



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:43 PM UTC

PDB ID : 4A51 / pdb_00004a51
Title : Crystal structure of human kinesin Eg5 in complex with 1-(3-(((2-Aminoethyl)thio)diphenylmethyl)phenyl)ethanone hydrochloride
Authors : Kaan, H.Y.K.; Kozielski, F.
Deposited on : 2011-10-24
Resolution : 2.75 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 : 4-5-2 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

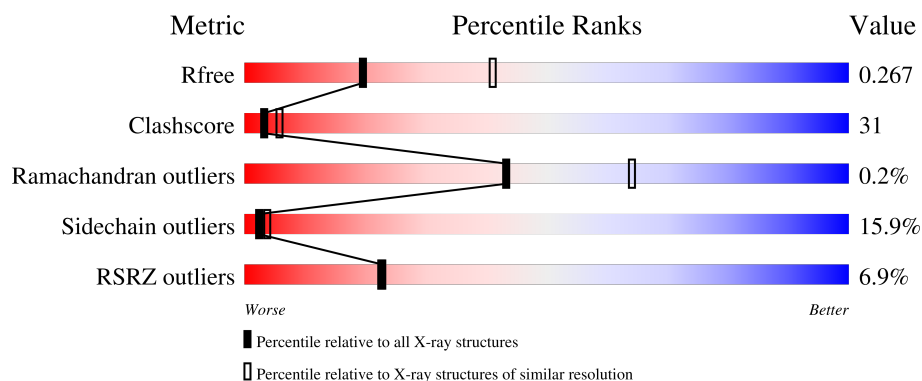
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	368	5% 46% 34% 7% 12%
1	B	368	3% 56% 26% 6% 12%
1	C	368	3% 48% 33% 5% 12%
1	D	368	4% 52% 31% . 12%
1	E	368	6% 43% 34% 9% 13%

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Mol	Chain	Length	Quality of chain
1	F	368	
1	G	368	

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
4	DQ8	E	801	-	-	X	-

2 Entry composition [i](#)

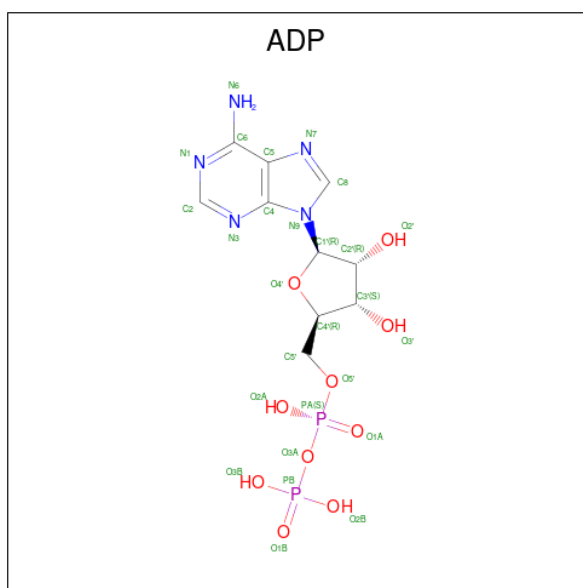
There are 7 unique types of molecules in this entry. The entry contains 18210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	1	0
			2522	1586	438	488	10			
1	B	324	Total	C	N	O	S	0	1	0
			2552	1602	446	494	10			
1	C	325	Total	C	N	O	S	0	1	0
			2551	1599	445	497	10			
1	D	322	Total	C	N	O	S	0	1	0
			2526	1585	438	493	10			
1	E	321	Total	C	N	O	S	0	0	0
			2504	1573	435	486	10			
1	F	319	Total	C	N	O	S	0	1	0
			2487	1559	433	486	9			
1	G	318	Total	C	N	O	S	0	0	0
			2446	1537	428	472	9			

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

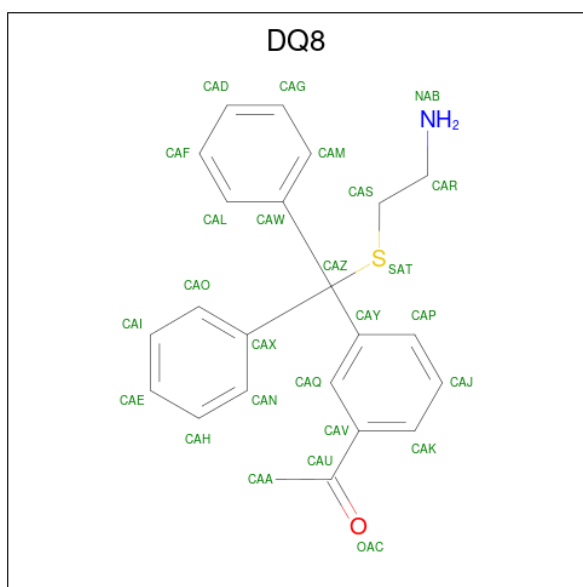


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 1-(3-{[(2-aminoethyl)sulfanyl](diphenyl)methyl}phenyl)ethanone (CCD ID: DQ8) (formula: C₂₃H₂₃NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	B	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	C	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	D	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	E	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	F	1	Total	C	N	O	S	0	0
			26	23	1	1	1		
4	G	1	Total	C	N	O	S	0	0
			26	23	1	1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

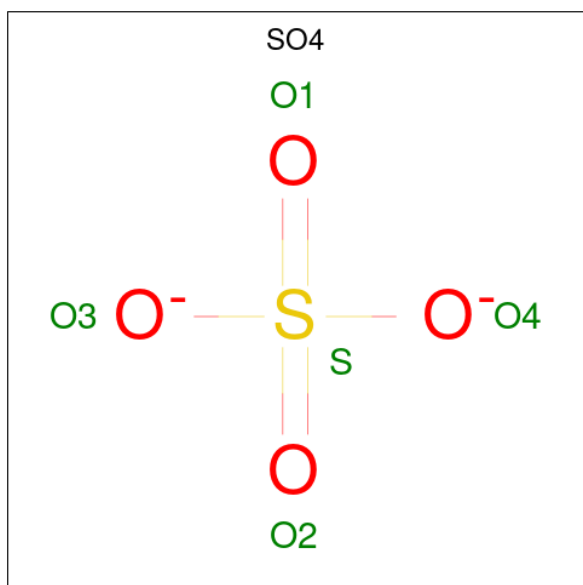
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Cl	0	0
			4	4		
5	B	2	Total	Cl	0	0
			2	2		
5	C	3	Total	Cl	0	0
			3	3		
5	D	2	Total	Cl	0	0
			2	2		
5	E	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Cl	0	0
			1	1		
5	G	1	Total	Cl	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	32	Total	O	0	0
			32	32		
7	B	34	Total	O	0	0
			34	34		
7	C	47	Total	O	0	0
			47	47		
7	D	46	Total	O	0	0
			46	46		
7	E	22	Total	O	0	0
			22	22		
7	F	25	Total	O	0	0
			25	25		

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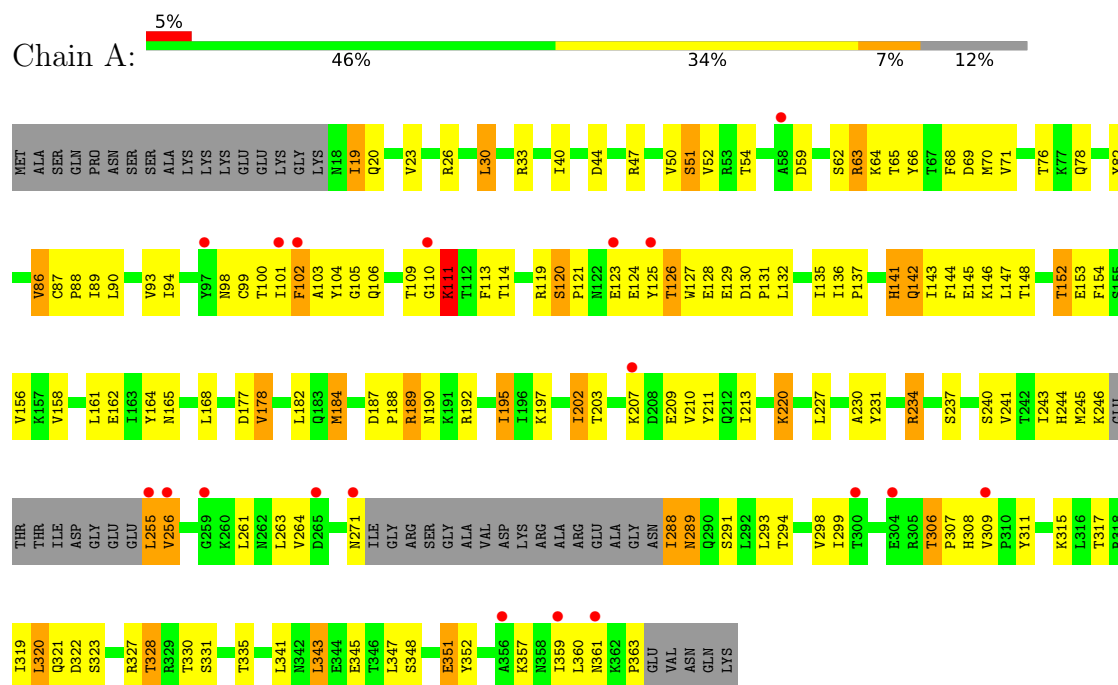
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	19	Total	O	0	0
			19	19		

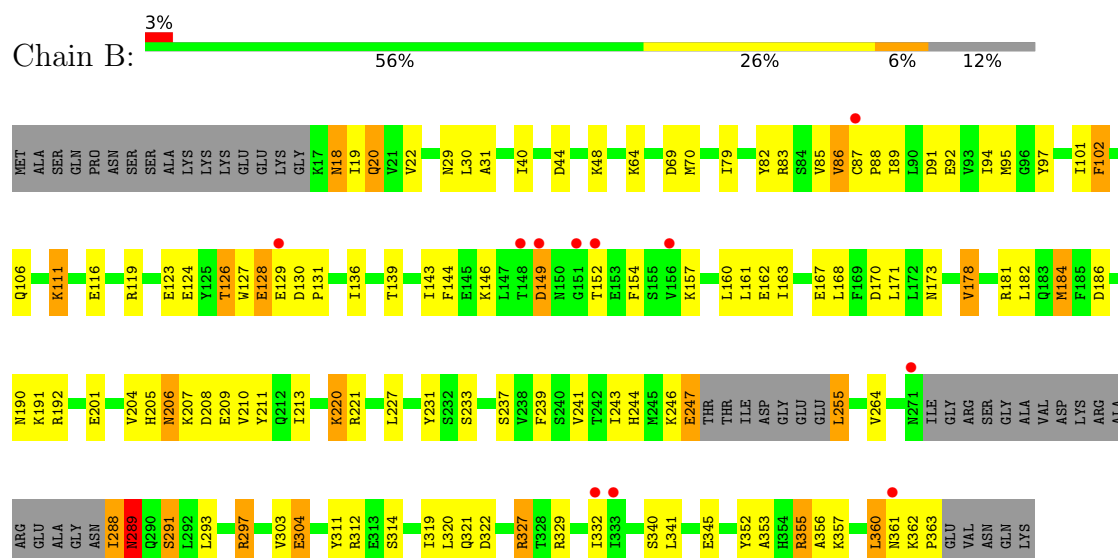
3 Residue-property plots

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: KINESIN-LIKE PROTEIN KIF11



• Molecule 1: KINESIN-LIKE PROTEIN KIF11



Chain C:

