



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:39 PM UTC

PDB ID : 5IK2 / pdb_00005ik2
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

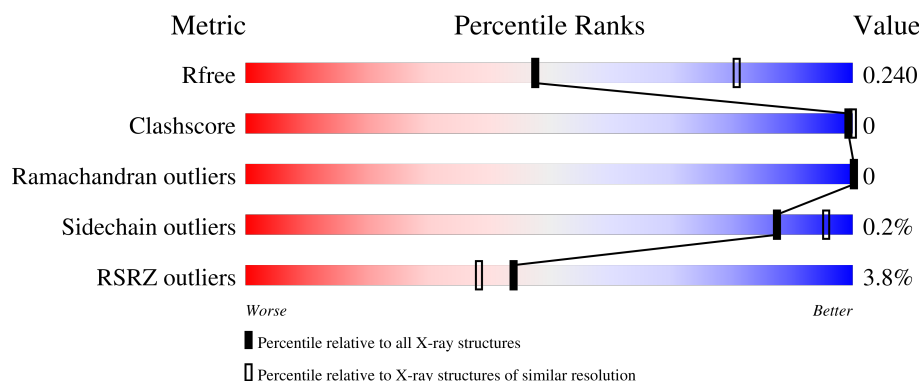
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	479	10% 99% ..
1	B	479	3% 98% .
1	C	479	3% 98% ..
1	I	479	6% 98% ..
1	J	479	3% 98% .

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Mol	Chain	Length	Quality of chain
1	K	479	% 98% ..
2	D	462	4% 100%
2	E	462	3% 98% .
2	F	462	2% 100%
2	L	462	2% 99% .
2	M	462	3% 99% .
2	N	462	3% 100%
3	G	285	4% 100%
3	O	285	3% 99% .
4	H	134	7% 97% ..
4	P	134	9% 99% .

2 Entry composition

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			

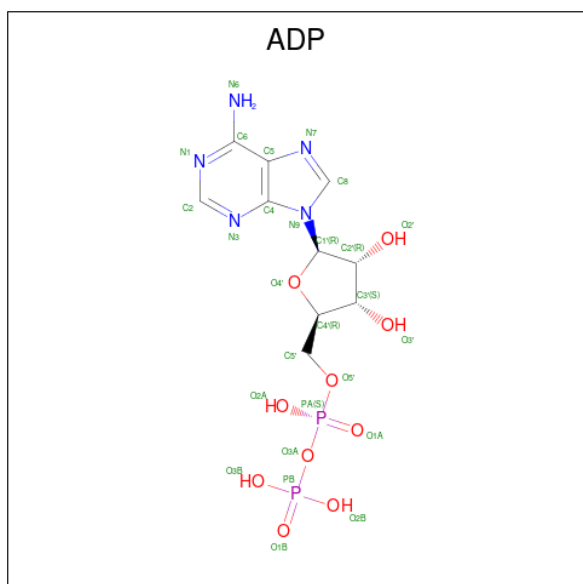
- Molecule 4 is a protein called ATP synthase epsilon chain.

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

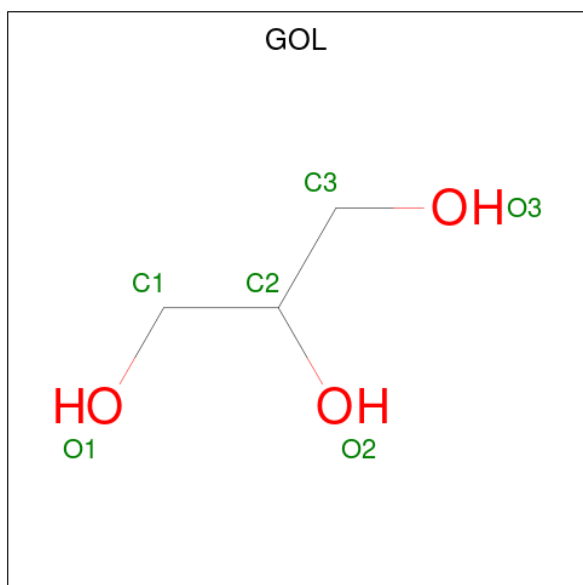
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		
6	K	1	Total	Mg	0	0
			1	1		

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



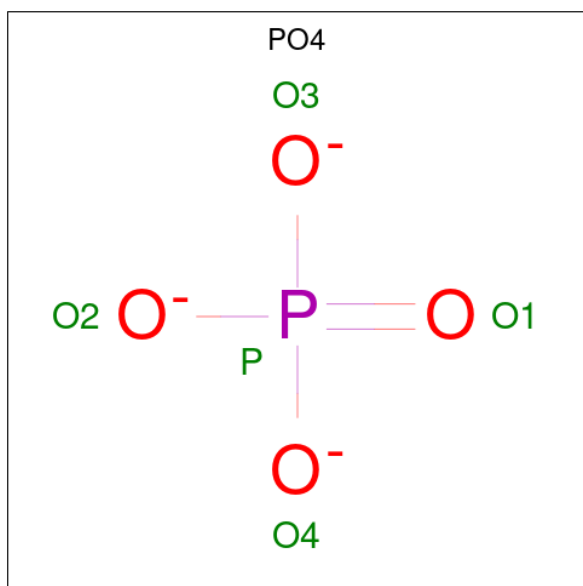
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total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

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

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

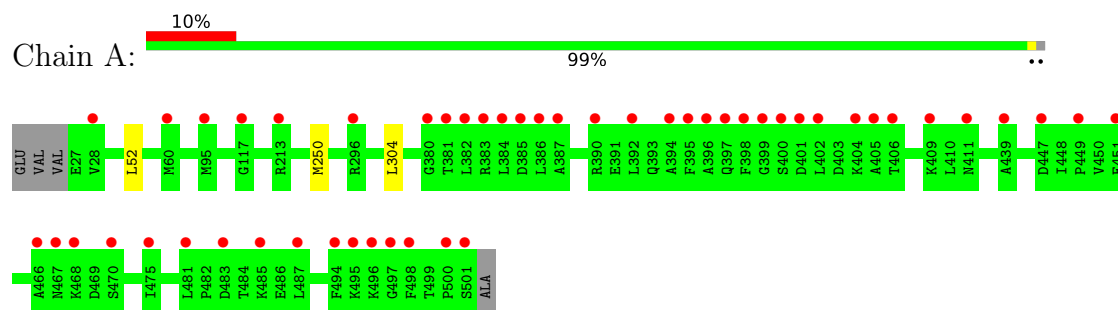
- Molecule 9 is water.

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

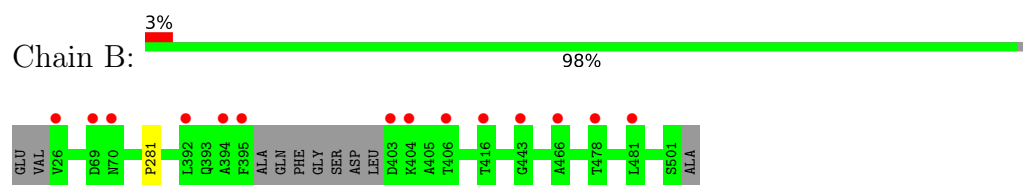
3 Residue-property plots

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.

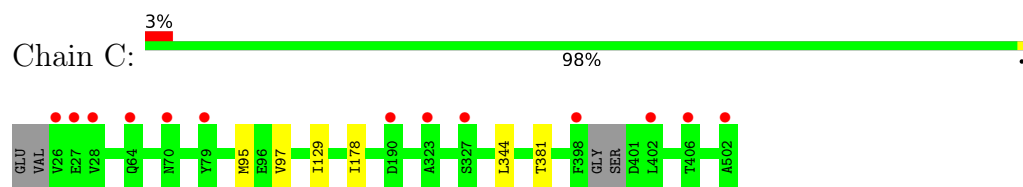
- Molecule 1: ATP synthase subunit alpha



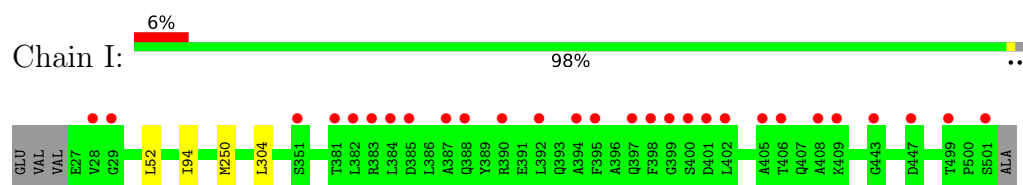
- Molecule 1: ATP synthase subunit alpha



- Molecule 1: ATP synthase subunit alpha

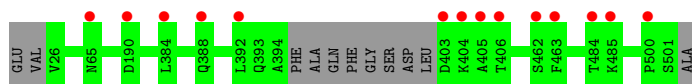


- Molecule 1: ATP synthase subunit alpha



- Molecule 1: ATP synthase subunit alpha

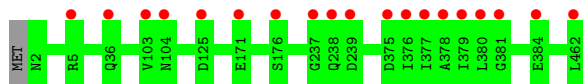




- Molecule 1: ATP synthase subunit alpha



- Molecule 2: ATP synthase subunit beta



- Molecule 2: ATP synthase subunit beta



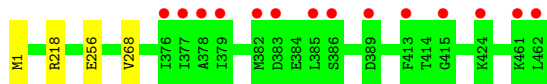
- Molecule 2: ATP synthase subunit beta



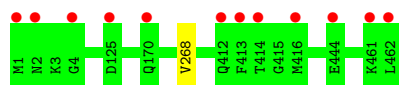
- Molecule 2: ATP synthase subunit beta



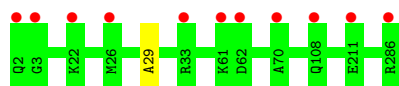
- Molecule 2: ATP synthase subunit beta



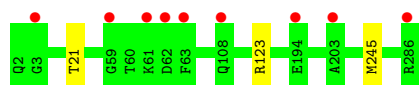
- Molecule 2: ATP synthase subunit beta



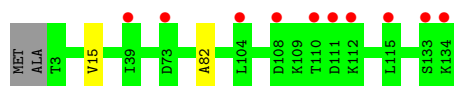
- Molecule 3: ATP synthase gamma chain



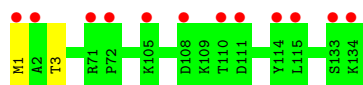
- Molecule 3: ATP synthase gamma chain



- Molecule 4: ATP synthase epsilon chain



- Molecule 4: ATP synthase epsilon chain



4 Data and refinement statistics

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 – 2.60 201.40 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.9 (201.40-2.60) 92.9 (201.40-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.67%)	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)	0.34 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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: ADP, GOL, PO4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.56	0/3716	0.76	0/5028
1	B	0.55	0/3659	0.76	0/4951
1	C	0.55	0/3706	0.76	0/5015
1	I	0.55	0/3705	0.76	0/5014
1	J	0.55	0/3647	0.76	0/4935
1	K	0.55	0/3710	0.76	0/5020
2	D	0.56	0/3581	0.76	0/4852
2	E	0.54	0/3601	0.76	0/4878
2	F	0.55	0/3589	0.76	0/4862
2	L	0.55	0/3589	0.76	0/4862
2	M	0.54	0/3601	0.75	0/4878
2	N	0.55	0/3589	0.76	0/4862
3	G	0.54	0/2263	0.81	0/3054
3	O	0.54	0/2263	0.81	0/3054
4	H	0.53	0/1033	0.72	0/1393
4	P	0.52	0/1046	0.71	0/1410
All	All	0.55	0/50298	0.76	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	1	0
1	B	3602	0	3642	1	0
1	C	3648	0	3684	2	0
1	I	3646	0	3679	1	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	4	0
2	F	3529	0	3541	0	0
2	L	3529	0	3541	2	0
2	M	3540	0	3550	2	0
2	N	3529	0	3541	0	0
3	G	2230	0	2269	1	0
3	O	2230	0	2269	2	0
4	H	1022	0	1082	1	0
4	P	1035	0	1099	1	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	17	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 (17) 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
3:O:21:THR:HG22	3:O:245:MET:HE3	1.86	0.57
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:M:1:MET:HE3	2:M:1:MET:HA	1.99	0.44
2:E:218:ARG:NH2	2:E:256:GLU:OE1	2.52	0.43
1:B:281:PRO:HD3	2:E:264:MET:HE1	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:250:MET:HE3	1:I:304:LEU:HG	2.02	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:A:250:MET:HE3	1:A:304:LEU:HG	2.03	0.41
1:K:280:PRO:HG2	2:L:259:ALA:HB1	2.03	0.40
4:P:1:MET:HE3	4:P:3:THR:CG2	2.51	0.40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	389 (100%)	1 (0%)	86	94
1	B	385/392 (98%)	385 (100%)	0	100	100
1	C	389/392 (99%)	387 (100%)	2 (0%)	81	92
1	I	389/392 (99%)	387 (100%)	2 (0%)	81	92
1	J	384/392 (98%)	384 (100%)	0	100	100
1	K	389/392 (99%)	387 (100%)	2 (0%)	81	92
2	D	375/376 (100%)	375 (100%)	0	100	100
2	E	377/376 (100%)	376 (100%)	1 (0%)	86	94
2	F	376/376 (100%)	375 (100%)	1 (0%)	86	94
2	L	376/376 (100%)	376 (100%)	0	100	100
2	M	377/376 (100%)	376 (100%)	1 (0%)	86	94
2	N	376/376 (100%)	375 (100%)	1 (0%)	86	94
3	G	238/238 (100%)	238 (100%)	0	100	100
3	O	238/238 (100%)	238 (100%)	0	100	100
4	H	109/110 (99%)	109 (100%)	0	100	100
4	P	110/110 (100%)	110 (100%)	0	100	100
All	All	5278/5304 (100%)	5267 (100%)	11 (0%)	87	95

