Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 11:00 pm GMT

PDB ID	:	5IK2
Title	:	Caldalaklibacillus thermarum F1-ATPase (epsilon mutant)
Authors	:	Ferguson, S.A.; Cook, G.M.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on	:	2016-03-03
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

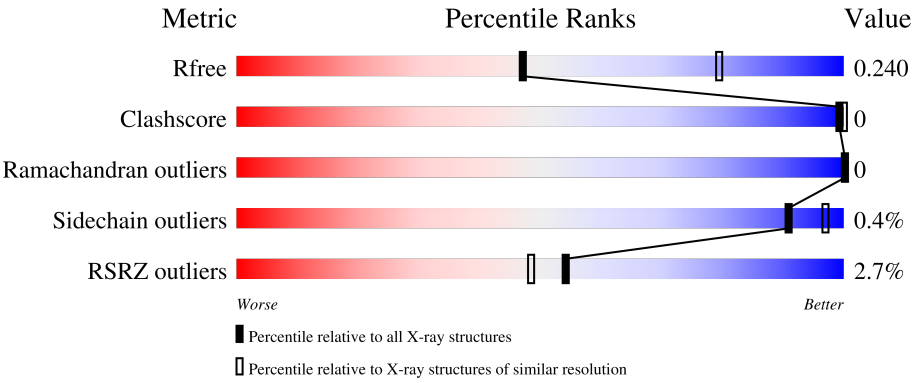
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	479	10% 99%
1	B	479	3% 98%
1	C	479	% 98%
1	I	479	4% 99%
1	J	479	3% 97%

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Mol	Chain	Length	Quality of chain
1	K	479	98%
2	D	462	4% 100%
2	E	462	99%
2	F	462	2% 100%
2	L	462	% 99%
2	M	462	% 99%
2	N	462	% 100%
3	G	285	4% 99%
3	O	285	2% 99%
4	H	134	2% 97%
4	P	134	4% 99%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 51018 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	1	0
			3654	2303	632	705	14			
1	B	469	Total	C	N	O	S	0	0	0
			3602	2271	622	695	14			
1	C	475	Total	C	N	O	S	0	0	0
			3648	2301	629	704	14			
1	I	475	Total	C	N	O	S	0	0	0
			3646	2298	629	705	14			
1	J	468	Total	C	N	O	S	0	0	0
			3591	2262	621	694	14			
1	K	476	Total	C	N	O	S	0	0	0
			3652	2303	630	705	14			

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	461	Total	C	N	O	S	0	0	0
			3521	2218	608	682	13			
2	E	462	Total	C	N	O	S	0	1	0
			3540	2232	610	684	14			
2	F	462	Total	C	N	O	S	0	0	0
			3529	2223	609	683	14			
2	L	462	Total	C	N	O	S	0	0	0
			3529	2223	609	683	14			
2	M	462	Total	C	N	O	S	0	1	0
			3540	2232	610	684	14			
2	N	462	Total	C	N	O	S	0	0	0
			3529	2223	609	683	14			

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	285	Total	C	N	O	S	0	0	0
			2230	1403	388	430	9			
3	O	285	Total	C	N	O	S	0	0	0
			2230	1403	388	430	9			

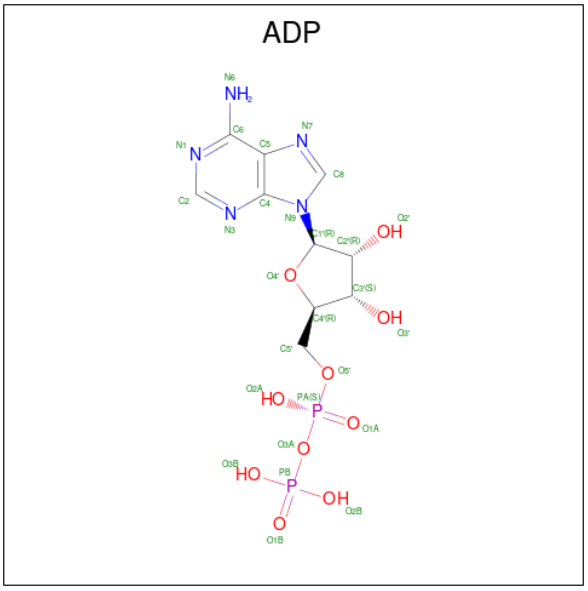
- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	132	Total	C	N	O	S	0	0	0
			1022	643	187	191	1			
4	P	134	Total	C	N	O	S	0	0	0
			1035	651	189	193	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	89	ALA	ASP	engineered mutation	UNP F5LA71
H	92	ALA	ARG	engineered mutation	UNP F5LA71
P	89	ALA	ASP	engineered mutation	UNP F5LA71
P	92	ALA	ARG	engineered mutation	UNP F5LA71

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		
6	K	1	Total	Mg	0	0
			1	1		

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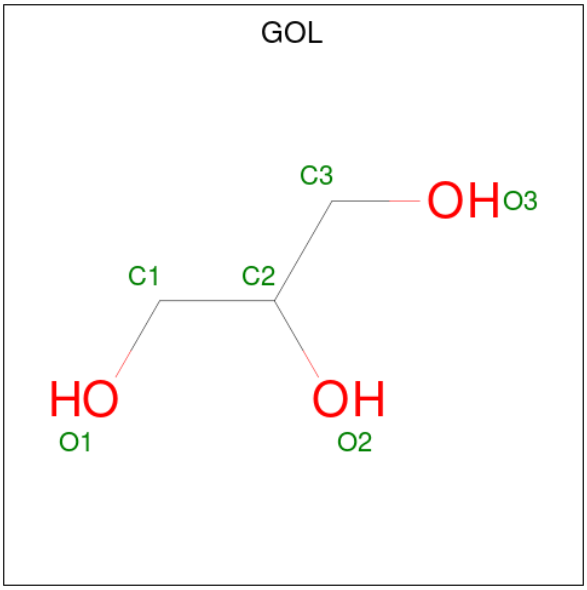
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total Mg 1 1	0	0
6	N	1	Total Mg 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	F	1	Total C O 6 3 3	0	0
7	I	1	Total C O 6 3 3	0	0
7	J	1	Total C O 6 3 3	0	0

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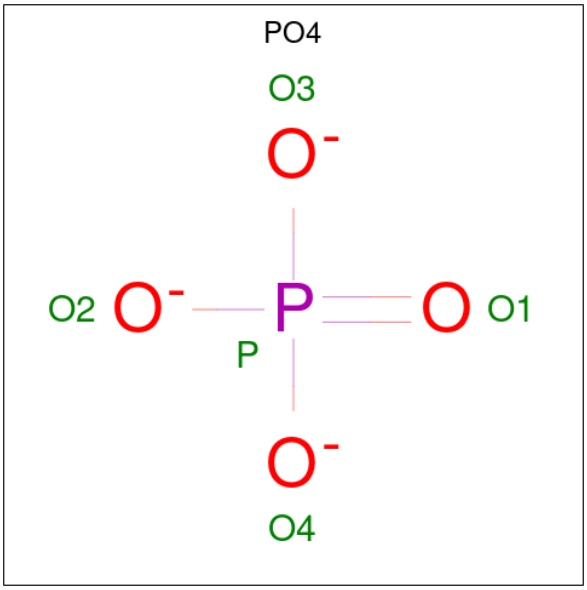
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	K	1	Total C O 6 3 3	0	0
7	M	1	Total C O 6 3 3	0	0
7	M	1	Total C O 6 3 3	0	0
7	M	1	Total C O 6 3 3	0	0
7	M	1	Total C O 6 3 3	0	0
7	N	1	Total C O 6 3 3	0	0
7	N	1	Total C O 6 3 3	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total O P 5 4 1	0	0
8	M	1	Total O P 5 4 1	0	0

- Molecule 9 is water.

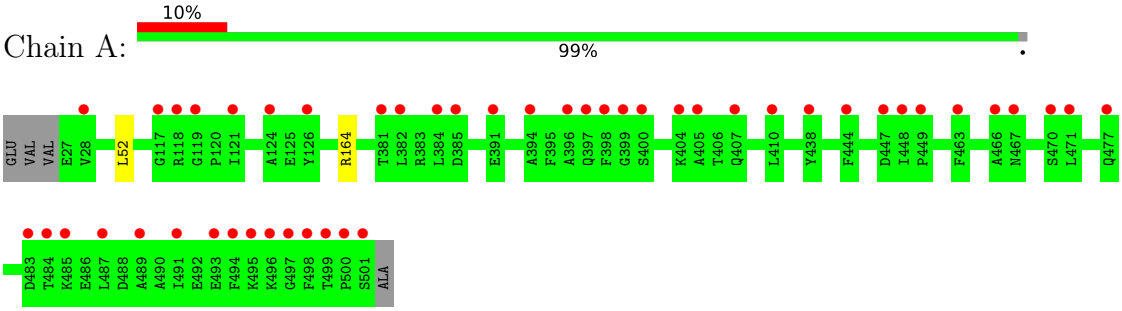
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	68	Total O 68 68	0	0
9	B	96	Total O 96 96	0	0
9	C	64	Total O 64 64	0	0
9	D	74	Total O 74 74	0	0
9	E	91	Total O 91 91	0	0
9	F	87	Total O 87 87	0	0
9	G	25	Total O 25 25	0	0
9	H	13	Total O 13 13	0	0
9	I	78	Total O 78 78	0	0
9	J	68	Total O 68 68	0	0
9	K	94	Total O 94 94	0	0
9	L	100	Total O 100 100	0	0
9	M	99	Total O 99 99	0	0
9	N	87	Total O 87 87	0	0
9	O	26	Total O 26 26	0	0
9	P	10	Total O 10 10	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.

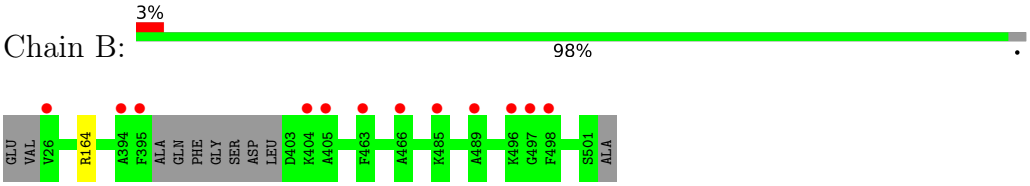
• Molecule 1: ATP synthase subunit alpha

Chain A:



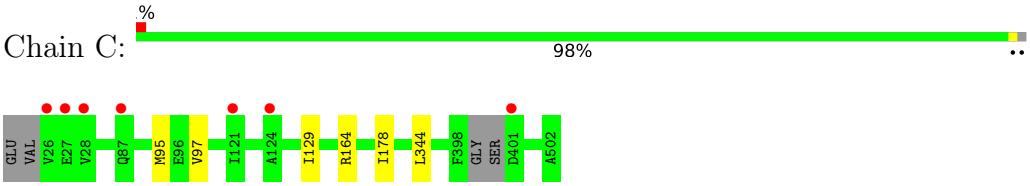
• Molecule 1: ATP synthase subunit alpha

Chain B:



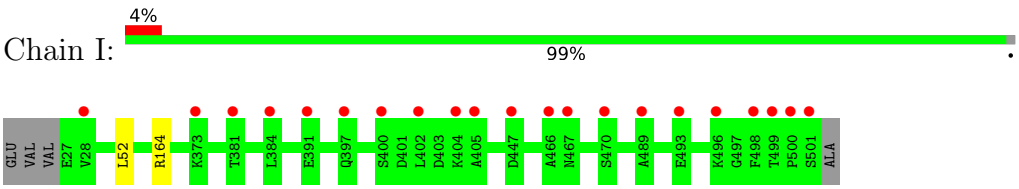
• Molecule 1: ATP synthase subunit alpha

Chain C:



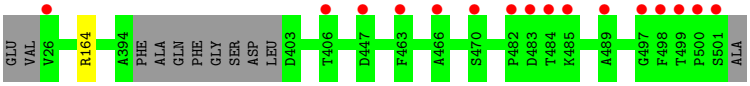
• Molecule 1: ATP synthase subunit alpha

Chain I:



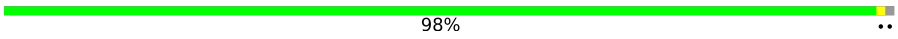
• Molecule 1: ATP synthase subunit alpha

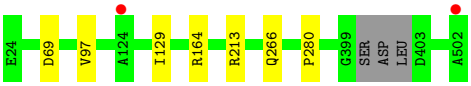
Chain J:



• Molecule 1: ATP synthase subunit alpha

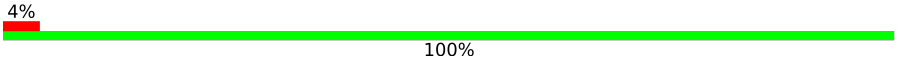
Chain K:

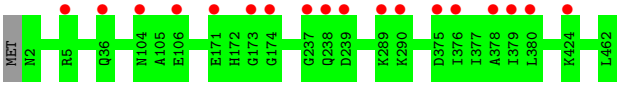




• Molecule 2: ATP synthase subunit beta

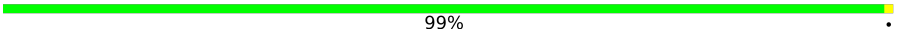
Chain D:





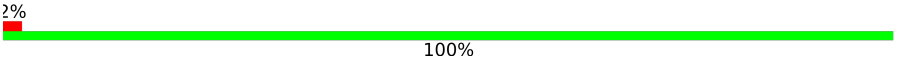
• Molecule 2: ATP synthase subunit beta

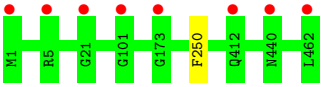
Chain E:



• Molecule 2: ATP synthase subunit beta

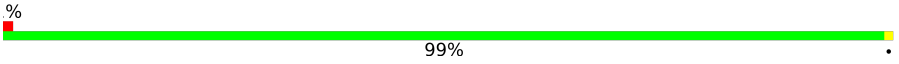
Chain F:

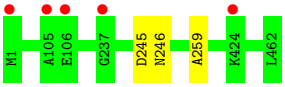




• Molecule 2: ATP synthase subunit beta

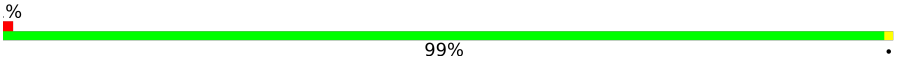
Chain L:

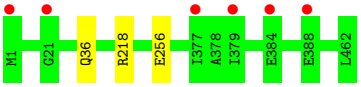




• Molecule 2: ATP synthase subunit beta

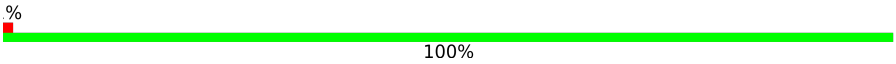
Chain M:

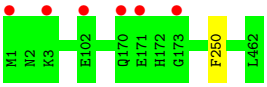




• Molecule 2: ATP synthase subunit beta

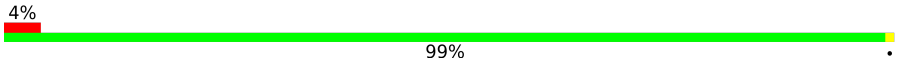
Chain N:

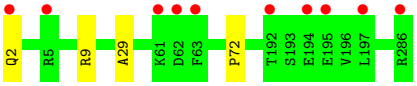




• Molecule 3: ATP synthase gamma chain

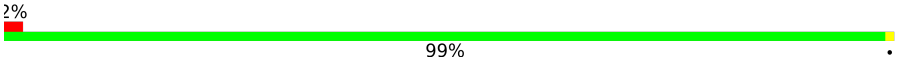
Chain G:





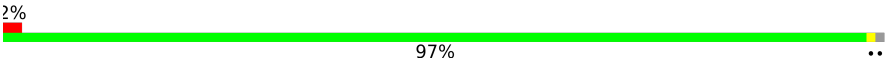
• Molecule 3: ATP synthase gamma chain

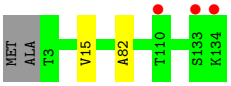
Chain O:



• Molecule 4: ATP synthase epsilon chain

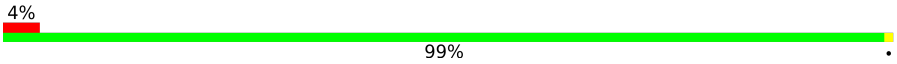
Chain H:

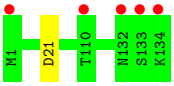




• Molecule 4: ATP synthase epsilon chain

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	148.24Å 131.29Å 212.01Å 90.00° 108.20° 90.00°	Depositor
Resolution (Å)	201.40 – 2.60 46.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.9 (201.40-2.60) 92.9 (46.94-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.213 , 0.238 0.216 , 0.240	Depositor DCC
R_{free} test set	11066 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	51018	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.36	0/3716	0.55	0/5028
1	B	0.36	0/3659	0.55	0/4951
1	C	0.36	0/3706	0.55	0/5015
1	I	0.36	0/3705	0.55	0/5014
1	J	0.35	0/3647	0.55	0/4935
1	K	0.35	0/3710	0.55	0/5020
2	D	0.35	0/3581	0.55	0/4852
2	E	0.35	0/3601	0.55	0/4878
2	F	0.35	0/3589	0.55	0/4862
2	L	0.35	0/3589	0.55	0/4862
2	M	0.35	0/3601	0.55	0/4878
2	N	0.35	0/3589	0.55	0/4862
3	G	0.35	0/2263	0.52	0/3054
3	O	0.35	0/2263	0.53	0/3054
4	H	0.33	0/1033	0.55	0/1393
4	P	0.33	0/1046	0.54	0/1410
All	All	0.35	0/50298	0.55	0/68068

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3654	0	3692	0	0
1	B	3602	0	3642	0	0
1	C	3648	0	3684	2	0
1	I	3646	0	3679	0	0
1	J	3591	0	3633	0	0
1	K	3652	0	3687	2	0
2	D	3521	0	3529	0	0
2	E	3540	0	3550	3	0
2	F	3529	0	3541	0	0
2	L	3529	0	3541	2	0
2	M	3540	0	3550	1	0
2	N	3529	0	3541	0	0
3	G	2230	0	2269	1	0
3	O	2230	0	2269	1	0
4	H	1022	0	1082	1	0
4	P	1035	0	1099	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
5	C	27	0	12	0	0
5	D	27	0	12	0	0
5	E	27	0	12	0	0
5	F	27	0	12	0	0
5	I	27	0	12	0	0
5	J	27	0	12	0	0
5	K	27	0	12	0	0
5	L	27	0	12	0	0
5	M	27	0	12	0	0
5	N	27	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	N	1	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
7	C	6	0	8	0	0
7	E	18	0	24	0	0
7	F	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	6	0	8	0	0
7	J	6	0	8	0	0
7	K	6	0	8	0	0
7	M	24	0	32	0	0
7	N	12	0	16	0	0
8	E	5	0	0	0	0
8	M	5	0	0	0	0
9	A	68	0	0	0	0
9	B	96	0	0	0	0
9	C	64	0	0	0	0
9	D	74	0	0	0	0
9	E	91	0	0	0	0
9	F	87	0	0	0	0
9	G	25	0	0	0	0
9	H	13	0	0	0	0
9	I	78	0	0	0	0
9	J	68	0	0	0	0
9	K	94	0	0	0	0
9	L	100	0	0	0	0
9	M	99	0	0	0	0
9	N	87	0	0	0	0
9	O	26	0	0	1	0
9	P	10	0	0	0	0
All	All	51018	0	50260	11	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 0.

All (11) 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)
3:O:123:ARG:NH1	9:O:801:HOH:O	2.33	0.60
1:C:97:VAL:HG13	1:C:129:ILE:HD11	1.86	0.57
4:H:15:VAL:HG21	4:H:82:ALA:HB3	1.96	0.47
2:E:380:LEU:HD21	3:G:29:ALA:HB1	1.97	0.45
2:E:218:ARG:NH2	2:E:256:GLU:OE1	2.52	0.43
1:K:97:VAL:HG13	1:K:129:ILE:HD11	2.02	0.42
2:M:218:ARG:NH2	2:M:256:GLU:OE1	2.52	0.42
2:E:79:VAL:HG11	2:E:224:THR:HG23	2.03	0.41
2:L:245:ASP:HA	2:L:246:ASN:HA	1.93	0.41
1:K:280:PRO:HG2	2:L:259:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ILE:HD12	1:C:344:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/479 (99%)	469 (99%)	5 (1%)	0	100	100
1	B	465/479 (97%)	457 (98%)	8 (2%)	0	100	100
1	C	471/479 (98%)	467 (99%)	4 (1%)	0	100	100
1	I	473/479 (99%)	468 (99%)	5 (1%)	0	100	100
1	J	464/479 (97%)	455 (98%)	9 (2%)	0	100	100
1	K	472/479 (98%)	467 (99%)	5 (1%)	0	100	100
2	D	459/462 (99%)	446 (97%)	13 (3%)	0	100	100
2	E	461/462 (100%)	446 (97%)	15 (3%)	0	100	100
2	F	460/462 (100%)	442 (96%)	18 (4%)	0	100	100
2	L	460/462 (100%)	447 (97%)	13 (3%)	0	100	100
2	M	461/462 (100%)	448 (97%)	13 (3%)	0	100	100
2	N	460/462 (100%)	442 (96%)	18 (4%)	0	100	100
3	G	283/285 (99%)	278 (98%)	5 (2%)	0	100	100
3	O	283/285 (99%)	280 (99%)	3 (1%)	0	100	100
4	H	130/134 (97%)	125 (96%)	5 (4%)	0	100	100
4	P	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
All	All	6408/6484 (99%)	6264 (98%)	144 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	390/392 (100%)	388 (100%)	2 (0%)	88 96
1	B	385/392 (98%)	384 (100%)	1 (0%)	92 98
1	C	389/392 (99%)	387 (100%)	2 (0%)	88 96
1	I	389/392 (99%)	387 (100%)	2 (0%)	88 96
1	J	384/392 (98%)	383 (100%)	1 (0%)	92 98
1	K	389/392 (99%)	385 (99%)	4 (1%)	76 90
2	D	375/376 (100%)	375 (100%)	0	100 100
2	E	377/376 (100%)	376 (100%)	1 (0%)	92 98
2	F	376/376 (100%)	375 (100%)	1 (0%)	92 98
2	L	376/376 (100%)	376 (100%)	0	100 100
2	M	377/376 (100%)	376 (100%)	1 (0%)	92 98
2	N	376/376 (100%)	375 (100%)	1 (0%)	92 98
3	G	238/238 (100%)	235 (99%)	3 (1%)	69 86
3	O	238/238 (100%)	237 (100%)	1 (0%)	91 97
4	H	109/110 (99%)	109 (100%)	0	100 100
4	P	110/110 (100%)	109 (99%)	1 (1%)	78 91
All	All	5278/5304 (100%)	5257 (100%)	21 (0%)	91 97

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	164	ARG
1	B	164	ARG
1	C	95	MET
1	C	164	ARG
2	E	36	GLN
2	F	250	PHE
3	G	2	GLN

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Mol	Chain	Res	Type
3	G	9	ARG
3	G	72	PRO
1	I	52	LEU
1	I	164	ARG
1	J	164	ARG
1	K	69	ASP
1	K	164	ARG
1	K	213	ARG
1	K	266	GLN
2	M	36	GLN
2	N	250	PHE
3	O	72	PRO
4	P	21	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	440	ASN
2	E	51	ASN
2	E	210	GLN
4	H	132	ASN
1	K	266	GLN
2	M	210	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ADP	A	600	6	24,29,29	1.03	2 (8%)	29,45,45	1.42	5 (17%)
7	GOL	M	606	-	5,5,5	0.26	0	5,5,5	0.26	0
5	ADP	B	600	6	24,29,29	1.04	2 (8%)	29,45,45	1.34	5 (17%)
5	ADP	D	600	6	24,29,29	1.01	2 (8%)	29,45,45	1.27	3 (10%)
7	GOL	M	605	-	5,5,5	0.25	0	5,5,5	0.33	0
7	GOL	M	604	-	5,5,5	0.34	0	5,5,5	0.54	0
5	ADP	F	600	6	24,29,29	1.05	3 (12%)	29,45,45	1.35	4 (13%)
5	ADP	N	600	6	24,29,29	1.03	2 (8%)	29,45,45	1.33	5 (17%)
7	GOL	E	604	-	5,5,5	0.39	0	5,5,5	0.49	0
7	GOL	K	602	-	5,5,5	0.32	0	5,5,5	0.18	0
8	PO4	E	601	-	4,4,4	0.91	0	6,6,6	0.39	0
5	ADP	I	600	6	24,29,29	1.03	2 (8%)	29,45,45	1.33	5 (17%)
7	GOL	E	602	-	5,5,5	0.25	0	5,5,5	0.30	0
7	GOL	I	602	-	5,5,5	0.36	0	5,5,5	0.26	0
5	ADP	M	600	-	24,29,29	1.06	3 (12%)	29,45,45	1.32	5 (17%)
7	GOL	N	604	-	5,5,5	0.23	0	5,5,5	0.15	0
7	GOL	A	602	-	5,5,5	0.23	0	5,5,5	0.17	0
7	GOL	M	603	-	5,5,5	0.28	0	5,5,5	0.23	0
5	ADP	E	600	-	24,29,29	1.06	3 (12%)	29,45,45	1.34	5 (17%)
7	GOL	J	602	-	5,5,5	0.27	0	5,5,5	0.19	0
7	GOL	B	602	-	5,5,5	0.33	0	5,5,5	0.18	0
7	GOL	E	603	-	5,5,5	0.34	0	5,5,5	0.39	0
7	GOL	N	603	-	5,5,5	0.29	0	5,5,5	0.15	0
5	ADP	J	600	6	24,29,29	1.03	2 (8%)	29,45,45	1.32	4 (13%)
5	ADP	C	600	6	24,29,29	1.03	2 (8%)	29,45,45	1.36	3 (10%)
7	GOL	C	602	-	5,5,5	0.30	0	5,5,5	0.14	0
7	GOL	F	602	-	5,5,5	0.40	0	5,5,5	0.36	0
8	PO4	M	602	-	4,4,4	0.90	0	6,6,6	0.47	0
5	ADP	K	600	6	24,29,29	1.02	2 (8%)	29,45,45	1.34	4 (13%)
5	ADP	L	600	6	24,29,29	1.01	2 (8%)	29,45,45	1.32	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	600	6	-	3/12/32/32	0/3/3/3
7	GOL	M	606	-	-	2/4/4/4	-
5	ADP	B	600	6	-	0/12/32/32	0/3/3/3
5	ADP	D	600	6	-	3/12/32/32	0/3/3/3
7	GOL	M	605	-	-	0/4/4/4	-
7	GOL	M	604	-	-	4/4/4/4	-
5	ADP	F	600	6	-	2/12/32/32	0/3/3/3
5	ADP	N	600	6	-	3/12/32/32	0/3/3/3
7	GOL	E	604	-	-	4/4/4/4	-
7	GOL	K	602	-	-	2/4/4/4	-
5	ADP	I	600	6	-	0/12/32/32	0/3/3/3
7	GOL	E	602	-	-	1/4/4/4	-
7	GOL	I	602	-	-	1/4/4/4	-
5	ADP	M	600	-	-	0/12/32/32	0/3/3/3
7	GOL	N	604	-	-	2/4/4/4	-
7	GOL	A	602	-	-	0/4/4/4	-
7	GOL	M	603	-	-	0/4/4/4	-
5	ADP	E	600	-	-	0/12/32/32	0/3/3/3
7	GOL	J	602	-	-	2/4/4/4	-
7	GOL	B	602	-	-	2/4/4/4	-
7	GOL	E	603	-	-	2/4/4/4	-
7	GOL	N	603	-	-	0/4/4/4	-
5	ADP	J	600	6	-	0/12/32/32	0/3/3/3
5	ADP	C	600	6	-	1/12/32/32	0/3/3/3
7	GOL	C	602	-	-	2/4/4/4	-
7	GOL	F	602	-	-	2/4/4/4	-
5	ADP	K	600	6	-	0/12/32/32	0/3/3/3
5	ADP	L	600	6	-	1/12/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	600	ADP	C5-C4	2.70	1.48	1.40
5	A	600	ADP	C5-C4	2.67	1.48	1.40
5	E	600	ADP	C5-C4	2.66	1.48	1.40
5	M	600	ADP	C5-C4	2.64	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	ADP	C5-C4	2.63	1.47	1.40
5	F	600	ADP	C5-C4	2.59	1.47	1.40
5	J	600	ADP	C5-C4	2.59	1.47	1.40
5	K	600	ADP	C5-C4	2.57	1.47	1.40
5	N	600	ADP	C5-C4	2.56	1.47	1.40
5	D	600	ADP	C5-C4	2.54	1.47	1.40
5	C	600	ADP	C5-C4	2.54	1.47	1.40
5	L	600	ADP	C5-C4	2.52	1.47	1.40
5	M	600	ADP	C2-N3	2.20	1.35	1.32
5	A	600	ADP	C2-N3	2.17	1.35	1.32
5	B	600	ADP	C2-N3	2.16	1.35	1.32
5	E	600	ADP	C2-N3	2.15	1.35	1.32
5	C	600	ADP	C2-N3	2.13	1.35	1.32
5	I	600	ADP	C2-N3	2.13	1.35	1.32
5	M	600	ADP	O4'-C1'	2.13	1.44	1.41
5	J	600	ADP	C2-N3	2.12	1.35	1.32
5	N	600	ADP	C2-N3	2.11	1.35	1.32
5	F	600	ADP	O4'-C1'	2.10	1.44	1.41
5	D	600	ADP	C2-N3	2.06	1.35	1.32
5	E	600	ADP	O4'-C1'	2.06	1.44	1.41
5	L	600	ADP	O4'-C1'	2.03	1.43	1.41
5	F	600	ADP	C2-N3	2.02	1.35	1.32
5	K	600	ADP	C2-N3	2.01	1.35	1.32