3% 48% 33% 5% 12%

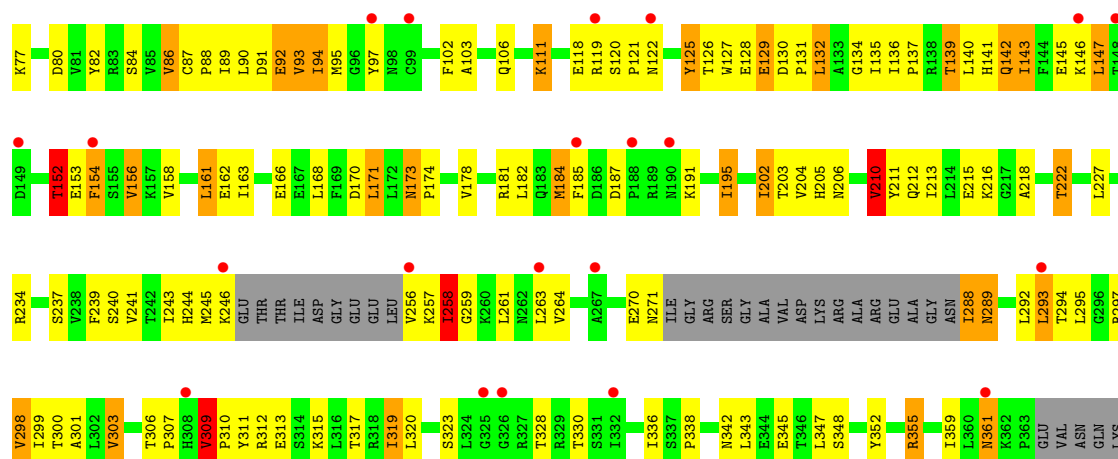
MET ALA SER GLN PRO ASN SER SER ALA LYS LYS LYS GLU GLU LYS GLY LYS N18 N19 V22 V23 R24 C25 R26 P27 F28 N29 L30 R33 K34 S39 I40 V41 E42 C43 D44 V50 T54 D59 S62 R63 R64 T67 F68 D69 M70 V71 F72 G73 A74 S75 T76 K77 Y82 W85 W86 C87 P88 V178 E92 Y93 I94 Y97 T100 I101 F102 A103 Y104 M115 E116 G117 E118 R119 S120 P121 T126 W127 E128 E129 D130 I135 I136 C142 F144 E145 K146 D149 N150 G151 T152 S159 I160 L161 E162 I163 K164 N165 E166 E167 F168 D170 N173 V178 D186 D187 P188 R189 A190 K191 R192 L199 T203 N206 K207 D208 E209 V210 Y211 Q212 K216 K220 L227 Y231 S232 S233 R234 V238 I243 H244 M245 K245 GLU THR THR ILE ASP GLY GLU GLU LEU V256 K257 L258 L261 N262 L263 V264 D265 L266 E270 N271 ILE GLY ARG SER ARG GLY ALA VAL ASP LYS ARG ALA ARG GLU ALA GLY N287 I288 N289 L292 L293 R297 V298 L299 T300 A301 L302 V303 T306 P307 H308 V309 P310 P311 Y311 R312 L316 L320 Q321 D322 S323 L324 R327 T328 S337 R338 A339 S340 L341 N342 L343 E344 E351 V352 A353 H354 K355 A356 K357 N358 I359 L360 N361 K362 P363 E364 V365 N366 GLN LYS

Chain D:

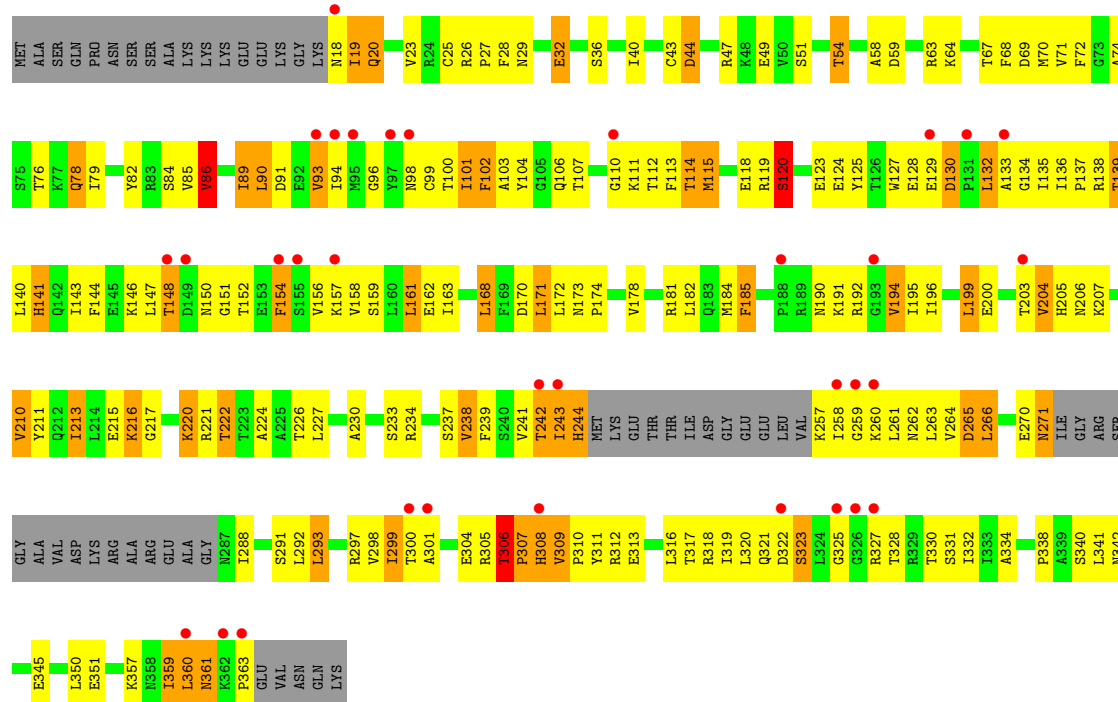
4% 52% 31% 12%

MET SER GLN PRO ASN LYS ALA LYS LYS GLU GLU LYS GLY LYS N18 I19 V22 C25 R26 P27 L30 A31 E32 R33 R34 A35 S36 I40 D44 S51 V52 R53 T54 G55 G56 K64 T65 V66 T67 M70 V71 A74 K77 Q78 I79 S82

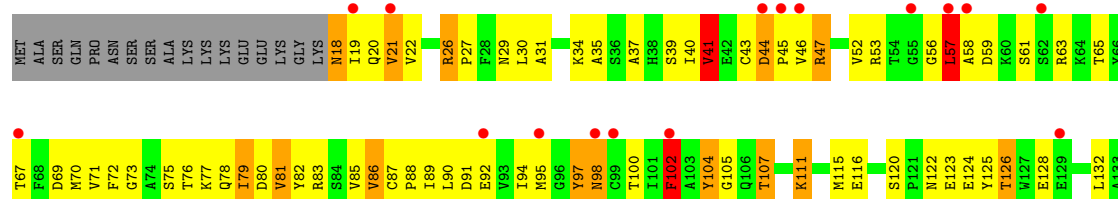
Chain E:

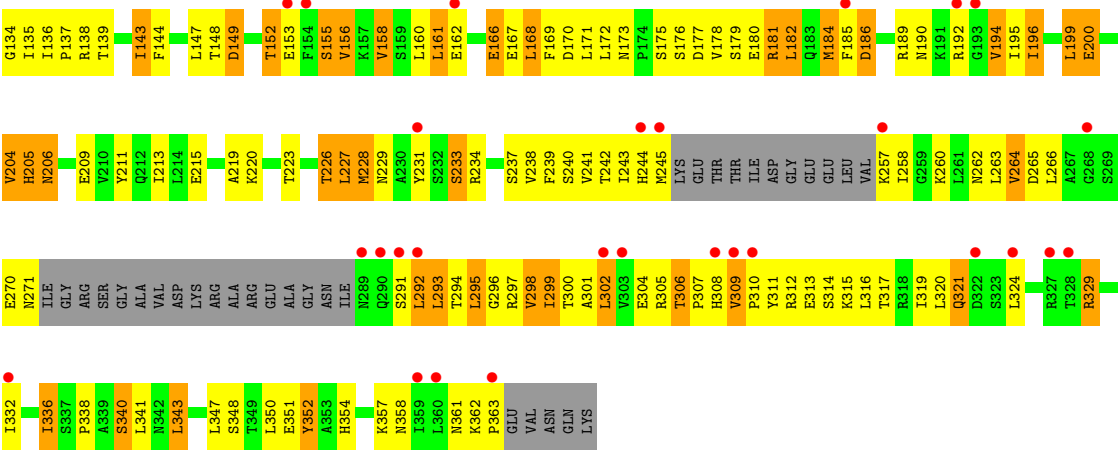


• Molecule 1: KINESIN-LIKE PROTEIN KIF11



• Molecule 1: KINESIN-LIKE PROTEIN KIF11





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.84Å 156.40Å 170.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.75 29.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.99-2.75) 97.3 (29.99-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.280 0.210 , 0.267	Depositor DCC
R_{free} test set	4939 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18210	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.91% 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, SO4, MG, CL, DQ8

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	0.85	0/2563	1.22	11/3467 (0.3%)
1	B	0.84	1/2593 (0.0%)	1.14	9/3505 (0.3%)
1	C	0.85	0/2589	1.21	23/3503 (0.7%)
1	D	0.84	0/2566	1.14	8/3471 (0.2%)
1	E	0.68	0/2542	1.09	17/3440 (0.5%)
1	F	0.72	0/2527	1.19	19/3421 (0.6%)
1	G	0.67	0/2483	1.13	17/3364 (0.5%)
All	All	0.78	1/17863 (0.0%)	1.16	104/24171 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	ILE	CA-CB	-6.24	1.50	1.54

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	210	VAL	N-CA-C	9.27	119.81	110.82
1	A	105	GLY	N-CA-C	8.89	121.54	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	VAL	N-CA-C	8.72	120.51	111.00
1	C	190	ASN	N-CA-C	-8.64	92.40	110.80
1	E	93	VAL	N-CA-C	-8.30	102.33	110.72

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	GLU	Peptide
1	C	189	ARG	Peptide
1	F	304	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2522	0	2550	146	0
1	B	2552	0	2584	87	0
1	C	2551	0	2563	127	0
1	D	2526	0	2539	95	0
1	E	2504	0	2520	146	0
1	F	2487	0	2494	233	0
1	G	2446	0	2442	243	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	4	0
2	D	27	0	12	5	0
2	E	27	0	12	5	0
2	F	27	0	12	3	0
2	G	27	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	26	0	23	7	0
4	B	26	0	23	8	0
4	C	26	0	23	2	0
4	D	26	0	23	4	0
4	E	26	0	23	9	0
4	F	26	0	23	7	0
4	G	26	0	23	7	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	D	5	0	0	0	0
7	A	32	0	0	2	0
7	B	34	0	0	0	0
7	C	47	0	0	2	0
7	D	46	0	0	2	0
7	E	22	0	0	1	0
7	F	25	0	0	1	0
7	G	19	0	0	0	0
All	All	18210	0	17937	1104	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 31.

The worst 5 of 1104 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:E:82:TYR:CE2	1:E:86:VAL:HG21	1.82	1.12
1:F:89:ILE:HD12	1:F:101:ILE:HD11	1.23	1.12
1:A:141:HIS:O	1:A:207:LYS:NZ	1.83	1.11
1:F:136:ILE:HD13	1:F:263:LEU:HD12	1.29	1.09
1:F:171:LEU:HD12	1:F:220:LYS:HB3	1.34	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/368 (86%)	300 (95%)	17 (5%)	0	100	100
1	B	319/368 (87%)	308 (97%)	11 (3%)	0	100	100
1	C	320/368 (87%)	302 (94%)	17 (5%)	1 (0%)	36	56
1	D	317/368 (86%)	303 (96%)	14 (4%)	0	100	100
1	E	315/368 (86%)	300 (95%)	15 (5%)	0	100	100
1	F	314/368 (85%)	286 (91%)	27 (9%)	1 (0%)	36	56
1	G	312/368 (85%)	277 (89%)	33 (11%)	2 (1%)	21	38
All	All	2214/2576 (86%)	2076 (94%)	134 (6%)	4 (0%)	43	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	206	ASN
1	G	97	TYR
1	C	190	ASN
1	F	307	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/322 (88%)	243 (86%)	41 (14%)	3	5
1	B	288/322 (89%)	257 (89%)	31 (11%)	6	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	287/322 (89%)	249 (87%)	38 (13%)	4	7
1	D	284/322 (88%)	251 (88%)	33 (12%)	5	10
1	E	281/322 (87%)	233 (83%)	48 (17%)	2	3
1	F	279/322 (87%)	225 (81%)	54 (19%)	1	2
1	G	269/322 (84%)	200 (74%)	69 (26%)	0	1
All	All	1972/2254 (88%)	1658 (84%)	314 (16%)	2	4

5 of 314 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	271	ASN
1	G	204	VAL
1	F	309	VAL
1	G	102	PHE
1	G	293	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	290	GLN
1	F	290	GLN
1	F	78	GLN
1	G	142	GLN
1	B	308	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 21 are monoatomic - leaving 15 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	DQ8	B	801	-	28,28,28	0.67	0	38,38,38	1.05	2 (5%)
4	DQ8	F	801	-	28,28,28	0.76	1 (3%)	38,38,38	1.09	3 (7%)
6	SO4	D	1362	-	4,4,4	0.33	0	6,6,6	0.38	0
2	ADP	A	601	3	28,29,29	1.47	6 (21%)	43,45,45	1.99	13 (30%)
4	DQ8	E	801	-	28,28,28	0.71	1 (3%)	38,38,38	1.08	4 (10%)
2	ADP	G	601	3	28,29,29	1.47	3 (10%)	43,45,45	2.06	10 (23%)
4	DQ8	A	801	-	28,28,28	0.85	1 (3%)	38,38,38	1.12	1 (2%)
4	DQ8	G	801	-	28,28,28	0.91	2 (7%)	38,38,38	1.26	5 (13%)
4	DQ8	D	801	-	28,28,28	0.97	1 (3%)	38,38,38	1.37	5 (13%)
4	DQ8	C	801	-	28,28,28	0.77	0	38,38,38	1.32	6 (15%)
2	ADP	F	601	3	28,29,29	1.60	6 (21%)	43,45,45	1.66	8 (18%)
2	ADP	E	601	3	28,29,29	1.49	6 (21%)	43,45,45	1.79	10 (23%)
2	ADP	C	601	3	28,29,29	1.56	5 (17%)	43,45,45	1.84	12 (27%)
2	ADP	B	601	3	28,29,29	1.34	4 (14%)	43,45,45	2.12	14 (32%)
2	ADP	D	601	3	28,29,29	1.38	4 (14%)	43,45,45	1.97	13 (30%)

