



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 12, 2024 – 03:34 AM EST

PDB ID : 2Q14
Title : Crystal structure of Phosphohydrolase (BT4208) from *Bacteroides thetaio-*
taomicron VPI-5482 at 2.20 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-05-23
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

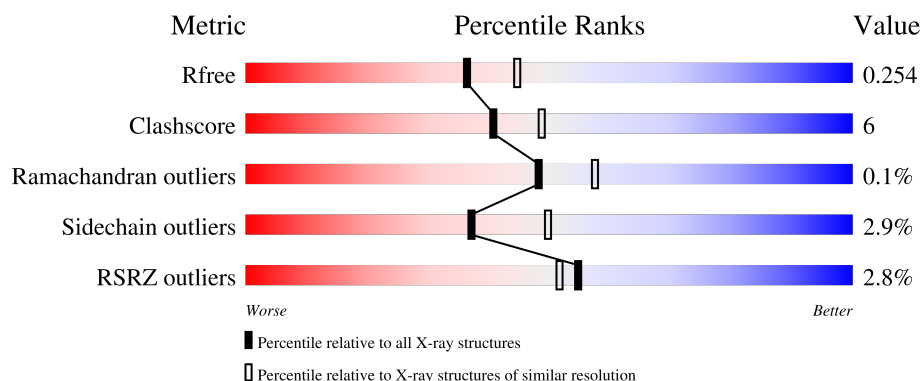
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	410	<div> <div>0%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	B	410	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
1	C	410	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	D	410	<div> <div>4%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
1	E	410	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	410	
1	G	410	
1	H	410	

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
5	GOL	D	502	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27697 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 Phosphohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	Se	0	2	0
			3233	2069	543	606	2	13			
1	B	400	Total	C	N	O	S	Se	0	3	0
			3189	2042	533	599	2	13			
1	C	406	Total	C	N	O	S	Se	0	2	0
			3246	2078	547	605	2	14			
1	D	403	Total	C	N	O	S	Se	0	3	0
			3223	2070	539	598	2	14			
1	E	403	Total	C	N	O	S	Se	0	5	0
			3246	2079	547	604	2	14			
1	F	400	Total	C	N	O	S	Se	0	11	0
			3242	2079	543	604	2	14			
1	G	403	Total	C	N	O	S	Se	0	5	0
			3236	2072	545	604	2	13			
1	H	398	Total	C	N	O	S	Se	0	11	0
			3197	2052	530	600	2	13			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	cloning artifact	UNP Q8A013
A	1	MSE	MET	modified residue	UNP Q8A013
A	66	MSE	MET	modified residue	UNP Q8A013
A	122	MSE	MET	modified residue	UNP Q8A013
A	124	MSE	MET	modified residue	UNP Q8A013
A	127	MSE	MET	modified residue	UNP Q8A013
A	131	MSE	MET	modified residue	UNP Q8A013
A	161	MSE	MET	modified residue	UNP Q8A013
A	189	MSE	MET	modified residue	UNP Q8A013
A	217	MSE	MET	modified residue	UNP Q8A013
A	233	MSE	MET	modified residue	UNP Q8A013
A	310	MSE	MET	modified residue	UNP Q8A013
A	361	MSE	MET	modified residue	UNP Q8A013

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Chain	Residue	Modelled	Actual	Comment	Reference
A	387	MSE	MET	modified residue	UNP Q8A013
B	0	GLY	-	cloning artifact	UNP Q8A013
B	1	MSE	MET	modified residue	UNP Q8A013
B	66	MSE	MET	modified residue	UNP Q8A013
B	122	MSE	MET	modified residue	UNP Q8A013
B	124	MSE	MET	modified residue	UNP Q8A013
B	127	MSE	MET	modified residue	UNP Q8A013
B	131	MSE	MET	modified residue	UNP Q8A013
B	161	MSE	MET	modified residue	UNP Q8A013
B	189	MSE	MET	modified residue	UNP Q8A013
B	217	MSE	MET	modified residue	UNP Q8A013
B	233	MSE	MET	modified residue	UNP Q8A013
B	310	MSE	MET	modified residue	UNP Q8A013
B	361	MSE	MET	modified residue	UNP Q8A013
B	387	MSE	MET	modified residue	UNP Q8A013
C	0	GLY	-	cloning artifact	UNP Q8A013
C	1	MSE	MET	modified residue	UNP Q8A013
C	66	MSE	MET	modified residue	UNP Q8A013
C	122	MSE	MET	modified residue	UNP Q8A013
C	124	MSE	MET	modified residue	UNP Q8A013
C	127	MSE	MET	modified residue	UNP Q8A013
C	131	MSE	MET	modified residue	UNP Q8A013
C	161	MSE	MET	modified residue	UNP Q8A013
C	189	MSE	MET	modified residue	UNP Q8A013
C	217	MSE	MET	modified residue	UNP Q8A013
C	233	MSE	MET	modified residue	UNP Q8A013
C	310	MSE	MET	modified residue	UNP Q8A013
C	361	MSE	MET	modified residue	UNP Q8A013
C	387	MSE	MET	modified residue	UNP Q8A013
D	0	GLY	-	cloning artifact	UNP Q8A013
D	1	MSE	MET	modified residue	UNP Q8A013
D	66	MSE	MET	modified residue	UNP Q8A013
D	122	MSE	MET	modified residue	UNP Q8A013
D	124	MSE	MET	modified residue	UNP Q8A013
D	127	MSE	MET	modified residue	UNP Q8A013
D	131	MSE	MET	modified residue	UNP Q8A013
D	161	MSE	MET	modified residue	UNP Q8A013
D	189	MSE	MET	modified residue	UNP Q8A013
D	217	MSE	MET	modified residue	UNP Q8A013
D	233	MSE	MET	modified residue	UNP Q8A013
D	310	MSE	MET	modified residue	UNP Q8A013
D	361	MSE	MET	modified residue	UNP Q8A013

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Chain	Residue	Modelled	Actual	Comment	Reference
D	387	MSE	MET	modified residue	UNP Q8A013
E	0	GLY	-	cloning artifact	UNP Q8A013
E	1	MSE	MET	modified residue	UNP Q8A013
E	66	MSE	MET	modified residue	UNP Q8A013
E	122	MSE	MET	modified residue	UNP Q8A013
E	124	MSE	MET	modified residue	UNP Q8A013
E	127	MSE	MET	modified residue	UNP Q8A013
E	131	MSE	MET	modified residue	UNP Q8A013
E	161	MSE	MET	modified residue	UNP Q8A013
E	189	MSE	MET	modified residue	UNP Q8A013
E	217	MSE	MET	modified residue	UNP Q8A013
E	233	MSE	MET	modified residue	UNP Q8A013
E	310	MSE	MET	modified residue	UNP Q8A013
E	361	MSE	MET	modified residue	UNP Q8A013
E	387	MSE	MET	modified residue	UNP Q8A013
F	0	GLY	-	cloning artifact	UNP Q8A013
F	1	MSE	MET	modified residue	UNP Q8A013
F	66	MSE	MET	modified residue	UNP Q8A013
F	122	MSE	MET	modified residue	UNP Q8A013
F	124	MSE	MET	modified residue	UNP Q8A013
F	127	MSE	MET	modified residue	UNP Q8A013
F	131	MSE	MET	modified residue	UNP Q8A013
F	161	MSE	MET	modified residue	UNP Q8A013
F	189	MSE	MET	modified residue	UNP Q8A013
F	217	MSE	MET	modified residue	UNP Q8A013
F	233	MSE	MET	modified residue	UNP Q8A013
F	310	MSE	MET	modified residue	UNP Q8A013
F	361	MSE	MET	modified residue	UNP Q8A013
F	387	MSE	MET	modified residue	UNP Q8A013
G	0	GLY	-	cloning artifact	UNP Q8A013
G	1	MSE	MET	modified residue	UNP Q8A013
G	66	MSE	MET	modified residue	UNP Q8A013
G	122	MSE	MET	modified residue	UNP Q8A013
G	124	MSE	MET	modified residue	UNP Q8A013
G	127	MSE	MET	modified residue	UNP Q8A013
G	131	MSE	MET	modified residue	UNP Q8A013
G	161	MSE	MET	modified residue	UNP Q8A013
G	189	MSE	MET	modified residue	UNP Q8A013
G	217	MSE	MET	modified residue	UNP Q8A013
G	233	MSE	MET	modified residue	UNP Q8A013
G	310	MSE	MET	modified residue	UNP Q8A013
G	361	MSE	MET	modified residue	UNP Q8A013

