-	2/13/13/13	-
3	GST	G	501	2	-	1/13/19/19	-
3	GST	H	501	2	-	1/13/19/19	-
4	DMA	H	502	2	-	3/13/13/13	-
3	GST	F	501	2	-	2/13/19/19	-
4	DMA	D	502	2	-	2/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GST	C	501	2	-	2/13/19/19	-
3	GST	A	501	2	-	4/13/19/19	-
4	DMA	G	502[B]	2	-	5/13/13/13	-
4	DMA	E	502[B]	2	-	3/13/13/13	-
4	DMA	G	502[A]	-	-	6/13/13/13	-
3	GST	E	501	2	-	4/13/19/19	-
4	DMA	F	502	2	-	2/13/13/13	-
4	DMA	E	502[A]	2	-	7/13/13/13	-
3	GST	B	501	2	-	2/13/19/19	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	502	DMA	O1-C1	-2.59	1.39	1.43
4	D	502	DMA	O1-C1	-2.57	1.39	1.43
4	F	502	DMA	O1-C1	-2.56	1.39	1.43
4	B	502	DMA	O1-C1	-2.52	1.40	1.43
3	B	501	GST	C1-S1	-2.41	1.81	1.84
3	E	501	GST	C1-S1	-2.32	1.81	1.84
4	E	502[A]	DMA	O1-C1	-2.31	1.40	1.43
4	E	502[B]	DMA	O1-C1	-2.31	1.40	1.43
3	H	501	GST	C1-S1	-2.27	1.81	1.84
4	G	502[A]	DMA	O1-C1	-2.26	1.40	1.43
4	G	502[B]	DMA	O1-C1	-2.26	1.40	1.43
4	C	502[A]	DMA	O1-C1	-2.25	1.40	1.43
4	C	502[B]	DMA	O1-C1	-2.25	1.40	1.43
3	A	501	GST	PB-O3B	-2.19	1.51	1.56
3	C	501	GST	C1-S1	-2.19	1.81	1.84
3	E	501	GST	PB-O3B	-2.17	1.51	1.56
3	C	501	GST	PB-O3B	-2.16	1.51	1.56
4	A	502[A]	DMA	O1-C1	-2.11	1.40	1.43
4	A	502[B]	DMA	O1-C1	-2.11	1.40	1.43
3	A	501	GST	C1-S1	-2.11	1.81	1.84
3	F	501	GST	C1-S1	-2.11	1.81	1.84
3	B	501	GST	PB-O3B	-2.10	1.51	1.56
3	F	501	GST	PB-O3B	-2.09	1.51	1.56
3	D	501	GST	PB-O3B	-2.01	1.51	1.56
3	H	501	GST	PB-O3B	-2.00	1.51	1.56

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	502[A]	DMA	C1-C2-C3	-3.64	120.86	126.75
4	C	502[B]	DMA	C1-C2-C3	-3.64	120.86	126.75
3	A	501	GST	C10-C3-C4	3.58	121.29	115.27
4	G	502[A]	DMA	C1-C2-C3	-3.54	121.03	126.75
4	G	502[B]	DMA	C1-C2-C3	-3.54	121.03	126.75
3	E	501	GST	C10-C3-C4	3.53	121.22	115.27
4	F	502	DMA	C1-C2-C3	-3.52	121.06	126.75
4	E	502[A]	DMA	C1-C2-C3	-3.52	121.06	126.75
4	E	502[B]	DMA	C1-C2-C3	-3.52	121.06	126.75
4	A	502[A]	DMA	C1-C2-C3	-3.40	121.25	126.75
4	A	502[B]	DMA	C1-C2-C3	-3.40	121.25	126.75
3	C	501	GST	C10-C3-C4	3.15	120.57	115.27
4	B	502	DMA	C1-C2-C3	-3.12	121.71	126.75
3	B	501	GST	C10-C3-C4	3.02	120.35	115.27
4	C	502[B]	DMA	PA-O3A-PB	-3.00	122.54	132.83
3	G	501	GST	C10-C3-C4	2.98	120.29	115.27
4	H	502	DMA	C1-C2-C3	-2.92	122.03	126.75
4	E	502[B]	DMA	PA-O3A-PB	-2.89	122.92	132.83
4	D	502	DMA	C1-C2-C3	-2.85	122.15	126.75
3	H	501	GST	C10-C3-C4	2.77	119.93	115.27
4	G	502[B]	DMA	PA-O3A-PB	-2.73	123.44	132.83
3	F	501	GST	C10-C3-C4	2.70	119.81	115.27
4	F	502	DMA	PA-O3A-PB	-2.69	123.59	132.83
3	A	501	GST	C8-C7-C9	2.69	120.53	114.60
3	D	501	GST	C5-C6-C7	-2.68	118.58	127.75
3	B	501	GST	C8-C7-C9	2.62	120.39	114.60
4	H	502	DMA	C5-C3-C4	2.58	120.30	114.60
3	E	501	GST	C8-C7-C9	2.58	120.29	114.60
3	B	501	GST	C5-C6-C7	-2.53	119.09	127.75
4	B	502	DMA	C5-C3-C4	2.53	120.19	114.60
3	D	501	GST	C10-C3-C4	2.52	119.50	115.27
4	F	502	DMA	C5-C3-C4	2.45	120.02	114.60
3	H	501	GST	C5-C6-C7	-2.43	119.43	127.75
3	D	501	GST	C8-C7-C9	2.43	119.98	114.60
3	C	501	GST	C8-C7-C9	2.39	119.89	114.60
4	A	502[B]	DMA	PA-O3A-PB	-2.35	124.78	132.83
4	G	502[A]	DMA	C5-C3-C4	2.34	119.78	114.60
4	G	502[B]	DMA	C5-C3-C4	2.34	119.78	114.60
3	F	501	GST	C5-C6-C7	-2.33	119.78	127.75
4	E	502[A]	DMA	C5-C3-C4	2.30	119.67	114.60
4	E	502[B]	DMA	C5-C3-C4	2.30	119.67	114.60
4	B	502	DMA	PA-O3A-PB	-2.29	124.96	132.83
3	F	501	GST	C8-C7-C9	2.29	119.66	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	502[A]	DMA	C5-C3-C4	2.26	119.60	114.60
4	C	502[B]	DMA	C5-C3-C4	2.26	119.60	114.60
3	G	501	GST	C8-C7-C9	2.24	119.55	114.60
4	A	502[A]	DMA	C5-C3-C4	2.23	119.53	114.60
4	A	502[B]	DMA	C5-C3-C4	2.23	119.53	114.60
3	E	501	GST	C5-C6-C7	-2.21	120.19	127.75
3	H	501	GST	C8-C7-C9	2.20	119.47	114.60
4	E	502[A]	DMA	PA-O3A-PB	-2.14	125.48	132.83
3	A	501	GST	C5-C6-C7	-2.12	120.50	127.75
4	D	502	DMA	C5-C3-C4	2.12	119.28	114.60
4	H	502	DMA	PA-O3A-PB	-2.09	125.67	132.83
4	A	502[A]	DMA	PA-O3A-PB	-2.08	125.67	132.83

