WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 05:16 am GMT

PDB ID	:	5L3K
Title	:	Structure of Mycobacterium thermoresistibile trehalose-6-phosphate synthase in a ternary complex with ADP and fructose-6-phosphate
Authors	:	Mendes, V.; Verma, N.; Blaszczyk, M.; Blundell, T.L.
Deposited on	:	2016-05-23
Resolution	:	2.31 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.31 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		0.209
Clashscore		8
Ramachandran outliers		0.3%
Sidechain outliers		2.0%
RSRZ outliers		0.7%

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	487	72% 19% · 8%
1	B	487	77% 16% · 6%
1	C	487	69% 21% · 9%
1	D	487	82% 13% 5%
1	E	487	80% 14% 5%

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Mol	Chain	Length	Quality of chain
1	F	487	78% 15% 7%
1	G	487	% 67% 18% · 14%
1	H	487	2% 77% 15% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 29978 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.
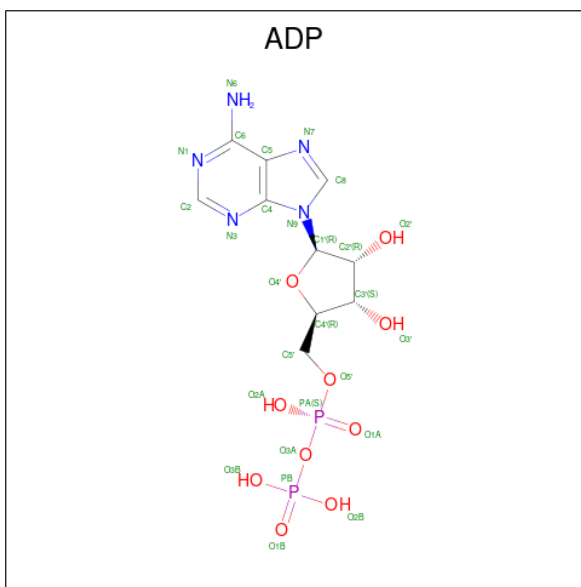
- Molecule 1 is a protein called Alpha,alpha-trehalose-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3467	2211	622	627	7			
1	B	458	Total	C	N	O	S	0	0	0
			3583	2286	654	636	7			
1	C	444	Total	C	N	O	S	0	0	0
			3449	2198	625	619	7			
1	D	462	Total	C	N	O	S	0	0	0
			3607	2301	657	642	7			
1	E	461	Total	C	N	O	S	0	0	0
			3625	2305	660	653	7			
1	F	455	Total	C	N	O	S	0	0	0
			3558	2267	646	638	7			
1	G	419	Total	C	N	O	S	0	0	0
			3262	2086	581	588	7			
1	H	450	Total	C	N	O	S	0	0	0
			3511	2235	642	627	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A117IMA6
B	0	SER	-	expression tag	UNP A0A117IMA6
C	0	SER	-	expression tag	UNP A0A117IMA6
D	0	SER	-	expression tag	UNP A0A117IMA6
E	0	SER	-	expression tag	UNP A0A117IMA6
F	0	SER	-	expression tag	UNP A0A117IMA6
G	0	SER	-	expression tag	UNP A0A117IMA6
H	0	SER	-	expression tag	UNP A0A117IMA6

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP
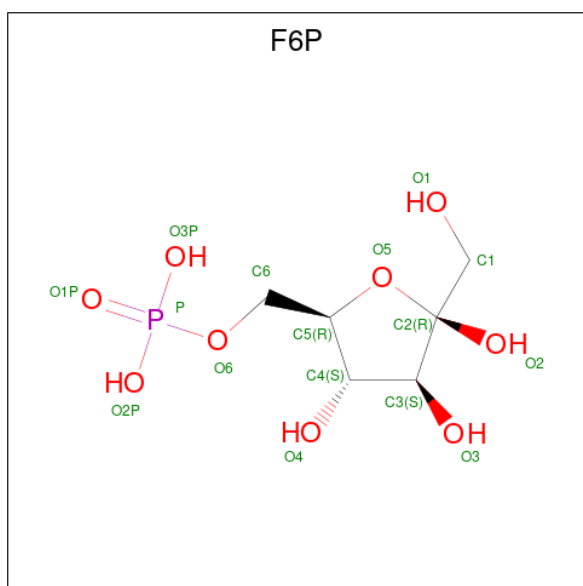
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO
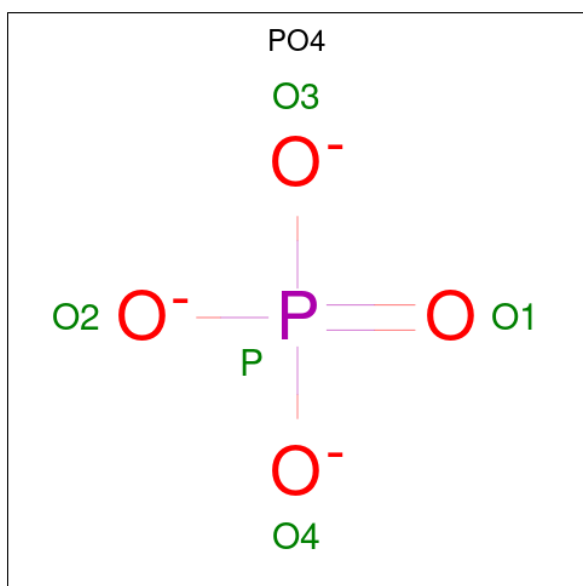
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0

- Molecule 4 is 6-O-phosphono-beta-D-fructofuranose (three-letter code: F6P) (formula: $C_6H_{13}O_9P$).

F6P

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 16	C 6	O 9	P 1	0	0
4	C	1	Total 16	C 6	O 9	P 1	0	0
4	D	1	Total 16	C 6	O 9	P 1	0	0
4	E	1	Total 16	C 6	O 9	P 1	0	0
4	F	1	Total 16	C 6	O 9	P 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 5	O 4	P 1	0	0
5	D	1	Total 5	O 4	P 1	0	0
5	D	1	Total 5	O 4	P 1	0	0
5	F	1	Total 5	O 4	P 1	0	0
5	H	1	Total 5	O 4	P 1	0	0
5	H	1	Total 5	O 4	P 1	0	0
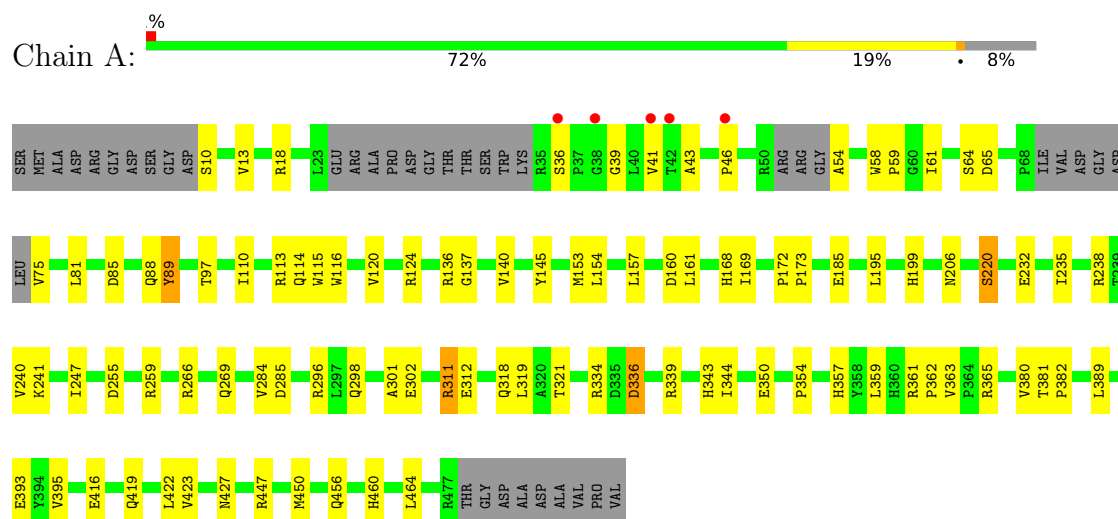
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total 148	O 148	0	0
6	B	215	Total 215	O 215	0	0
6	C	172	Total 172	O 172	0	0
6	D	230	Total 230	O 230	0	0
6	E	259	Total 259	O 259	0	0
6	F	188	Total 188	O 188	0	0
6	G	134	Total 134	O 134	0	0
6	H	232	Total 232	O 232	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.
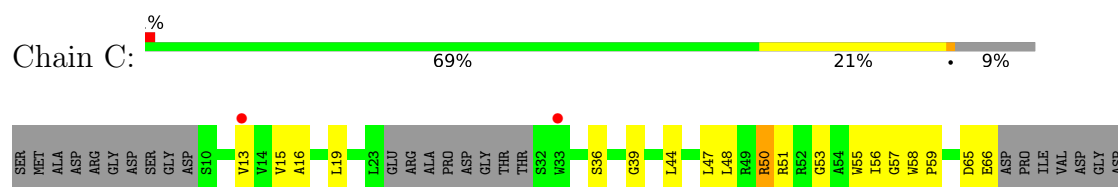
- Molecule 1: Alpha,alpha-trehalose-phosphate synthase
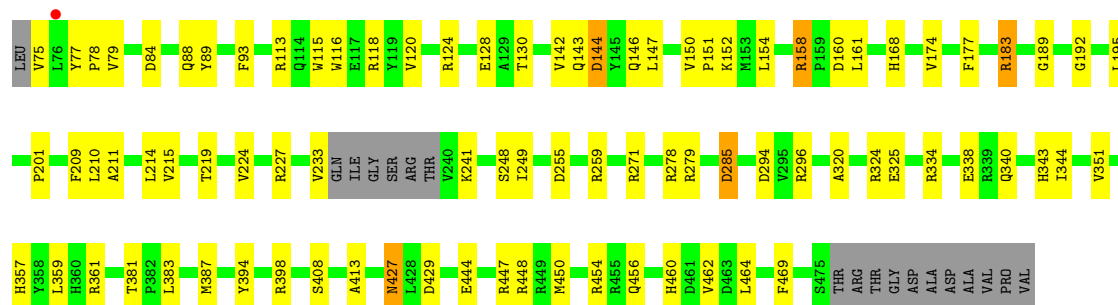
Chain A:

- Molecule 1: Alpha,alpha-trehalose-phosphate synthase
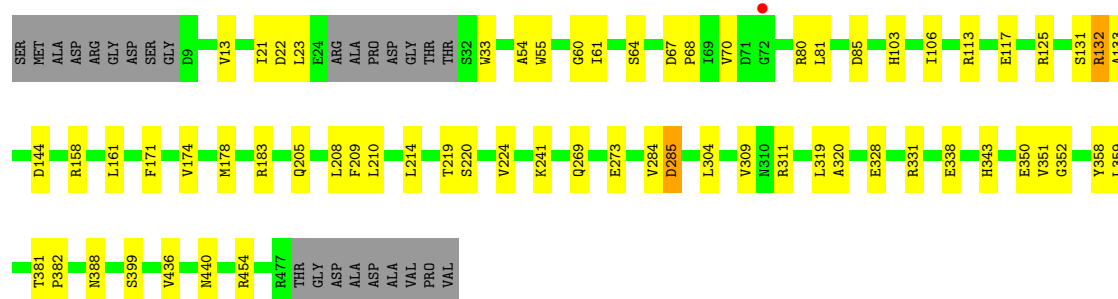
Chain B:

- Molecule 1: Alpha,alpha-trehalose-phosphate synthase
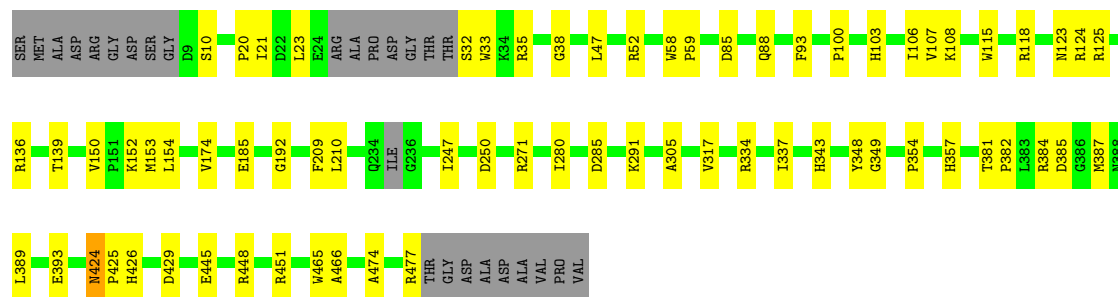
Chain C:

• Molecule 1: Alpha,alpha-trehalose-phosphate synthase

Chain D:

82%   13%   5%
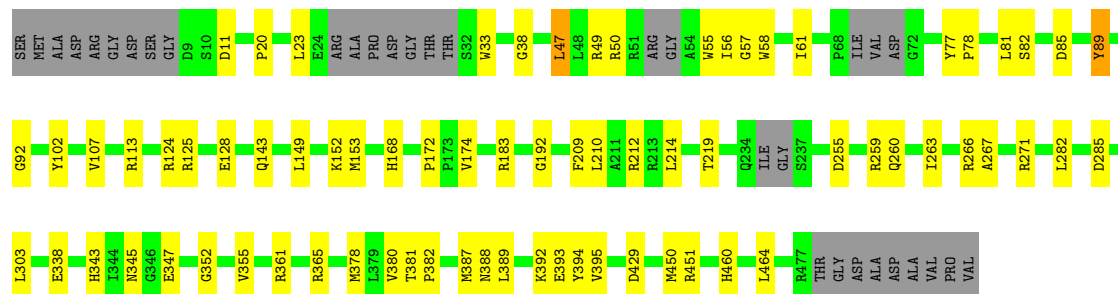
• Molecule 1: Alpha,alpha-trehalose-phosphate synthase

Chain E:

80%   14%   5%
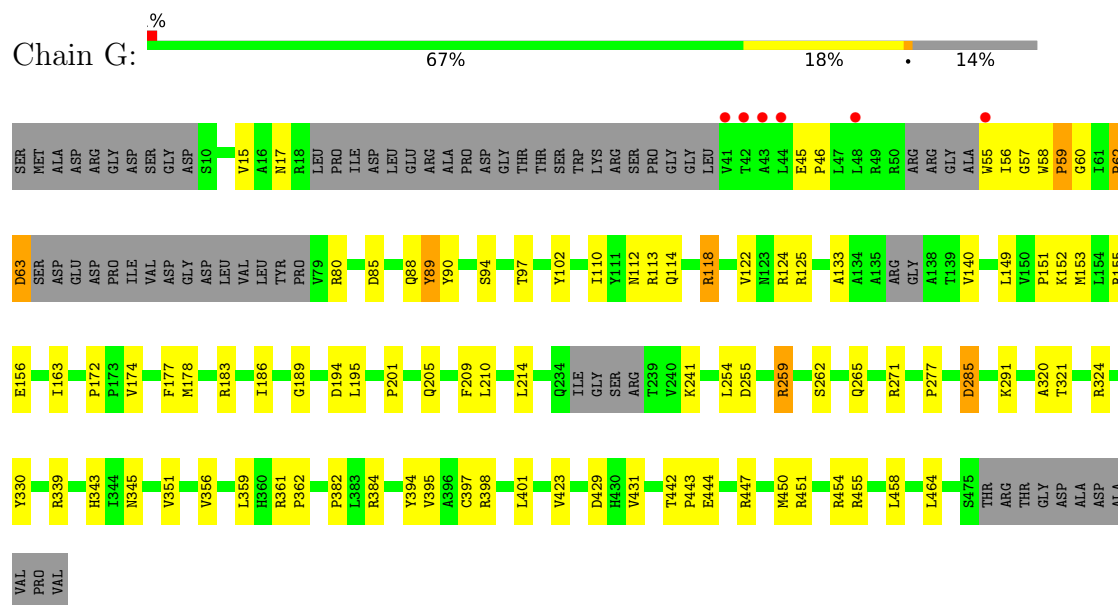
• Molecule 1: Alpha,alpha-trehalose-phosphate synthase
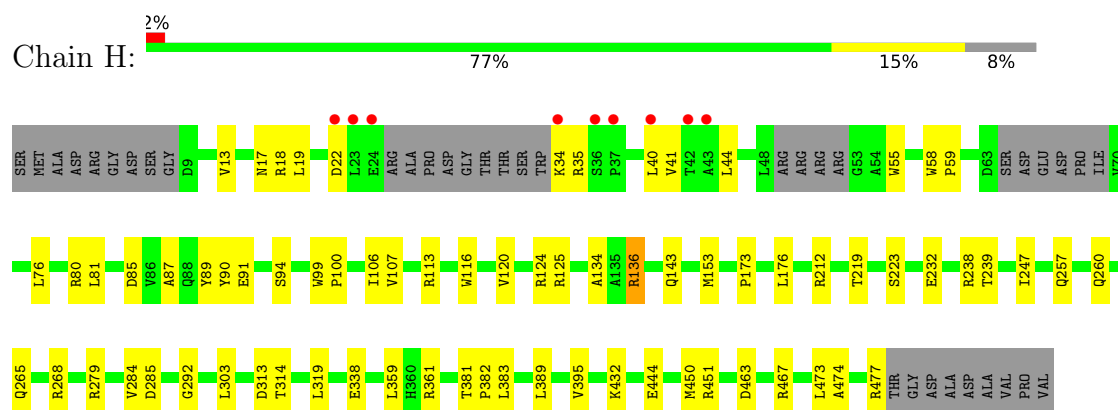
Chain F:

78%   15%   7%

• Molecule 1: Alpha,alpha-trehalose-phosphate synthase

Chain G:

• Molecule 1: Alpha,alpha-trehalose-phosphate synthase

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	216.96Å 216.96Å 159.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	121.74 – 2.31 121.74 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (121.74-2.31) 100.0 (121.74-2.31)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.153 , 0.213 0.151 , 0.209	Depositor DCC
R_{free} test set	9365 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.0	EDS
L-test for twinning [2]	$< |L| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.277 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.300 for h,-h-k,-l	Depositor
Outliers	0 of 187654 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	29978	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PO4, ADP, F6P