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	DQ8	B	801	-	-	2/27/27/27	0/3/3/3
4	DQ8	F	801	-	-	0/27/27/27	0/3/3/3
2	ADP	A	601	3	-	2/16/32/32	0/3/3/3
4	DQ8	E	801	-	-	2/27/27/27	0/3/3/3
2	ADP	G	601	3	-	1/16/32/32	0/3/3/3
4	DQ8	A	801	-	-	0/27/27/27	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DQ8	G	801	-	-	2/27/27/27	0/3/3/3
4	DQ8	D	801	-	-	2/27/27/27	0/3/3/3
4	DQ8	C	801	-	-	2/27/27/27	0/3/3/3
2	ADP	F	601	3	-	2/16/32/32	0/3/3/3
2	ADP	E	601	3	-	5/16/32/32	0/3/3/3
2	ADP	C	601	3	-	3/16/32/32	0/3/3/3
2	ADP	B	601	3	-	2/16/32/32	0/3/3/3
2	ADP	D	601	3	-	1/16/32/32	0/3/3/3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	ADP	C5-C4	5.11	1.48	1.39
2	F	601	ADP	C5-C4	5.06	1.48	1.39
2	C	601	ADP	C5-C4	4.83	1.47	1.39
2	E	601	ADP	C5-C4	4.67	1.47	1.39
2	A	601	ADP	C5-C4	4.52	1.47	1.39

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5-C4-N3	-6.63	117.59	126.72
2	G	601	ADP	C5-C4-N3	-6.26	118.10	126.72
2	A	601	ADP	C5-C4-N3	-5.80	118.74	126.72
2	G	601	ADP	N3-C4-N9	5.60	136.69	127.17
2	D	601	ADP	C5-C4-N3	-5.41	119.26	126.72

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	ADP	PA-O3A-PB-O2B
2	E	601	ADP	C5'-O5'-PA-O2A
2	E	601	ADP	C3'-C4'-C5'-O5'
2	B	601	ADP	PA-O3A-PB-O1B
2	C	601	ADP	PA-O3A-PB-O2B

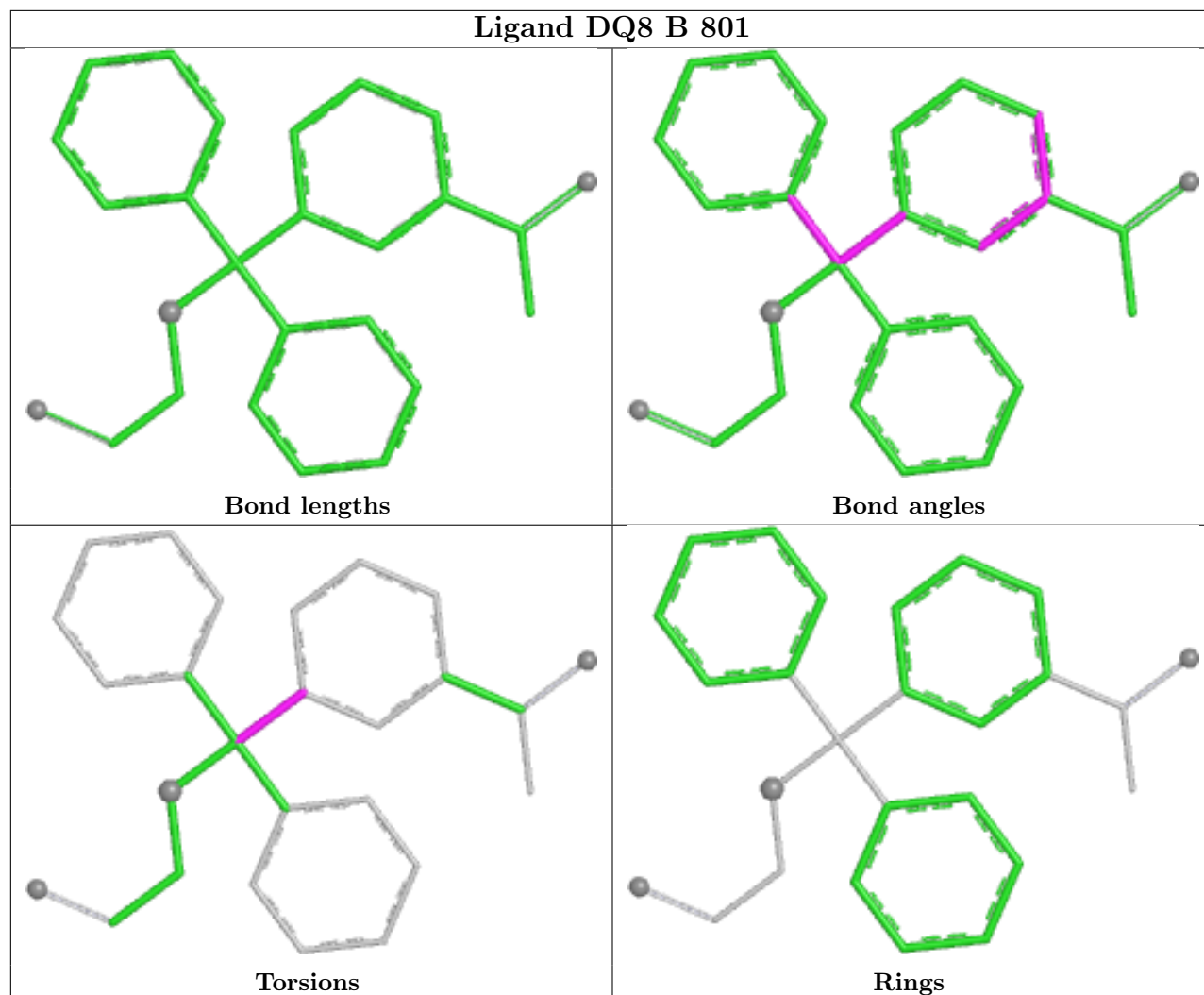
There are no ring outliers.

12 monomers are involved in 63 short contacts:

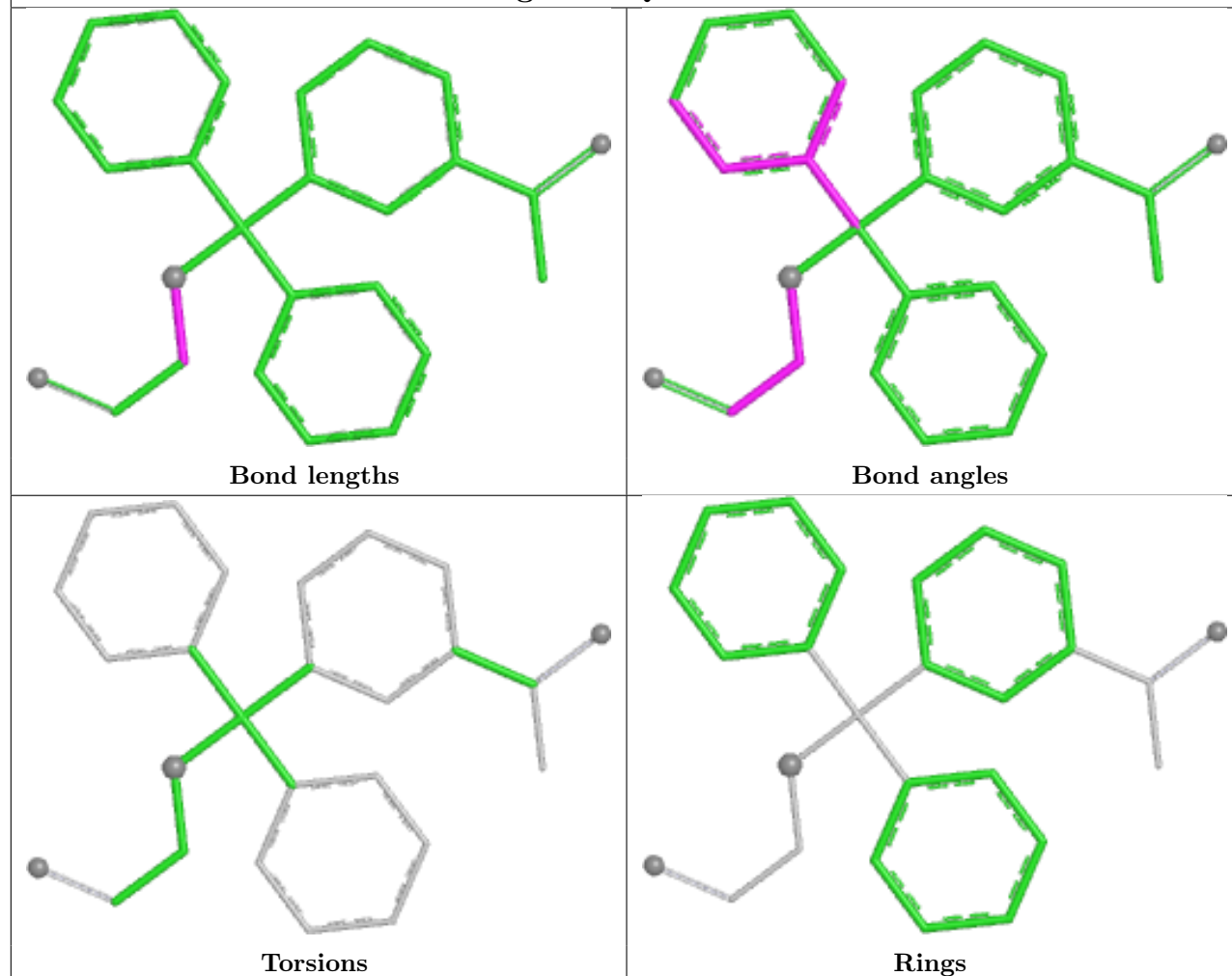
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	DQ8	8	0
4	F	801	DQ8	7	0
4	E	801	DQ8	9	0
2	G	601	ADP	2	0
4	A	801	DQ8	7	0
4	G	801	DQ8	7	0
4	D	801	DQ8	4	0
4	C	801	DQ8	2	0
2	F	601	ADP	3	0
2	E	601	ADP	5	0
2	C	601	ADP	4	0
2	D	601	ADP	5	0

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.