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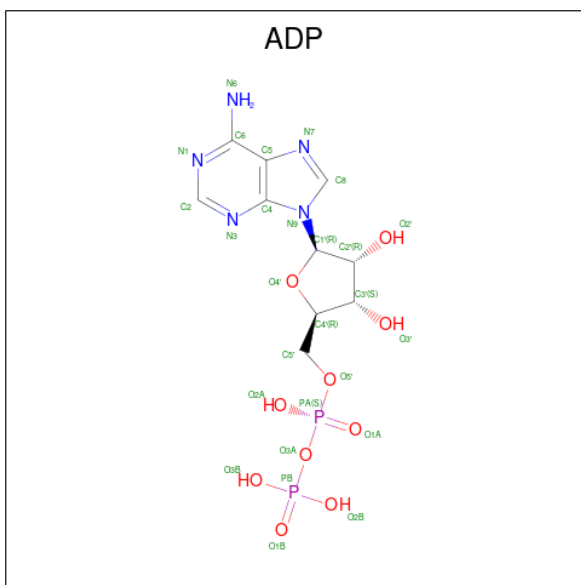
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Chain	Residue	Modelled	Actual	Comment	Reference
G	387	MSE	MET	modified residue	UNP Q8A013
H	0	GLY	-	cloning artifact	UNP Q8A013
H	1	MSE	MET	modified residue	UNP Q8A013
H	66	MSE	MET	modified residue	UNP Q8A013
H	122	MSE	MET	modified residue	UNP Q8A013
H	124	MSE	MET	modified residue	UNP Q8A013
H	127	MSE	MET	modified residue	UNP Q8A013
H	131	MSE	MET	modified residue	UNP Q8A013
H	161	MSE	MET	modified residue	UNP Q8A013
H	189	MSE	MET	modified residue	UNP Q8A013
H	217	MSE	MET	modified residue	UNP Q8A013
H	233	MSE	MET	modified residue	UNP Q8A013
H	310	MSE	MET	modified residue	UNP Q8A013
H	361	MSE	MET	modified residue	UNP Q8A013
H	387	MSE	MET	modified residue	UNP Q8A013

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

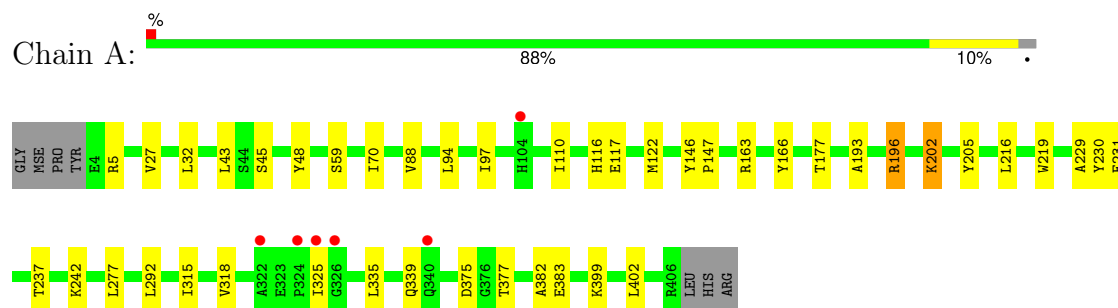
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	262	Total	O	0	0
			262	262		
6	B	259	Total	O	0	0
			259	259		
6	C	198	Total	O	0	0
			198	198		
6	D	182	Total	O	0	0
			182	182		
6	E	203	Total	O	0	0
			203	203		
6	F	236	Total	O	0	0
			236	236		
6	G	181	Total	O	0	0
			181	181		
6	H	103	Total	O	0	0
			103	103		

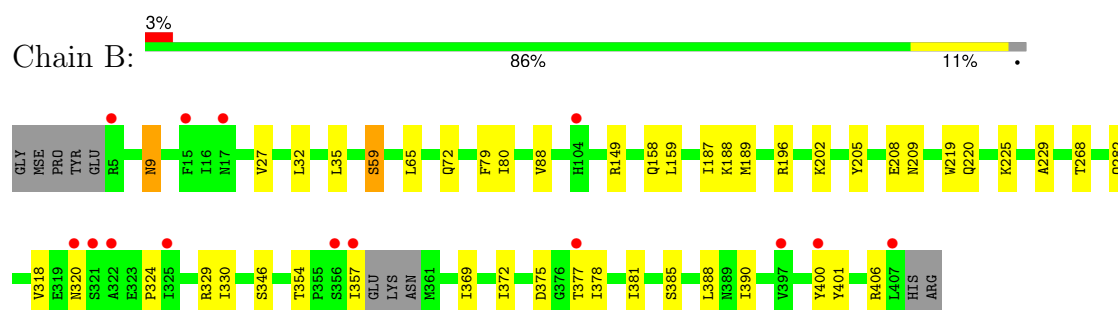
3 Residue-property plots [i](#)

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.

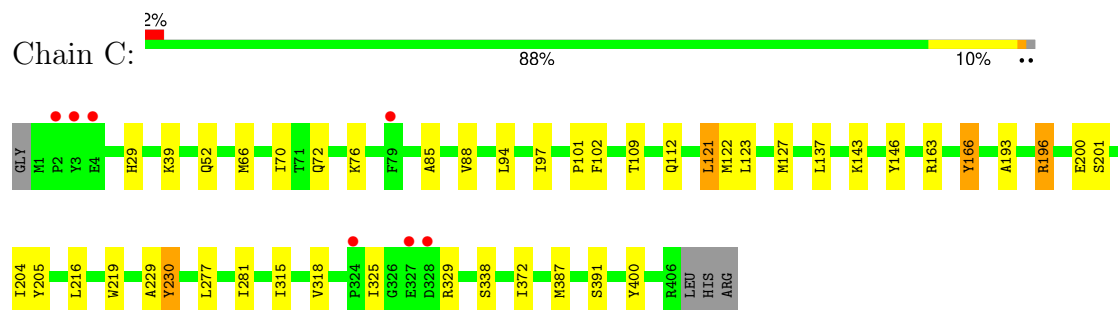
• Molecule 1: Phosphohydrolase



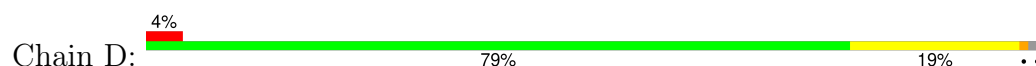
• Molecule 1: Phosphohydrolase

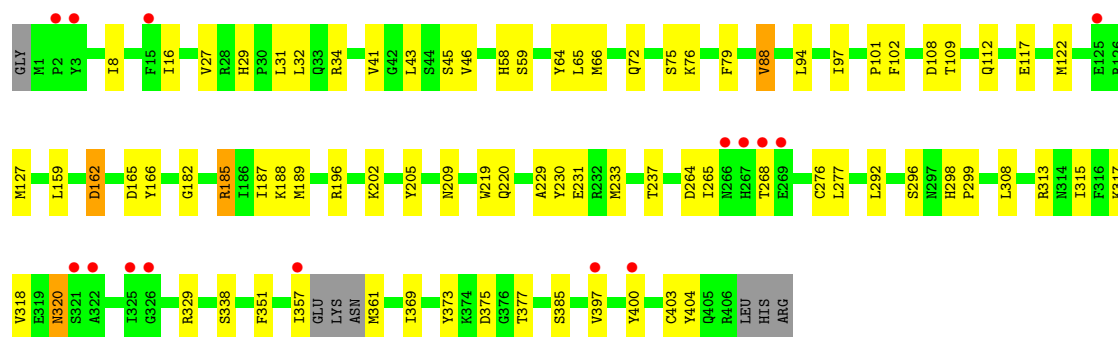


• Molecule 1: Phosphohydrolase

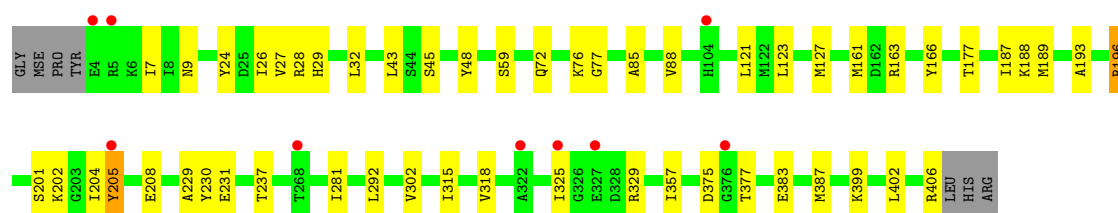
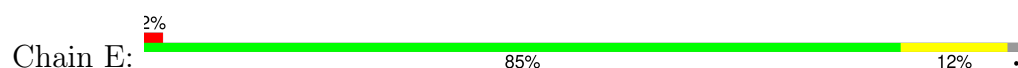


• Molecule 1: Phosphohydrolase

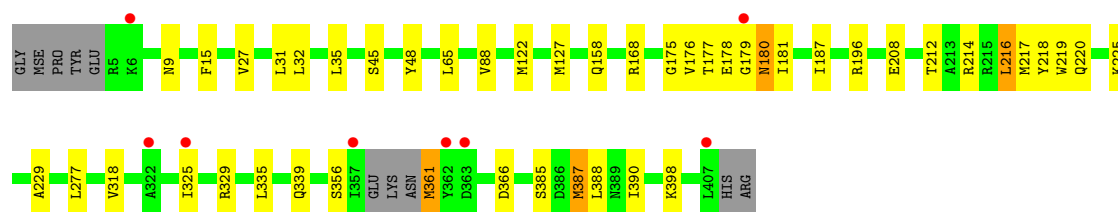
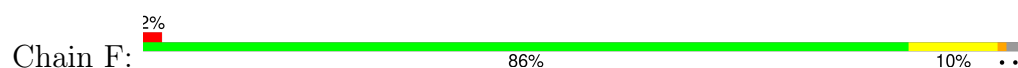




