W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2023 – 02:37 AM EDT

PDB ID	:	4QPZ
Title	:	Crystal structure of the formolase FLS_v2 in space group P 21
Authors	:	Shen, B.W.; Siegel, J.B.; Stoddard, B.L.; Baker, D.
Deposited on	:	2014-06-25
Resolution	:	3.00 Å(reported)

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

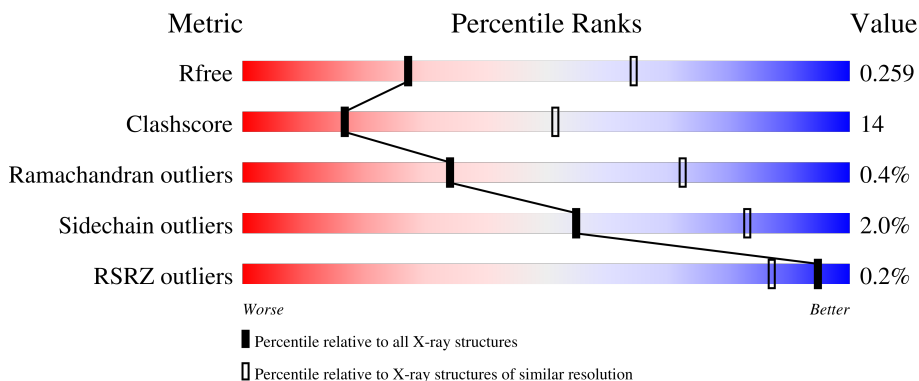|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1　Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.00 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.259
Clashscore		14
Ramachandran outliers		0.4%
Sidechain outliers		2.0%
RSRZ outliers		0.2%

Worse　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	582	69% · · · · 27% · ·
1	B	582	74% · · · · 22% · ·
1	C	582	75% · · · · 21% ·
1	D	582	70% · · · · 26% · ·
1	E	582	73% · · · · 23% ·