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	501	GST	C2-C3-C4-C5
3	E	501	GST	C10-C3-C4-C5
3	F	501	GST	PB-O1B-PA-O3A
4	A	502[A]	DMA	C1-O1-PA-O1A
4	A	502[A]	DMA	C1-O1-PA-O2A
4	A	502[A]	DMA	PA-O3A-PB-O2B
4	A	502[A]	DMA	PA-O3A-PB-O3B
4	A	502[B]	DMA	C1-O1-PA-O1A
4	A	502[B]	DMA	C1-O1-PA-O2A
4	A	502[B]	DMA	C1-O1-PA-O3A
4	A	502[B]	DMA	PA-O3A-PB-O2B
4	A	502[B]	DMA	PA-O3A-PB-O3B
4	B	502	DMA	C1-O1-PA-O3A
4	C	502[A]	DMA	C1-O1-PA-O1A
4	C	502[A]	DMA	C1-O1-PA-O2A
4	C	502[A]	DMA	PA-O3A-PB-O3B
4	C	502[B]	DMA	C1-O1-PA-O1A
4	C	502[B]	DMA	C1-O1-PA-O2A
4	D	502	DMA	C1-O1-PA-O3A
4	E	502[A]	DMA	C1-O1-PA-O1A
4	E	502[A]	DMA	C1-O1-PA-O2A
4	E	502[A]	DMA	PA-O3A-PB-O2B
4	E	502[B]	DMA	C1-O1-PA-O1A
4	E	502[B]	DMA	C1-O1-PA-O2A
4	F	502	DMA	C1-O1-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	G	502[A]	DMA	C1-O1-PA-O1A
4	G	502[A]	DMA	C1-O1-PA-O2A
4	G	502[A]	DMA	PA-O3A-PB-O2B
4	G	502[A]	DMA	PA-O3A-PB-O3B
4	G	502[B]	DMA	C1-O1-PA-O1A
4	G	502[B]	DMA	C1-O1-PA-O2A
4	G	502[B]	DMA	PB-O3A-PA-O1
4	H	502	DMA	C1-O1-PA-O2A
4	H	502	DMA	C1-O1-PA-O3A
3	A	501	GST	C10-C3-C4-C5
3	B	501	GST	C3-C4-C5-C6
3	H	501	GST	C3-C4-C5-C6
3	A	501	GST	C2-C3-C4-C5
3	D	501	GST	C3-C4-C5-C6
3	F	501	GST	C3-C4-C5-C6
4	A	502[B]	DMA	C2-C1-O1-PA
4	G	502[B]	DMA	PA-O3A-PB-O1B
4	E	502[A]	DMA	PA-O3A-PB-O1B
4	C	502[B]	DMA	C1-O1-PA-O3A
4	E	502[B]	DMA	C1-O1-PA-O3A
4	G	502[B]	DMA	C1-O1-PA-O3A
3	A	501	GST	PA-O1B-PB-O3B
3	E	501	GST	PA-O1B-PB-O3B
3	G	501	GST	PA-O1B-PB-O3B
4	C	502[A]	DMA	PB-O3A-PA-O2A
4	E	502[A]	DMA	PB-O3A-PA-O2A
4	B	502	DMA	C1-O1-PA-O2A
4	D	502	DMA	C1-O1-PA-O1A
4	F	502	DMA	C1-O1-PA-O2A
4	H	502	DMA	C1-O1-PA-O1A
3	C	501	GST	PA-O1B-PB-O3B
4	G	502[A]	DMA	PB-O3A-PA-O2A
4	A	502[A]	DMA	PA-O3A-PB-O1B
4	A	502[B]	DMA	PA-O3A-PB-O1B
4	C	502[A]	DMA	PA-O3A-PB-O1B
3	B	501	GST	PB-O1B-PA-O3A
4	C	502[A]	DMA	PA-O3A-PB-O2B
4	A	502[A]	DMA	C2-C1-O1-PA
4	E	502[A]	DMA	C2-C1-O1-PA
4	A	502[A]	DMA	C1-O1-PA-O3A
4	C	502[A]	DMA	C1-O1-PA-O3A
4	E	502[A]	DMA	C1-O1-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	G	502[A]	DMA	C1-O1-PA-O3A
3	A	501	GST	PA-O1B-PB-O2B
3	C	501	GST	PA-O1B-PB-O2B
3	E	501	GST	PA-O1B-PB-O2B

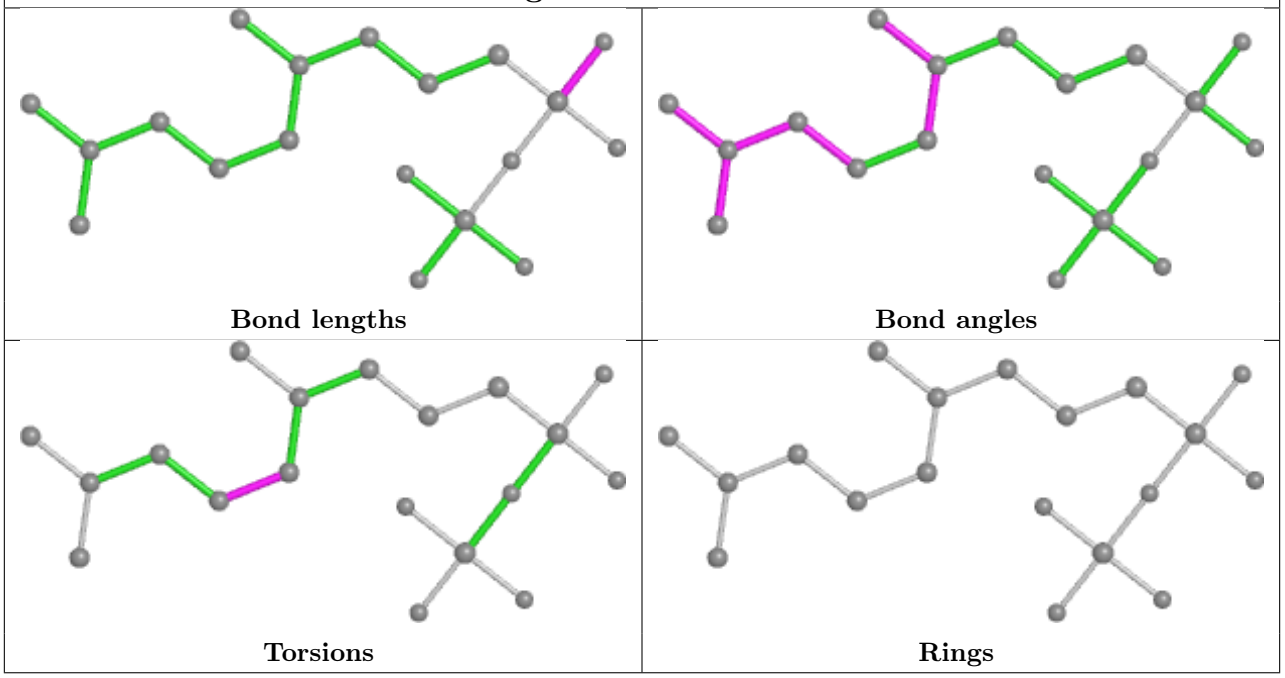
There are no ring outliers.