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	600	ADP	N3-C2-N1	-3.93	122.53	128.68
5	J	600	ADP	N3-C2-N1	-3.93	122.53	128.68
5	L	600	ADP	N3-C2-N1	-3.91	122.57	128.68
5	B	600	ADP	N3-C2-N1	-3.84	122.68	128.68
5	K	600	ADP	N3-C2-N1	-3.83	122.70	128.68
5	F	600	ADP	N3-C2-N1	-3.82	122.70	128.68
5	N	600	ADP	N3-C2-N1	-3.78	122.77	128.68
5	E	600	ADP	N3-C2-N1	-3.77	122.78	128.68
5	C	600	ADP	N3-C2-N1	-3.77	122.78	128.68
5	I	600	ADP	N3-C2-N1	-3.77	122.79	128.68
5	A	600	ADP	N3-C2-N1	-3.76	122.80	128.68
5	M	600	ADP	N3-C2-N1	-3.71	122.88	128.68
5	A	600	ADP	C3'-C2'-C1'	2.95	105.41	100.98
5	C	600	ADP	C4-C5-N7	-2.87	106.41	109.40
5	B	600	ADP	C4-C5-N7	-2.78	106.50	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	600	ADP	C4-C5-N7	-2.75	106.53	109.40
5	I	600	ADP	C4-C5-N7	-2.71	106.58	109.40
5	N	600	ADP	C4-C5-N7	-2.71	106.58	109.40
5	L	600	ADP	C4-C5-N7	-2.70	106.58	109.40
5	F	600	ADP	C4-C5-N7	-2.70	106.58	109.40
5	A	600	ADP	PA-O3A-PB	-2.70	123.57	132.83
5	D	600	ADP	C4-C5-N7	-2.67	106.62	109.40
5	M	600	ADP	PA-O3A-PB	-2.65	123.73	132.83
5	M	600	ADP	C4-C5-N7	-2.62	106.67	109.40
5	E	600	ADP	PA-O3A-PB	-2.59	123.93	132.83
5	J	600	ADP	C4-C5-N7	-2.57	106.72	109.40
5	A	600	ADP	C4-C5-N7	-2.55	106.74	109.40
5	E	600	ADP	C4-C5-N7	-2.54	106.75	109.40
5	K	600	ADP	PA-O3A-PB	-2.49	124.29	132.83
5	C	600	ADP	PA-O3A-PB	-2.48	124.32	132.83
5	F	600	ADP	PA-O3A-PB	-2.45	124.44	132.83
5	N	600	ADP	C3'-C2'-C1'	2.42	104.62	100.98
5	I	600	ADP	PA-O3A-PB	-2.38	124.65	132.83
5	L	600	ADP	C2-N1-C6	2.35	122.78	118.75
5	I	600	ADP	C3'-C2'-C1'	2.33	104.48	100.98
5	E	600	ADP	C3'-C2'-C1'	2.30	104.44	100.98
5	B	600	ADP	PA-O3A-PB	-2.29	124.97	132.83
5	B	600	ADP	C3'-C2'-C1'	2.24	104.34	100.98
5	M	600	ADP	C3'-C2'-C1'	2.23	104.34	100.98
5	D	600	ADP	C2-N1-C6	2.23	122.57	118.75
5	F	600	ADP	C2-N1-C6	2.23	122.56	118.75
5	J	600	ADP	C2-N1-C6	2.14	122.41	118.75
5	L	600	ADP	PA-O3A-PB	-2.11	125.60	132.83
5	K	600	ADP	C2-N1-C6	2.08	122.31	118.75
5	A	600	ADP	C2-N1-C6	2.07	122.30	118.75
5	E	600	ADP	C2-N1-C6	2.07	122.30	118.75
5	J	600	ADP	PA-O3A-PB	-2.07	125.73	132.83
5	N	600	ADP	C2-N1-C6	2.05	122.26	118.75
5	B	600	ADP	C2-N1-C6	2.04	122.24	118.75
5	I	600	ADP	C2-N1-C6	2.01	122.19	118.75
5	M	600	ADP	C2-N1-C6	2.01	122.19	118.75
5	N	600	ADP	PA-O3A-PB	-2.00	125.96	132.83

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	600	ADP	PA-O3A-PB-O2B
5	L	600	ADP	PA-O3A-PB-O2B
5	N	600	ADP	PA-O3A-PB-O2B
7	B	602	GOL	O1-C1-C2-C3
7	C	602	GOL	C1-C2-C3-O3
7	C	602	GOL	O2-C2-C3-O3
7	E	603	GOL	O1-C1-C2-C3
7	F	602	GOL	O1-C1-C2-O2
7	F	602	GOL	O1-C1-C2-C3
7	J	602	GOL	C1-C2-C3-O3
7	K	602	GOL	C1-C2-C3-O3
7	K	602	GOL	O2-C2-C3-O3
7	M	604	GOL	O1-C1-C2-C3
7	M	604	GOL	C1-C2-C3-O3
7	M	604	GOL	O2-C2-C3-O3
7	M	606	GOL	C1-C2-C3-O3
7	M	606	GOL	O2-C2-C3-O3
7	N	604	GOL	O1-C1-C2-C3
7	B	602	GOL	O1-C1-C2-O2
7	N	604	GOL	O1-C1-C2-O2
7	E	604	GOL	C1-C2-C3-O3
7	E	603	GOL	O1-C1-C2-O2
7	J	602	GOL	O2-C2-C3-O3
7	M	604	GOL	O1-C1-C2-O2
5	C	600	ADP	PA-O3A-PB-O1B
5	D	600	ADP	PA-O3A-PB-O1B
7	E	604	GOL	O1-C1-C2-O2
5	A	600	ADP	O4'-C4'-C5'-O5'
5	A	600	ADP	PB-O3A-PA-O1A
7	E	602	GOL	C1-C2-C3-O3
5	F	600	ADP	PA-O3A-PB-O1B
5	N	600	ADP	PA-O3A-PB-O1B
5	D	600	ADP	PA-O3A-PB-O2B
5	D	600	ADP	PA-O3A-PB-O3B
5	N	600	ADP	PA-O3A-PB-O3B
7	E	604	GOL	O2-C2-C3-O3
5	A	600	ADP	PB-O3A-PA-O2A
7	E	604	GOL	O1-C1-C2-C3
7	I	602	GOL	O1-C1-C2-C3

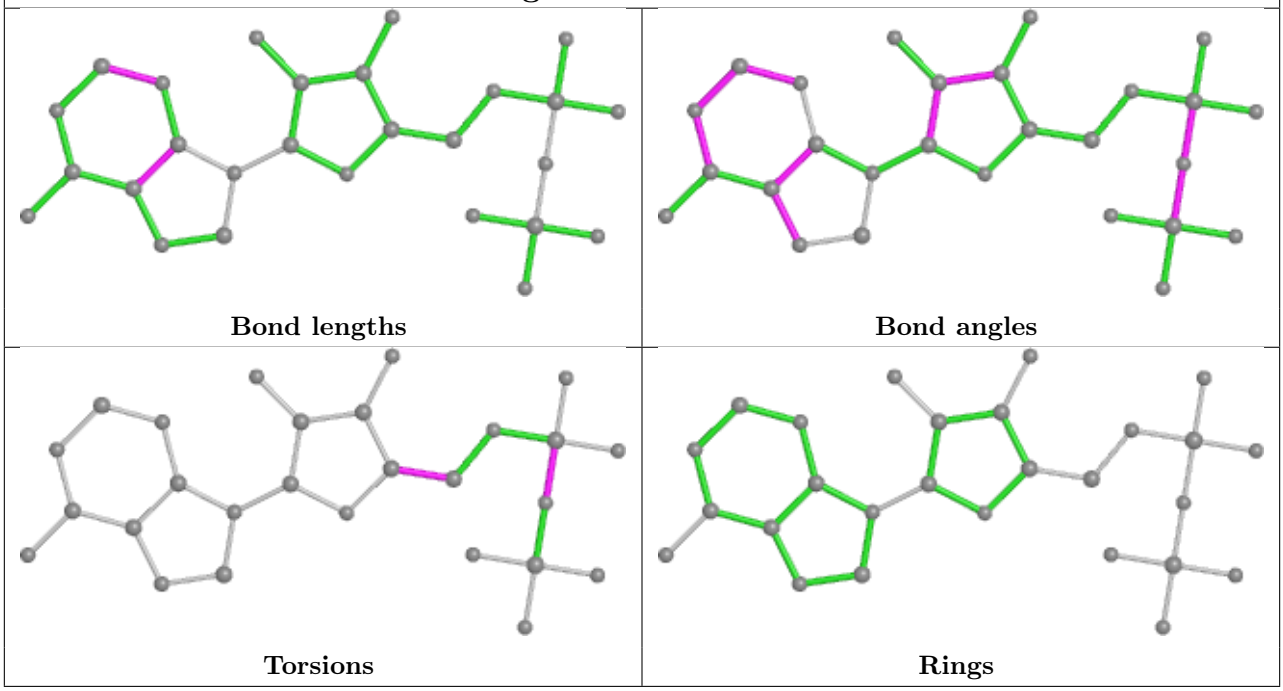
There are no ring outliers.

No monomer is involved in short contacts.