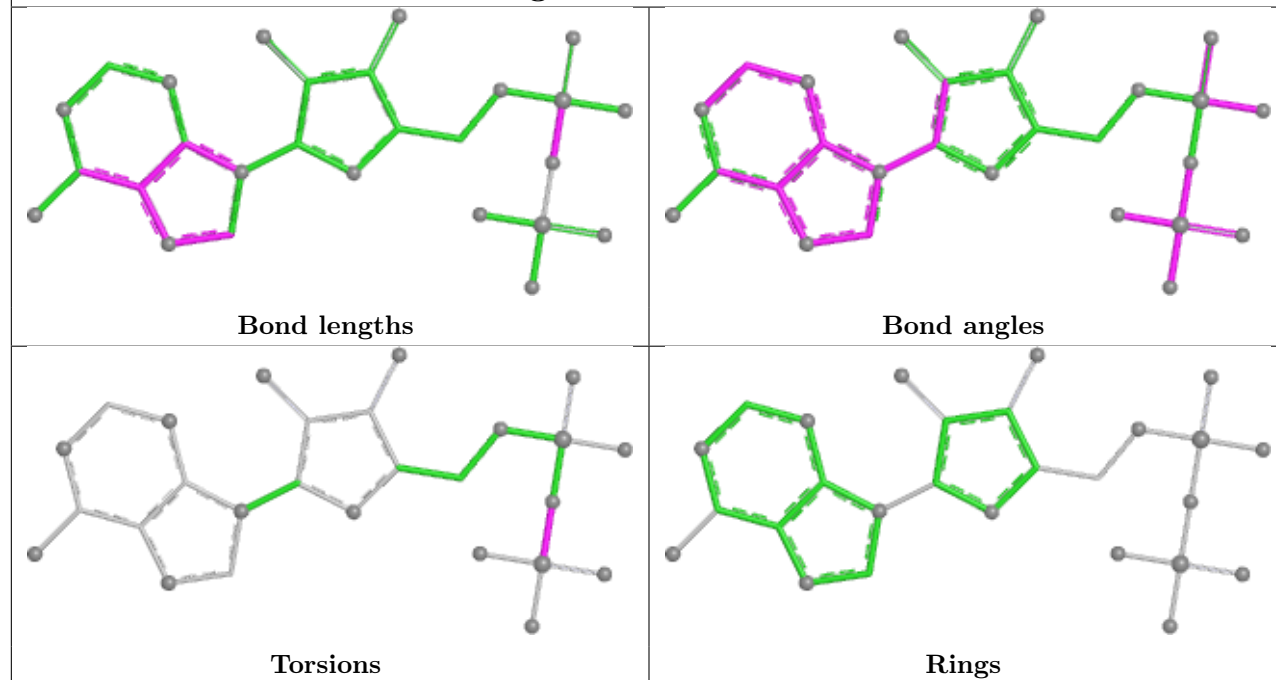
Ligand DQ8 B 801



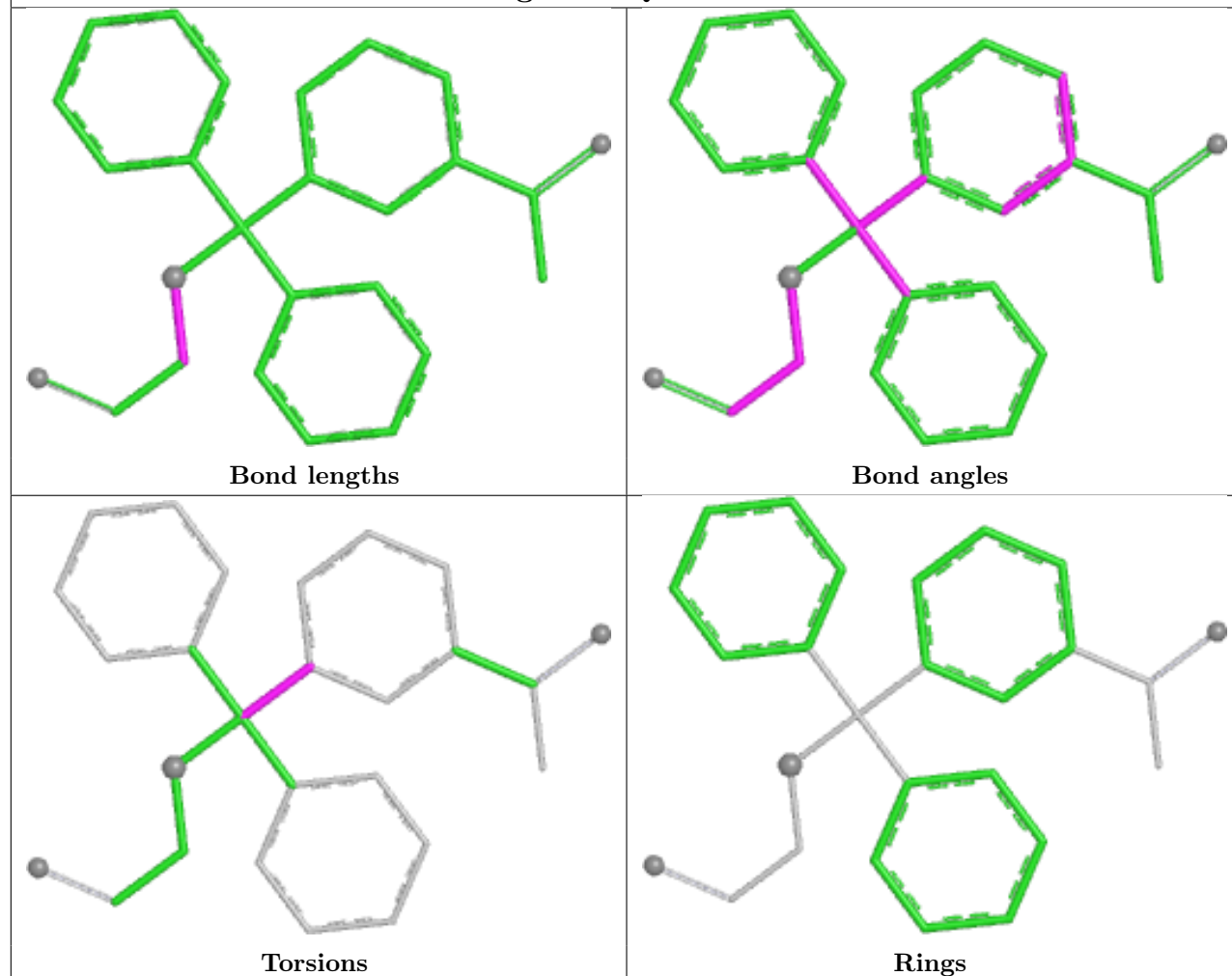
Ligand DQ8 F 801



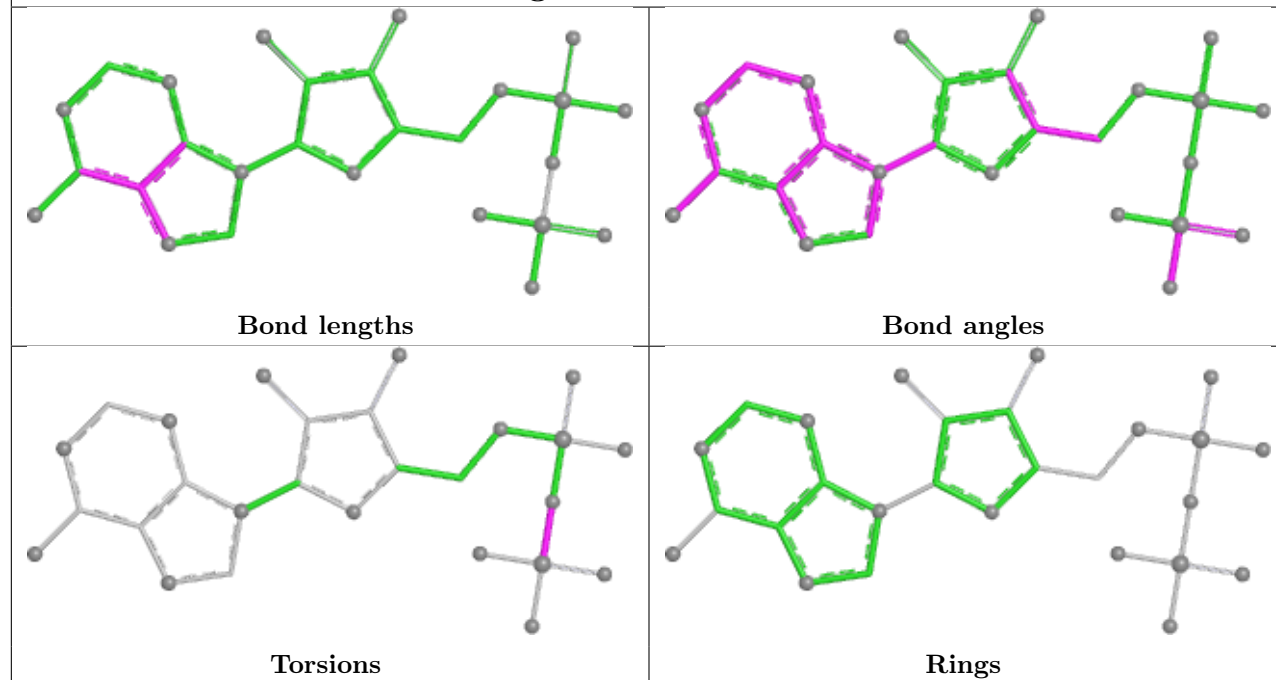
Ligand ADP A 601



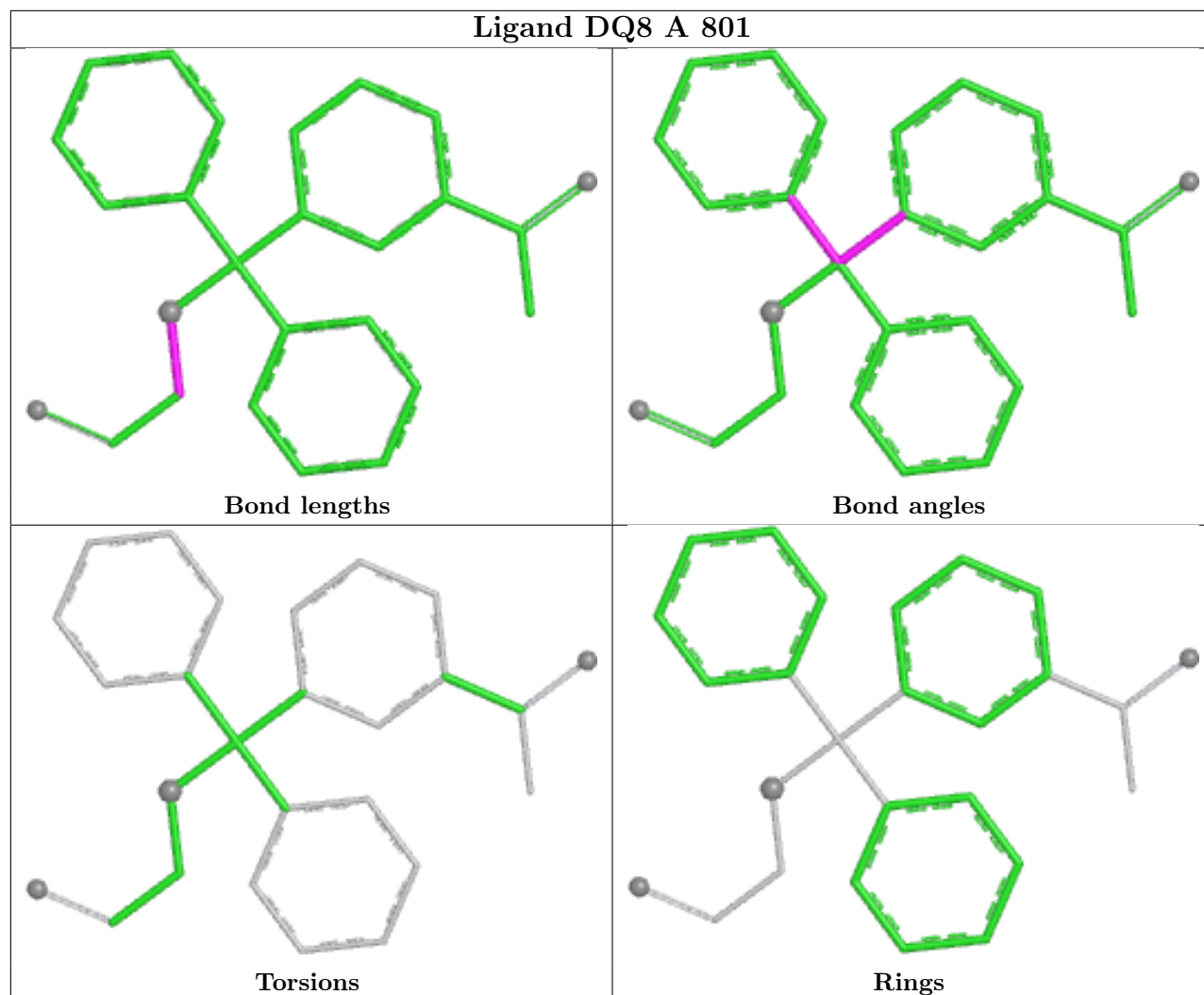
Ligand DQ8 E 801



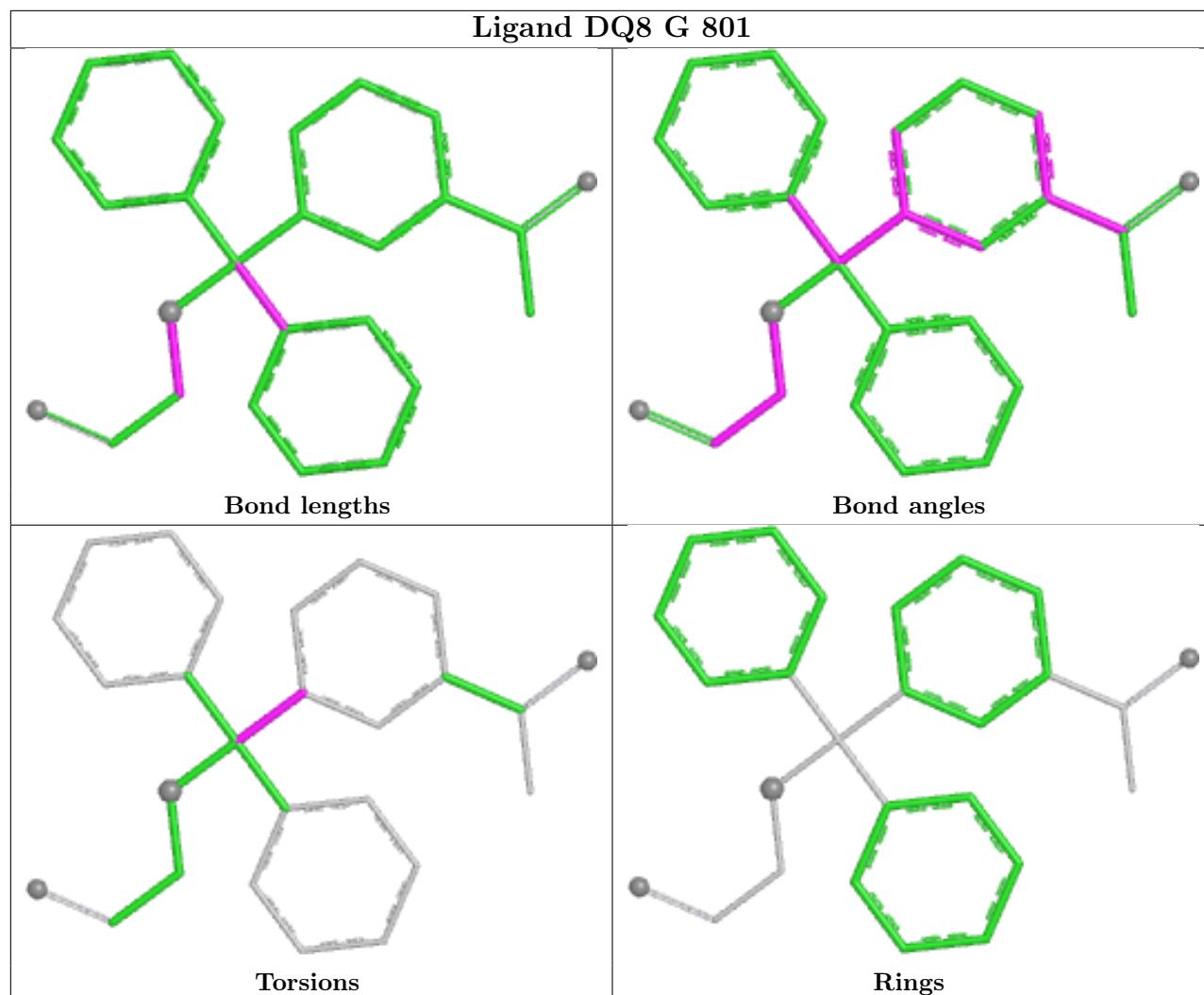
Ligand ADP G 601



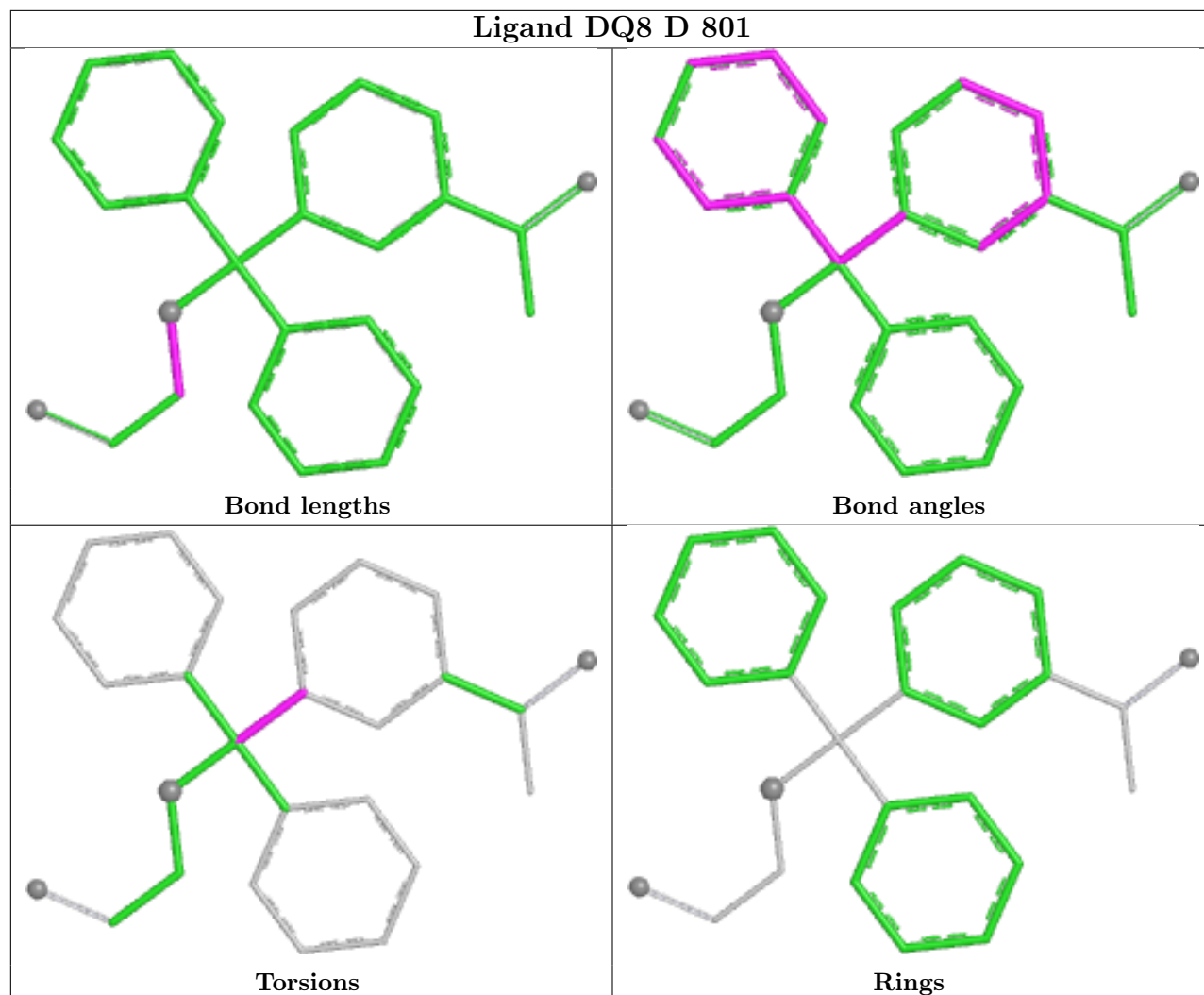
Ligand DQ8 A 801



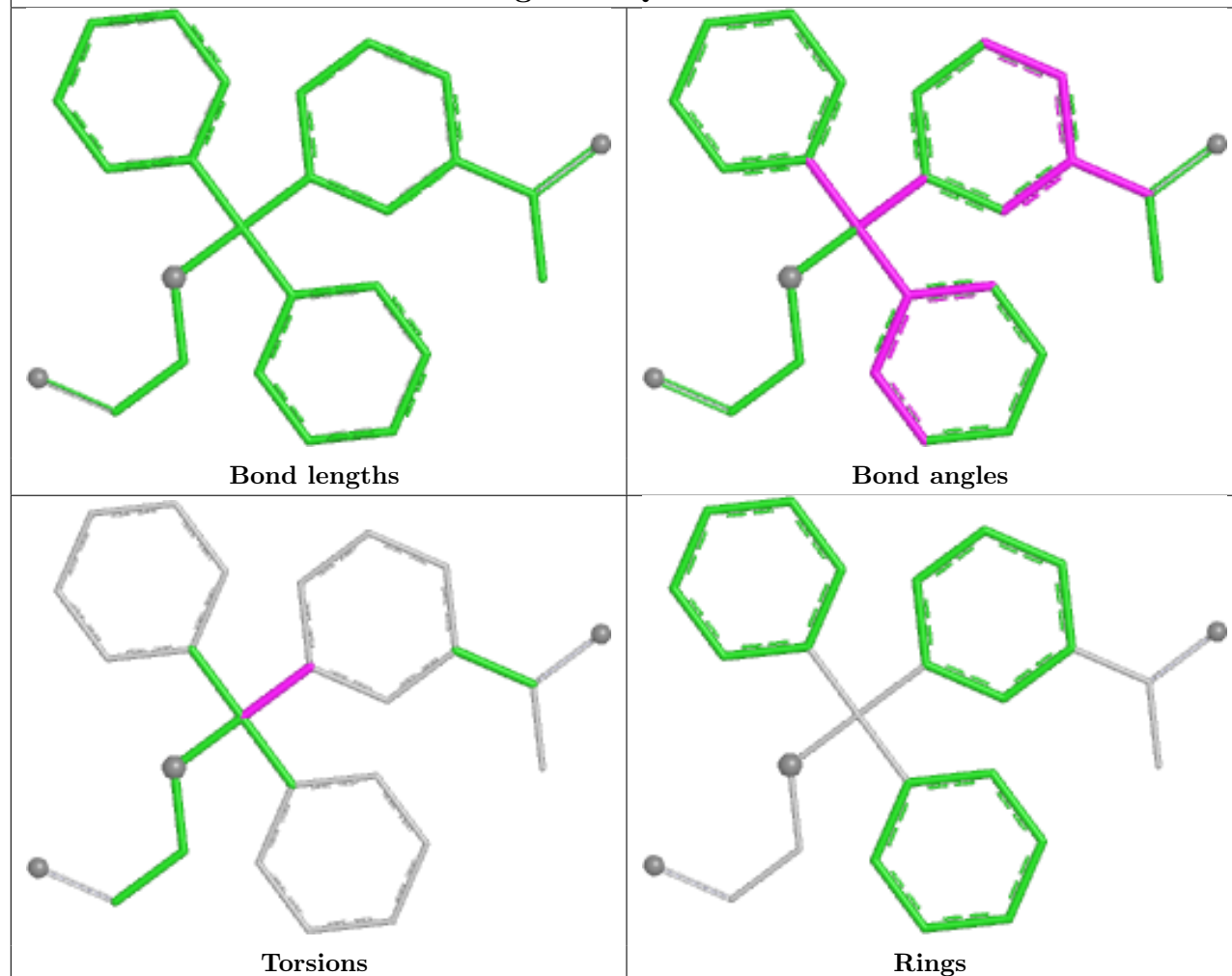
Ligand DQ8 G 801



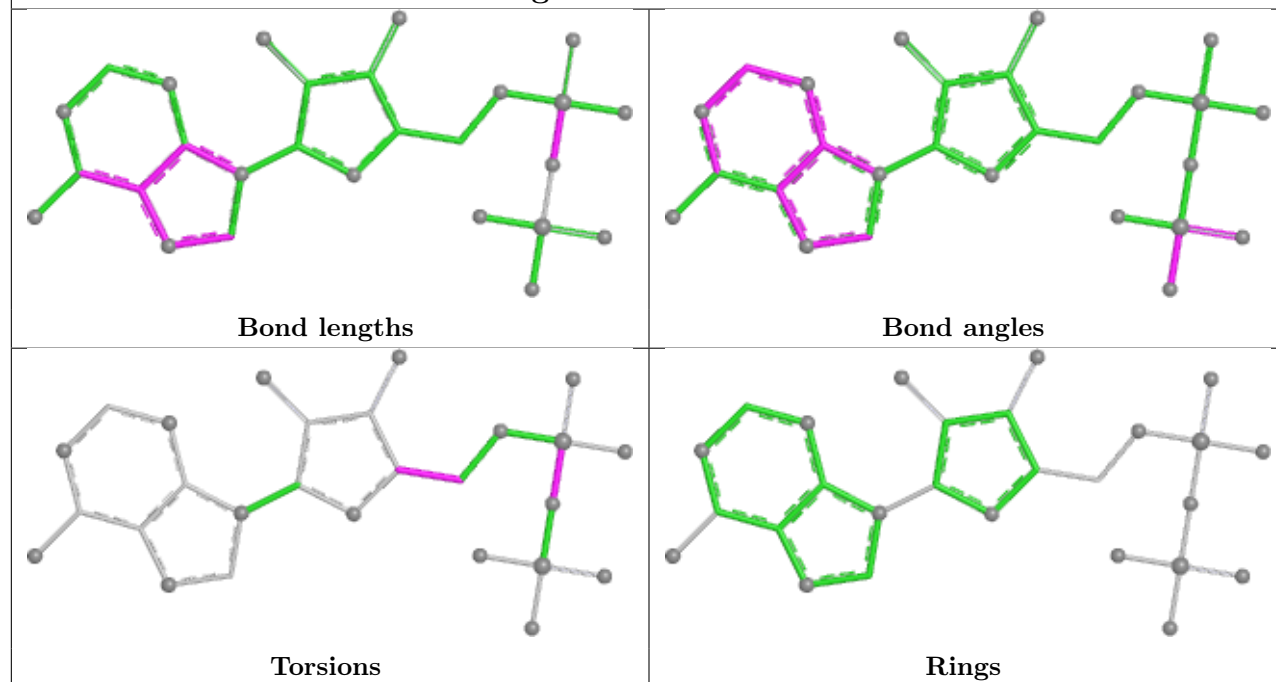
Ligand DQ8 D 801

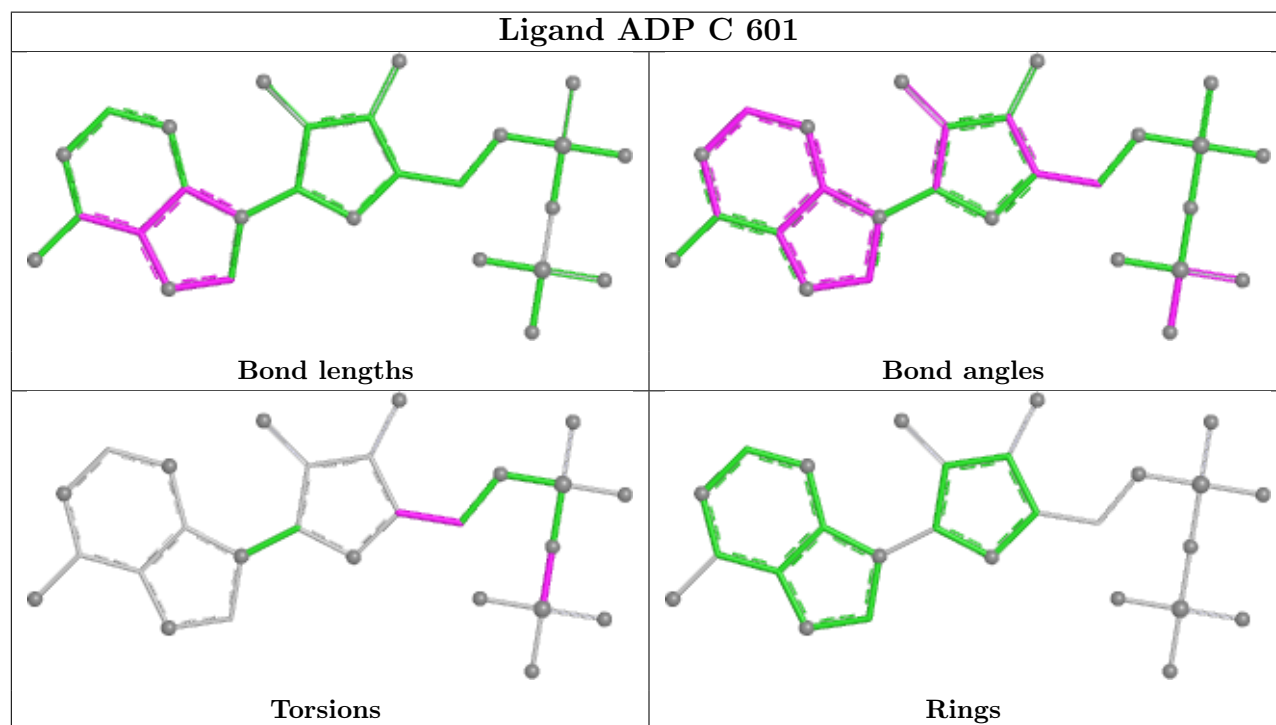
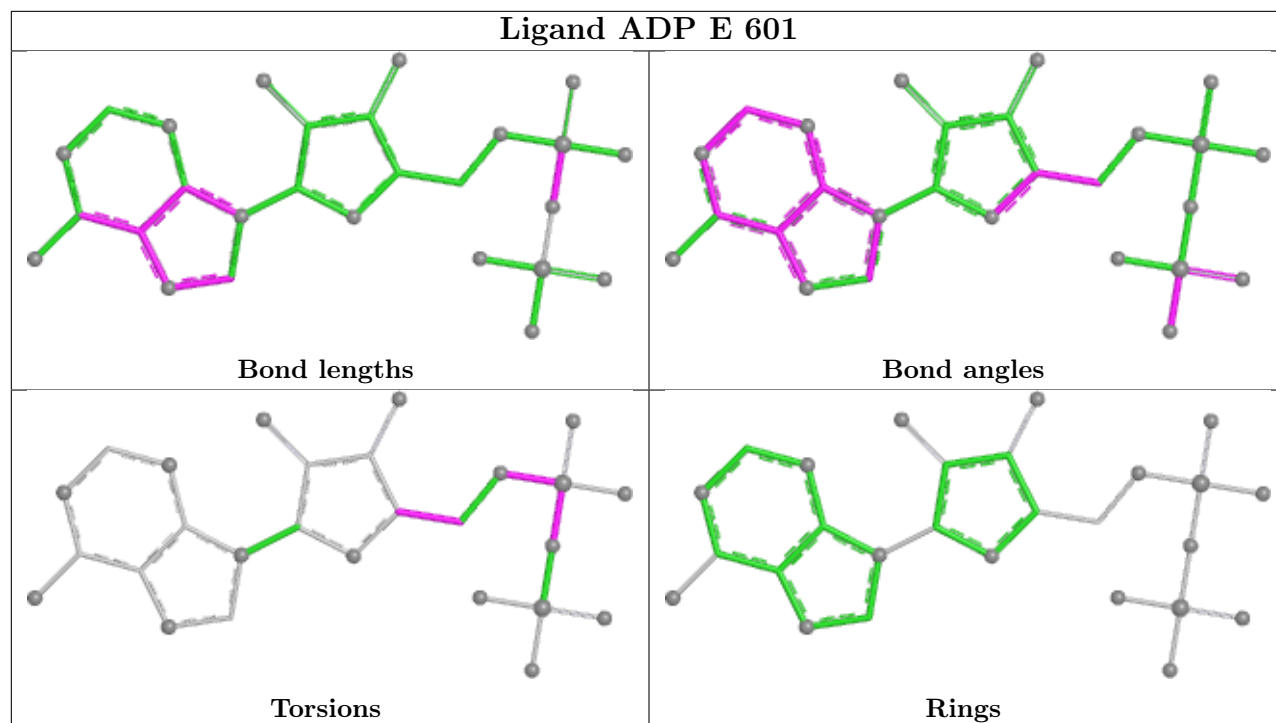


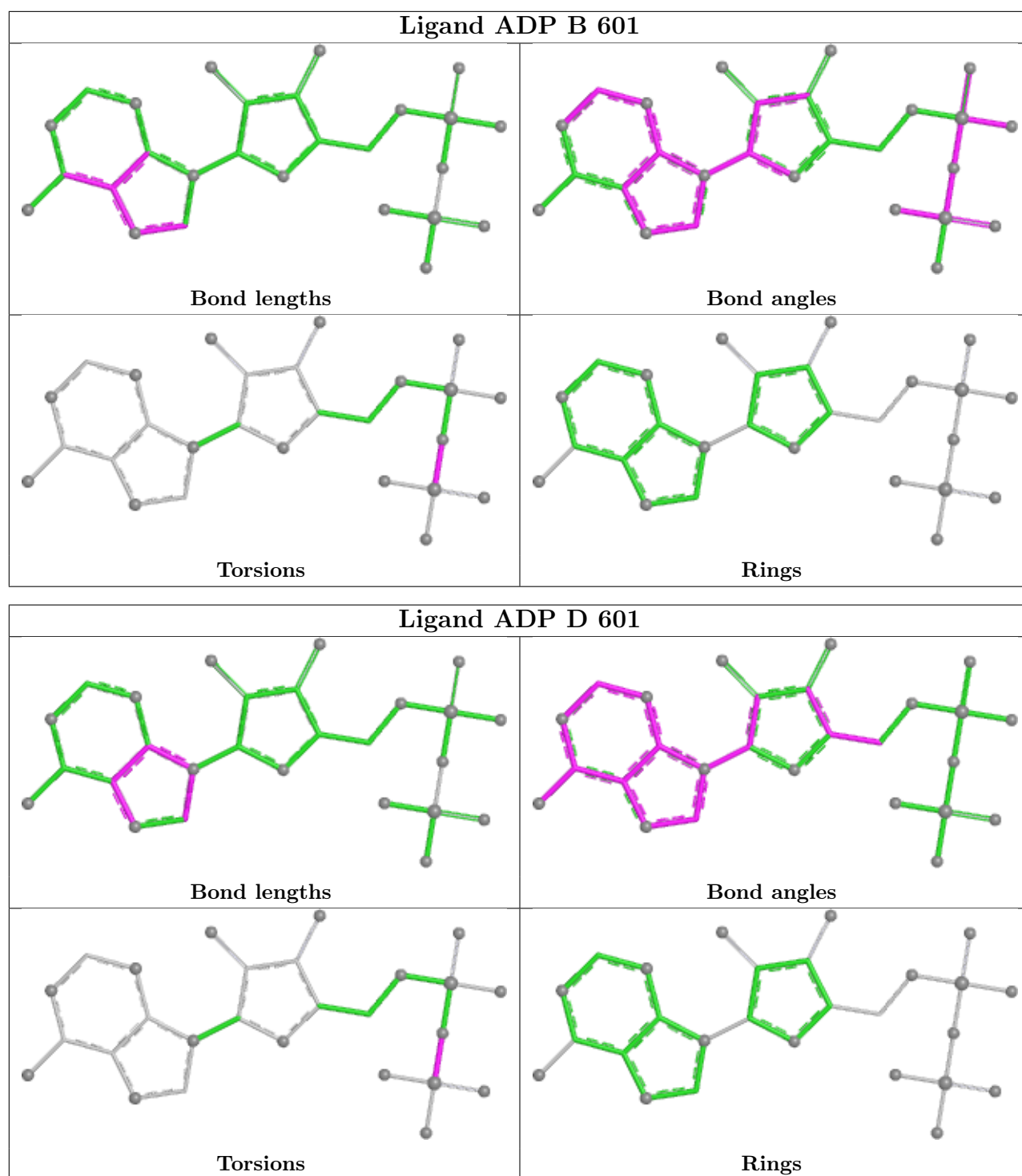
Ligand DQ8 C 801



Ligand ADP F 601







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 [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	322/368 (87%)	0.30	19 (5%)	28 28	25, 54, 90, 112	1 (0%)
1	B	324/368 (88%)	0.18	11 (3%)	48 46	22, 53, 92, 104	1 (0%)
1	C	325/368 (88%)	0.06	10 (3%)	51 49	28, 50, 86, 113	1 (0%)
1	D	322/368 (87%)	0.21	16 (4%)	34 34	20, 50, 92, 114	1 (0%)
1	E	321/368 (87%)	0.54	23 (7%)	21 21	42, 67, 99, 119	0