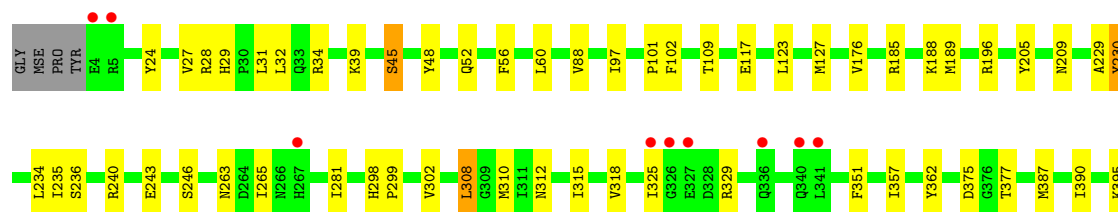
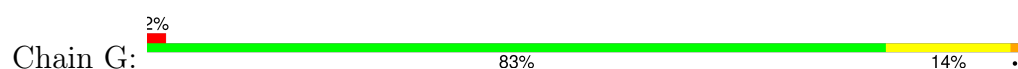
• Molecule 1: Phosphohydrolase



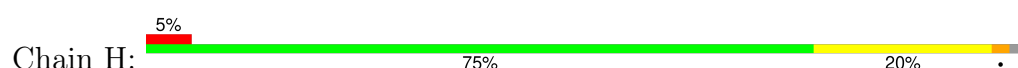
• Molecule 1: Phosphohydrolase

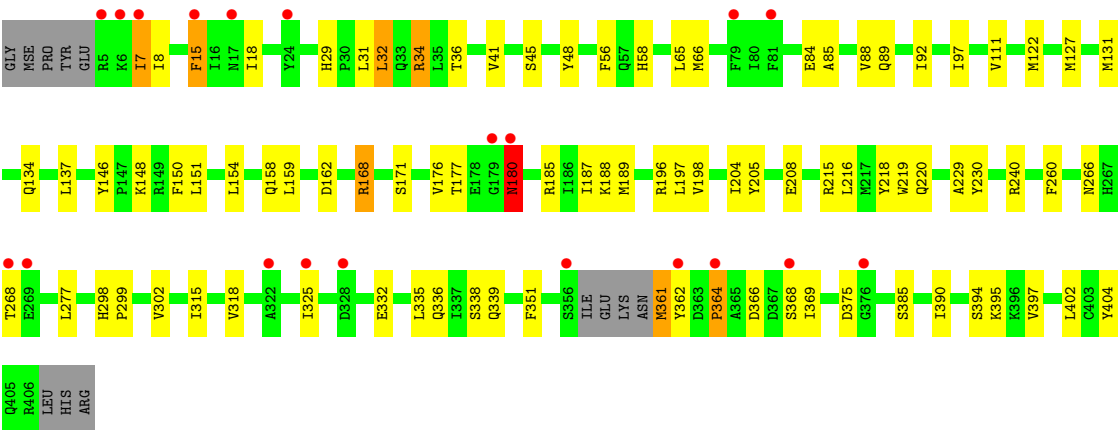


• Molecule 1: Phosphohydrolase



• Molecule 1: Phosphohydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.44Å 137.50Å 279.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 2.20 49.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.03-2.20) 98.7 (49.03-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.207 , 0.252 0.212 , 0.254	Depositor DCC
R_{free} test set	11153 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27697	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 35.59 % 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 5.6995e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.68	0/3292	0.71	0/4437
1	B	0.68	0/3251	0.71	0/4389
1	C	0.70	0/3305	0.68	0/4455
1	D	0.72	0/3287	0.73	2/4434 (0.0%)
1	E	0.66	0/3314	0.70	0/4465
1	F	0.67	0/3308	0.72	1/4464 (0.0%)
1	G	0.66	0/3303	0.67	1/4452 (0.0%)
1	H	3.07	2/3262 (0.1%)	0.92	4/4408 (0.1%)
All	All	1.25	2/26322 (0.0%)	0.73	8/35504 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	180[A]	ASN	CB-CG	120.09	4.27	1.51
1	H	180[B]	ASN	CB-CG	120.09	4.27	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	180[A]	ASN	CB-CG-OD1	-22.50	76.60	121.60
1	H	180[B]	ASN	CB-CG-OD1	-22.50	76.60	121.60
1	H	180[A]	ASN	CB-CG-ND2	9.80	140.22	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	180[B]	ASN	CB-CG-ND2	9.80	140.22	116.70
1	F	216	LEU	CB-CG-CD2	7.10	123.06	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	406	ARG	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	3233	0	3206	30	0
1	B	3189	0	3132	30	0
1	C	3246	0	3225	31	0
1	D	3223	0	3193	60	0
1	E	3246	0	3229	52	0
1	F	3242	0	3200	40	0
1	G	3236	0	3213	44	0
1	H	3197	0	3125	80	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	1	0
3	H	27	0	12	0	0
4	A	8	0	12	1	0
4	C	4	0	6	0	0
4	E	4	0	6	0	0
4	G	8	0	12	0	0
5	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	6	0	8	4	0
5	H	6	0	8	0	0
6	A	262	0	0	3	0
6	B	259	0	0	3	0
6	C	198	0	0	1	0
6	D	182	0	0	5	0
6	E	203	0	0	2	0
6	F	236	0	0	4	0
6	G	181	0	0	3	0
6	H	103	0	0	1	0
All	All	27697	0	25679	332	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 6.

The worst 5 of 332 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:H:168:ARG:HH11	1:H:180[A]:ASN:CB	1.63	1.11
1:E:123:LEU:HD21	1:E:281:ILE:HD11	1.34	1.10
1:B:375:ASP:OD1	1:B:377:THR:HG22	1.52	1.10
1:D:375:ASP:OD1	1:D:377:THR:HG22	1.52	1.10
1:G:375:ASP:OD1	1:G:377:THR:HG22	1.50	1.09

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	403/410 (98%)	397 (98%)	6 (2%)	0	100	100
1	B	399/410 (97%)	391 (98%)	7 (2%)	1 (0%)	37	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	406/410 (99%)	396 (98%)	10 (2%)	0	100	100
1	D	402/410 (98%)	389 (97%)	13 (3%)	0	100	100
1	E	406/410 (99%)	399 (98%)	7 (2%)	0	100	100
1	F	407/410 (99%)	397 (98%)	9 (2%)	1 (0%)	44	52
1	G	406/410 (99%)	394 (97%)	11 (3%)	1 (0%)	44	52
1	H	405/410 (99%)	388 (96%)	16 (4%)	1 (0%)	44	52
All	All	3234/3280 (99%)	3151 (97%)	79 (2%)	4 (0%)	48	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	356	SER
1	G	176	VAL
1	H	364	PRO
1	B	324	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/354 (100%)	350 (99%)	5 (1%)	62	77
1	B	347/354 (98%)	335 (96%)	12 (4%)	31	41
1	C	355/354 (100%)	346 (98%)	9 (2%)	42	56
1	D	350/354 (99%)	333 (95%)	17 (5%)	21	27
1	E	356/354 (101%)	348 (98%)	8 (2%)	47	61
1	F	353/354 (100%)	342 (97%)	11 (3%)	35	47
1	G	354/354 (100%)	344 (97%)	10 (3%)	38	51
1	H	344/354 (97%)	329 (96%)	15 (4%)	24	31
All	All	2814/2832 (99%)	2727 (97%)	87 (3%)	37	47