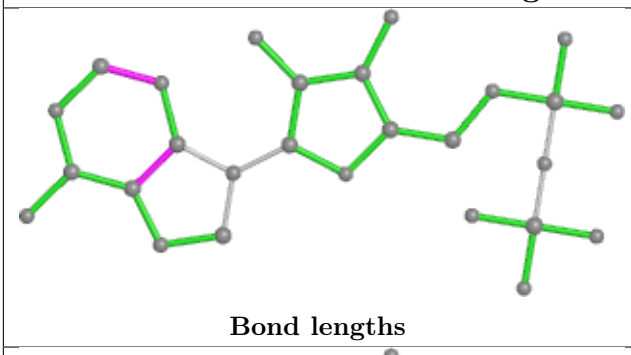
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

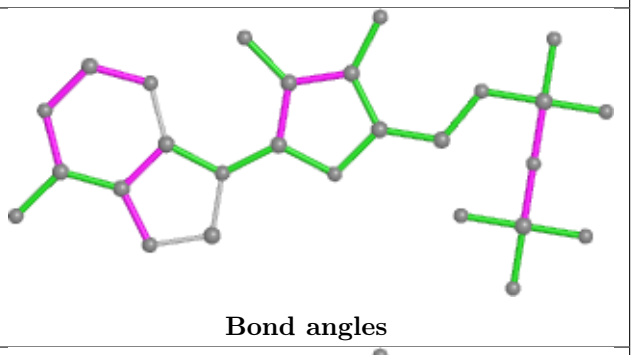
Ligand ADP A 600



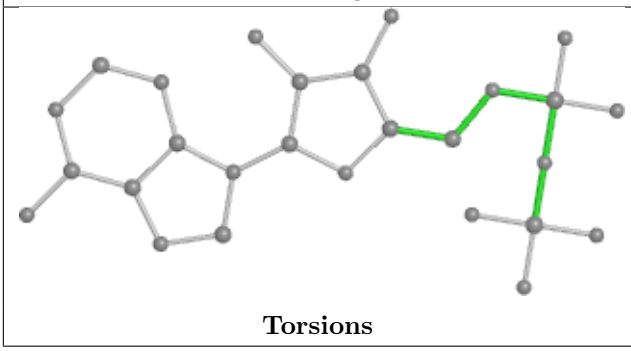
Ligand ADP B 600



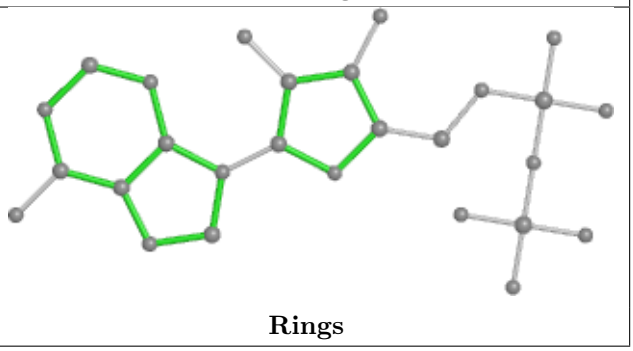
Bond lengths



Bond angles

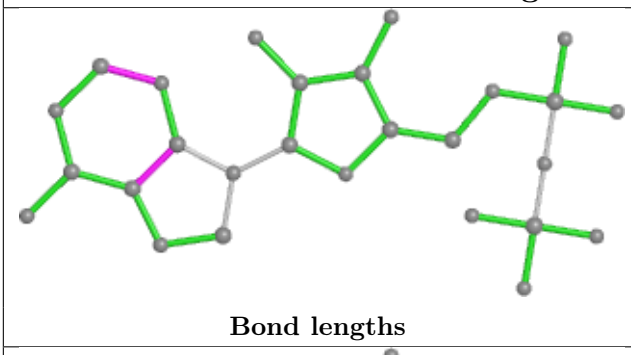


Torsions

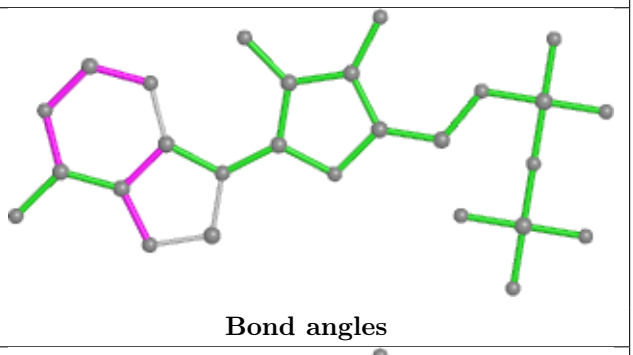


Rings

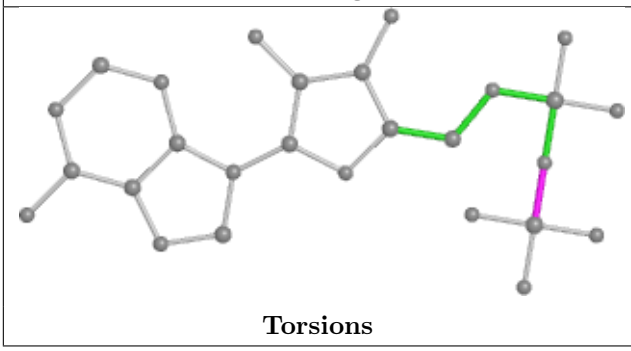
Ligand ADP D 600



Bond lengths



Bond angles



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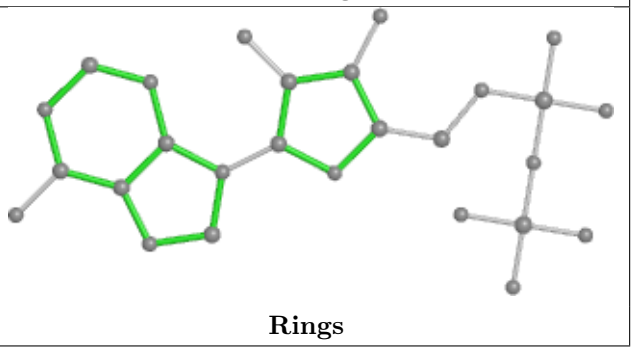
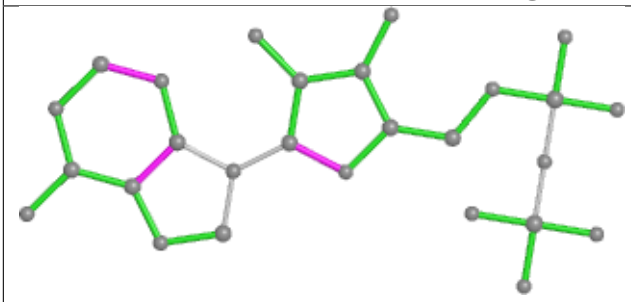


Rings

Ligand ADP F 600



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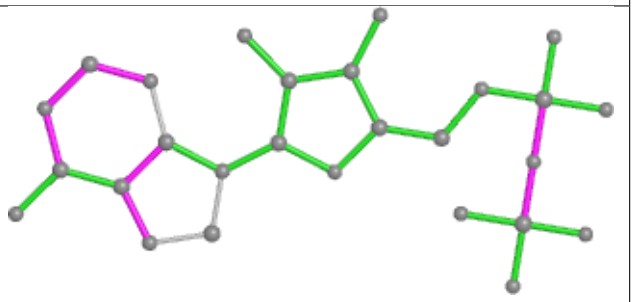
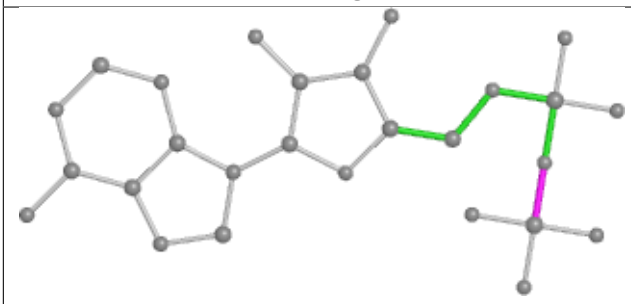
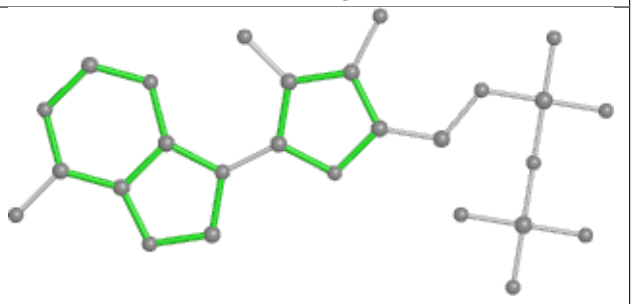


Bond angles

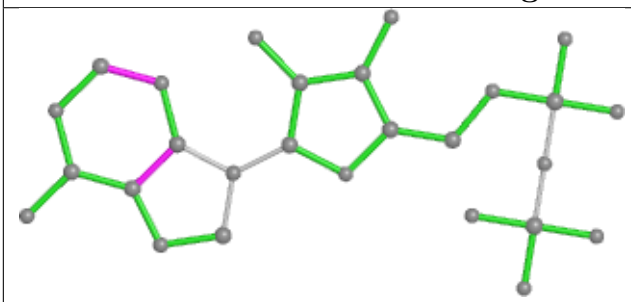


Torsions

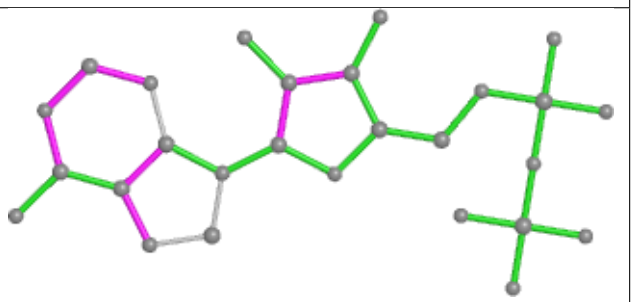


Rings

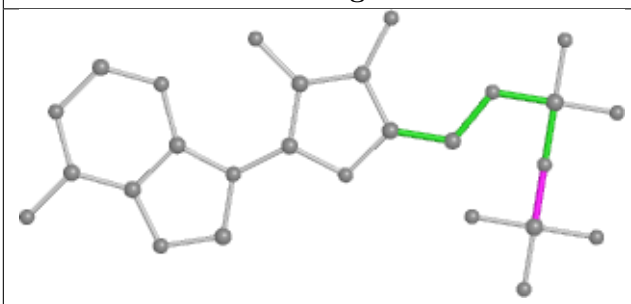
Ligand ADP N 600



Bond lengths



Bond angles



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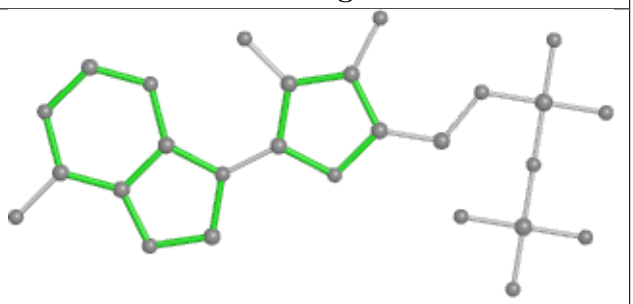
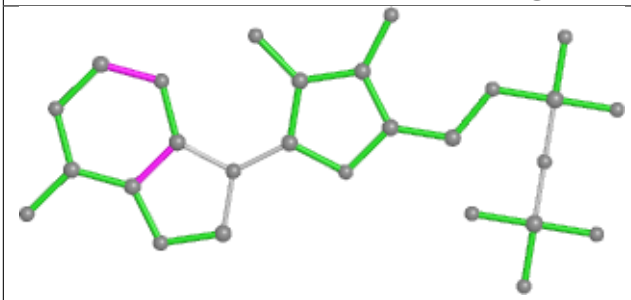


Rings

Ligand ADP I 600



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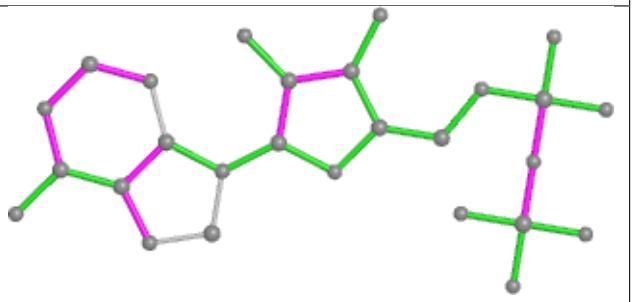
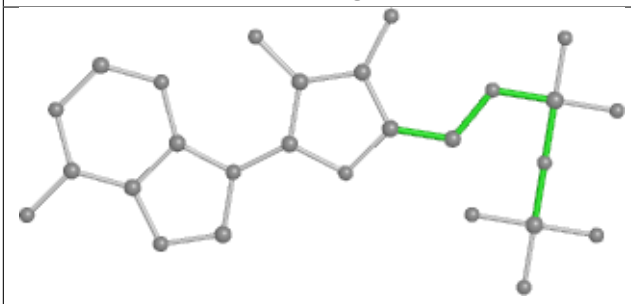


Bond angles



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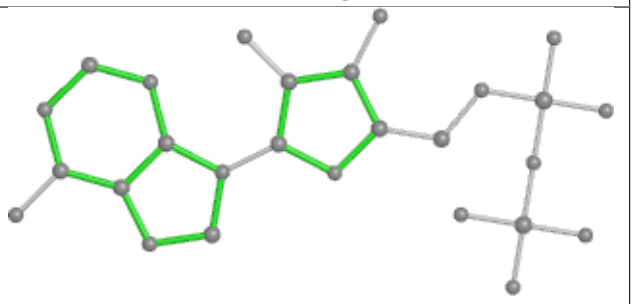

Rings

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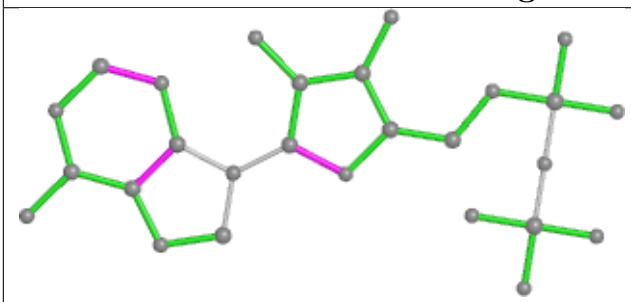

