



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2024 – 07:43 PM EST

PDB ID : 1S4E
Title : Pyrococcus furiosus galactokinase in complex with galactose, ADP and magnesium
Authors : Hartley, A.; Glynn, S.E.; Barynin, V.; Baker, P.J.; Sedelnikova, S.E.; Verhees, C.; de Geus, D.; van der Oost, J.; Timson, D.J.; Reece, R.J.; Rice, D.W.
Deposited on : 2004-01-16
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

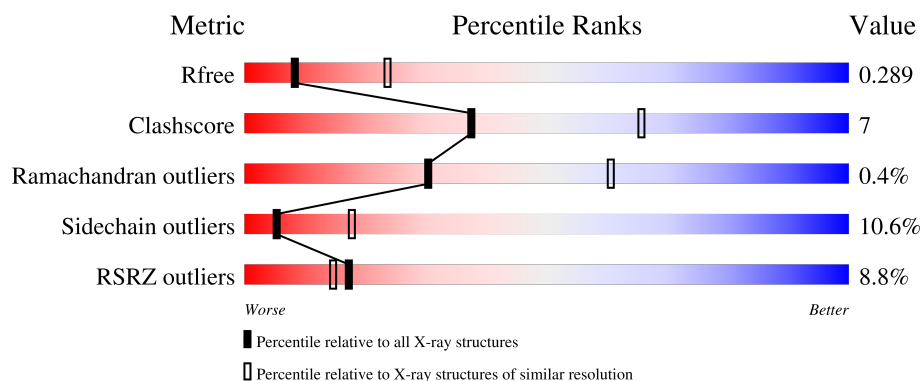
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	352	
1	B	352	
1	C	352	
1	D	352	

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Mol	Chain	Length	Quality of chain
1	E	352	
1	F	352	
1	G	352	
1	H	352	
1	I	352	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLA	E	4500	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22711 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 Galactokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	Se	0	0	0
			2554	1660	410	479	2	3			
1	B	310	Total	C	N	O	S	Se	0	0	0
			2266	1463	368	430	2	3			
1	C	337	Total	C	N	O	S	Se	0	0	0
			2419	1564	396	454	2	3			
1	D	349	Total	C	N	O	S	Se	0	0	0
			2643	1715	420	503	2	3			
1	E	346	Total	C	N	O	S	Se	0	0	0
			2616	1703	414	494	2	3			
1	F	351	Total	C	N	O	S	Se	0	0	0
			2722	1769	433	515	2	3			
1	G	255	Total	C	N	O	S	Se	0	0	0
			1811	1157	303	346	2	3			
1	H	347	Total	C	N	O	S	Se	0	0	0
			2652	1728	422	497	2	3			
1	I	351	Total	C	N	O	S	Se	0	0	0
			2668	1741	416	506	2	3			

There are 36 discrepancies between the modelled and reference sequences:

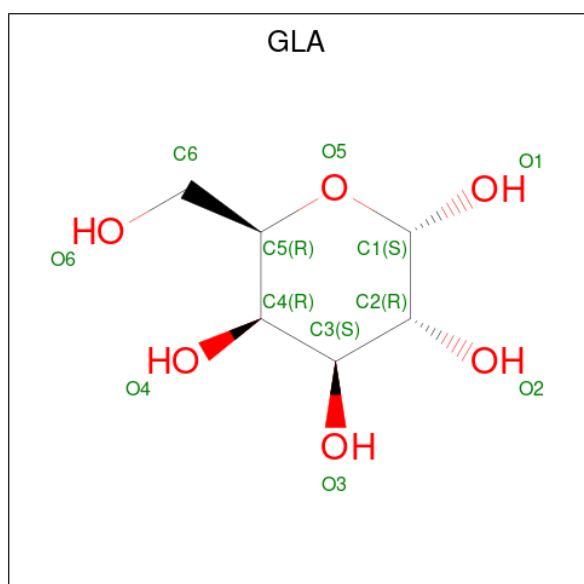
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9HHB6
A	27	MSE	MET	modified residue	UNP Q9HHB6
A	29	MSE	MET	modified residue	UNP Q9HHB6
A	293	MSE	MET	modified residue	UNP Q9HHB6
B	1	MSE	MET	modified residue	UNP Q9HHB6
B	27	MSE	MET	modified residue	UNP Q9HHB6
B	29	MSE	MET	modified residue	UNP Q9HHB6
B	293	MSE	MET	modified residue	UNP Q9HHB6
C	1	MSE	MET	modified residue	UNP Q9HHB6
C	27	MSE	MET	modified residue	UNP Q9HHB6
C	29	MSE	MET	modified residue	UNP Q9HHB6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	293	MSE	MET	modified residue	UNP Q9HHB6
D	1	MSE	MET	modified residue	UNP Q9HHB6
D	27	MSE	MET	modified residue	UNP Q9HHB6
D	29	MSE	MET	modified residue	UNP Q9HHB6
D	293	MSE	MET	modified residue	UNP Q9HHB6
E	1	MSE	MET	modified residue	UNP Q9HHB6
E	27	MSE	MET	modified residue	UNP Q9HHB6
E	29	MSE	MET	modified residue	UNP Q9HHB6
E	293	MSE	MET	modified residue	UNP Q9HHB6
F	1	MSE	MET	modified residue	UNP Q9HHB6
F	27	MSE	MET	modified residue	UNP Q9HHB6
F	29	MSE	MET	modified residue	UNP Q9HHB6
F	293	MSE	MET	modified residue	UNP Q9HHB6
G	1	MSE	MET	modified residue	UNP Q9HHB6
G	27	MSE	MET	modified residue	UNP Q9HHB6
G	29	MSE	MET	modified residue	UNP Q9HHB6
G	293	MSE	MET	modified residue	UNP Q9HHB6
H	1	MSE	MET	modified residue	UNP Q9HHB6
H	27	MSE	MET	modified residue	UNP Q9HHB6
H	29	MSE	MET	modified residue	UNP Q9HHB6
H	293	MSE	MET	modified residue	UNP Q9HHB6
I	1	MSE	MET	modified residue	UNP Q9HHB6
I	27	MSE	MET	modified residue	UNP Q9HHB6
I	29	MSE	MET	modified residue	UNP Q9HHB6
I	293	MSE	MET	modified residue	UNP Q9HHB6

- Molecule 2 is alpha-D-galactopyranose (three-letter code: GLA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0
2	E	1	Total C O 12 6 6	0	0
2	F	1	Total C O 12 6 6	0	0
2	G	1	Total C O 12 6 6	0	0
2	H	1	Total C O 12 6 6	0	0
2	I	1	Total C O 12 6 6	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

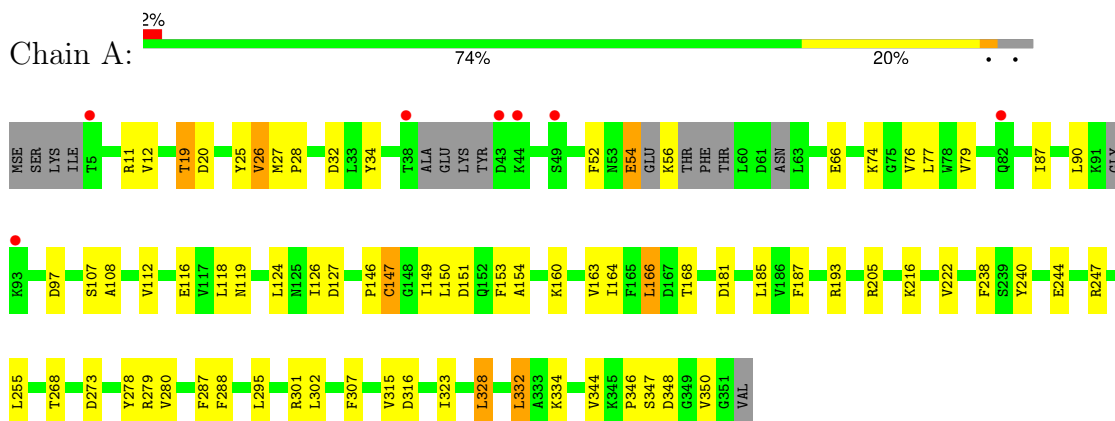


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G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

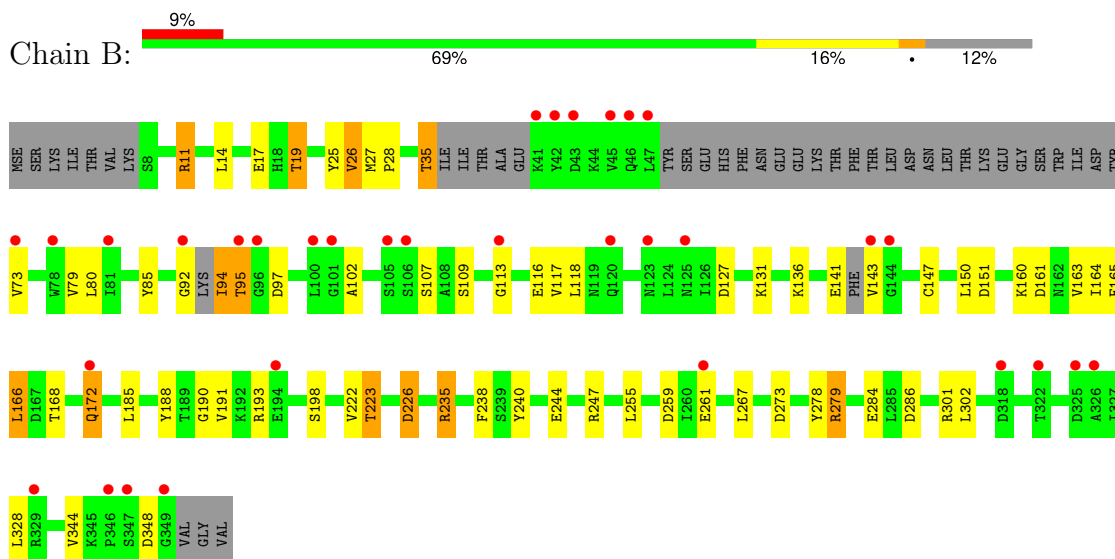
3 Residue-property plots

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.