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	329	ARG
1	G	406	ARG
1	F	385	SER
1	G	196	ARG
1	H	32	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	263	ASN
1	G	312	ASN
1	H	263	ASN
1	D	336	GLN
1	E	9	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 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	EDO	G	503	-	3,3,3	0.64	0	2,2,2	0.43	0
4	EDO	E	502	-	3,3,3	0.41	0	2,2,2	0.51	0
5	GOL	B	502	-	5,5,5	0.53	0	5,5,5	0.52	0
5	GOL	H	502	-	5,5,5	0.46	0	5,5,5	0.75	0
3	ADP	A	501	-	24,29,29	1.00	2 (8%)	29,45,45	1.29	3 (10%)
3	ADP	C	501	-	24,29,29	1.04	2 (8%)	29,45,45	1.28	3 (10%)
3	ADP	B	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.25	3 (10%)
3	ADP	G	501	-	24,29,29	1.02	2 (8%)	29,45,45	1.26	2 (6%)
3	ADP	D	501	-	24,29,29	1.23	3 (12%)	29,45,45	1.31	4 (13%)
3	ADP	H	501	-	24,29,29	1.04	2 (8%)	29,45,45	1.32	3 (10%)
4	EDO	A	502	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	G	502	-	3,3,3	0.54	0	2,2,2	0.17	0
3	ADP	F	501	-	24,29,29	1.11	3 (12%)	29,45,45	1.27	3 (10%)
4	EDO	C	502	-	3,3,3	0.44	0	2,2,2	0.32	0
4	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.17	0
3	ADP	E	501	-	24,29,29	1.00	1 (4%)	29,45,45	1.30	4 (13%)
5	GOL	D	502	-	5,5,5	0.36	0	5,5,5	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	G	503	-	-	0/1/1/1	-
4	EDO	E	502	-	-	0/1/1/1	-
5	GOL	B	502	-	-	3/4/4/4	-
5	GOL	H	502	-	-	2/4/4/4	-
3	ADP	A	501	-	-	4/12/32/32	0/3/3/3
3	ADP	C	501	-	-	4/12/32/32	0/3/3/3
3	ADP	B	501	-	-	4/12/32/32	0/3/3/3
3	ADP	G	501	-	-	4/12/32/32	0/3/3/3
3	ADP	D	501	-	-	4/12/32/32	0/3/3/3
3	ADP	H	501	-	-	4/12/32/32	0/3/3/3
4	EDO	A	502	-	-	1/1/1/1	-
4	EDO	G	502	-	-	1/1/1/1	-
3	ADP	F	501	-	-	4/12/32/32	0/3/3/3
4	EDO	C	502	-	-	1/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	E	501	-	-	4/12/32/32	0/3/3/3
5	GOL	D	502	-	-	2/4/4/4	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	ADP	PA-O3A	3.74	1.63	1.59
3	F	501	ADP	PA-O3A	3.30	1.63	1.59
3	C	501	ADP	PA-O3A	3.06	1.62	1.59
3	H	501	ADP	PA-O3A	3.00	1.62	1.59
3	E	501	ADP	PA-O3A	2.94	1.62	1.59

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	501	ADP	N3-C2-N1	-4.37	122.74	128.67
3	D	501	ADP	N3-C2-N1	-4.14	123.06	128.67
3	F	501	ADP	N3-C2-N1	-4.03	123.20	128.67
3	H	501	ADP	N3-C2-N1	-4.02	123.22	128.67
3	C	501	ADP	N3-C2-N1	-4.00	123.24	128.67

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

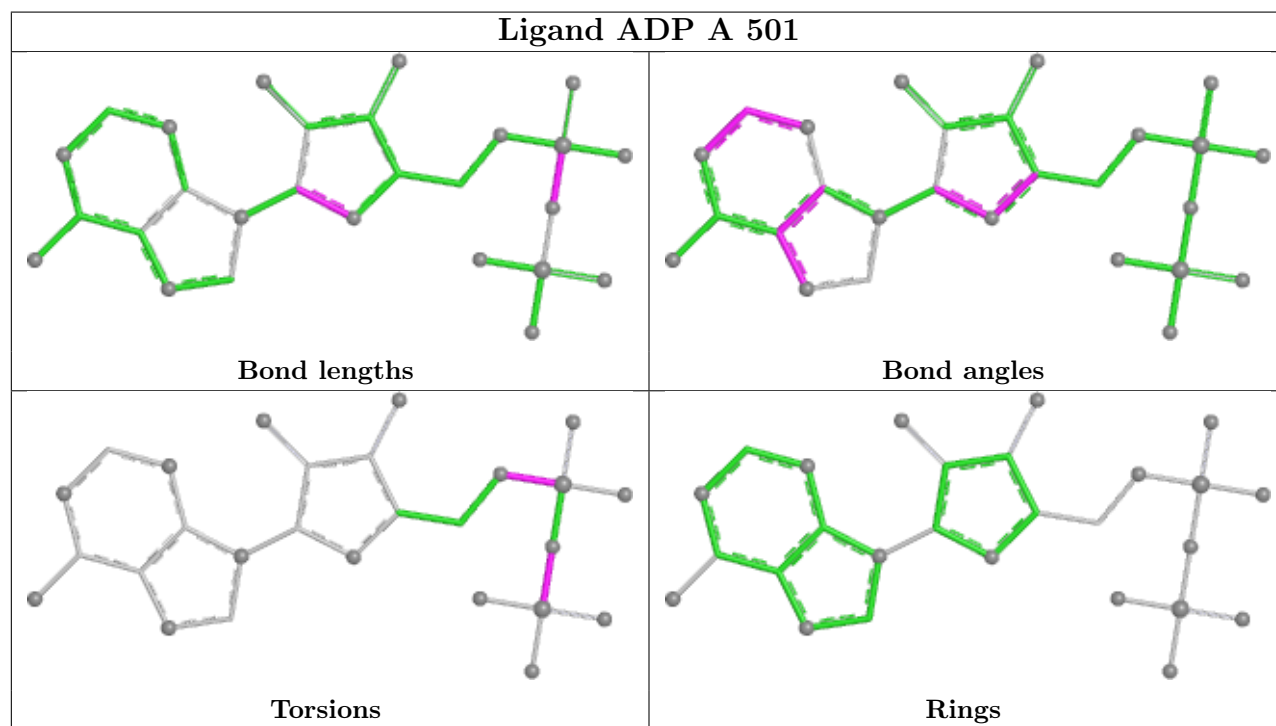
Mol	Chain	Res	Type	Atoms
3	A	501	ADP	C5'-O5'-PA-O2A
3	A	501	ADP	C5'-O5'-PA-O3A
3	B	501	ADP	PA-O3A-PB-O2B
3	B	501	ADP	C5'-O5'-PA-O2A
3	B	501	ADP	C5'-O5'-PA-O3A

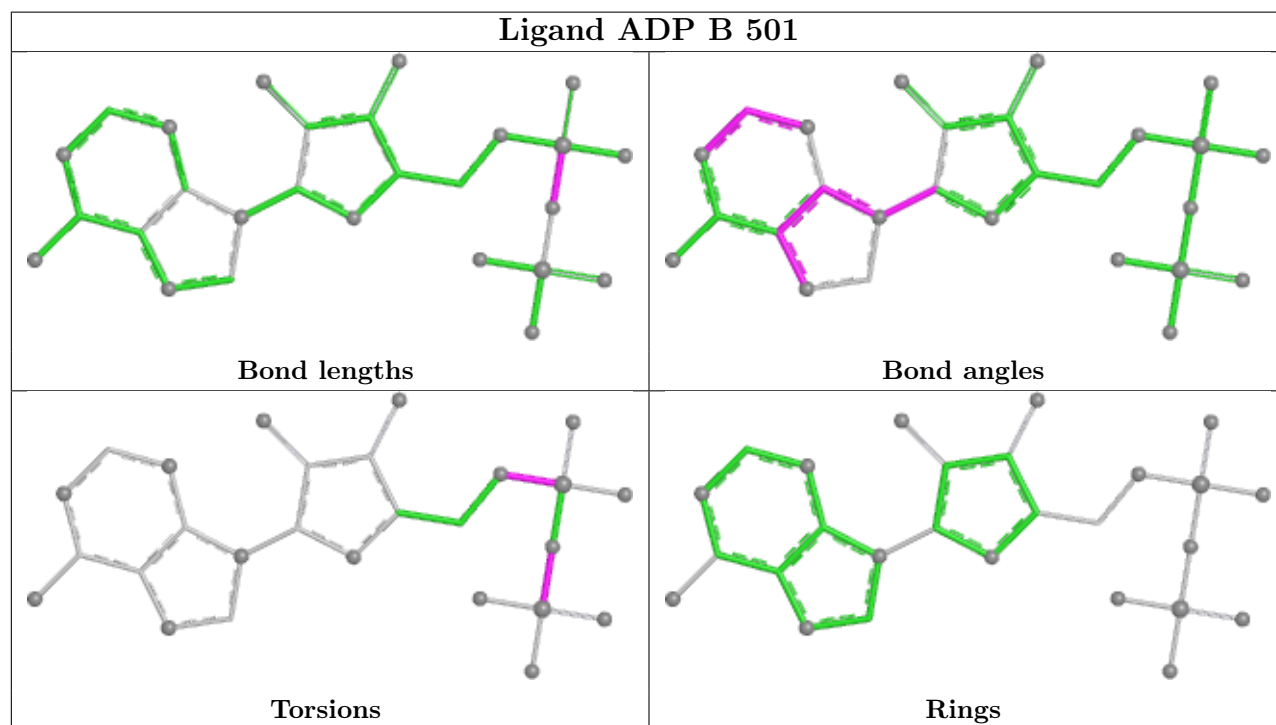
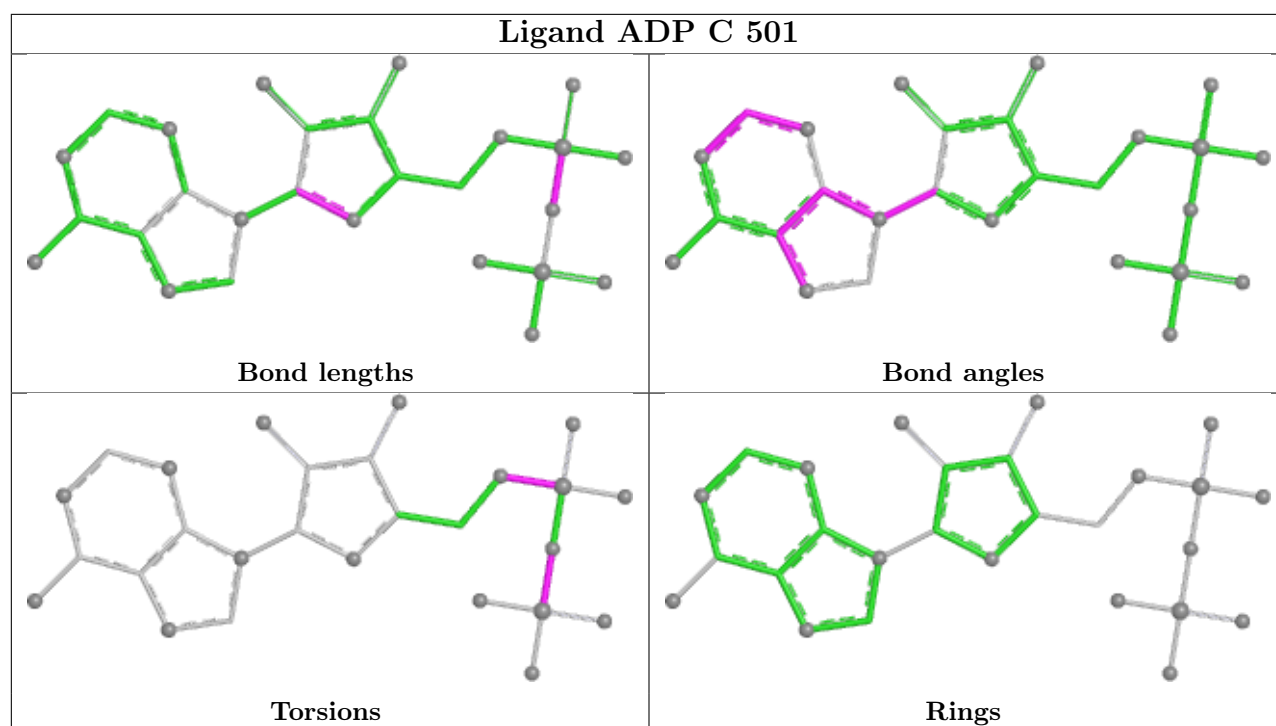
There are no ring outliers.