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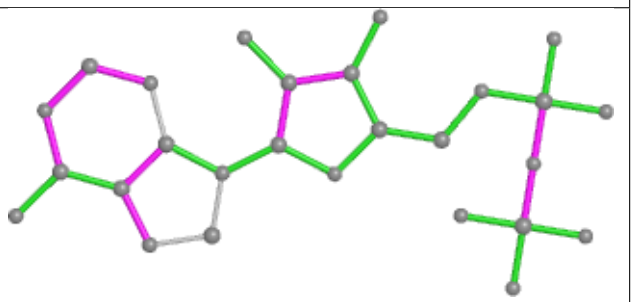
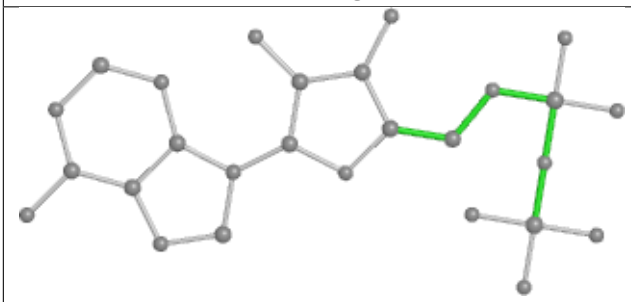


Bond angles



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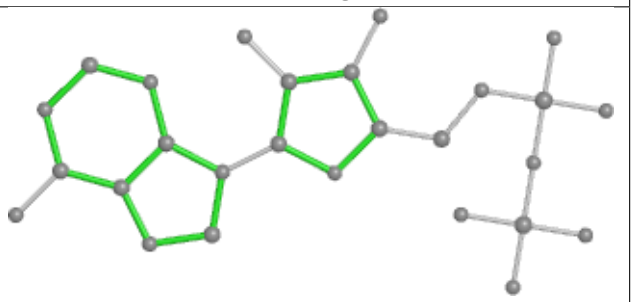
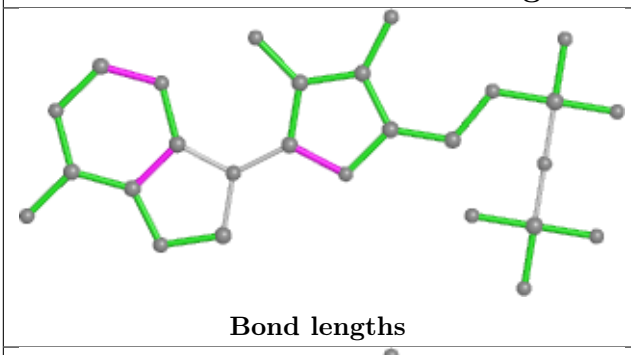
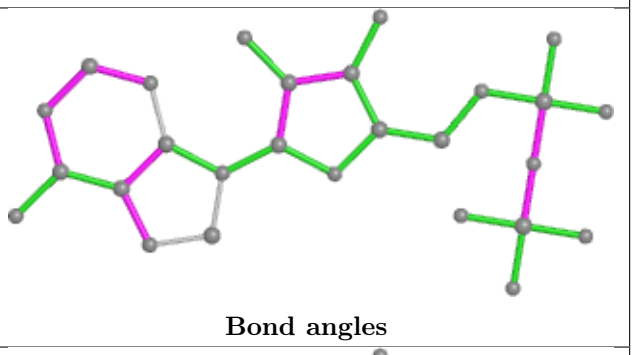


Rings

Ligand ADP E 600



Bond lengths



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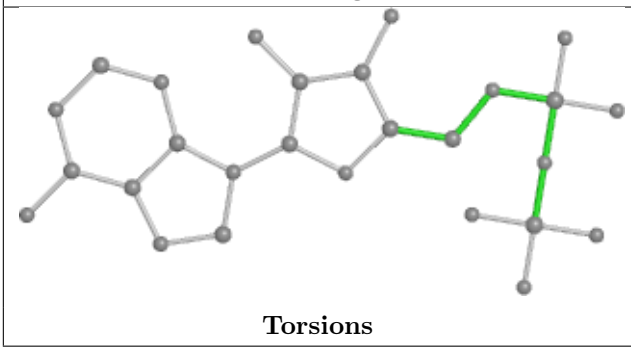

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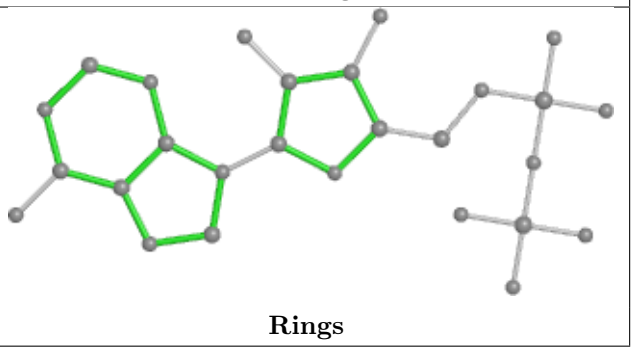
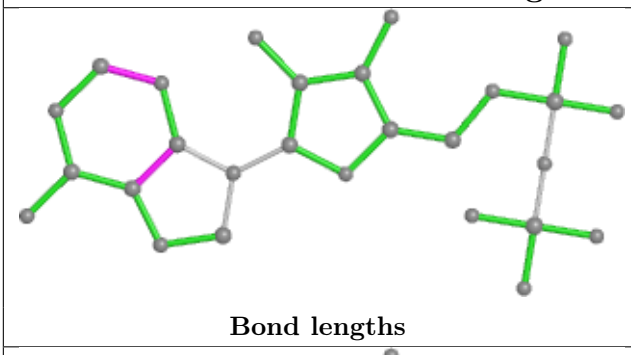
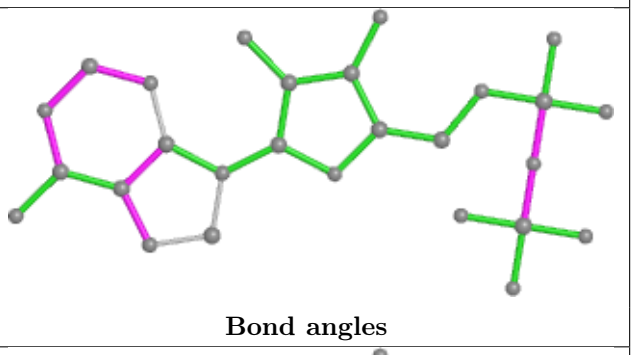


Rings

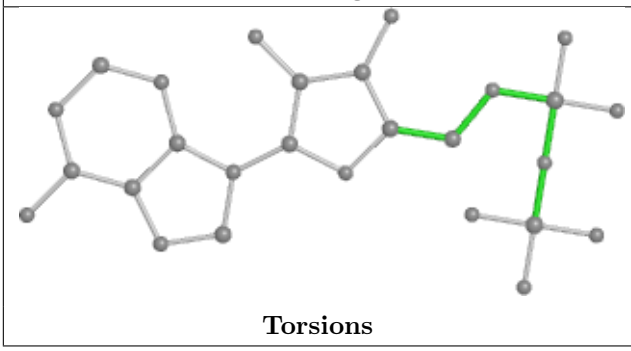
Ligand ADP J 600



Bond lengths



Bond angles



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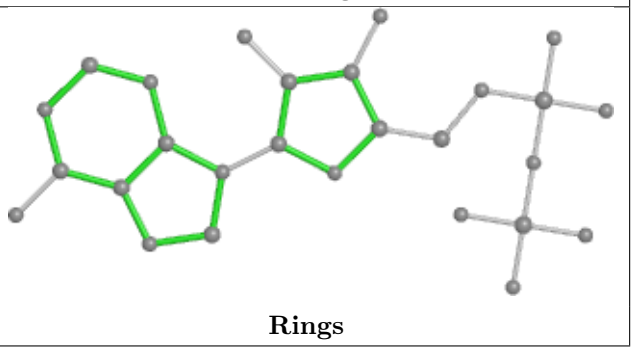
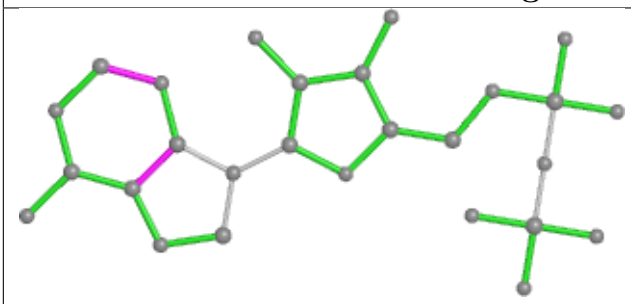
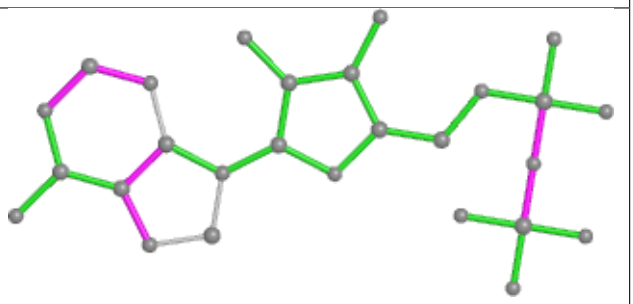


Rings

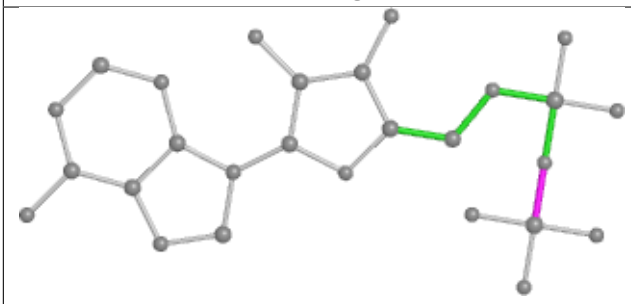
Ligand ADP C 600



Bond lengths



Bond angles



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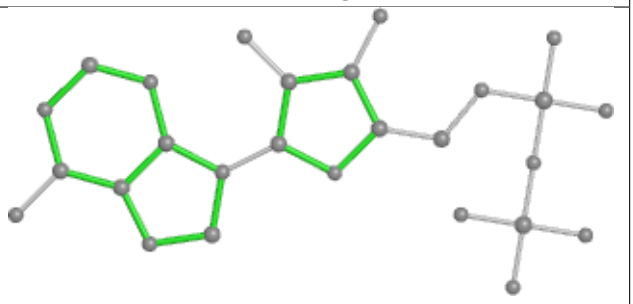
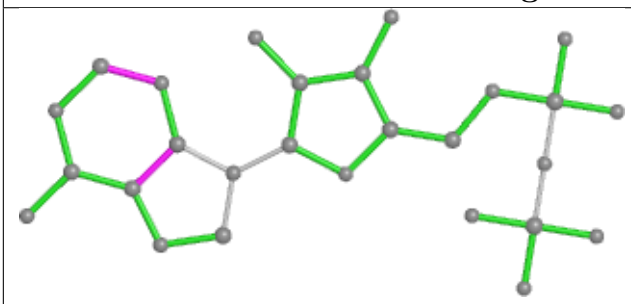


Rings

Ligand ADP K 600



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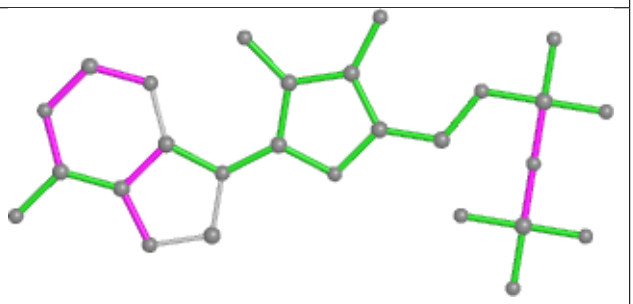
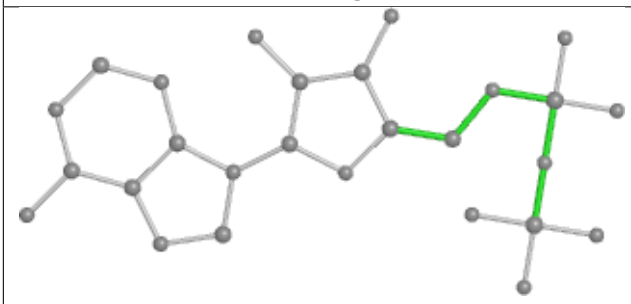
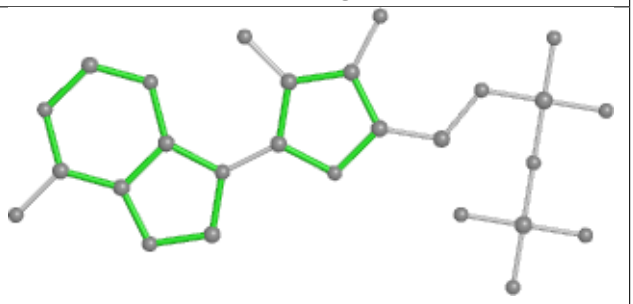


Bond angles



Torsions



Rings

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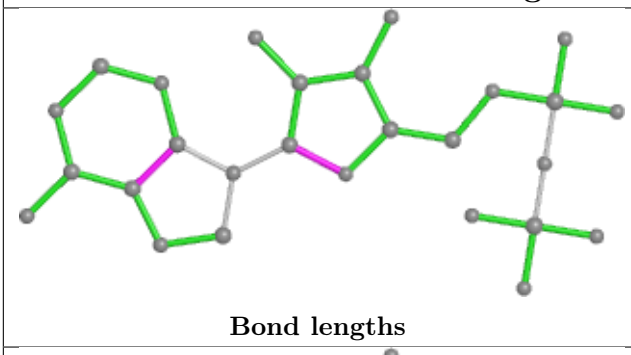