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	C	95	MET
1	C	381	THR
2	E	268	VAL
2	F	268	VAL
1	I	52	LEU
1	I	94	ILE
1	K	266	GLN
1	K	381	THR
2	M	268	VAL
2	N	268	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	186	GLN
1	B	172	GLN
1	B	186	GLN
1	B	322	GLN
1	C	33	GLN
1	C	200	GLN
1	C	322	GLN
1	C	407	GLN
2	D	2	ASN
2	D	8	GLN
2	D	22	GLN
2	D	51	ASN
2	D	170	GLN
2	D	374	GLN
2	D	440	ASN
2	E	28	ASN
2	E	36	GLN
2	E	189	ASN
2	E	193	HIS
2	E	210	GLN
2	E	356	HIS
2	F	189	ASN
2	F	193	HIS
2	F	374	GLN
4	H	132	ASN
1	I	64	GLN
1	J	172	GLN

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Mol	Chain	Res	Type
1	J	186	GLN
1	K	172	GLN
1	K	266	GLN
1	K	322	GLN
1	K	407	GLN
2	L	2	ASN
2	L	22	GLN
2	L	51	ASN
2	L	170	GLN
2	L	374	GLN
2	M	36	GLN
2	M	104	ASN
2	M	189	ASN
2	M	193	HIS
2	M	210	GLN
2	M	400	GLN
2	N	189	ASN
2	N	193	HIS
2	N	374	GLN
4	P	5	GLN
4	P	17	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 oligosaccharides 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
7	GOL	N	604	-	5,5,5	0.23	0	5,5,5	0.17	0
5	ADP	E	600	-	28,29,29	1.50	5 (17%)	43,45,45	1.83	9 (20%)
7	GOL	M	604	-	5,5,5	0.35	0	5,5,5	0.56	0
7	GOL	N	603	-	5,5,5	0.30	0	5,5,5	0.16	0
7	GOL	E	602	-	5,5,5	0.26	0	5,5,5	0.33	0
7	GOL	E	603	-	5,5,5	0.35	0	5,5,5	0.41	0
7	GOL	M	606	-	5,5,5	0.27	0	5,5,5	0.28	0
7	GOL	J	602	-	5,5,5	0.28	0	5,5,5	0.22	0
7	GOL	B	602	-	5,5,5	0.34	0	5,5,5	0.19	0
5	ADP	D	600	6	28,29,29	1.47	5 (17%)	43,45,45	1.84	11 (25%)
7	GOL	A	602	-	5,5,5	0.24	0	5,5,5	0.20	0
5	ADP	J	600	6	28,29,29	1.52	5 (17%)	43,45,45	1.82	10 (23%)
5	ADP	L	600	6	28,29,29	1.48	6 (21%)	43,45,45	1.81	12 (27%)
8	PO4	E	601	-	4,4,4	0.95	0	6,6,6	0.42	0
5	ADP	B	600	6	28,29,29	1.53	5 (17%)	43,45,45	1.84	9 (20%)
5	ADP	A	600	6	28,29,29	1.48	4 (14%)	43,45,45	1.84	10 (23%)
5	ADP	F	600	6	28,29,29	1.48	4 (14%)	43,45,45	1.82	9 (20%)
7	GOL	F	602	-	5,5,5	0.41	0	5,5,5	0.36	0
7	GOL	M	605	-	5,5,5	0.25	0	5,5,5	0.36	0
7	GOL	E	604	-	5,5,5	0.40	0	5,5,5	0.51	0
5	ADP	M	600	-	28,29,29	1.51	5 (17%)	43,45,45	1.83	9 (20%)
5	ADP	K	600	6	28,29,29	1.50	5 (17%)	43,45,45	1.83	10 (23%)
7	GOL	C	602	-	5,5,5	0.30	0	5,5,5	0.16	0
5	ADP	C	600	6	28,29,29	1.48	5 (17%)	43,45,45	1.88	9 (20%)
7	GOL	K	602	-	5,5,5	0.33	0	5,5,5	0.19	0
5	ADP	N	600	6	28,29,29	1.48	5 (17%)	43,45,45	1.85	10 (23%)
8	PO4	M	602	-	4,4,4	0.95	0	6,6,6	0.50	0
7	GOL	I	602	-	5,5,5	0.37	0	5,5,5	0.27	0
7	GOL	M	603	-	5,5,5	0.29	0	5,5,5	0.25	0
5	ADP	I	600	6	28,29,29	1.53	5 (17%)	43,45,45	1.83	10 (23%)

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
7	GOL	N	604	-	-	2/4/4/4	-
5	ADP	E	600	-	-	0/16/32/32	0/3/3/3
7	GOL	M	604	-	-	4/4/4/4	-
7	GOL	N	603	-	-	0/4/4/4	-
7	GOL	E	602	-	-	2/4/4/4	-
7	GOL	E	603	-	-	2/4/4/4	-
7	GOL	M	606	-	-	2/4/4/4	-
7	GOL	J	602	-	-	2/4/4/4	-
7	GOL	B	602	-	-	2/4/4/4	-
5	ADP	D	600	6	-	3/16/32/32	0/3/3/3
7	GOL	A	602	-	-	0/4/4/4	-
5	ADP	J	600	6	-	0/16/32/32	0/3/3/3
5	ADP	L	600	6	-	1/16/32/32	0/3/3/3
5	ADP	B	600	6	-	0/16/32/32	0/3/3/3
5	ADP	A	600	6	-	3/16/32/32	0/3/3/3
5	ADP	F	600	6	-	2/16/32/32	0/3/3/3
7	GOL	F	602	-	-	2/4/4/4	-
7	GOL	M	605	-	-	1/4/4/4	-
7	GOL	E	604	-	-	3/4/4/4	-
5	ADP	M	600	-	-	0/16/32/32	0/3/3/3
5	ADP	K	600	6	-	0/16/32/32	0/3/3/3
7	GOL	C	602	-	-	2/4/4/4	-
5	ADP	C	600	6	-	1/16/32/32	0/3/3/3
7	GOL	K	602	-	-	2/4/4/4	-
5	ADP	N	600	6	-	3/16/32/32	0/3/3/3
7	GOL	I	602	-	-	0/4/4/4	-
7	GOL	M	603	-	-	0/4/4/4	-
5	ADP	I	600	6	-	0/16/32/32	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	600	ADP	C5-C4	5.04	1.48	1.39
5	A	600	ADP	C5-C4	5.00	1.48	1.39
5	E	600	ADP	C5-C4	4.98	1.48	1.39
5	M	600	ADP	C5-C4	4.94	1.47	1.39
5	B	600	ADP	C5-C4	4.94	1.47	1.39
5	F	600	ADP	C5-C4	4.88	1.47	1.39
5	J	600	ADP	C5-C4	4.87	1.47	1.39
5	K	600	ADP	C5-C4	4.85	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	600	ADP	C5-C4	4.83	1.47	1.39
5	D	600	ADP	C5-C4	4.80	1.47	1.39
5	C	600	ADP	C5-C4	4.79	1.47	1.39
5	L	600	ADP	C5-C4	4.77	1.47	1.39
5	B	600	ADP	C5-C6	2.98	1.49	1.41
5	K	600	ADP	C5-C6	2.94	1.49	1.41
5	J	600	ADP	C5-C6	2.93	1.49	1.41
5	C	600	ADP	C5-C6	2.90	1.49	1.41
5	F	600	ADP	C5-C6	2.88	1.49	1.41
5	I	600	ADP	C5-C6	2.87	1.49	1.41
5	N	600	ADP	C5-C6	2.83	1.48	1.41
5	M	600	ADP	C5-C6	2.82	1.48	1.41
5	A	600	ADP	C5-C6	2.79	1.48	1.41
5	E	600	ADP	C5-C6	2.76	1.48	1.41
5	J	600	ADP	PA-O3A	2.71	1.62	1.59
5	B	600	ADP	PA-O3A	2.71	1.62	1.59
5	L	600	ADP	C5-C6	2.70	1.48	1.41
5	D	600	ADP	C5-C6	2.69	1.48	1.41
5	I	600	ADP	PA-O3A	2.60	1.62	1.59
5	C	600	ADP	C8-N7	2.52	1.36	1.31
5	E	600	ADP	C5-N7	-2.51	1.34	1.39
5	M	600	ADP	C5-N7	-2.49	1.34	1.39
5	K	600	ADP	C8-N7	2.48	1.36	1.31
5	I	600	ADP	C8-N7	2.44	1.36	1.31
5	F	600	ADP	C5-N7	-2.42	1.34	1.39
5	K	600	ADP	PA-O3A	2.41	1.62	1.59
5	D	600	ADP	C5-N7	-2.40	1.34	1.39
5	L	600	ADP	C8-N7	2.40	1.36	1.31
5	L	600	ADP	C5-N7	-2.40	1.34	1.39
5	A	600	ADP	C8-N7	2.39	1.36	1.31
5	N	600	ADP	PA-O3A	2.37	1.62	1.59
5	D	600	ADP	PA-O3A	2.37	1.62	1.59
5	J	600	ADP	C8-N7	2.37	1.36	1.31
5	A	600	ADP	C5-N7	-2.36	1.34	1.39
5	C	600	ADP	C5-N7	-2.33	1.34	1.39
5	M	600	ADP	PA-O3A	2.33	1.62	1.59
5	B	600	ADP	C5-N7	-2.33	1.34	1.39
5	N	600	ADP	C5-N7	-2.32	1.34	1.39
5	N	600	ADP	C8-N7	2.32	1.36	1.31
5	B	600	ADP	C8-N7	2.32	1.36	1.31
5	I	600	ADP	C5-N7	-2.31	1.34	1.39
5	E	600	ADP	C8-N7	2.29	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	600	ADP	C5-N7	-2.28	1.34	1.39
5	D	600	ADP	C8-N7	2.26	1.36	1.31
5	M	600	ADP	C8-N7	2.24	1.36	1.31
5	L	600	ADP	PA-O3A	2.24	1.61	1.59
5	F	600	ADP	C8-N7	2.23	1.36	1.31
5	K	600	ADP	C5-N7	-2.17	1.35	1.39
5	L	600	ADP	C4-N9	-2.08	1.33	1.37
5	C	600	ADP	PA-O3A	2.06	1.61	1.59
5	E	600	ADP	PA-O3A	2.04	1.61	1.59