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Mol	Chain	Length	Quality of chain
1	F	582	72% 23%
1	G	582	69% 26%
1	H	582	73% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TPP	C	602	-	-	X	-
3	TPP	F	602	-	-	X	-
3	TPP	G	602	-	-	X	-
3	TPP	H	602	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 33455 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 Formolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4157	2630	734	776	17			
1	B	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	C	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	D	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	E	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	F	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	G	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			
1	H	562	Total	C	N	O	S	0	0	0
			4153	2628	733	775	17			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ILE	ALA	conflict	UNP Q9F4L3
A	394	GLY	ALA	conflict	UNP Q9F4L3
A	419	ASN	GLY	conflict	UNP Q9F4L3
A	480	TRP	ALA	conflict	UNP Q9F4L3
A	564	GLY	-	expression tag	UNP Q9F4L3
A	565	SER	-	expression tag	UNP Q9F4L3
A	566	THR	-	expression tag	UNP Q9F4L3
A	567	GLU	-	expression tag	UNP Q9F4L3
A	568	ASN	-	expression tag	UNP Q9F4L3
A	569	LEU	-	expression tag	UNP Q9F4L3
A	570	TYR	-	expression tag	UNP Q9F4L3
A	571	PHE	-	expression tag	UNP Q9F4L3
A	572	GLN	-	expression tag	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	573	SER	-	expression tag	UNP Q9F4L3
A	574	GLY	-	expression tag	UNP Q9F4L3
A	575	ALA	-	expression tag	UNP Q9F4L3
A	576	LEU	-	expression tag	UNP Q9F4L3
A	577	GLU	-	expression tag	UNP Q9F4L3
A	578	HIS	-	expression tag	UNP Q9F4L3
A	579	HIS	-	expression tag	UNP Q9F4L3
A	580	HIS	-	expression tag	UNP Q9F4L3
A	581	HIS	-	expression tag	UNP Q9F4L3
A	582	HIS	-	expression tag	UNP Q9F4L3
A	583	HIS	-	expression tag	UNP Q9F4L3
B	28	ILE	ALA	conflict	UNP Q9F4L3
B	394	GLY	ALA	conflict	UNP Q9F4L3
B	419	ASN	GLY	conflict	UNP Q9F4L3
B	480	TRP	ALA	conflict	UNP Q9F4L3
B	564	GLY	-	expression tag	UNP Q9F4L3
B	565	SER	-	expression tag	UNP Q9F4L3
B	566	THR	-	expression tag	UNP Q9F4L3
B	567	GLU	-	expression tag	UNP Q9F4L3
B	568	ASN	-	expression tag	UNP Q9F4L3
B	569	LEU	-	expression tag	UNP Q9F4L3
B	570	TYR	-	expression tag	UNP Q9F4L3
B	571	PHE	-	expression tag	UNP Q9F4L3
B	572	GLN	-	expression tag	UNP Q9F4L3
B	573	SER	-	expression tag	UNP Q9F4L3
B	574	GLY	-	expression tag	UNP Q9F4L3
B	575	ALA	-	expression tag	UNP Q9F4L3
B	576	LEU	-	expression tag	UNP Q9F4L3
B	577	GLU	-	expression tag	UNP Q9F4L3
B	578	HIS	-	expression tag	UNP Q9F4L3
B	579	HIS	-	expression tag	UNP Q9F4L3
B	580	HIS	-	expression tag	UNP Q9F4L3
B	581	HIS	-	expression tag	UNP Q9F4L3
B	582	HIS	-	expression tag	UNP Q9F4L3
B	583	HIS	-	expression tag	UNP Q9F4L3
C	28	ILE	ALA	conflict	UNP Q9F4L3
C	394	GLY	ALA	conflict	UNP Q9F4L3
C	419	ASN	GLY	conflict	UNP Q9F4L3
C	480	TRP	ALA	conflict	UNP Q9F4L3
C	564	GLY	-	expression tag	UNP Q9F4L3
C	565	SER	-	expression tag	UNP Q9F4L3
C	566	THR	-	expression tag	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	567	GLU	-	expression tag	UNP Q9F4L3
C	568	ASN	-	expression tag	UNP Q9F4L3
C	569	LEU	-	expression tag	UNP Q9F4L3
C	570	TYR	-	expression tag	UNP Q9F4L3
C	571	PHE	-	expression tag	UNP Q9F4L3
C	572	GLN	-	expression tag	UNP Q9F4L3
C	573	SER	-	expression tag	UNP Q9F4L3
C	574	GLY	-	expression tag	UNP Q9F4L3
C	575	ALA	-	expression tag	UNP Q9F4L3
C	576	LEU	-	expression tag	UNP Q9F4L3
C	577	GLU	-	expression tag	UNP Q9F4L3
C	578	HIS	-	expression tag	UNP Q9F4L3
C	579	HIS	-	expression tag	UNP Q9F4L3
C	580	HIS	-	expression tag	UNP Q9F4L3
C	581	HIS	-	expression tag	UNP Q9F4L3
C	582	HIS	-	expression tag	UNP Q9F4L3
C	583	HIS	-	expression tag	UNP Q9F4L3
D	28	ILE	ALA	conflict	UNP Q9F4L3
D	394	GLY	ALA	conflict	UNP Q9F4L3
D	419	ASN	GLY	conflict	UNP Q9F4L3
D	480	TRP	ALA	conflict	UNP Q9F4L3
D	564	GLY	-	expression tag	UNP Q9F4L3
D	565	SER	-	expression tag	UNP Q9F4L3
D	566	THR	-	expression tag	UNP Q9F4L3
D	567	GLU	-	expression tag	UNP Q9F4L3
D	568	ASN	-	expression tag	UNP Q9F4L3
D	569	LEU	-	expression tag	UNP Q9F4L3
D	570	TYR	-	expression tag	UNP Q9F4L3
D	571	PHE	-	expression tag	UNP Q9F4L3
D	572	GLN	-	expression tag	UNP Q9F4L3
D	573	SER	-	expression tag	UNP Q9F4L3
D	574	GLY	-	expression tag	UNP Q9F4L3
D	575	ALA	-	expression tag	UNP Q9F4L3
D	576	LEU	-	expression tag	UNP Q9F4L3
D	577	GLU	-	expression tag	UNP Q9F4L3
D	578	HIS	-	expression tag	UNP Q9F4L3
D	579	HIS	-	expression tag	UNP Q9F4L3
D	580	HIS	-	expression tag	UNP Q9F4L3
D	581	HIS	-	expression tag	UNP Q9F4L3
D	582	HIS	-	expression tag	UNP Q9F4L3
D	583	HIS	-	expression tag	UNP Q9F4L3
E	28	ILE	ALA	conflict	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	394	GLY	ALA	conflict	UNP Q9F4L3
E	419	ASN	GLY	conflict	UNP Q9F4L3
E	480	TRP	ALA	conflict	UNP Q9F4L3
E	564	GLY	-	expression tag	UNP Q9F4L3
E	565	SER	-	expression tag	UNP Q9F4L3
E	566	THR	-	expression tag	UNP Q9F4L3
E	567	GLU	-	expression tag	UNP Q9F4L3
E	568	ASN	-	expression tag	UNP Q9F4L3
E	569	LEU	-	expression tag	UNP Q9F4L3
E	570	TYR	-	expression tag	UNP Q9F4L3
E	571	PHE	-	expression tag	UNP Q9F4L3
E	572	GLN	-	expression tag	UNP Q9F4L3
E	573	SER	-	expression tag	UNP Q9F4L3
E	574	GLY	-	expression tag	UNP Q9F4L3
E	575	ALA	-	expression tag	UNP Q9F4L3
E	576	LEU	-	expression tag	UNP Q9F4L3
E	577	GLU	-	expression tag	UNP Q9F4L3
E	578	HIS	-	expression tag	UNP Q9F4L3
E	579	HIS	-	expression tag	UNP Q9F4L3
E	580	HIS	-	expression tag	UNP Q9F4L3
E	581	HIS	-	expression tag	UNP Q9F4L3
E	582	HIS	-	expression tag	UNP Q9F4L3
E	583	HIS	-	expression tag	UNP Q9F4L3
F	28	ILE	ALA	conflict	UNP Q9F4L3
F	394	GLY	ALA	conflict	UNP Q9F4L3
F	419	ASN	GLY	conflict	UNP Q9F4L3
F	480	TRP	ALA	conflict	UNP Q9F4L3
F	564	GLY	-	expression tag	UNP Q9F4L3
F	565	SER	-	expression tag	UNP Q9F4L3
F	566	THR	-	expression tag	UNP Q9F4L3
F	567	GLU	-	expression tag	UNP Q9F4L3
F	568	ASN	-	expression tag	UNP Q9F4L3
F	569	LEU	-	expression tag	UNP Q9F4L3
F	570	TYR	-	expression tag	UNP Q9F4L3
F	571	PHE	-	expression tag	UNP Q9F4L3
F	572	GLN	-	expression tag	UNP Q9F4L3
F	573	SER	-	expression tag	UNP Q9F4L3
F	574	GLY	-	expression tag	UNP Q9F4L3
F	575	ALA	-	expression tag	UNP Q9F4L3
F	576	LEU	-	expression tag	UNP Q9F4L3
F	577	GLU	-	expression tag	UNP Q9F4L3
F	578	HIS	-	expression tag	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	579	HIS	-	expression tag	UNP Q9F4L3
F	580	HIS	-	expression tag	UNP Q9F4L3
F	581	HIS	-	expression tag	UNP Q9F4L3
F	582	HIS	-	expression tag	UNP Q9F4L3
F	583	HIS	-	expression tag	UNP Q9F4L3
G	28	ILE	ALA	conflict	UNP Q9F4L3
G	394	GLY	ALA	conflict	UNP Q9F4L3
G	419	ASN	GLY	conflict	UNP Q9F4L3
G	480	TRP	ALA	conflict	UNP Q9F4L3
G	564	GLY	-	expression tag	UNP Q9F4L3
G	565	SER	-	expression tag	UNP Q9F4L3
G	566	THR	-	expression tag	UNP Q9F4L3
G	567	GLU	-	expression tag	UNP Q9F4L3
G	568	ASN	-	expression tag	UNP Q9F4L3
G	569	LEU	-	expression tag	UNP Q9F4L3
G	570	TYR	-	expression tag	UNP Q9F4L3
G	571	PHE	-	expression tag	UNP Q9F4L3
G	572	GLN	-	expression tag	UNP Q9F4L3
G	573	SER	-	expression tag	UNP Q9F4L3
G	574	GLY	-	expression tag	UNP Q9F4L3
G	575	ALA	-	expression tag	UNP Q9F4L3
G	576	LEU	-	expression tag	UNP Q9F4L3
G	577	GLU	-	expression tag	UNP Q9F4L3
G	578	HIS	-	expression tag	UNP Q9F4L3
G	579	HIS	-	expression tag	UNP Q9F4L3
G	580	HIS	-	expression tag	UNP Q9F4L3
G	581	HIS	-	expression tag	UNP Q9F4L3
G	582	HIS	-	expression tag	UNP Q9F4L3
G	583	HIS	-	expression tag	UNP Q9F4L3
H	28	ILE	ALA	conflict	UNP Q9F4L3
H	394	GLY	ALA	conflict	UNP Q9F4L3
H	419	ASN	GLY	conflict	UNP Q9F4L3
H	480	TRP	ALA	conflict	UNP Q9F4L3
H	564	GLY	-	expression tag	UNP Q9F4L3
H	565	SER	-	expression tag	UNP Q9F4L3
H	566	THR	-	expression tag	UNP Q9F4L3
H	567	GLU	-	expression tag	UNP Q9F4L3
H	568	ASN	-	expression tag	UNP Q9F4L3
H	569	LEU	-	expression tag	UNP Q9F4L3
H	570	TYR	-	expression tag	UNP Q9F4L3
H	571	PHE	-	expression tag	UNP Q9F4L3
H	572	GLN	-	expression tag	UNP Q9F4L3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	573	SER	-	expression tag	UNP Q9F4L3
H	574	GLY	-	expression tag	UNP Q9F4L3
H	575	ALA	-	expression tag	UNP Q9F4L3
H	576	LEU	-	expression tag	UNP Q9F4L3
H	577	GLU	-	expression tag	UNP Q9F4L3
H	578	HIS	-	expression tag	UNP Q9F4L3
H	579	HIS	-	expression tag	UNP Q9F4L3
H	580	HIS	-	expression tag	UNP Q9F4L3
H	581	HIS	-	expression tag	UNP Q9F4L3
H	582	HIS	-	expression tag	UNP Q9F4L3
H	583	HIS	-	expression tag	UNP Q9F4L3