13 monomers are involved in 23 short contacts:

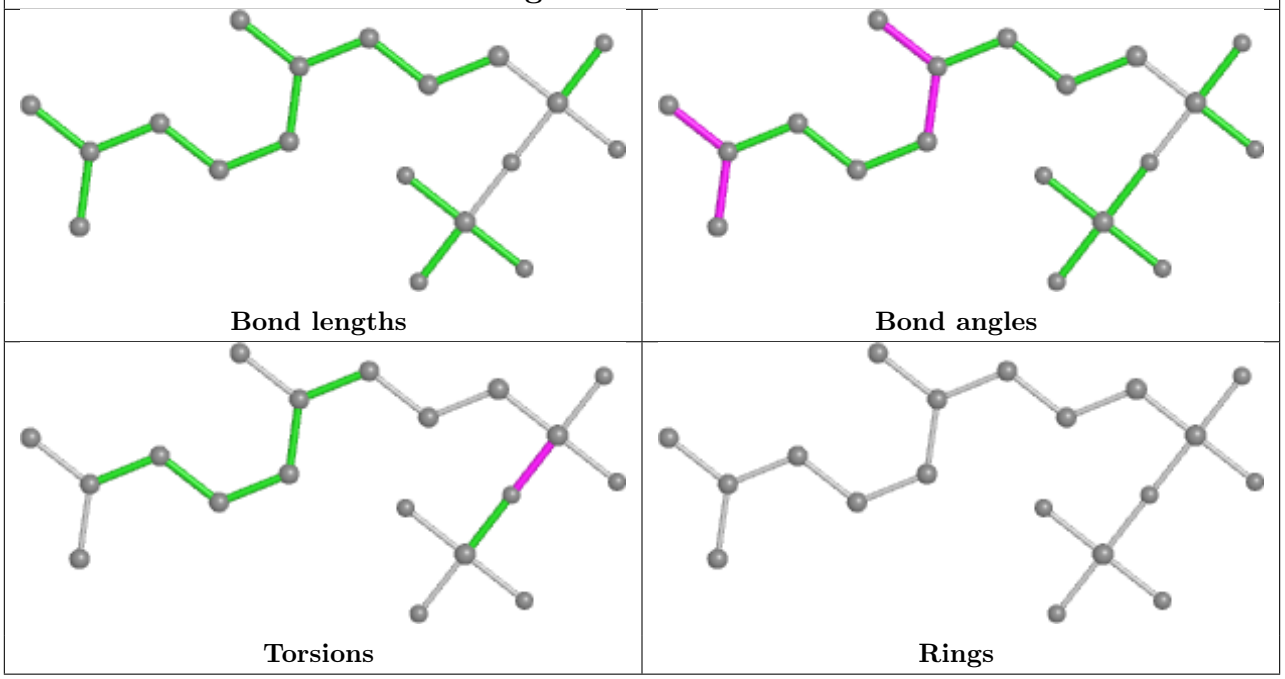
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	GST	2	0
4	B	502	DMA	2	0
3	G	501	GST	3	0
3	H	501	GST	1	0
4	H	502	DMA	1	0
4	D	502	DMA	2	0
3	C	501	GST	2	0
3	A	501	GST	1	0
4	G	502[B]	DMA	1	0
3	E	501	GST	4	0
4	F	502	DMA	2	0
4	E	502[A]	DMA	1	0
3	B	501	GST	2	0

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.