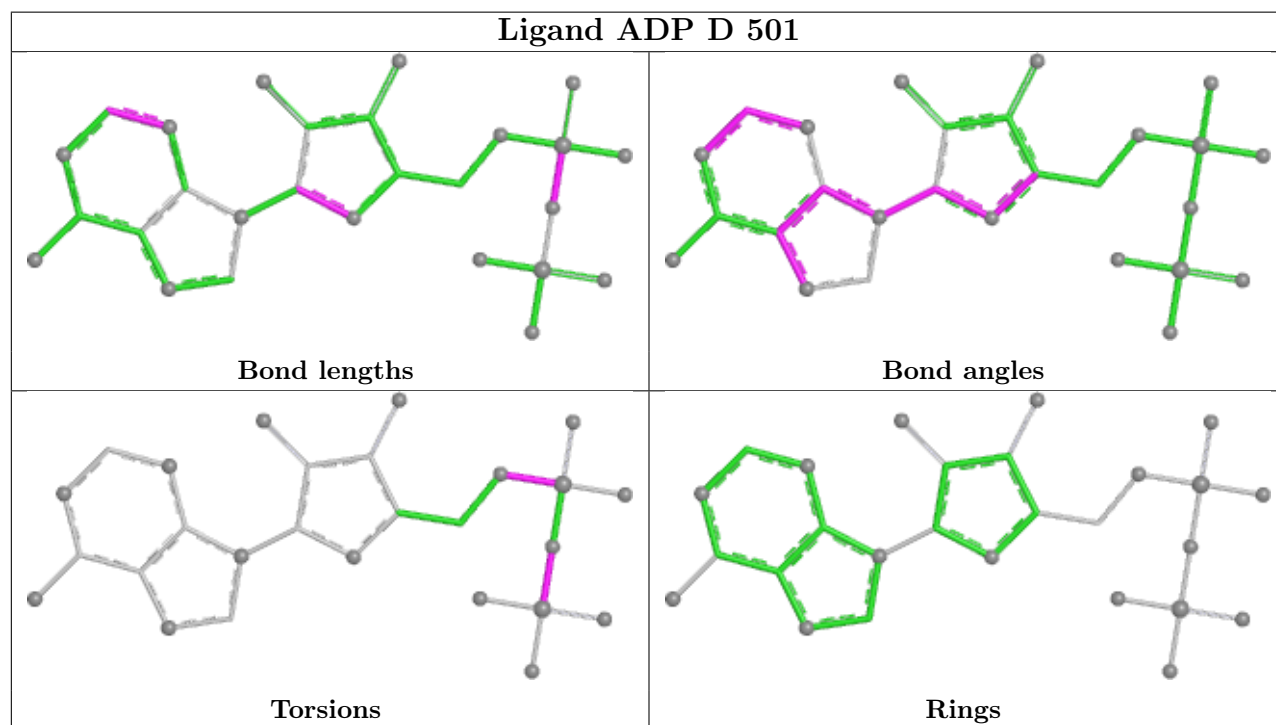
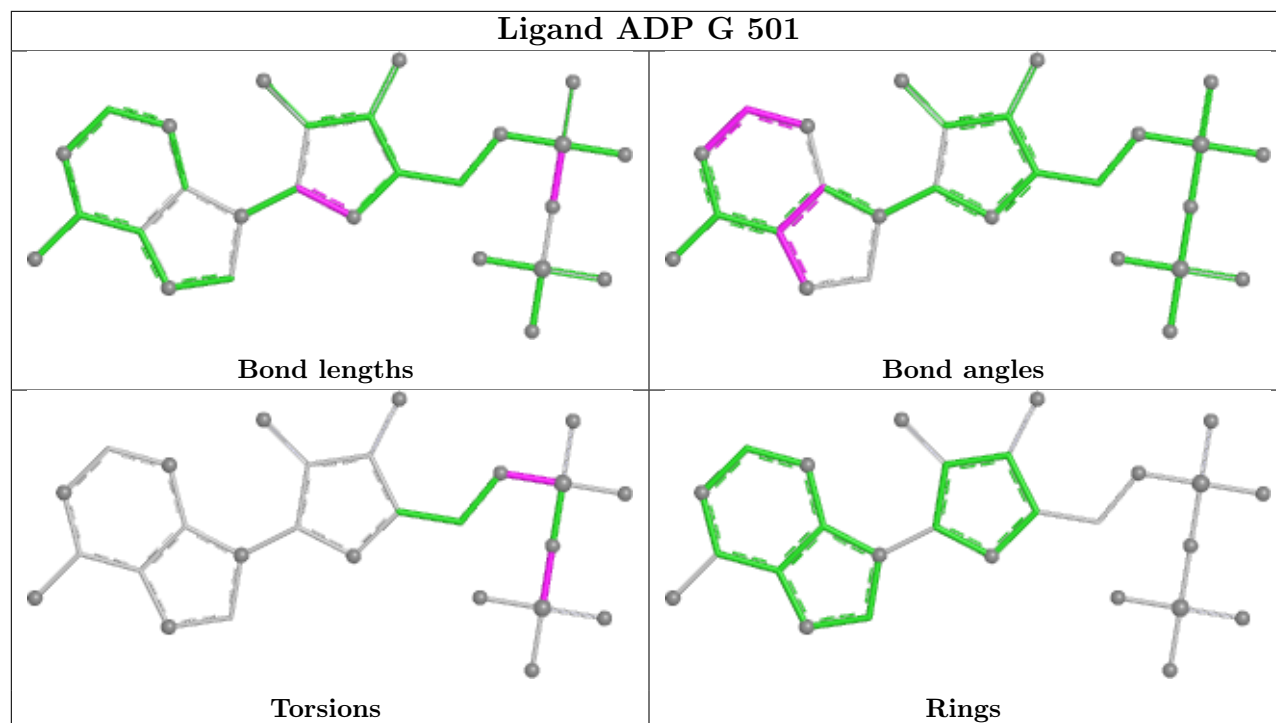
5 monomers are involved in 8 short contacts:

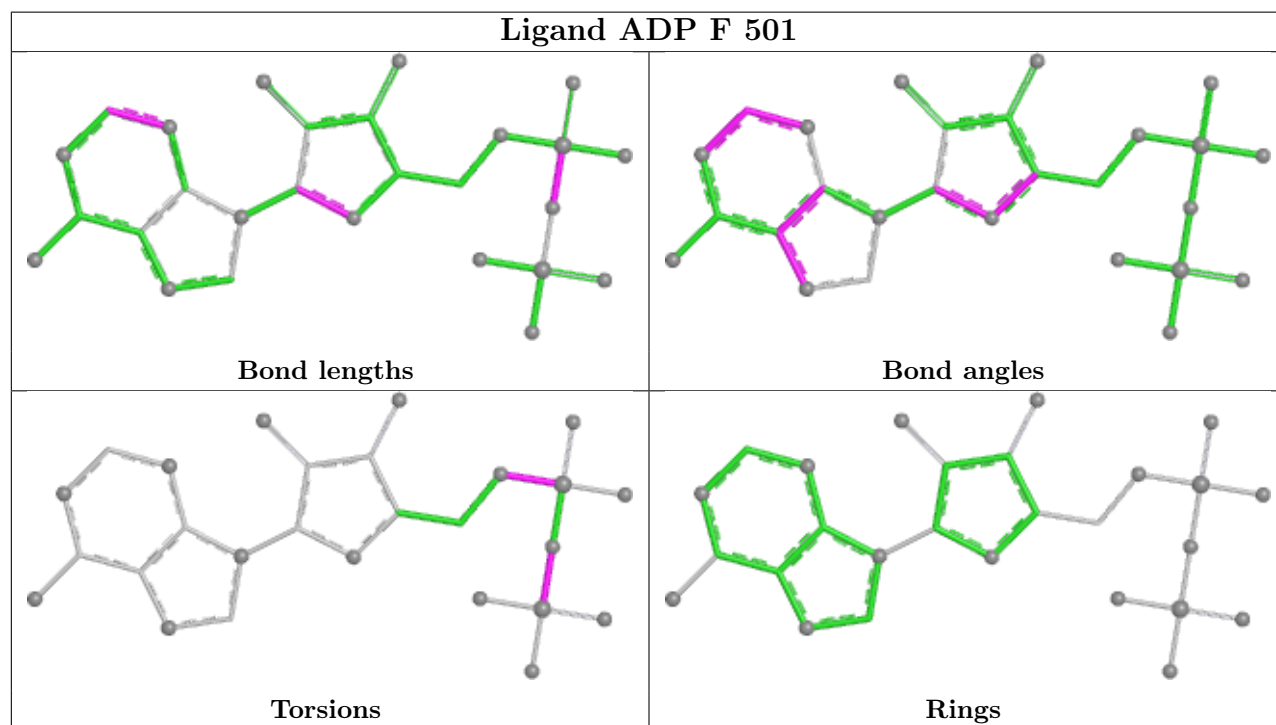
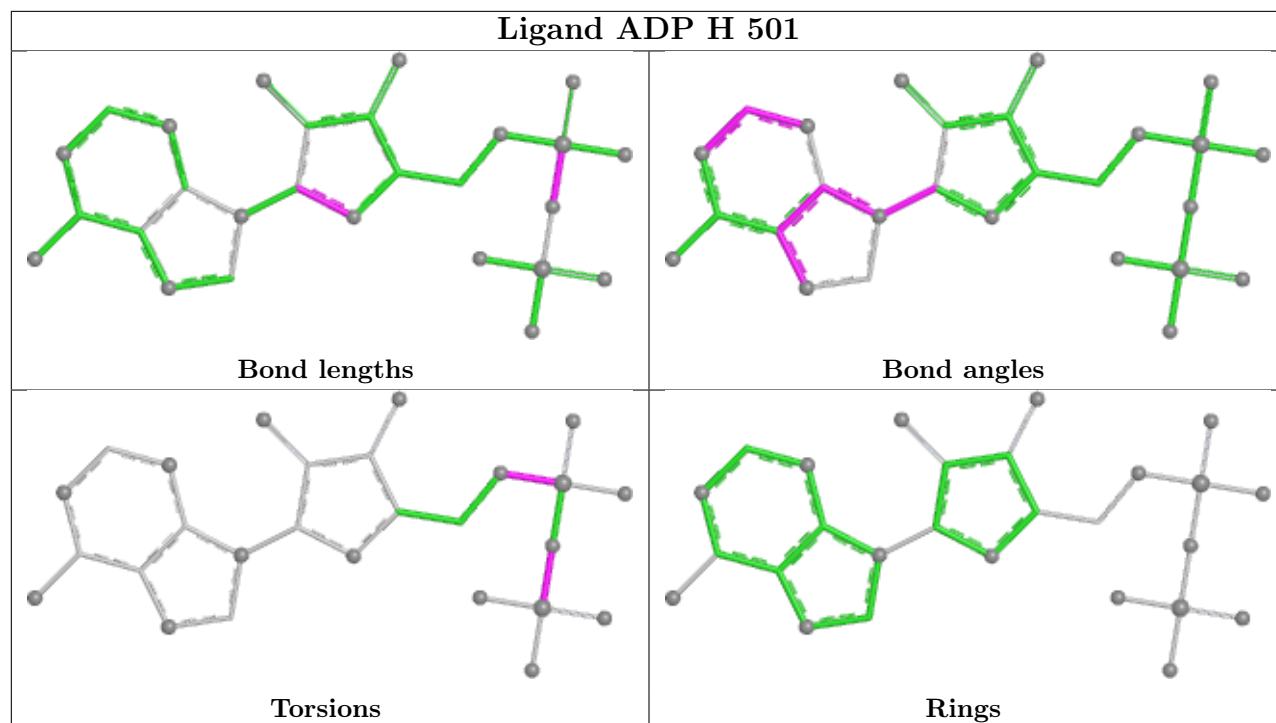
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	ADP	1	0
3	G	501	ADP	1	0
3	D	501	ADP	1	0
4	A	502	EDO	1	0
5	D	502	GOL	4	0

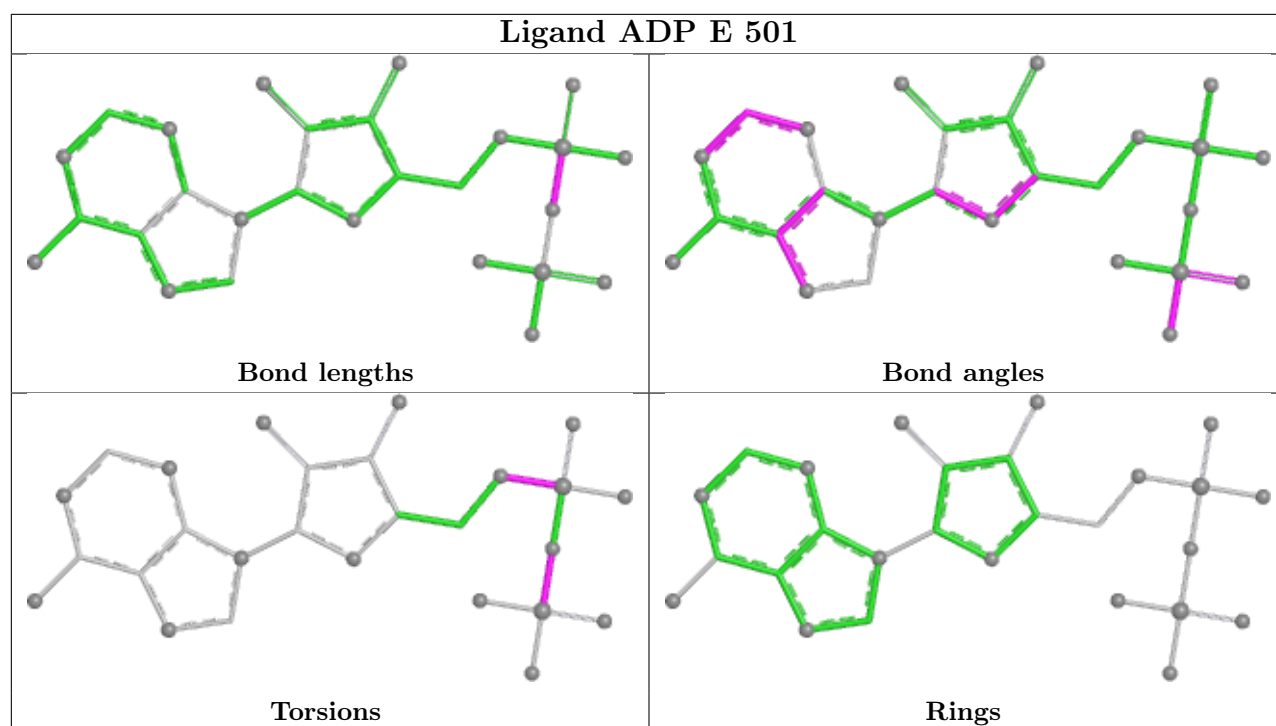
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	391/410 (95%)	-0.04	6 (1%) 71 68	16, 30, 53, 62	1 (0%)
1	B	388/410 (94%)	0.10	14 (3%) 46 43	15, 31, 54, 73	2 (0%)
1	C	393/410 (95%)	0.14	7 (1%) 67 64	18, 32, 55, 69	1 (0%)
1	D	390/410 (95%)	0.25	15 (3%) 44 41	13, 32, 54, 79	2 (0%)
1	E	391/410 (95%)	-0.08	9 (2%) 61 57	17, 31, 53, 63	3 (0%)
1	F	388/410 (94%)	0.06	8 (2%) 63 59	10, 30, 54, 62	9 (2%)
1	G	391/410 (95%)	0.07	9 (2%) 61 57	14, 31, 53, 63	4 (1%)
1	H	386/410 (94%)	0.38	20 (5%) 34 30	10, 32, 53, 61	10 (2%)
All	All	3118/3280 (95%)	0.11	88 (2%) 55 52	10, 31, 54, 79	32 (1%)