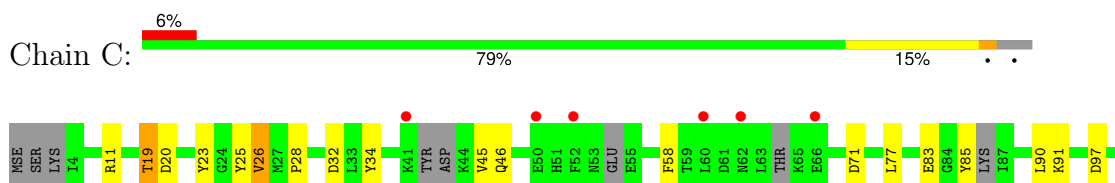
• Molecule 1: Galactokinase

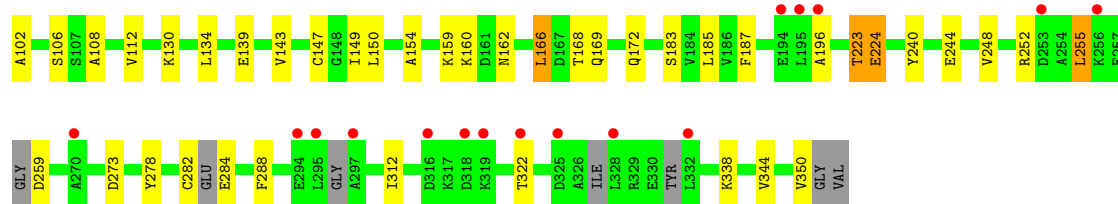


• Molecule 1: Galactokinase

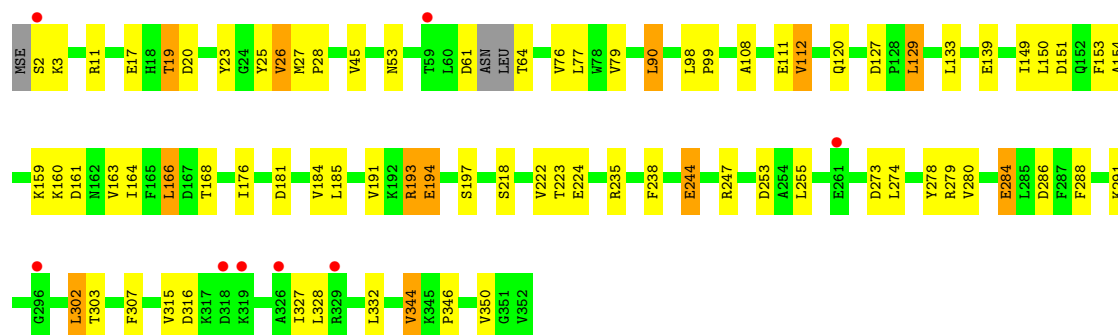
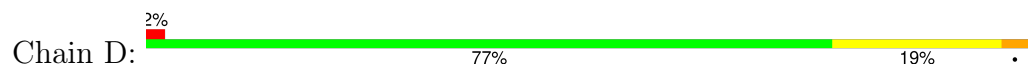


• Molecule 1: Galactokinase

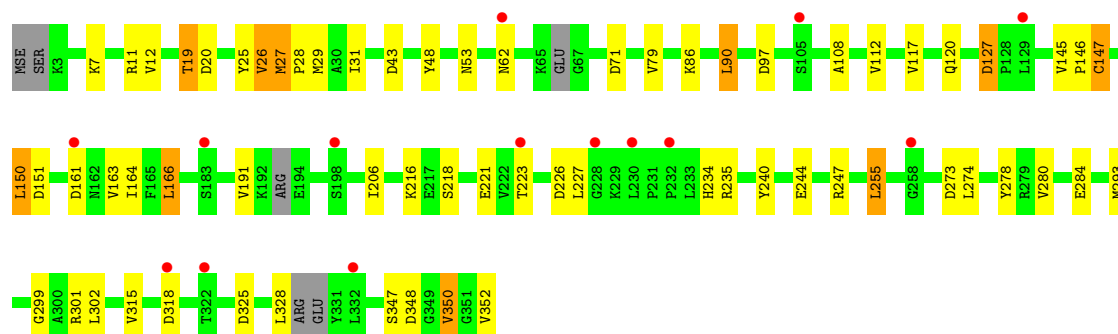




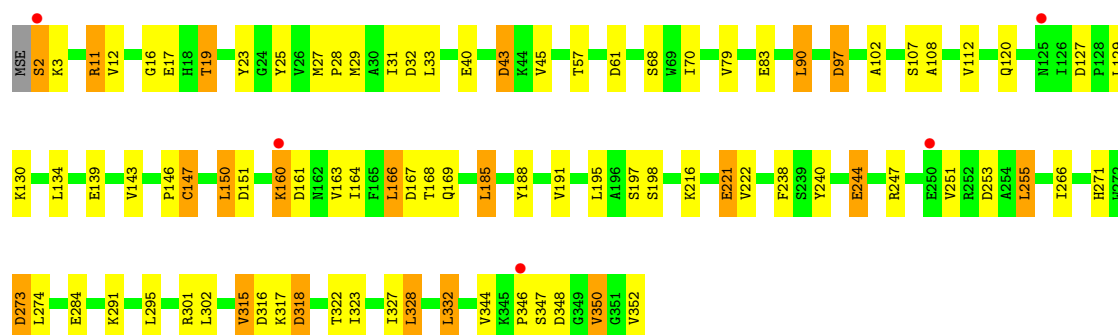
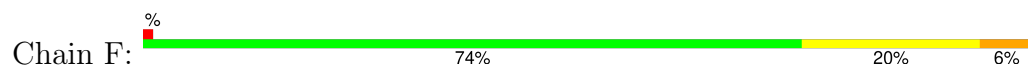
• Molecule 1: Galactokinase