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

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

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

TPP
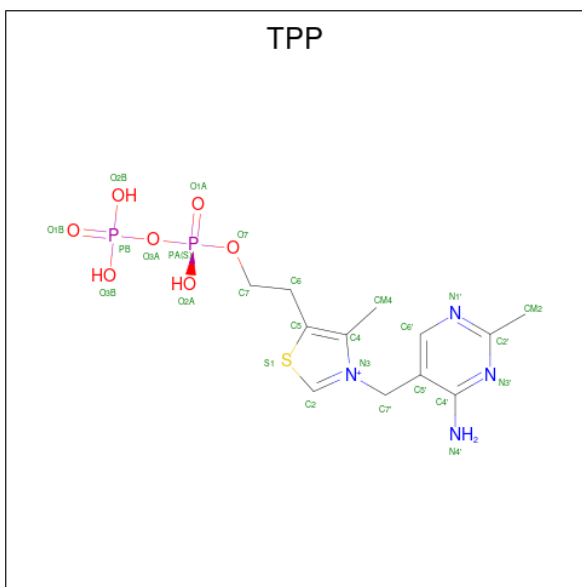
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S		0	0
			26	12	4	7	2	1			
3	B	1	Total	C	N	O	P	S		0	0
			26	12	4	7	2	1			
3	C	1	Total	C	N	O	P	S		0	0
			26	12	4	7	2	1			
3	D	1	Total	C	N	O	P	S		0	0
			26	12	4	7	2	1			
3	E	1	Total	C	N	O	P	S		0	0
			26	12	4	7	2	1			
3	F	1	Total	C	N	O	P	S		0	0
			26	12	4	7	2	1			
3	G	1	Total	C	N	O	P	S		0	0
			26	12	4	7	2	1			
3	H	1	Total	C	N	O	P	S		0	0
			26	12	4	7	2	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		
4	E	3	Total	O	0	0
			3	3		
4	F	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Formolase
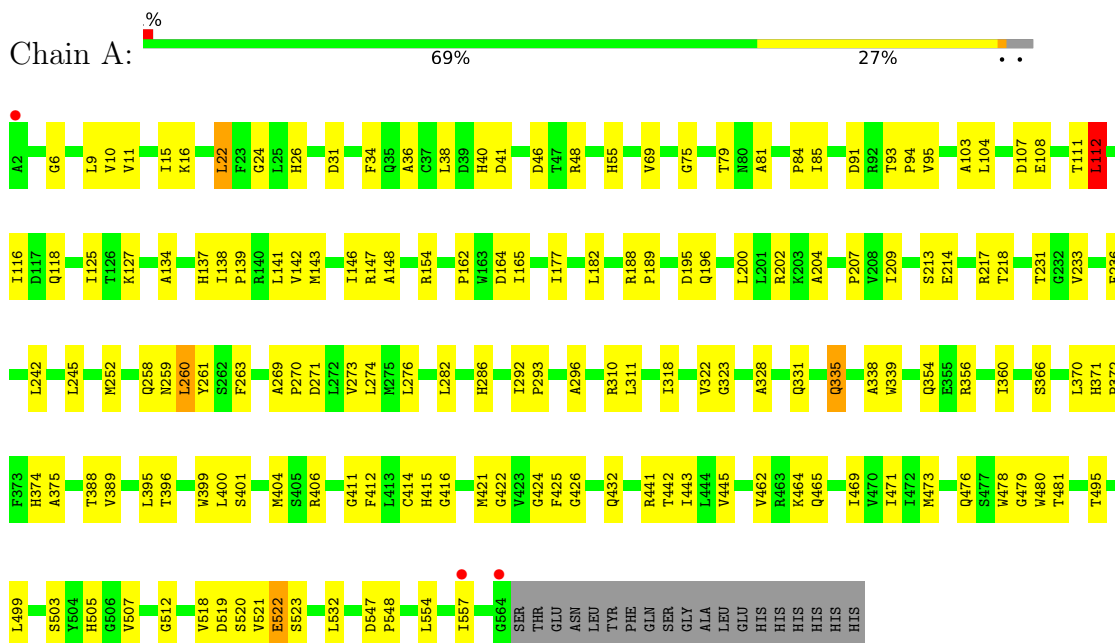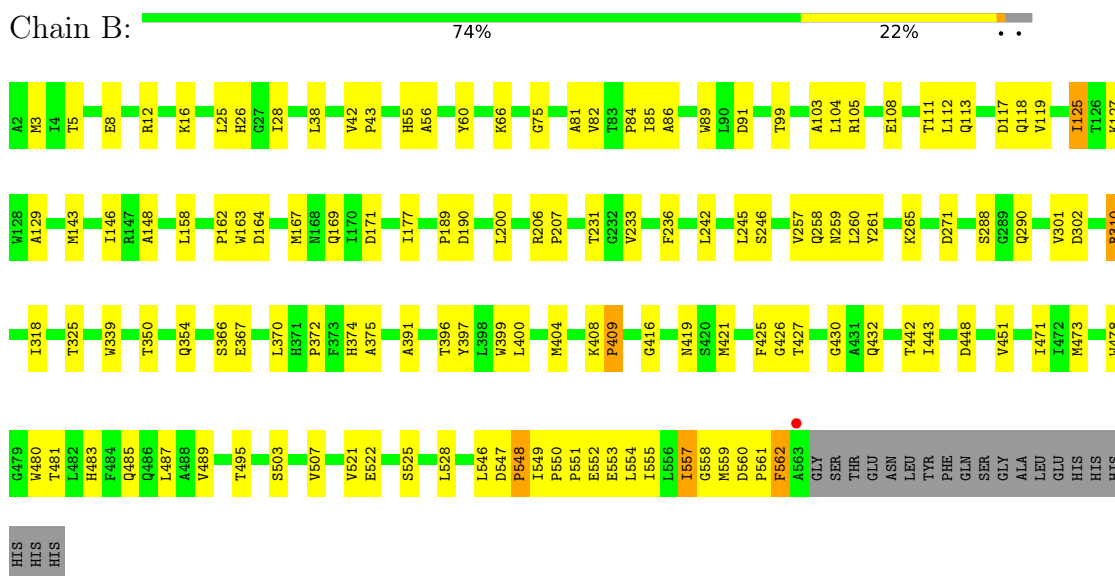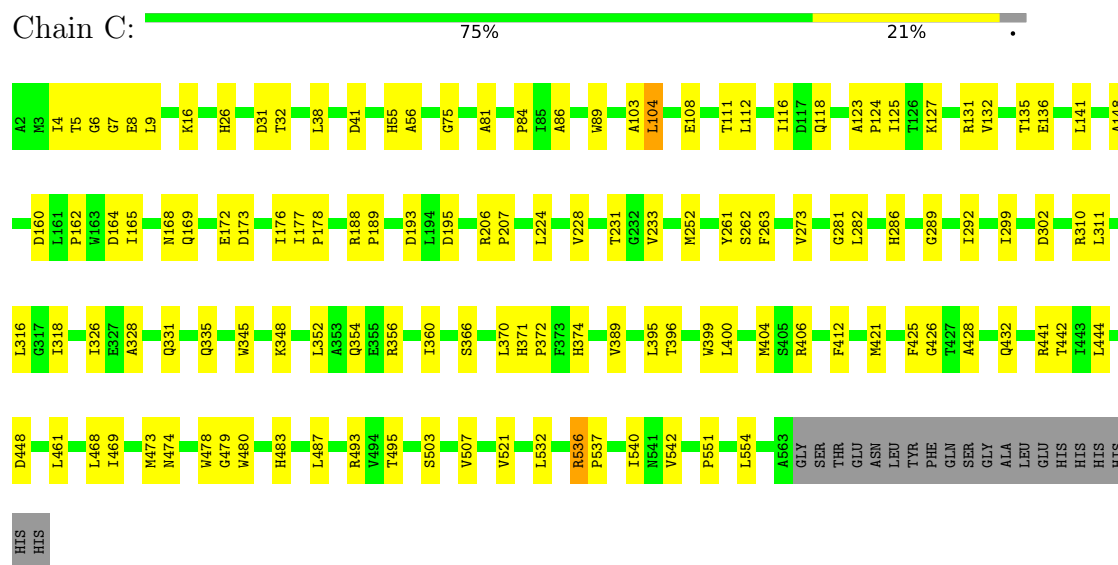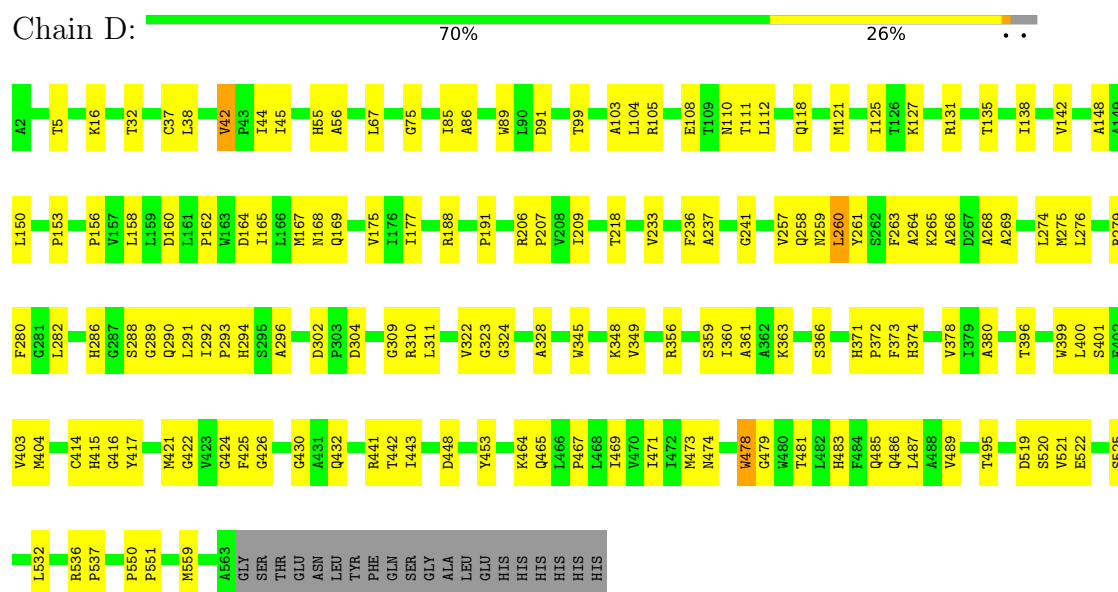
- Molecule 1: Formolase