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	TYR	5.5
1	B	357	ILE	5.1
1	D	357	ILE	4.9
1	F	407	LEU	3.9
1	H	15[A]	PHE	3.8

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 ⓘ

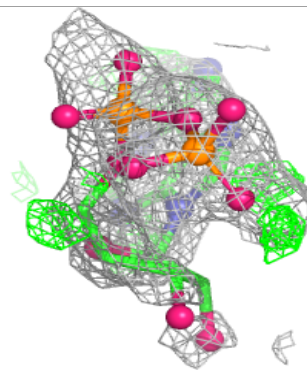
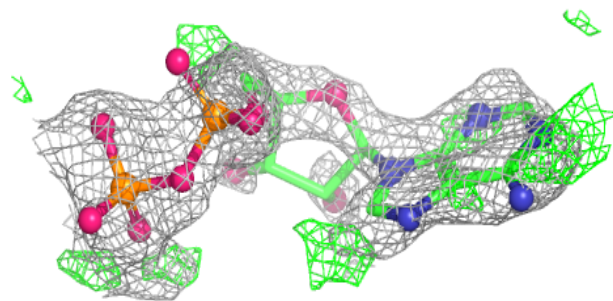
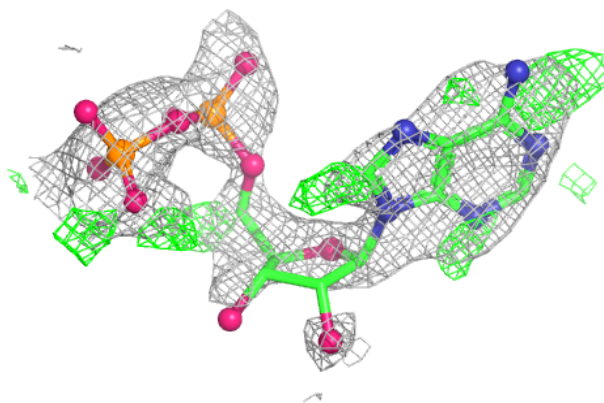
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	ADP	D	501	27/27	0.75	0.25	55,59,62,63	27
3	ADP	B	501	27/27	0.79	0.25	55,59,62,63	27
3	ADP	C	501	27/27	0.80	0.23	55,59,62,63	27
3	ADP	H	501	27/27	0.80	0.24	55,59,62,63	27
3	ADP	G	501	27/27	0.81	0.24	56,59,62,63	27
3	ADP	A	501	27/27	0.81	0.26	55,59,62,63	27
3	ADP	E	501	27/27	0.82	0.26	55,59,62,63	27
3	ADP	F	501	27/27	0.82	0.22	56,59,62,63	27
4	EDO	A	503	4/4	0.82	0.18	49,53,55,56	0
4	EDO	G	503	4/4	0.83	0.15	40,44,45,49	0
2	CL	C	410	1/1	0.86	0.20	72,72,72,72	0
4	EDO	C	502	4/4	0.89	0.18	39,44,45,48	0
5	GOL	H	502	6/6	0.89	0.15	32,55,57,59	0
2	CL	D	410	1/1	0.91	0.10	59,59,59,59	0
5	GOL	B	502	6/6	0.91	0.13	28,50,55,57	0
4	EDO	E	502	4/4	0.91	0.13	18,40,41,51	0
5	GOL	D	502	6/6	0.92	0.16	25,50,54,60	0
4	EDO	G	502	4/4	0.94	0.13	20,35,43,53	0
4	EDO	A	502	4/4	0.96	0.10	13,39,40,40	0
2	CL	A	410	1/1	0.99	0.03	28,28,28,28	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.

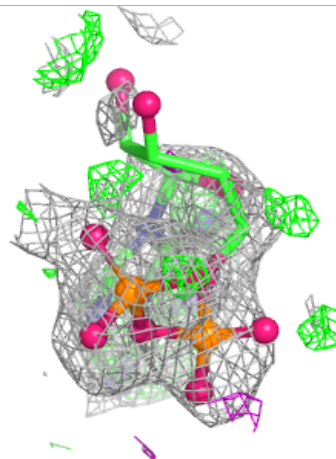
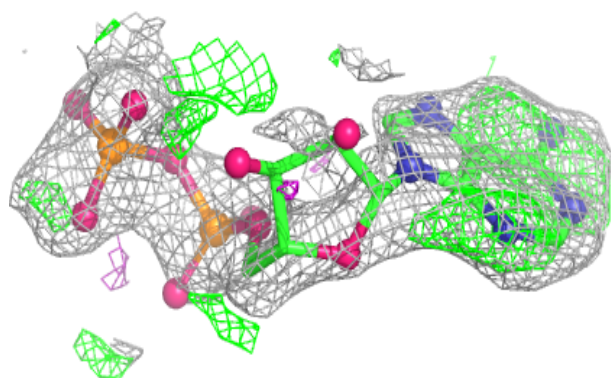
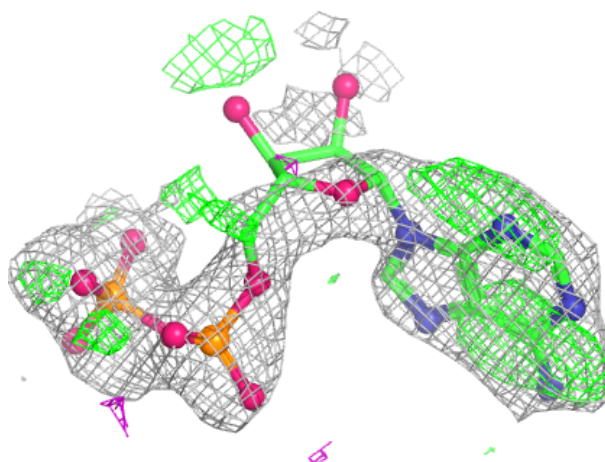
Electron density around ADP D 501:

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



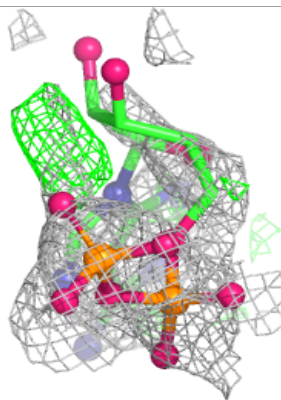
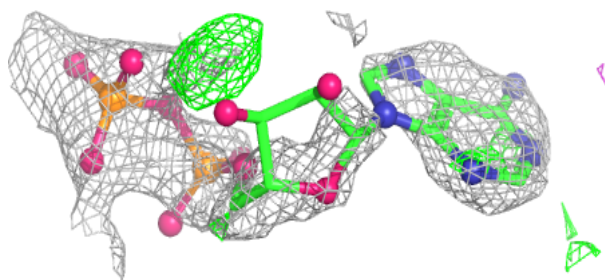
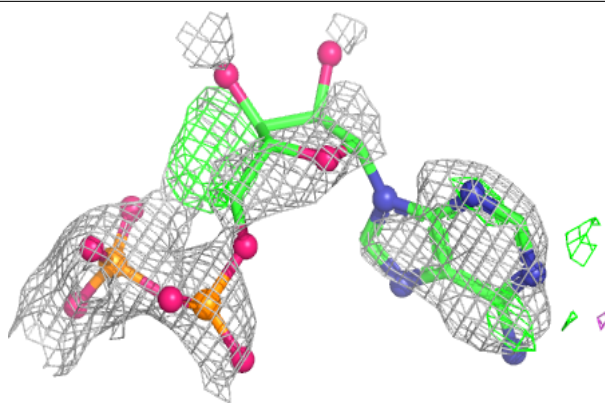
Electron density around ADP B 501:

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

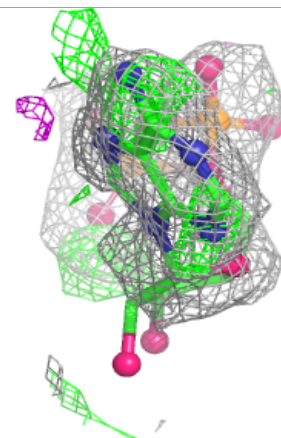
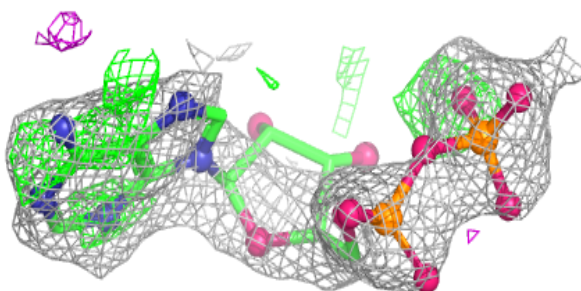
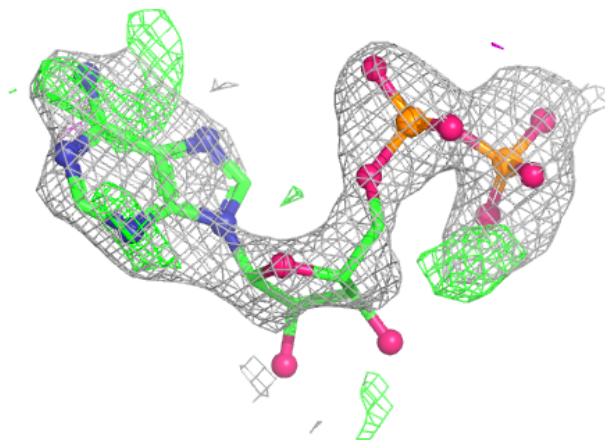