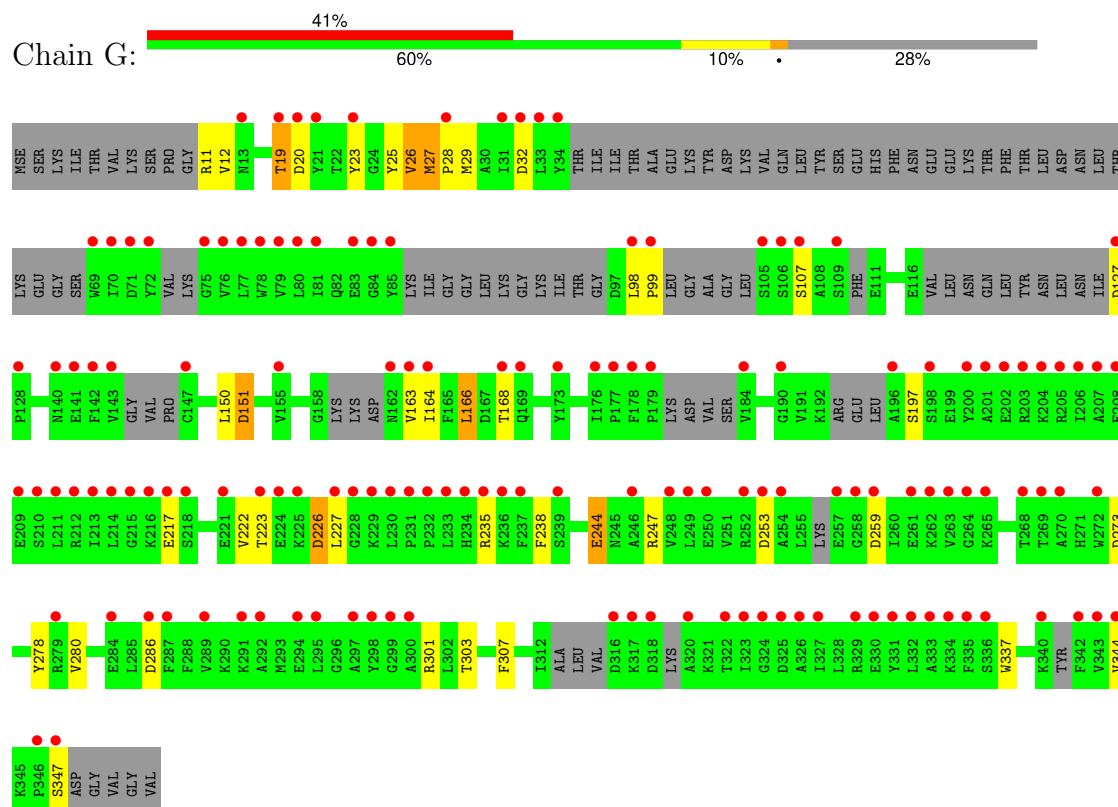
• Molecule 1: Galactokinase



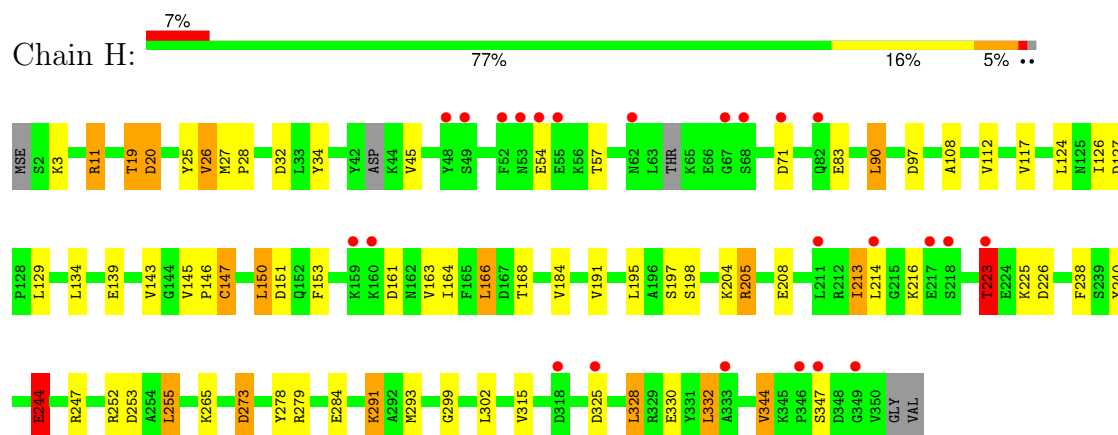
• Molecule 1: Galactokinase



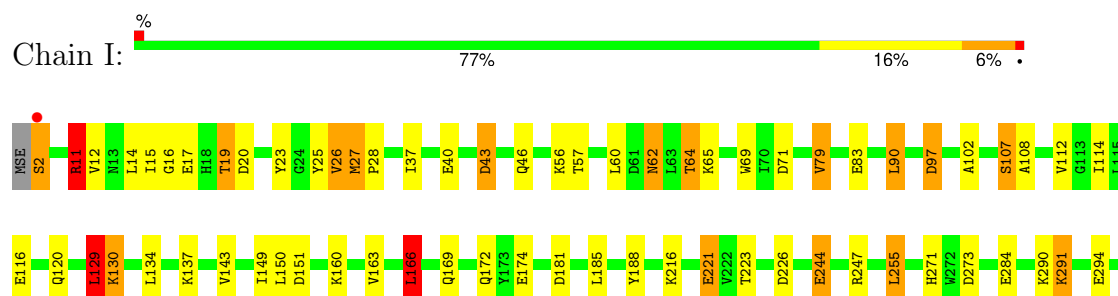
- Molecule 1: Galactokinase

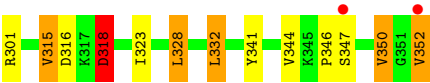


- Molecule 1: Galactokinase



- Molecule 1: Galactokinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.97Å 355.67Å 165.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-2.90) 97.3 (10.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.230 , 0.270 0.258 , 0.289	Depositor DCC
R_{free} test set	6821 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.007 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22711	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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, GLA, 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	0.67	0/2599	0.89	7/3513 (0.2%)
1	B	0.67	1/2301 (0.0%)	0.86	9/3116 (0.3%)
1	C	0.53	0/2457	0.76	5/3336 (0.1%)
1	D	0.60	0/2694	0.85	11/3659 (0.3%)
1	E	0.55	0/2665	0.82	10/3616 (0.3%)
1	F	0.80	1/2774 (0.0%)	1.00	16/3752 (0.4%)
1	G	0.54	0/1828	0.78	9/2464 (0.4%)
1	H	0.78	0/2701	0.96	15/3656 (0.4%)
1	I	0.88	2/2720 (0.1%)	1.03	21/3689 (0.6%)
All	All	0.69	4/22739 (0.0%)	0.89	103/30801 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	I	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	97	ASP	CB-CG	-8.05	1.34	1.51
1	I	221	GLU	CG-CD	5.92	1.60	1.51
1	B	92	GLY	CA-C	5.67	1.60	1.51
1	I	2	SER	CA-CB	5.14	1.60	1.52

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	97	ASP	CB-CG-OD1	-11.48	107.97	118.30
1	I	316	ASP	CB-CG-OD2	9.94	127.24	118.30
1	F	97	ASP	CB-CG-OD2	9.76	127.08	118.30
1	A	193	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	A	273	ASP	CB-CG-OD2	8.75	126.18	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	221	GLU	Peptide
1	I	221	GLU	Peptide

5.2 Too-close contacts [i](#)

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	2554	0	2465	37	0
1	B	2266	0	2131	36	0
1	C	2419	0	2187	26	0
1	D	2643	0	2524	33	0
1	E	2616	0	2499	28	0
1	F	2722	0	2687	51	0
1	G	1811	0	1608	16	0
1	H	2652	0	2592	38	0
1	I	2668	0	2578	44	0
2	A	12	0	12	0	0
2	B	12	0	12	1	0
2	C	12	0	12	0	0
2	D	12	0	12	1	0
2	E	12	0	12	1	0
2	F	12	0	12	1	0
2	G	12	0	12	0	0
2	H	12	0	12	0	0
2	I	12	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
4	G	27	0	12	1	0
4	H	27	0	12	0	0
4	I	27	0	12	1	0
All	All	22711	0	21487	306	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 7.

The worst 5 of 306 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:THR:HG21	1:F:25:TYR:O	1.56	1.04
1:A:19:THR:HG21	1:A:25:TYR:O	1.59	1.02
1:C:19:THR:HG21	1:C:25:TYR:O	1.66	0.95
1:B:172:GLN:HA	1:B:172:GLN:NE2	1.82	0.93
1:F:244:GLU:HG2	1:F:247:ARG:NH1	1.83	0.92

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	326/352 (93%)	311 (95%)	14 (4%)	1 (0%)	37	66
1	B	300/352 (85%)	282 (94%)	16 (5%)	2 (1%)	19	49
1	C	317/352 (90%)	292 (92%)	22 (7%)	3 (1%)	14	43
1	D	345/352 (98%)	336 (97%)	8 (2%)	1 (0%)	37	66
1	E	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	37	66
1	F	349/352 (99%)	329 (94%)	18 (5%)	2 (1%)	22	52
1	G	225/352 (64%)	210 (93%)	13 (6%)	2 (1%)	14	43
1	H	341/352 (97%)	328 (96%)	12 (4%)	1 (0%)	37	66
1	I	349/352 (99%)	332 (95%)	17 (5%)	0	100	100
All	All	2890/3168 (91%)	2736 (95%)	141 (5%)	13 (0%)	30	60

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	TYR
1	D	194	GLU
1	E	147	CYS
1	F	147	CYS
1	B	160	LYS

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	251/293 (86%)	229 (91%)	22 (9%)	8	26
1	B	210/293 (72%)	187 (89%)	23 (11%)	5	16
1	C	212/293 (72%)	193 (91%)	19 (9%)	8	25
1	D	260/293 (89%)	231 (89%)	29 (11%)	5	16
1	E	254/293 (87%)	230 (91%)	24 (9%)	7	23
1	F	278/293 (95%)	247 (89%)	31 (11%)	5	16
1	G	157/293 (54%)	140 (89%)	17 (11%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	264/293 (90%)	236 (89%)	28 (11%)	5	18
1	I	262/293 (89%)	227 (87%)	35 (13%)	3	9
All	All	2148/2637 (82%)	1920 (89%)	228 (11%)	5	18

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	347	SER
1	I	328	LEU
1	F	332	LEU
1	I	315	VAL
1	I	62	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	162	ASN
1	I	51	HIS
1	I	123	ASN
1	I	62	ASN
1	E	62	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ADP	F	5400	3	24,29,29	1.35	2 (8%)	29,45,45	1.70	5 (17%)
2	GLA	E	4500	-	12,12,12	0.74	0	17,17,17	2.51	10 (58%)
4	ADP	C	2400	3	24,29,29	1.44	2 (8%)	29,45,45	1.71	4 (13%)
4	ADP	I	8400	3	24,29,29	1.37	2 (8%)	29,45,45	2.03	11 (37%)
4	ADP	H	7400	3	24,29,29	1.42	2 (8%)	29,45,45	1.81	4 (13%)
2	GLA	H	7500	-	12,12,12	0.59	0	17,17,17	2.19	6 (35%)
2	GLA	C	2500	-	12,12,12	0.82	1 (8%)	17,17,17	2.53	4 (23%)
4	ADP	E	4400	3	24,29,29	1.15	2 (8%)	29,45,45	1.60	3 (10%)
2	GLA	F	5500	-	12,12,12	0.99	0	17,17,17	1.45	3 (17%)
4	ADP	B	1400	3	24,29,29	1.58	4 (16%)	29,45,45	1.47	2 (6%)
2	GLA	I	8500	-	12,12,12	0.66	0	17,17,17	1.18	2 (11%)
2	GLA	A	500	-	12,12,12	0.39	0	17,17,17	1.07	1 (5%)
2	GLA	G	6500	-	12,12,12	0.79	0	17,17,17	1.98	3 (17%)
4	ADP	A	400	3	24,29,29	1.50	3 (12%)	29,45,45	1.68	3 (10%)
4	ADP	D	3400	3	24,29,29	1.45	2 (8%)	29,45,45	1.62	3 (10%)
4	ADP	G	6400	3	24,29,29	1.95	4 (16%)	29,45,45	1.80	4 (13%)
2	GLA	B	1500	-	12,12,12	0.55	0	17,17,17	1.91	5 (29%)
2	GLA	D	3500	-	12,12,12	0.53	0	17,17,17	1.19	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	F	5400	3	-	7/12/32/32	0/3/3/3
2	GLA	E	4500	-	1/1/5/5	1/2/22/22	0/1/1/1
4	ADP	C	2400	3	-	4/12/32/32	0/3/3/3
4	ADP	I	8400	3	-	5/12/32/32	0/3/3/3
4	ADP	H	7400	3	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	H	7500	-	-	2/2/22/22	0/1/1/1
2	GLA	C	2500	-	-	2/2/22/22	0/1/1/1
4	ADP	E	4400	3	-	7/12/32/32	0/3/3/3
2	GLA	F	5500	-	-	2/2/22/22	0/1/1/1
4	ADP	B	1400	3	-	5/12/32/32	0/3/3/3
2	GLA	I	8500	-	-	2/2/22/22	0/1/1/1
2	GLA	A	500	-	-	1/2/22/22	0/1/1/1
2	GLA	G	6500	-	-	1/2/22/22	0/1/1/1
4	ADP	A	400	3	-	4/12/32/32	0/3/3/3
4	ADP	D	3400	3	-	7/12/32/32	0/3/3/3
4	ADP	G	6400	3	-	3/12/32/32	0/3/3/3
2	GLA	B	1500	-	-	2/2/22/22	0/1/1/1
2	GLA	D	3500	-	-	2/2/22/22	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	6400	ADP	C2-N3	5.73	1.41	1.32
4	H	7400	ADP	C2-N3	4.98	1.39	1.32
4	B	1400	ADP	C2-N3	4.98	1.39	1.32
4	A	400	ADP	C2-N3	4.69	1.39	1.32
4	C	2400	ADP	C2-N3	4.62	1.39	1.32