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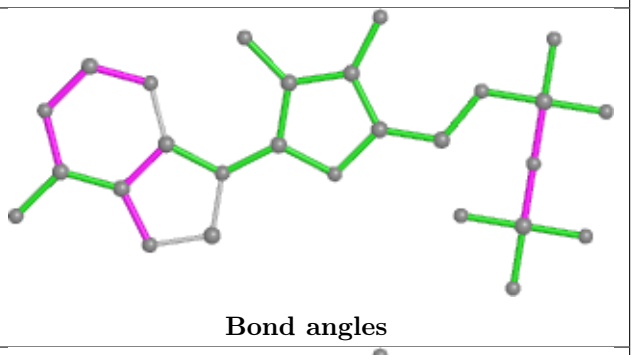

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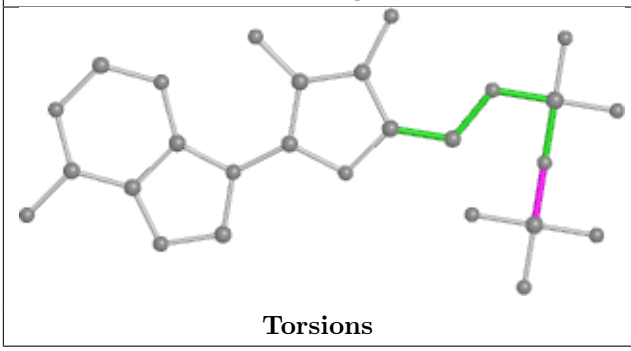
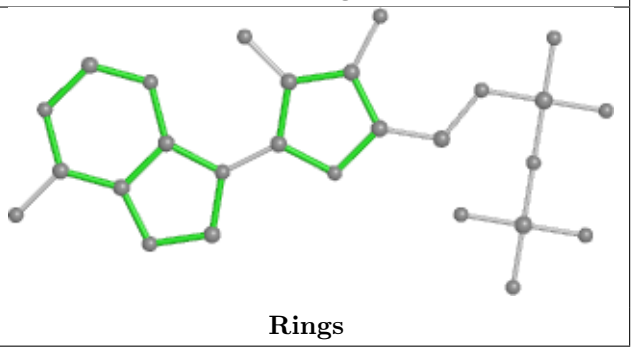


Torsions



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	475/479 (99%)	0.32	48 (10%) 7 4	21, 40, 86, 115	0
1	B	469/479 (97%)	0.01	12 (2%) 56 50	20, 34, 60, 71	0
1	C	475/479 (99%)	-0.13	7 (1%) 73 70	22, 33, 57, 84	0
1	I	475/479 (99%)	0.05	21 (4%) 34 27	19, 33, 72, 98	0
1	J	468/479 (97%)	0.02	16 (3%) 45 38	19, 33, 64, 77	0
1	K	476/479 (99%)	-0.31	2 (0%) 92 91	21, 30, 44, 53	0
2	D	461/462 (99%)	0.04	18 (3%) 39 32	27, 39, 59, 83	0
2	E	462/462 (100%)	-0.25	1 (0%) 95 95	21, 32, 53, 73	0
2	F	462/462 (100%)	-0.05	8 (1%) 70 66	22, 34, 55, 67	0
2	L	462/462 (100%)	-0.16	5 (1%) 80 78	21, 33, 53, 67	0
2	M	462/462 (100%)	-0.19	6 (1%) 77 73	19, 30, 55, 76	0
2	N	462/462 (100%)	-0.11	6 (1%) 77 73	20, 32, 54, 66	0
3	G	285/285 (100%)	0.08	10 (3%) 44 36	24, 38, 57, 75	0
3	O	285/285 (100%)	-0.04	6 (2%) 63 58	24, 34, 55, 72	0
4	H	132/134 (98%)	0.02	3 (2%) 60 54	27, 37, 63, 72	0
4	P	134/134 (100%)	0.34	5 (3%) 41 34	33, 43, 66, 76	0
All	All	6445/6484 (99%)	-0.04	174 (2%) 54 48	19, 34, 60, 115	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	VAL	6.3
2	D	378	ALA	6.1
2	D	375	ASP	5.8
1	A	399	GLY	5.4
1	A	496	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
4	P	1	MET	5.0
2	D	376	ILE	4.8
1	A	400	SER	4.7
3	O	61	LYS	4.5
1	A	498	PHE	4.4
1	A	404	LYS	4.4
1	I	466	ALA	4.2
1	J	26	VAL	4.1
4	P	134	LYS	4.0
2	N	1	MET	4.0
1	A	466	ALA	4.0
1	B	497	GLY	4.0
1	A	381	THR	3.9
1	I	496	LYS	3.9
1	A	485	LYS	3.8
2	L	1	MET	3.8
1	I	381	THR	3.7
1	A	497	GLY	3.6
1	C	28	VAL	3.6
1	A	398	PHE	3.5
1	J	406	THR	3.5
4	H	134	LYS	3.5
4	P	133	SER	3.5
2	M	379	ILE	3.5
1	J	498	PHE	3.5
1	B	26	VAL	3.5
1	A	489	ALA	3.4
1	A	396	ALA	3.4
2	F	462	LEU	3.4
1	I	400	SER	3.3
1	A	405	ALA	3.3
1	I	405	ALA	3.2
1	A	500	PRO	3.2
1	A	487	LEU	3.2
2	D	237	GLY	3.2
2	N	170	GLN	3.1
1	A	483	ASP	3.1
3	G	61	LYS	3.1
1	B	498	PHE	3.1
1	J	463	PHE	3.1
1	J	484	THR	3.1
3	G	2	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	407	GLN	3.1
4	H	110	THR	3.0
2	D	238	GLN	3.0
2	D	379	ILE	3.0
1	A	494	PHE	3.0
1	K	502	ALA	3.0
2	D	289	LYS	3.0
2	M	384	GLU	3.0
4	H	133	SER	3.0
3	O	63	PHE	3.0
1	K	124	ALA	3.0
3	G	286	ARG	2.9
1	A	121	ILE	2.9
1	J	485	LYS	2.9
1	A	384	LEU	2.9
2	F	440	ASN	2.9
1	A	410	LEU	2.9
2	L	237	GLY	2.9
1	A	397	GLN	2.8
1	B	489	ALA	2.8
1	A	501	SER	2.8
1	B	395	PHE	2.8
1	A	382	LEU	2.8
1	A	495	LYS	2.8
1	J	482	PRO	2.8
1	I	384	LEU	2.8
1	A	394	ALA	2.8
1	A	470	SER	2.8
1	I	447	ASP	2.8
1	I	404	LYS	2.8
1	I	498	PHE	2.8
1	I	501	SER	2.8
2	N	102	GLU	2.8
1	A	447	ASP	2.7
1	A	438	TYR	2.7
2	L	424	LYS	2.7
1	A	391	GLU	2.7
2	N	171	GLU	2.7
1	I	489	ALA	2.7
3	O	62	ASP	2.7
1	A	477	GLN	2.7
2	M	1	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	124	ALA	2.7
1	J	483	ASP	2.7
2	D	174	GLY	2.6
1	C	401	ASP	2.6
2	F	21	GLY	2.6
2	D	36	GLN	2.6
2	M	377	ILE	2.6
1	A	448	ILE	2.6
1	J	447	ASP	2.6
1	A	119	GLY	2.6
1	J	466	ALA	2.6
1	I	397	GLN	2.6
1	A	385	ASP	2.6
2	D	380	LEU	2.6
2	E	1	MET	2.6
1	A	463	PHE	2.6
2	D	173	GLY	2.6
2	D	104	ASN	2.6
3	G	192	THR	2.6
1	C	87	GLN	2.6
2	F	101	GLY	2.6
2	N	173	GLY	2.6
4	P	132	ASN	2.5
1	J	489	ALA	2.5
3	G	194	GLU	2.5
1	I	499	THR	2.5
1	J	497	GLY	2.5
3	G	5	ARG	2.5
1	A	28	VAL	2.5
1	C	27	GLU	2.4
2	F	173	GLY	2.4
1	B	405	ALA	2.4
2	M	388	GLU	2.4
1	I	28	VAL	2.4
1	A	467	ASN	2.4
2	N	3	LYS	2.4
3	G	63	PHE	2.4
1	B	485	LYS	2.4
1	I	493	GLU	2.3
1	J	501	SER	2.3
1	A	449	PRO	2.3
1	B	496	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	493	GLU	2.2
2	F	1	MET	2.2
3	O	108	GLN	2.2
1	A	491	ILE	2.2
3	G	197	LEU	2.2
2	F	412	GLN	2.2
1	J	470	SER	2.2
3	O	286	ARG	2.2
1	A	471	LEU	2.2
2	L	106	GLU	2.1
1	A	124	ALA	2.1
3	O	211	GLU	2.1
2	M	21	GLY	2.1
1	A	499	THR	2.1
1	A	444	PHE	2.1
1	I	402	LEU	2.1
1	B	466	ALA	2.1
1	I	391	GLU	2.1
1	C	121	ILE	2.1
4	P	110	THR	2.1
3	G	62	ASP	2.1
2	D	290	LYS	2.1
2	D	5	ARG	2.1
3	G	195	GLU	2.1
1	A	126	TYR	2.1
2	L	105	ALA	2.1
2	D	239	ASP	2.1
1	I	500	PRO	2.1
1	J	500	PRO	2.1
2	D	171	GLU	2.1
1	B	394	ALA	2.0
2	F	5	ARG	2.0
1	I	467	ASN	2.0
2	D	106	GLU	2.0
1	B	404	LYS	2.0
1	A	118	ARG	2.0
1	A	484	THR	2.0
1	I	470	SER	2.0
1	B	463	PHE	2.0
1	I	373	LYS	2.0
1	A	117	GLY	2.0
1	J	499	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	424	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	C	601	1/1	0.71	0.19	24,24,24,24	0
7	GOL	E	604	6/6	0.81	0.25	42,43,44,44	0
6	MG	I	601	1/1	0.86	0.26	23,23,23,23	0
6	MG	J	601	1/1	0.86	0.25	23,23,23,23	0
6	MG	F	601	1/1	0.86	0.33	22,22,22,22	0
7	GOL	N	603	6/6	0.87	0.22	40,40,41,41	0
6	MG	D	601	1/1	0.89	0.40	30,30,30,30	0
6	MG	N	602	1/1	0.89	0.37	22,22,22,22	0
7	GOL	N	604	6/6	0.89	0.21	32,32,32,32	0
7	GOL	E	603	6/6	0.90	0.21	37,37,37,37	0
6	MG	K	601	1/1	0.91	0.30	20,20,20,20	0
7	GOL	A	602	6/6	0.91	0.20	26,26,26,27	0
7	GOL	F	602	6/6	0.92	0.21	29,29,30,30	0
7	GOL	J	602	6/6	0.92	0.20	38,39,39,39	0
7	GOL	M	606	6/6	0.92	0.22	23,23,23,24	0
6	MG	A	601	1/1	0.92	0.17	31,31,31,31	0
7	GOL	E	602	6/6	0.92	0.21	28,29,29,29	0
7	GOL	M	604	6/6	0.94	0.21	27,27,27,27	0
7	GOL	C	602	6/6	0.94	0.20	34,35,35,36	0
7	GOL	B	602	6/6	0.94	0.16	34,35,35,35	0
7	GOL	M	603	6/6	0.94	0.15	36,36,37,37	0
5	ADP	M	600	27/27	0.95	0.15	40,41,42,42	0

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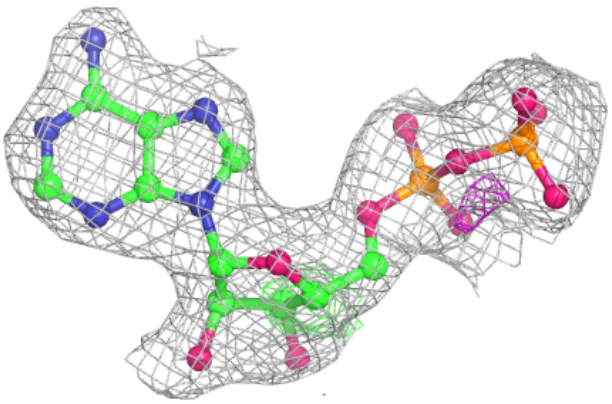
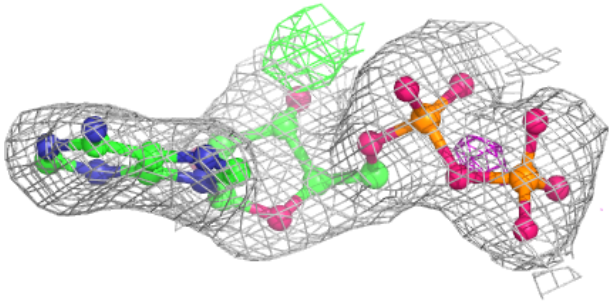
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	L	601	1/1	0.95	0.37	25,25,25,25	0
8	PO4	M	602	5/5	0.95	0.15	48,48,49,49	0
7	GOL	M	605	6/6	0.96	0.18	28,28,28,28	0
5	ADP	A	600	27/27	0.96	0.16	31,34,36,36	0
7	GOL	K	602	6/6	0.96	0.20	31,32,32,32	0
5	ADP	E	600	27/27	0.96	0.12	36,36,38,38	0
6	MG	B	601	1/1	0.96	0.16	23,23,23,23	0
5	ADP	L	600	27/27	0.97	0.13	25,26,26,26	0
5	ADP	C	600	27/27	0.97	0.14	22,22,23,23	0
5	ADP	D	600	27/27	0.97	0.16	28,29,29,29	0
5	ADP	B	600	27/27	0.97	0.14	23,24,25,25	0
5	ADP	F	600	27/27	0.97	0.14	22,24,25,25	0
5	ADP	I	600	27/27	0.97	0.13	24,27,28,28	0
8	PO4	E	601	5/5	0.97	0.12	55,55,56,56	0
5	ADP	J	600	27/27	0.97	0.13	23,24,25,26	0
5	ADP	K	600	27/27	0.98	0.12	20,20,20,20	0
7	GOL	I	602	6/6	0.98	0.13	18,18,18,18	0
5	ADP	N	600	27/27	0.98	0.14	22,24,25,26	0