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	600	ADP	C5-C4-N3	-5.92	118.57	126.72
5	B	600	ADP	C5-C4-N3	-5.90	118.59	126.72
5	C	600	ADP	C5-C4-N3	-5.89	118.61	126.72
5	N	600	ADP	C5-C4-N3	-5.77	118.78	126.72
5	E	600	ADP	C5-C4-N3	-5.76	118.78	126.72
5	I	600	ADP	C5-C4-N3	-5.76	118.79	126.72
5	A	600	ADP	C5-C4-N3	-5.72	118.84	126.72
5	J	600	ADP	C5-C4-N3	-5.71	118.86	126.72
5	F	600	ADP	C5-C4-N3	-5.62	118.98	126.72
5	K	600	ADP	C5-C4-N3	-5.58	119.03	126.72
5	D	600	ADP	C5-C4-N3	-5.51	119.13	126.72
5	L	600	ADP	C5-C4-N3	-5.05	119.76	126.72
5	M	600	ADP	N3-C4-N9	4.72	135.19	127.17
5	E	600	ADP	N3-C4-N9	4.68	135.13	127.17
5	C	600	ADP	N3-C4-N9	4.62	135.02	127.17
5	B	600	ADP	N3-C4-N9	4.61	135.00	127.17
5	I	600	ADP	N3-C4-N9	4.61	135.00	127.17
5	A	600	ADP	N3-C4-N9	4.61	135.00	127.17
5	J	600	ADP	N3-C4-N9	4.58	134.96	127.17
5	N	600	ADP	N3-C4-N9	4.55	134.91	127.17
5	F	600	ADP	N3-C4-N9	4.47	134.76	127.17
5	K	600	ADP	N3-C4-N9	4.46	134.75	127.17
5	D	600	ADP	N3-C4-N9	4.39	134.64	127.17
5	D	600	ADP	N3-C2-N1	-4.00	122.53	128.58
5	J	600	ADP	N3-C2-N1	-4.00	122.53	128.58
5	B	600	ADP	C2-N3-C4	3.99	121.58	111.83
5	C	600	ADP	C2-N3-C4	3.98	121.55	111.83
5	J	600	ADP	C2-N3-C4	3.97	121.53	111.83
5	L	600	ADP	N3-C2-N1	-3.97	122.57	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	600	ADP	N3-C4-N9	3.92	133.83	127.17
5	I	600	ADP	C2-N3-C4	3.91	121.37	111.83
5	B	600	ADP	N3-C2-N1	-3.90	122.68	128.58
5	M	600	ADP	C2-N3-C4	3.89	121.34	111.83
5	K	600	ADP	C2-N3-C4	3.89	121.34	111.83
5	N	600	ADP	C2-N3-C4	3.89	121.33	111.83
5	K	600	ADP	N3-C2-N1	-3.89	122.70	128.58
5	F	600	ADP	N3-C2-N1	-3.88	122.70	128.58
5	E	600	ADP	C2-N3-C4	3.86	121.25	111.83
5	N	600	ADP	N3-C2-N1	-3.84	122.77	128.58
5	A	600	ADP	C2-N3-C4	3.84	121.21	111.83
5	E	600	ADP	N3-C2-N1	-3.83	122.78	128.58
5	F	600	ADP	C2-N3-C4	3.83	121.19	111.83
5	C	600	ADP	N3-C2-N1	-3.83	122.78	128.58
5	I	600	ADP	N3-C2-N1	-3.82	122.79	128.58
5	A	600	ADP	N3-C2-N1	-3.82	122.80	128.58
5	D	600	ADP	C2-N3-C4	3.81	121.14	111.83
5	M	600	ADP	N3-C2-N1	-3.76	122.88	128.58
5	L	600	ADP	C2-N3-C4	3.66	120.77	111.83
5	C	600	ADP	C4-C5-N7	-3.65	106.41	110.58
5	B	600	ADP	C4-C5-N7	-3.57	106.50	110.58
5	K	600	ADP	C4-C5-N7	-3.54	106.53	110.58
5	I	600	ADP	C4-C5-N7	-3.50	106.58	110.58
5	N	600	ADP	C4-C5-N7	-3.50	106.58	110.58
5	L	600	ADP	C4-C5-N7	-3.50	106.58	110.58
5	F	600	ADP	C4-C5-N7	-3.50	106.58	110.58
5	D	600	ADP	C4-C5-N7	-3.47	106.62	110.58
5	M	600	ADP	C4-C5-N7	-3.42	106.67	110.58
5	J	600	ADP	C4-C5-N7	-3.38	106.72	110.58
5	A	600	ADP	C4-C5-N7	-3.36	106.74	110.58
5	E	600	ADP	C4-C5-N7	-3.35	106.75	110.58
5	K	600	ADP	C4-N9-C8	2.93	108.81	105.74
5	C	600	ADP	C5-N7-C8	2.81	107.86	103.45
5	C	600	ADP	C4-N9-C8	2.79	108.67	105.74
5	L	600	ADP	C4-N9-C8	2.71	108.59	105.74
5	I	600	ADP	C4-N9-C8	2.70	108.57	105.74
5	B	600	ADP	C5-N7-C8	2.70	107.69	103.45
5	D	600	ADP	C4-N9-C8	2.67	108.54	105.74
5	N	600	ADP	C5-N7-C8	2.66	107.63	103.45
5	K	600	ADP	C5-N7-C8	2.66	107.63	103.45
5	D	600	ADP	C5-N7-C8	2.65	107.61	103.45
5	I	600	ADP	C5-N7-C8	2.65	107.61	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	600	ADP	C4-N9-C8	2.64	108.51	105.74
5	F	600	ADP	C5-N7-C8	2.63	107.58	103.45
5	L	600	ADP	C5-N7-C8	2.61	107.56	103.45
5	A	600	ADP	C5-N7-C8	2.60	107.54	103.45
5	J	600	ADP	C5-N7-C8	2.59	107.52	103.45
5	A	600	ADP	C4-N9-C8	2.56	108.43	105.74
5	N	600	ADP	C4-N9-C8	2.55	108.42	105.74
5	D	600	ADP	C2'-C1'-N9	-2.54	107.00	113.30
5	M	600	ADP	C5-N7-C8	2.53	107.43	103.45
5	E	600	ADP	C5-N7-C8	2.53	107.42	103.45
5	E	600	ADP	C4-N9-C8	2.49	108.36	105.74
5	F	600	ADP	C4-N9-C8	2.47	108.33	105.74
5	L	600	ADP	C2-N1-C6	2.47	122.78	118.73
5	K	600	ADP	C6-C5-N7	2.46	136.83	132.09
5	L	600	ADP	C2'-C1'-N9	-2.45	107.20	113.30
5	L	600	ADP	C6-C5-N7	2.43	136.77	132.09
5	B	600	ADP	C4-N9-C8	2.39	108.25	105.74
5	M	600	ADP	C4-N9-C8	2.36	108.22	105.74
5	D	600	ADP	C2-N1-C6	2.34	122.57	118.73
5	F	600	ADP	C2-N1-C6	2.33	122.56	118.73
5	C	600	ADP	C6-C5-N7	2.31	136.54	132.09
5	C	600	ADP	N9-C8-N7	-2.29	110.69	113.94
5	I	600	ADP	C6-C5-N7	2.26	136.45	132.09
5	J	600	ADP	C2-N1-C6	2.24	122.41	118.73
5	D	600	ADP	C6-C5-N7	2.24	136.40	132.09
5	B	600	ADP	C6-C5-N7	2.23	136.39	132.09
5	J	600	ADP	C6-C5-N7	2.22	136.37	132.09
5	K	600	ADP	N9-C8-N7	-2.20	110.81	113.94
5	F	600	ADP	C6-C5-N7	2.19	136.31	132.09
5	K	600	ADP	C2-N1-C6	2.18	122.31	118.73
5	A	600	ADP	C2-N1-C6	2.17	122.30	118.73
5	E	600	ADP	C2-N1-C6	2.17	122.30	118.73
5	N	600	ADP	C6-C5-N7	2.17	136.28	132.09
5	L	600	ADP	N9-C8-N7	-2.17	110.86	113.94
5	N	600	ADP	C2-N1-C6	2.15	122.26	118.73
5	B	600	ADP	C2-N1-C6	2.14	122.24	118.73
5	A	600	ADP	C6-C5-N7	2.10	136.15	132.09
5	I	600	ADP	C2-N1-C6	2.10	122.19	118.73
5	M	600	ADP	C2-N1-C6	2.10	122.19	118.73
5	A	600	ADP	C3'-C2'-C1'	2.09	105.41	101.46
5	E	600	ADP	C6-C5-N7	2.08	136.10	132.09
5	D	600	ADP	N9-C8-N7	-2.07	111.00	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	600	ADP	N9-C8-N7	-2.05	111.03	113.94
5	M	600	ADP	C6-C5-N7	2.05	136.04	132.09
5	N	600	ADP	N9-C8-N7	-2.03	111.06	113.94
5	J	600	ADP	N9-C8-N7	-2.02	111.06	113.94
5	L	600	ADP	O4'-C1'-N9	2.00	111.93	108.09

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
7	E	604	GOL	O1-C1-C2-O2
5	C	600	ADP	PA-O3A-PB-O1B
5	D	600	ADP	PA-O3A-PB-O1B
5	A	600	ADP	PB-O3A-PA-O1A
7	E	602	GOL	C1-C2-C3-O3
7	E	604	GOL	O2-C2-C3-O3
5	A	600	ADP	O4'-C4'-C5'-O5'
5	F	600	ADP	PA-O3A-PB-O1B

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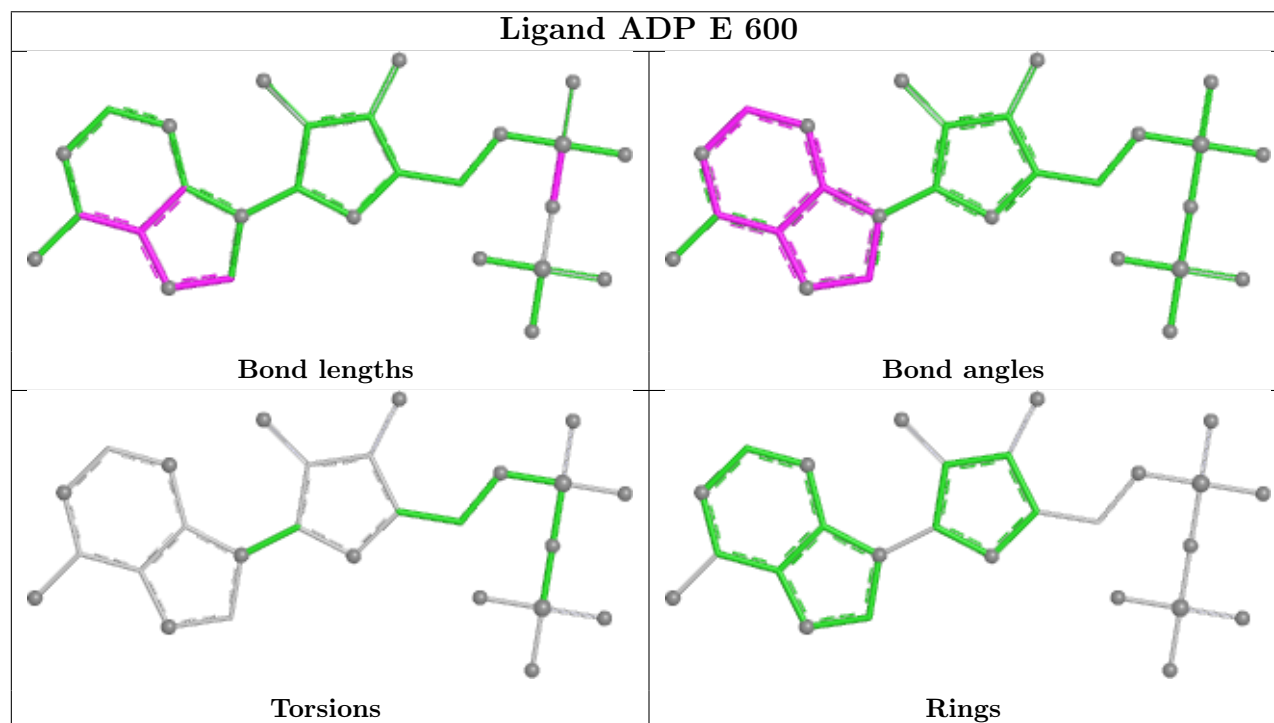
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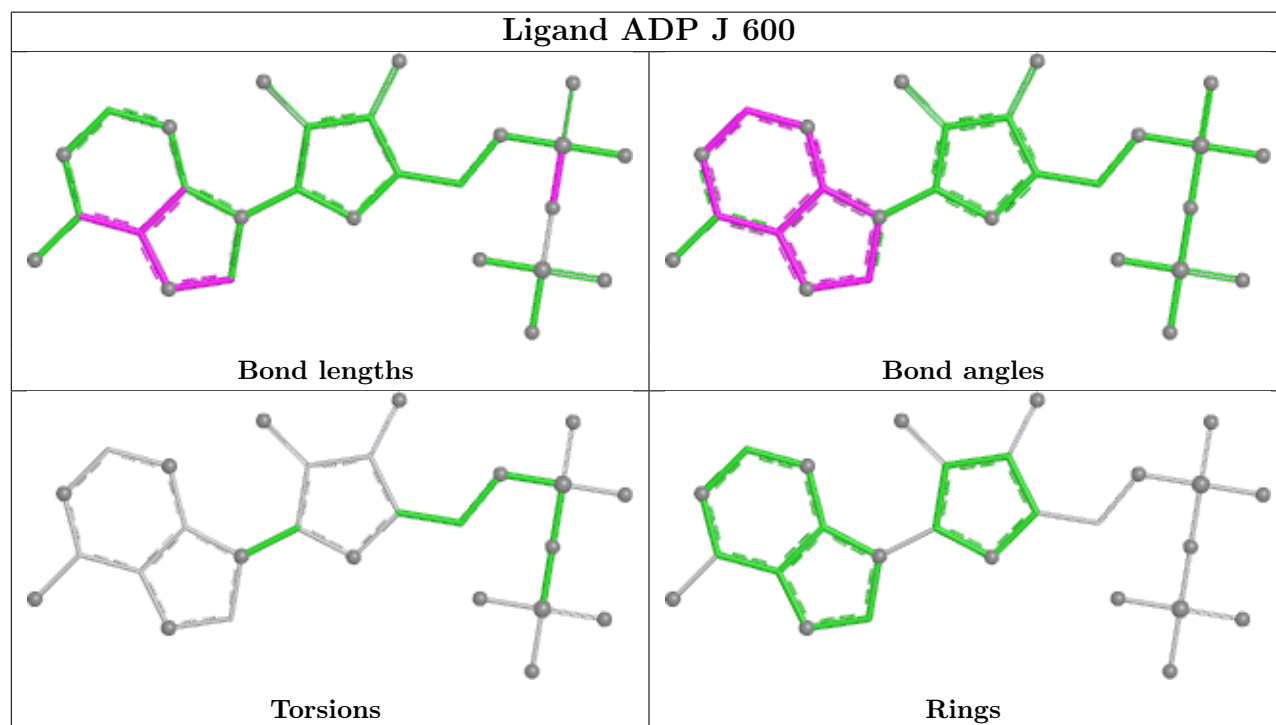
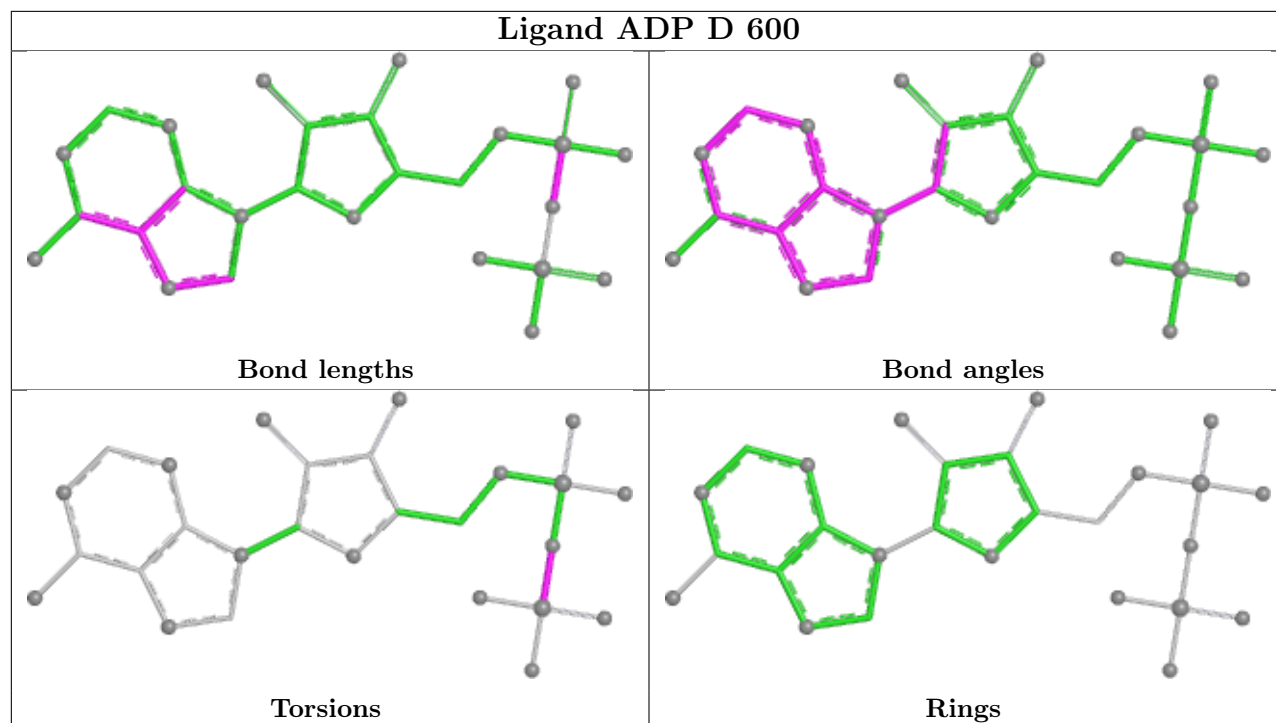
Mol	Chain	Res	Type	Atoms
5	N	600	ADP	PA-O3A-PB-O1B
5	D	600	ADP	PA-O3A-PB-O2B
5	D	600	ADP	PA-O3A-PB-O3B
5	N	600	ADP	PA-O3A-PB-O3B
5	A	600	ADP	PB-O3A-PA-O2A
7	M	605	GOL	O1-C1-C2-C3
7	E	602	GOL	O2-C2-C3-O3