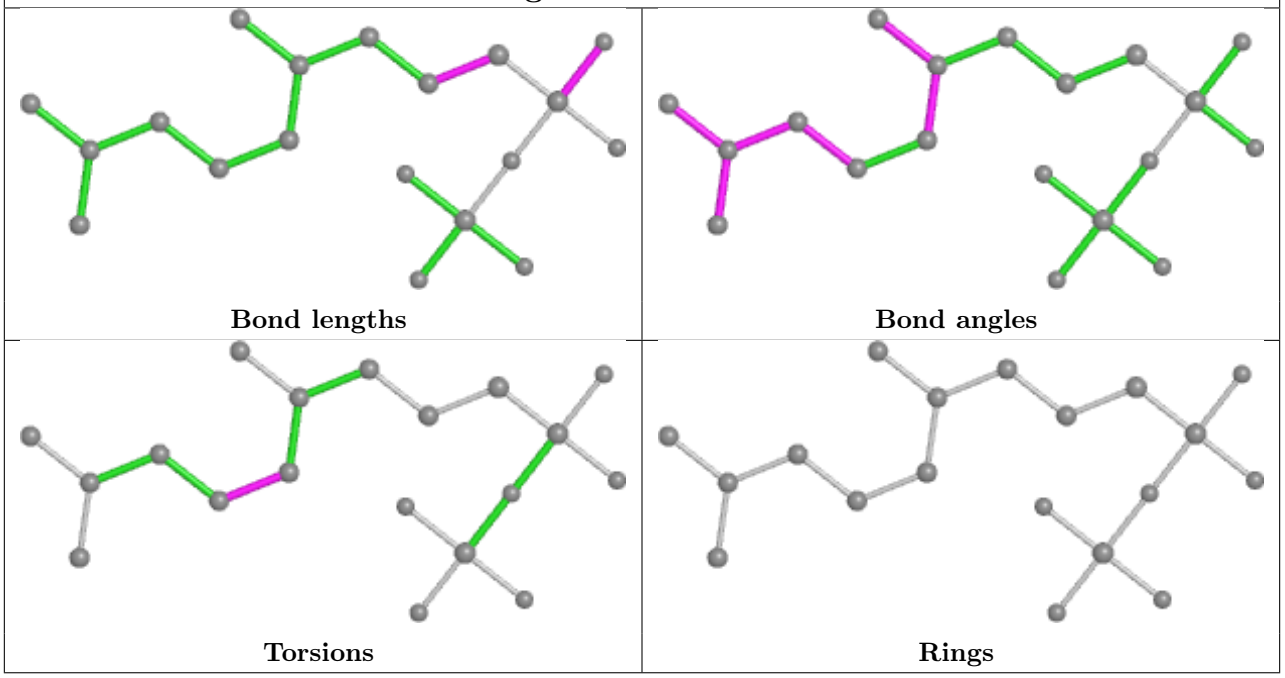
Ligand GST D 501



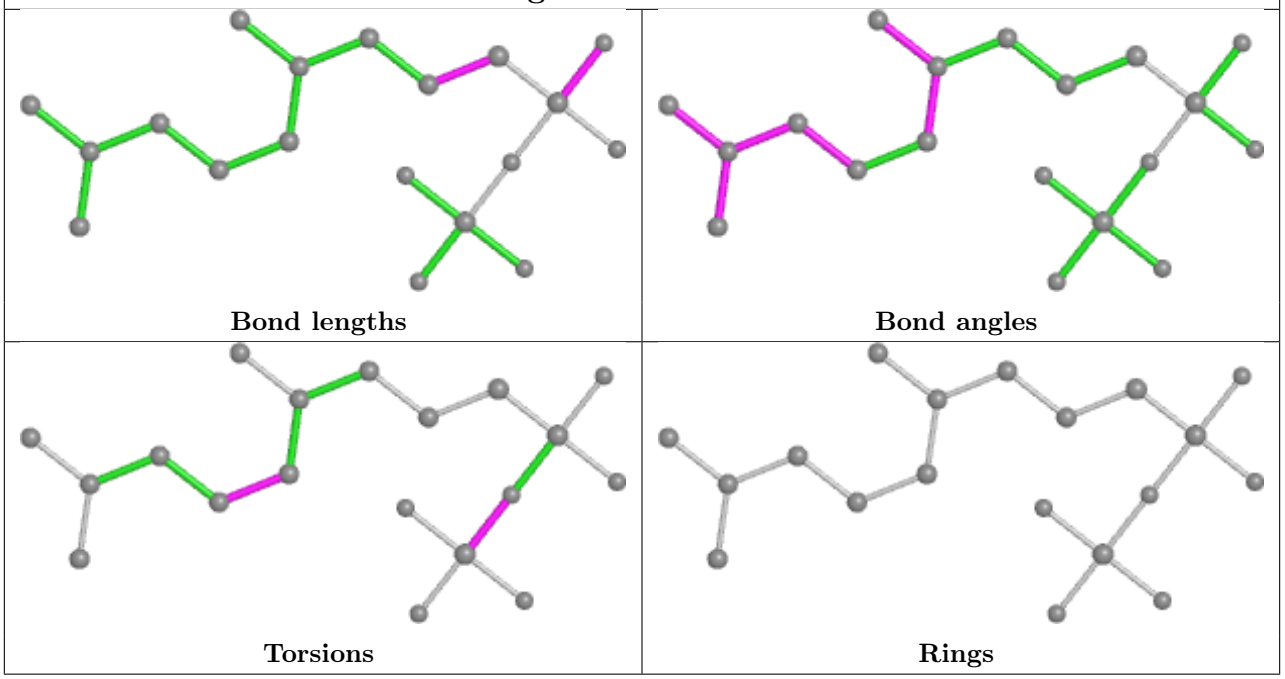
Ligand GST G 501



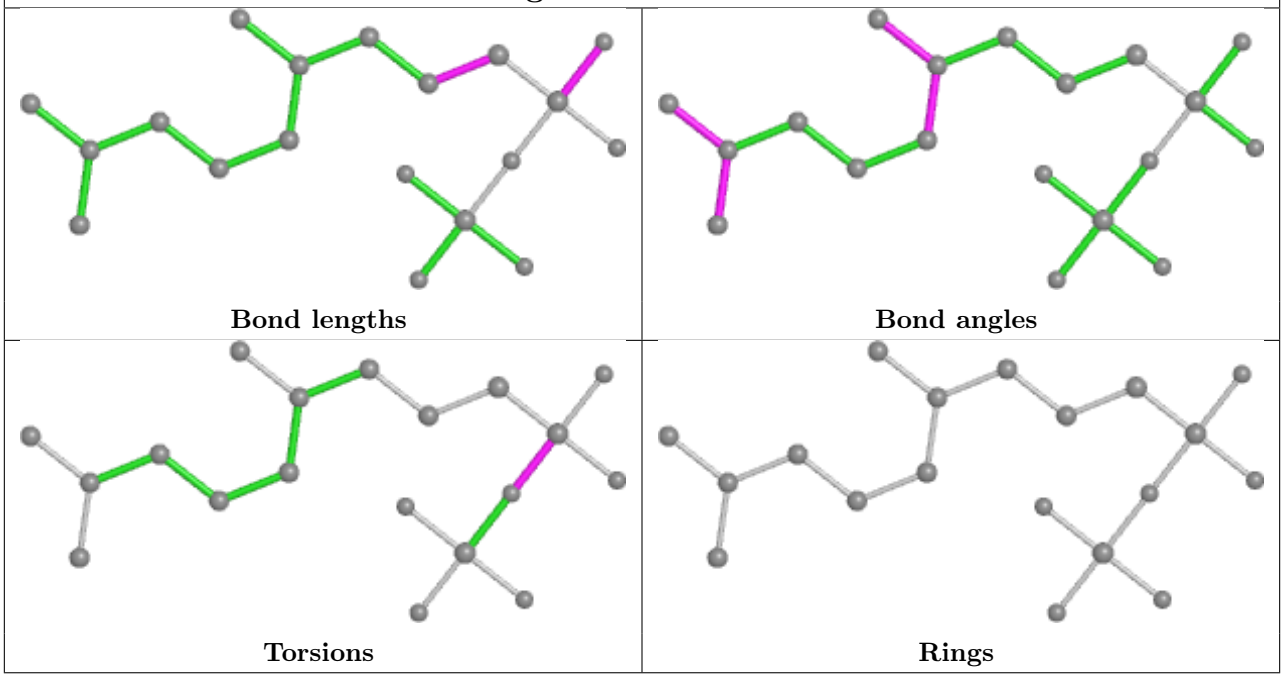
Ligand GST H 501



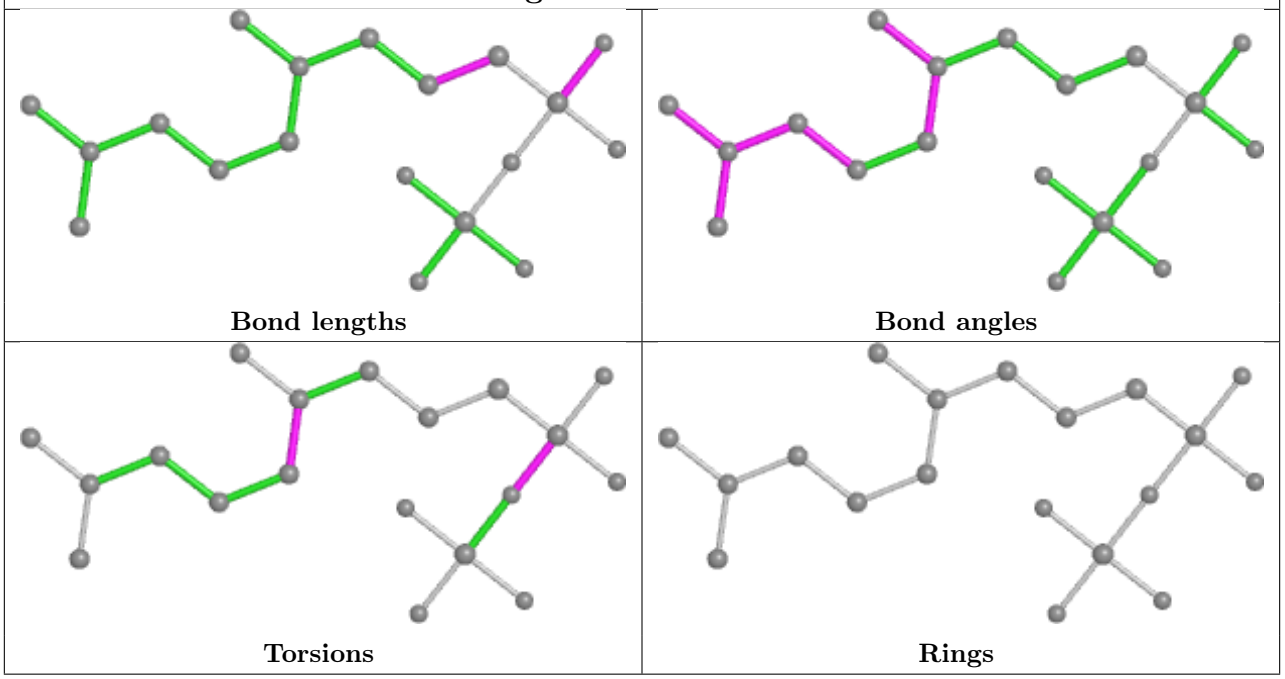
Ligand GST F 501



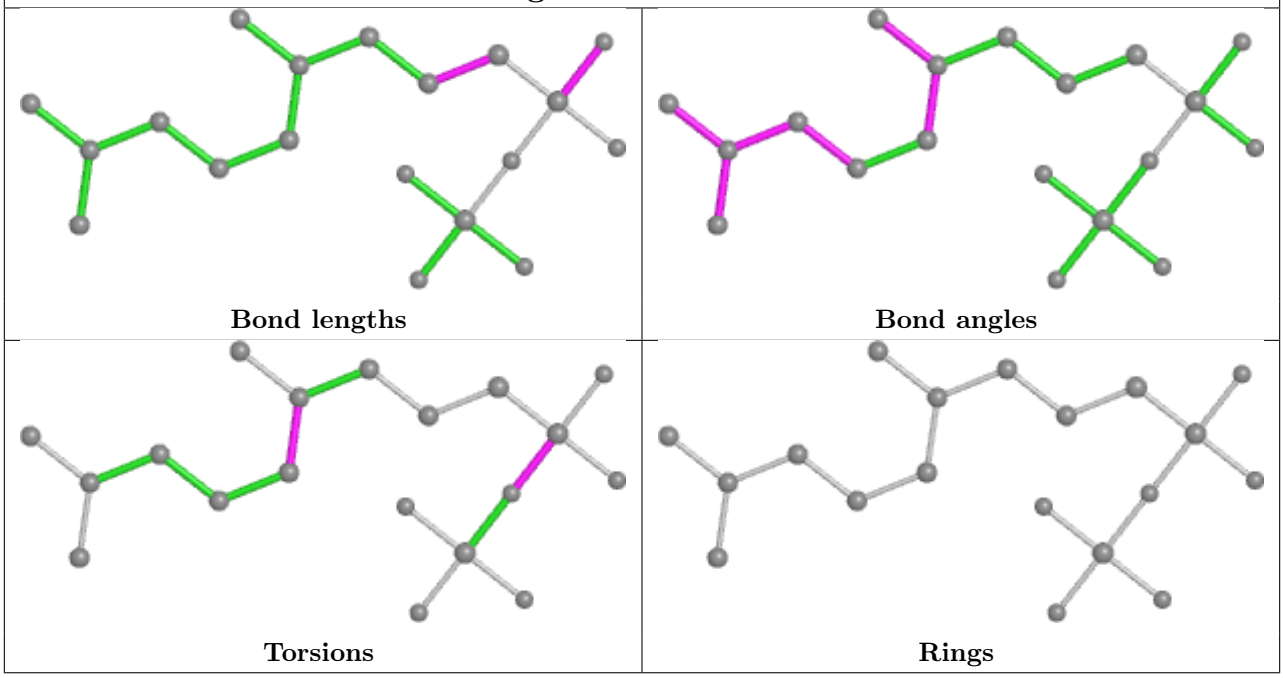
Ligand GST C 501



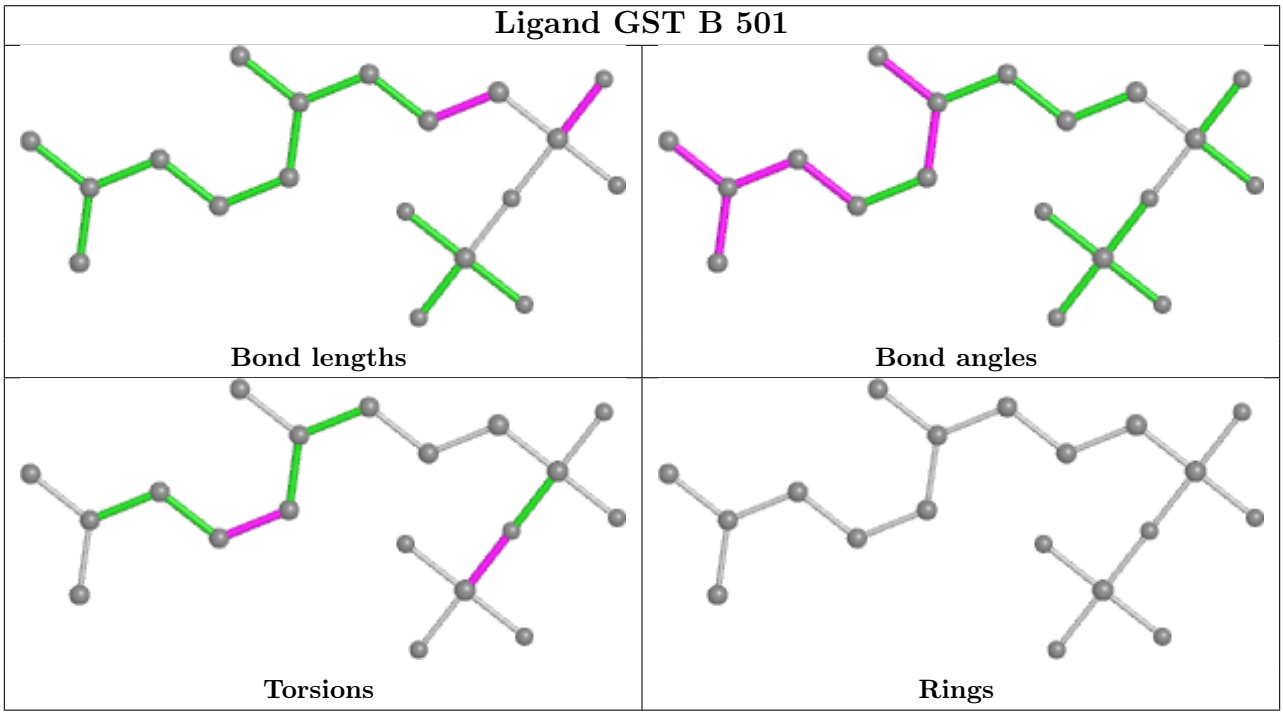
Ligand GST A 501



Ligand GST E 501



Ligand GST B 501



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	214/232 (92%)	1.05	24 (11%) 5 6	21, 32, 51, 65	0
1	B	209/232 (90%)	1.00	22 (10%) 6 8	23, 30, 48, 62	0
1	C	218/232 (93%)	0.95	21 (9%) 8 10	21, 28, 46, 102	0
1	D	209/232 (90%)	0.93	14 (6%) 17 22	21, 29, 43, 63	0
1	E	214/232 (92%)	1.10	26 (12%) 4 5	22, 32, 49, 70	0
1	F	209/232 (90%)	0.92	16 (7%) 13 17	20, 31, 48, 69	0
1	G	217/232 (93%)	0.97	22 (10%) 7 9	19, 28, 45, 79	0
1	H	208/232 (89%)	0.93	16 (7%) 13 17	21, 30, 45, 77	0
All	All	1698/1856 (91%)	0.98	161 (9%) 8 11	19, 30, 48, 102	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	VAL	11.6
1	B	0	MET	7.8
1	C	0	MET	5.8
1	G	1	MET	5.6
1	G	0	MET	5.5
1	E	1	MET	5.0
1	E	212	TYR	4.8
1	A	214	LEU	4.8
1	D	82	THR	4.5
1	A	1	MET	4.2
1	E	145	GLU	3.9
1	H	112	GLN	3.9
1	D	16	GLN	3.8
1	H	1	MET	3.7
1	F	81	ASP	3.6
1	F	62	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	22	LEU	3.5
1	A	112	GLN	3.5
1	A	22	LEU	3.5
1	F	147	LEU	3.5
1	A	212	TYR	3.5
1	A	79	CYS	3.4
1	A	107	ALA	3.4
1	C	81	ASP	3.4
1	G	216	PRO	3.4
1	C	216	PRO	3.4
1	H	23	ASP	3.3
1	E	2	THR	3.3
1	E	122	GLY	3.3
1	C	112	GLN	3.3
1	H	20	ILE	3.3
1	E	62	GLU	3.2
1	E	114	ASP	3.2
1	E	147	LEU	3.1
1	E	162	ILE	3.1
1	G	36	PHE	3.1
1	F	22	LEU	3.1
1	B	62	GLU	3.0
1	C	144	THR	3.0
1	H	79	CYS	3.0
1	D	1	MET	3.0
1	B	91	LEU	3.0