1	F	319/368 (86%)	0.74	33 (10%)	12 11	41, 71, 106, 117	1 (0%)
1	G	318/368 (86%)	0.91	44 (13%)	6 5	46, 81, 122, 140	0
All	All	2251/2576 (87%)	0.42	156 (6%)	23 22	20, 61, 105, 140	5 (0%)

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	289	ASN	6.2
1	B	129	GLU	5.2
1	F	93	VAL	5.2
1	G	327	ARG	4.8
1	G	322	ASP	4.5

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 oligosaccharides in this entry.

6.4 Ligands

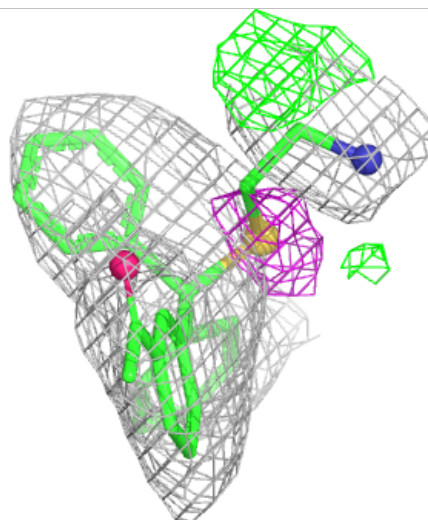
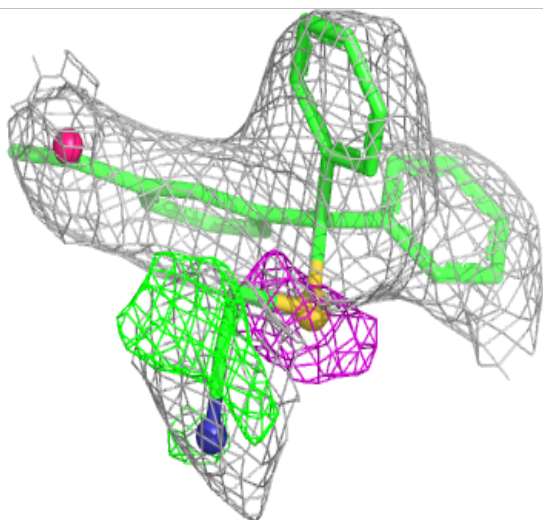
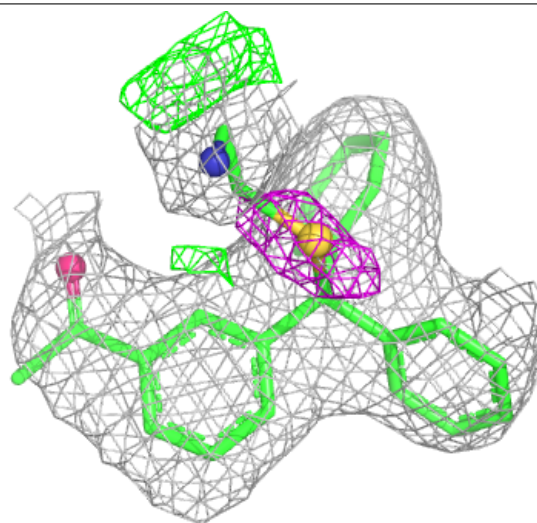
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	G	1364	1/1	0.82	0.12	106,106,106,106	0
5	CL	A	1365	1/1	0.83	0.12	95,95,95,95	0
4	DQ8	F	801	26/26	0.83	0.16	60,75,84,110	0
4	DQ8	E	801	26/26	0.87	0.13	57,67,77,98	0
5	CL	A	1366	1/1	0.88	0.13	89,89,89,89	0
4	DQ8	C	801	26/26	0.90	0.13	39,49,61,83	0
4	DQ8	D	801	26/26	0.91	0.12	38,47,60,79	0
4	DQ8	A	801	26/26	0.91	0.12	43,54,63,85	0
4	DQ8	B	801	26/26	0.92	0.12	44,53,67,82	0
5	CL	B	1365	1/1	0.92	0.13	78,78,78,78	0
5	CL	D	1364	1/1	0.92	0.18	77,77,77,77	0