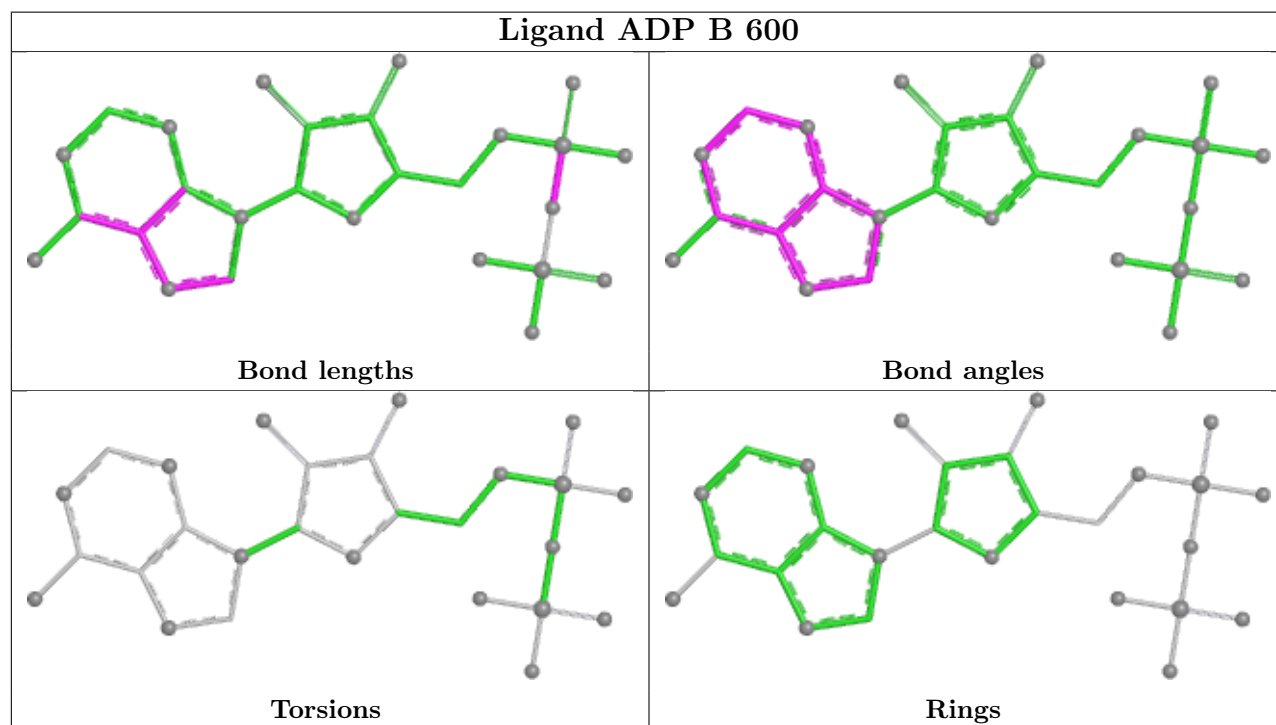
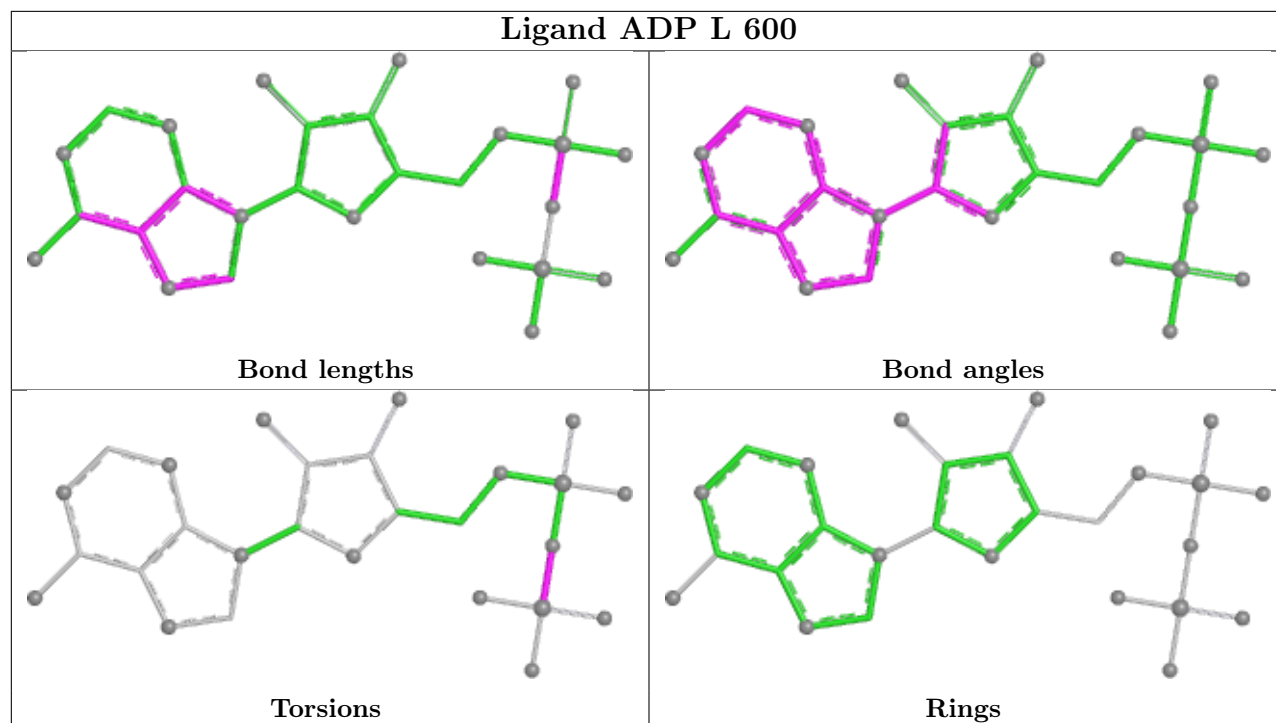
There are no ring outliers.

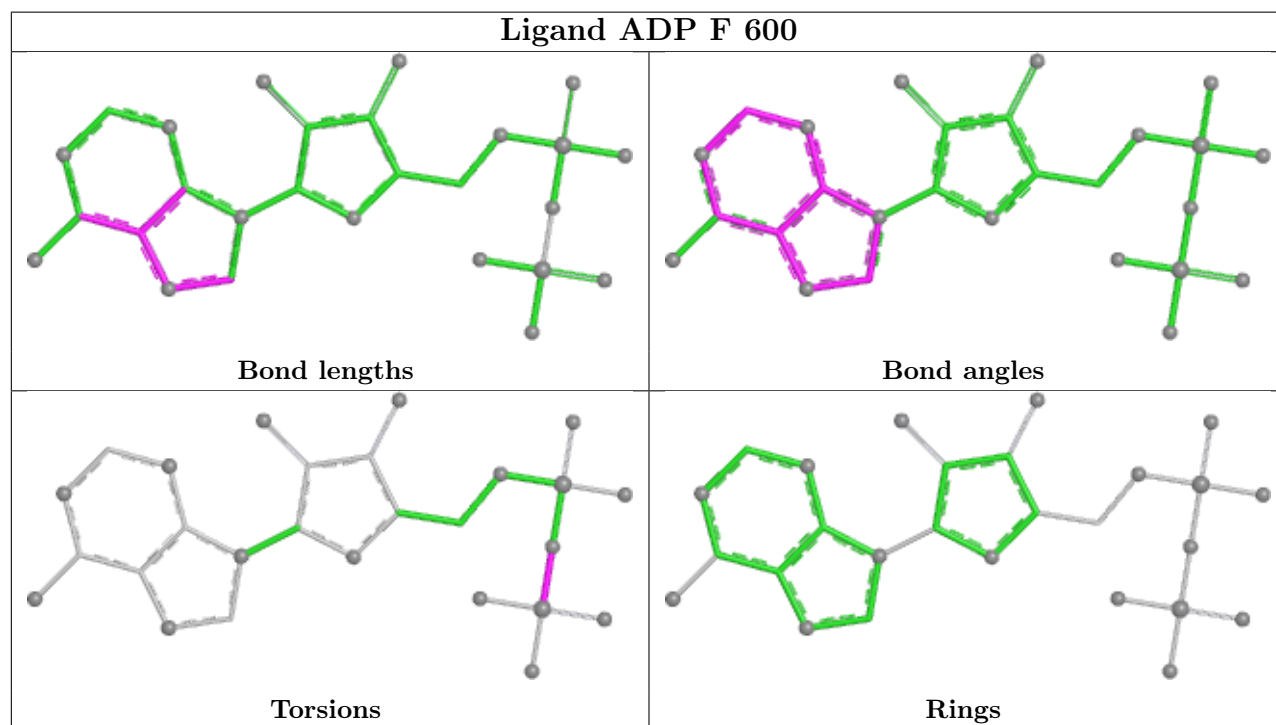
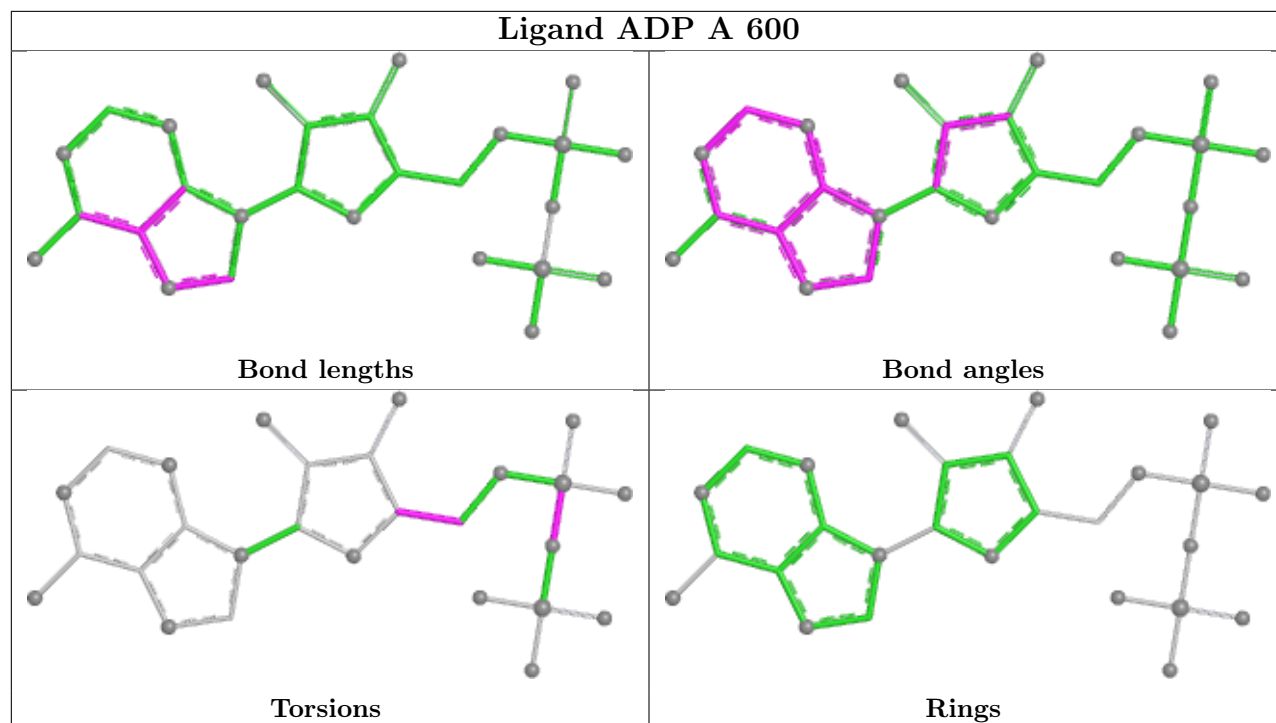
No monomer is involved in short contacts.