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	0.40	0/3544	0.59	1/4829 (0.0%)
1	B	0.43	0/3664	0.62	1/4989 (0.0%)
1	C	0.49	3/3525 (0.1%)	0.64	4/4801 (0.1%)
1	D	0.43	0/3689	0.59	0/5024
1	E	0.44	0/3706	0.63	0/5045
1	F	0.44	0/3637	0.62	3/4950 (0.1%)
1	G	0.51	4/3333 (0.1%)	0.67	5/4539 (0.1%)
1	H	0.43	0/3588	0.62	0/4884
All	All	0.45	7/28686 (0.0%)	0.62	14/39061 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	H	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	63	ASP	N-CA	-8.64	1.29	1.46
1	G	63	ASP	CA-CB	-7.98	1.36	1.53
1	C	158	ARG	NE-CZ	-7.91	1.22	1.33
1	C	158	ARG	CZ-NH1	-7.49	1.23	1.33
1	G	80	ARG	NE-CZ	6.21	1.41	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	63	ASP	CB-CG-OD1	-12.46	107.09	118.30
1	C	448	ARG	NE-CZ-NH1	-11.40	114.60	120.30
1	G	80	ARG	NE-CZ-NH2	10.44	125.52	120.30
1	F	47	LEU	CA-CB-CG	9.35	136.81	115.30
1	C	448	ARG	NE-CZ-NH2	6.81	123.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	63	ASP	Sidechain
1	H	143	GLN	Peptide

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	3467	0	3381	63	0
1	B	3583	0	3541	57	0
1	C	3449	0	3376	80	0
1	D	3607	0	3564	43	0
1	E	3625	0	3569	46	0
1	F	3558	0	3490	46	0
1	G	3262	0	3179	57	0
1	H	3511	0	3457	47	0
2	A	27	0	11	2	0
2	B	27	0	11	1	0
2	C	27	0	11	3	0
2	D	27	0	11	1	0
2	E	27	0	11	1	0
2	F	27	0	11	1	0
2	G	27	0	11	1	0
2	H	27	0	11	1	0
3	A	4	0	6	1	0
3	C	4	0	6	2	0
3	H	4	0	6	0	0
4	B	16	0	11	2	0
4	C	16	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	16	0	11	0	0
4	E	16	0	11	1	0
4	F	16	0	11	1	0
5	B	5	0	0	0	0
5	D	10	0	0	0	0
5	F	5	0	0	1	0
5	H	10	0	0	0	0
6	A	148	0	0	7	0
6	B	215	0	0	6	0
6	C	172	0	0	3	0
6	D	230	0	0	2	1
6	E	259	0	0	3	1
6	F	188	0	0	1	0
6	G	134	0	0	3	0
6	H	232	0	0	4	0
All	All	29978	0	27717	428	1

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 8.

The worst 5 of 428 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)
2:F:501:ADP:C1'	2:F:501:ADP:O4'	1.66	1.27
2:G:501:ADP:O4'	2:G:501:ADP:C1'	1.65	1.27
2:A:501:ADP:O4'	2:A:501:ADP:C1'	1.66	1.26
2:B:501:ADP:O4'	2:B:501:ADP:C1'	1.64	1.22
2:C:501:ADP:O4'	2:C:501:ADP:C1'	1.65	1.19

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:751:HOH:O	6:E:728:HOH:O[2_755]	2.13	0.07

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	440/487 (90%)	416 (94%)	23 (5%)	1 (0%)	47	58
1	B	452/487 (93%)	429 (95%)	22 (5%)	1 (0%)	47	58
1	C	436/487 (90%)	414 (95%)	21 (5%)	1 (0%)	47	58
1	D	458/487 (94%)	432 (94%)	24 (5%)	2 (0%)	34	42
1	E	455/487 (93%)	434 (95%)	21 (5%)	0	100	100
1	F	445/487 (91%)	425 (96%)	18 (4%)	2 (0%)	34	42
1	G	407/487 (84%)	378 (93%)	25 (6%)	4 (1%)	15	17
1	H	442/487 (91%)	419 (95%)	23 (5%)	0	100	100
All	All	3535/3896 (91%)	3347 (95%)	177 (5%)	11 (0%)	41	50

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	50	ARG
1	G	62	PRO
1	G	133	ALA
1	B	144	ASP
1	D	388	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/402 (87%)	338 (97%)	11 (3%)	39	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	B	364/402 (90%)	358 (98%)	6 (2%)		62	78
1	C	347/402 (86%)	336 (97%)	11 (3%)		39	54
1	D	366/402 (91%)	363 (99%)	3 (1%)		81	91
1	E	371/402 (92%)	362 (98%)	9 (2%)		49	66
1	F	361/402 (90%)	355 (98%)	6 (2%)		60	76
1	G	329/402 (82%)	324 (98%)	5 (2%)		65	79
1	H	356/402 (89%)	350 (98%)	6 (2%)		60	76
All	All	2843/3216 (88%)	2786 (98%)	57 (2%)		55	72

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	132	ARG
1	H	451	ARG
1	E	154	LEU
1	H	285	ASP
1	G	285	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	17	ASN
1	G	345	ASN
1	B	426	HIS
1	B	318	GLN
1	H	234	GLN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

22 ligands are modelled in this entry.

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	EDO	A	502	-	3,3,3	0.48	0	2,2,2	0.33	0
2	ADP	C	501	-	24,29,29	4.69	6 (25%)	29,45,45	1.55	4 (13%)
4	F6P	F	502	-	15,16,16	0.85	1 (6%)	17,25,25	0.93	1 (5%)
3	EDO	H	502	-	3,3,3	0.36	0	2,2,2	0.65	0
2	ADP	A	501	-	24,29,29	4.80	6 (25%)	29,45,45	1.63	4 (13%)
5	PO4	B	503	-	4,4,4	0.89	0	6,6,6	0.47	0
2	ADP	D	501	-	24,29,29	4.71	6 (25%)	29,45,45	1.63	5 (17%)
4	F6P	C	502	-	15,16,16	0.91	1 (6%)	17,25,25	1.48	4 (23%)
5	PO4	D	504	-	4,4,4	0.88	0	6,6,6	0.40	0
2	ADP	E	501	-	24,29,29	4.60	6 (25%)	29,45,45	1.29	3 (10%)
2	ADP	B	501	-	24,29,29	4.55	6 (25%)	29,45,45	1.56	5 (17%)
4	F6P	D	502	-	15,16,16	0.88	1 (6%)	17,25,25	1.53	4 (23%)
4	F6P	B	502	-	15,16,16	0.90	1 (6%)	17,25,25	1.43	4 (23%)
3	EDO	C	503	-	3,3,3	0.51	0	2,2,2	0.27	0
2	ADP	G	501	-	24,29,29	4.76	7 (29%)	29,45,45	1.30	3 (10%)
5	PO4	F	503	-	4,4,4	0.87	0	6,6,6	0.42	0
5	PO4	D	503	-	4,4,4	0.94	0	6,6,6	0.40	0
2	ADP	H	501	-	24,29,29	4.68	6 (25%)	29,45,45	1.39	2 (6%)
2	ADP	F	501	-	24,29,29	4.81	6 (25%)	29,45,45	1.64	5 (17%)
5	PO4	H	504	-	4,4,4	0.96	0	6,6,6	0.61	0
4	F6P	E	502	-	15,16,16	1.02	1 (6%)	17,25,25	1.79	5 (29%)
5	PO4	H	503	-	4,4,4	0.88	0	6,6,6	0.55	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
3	EDO	A	502	-	-	0/1/1/1	-
2	ADP	C	501	-	-	3/12/32/32	0/3/3/3
2	ADP	B	501	-	-	4/12/32/32	0/3/3/3
2	ADP	H	501	-	-	3/12/32/32	0/3/3/3
2	ADP	F	501	-	-	3/12/32/32	0/3/3/3
2	ADP	D	501	-	-	3/12/32/32	0/3/3/3
4	F6P	C	502	-	-	5/9/28/28	0/1/1/1
4	F6P	F	502	-	-	0/9/28/28	0/1/1/1
4	F6P	D	502	-	-	4/9/28/28	0/1/1/1
4	F6P	E	502	-	-	7/9/28/28	0/1/1/1
4	F6P	B	502	-	-	5/9/28/28	0/1/1/1
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	H	502	-	-	0/1/1/1	-
2	ADP	E	501	-	-	2/12/32/32	0/3/3/3
2	ADP	A	501	-	-	5/12/32/32	0/3/3/3
2	ADP	G	501	-	-	3/12/32/32	0/3/3/3

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	ADP	O4'-C1'	18.50	1.66	1.41
2	A	501	ADP	O4'-C1'	18.16	1.66	1.41
2	D	501	ADP	O4'-C1'	17.95	1.66	1.41
2	H	501	ADP	O4'-C1'	17.63	1.65	1.41
2	G	501	ADP	O4'-C1'	17.45	1.65	1.41

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ADP	N3-C2-N1	-5.10	120.70	128.68
2	E	501	ADP	N3-C2-N1	-4.95	120.94	128.68
2	H	501	ADP	N3-C2-N1	-4.66	121.39	128.68
2	A	501	ADP	N3-C2-N1	-4.66	121.40	128.68
2	B	501	ADP	N3-C2-N1	-4.61	121.47	128.68

There are no chirality outliers.