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2500	GLA	O5-C1-C2	8.81	125.78	110.30
4	H	7400	ADP	N3-C2-N1	-6.94	119.26	128.67
4	I	8400	ADP	N3-C2-N1	-6.70	119.58	128.67
4	C	2400	ADP	N3-C2-N1	-6.49	119.86	128.67
4	A	400	ADP	N3-C2-N1	-6.41	119.97	128.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	4500	GLA	C1

5 of 58 torsion outliers are listed below:

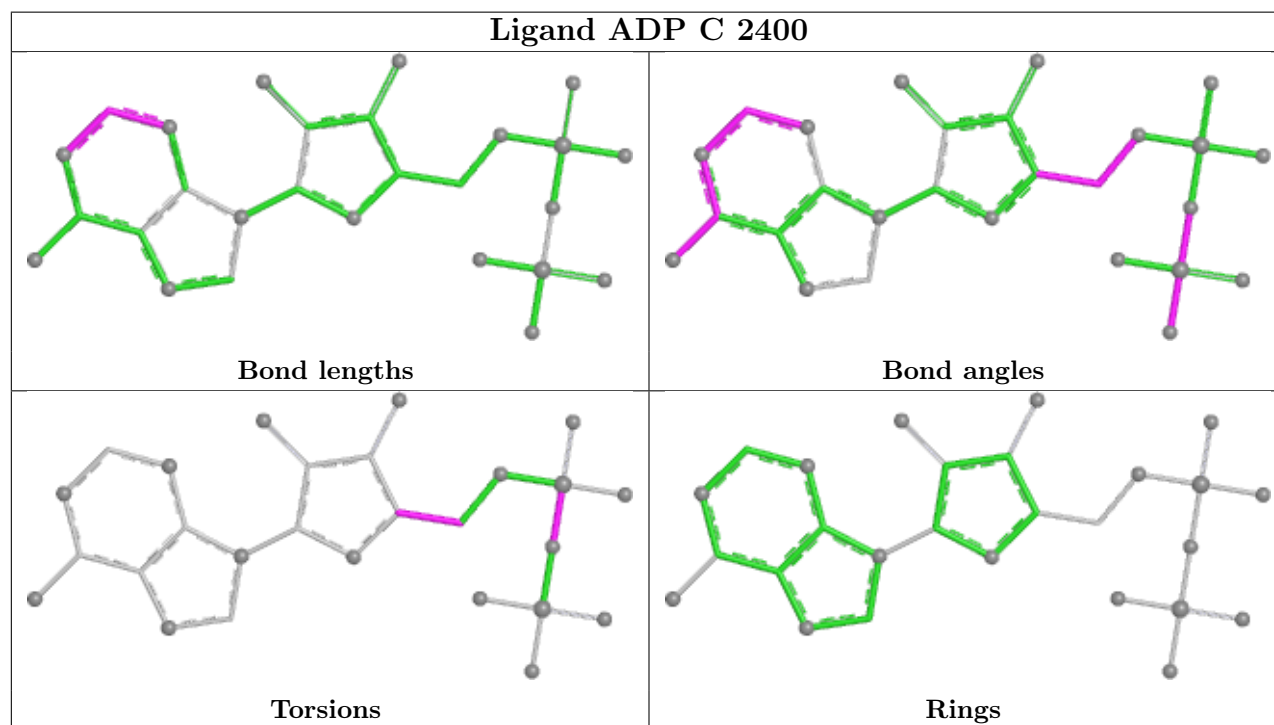
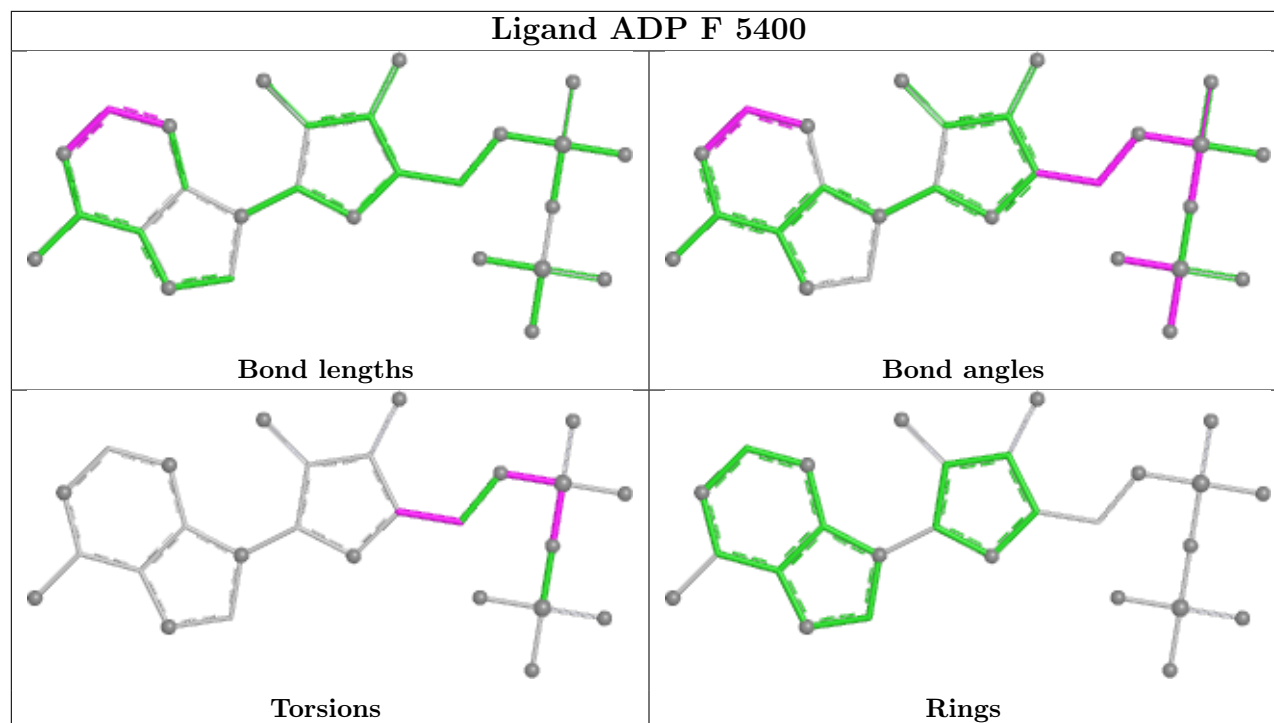
Mol	Chain	Res	Type	Atoms
4	A	400	ADP	PA-O3A-PB-O2B
4	B	1400	ADP	C5'-O5'-PA-O1A
4	B	1400	ADP	C5'-O5'-PA-O2A
4	B	1400	ADP	C5'-O5'-PA-O3A
4	C	2400	ADP	O4'-C4'-C5'-O5'