5	CL	E	1364	1/1	0.92	0.10	90,90,90,90	0
5	CL	F	1364	1/1	0.92	0.18	89,89,89,89	0
3	MG	C	701	1/1	0.92	0.09	40,40,40,40	0
4	DQ8	G	801	26/26	0.93	0.12	49,57,68,85	0
5	CL	C	1367	1/1	0.94	0.24	62,62,62,62	0
5	CL	C	1369	1/1	0.94	0.10	97,97,97,97	0
6	SO4	D	1362	5/5	0.94	0.09	54,54,63,68	0
5	CL	A	1364	1/1	0.95	0.12	75,75,75,75	0
3	MG	G	701	1/1	0.95	0.14	45,45,45,45	0
2	ADP	E	601	27/27	0.95	0.09	45,54,61,71	0
5	CL	B	1364	1/1	0.95	0.27	80,80,80,80	0
5	CL	A	1367	1/1	0.96	0.18	73,73,73,73	0
5	CL	C	1368	1/1	0.96	0.06	56,56,56,56	0
2	ADP	F	601	27/27	0.96	0.07	45,55,70,77	0
3	MG	B	701	1/1	0.96	0.08	37,37,37,37	0
2	ADP	B	601	27/27	0.97	0.07	35,42,48,58	0
2	ADP	D	601	27/27	0.97	0.06	28,40,45,51	0
2	ADP	G	601	27/27	0.97	0.06	46,54,59,64	0
5	CL	D	1363	1/1	0.98	0.15	79,79,79,79	0
3	MG	D	701	1/1	0.98	0.08	35,35,35,35	0
3	MG	E	701	1/1	0.98	0.06	50,50,50,50	0
3	MG	F	701	1/1	0.98	0.06	50,50,50,50	0
2	ADP	A	601	27/27	0.98	0.06	34,41,47,50	0
2	ADP	C	601	27/27	0.98	0.06	28,38,42,48	0
3	MG	A	701	1/1	0.99	0.04	35,35,35,35	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.