1	H	63	GLU	3.0
1	H	157	PRO	3.0
1	G	17	LYS	2.9
1	D	36	PHE	2.9
1	E	21	SER	2.9
1	H	43	GLU	2.9
1	E	190	LEU	2.9
1	B	96	GLU	2.9
1	A	56	ALA	2.9
1	G	81	ASP	2.8
1	C	16	GLN	2.8
1	C	20	ILE	2.8
1	A	75	VAL	2.8
1	B	93	VAL	2.8
1	G	179	PRO	2.8
1	A	136	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	79	CYS	2.8
1	G	16	GLN	2.8
1	G	161	LEU	2.8
1	C	1	MET	2.7
1	E	4	LEU	2.7
1	A	23	ASP	2.7
1	H	202	LEU	2.7
1	G	181	ALA	2.7
1	B	176	LEU	2.7
1	G	79	CYS	2.7
1	G	143	LEU	2.7
1	F	0	MET	2.7
1	F	33	LEU	2.7
1	E	87	TYR	2.6
1	A	16	GLN	2.6
1	B	112	GLN	2.6
1	C	147	LEU	2.6
1	H	19	GLY	2.6
1	C	79	CYS	2.6
1	E	59	SER	2.6
1	E	112	GLN	2.6
1	G	24	ASP	2.5
1	F	55	VAL	2.5
1	D	22	LEU	2.5
1	D	104	ALA	2.5
1	C	62	GLU	2.5
1	H	207	GLU	2.5
1	E	207	GLU	2.5
1	A	34	VAL	2.4
1	B	103	GLU	2.4
1	B	89	GLY	2.4
1	G	26	TYR	2.4
1	H	173	PHE	2.4
1	B	147	LEU	2.4
1	G	65	VAL	2.4
1	G	62	GLU	2.4
1	B	22	LEU	2.4
1	B	16	GLN	2.4
1	A	4	LEU	2.4
1	D	96	GLU	2.4
1	G	73	THR	2.4
1	G	215	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	148	LEU	2.3
1	F	16	GLN	2.3
1	D	132	ILE	2.3
1	E	14	TRP	2.3
1	B	185	PHE	2.3
1	G	198	PHE	2.3
1	B	8	PRO	2.3
1	C	36	PHE	2.3
1	A	81	ASP	2.3
1	D	114	ASP	2.3
1	D	97	ARG	2.3
1	E	45	PHE	2.3
1	F	1	MET	2.3
1	G	142	ALA	2.3
1	H	98	TRP	2.3
1	E	79	CYS	2.3
1	A	106	ARG	2.3
1	B	114	ASP	2.2
1	A	103	GLU	2.2
1	B	63	GLU	2.2
1	E	64	GLN	2.2
1	F	15	SER	2.2
1	F	98	TRP	2.2
1	A	209	ASP	2.2
1	B	23	ASP	2.2
1	B	97	ARG	2.2
1	G	96	GLU	2.2
1	D	100	THR	2.2
1	E	210	ARG	2.2
1	C	202	LEU	2.2
1	B	34	VAL	2.2
1	C	63	GLU	2.2
1	C	207	GLU	2.2
1	B	20	ILE	2.1
1	B	3	ASN	2.1
1	H	37	THR	2.1
1	G	200	VAL	2.1
1	A	19	GLY	2.1
1	A	2	THR	2.1
1	A	207	GLU	2.1
1	A	7	LEU	2.1
1	E	65	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	121	MET	2.1
1	H	36	PHE	2.1