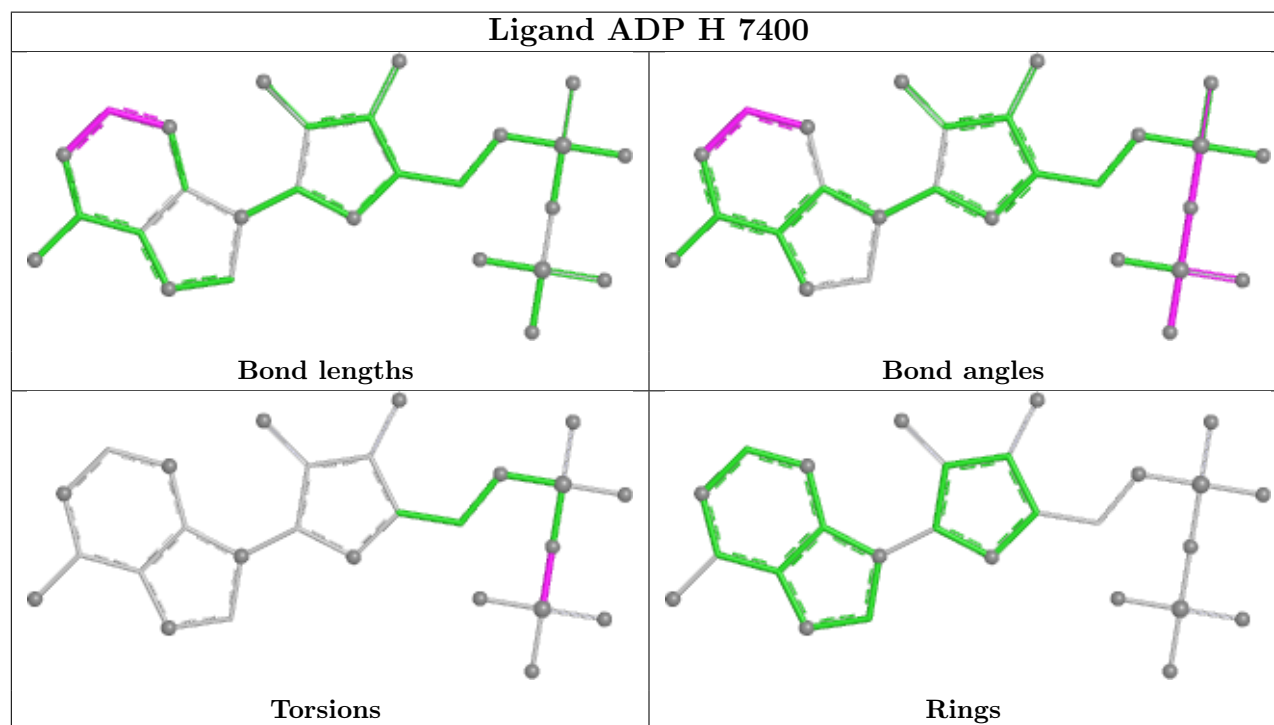
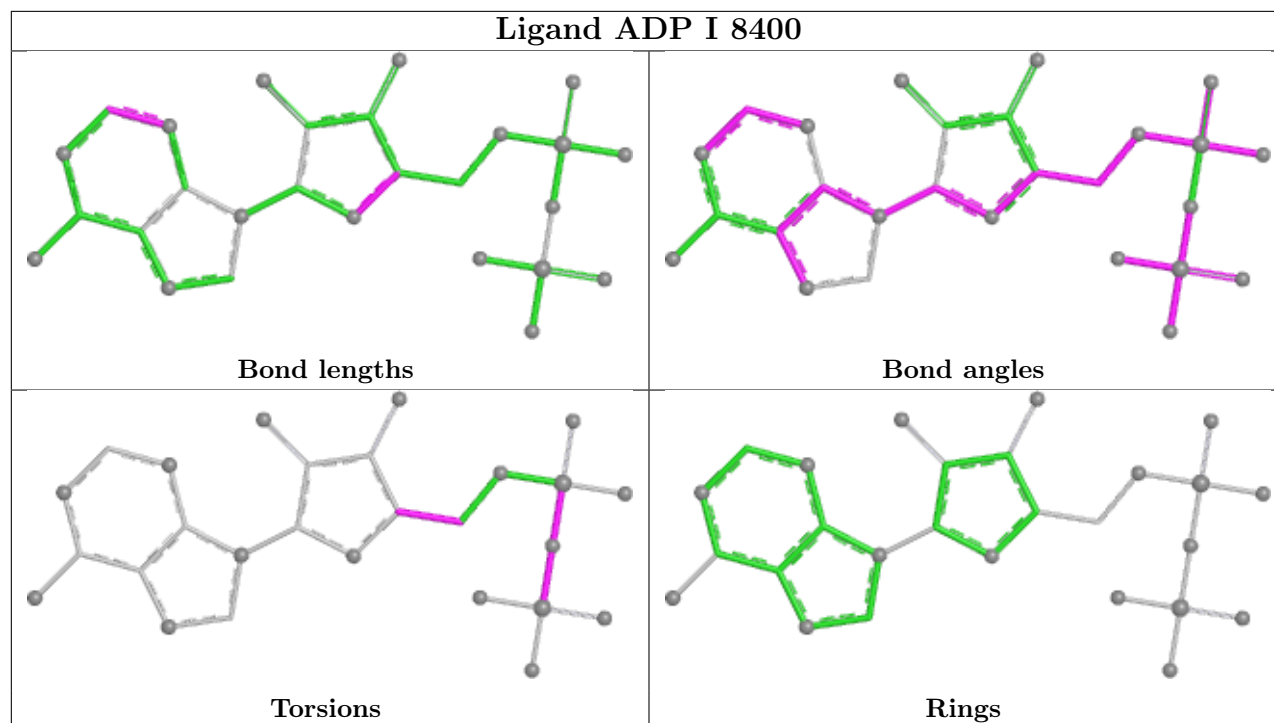
There are no ring outliers.

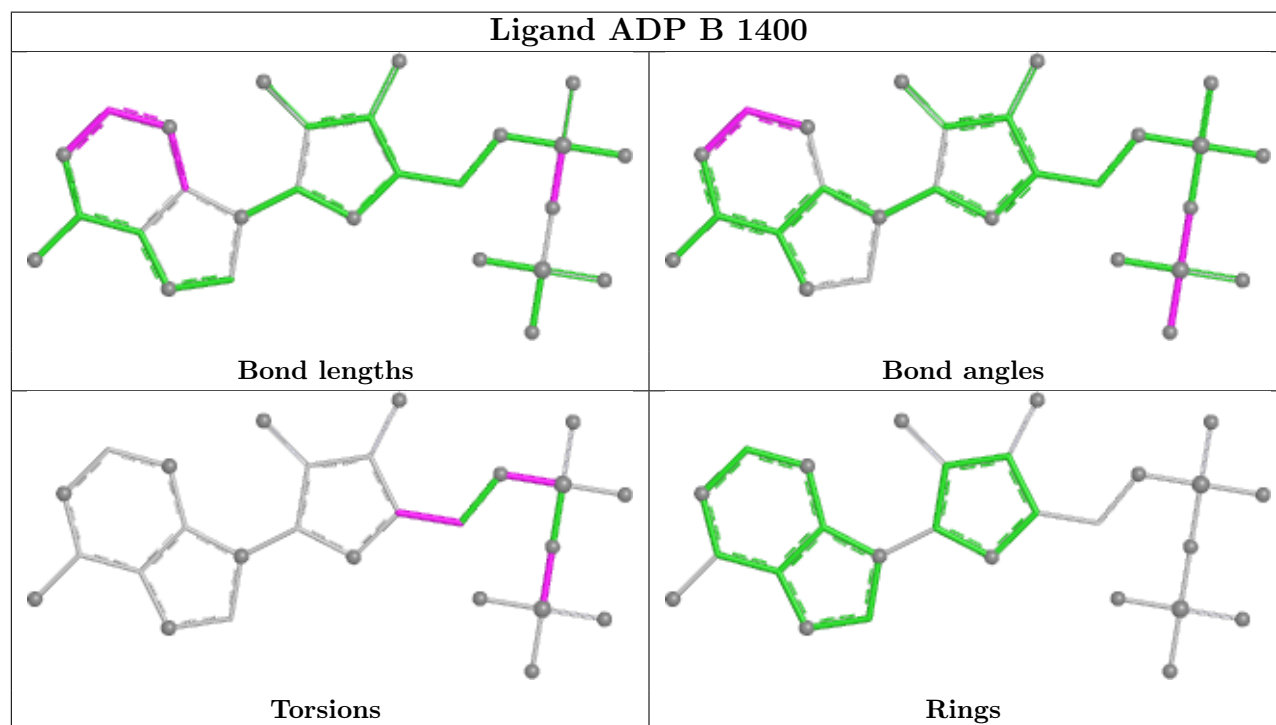
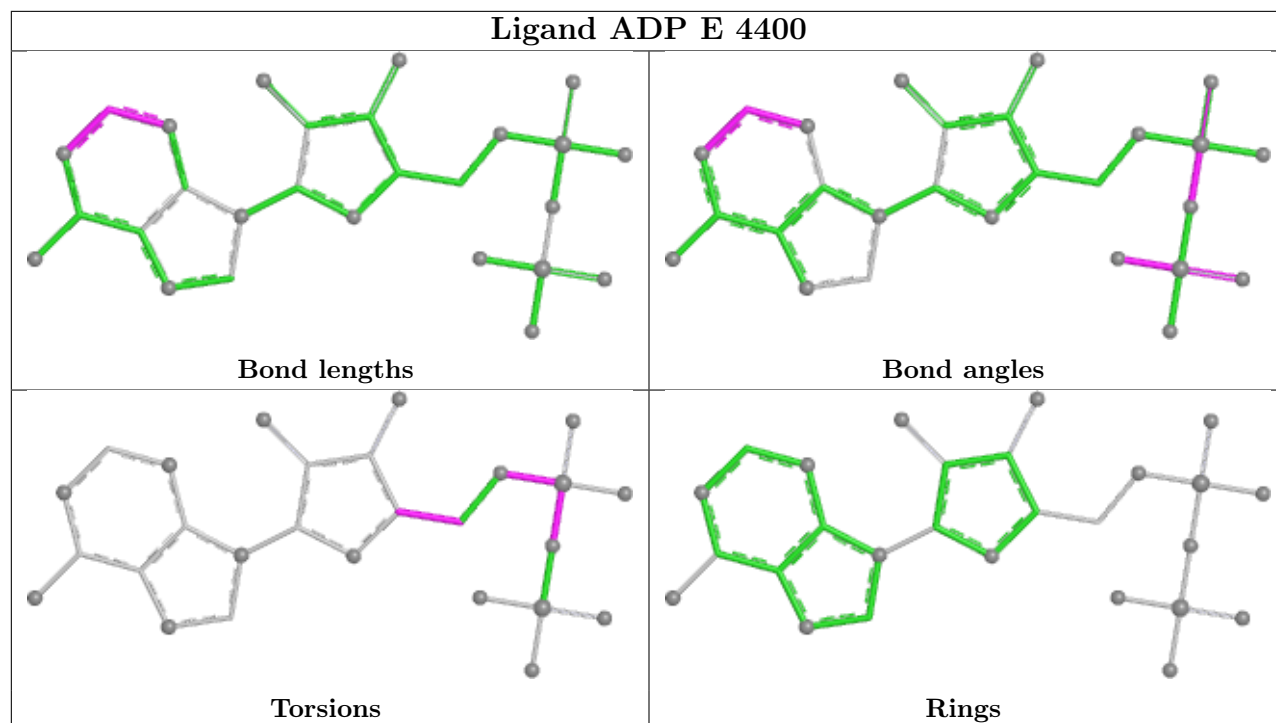
8 monomers are involved in 8 short contacts:

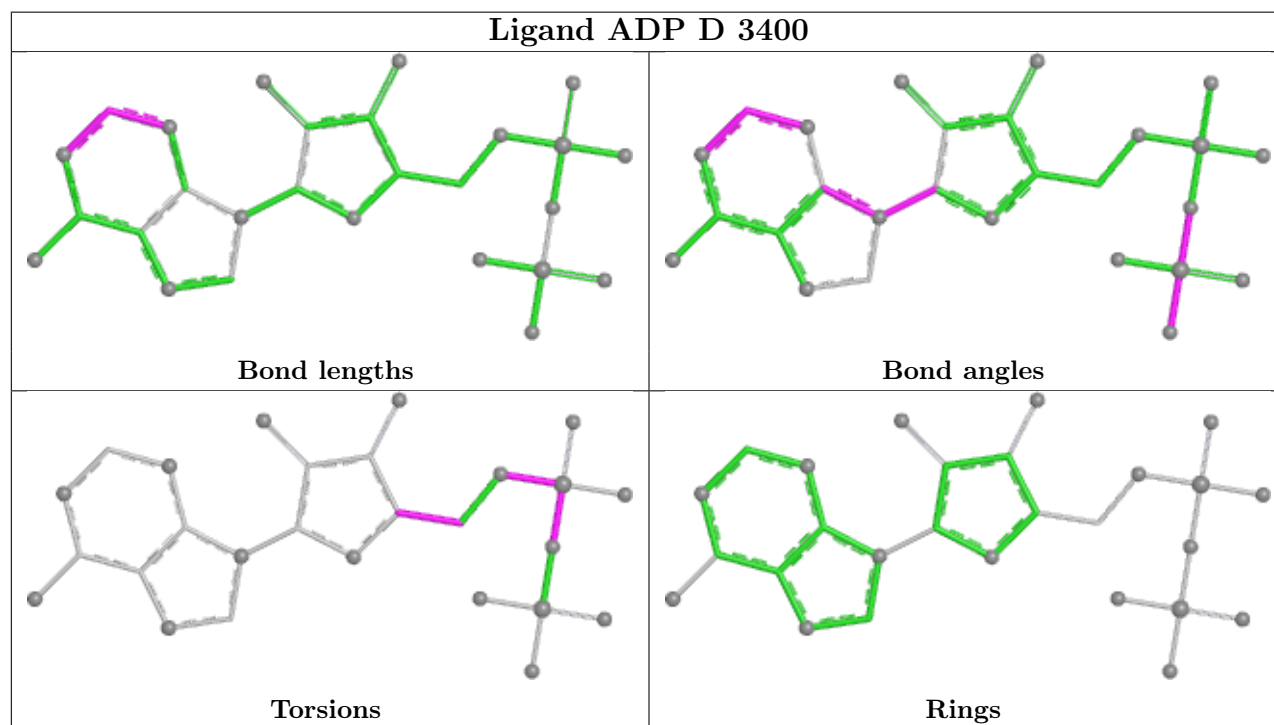
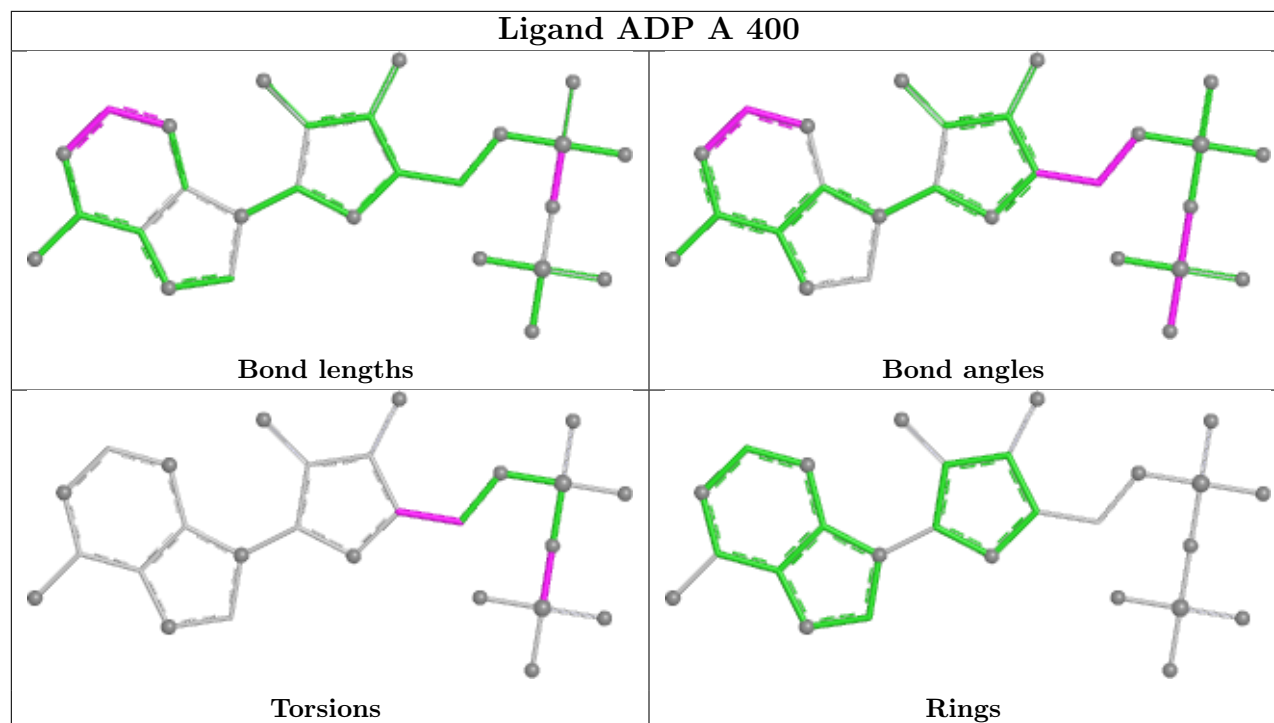
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4500	GLA	1	0
4	C	2400	ADP	1	0
4	I	8400	ADP	1	0
2	F	5500	GLA	1	0
4	B	1400	ADP	1	0
4	G	6400	ADP	1	0
2	B	1500	GLA	1	0
2	D	3500	GLA	1	0

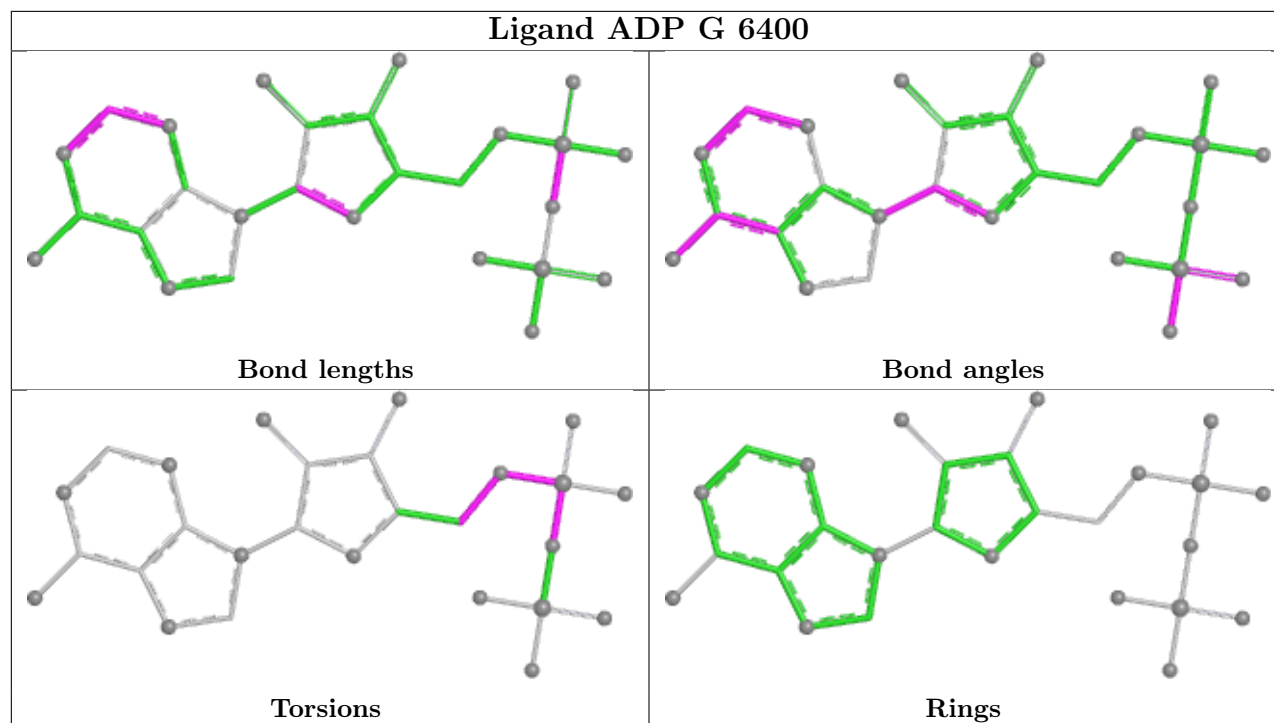
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/352 (94%)	-0.39	7 (2%) 63 57	33, 54, 108, 137	0
1	B	307/352 (87%)	0.19	33 (10%) 12 11	31, 78, 137, 173	0
1	C	334/352 (94%)	0.18	22 (6%) 26 22	50, 78, 126, 151	0
1	D	346/352 (98%)	-0.24	8 (2%) 61 54	46, 65, 93, 105	0
1	E	343/352 (97%)	0.26	14 (4%) 42 35	47, 66, 95, 108	0
1	F	348/352 (98%)	-0.28	5 (1%) 73 68	26, 42, 55, 70	0
1	G	252/352 (71%)	2.51	143 (56%) 0 0	45, 94, 148, 201	0
1	H	344/352 (97%)	0.28	24 (6%) 24 20	24, 46, 73, 103	0
1	I	348/352 (98%)	-0.31	3 (0%) 81 76	23, 36, 56, 69	0
All	All	2956/3168 (93%)	0.18	259 (8%) 17 15	23, 58, 116, 201	0

The worst 5 of 259 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	198	SER	8.2
1	G	294	GLU	7.8
1	G	105	SER	7.8
1	G	106	SER	7.2
1	G	127	ASP	6.5