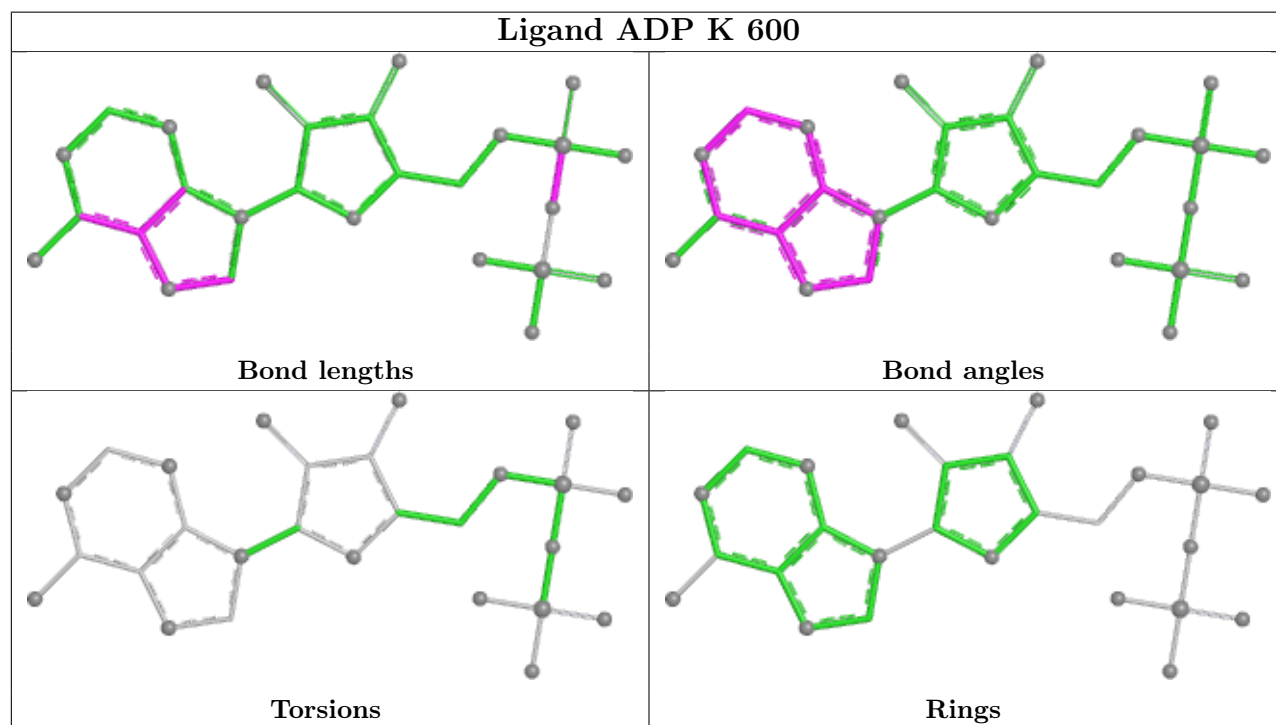
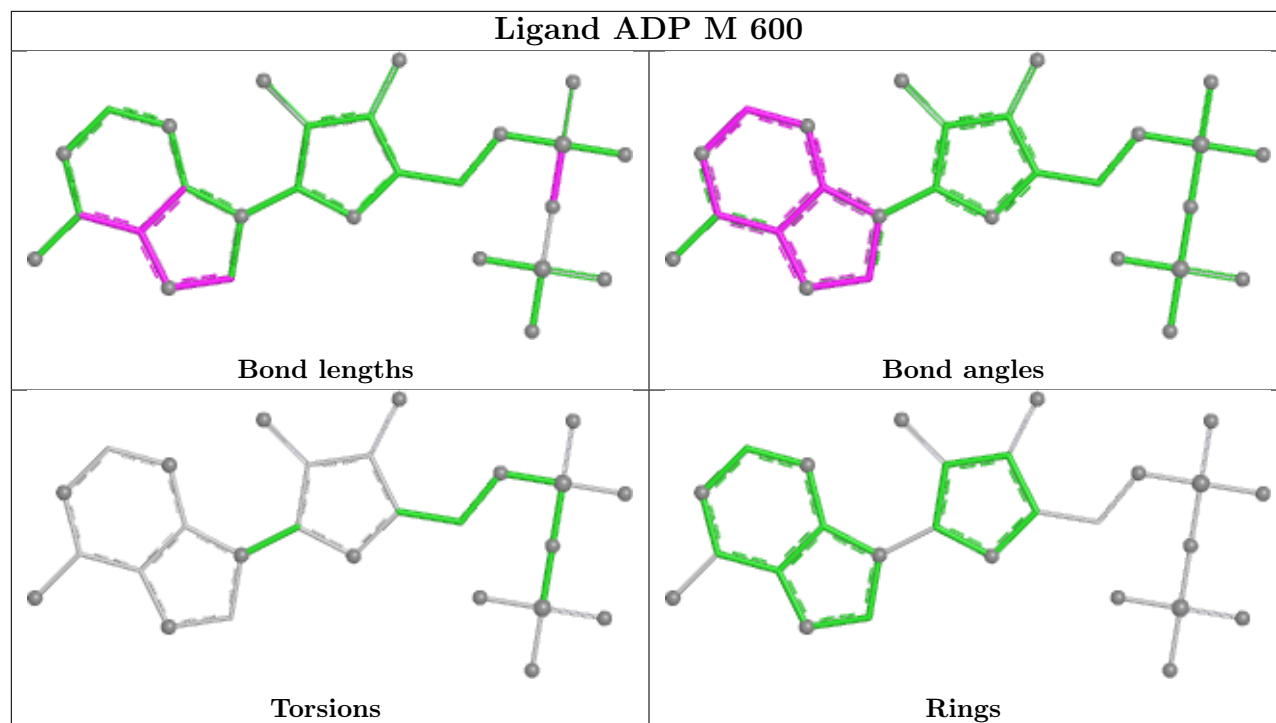
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

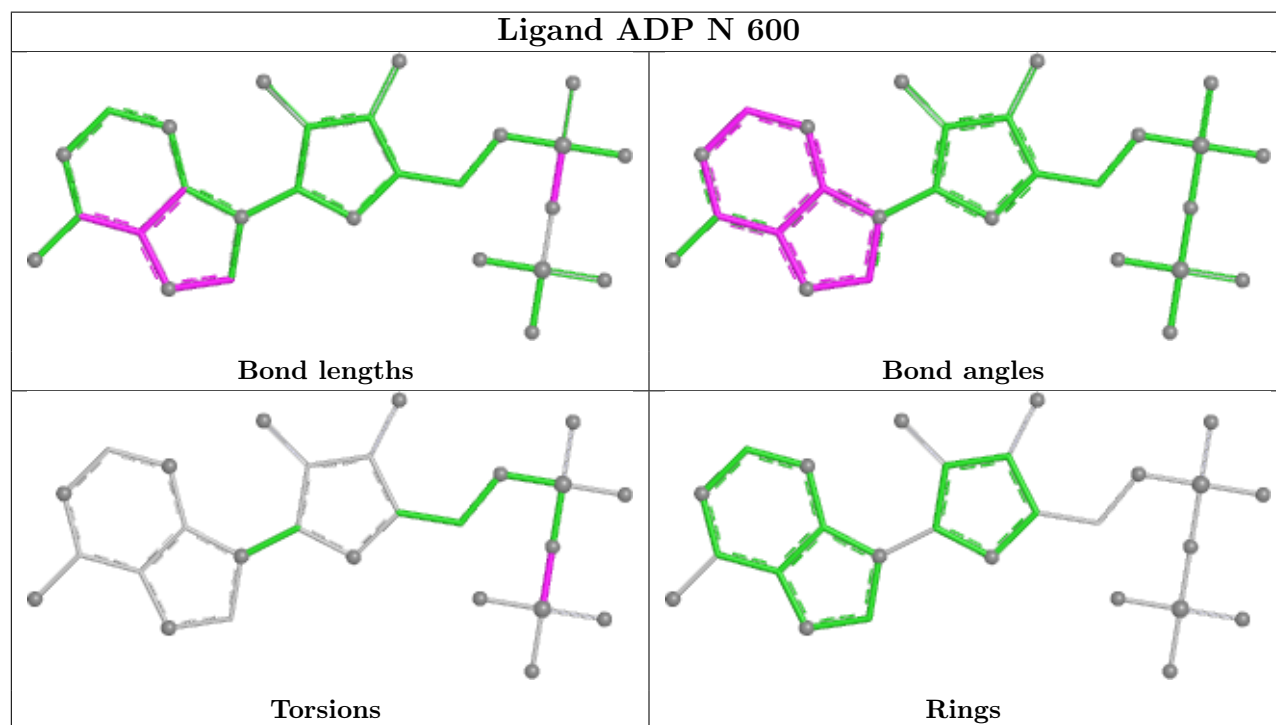
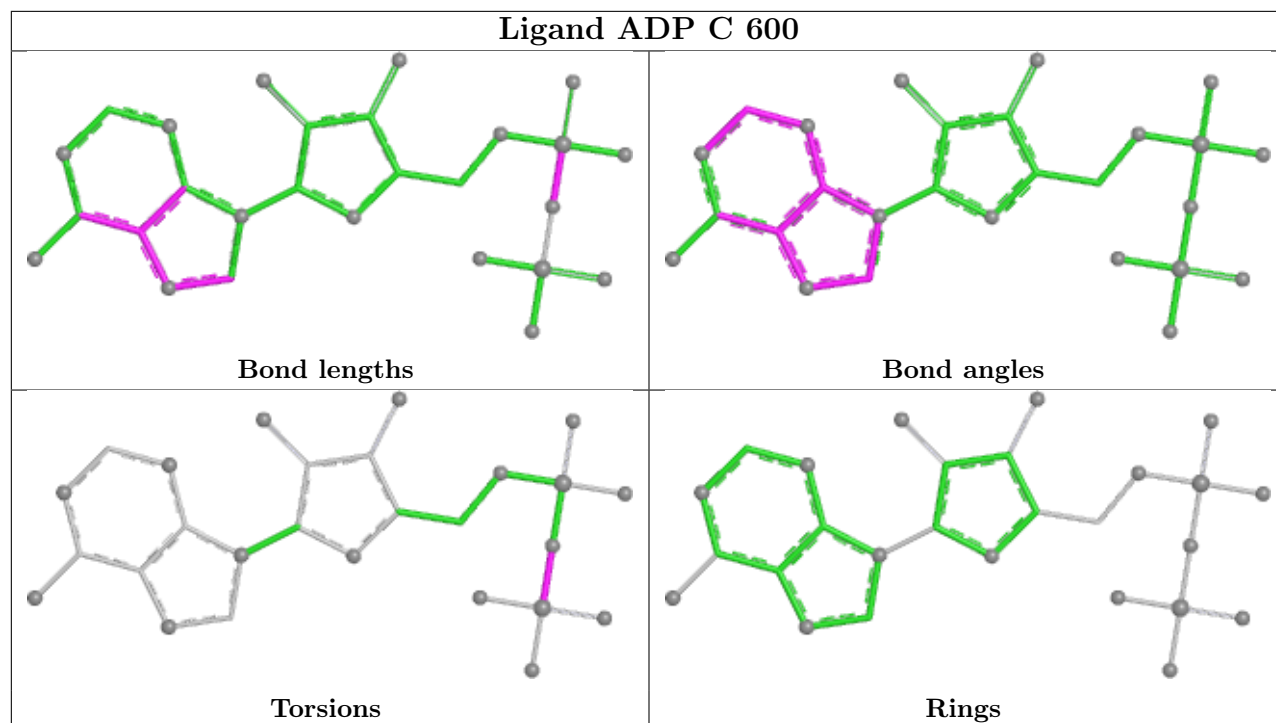