1	A	20	ILE	2.1
1	C	7	LEU	2.1
1	F	158	VAL	2.1
1	A	127	HIS	2.1
1	D	145	GLU	2.1
1	C	162	ILE	2.1
1	B	105	LEU	2.1
1	E	180	PHE	2.1
1	C	161	LEU	2.0
1	F	112	GLN	2.0
1	E	198	PHE	2.0
1	F	24	ASP	2.0
1	D	148	LEU	2.0
1	H	18	GLN	2.0
1	D	103	GLU	2.0
1	C	93	VAL	2.0
1	E	106	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
2	MG	A	500	1/1	0.54	0.19	40,40,40,40	0
2	MG	G	500	1/1	0.54	0.27	84,84,84,84	0
4	DMA	C	502[A]	14/14	0.70	0.25	34,41,42,42	8
4	DMA	C	502[B]	14/14	0.70	0.25	34,41,42,42	8

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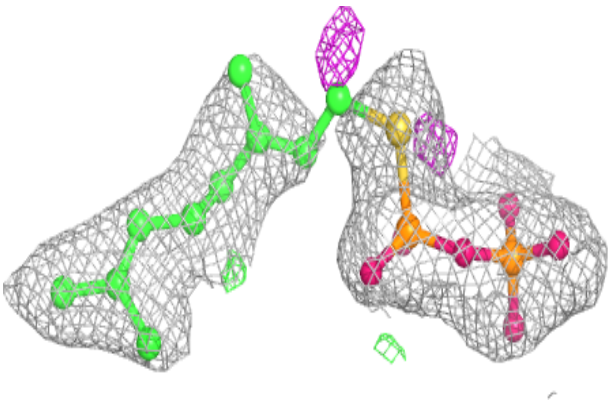
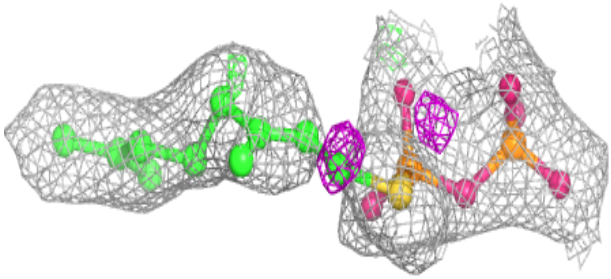
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMA	G	502[A]	14/14	0.75	0.28	42,43,45,45	8
4	DMA	G	502[B]	14/14	0.75	0.28	36,43,45,45	8
4	DMA	A	502[A]	14/14	0.76	0.25	40,41,42,42	8
4	DMA	A	502[B]	14/14	0.76	0.25	39,40,42,42	8
2	MG	F	500	1/1	0.77	0.14	38,38,38,38	0
4	DMA	F	502	14/14	0.81	0.22	42,45,47,47	0
4	DMA	E	502[B]	14/14	0.85	0.19	38,40,41,41	8
4	DMA	E	502[A]	14/14	0.85	0.19	39,40,41,41	8
4	DMA	B	502	14/14	0.86	0.25	48,52,56,57	0
2	MG	D	500	1/1	0.87	0.09	32,32,32,32	0
3	GST	D	501	19/19	0.90	0.18	27,32,38,39	0
3	GST	H	501	19/19	0.90	0.22	32,36,40,40	0
2	MG	E	500	1/1	0.90	0.07	40,40,40,40	0
3	GST	E	501	19/19	0.91	0.20	36,39,41,41	0
3	GST	B	501	19/19	0.91	0.19	36,42,46,47	0
3	GST	G	501	19/19	0.92	0.15	33,35,38,40	0
3	GST	A	501	19/19	0.92	0.19	37,40,44,44	0
3	GST	C	501	19/19	0.92	0.21	34,37,40,41	0
3	GST	F	501	19/19	0.92	0.28	41,46,50,50	0
2	MG	B	500	1/1	0.93	0.07	40,40,40,40	0
4	DMA	H	502	14/14	0.93	0.19	28,32,38,38	0
2	MG	H	500	1/1	0.94	0.11	35,35,35,35	0
4	DMA	D	502	14/14	0.95	0.16	26,30,36,36	0
2	MG	C	500	1/1	0.97	0.13	31,31,31,31	0