5 of 48 torsion outliers are listed below:
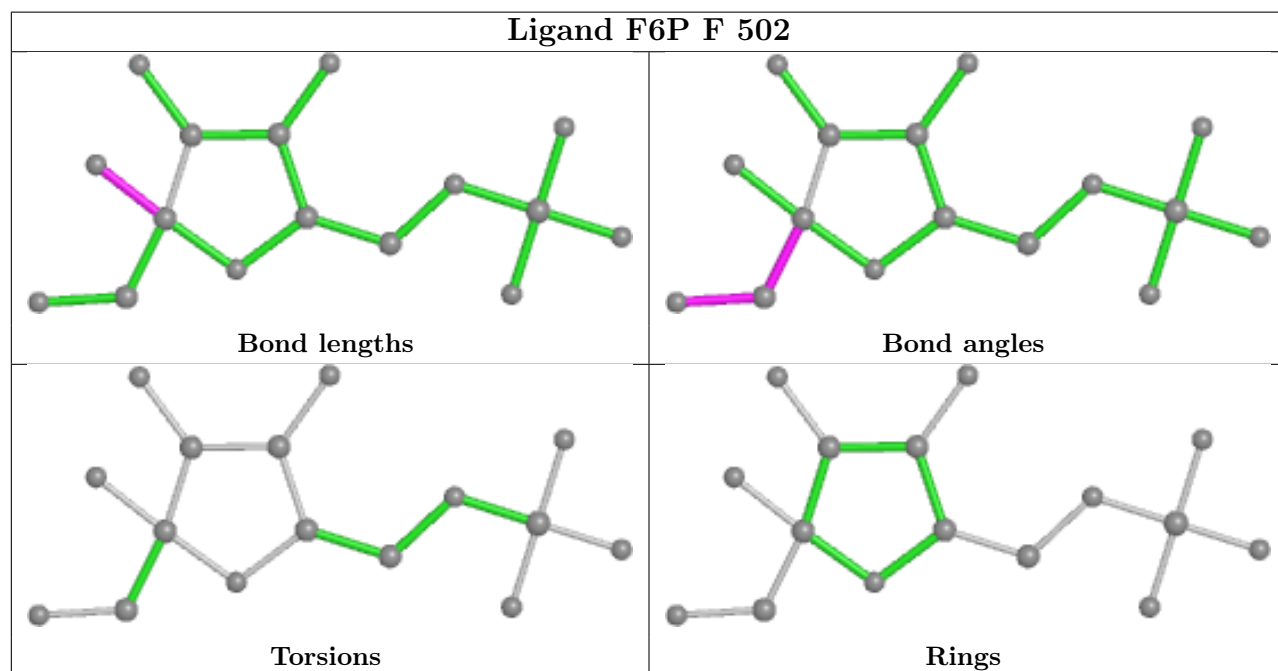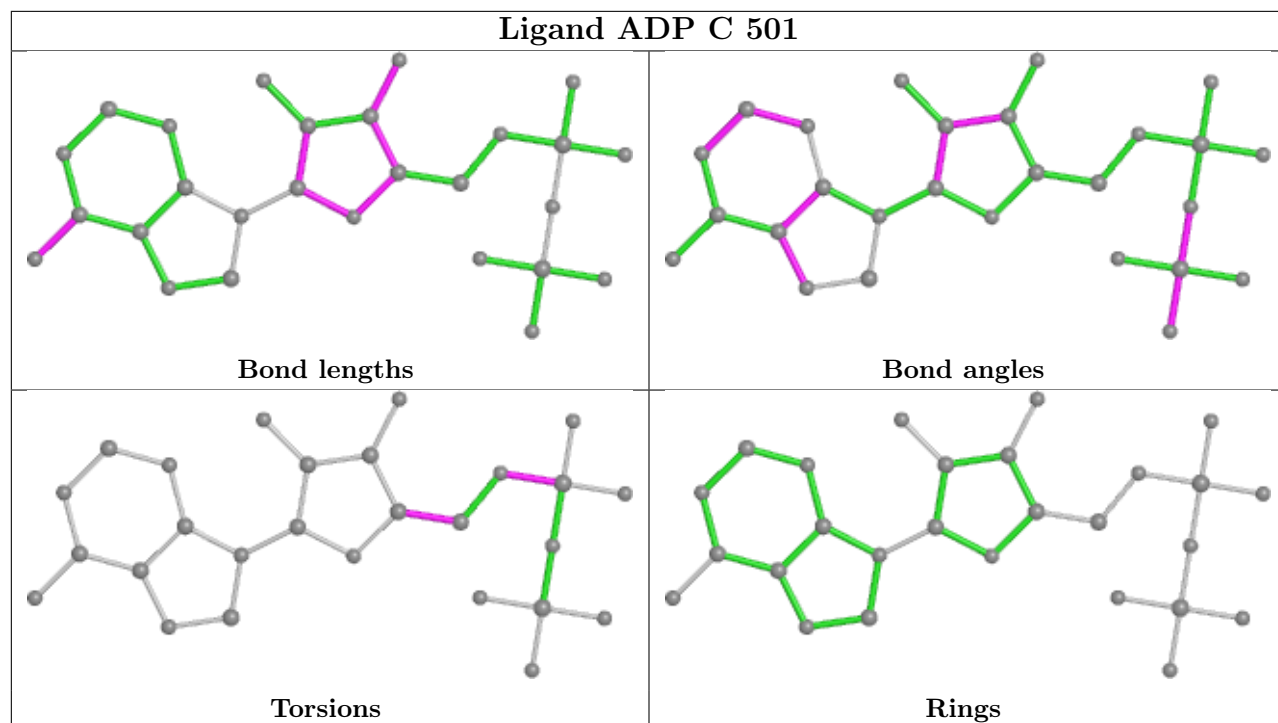
Mol	Chain	Res	Type	Atoms
2	A	501	ADP	C5'-O5'-PA-O2A
2	A	501	ADP	C5'-O5'-PA-O3A
2	C	501	ADP	C5'-O5'-PA-O1A
2	C	501	ADP	O4'-C4'-C5'-O5'
2	E	501	ADP	PB-O3A-PA-O5'
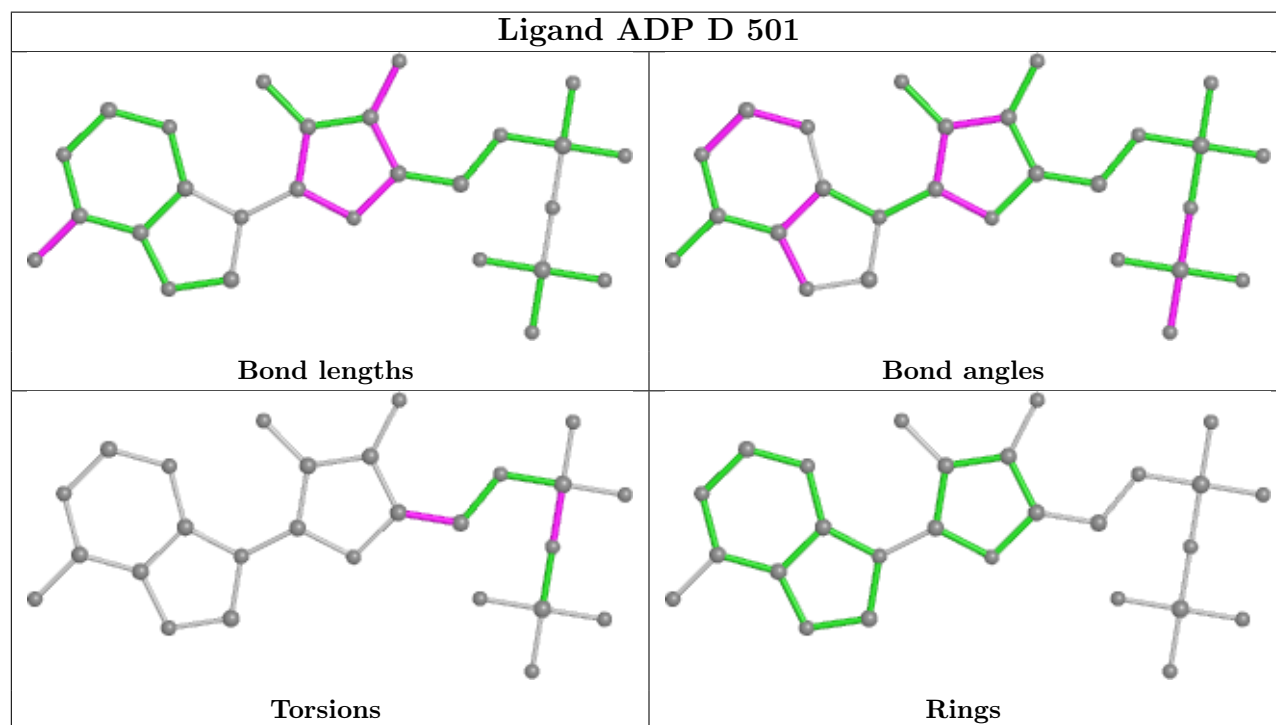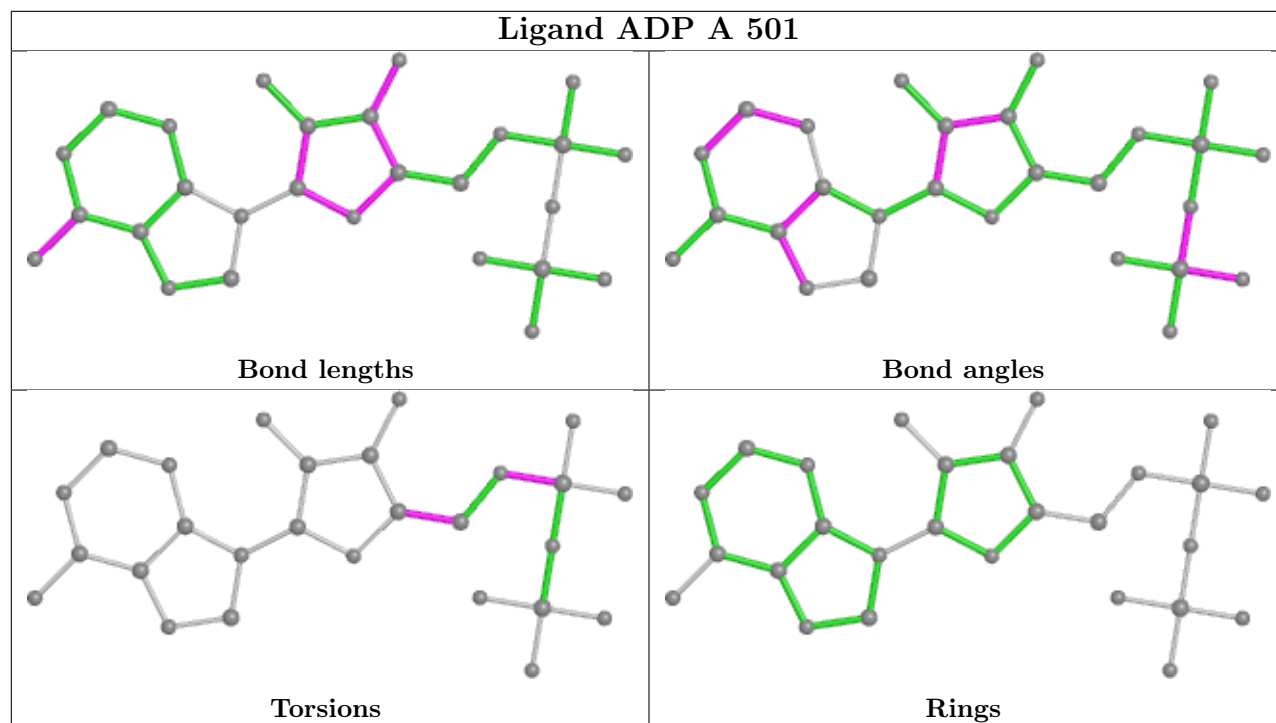
There are no ring outliers.