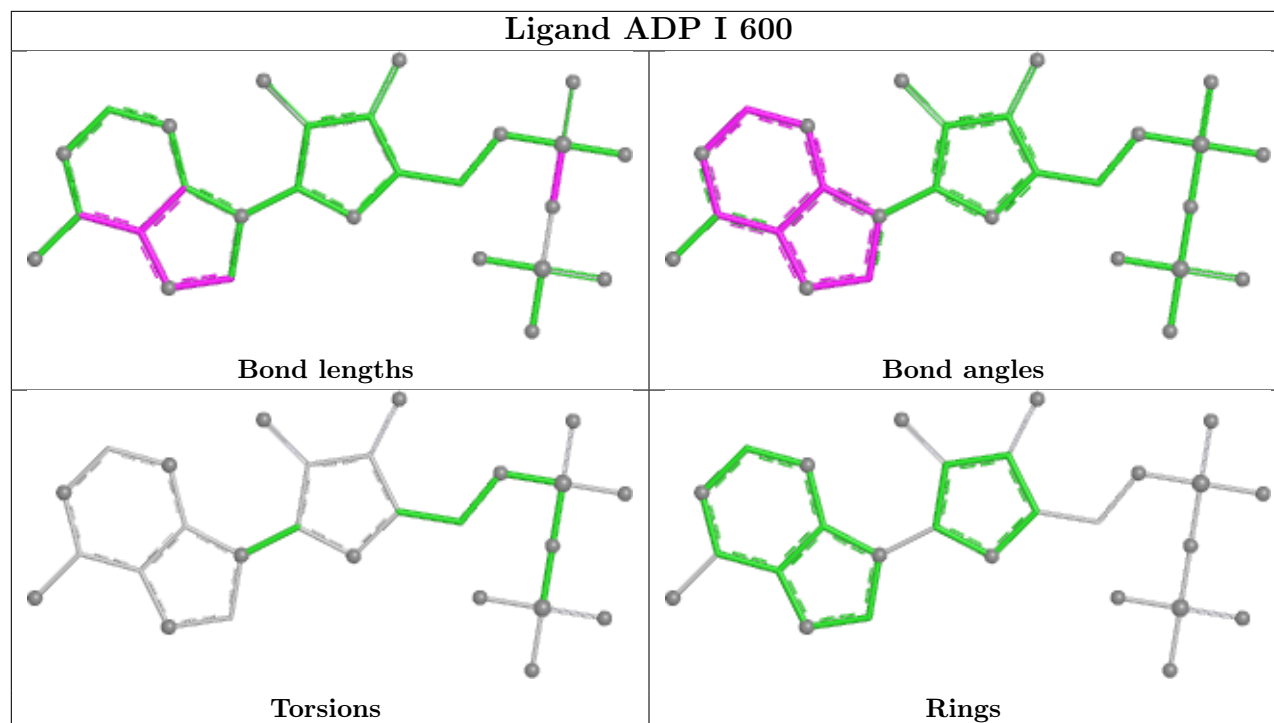












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	475/479 (99%)	0.64	50 (10%) 11 9	16, 40, 86, 115	1 (0%)
1	B	469/479 (97%)	0.24	14 (2%) 52 47	20, 34, 60, 71	0
1	C	475/479 (99%)	0.23	13 (2%) 56 50	22, 33, 57, 84	0
1	I	475/479 (99%)	0.30	28 (5%) 28 23	19, 33, 72, 98	0
1	J	468/479 (97%)	0.24	14 (2%) 52 47	19, 33, 64, 77	0
1	K	476/479 (99%)	-0.01	4 (0%) 82 80	21, 30, 44, 53	0
2	D	461/462 (99%)	0.39	19 (4%) 41 36	27, 39, 59, 83	0
2	E	462/462 (100%)	0.16	12 (2%) 57 51	14, 32, 53, 73	1 (0%)
2	F	462/462 (100%)	0.21	11 (2%) 59 54	22, 34, 55, 67	0
2	L	462/462 (100%)	0.20	11 (2%) 59 54	21, 33, 53, 67	0
2	M	462/462 (100%)	0.06	14 (3%) 52 47	15, 30, 55, 76	1 (0%)
2	N	462/462 (100%)	0.17	12 (2%) 57 51	20, 32, 54, 66	0
3	G	285/285 (100%)	0.40	11 (3%) 43 38	24, 38, 57, 75	0
3	O	285/285 (100%)	0.32	9 (3%) 50 44	24, 34, 55, 72	0
4	H	132/134 (98%)	0.36	10 (7%) 20 16	27, 37, 63, 72	0
4	P	134/134 (100%)	0.60	12 (8%) 15 11	33, 43, 66, 76	0
All	All	6445/6484 (99%)	0.26	244 (3%) 44 38	14, 34, 60, 115	3 (0%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	P	1	MET	5.1
1	A	398	PHE	4.9
2	M	379	ILE	4.9
1	A	394	ALA	4.9
1	K	399	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	378	ALA	4.8
1	J	406	THR	4.7
2	F	412	GLN	4.5
1	C	26	VAL	4.4
1	A	395	PHE	4.3
2	D	376	ILE	4.3
4	P	72	PRO	4.1
1	A	399	GLY	4.0
2	L	376	ILE	4.0
2	L	375	ASP	4.0
1	I	384	LEU	3.9
1	A	384	LEU	3.9
1	A	396	ALA	3.9
2	D	375	ASP	3.8
1	C	402	LEU	3.7
2	D	381	GLY	3.7
2	L	379	ILE	3.7
1	I	406	THR	3.6
2	D	379	ILE	3.6
1	I	447	ASP	3.6
1	A	496	LYS	3.6
1	I	398	PHE	3.6
1	I	392	LEU	3.5
1	A	400	SER	3.5
1	B	395	PHE	3.5
4	H	110	THR	3.4
2	D	377	ILE	3.4
1	A	498	PHE	3.4
1	I	381	THR	3.4
1	I	405	ALA	3.3
1	B	26	VAL	3.3
2	E	379	ILE	3.3
2	N	412	GLN	3.3
1	A	383	ARG	3.2
2	L	237	GLY	3.2
2	D	36	GLN	3.2
1	I	400	SER	3.2
2	N	1	MET	3.1
1	A	380	GLY	3.1
3	O	3	GLY	3.1
2	L	5	ARG	3.1
2	M	378	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	404	LYS	3.1
1	I	402	LEU	3.1
2	F	414	THR	3.1
1	A	468	LYS	3.1
2	M	377	ILE	3.0
1	C	70	ASN	3.0
2	E	1	MET	3.0
1	B	443	GLY	3.0
1	A	494	PHE	3.0
1	C	327	SER	2.9
3	G	61	LYS	2.9
1	B	404	LYS	2.9
1	A	401	ASP	2.9
2	M	385	LEU	2.9
1	A	497	GLY	2.9
1	J	392	LEU	2.9
3	O	108	GLN	2.9
2	N	2	ASN	2.9
1	B	478	THR	2.9
1	A	405	ALA	2.9
2	E	380	LEU	2.9
1	A	213	ARG	2.8
1	A	390	ARG	2.8
1	I	395	PHE	2.8
4	H	134	LYS	2.8
1	I	501	SER	2.8
1	I	382	LEU	2.8
2	M	415	GLY	2.8
1	A	385	ASP	2.8
1	A	381	THR	2.8
1	J	484	THR	2.8
1	A	397	GLN	2.7
1	A	28	VAL	2.7
4	P	111	ASP	2.7
2	N	170	GLN	2.7
1	J	384	LEU	2.7
1	I	383	ARG	2.7
1	J	405	ALA	2.7
2	L	383	ASP	2.7
4	P	134	LYS	2.7
1	I	399	GLY	2.7
1	J	403	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
3	G	62	ASP	2.7
1	C	79	TYR	2.7
3	O	286	ARG	2.7
1	A	387	ALA	2.7
1	C	406	THR	2.7
1	A	402	LEU	2.6
1	B	392	LEU	2.6
1	J	462	SER	2.6
2	F	413	PHE	2.6
1	C	323	ALA	2.6
1	A	500	PRO	2.6
1	B	70	ASN	2.6
1	A	409	LYS	2.6
1	A	451	GLU	2.6
2	F	105	ALA	2.6
2	N	413	PHE	2.6
1	I	408	ALA	2.5
1	A	483	ASP	2.5
1	B	69	ASP	2.5
1	A	392	LEU	2.5
2	L	4	GLY	2.5
2	F	1	MET	2.5
2	E	388	GLU	2.5
2	N	4	GLY	2.5
2	L	1	MET	2.5
1	A	406	THR	2.5
2	M	461	LYS	2.5
4	H	111	ASP	2.5
3	O	59	GLY	2.5
1	A	386	LEU	2.4
2	D	176	SER	2.4
1	A	117	GLY	2.4
1	C	28	VAL	2.4
1	C	502	ALA	2.4
2	D	5	ARG	2.4
1	J	65	ASN	2.4
2	M	376	ILE	2.4
3	G	3	GLY	2.4
1	I	387	ALA	2.4
1	I	394	ALA	2.4
2	E	378	ALA	2.4
4	P	2	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	380	LEU	2.4
2	D	104	ASN	2.4
1	A	449	PRO	2.4
1	A	495	LYS	2.4
1	J	485	LYS	2.4
1	A	439	ALA	2.4
1	A	466	ALA	2.4
1	J	463	PHE	2.4
2	M	413	PHE	2.4
2	F	444	GLU	2.4
2	E	416	MET	2.4
1	J	404	LYS	2.4
1	I	443	GLY	2.4
3	O	63	PHE	2.4
2	N	462	LEU	2.3
2	D	384	GLU	2.3
2	D	125	ASP	2.3
4	H	108	ASP	2.3
2	D	238	GLN	2.3
3	G	2	GLN	2.3
2	L	385	LEU	2.3
3	O	61	LYS	2.3
1	A	470	SER	2.3
4	H	133	SER	2.3
1	I	390	ARG	2.3
1	C	398	PHE	2.3
2	F	440	ASN	2.3
1	A	501	SER	2.3
1	I	401	ASP	2.3
2	M	383	ASP	2.3
4	P	133	SER	2.3
2	L	100	GLN	2.3
2	E	423	VAL	2.3
1	A	475	ILE	2.3
3	O	194	GLU	2.3
1	A	296[A]	ARG	2.3
3	G	33	ARG	2.3
3	G	286	ARG	2.3
1	A	485	LYS	2.2
4	H	112	LYS	2.2
4	P	110	THR	2.2
2	N	444	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	2	ASN	2.2
1	I	385	ASP	2.2
2	D	237	GLY	2.2
2	M	382	MET	2.2
3	G	108	GLN	2.2
2	E	353	GLY	2.2
1	I	499	THR	2.2
4	P	71	ARG	2.2
2	E	104	ASN	2.2
1	A	447	ASP	2.2
1	I	409	LYS	2.2
2	F	101	GLY	2.2
4	P	115	LEU	2.2
1	A	411	ASN	2.2
1	A	467	ASN	2.2
1	K	397	GLN	2.2
2	N	461	LYS	2.2
2	M	462	LEU	2.2
2	D	239	ASP	2.2
2	M	389	ASP	2.2
2	D	171	GLU	2.1
2	F	106	GLU	2.1
1	A	382	LEU	2.1
3	G	26	MET	2.1
4	H	104	LEU	2.1
2	E	415	GLY	2.1
1	C	190	ASP	2.1
2	E	377	ILE	2.1
2	F	103	VAL	2.1
1	B	394	ALA	2.1
1	K	502	ALA	2.1
1	C	27	GLU	2.1
1	K	332	THR	2.1
3	G	22	LYS	2.1
4	P	105	LYS	2.1
1	I	397	GLN	2.1
1	A	487	LEU	2.1
2	D	462	LEU	2.1
2	N	416	MET	2.1
4	H	115	LEU	2.1
1	I	29	GLY	2.1
1	B	466	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	410	ALA	2.1
3	G	70	ALA	2.1
2	M	386	SER	2.1
3	G	211	GLU	2.1
3	O	203	ALA	2.1
2	M	424	LYS	2.1
1	B	406	THR	2.1
1	B	416	THR	2.1
2	N	414	THR	2.1
1	C	64	GLN	2.1
1	A	481	LEU	2.1
1	B	481	LEU	2.1
4	H	39	ILE	2.1
4	P	114	TYR	2.1
1	B	403	ASP	2.0
1	J	190	ASP	2.0
2	N	125	ASP	2.0
4	H	73	ASP	2.0
4	P	108	ASP	2.0
1	A	95	MET	2.0
1	J	500	PRO	2.0
2	F	416	MET	2.0
1	J	388	GLN	2.0
2	D	103	VAL	2.0
3	O	62	ASP	2.0
1	I	351	SER	2.0
1	A	60	MET	2.0
1	I	388	GLN	2.0
1	I	28	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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.