• Molecule 1: Formolase

Chain C:

• Molecule 1: Formolase

Chain D:

• Molecule 1: Formolase

Chain E:

S405 R406 V407 K408 P409 L413 G416 F425 G426 Q432 V433 R441 T442 I443 D448 V451 S454 E457 K464 Q465 L466 P467 L468 I469 V470 I471 I472 M473 N474 W478 G479 W480 T481 T495 V507 S525 L532 A563 GLY SER THR GLU ASN LEU

TYR PHE GLN SER GLY ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Formolase

Chain F:

• Molecule 1: Formolase

Chain G:

• Molecule 1: Formolase

Chain H:
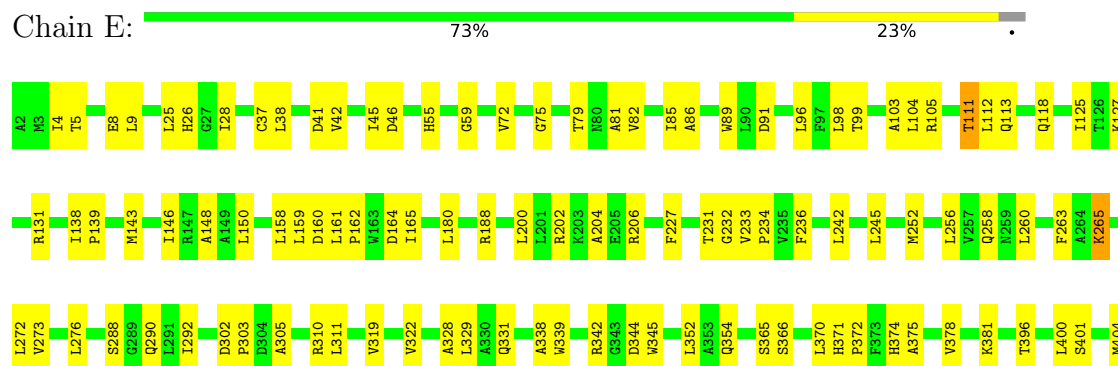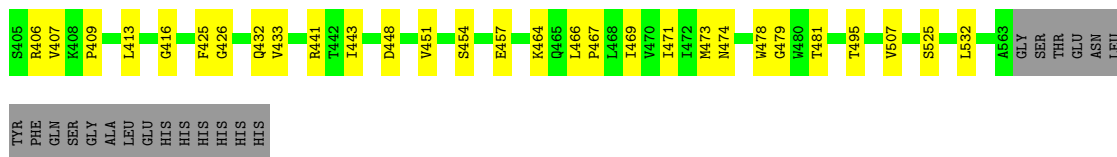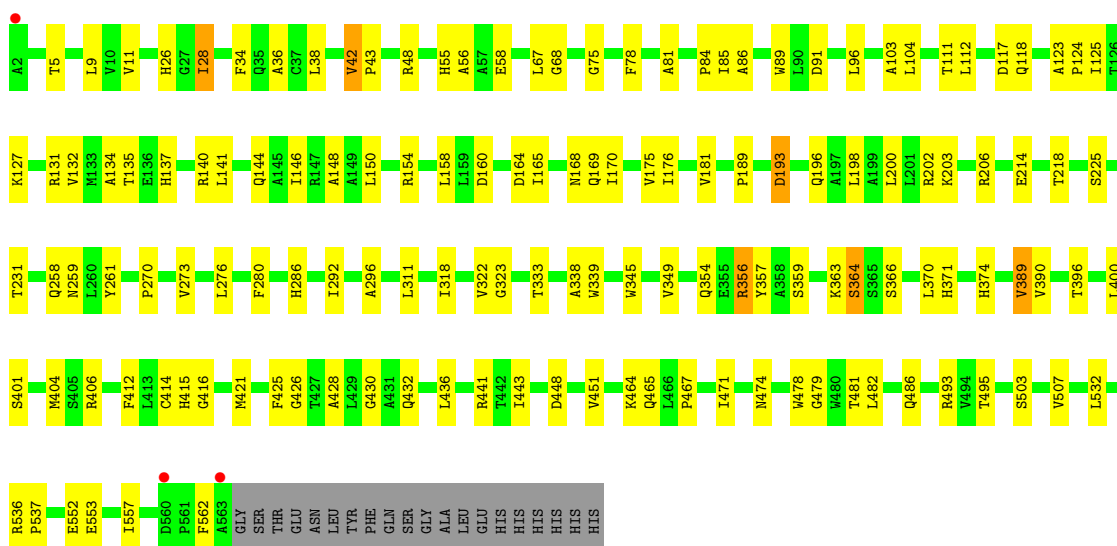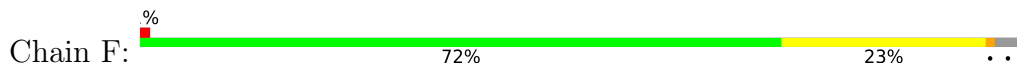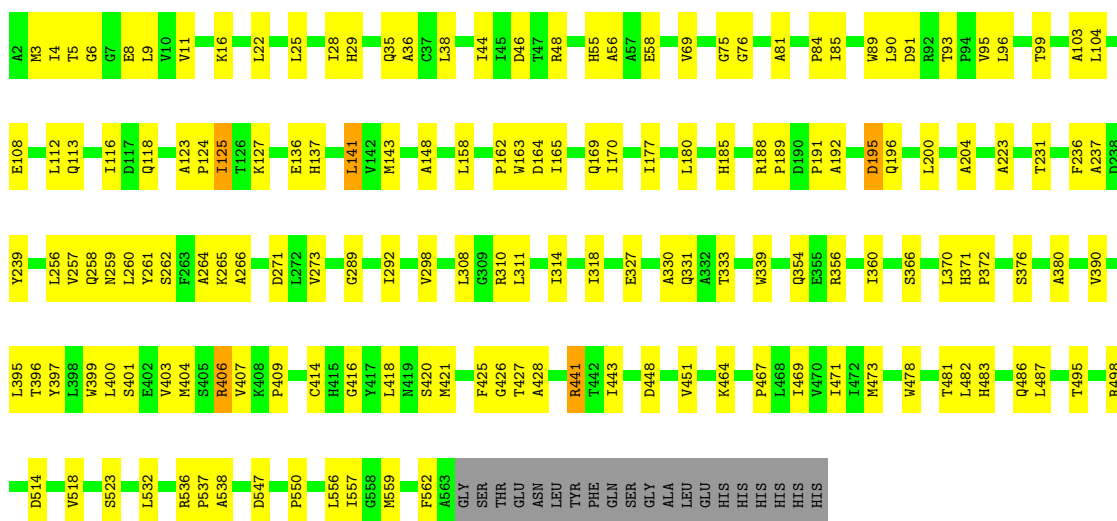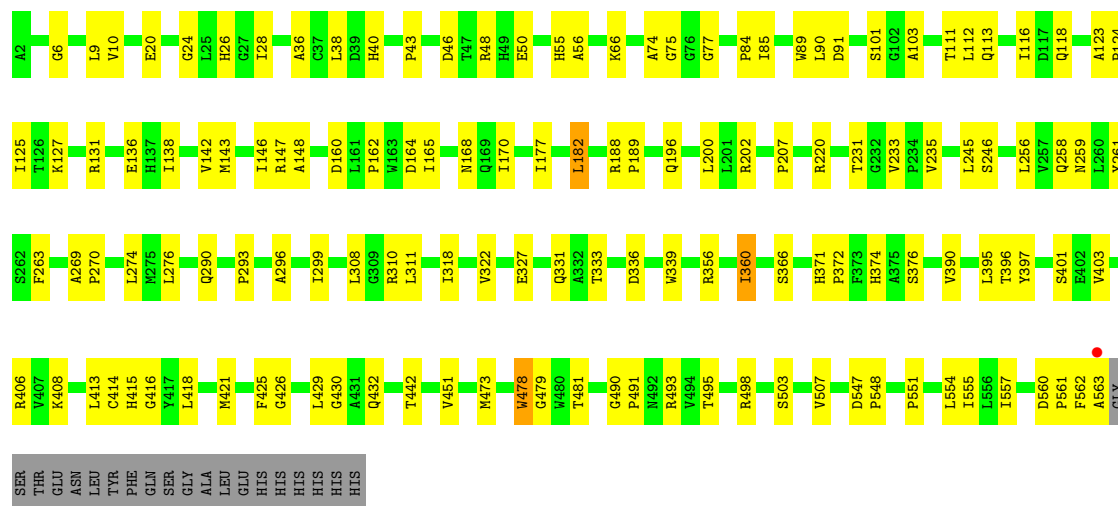
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.88Å 136.56Å 167.06Å 90.00° 95.36° 90.00°	Depositor
Resolution (Å)	166.33 – 3.00 48.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.4 (166.33-3.00) 89.5 (48.91-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.208 , 0.257 0.212 , 0.259	Depositor DCC
R_{free} test set	4028 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 30.0	EDS
L-test for twinning [2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	33455	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3419e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.50	0/4244	0.74	1/5789 (0.0%)
1	B	0.54	1/4240 (0.0%)	0.76	2/5784 (0.0%)
1	C	0.52	0/4240	0.77	0/5784
1	D	0.51	0/4240	0.74	0/5784
1	E	0.52	0/4240	0.76	1/5784 (0.0%)
1	F	0.51	0/4240	0.75	1/5784 (0.0%)
1	G	0.54	0/4240	0.76	1/5784 (0.0%)
1	H	0.53	0/4240	0.79	1/5784 (0.0%)
All	All	0.52	1/33924 (0.0%)	0.76	7/46277 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	PRO	N-CD	-5.57	1.40	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	LEU	CA-CB-CG	6.85	131.05	115.30
1	B	117	ASP	CB-CG-OD1	6.44	124.10	118.30
1	E	159	LEU	CB-CG-CD2	-5.84	101.07	111.00
1	H	429	LEU	CB-CG-CD1	-5.40	101.81	111.00