15 monomers are involved in 20 short contacts:
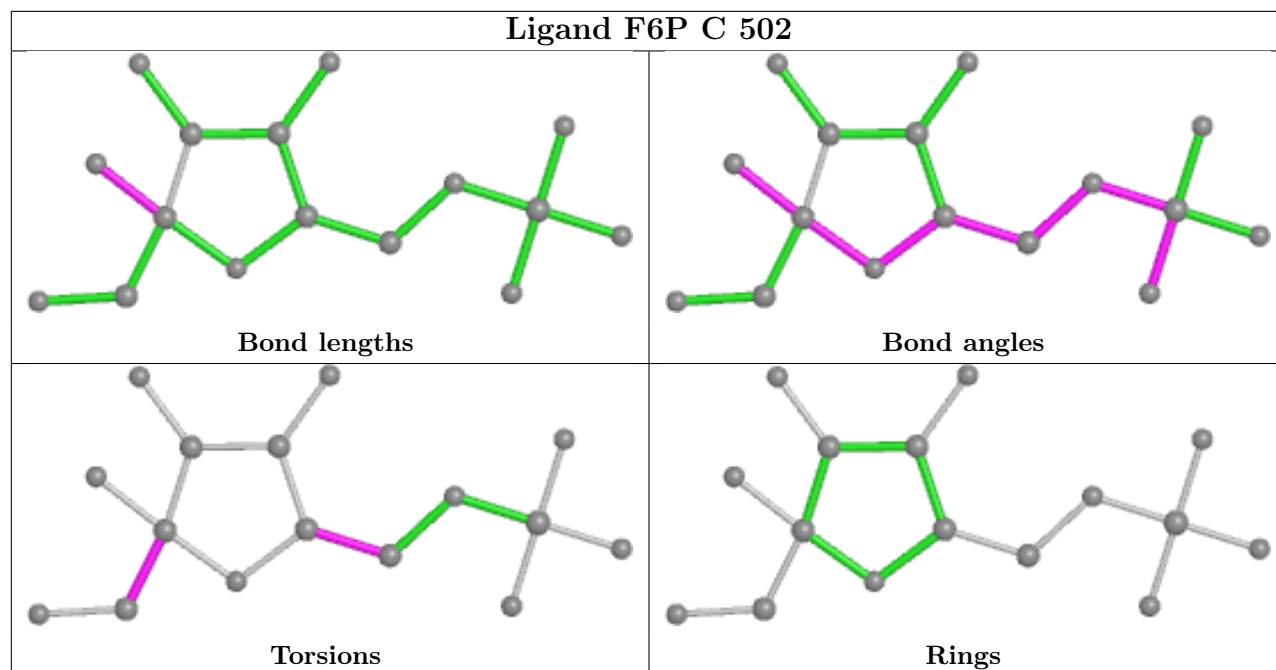
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	1	0
2	C	501	ADP	3	0
4	F	502	F6P	1	0
2	A	501	ADP	2	0
2	D	501	ADP	1	0
4	C	502	F6P	1	0
2	E	501	ADP	1	0
2	B	501	ADP	1	0
4	B	502	F6P	2	0
3	C	503	EDO	2	0
2	G	501	ADP	1	0
5	F	503	PO4	1	0
2	H	501	ADP	1	0
2	F	501	ADP	1	0
4	E	502	F6P	1	0

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 ADP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand F6P F 502

Bond lengths

Bond angles

Torsions

Rings

wwPDB X-ray Structure Validation Summary Report

Ligand ADP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand F6P C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand F6P D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand F6P B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP G 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP H 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP F 501

Bond lengths

Bond angles

Torsions

Rings

Ligand F6P E 502

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	448/487 (91%)	-0.53	5 (1%)	80	85	13, 32, 74, 118	0
1	B	458/487 (94%)	-0.70	0	100	100	13, 26, 55, 84	0
1	C	444/487 (91%)	-0.48	3 (0%)	87	91	16, 34, 74, 109	0
1	D	462/487 (94%)	-0.70	1 (0%)	95	96	12, 25, 53, 97	0
1	E	461/487 (94%)	-0.74	0	100	100	13, 24, 49, 78	0
1	F	455/487 (93%)	-0.65	0	100	100	14, 29, 64, 87	0
1	G	419/487 (86%)	-0.53	6 (1%)	75	80	16, 35, 74, 132	0
1	H	450/487 (92%)	-0.61	9 (2%)	65	71	13, 26, 63, 126	0
All	All	3597/3896 (92%)	-0.62	24 (0%)	87	91	12, 28, 66, 132	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	40	LEU	6.2
1	A	38	GLY	5.8
1	A	41	VAL	5.0
1	G	48	LEU	4.2
1	A	36	SER	4.1