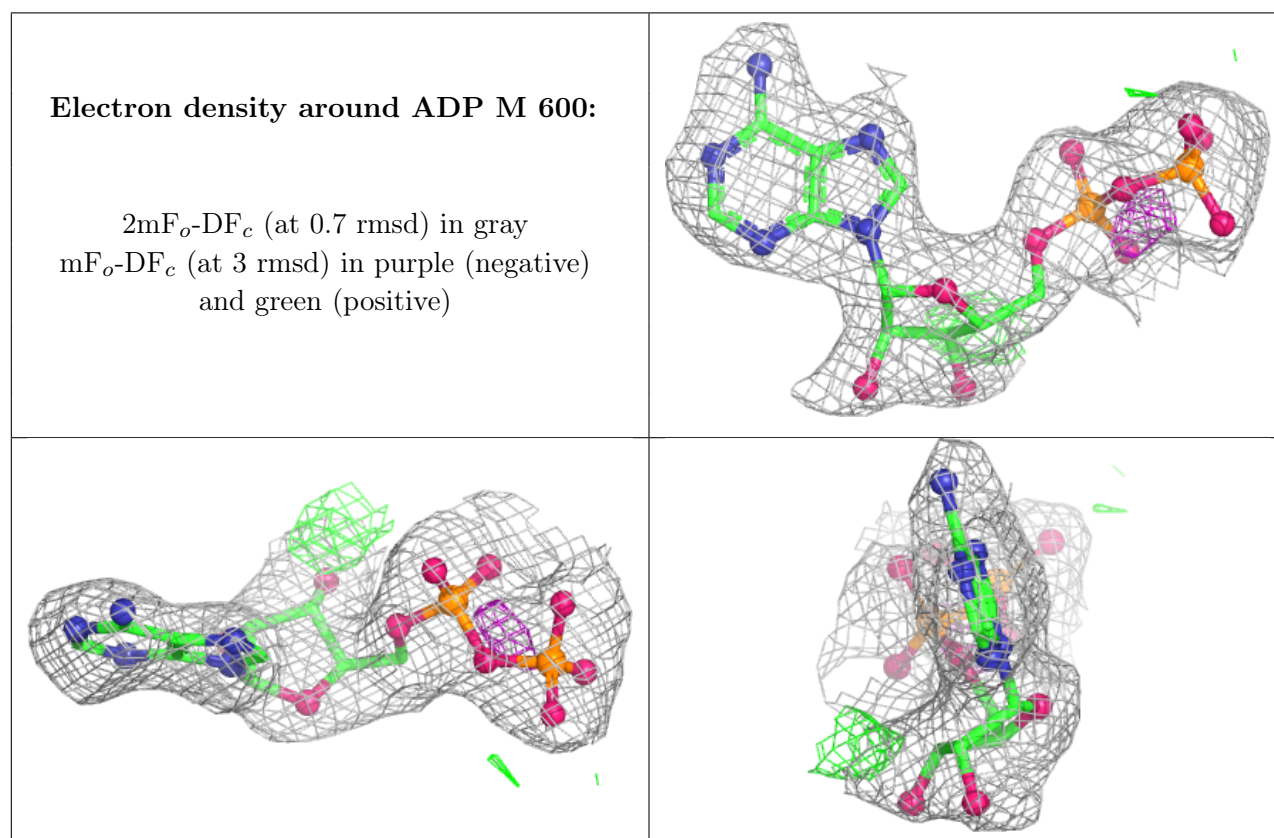
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	E	604	6/6	0.78	0.22	42,43,44,44	0
6	MG	C	601	1/1	0.81	0.13	24,24,24,24	0
6	MG	N	602	1/1	0.82	0.14	22,22,22,22	0
6	MG	K	601	1/1	0.83	0.17	20,20,20,20	0
7	GOL	N	604	6/6	0.84	0.17	32,32,32,32	0
7	GOL	M	604	6/6	0.85	0.14	27,27,27,27	0
6	MG	I	601	1/1	0.85	0.13	23,23,23,23	0
7	GOL	E	603	6/6	0.86	0.18	37,37,37,37	0
6	MG	J	601	1/1	0.86	0.17	23,23,23,23	0
7	GOL	A	602	6/6	0.87	0.12	26,26,26,27	0
8	PO4	M	602	5/5	0.87	0.15	48,48,49,49	0
7	GOL	E	602	6/6	0.88	0.14	28,29,29,29	0
6	MG	L	601	1/1	0.88	0.11	25,25,25,25	0
8	PO4	E	601	5/5	0.88	0.14	55,55,56,56	0
7	GOL	C	602	6/6	0.88	0.14	34,35,35,36	0
6	MG	F	601	1/1	0.89	0.20	22,22,22,22	0
7	GOL	J	602	6/6	0.89	0.15	38,39,39,39	0
7	GOL	N	603	6/6	0.90	0.13	40,40,41,41	0
7	GOL	M	603	6/6	0.90	0.11	36,36,37,37	0
6	MG	D	601	1/1	0.90	0.18	30,30,30,30	0
7	GOL	M	606	6/6	0.90	0.12	23,23,23,24	0
7	GOL	F	602	6/6	0.91	0.11	29,29,30,30	0
7	GOL	B	602	6/6	0.92	0.10	34,35,35,35	0
7	GOL	K	602	6/6	0.92	0.13	31,32,32,32	0
5	ADP	M	600	27/27	0.92	0.10	40,41,42,42	0
7	GOL	M	605	6/6	0.95	0.09	28,28,28,28	0
5	ADP	A	600	27/27	0.95	0.08	31,34,36,36	0
5	ADP	E	600	27/27	0.95	0.08	36,36,38,38	0
5	ADP	L	600	27/27	0.96	0.07	25,26,26,26	0
5	ADP	D	600	27/27	0.96	0.07	28,29,29,29	0
5	ADP	J	600	27/27	0.96	0.07	23,24,25,26	0
6	MG	A	601	1/1	0.97	0.05	31,31,31,31	0
7	GOL	I	602	6/6	0.97	0.06	18,18,18,18	0
5	ADP	I	600	27/27	0.97	0.06	24,27,28,28	0
5	ADP	B	600	27/27	0.97	0.07	23,24,25,25	0
5	ADP	C	600	27/27	0.97	0.07	22,22,23,23	0
5	ADP	F	600	27/27	0.97	0.07	22,24,25,25	0

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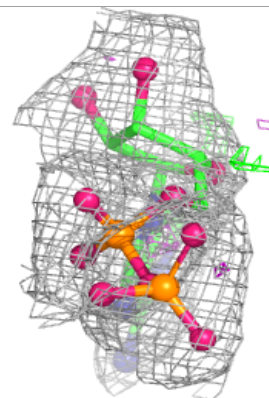
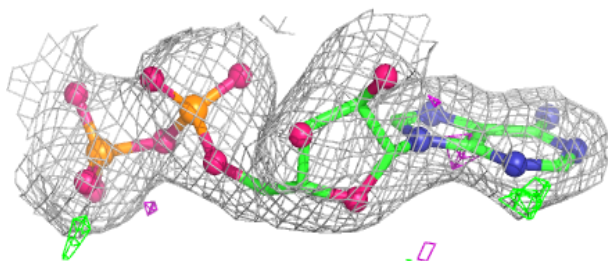
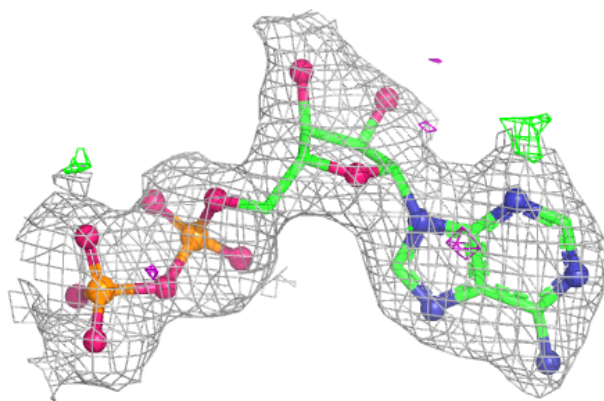
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ADP	N	600	27/27	0.98	0.06	22,24,25,26	0
5	ADP	K	600	27/27	0.98	0.06	20,20,20,20	0
6	MG	B	601	1/1	0.99	0.07	23,23,23,23	0

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.

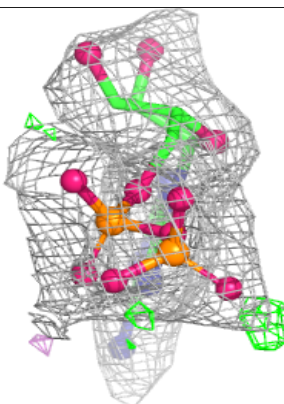
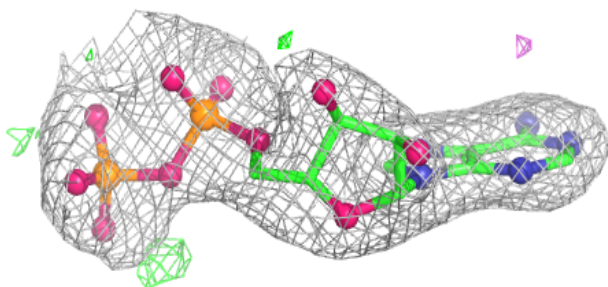
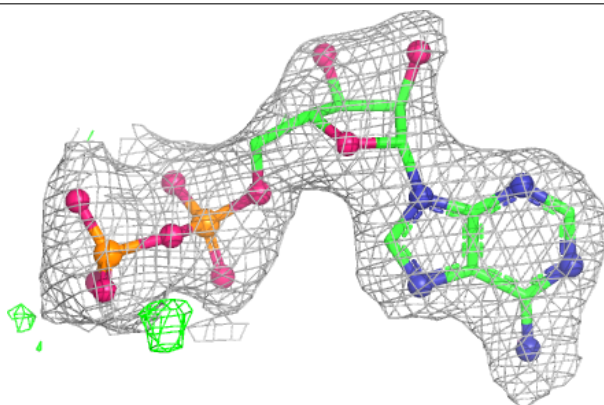


Electron density around ADP A 600:

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

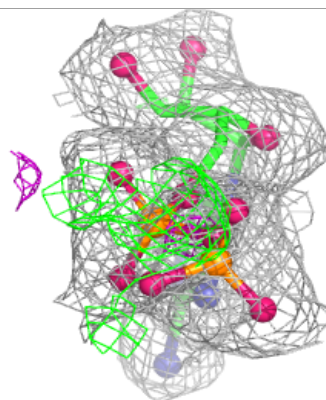
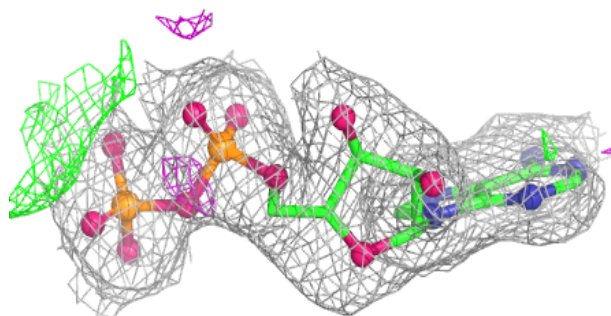
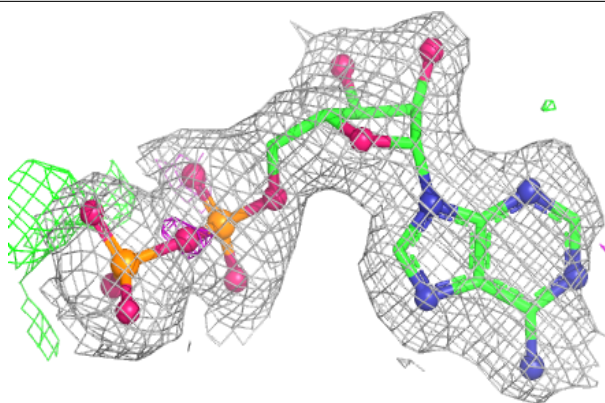
**Electron density around ADP E 600:**

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

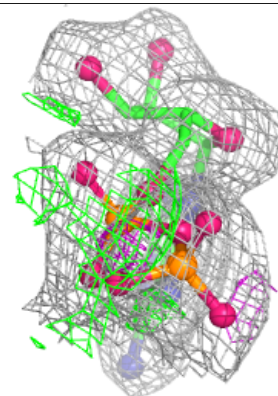
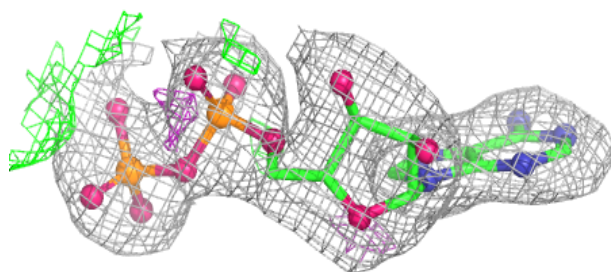
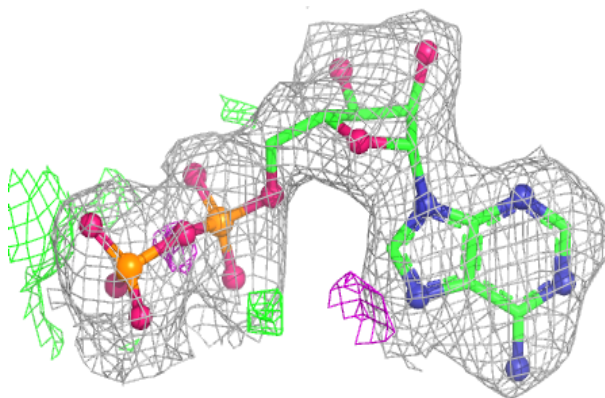


Electron density around ADP L 600:

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

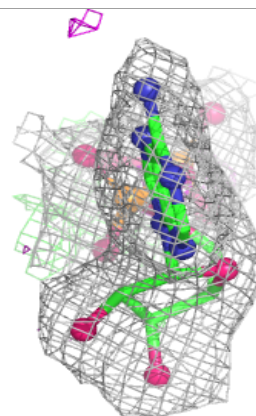
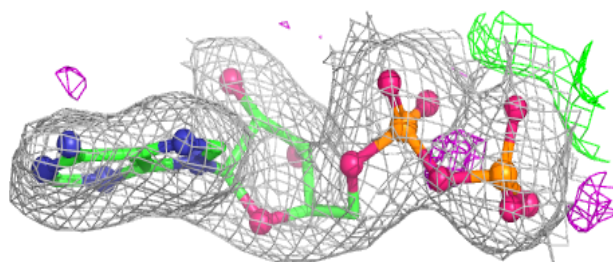
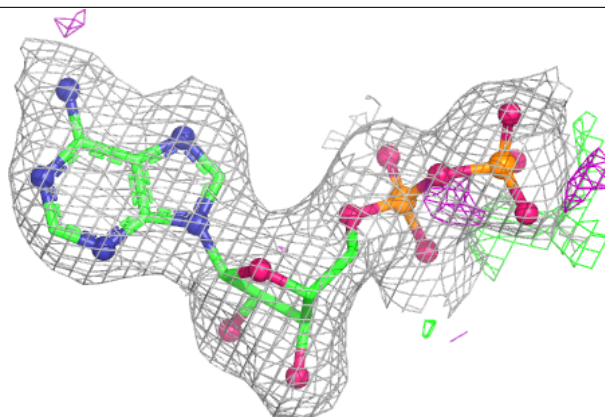
**Electron density around ADP D 600:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