1	F	96	LEU	CA-CB-CG	-5.19	103.36	115.30

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	4157	0	4143	141	0
1	B	4153	0	4140	115	0
1	C	4153	0	4140	109	0
1	D	4153	0	4140	138	0
1	E	4153	0	4140	121	0
1	F	4153	0	4140	116	0
1	G	4153	0	4140	131	0
1	H	4153	0	4140	112	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	26	0	16	8	0
3	B	26	0	16	7	0
3	C	26	0	16	9	0
3	D	26	0	16	6	0
3	E	26	0	16	5	0
3	F	26	0	16	9	0
3	G	26	0	16	10	0
3	H	26	0	16	9	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
4	G	3	0	0	0	0
All	All	33455	0	33251	941	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 14.

The worst 5 of 941 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:E:425:PHE:CZ	1:E:451:VAL:HG23	1.78	1.18
1:F:5:THR:HG22	1:F:169:GLN:HG2	1.27	1.13
1:F:196:GLN:O	1:F:200:LEU:HD13	1.50	1.11
1:G:38:LEU:HD13	1:H:495:THR:HG21	1.20	1.10
1:E:425:PHE:HZ	1:E:451:VAL:HG23	1.08	1.07

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	561/582 (96%)	524 (93%)	35 (6%)	2 (0%)	34	72
1	B	560/582 (96%)	522 (93%)	35 (6%)	3 (0%)	29	68
1	C	560/582 (96%)	529 (94%)	29 (5%)	2 (0%)	34	72
1	D	560/582 (96%)	517 (92%)	39 (7%)	4 (1%)	22	60
1	E	560/582 (96%)	532 (95%)	27 (5%)	1 (0%)	47	82
1	F	560/582 (96%)	531 (95%)	28 (5%)	1 (0%)	47	82
1	G	560/582 (96%)	528 (94%)	27 (5%)	5 (1%)	17	55
1	H	560/582 (96%)	530 (95%)	29 (5%)	1 (0%)	47	82
All	All	4481/4656 (96%)	4213 (94%)	249 (6%)	19 (0%)	34	72

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	PRO
1	C	41	ASP
1	D	265	LYS
1	D	290	GLN
1	F	117	ASP

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	421/438 (96%)	412 (98%)	9 (2%)	53	82
1	B	421/438 (96%)	412 (98%)	9 (2%)	53	82
1	C	421/438 (96%)	413 (98%)	8 (2%)	57	84
1	D	421/438 (96%)	416 (99%)	5 (1%)	71	90
1	E	421/438 (96%)	412 (98%)	9 (2%)	53	82
1	F	421/438 (96%)	411 (98%)	10 (2%)	49	79
1	G	421/438 (96%)	412 (98%)	9 (2%)	53	82
1	H	421/438 (96%)	414 (98%)	7 (2%)	60	85
All	All	3368/3504 (96%)	3302 (98%)	66 (2%)	55	83