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

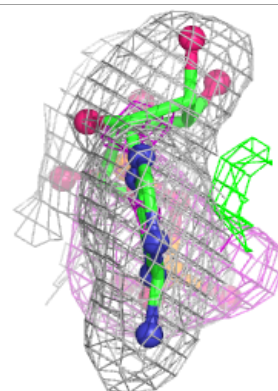
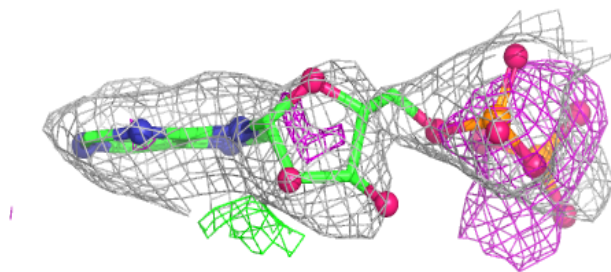
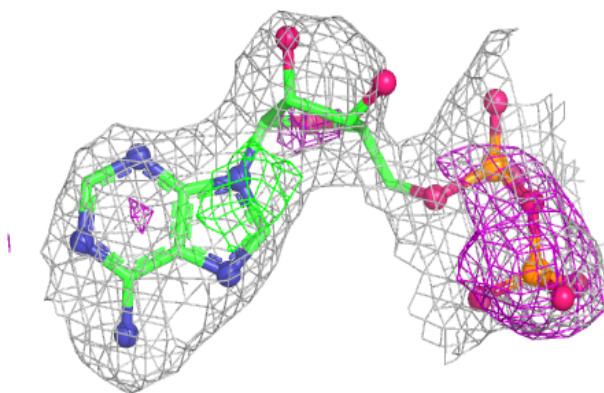
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	G	6600	1/1	0.31	0.14	60,60,60,60	0
3	MG	B	1600	1/1	0.38	0.20	55,55,55,55	0
3	MG	A	600	1/1	0.45	0.19	46,46,46,46	0
3	MG	E	4600	1/1	0.48	0.17	47,47,47,47	0
4	ADP	G	6400	27/27	0.58	0.16	67,71,73,76	0
3	MG	D	3600	1/1	0.60	0.18	44,44,44,44	0
3	MG	I	8600	1/1	0.64	0.18	35,35,35,35	0
3	MG	C	2600	1/1	0.76	0.11	51,51,51,51	0
3	MG	F	5600	1/1	0.80	0.17	32,32,32,32	0
2	GLA	G	6500	12/12	0.82	0.16	54,59,61,62	0
3	MG	H	7600	1/1	0.82	0.15	44,44,44,44	0
2	GLA	F	5500	12/12	0.84	0.13	51,54,56,56	0
2	GLA	E	4500	12/12	0.86	0.09	52,55,55,55	0
4	ADP	B	1400	27/27	0.87	0.11	63,68,70,70	0
2	GLA	B	1500	12/12	0.88	0.10	53,56,57,58	0
4	ADP	C	2400	27/27	0.92	0.09	58,60,61,63	0
4	ADP	A	400	27/27	0.93	0.08	50,54,58,59	0
2	GLA	A	500	12/12	0.94	0.07	42,46,49,50	0
2	GLA	H	7500	12/12	0.94	0.08	36,39,41,42	0
2	GLA	D	3500	12/12	0.94	0.07	43,49,51,52	0
2	GLA	I	8500	12/12	0.95	0.09	33,34,36,37	0
4	ADP	D	3400	27/27	0.95	0.07	48,50,53,54	0
4	ADP	E	4400	27/27	0.95	0.08	48,49,55,56	0
2	GLA	C	2500	12/12	0.95	0.05	45,49,50,51	0
4	ADP	H	7400	27/27	0.95	0.08	40,50,53,54	0
4	ADP	I	8400	27/27	0.95	0.09	31,37,39,42	0
4	ADP	F	5400	27/27	0.96	0.07	30,38,44,44	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.

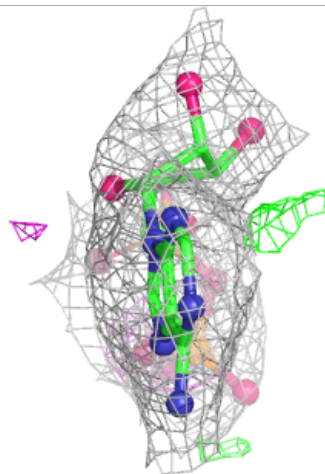
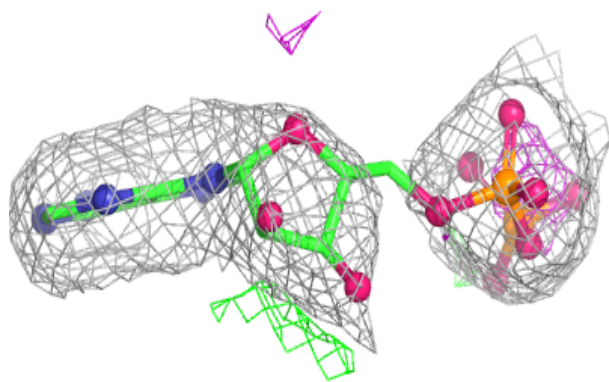
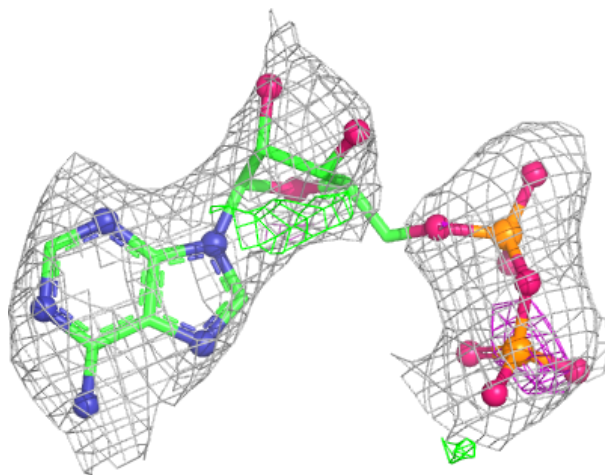
Electron density around ADP G 6400:

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



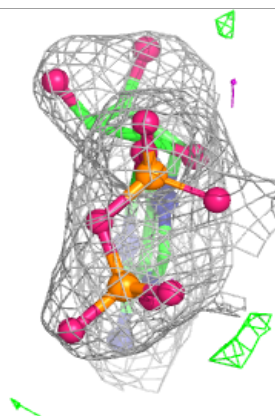
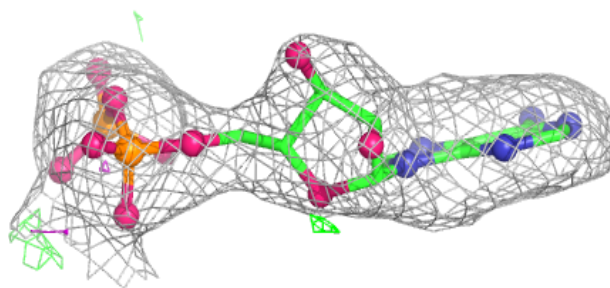
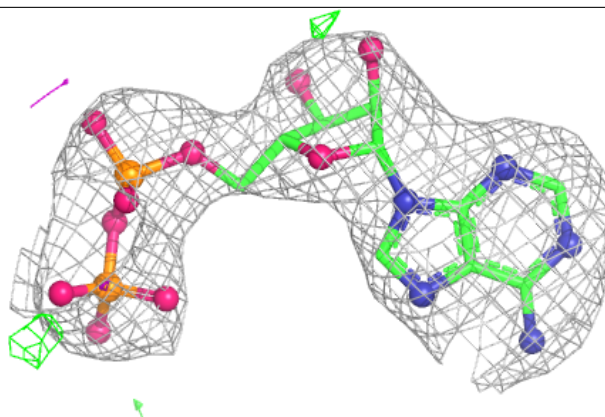
Electron density around ADP B 1400:

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

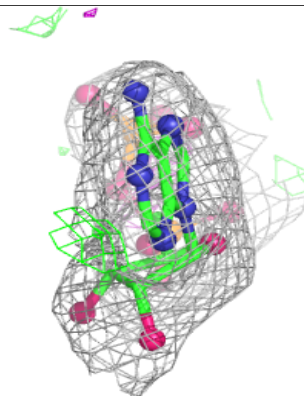
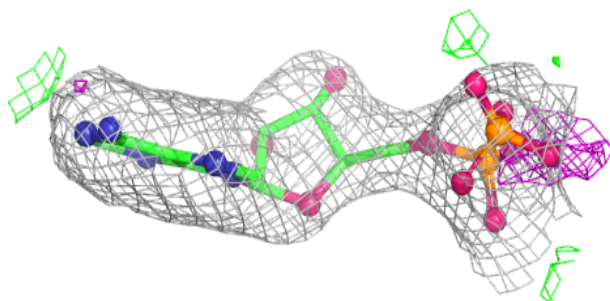
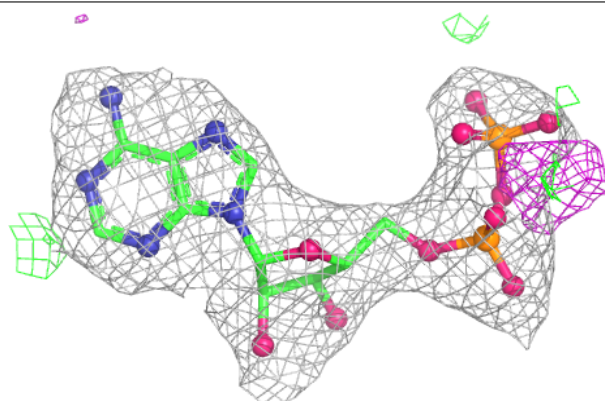


Electron density around ADP C 2400:

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

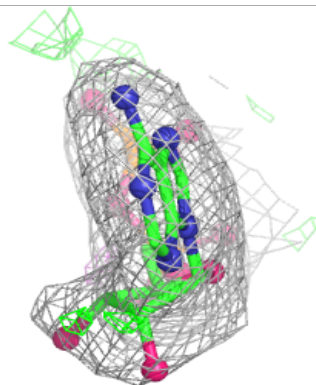
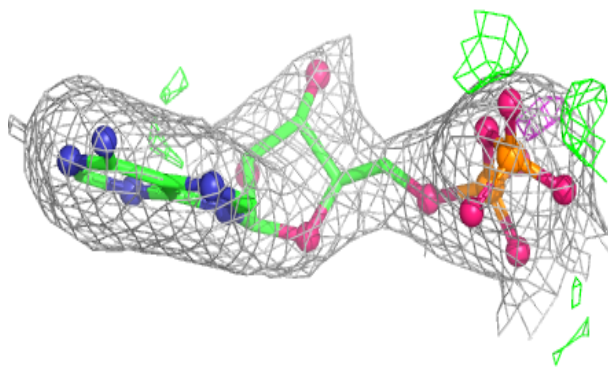
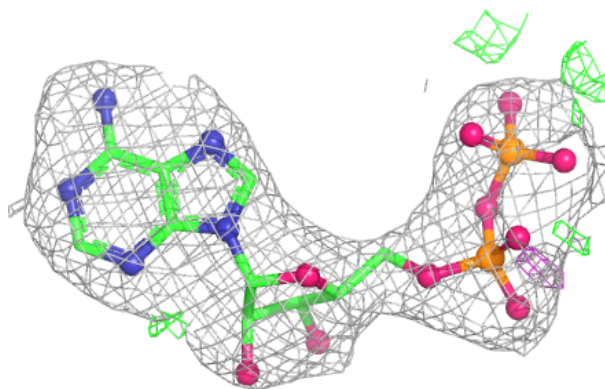
**Electron density around ADP A 400:**

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



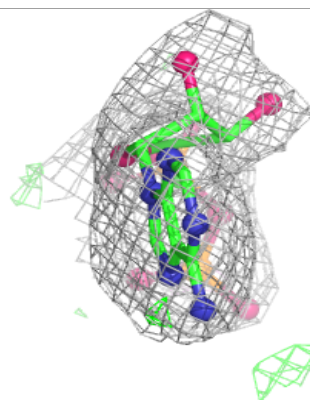
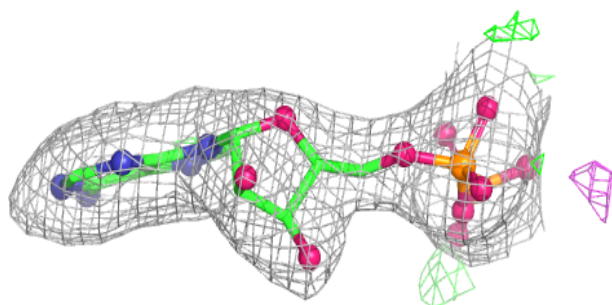
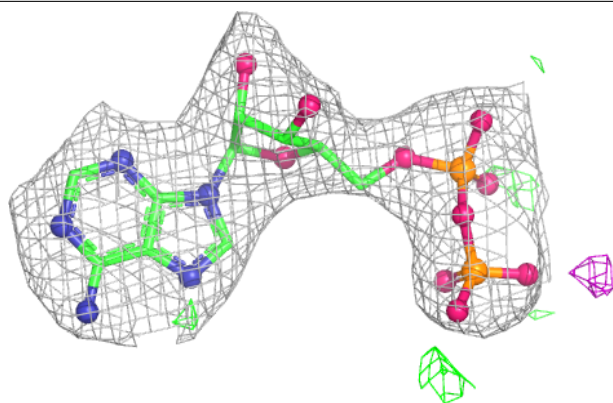
Electron density around ADP D 3400:

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and green (positive)

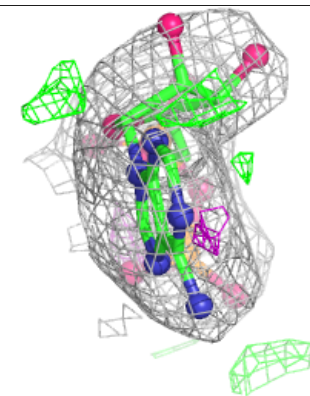
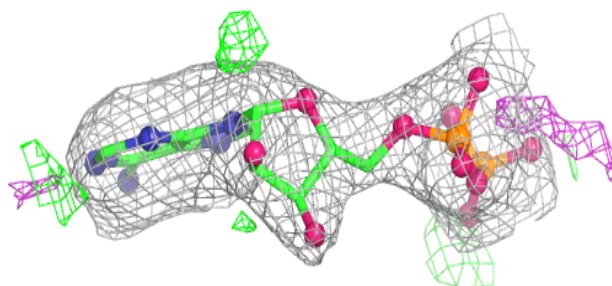
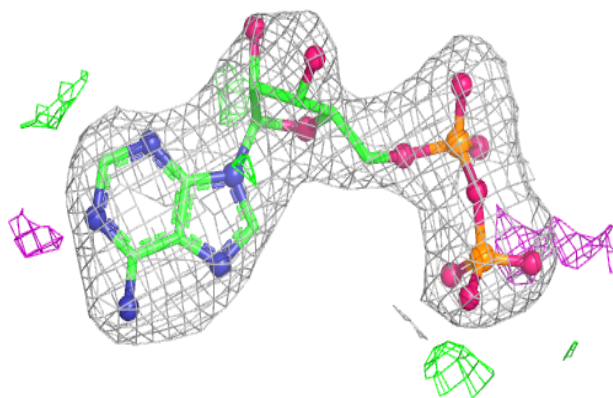


Electron density around ADP E 4400:

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

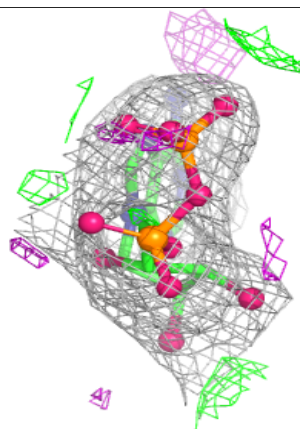
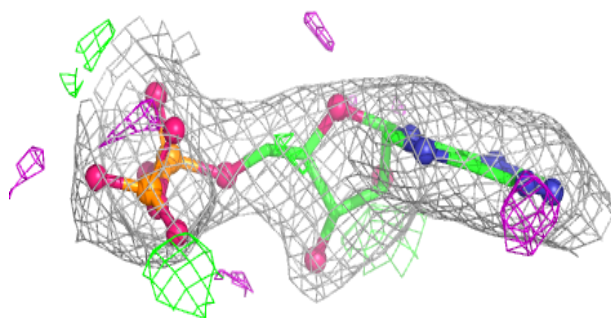
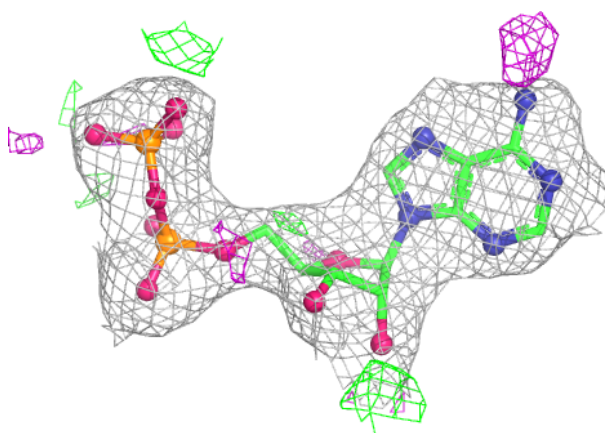
**Electron density around ADP H 7400:**

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

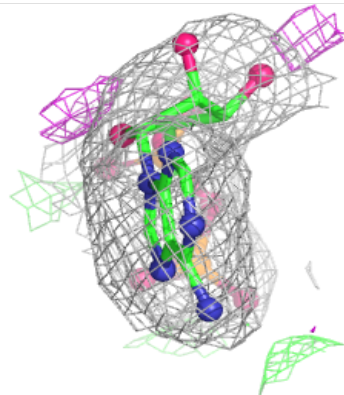
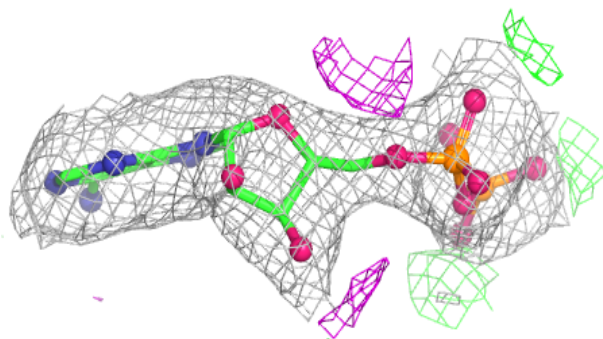
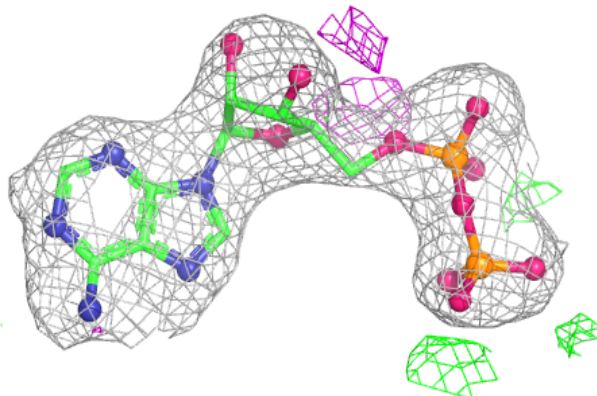


Electron density around ADP I 8400:

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

**Electron density around ADP F 5400:**

$2mF_o-DF_c$ (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.