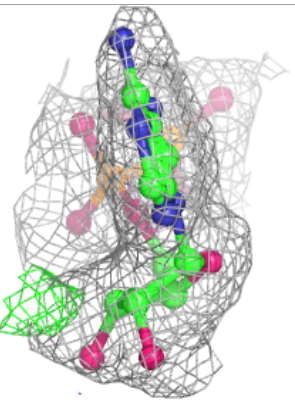
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP M 600:

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

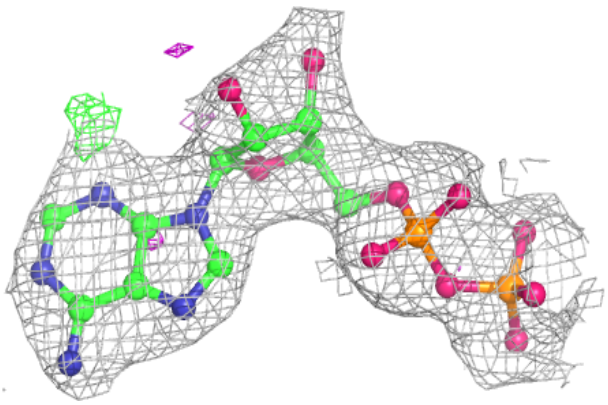


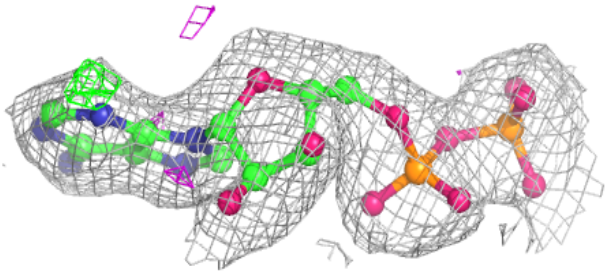


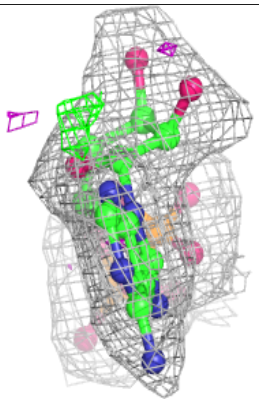


Electron density around ADP A 600:

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

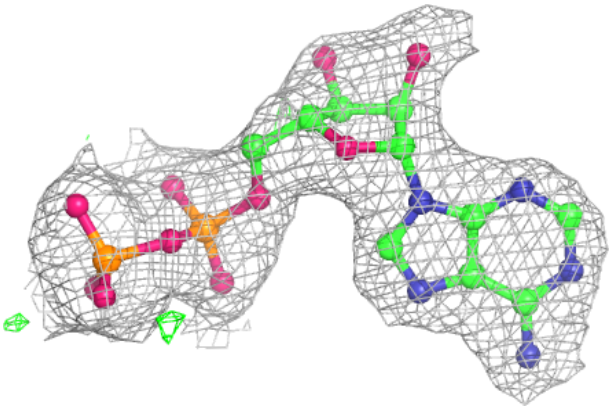


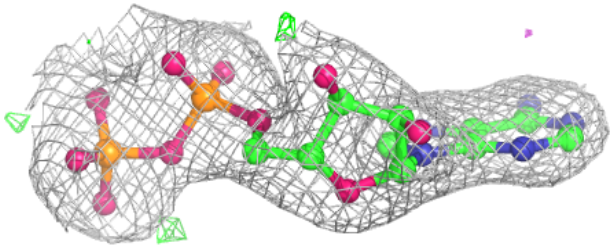




Electron density around ADP E 600:

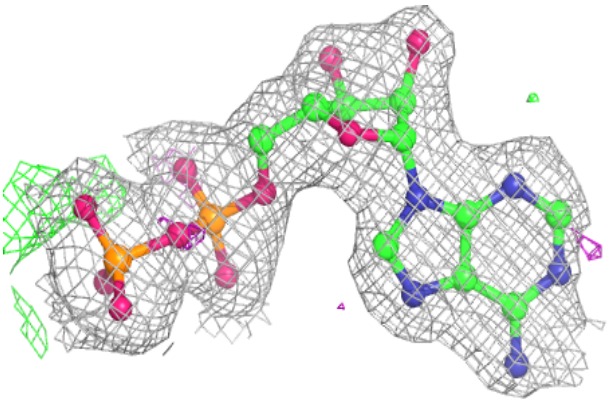
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

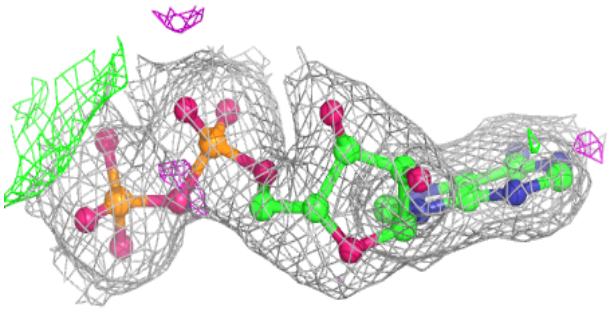




Electron density around ADP L 600:

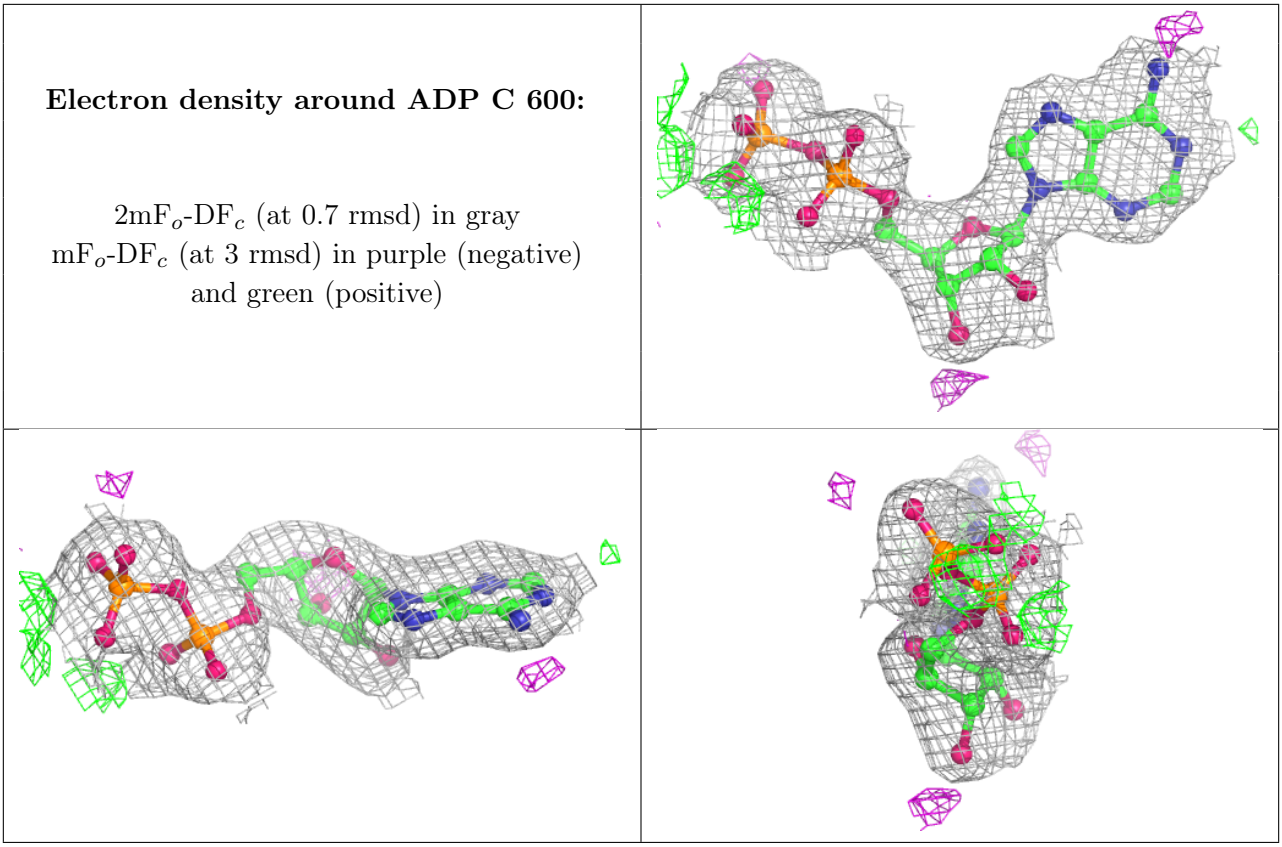
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





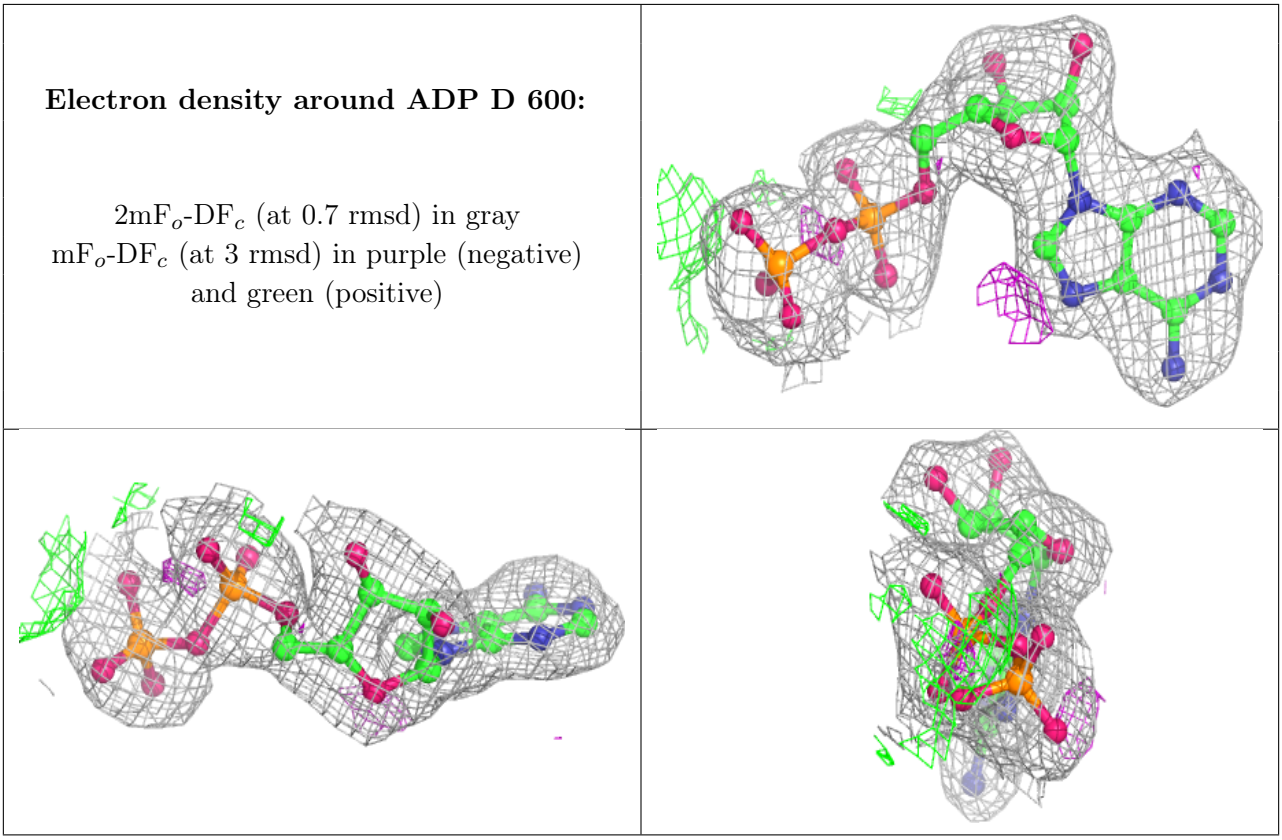
Electron density around ADP C 600:

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



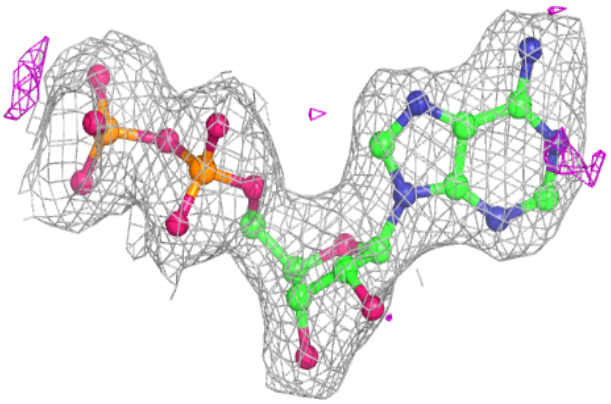
Electron density around ADP D 600:

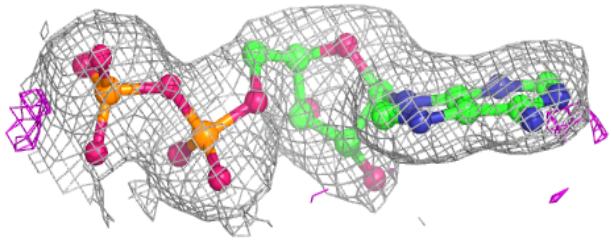
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

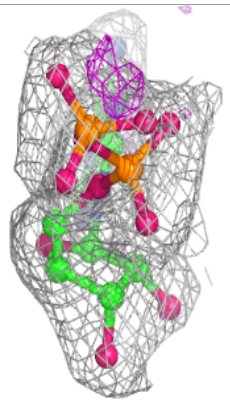


Electron density around ADP B 600:

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

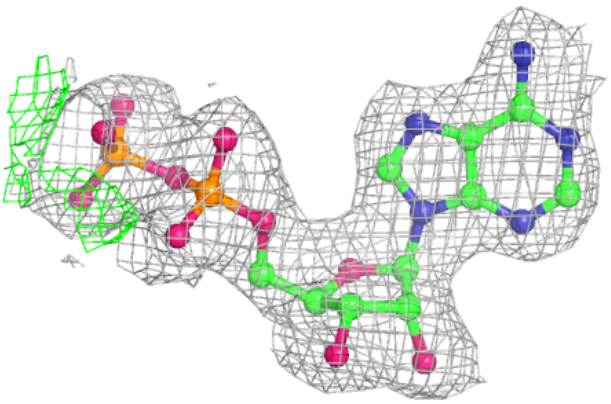


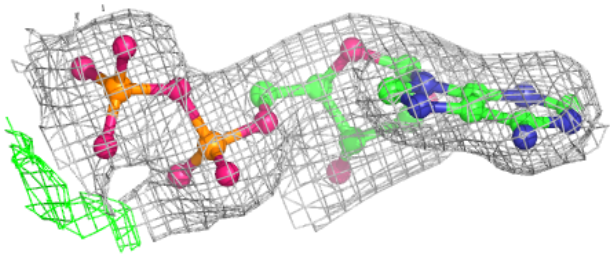


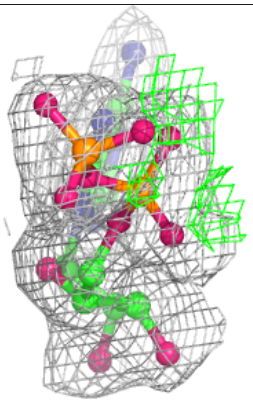


Electron density around ADP F 600:

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

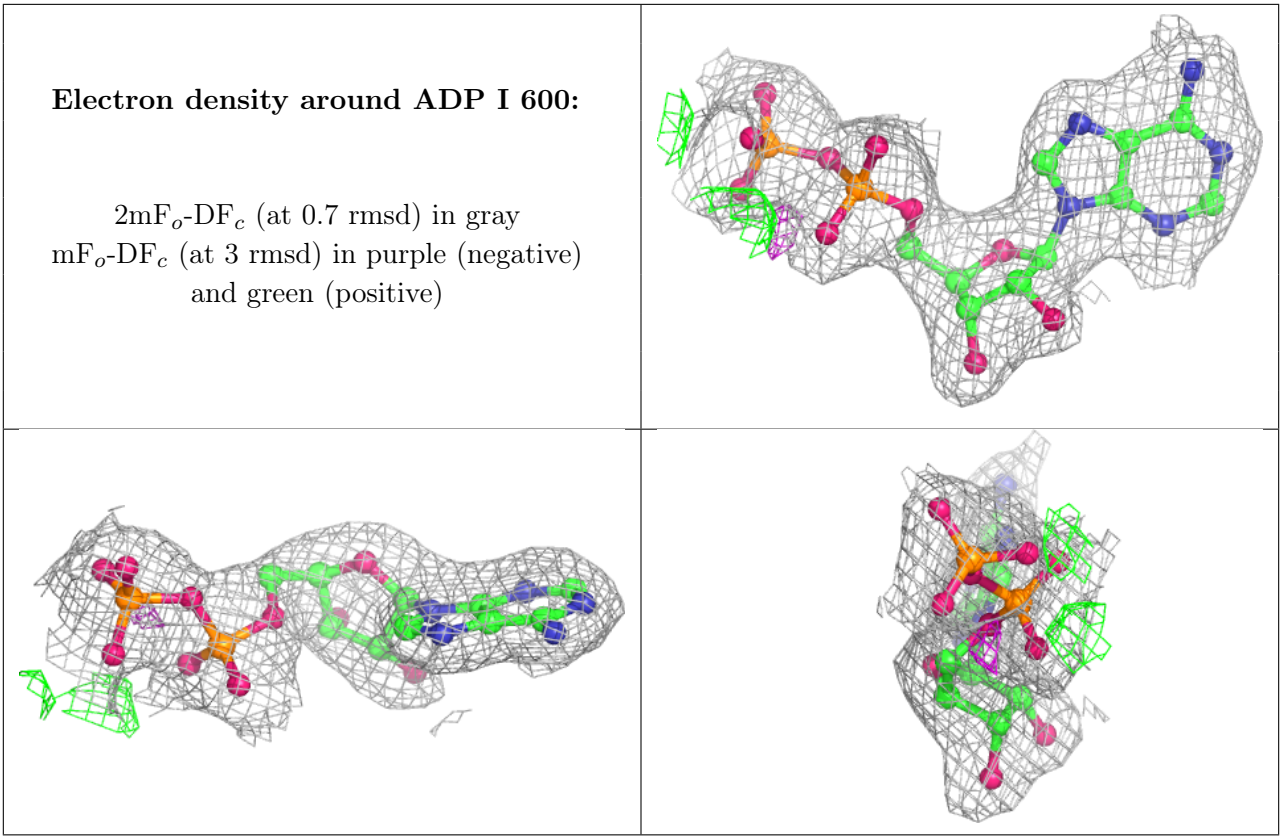






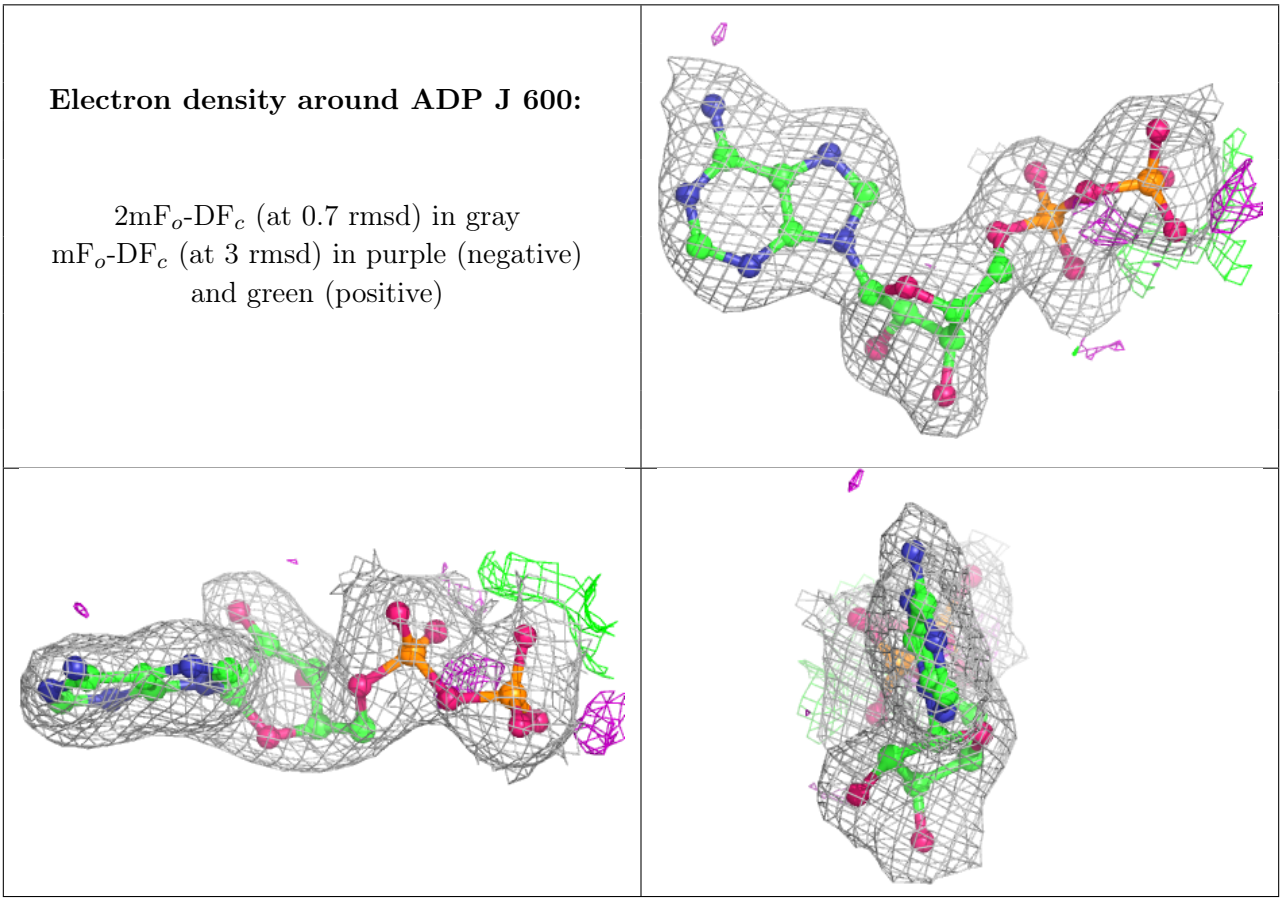
Electron density around ADP I 600:

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



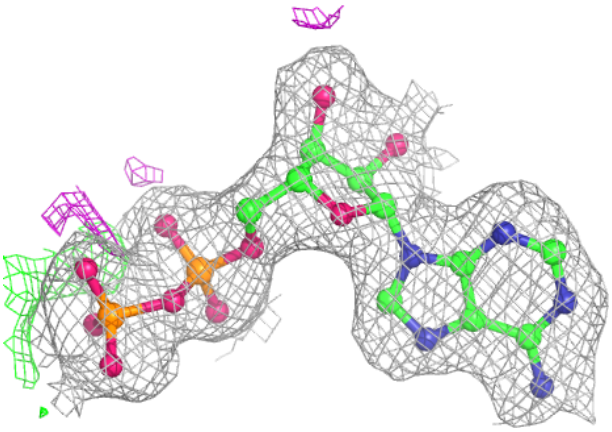
Electron density around ADP J 600:

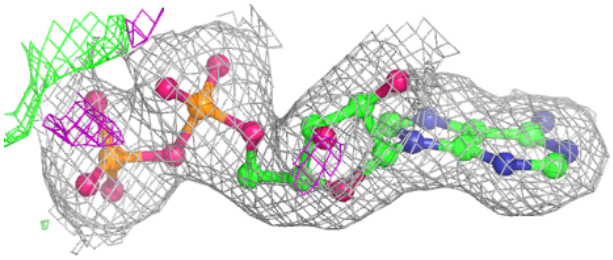
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

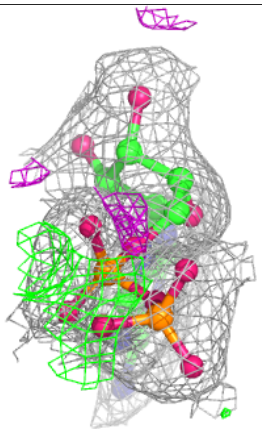


Electron density around ADP K 600:

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

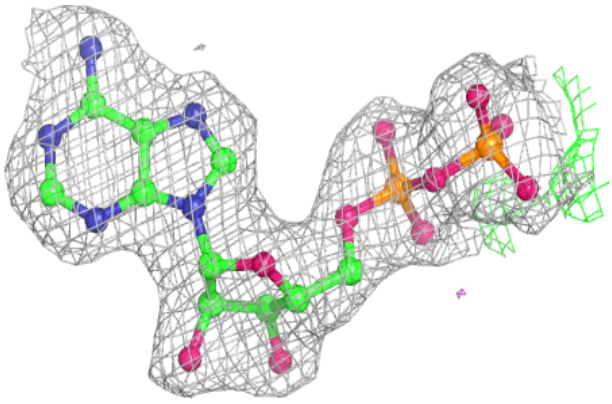


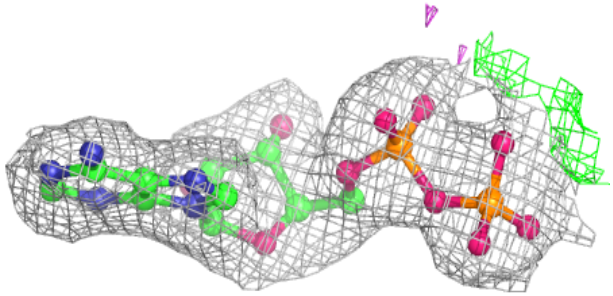


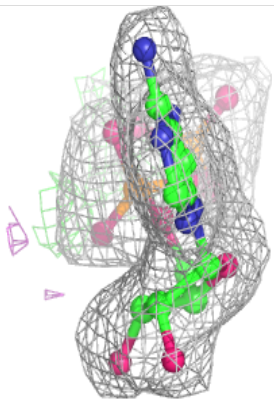


Electron density around ADP N 600:

$2mF_o$-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.