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	547	ASP
1	H	66	LYS
1	H	406	ARG
1	C	493	ARG
1	C	425	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	432	GLN
1	H	465	GLN
1	F	137	HIS
1	H	432	GLN
1	H	113	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	TPP	G	602	2	22,27,27	2.87	5 (22%)	29,40,40	2.13	10 (34%)
3	TPP	D	602	2	22,27,27	2.57	3 (13%)	29,40,40	2.12	9 (31%)
3	TPP	F	602	2	22,27,27	2.00	4 (18%)	29,40,40	1.98	11 (37%)
3	TPP	E	602	2	22,27,27	2.88	3 (13%)	29,40,40	1.81	10 (34%)
3	TPP	H	602	2	22,27,27	2.33	5 (22%)	29,40,40	2.15	10 (34%)
3	TPP	C	602	2	22,27,27	2.39	4 (18%)	29,40,40	1.81	9 (31%)
3	TPP	A	602	2	22,27,27	2.38	5 (22%)	29,40,40	2.17	10 (34%)
3	TPP	B	602	2	22,27,27	2.18	4 (18%)	29,40,40	2.26	12 (41%)

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

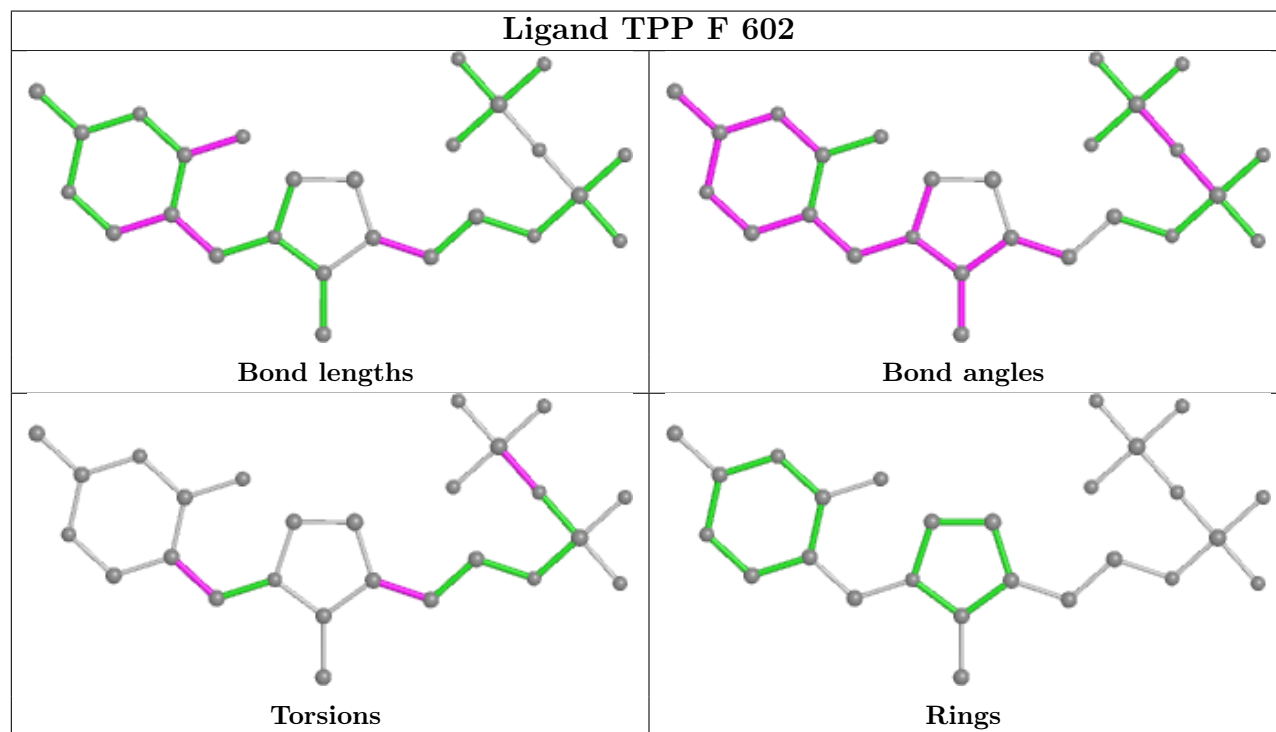| Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	G	602	2	-	2/16/17/17	0/2/2/2
3	TPP	D	602	2	-	5/16/17/17	0/2/2/2
3	TPP	F	602	2	-	4/16/17/17	0/2/2/2
3	TPP	E	602	2	-	2/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	H	602	2	-	4/16/17/17	0/2/2/2
3	TPP	C	602	2	-	4/16/17/17	0/2/2/2
3	TPP	A	602	2	-	3/16/17/17	0/2/2/2
3	TPP	B	602	2	-	4/16/17/17	0/2/2/2

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	TPP	C6-C5	12.27	1.56	1.50
3	G	602	TPP	C6-C5	11.90	1.56	1.50
3	D	602	TPP	C6-C5	10.65	1.55	1.50
3	C	602	TPP	C6-C5	9.02	1.54	1.50
3	A	602	TPP	C6-C5	8.81	1.54	1.50

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	TPP	C6-C5-C4	6.33	132.51	127.43
3	G	602	TPP	C6-C5-C4	6.19	132.40	127.43
3	B	602	TPP	C6-C5-C4	6.18	132.40	127.43
3	D	602	TPP	C6-C5-C4	5.53	131.88	127.43
3	H	602	TPP	C6-C5-C4	4.63	131.15	127.43

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	TPP	PA-O3A-PB-O3B
3	B	602	TPP	C6'-C5'-C7'-N3
3	B	602	TPP	PA-O3A-PB-O3B
3	C	602	TPP	PA-O3A-PB-O3B
3	D	602	TPP	C6'-C5'-C7'-N3

There are no ring outliers.

8 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	602	TPP	10	0
3	D	602	TPP	6	0
3	F	602	TPP	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	602	TPP	5	0
3	H	602	TPP	9	0
3	C	602	TPP	9	0
3	A	602	TPP	8	0
3	B	602	TPP	7	0

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

Ligand TPP G 602

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP D 602

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP F 602

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP E 602

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP H 602

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP C 602

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand TPP B 602

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	563/582 (96%)	-0.46	3 (0%)	91	75	31, 65, 89, 116	0
1	B	562/582 (96%)	-0.50	1 (0%)	95	87	28, 64, 110, 146	0
1	C	562/582 (96%)	-0.51	0	100	100	30, 60, 88, 116	0
1	D	562/582 (96%)	-0.47	0	100	100	32, 72, 112, 132	0
1	E	562/582 (96%)	-0.45	0	100	100	31, 69, 115, 149	0
1	F	562/582 (96%)	-0.42	3 (0%)	91	75	32, 66, 97, 136	0
1	G	562/582 (96%)	-0.48	0	100	100	22, 64, 116, 144	0
1	H	562/582 (96%)	-0.48	1 (0%)	95	87	26, 58, 97, 130	0
All	All	4497/4656 (96%)	-0.47	8 (0%)	95	87	22, 64, 107, 149	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	563	ALA	3.2
1	F	563	ALA	3.0
1	A	2	ALA	2.6
1	A	564	GLY	2.5
1	B	563	ALA	2.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	601	1/1	0.94	0.21	56,56,56,56	0
3	TPP	A	602	26/26	0.95	0.19	55,71,98,114	0
2	MG	D	601	1/1	0.96	0.11	75,75,75,75	0
3	TPP	B	602	26/26	0.96	0.17	77,95,120,126	0
3	TPP	D	602	26/26	0.96	0.18	73,92,112,123	0
3	TPP	E	602	26/26	0.96	0.17	66,73,93,100	0
3	TPP	F	602	26/26	0.96	0.16	61,82,112,119	0
3	TPP	G	602	26/26	0.96	0.17	55,75,91,94	0
3	TPP	H	602	26/26	0.96	0.19	52,84,108,121	0
3	TPP	C	602	26/26	0.97	0.16	60,80,103,108	0
2	MG	H	601	1/1	0.97	0.14	43,43,43,43	0
2	MG	G	601	1/1	0.98	0.16	36,36,36,36	0
2	MG	B	601	1/1	0.98	0.12	68,68,68,68	0
2	MG	E	601	1/1	0.99	0.16	62,62,62,62	0
2	MG	F	601	1/1	0.99	0.10	45,45,45,45	0
2	MG	C	601	1/1	0.99	0.15	49,49,49,49	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.