Electron density around ADP C 501:

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

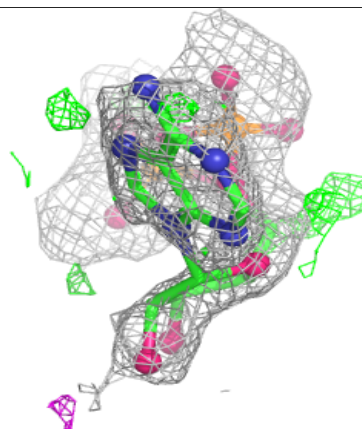
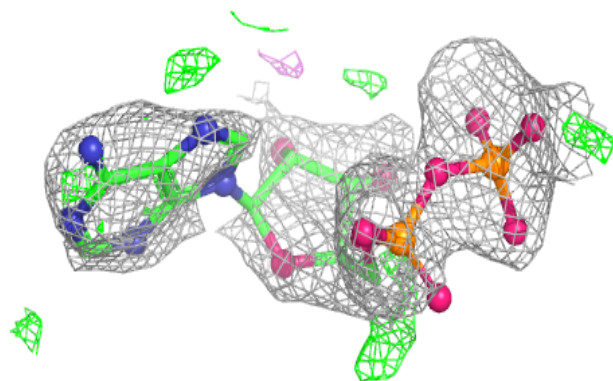
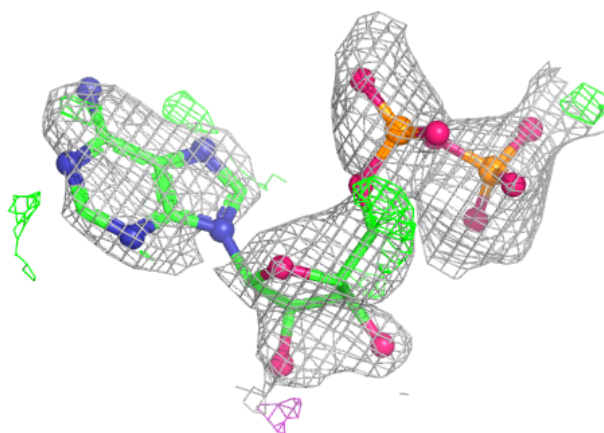
**Electron density around ADP H 501:**

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



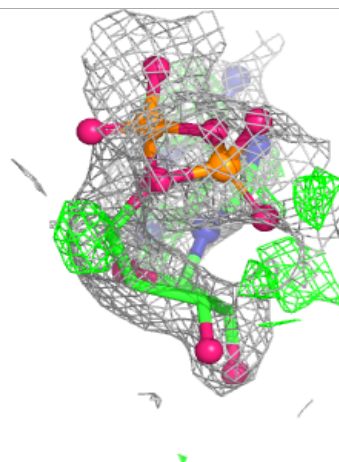
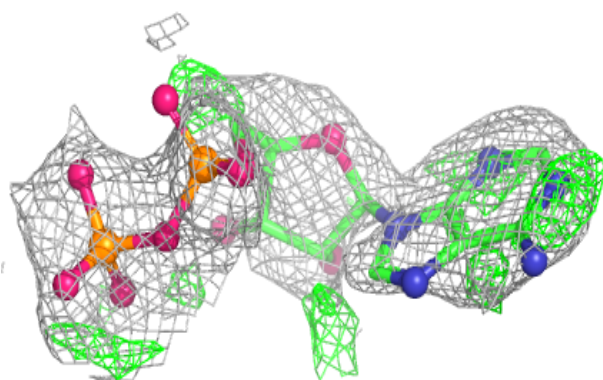
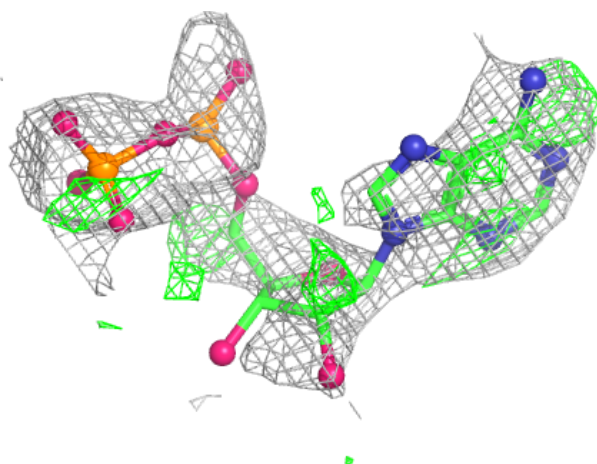
Electron density around ADP G 501:

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



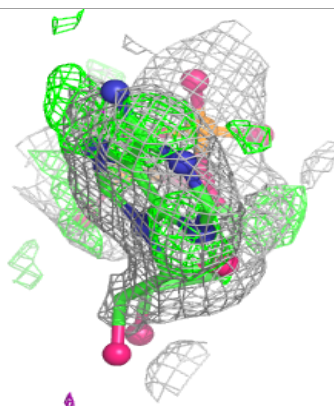
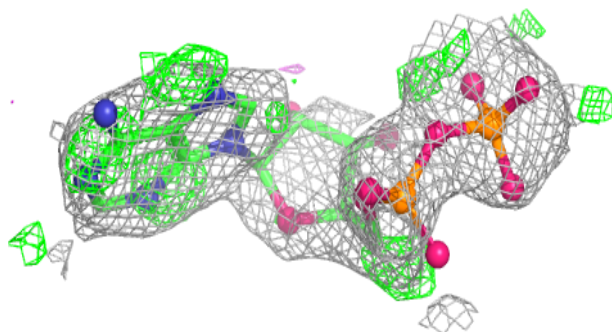
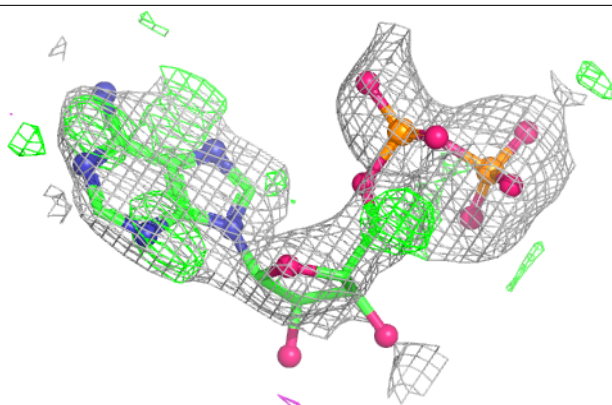
Electron density around ADP A 501:

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

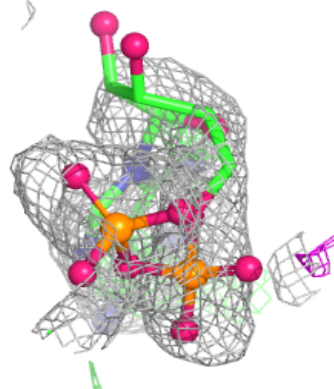
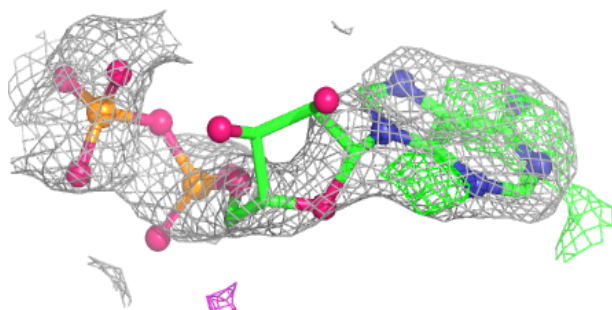
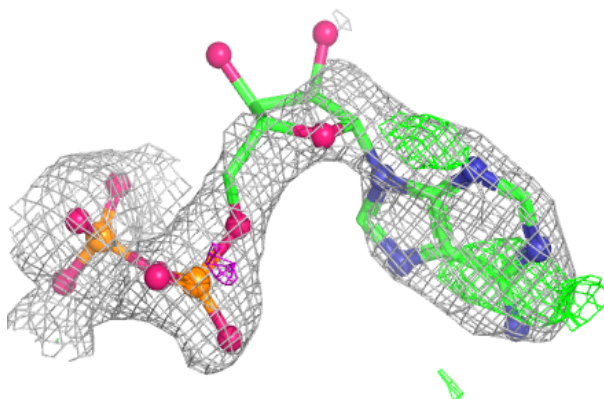


Electron density around ADP E 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.