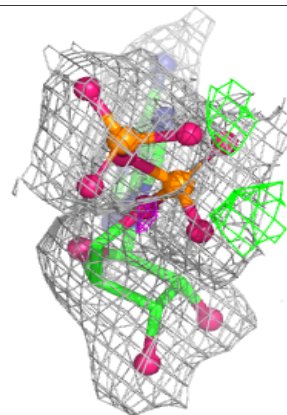
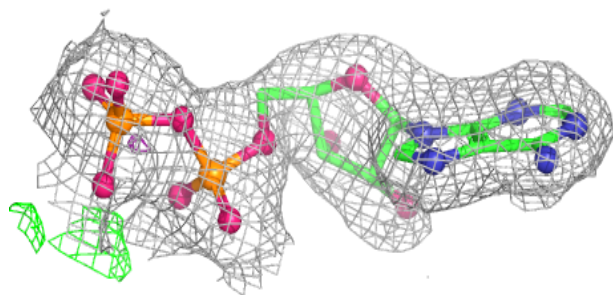
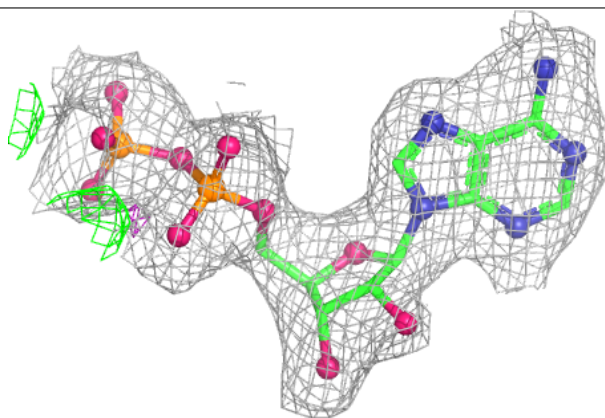


Electron density around ADP J 600:

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

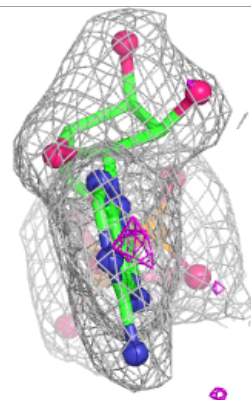
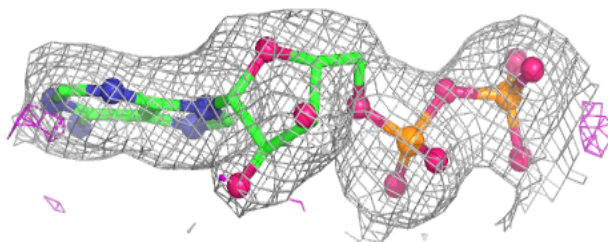
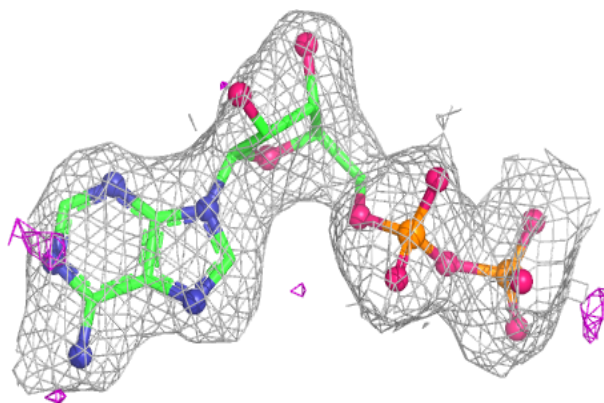
**Electron density around ADP I 600:**

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

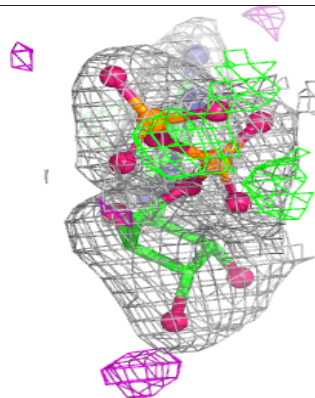
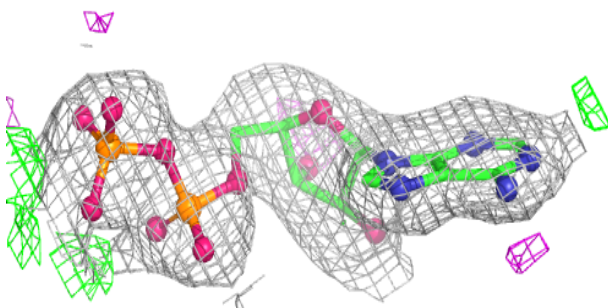
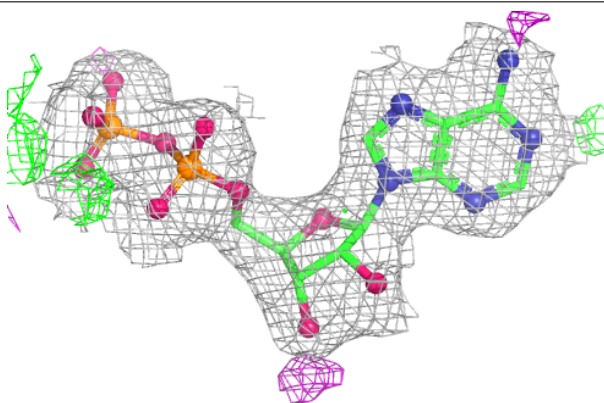


Electron density around ADP B 600:

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

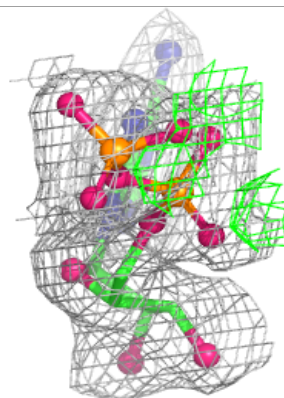
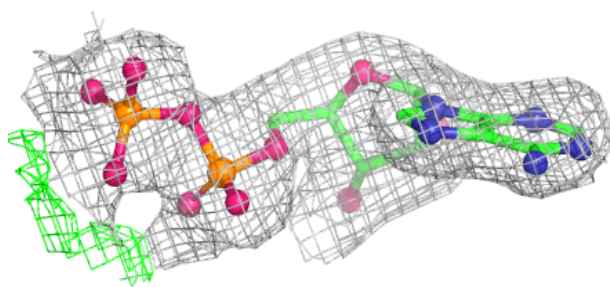
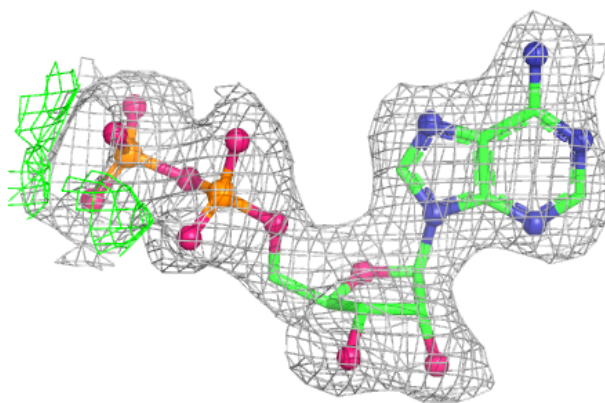
**Electron density around ADP C 600:**

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

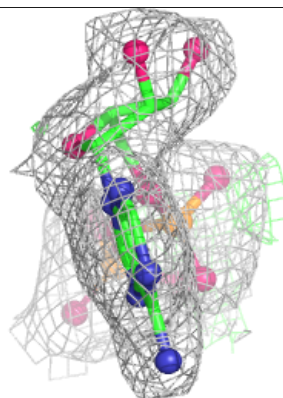
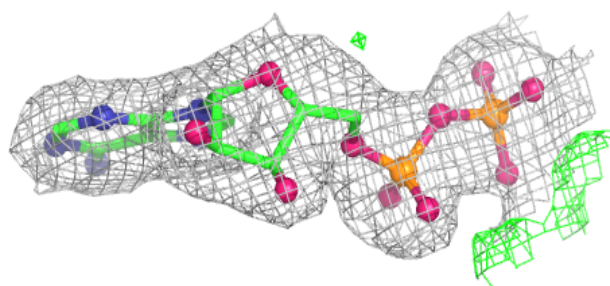
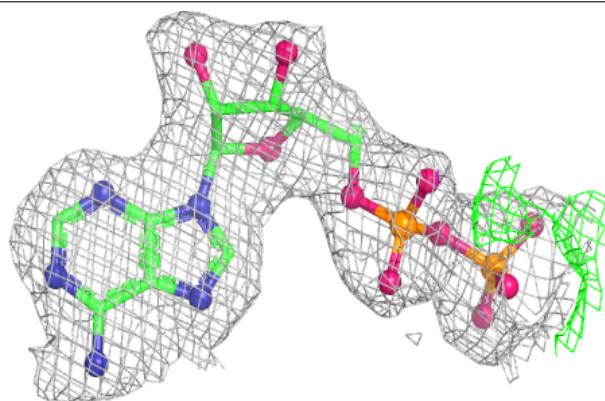


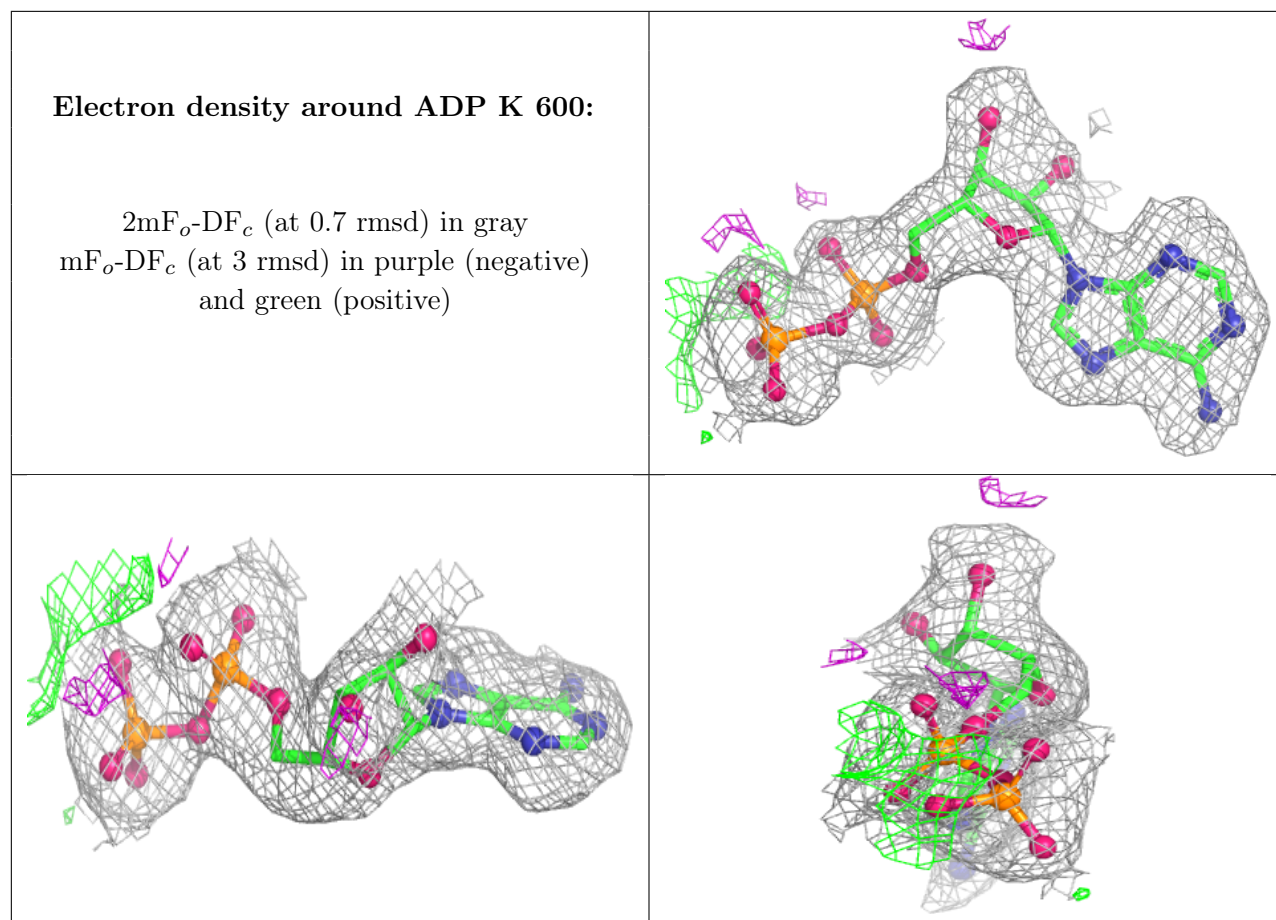
Electron density around ADP F 600:

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

**Electron density around ADP 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 ⓘ

There are no such residues in this entry.