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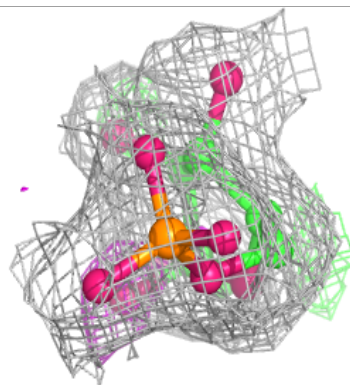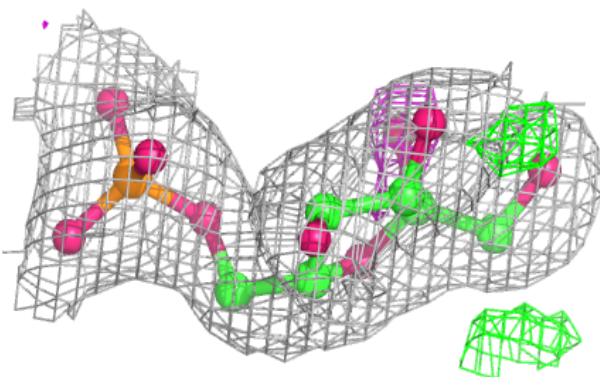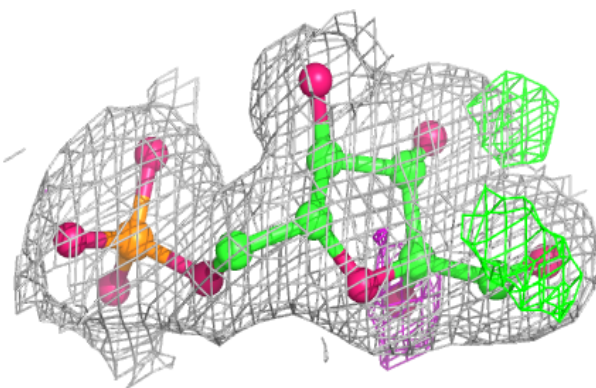
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	503	4/4	0.90	0.28	29,35,41,44	0
3	EDO	A	502	4/4	0.93	0.37	54,54,55,56	0
5	PO4	B	503	5/5	0.93	0.10	83,85,88,88	0
5	PO4	F	503	5/5	0.94	0.12	67,72,73,77	0
4	F6P	F	502	16/16	0.95	0.11	19,33,41,51	0
5	PO4	H	503	5/5	0.95	0.09	61,61,62,62	0
5	PO4	D	503	5/5	0.96	0.07	56,57,60,60	0
5	PO4	D	504	5/5	0.96	0.09	78,79,80,80	0
5	PO4	H	504	5/5	0.96	0.10	67,70,72,72	0
4	F6P	C	502	16/16	0.97	0.13	26,33,38,42	0
4	F6P	B	502	16/16	0.97	0.11	26,31,35,42	0
3	EDO	H	502	4/4	0.98	0.12	19,20,24,27	0
2	ADP	G	501	27/27	0.98	0.10	24,32,38,39	0
2	ADP	A	501	27/27	0.98	0.09	20,26,30,32	0
4	F6P	D	502	16/16	0.98	0.09	21,26,32,35	0
4	F6P	E	502	16/16	0.98	0.10	17,29,46,53	0
2	ADP	C	501	27/27	0.98	0.09	17,24,31,34	0
2	ADP	H	501	27/27	0.99	0.08	18,25,30,33	0
2	ADP	D	501	27/27	0.99	0.09	14,20,26,28	0
2	ADP	E	501	27/27	0.99	0.10	12,21,24,25	0
2	ADP	F	501	27/27	0.99	0.09	14,20,26,29	0
2	ADP	B	501	27/27	0.99	0.08	15,20,25,28	0
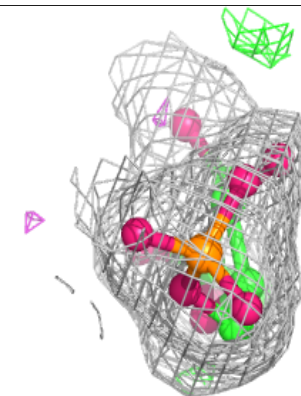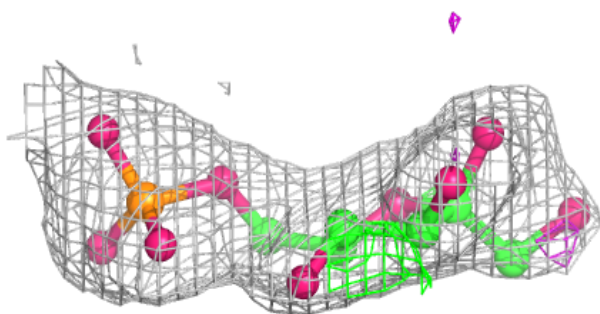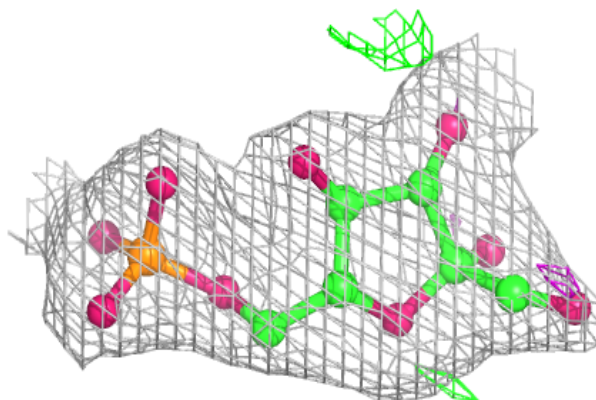
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around F6P F 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
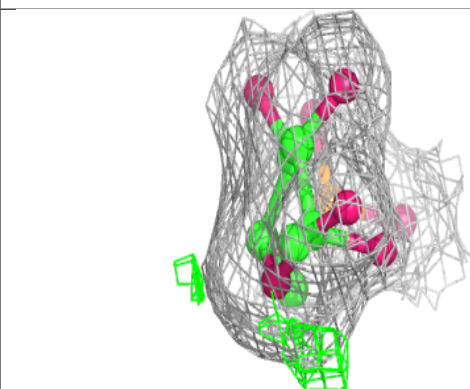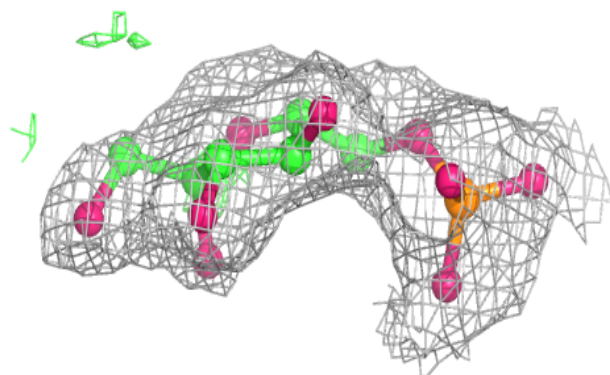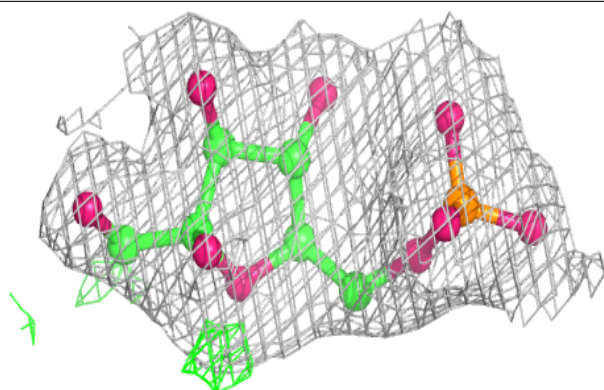
Electron density around F6P C 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
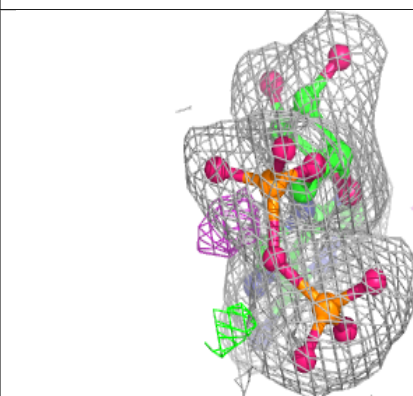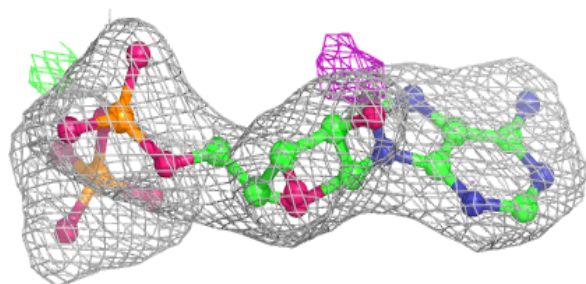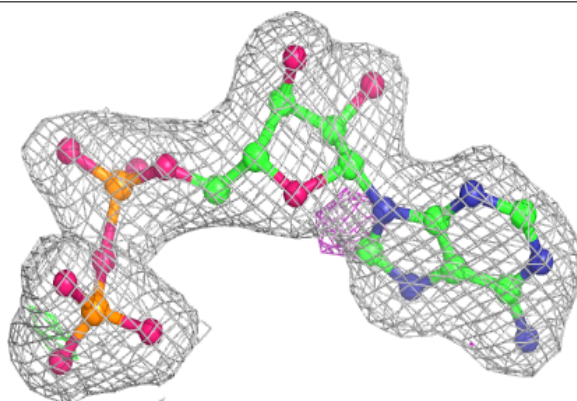
Electron density around F6P B 502:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
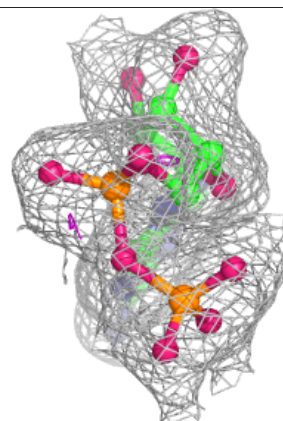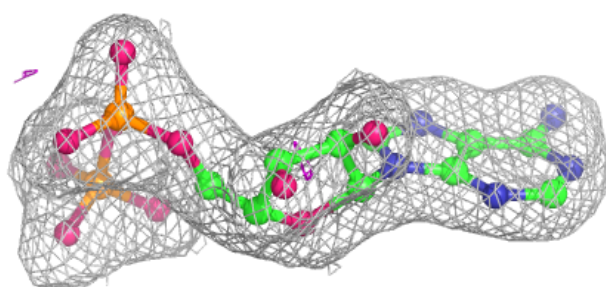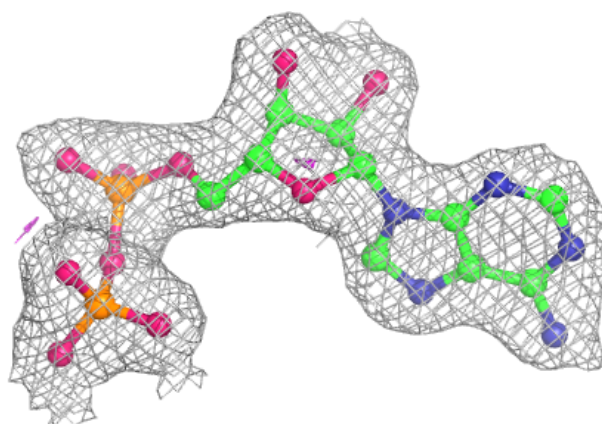
Electron density around ADP G 501:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
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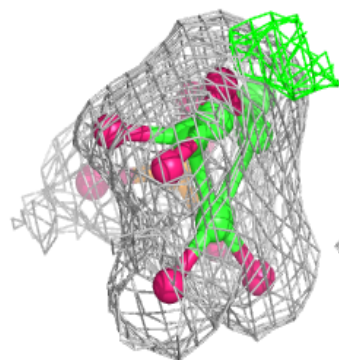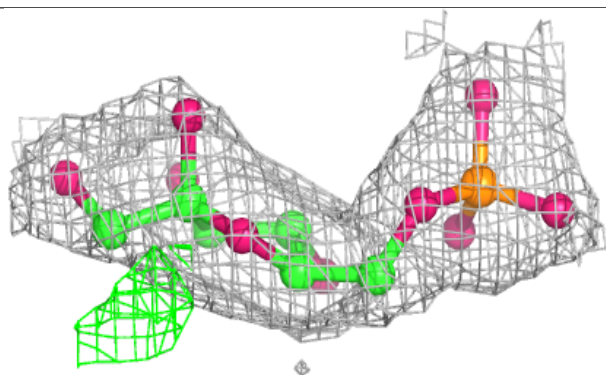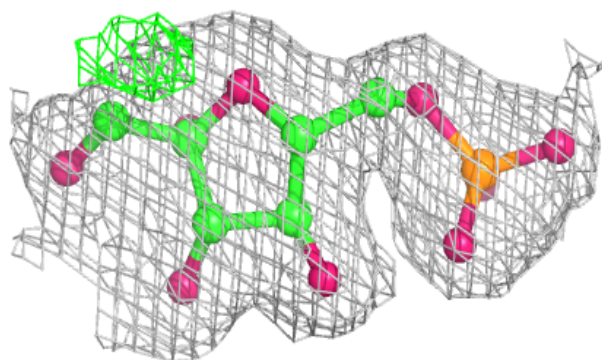
Electron density around ADP A 501:

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and green (positive)
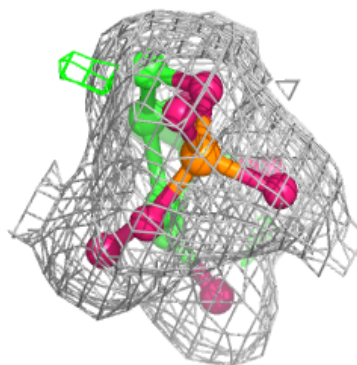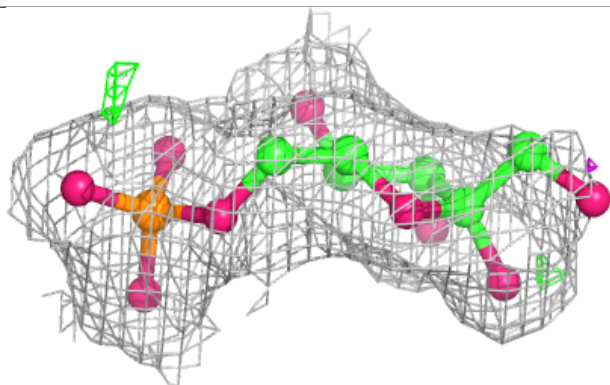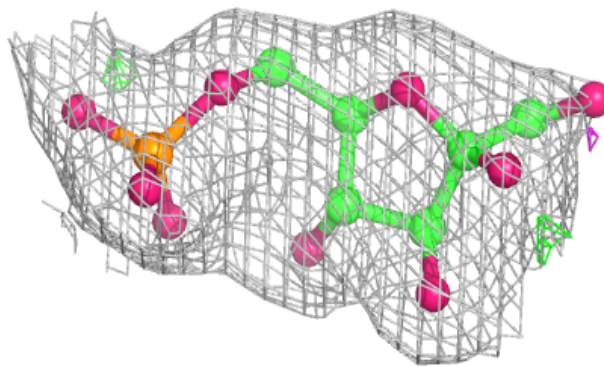
Electron density around F6P D 502:

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and green (positive)
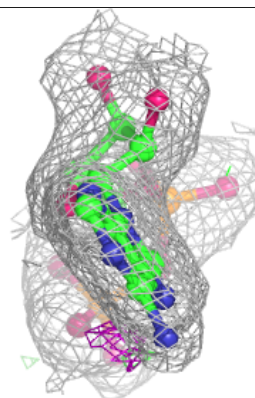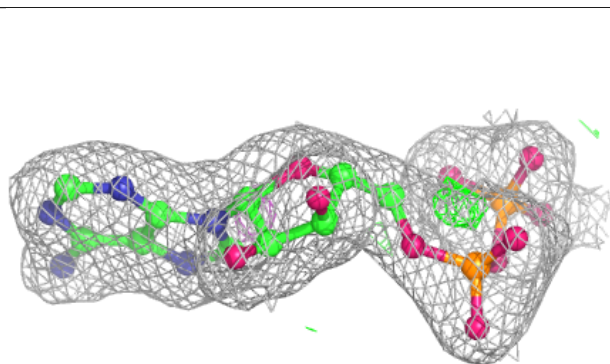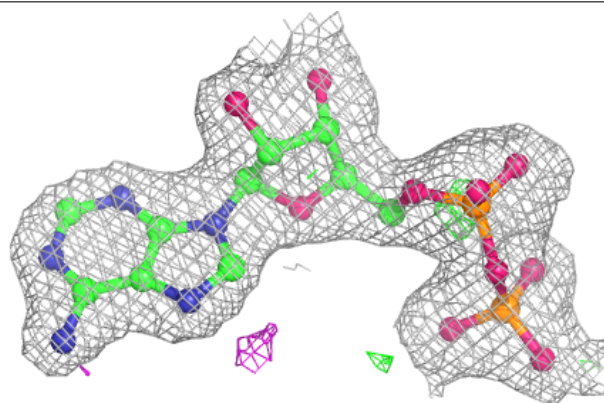
Electron density around F6P E 502:

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and green (positive)
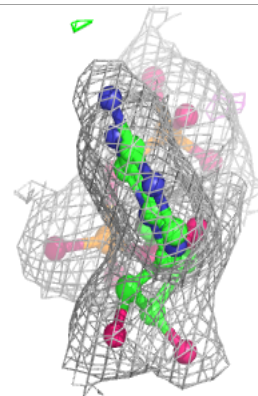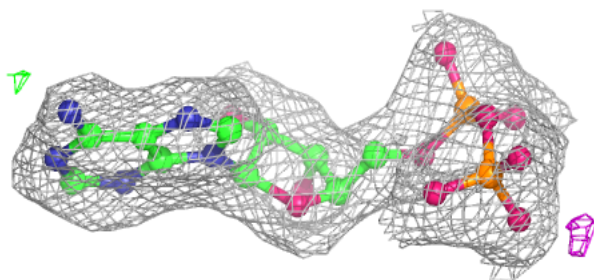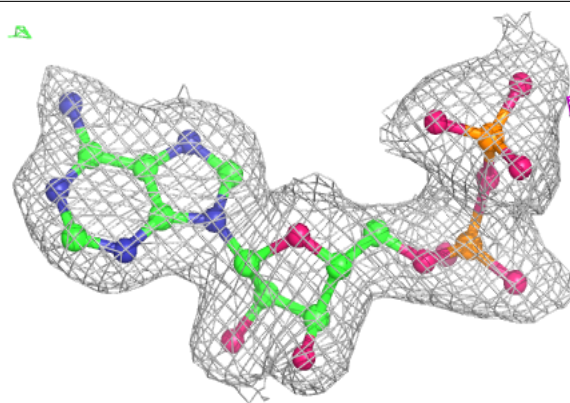
Electron density around ADP C 501:

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$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
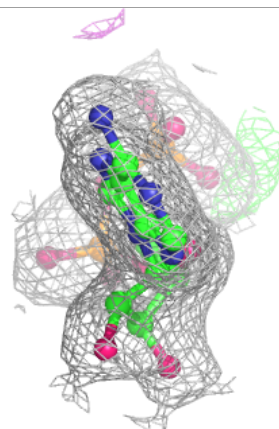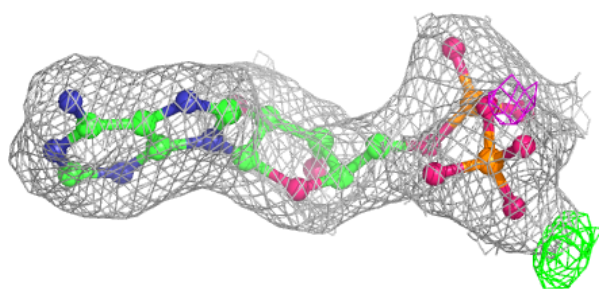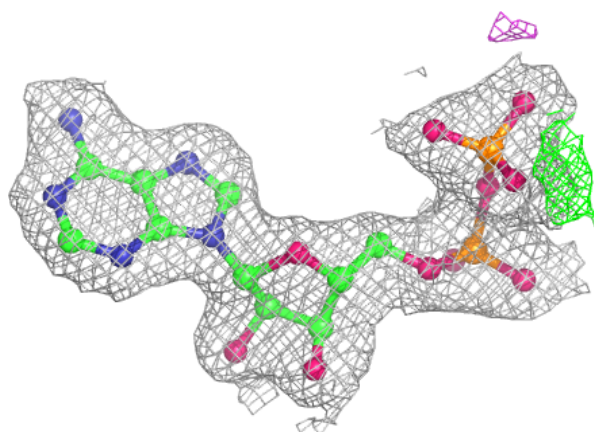
Electron density around ADP H 501:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
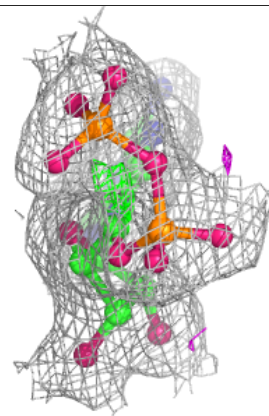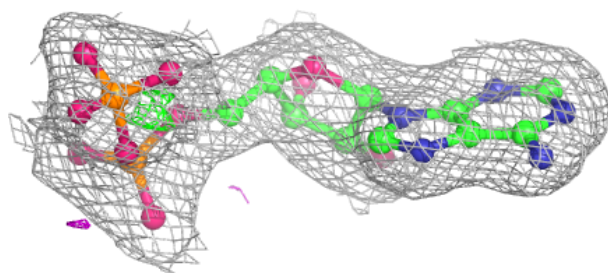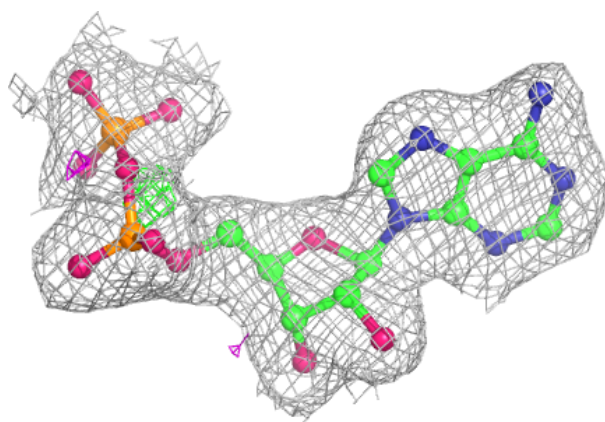
Electron density around ADP D 501:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
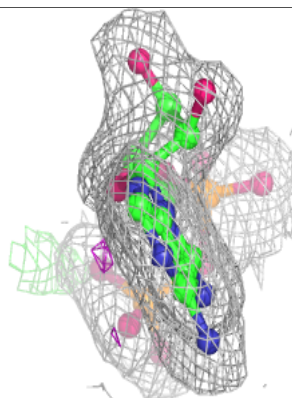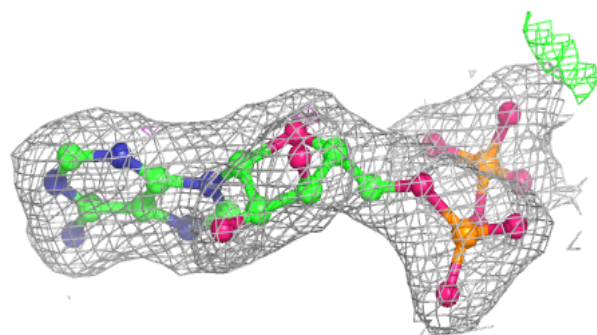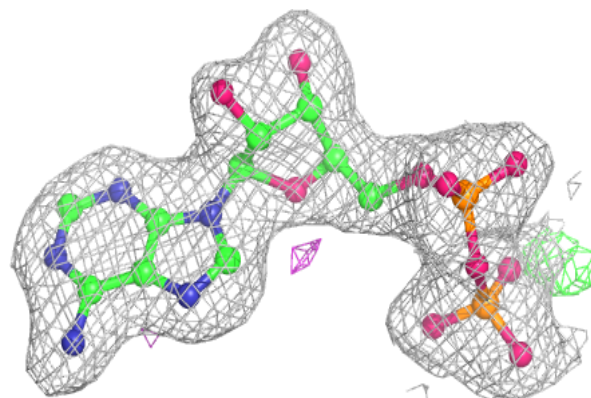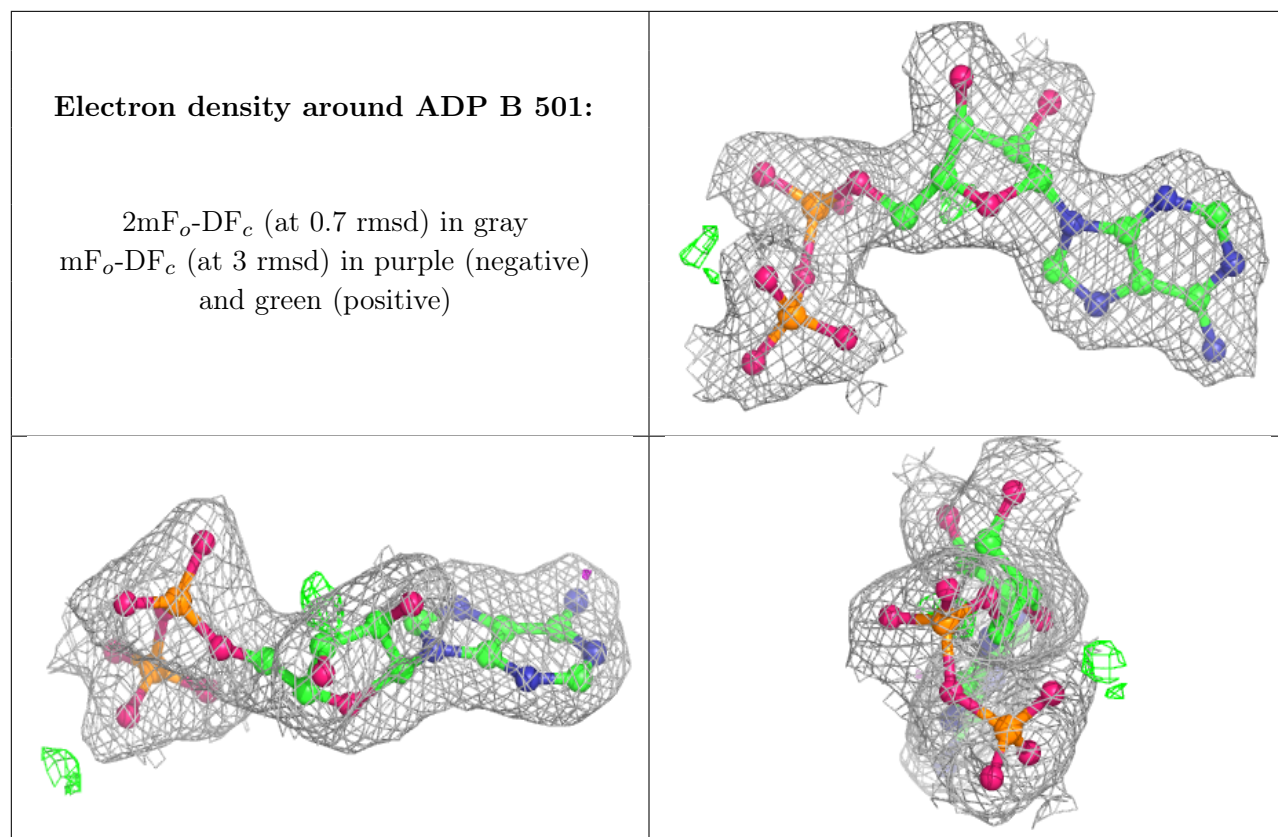
Electron density around ADP E 501:

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

Electron density around ADP 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)

Electron density around ADP 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)

6.5   Other polymers (i)

There are no such residues in this entry.