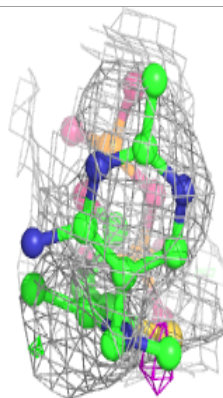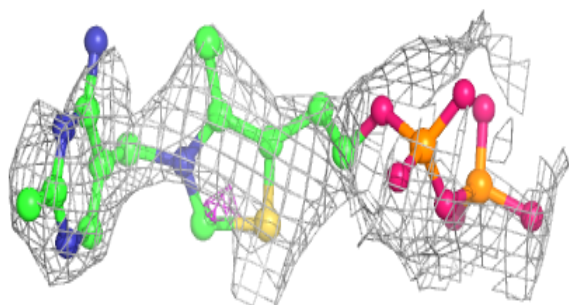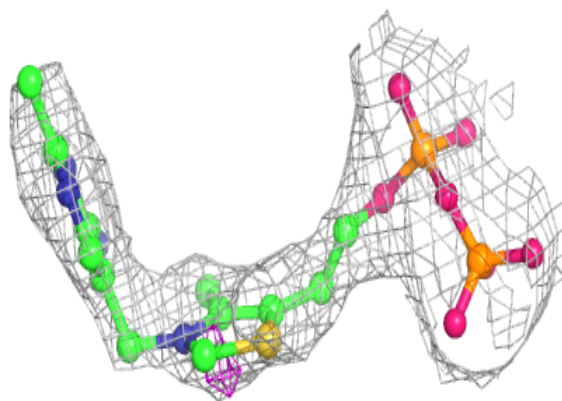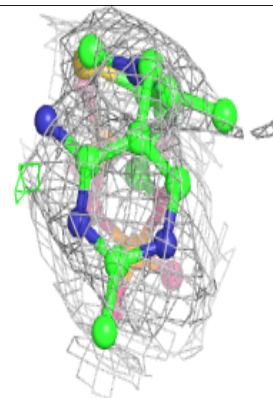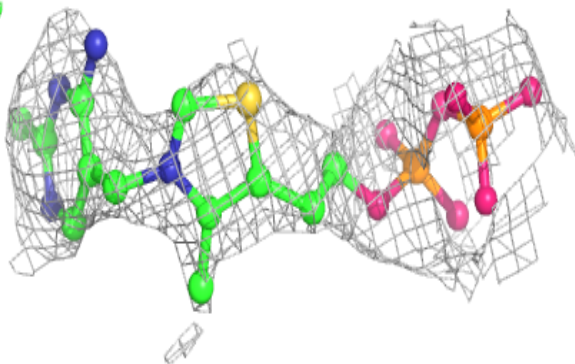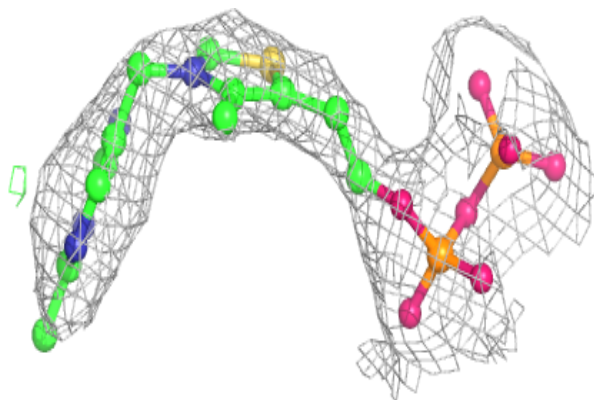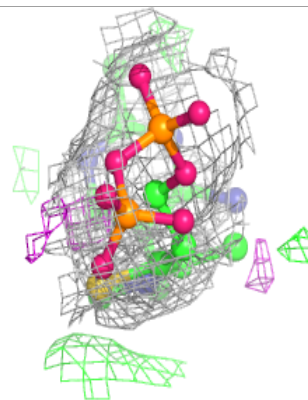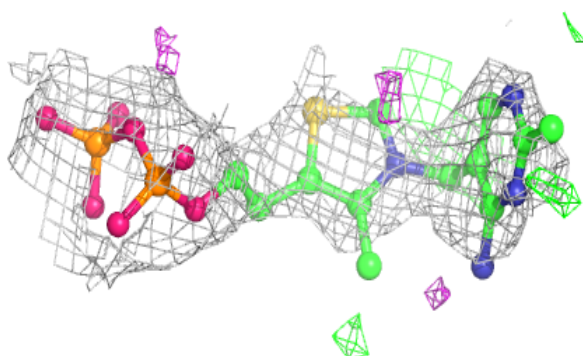**Electron density around TPP A 602:**

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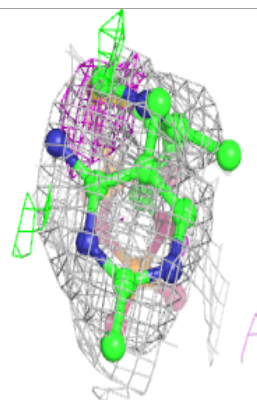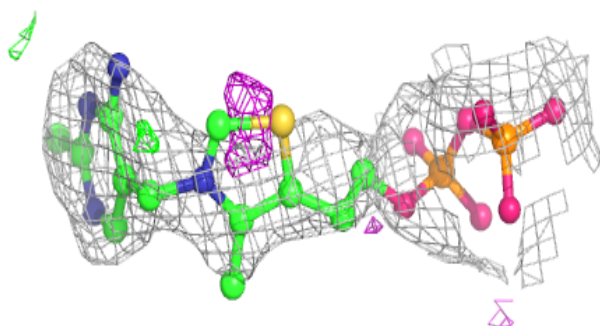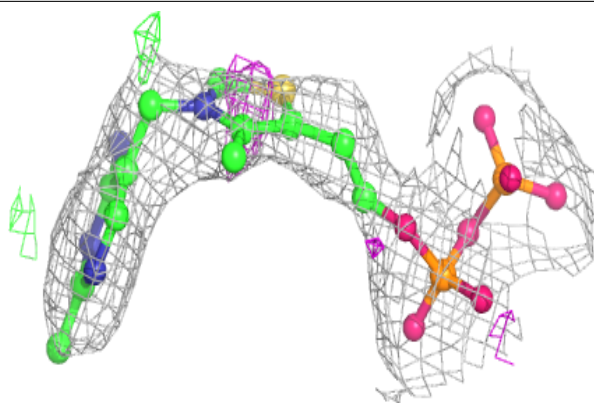
Electron density around TPP B 602:

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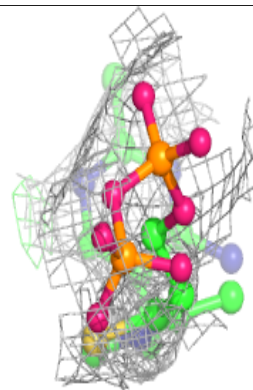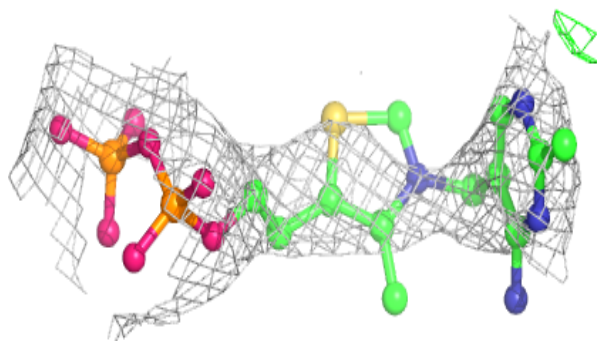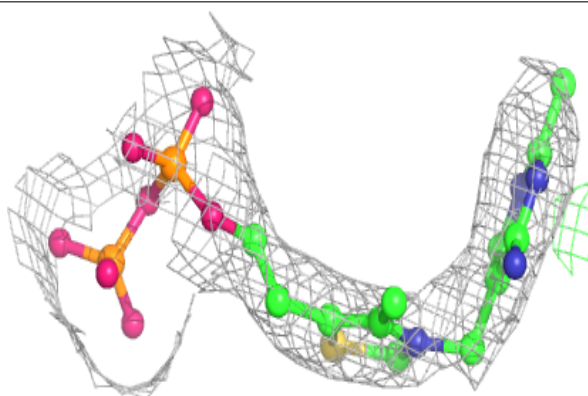
Electron density around TPP D 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
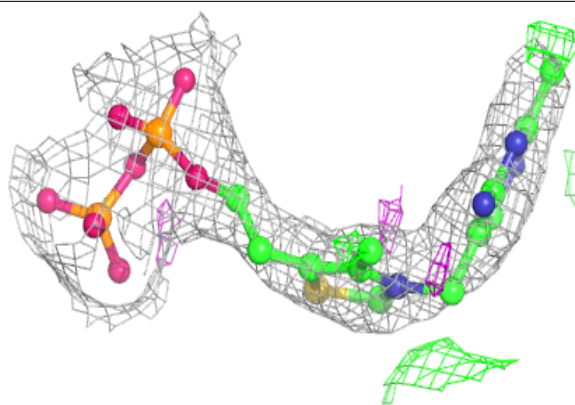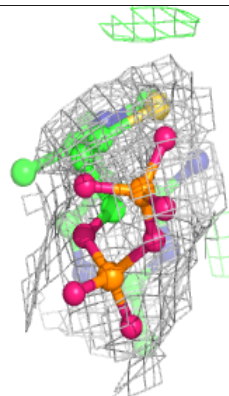and green (positive)
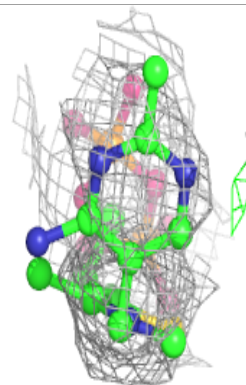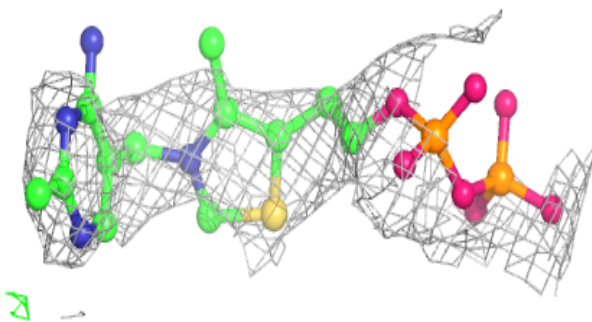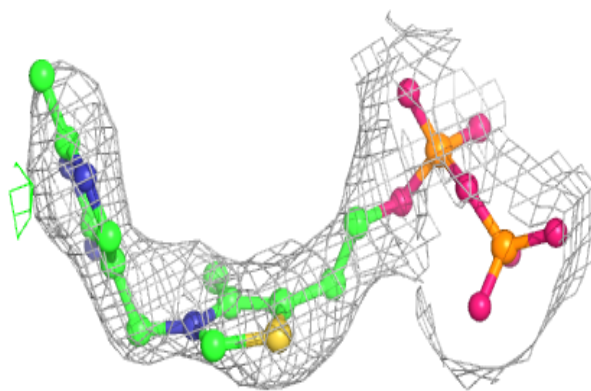
Electron density around TPP E 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
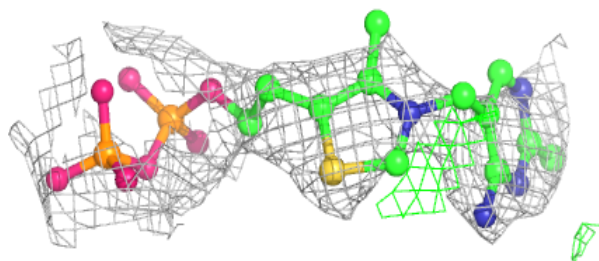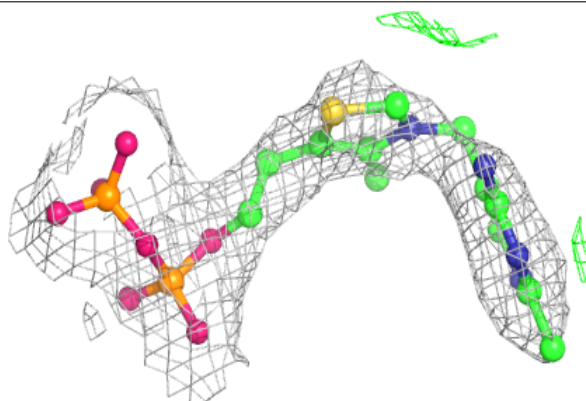and green (positive)
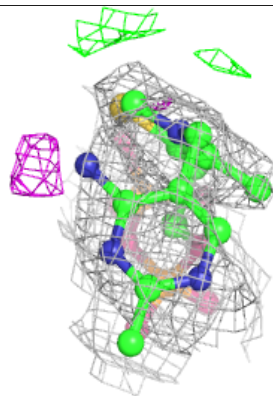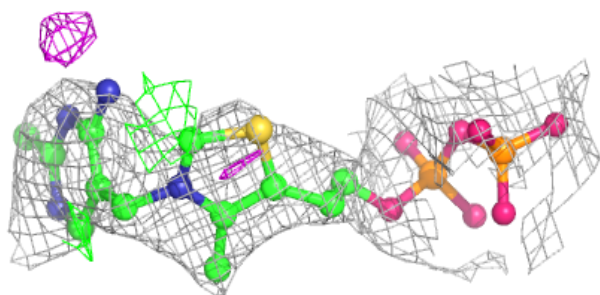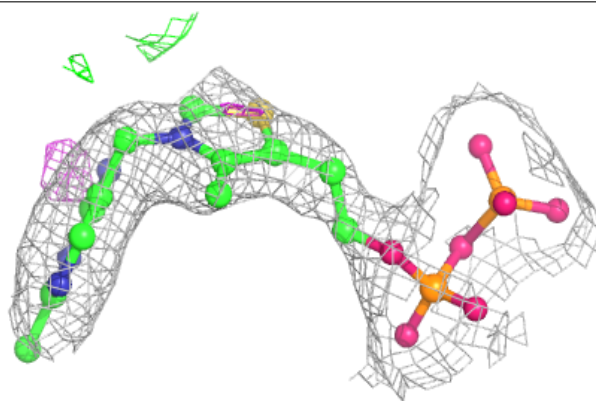
Electron density around TPP F 602:

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 G 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 H 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 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.