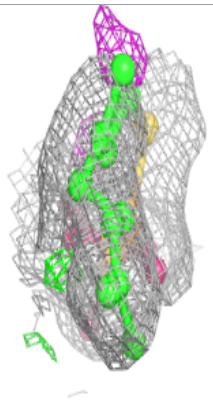
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GST D 501:

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

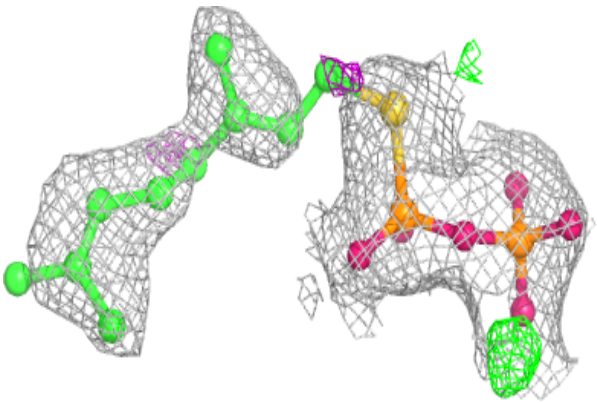


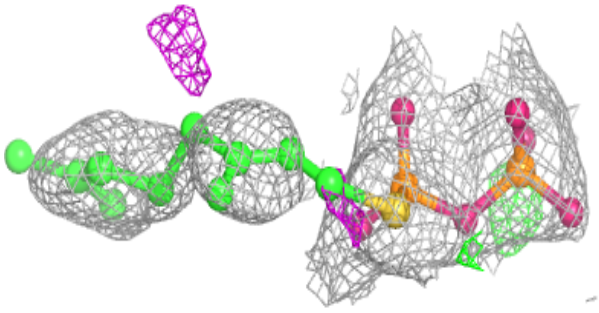


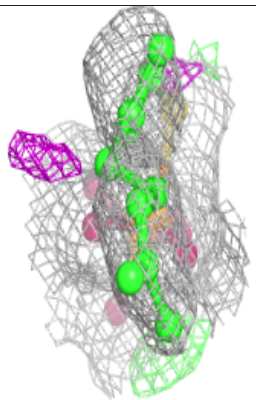


Electron density around GST H 501:

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

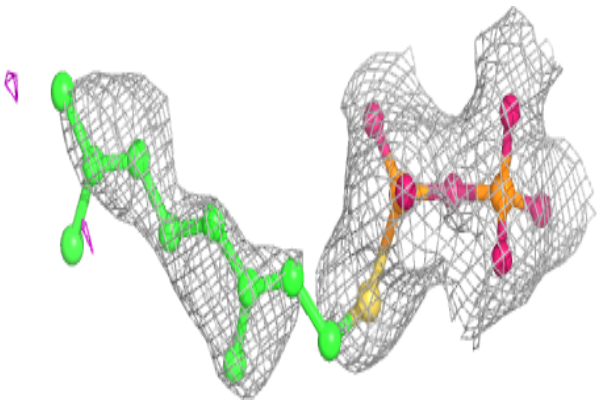


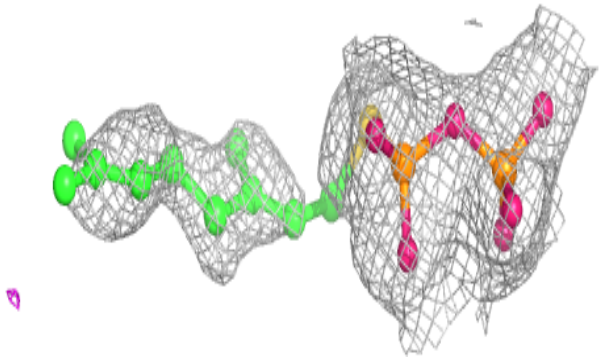


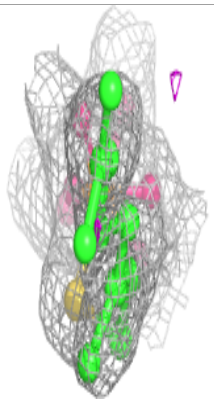


Electron density around GST E 501:

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

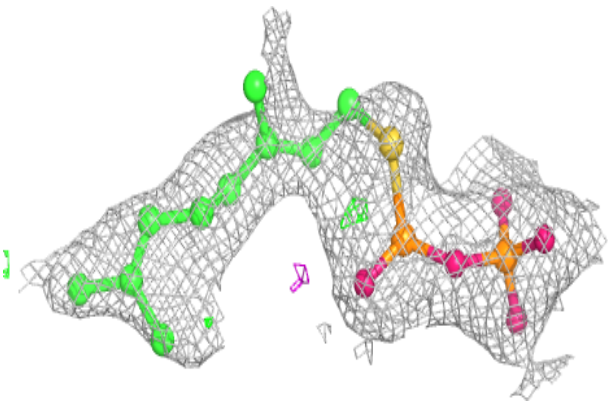


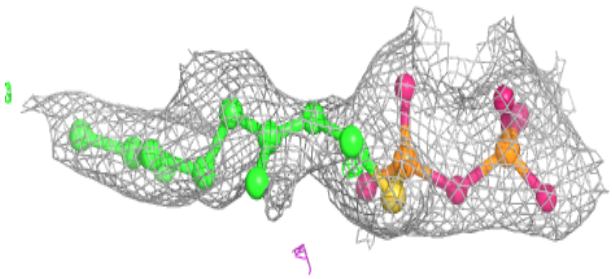


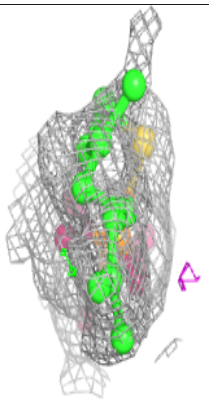


Electron density around GST B 501:

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

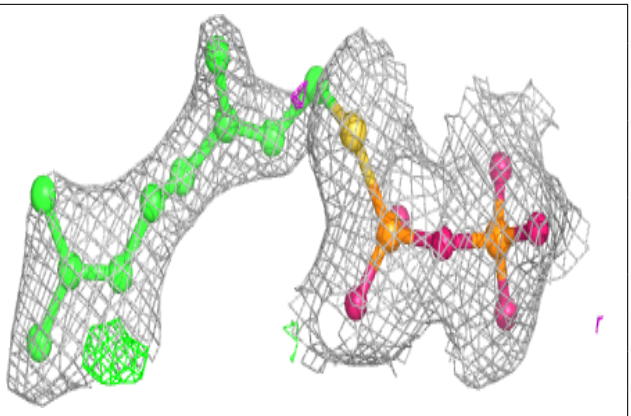


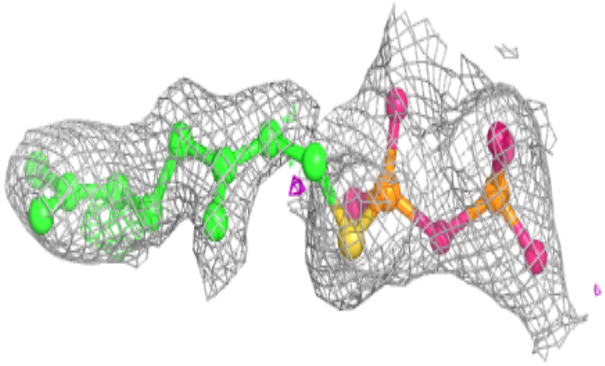


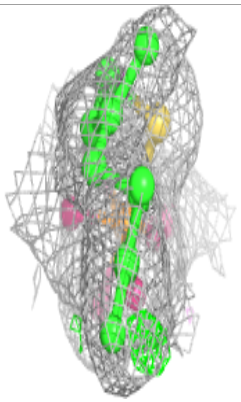


Electron density around GST G 501:

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

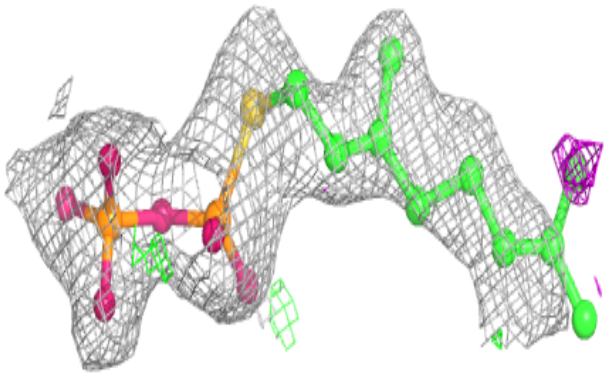


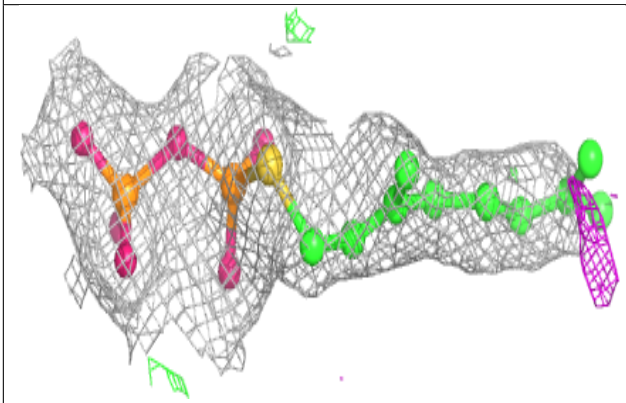


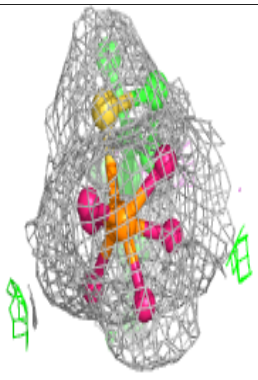


Electron density around GST A 501:

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

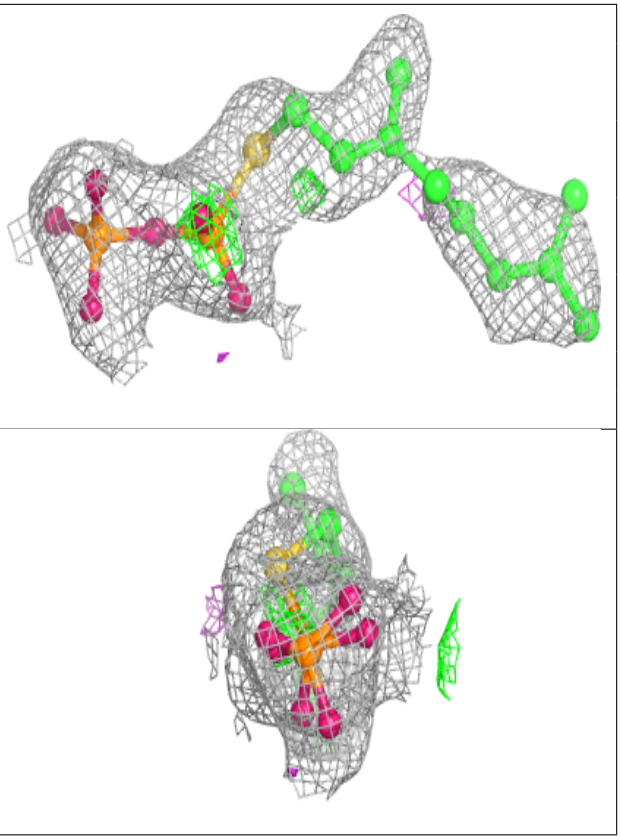






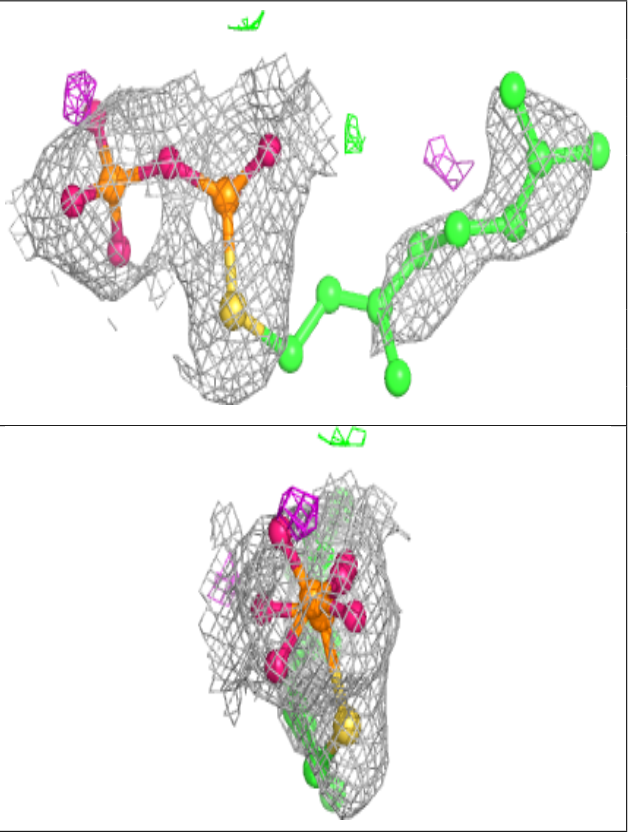
Electron density around GST C 501:

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



Electron density around GST F 501:

$2mF_o$-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.