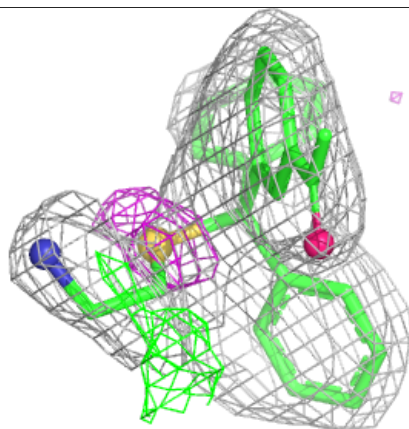
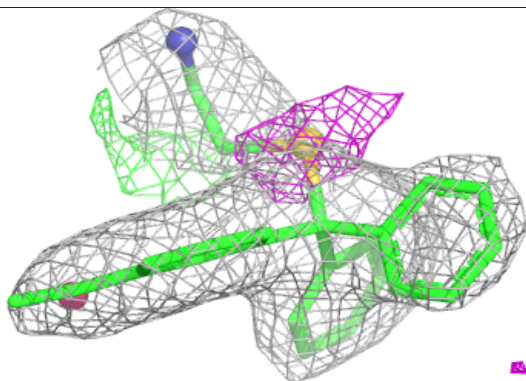
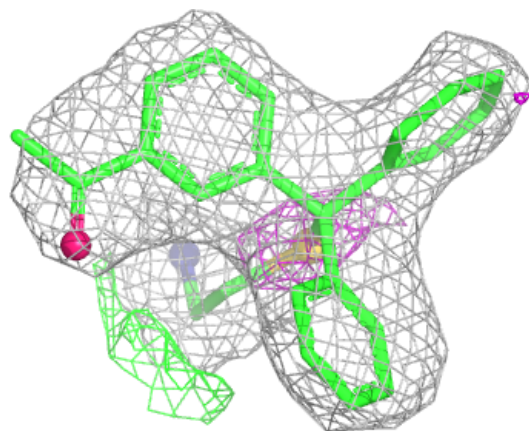
Electron density around DQ8 F 801:

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



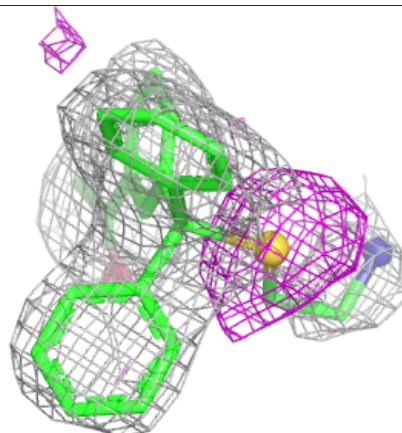
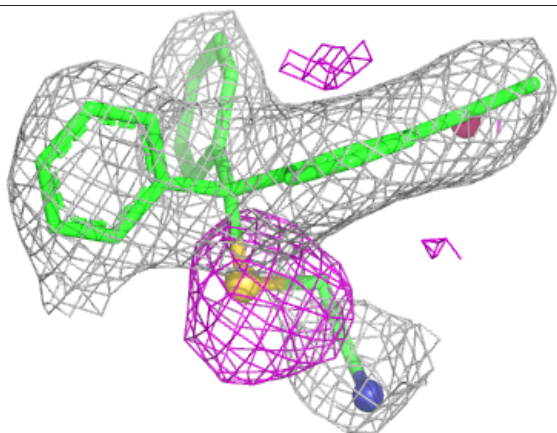
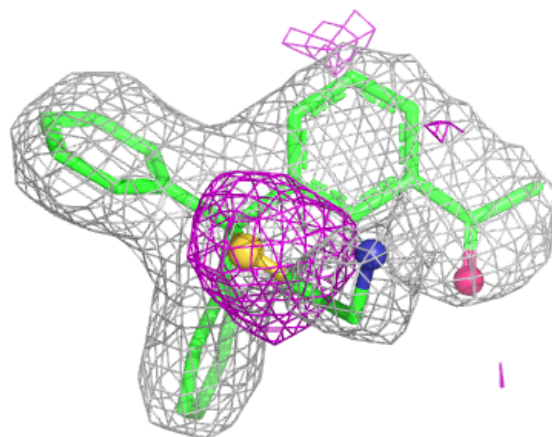
Electron density around DQ8 E 801:

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and green (positive)



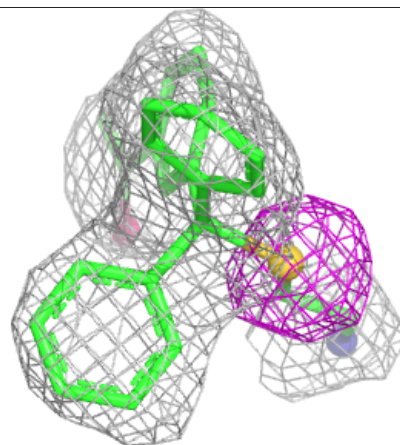
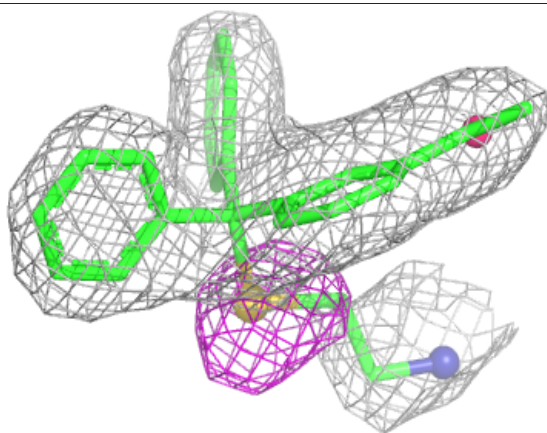
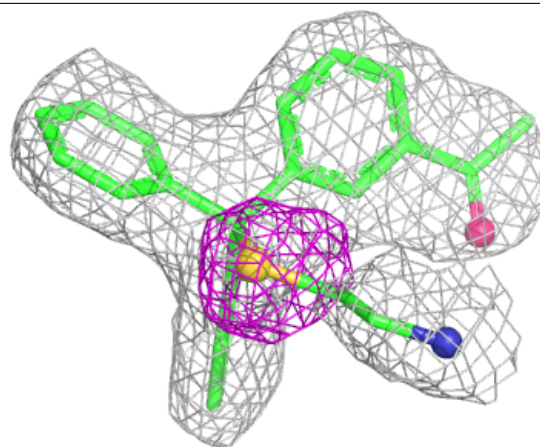
Electron density around DQ8 C 801:

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and green (positive)



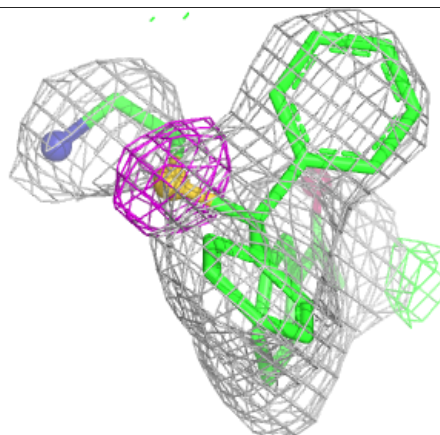
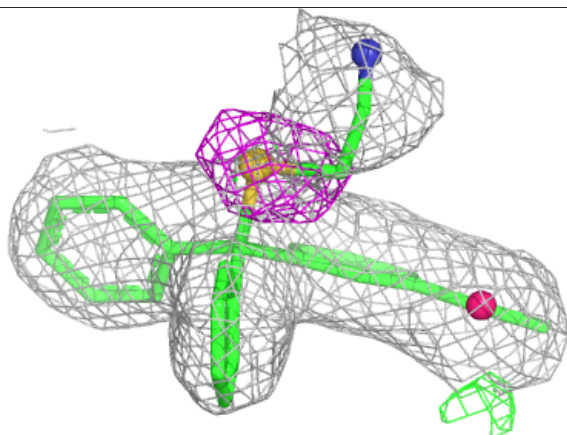
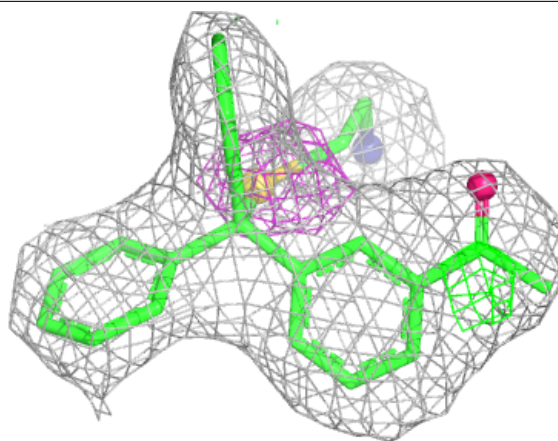
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and green (positive)



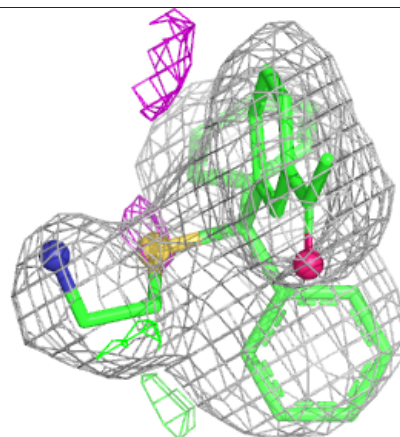
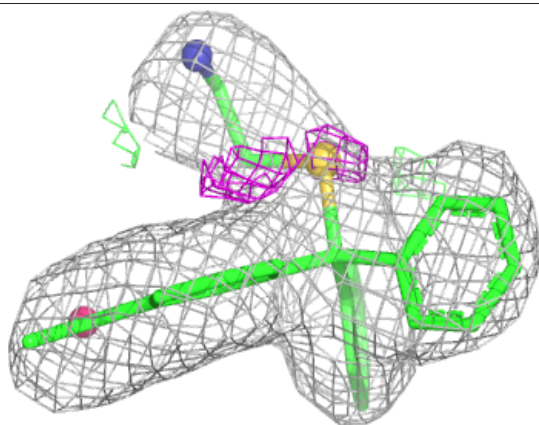
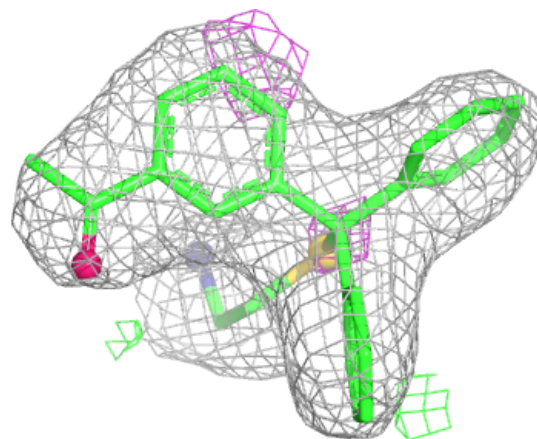
Electron density around DQ8 A 801:

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and green (positive)



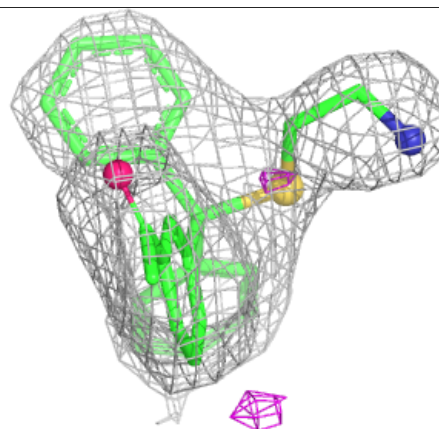
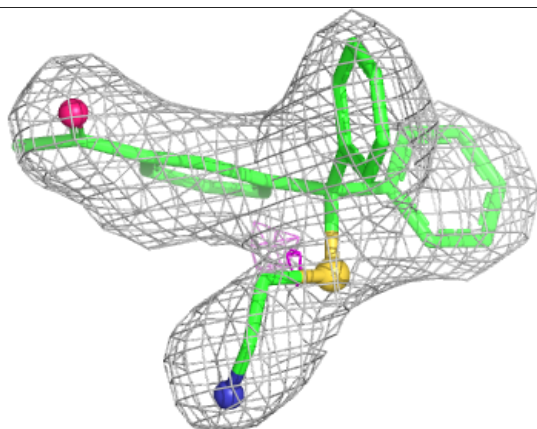
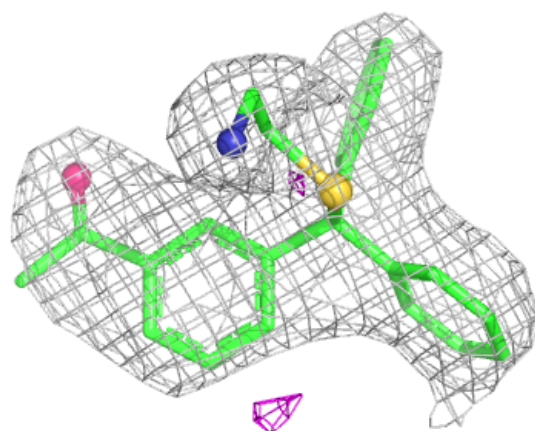
Electron density around DQ8 B 801:

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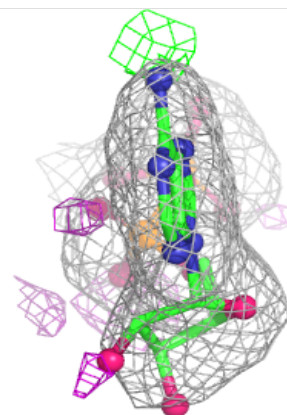
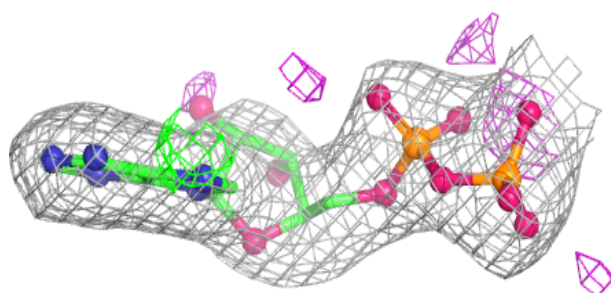
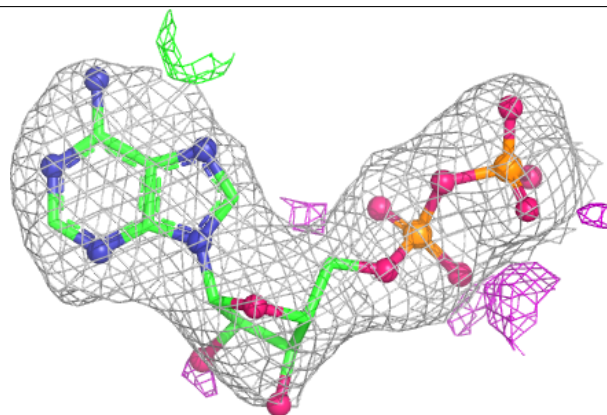


Electron density around DQ8 G 801:

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and green (positive)

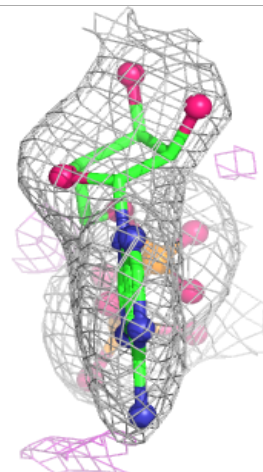
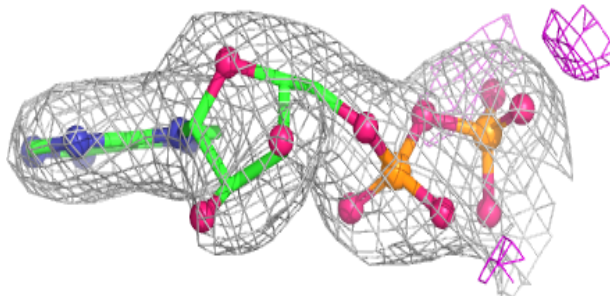
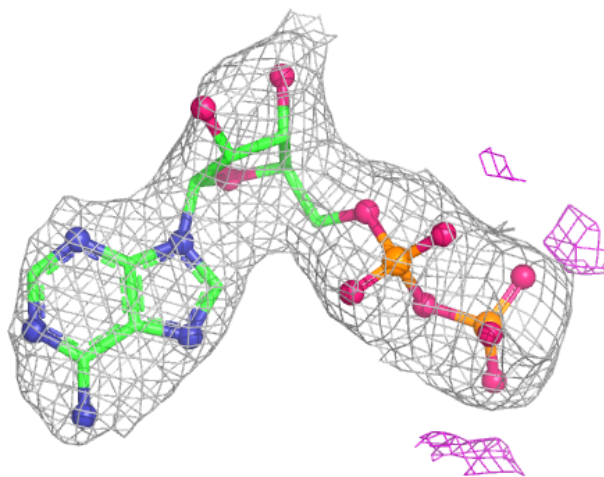
**Electron density around ADP E 601:**

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



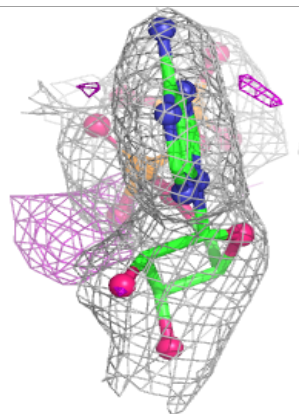
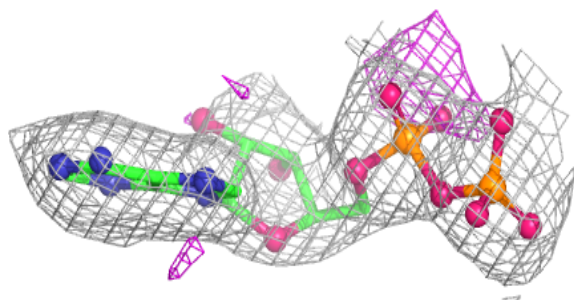
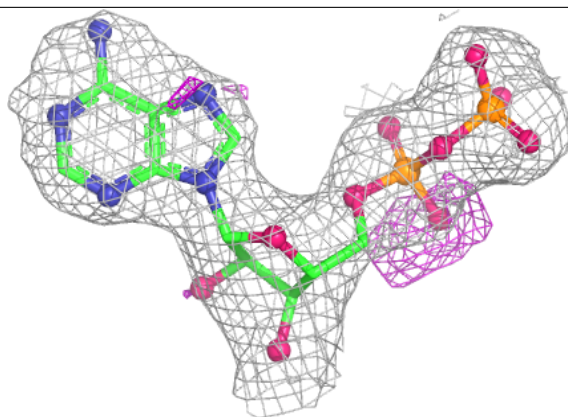
Electron density around ADP F 601:

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

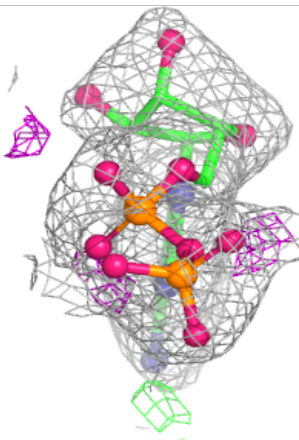
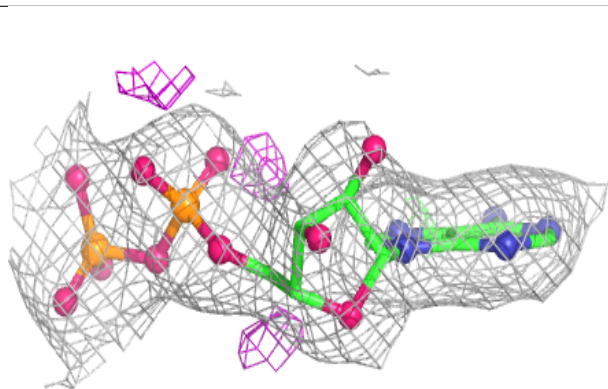
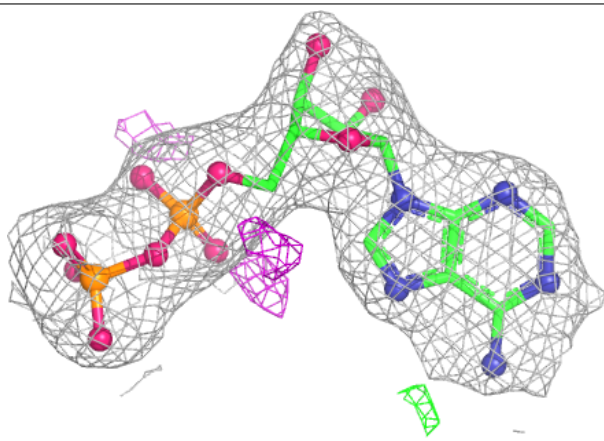


Electron density around ADP B 601:

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

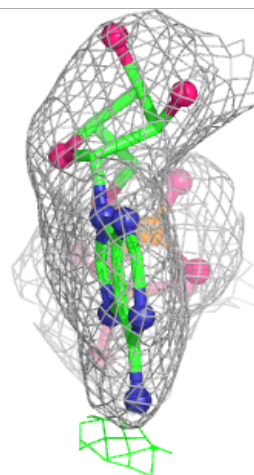
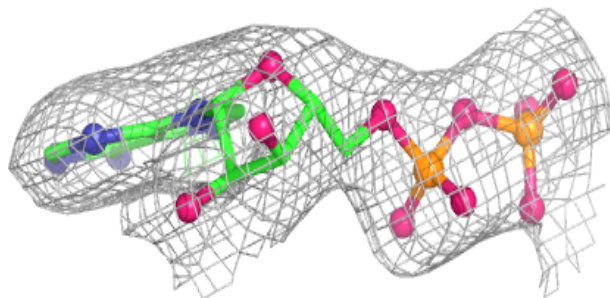
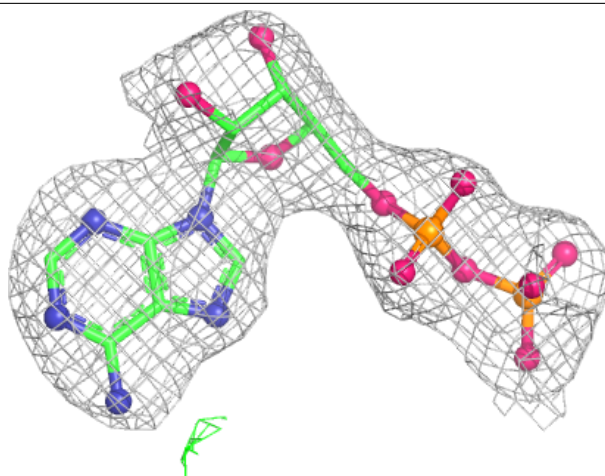
**Electron density around ADP D 601:**

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



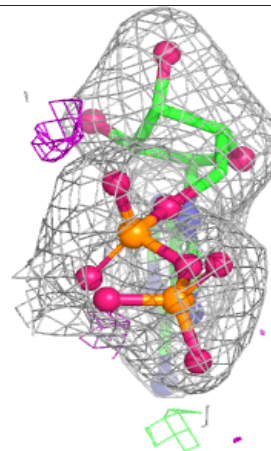
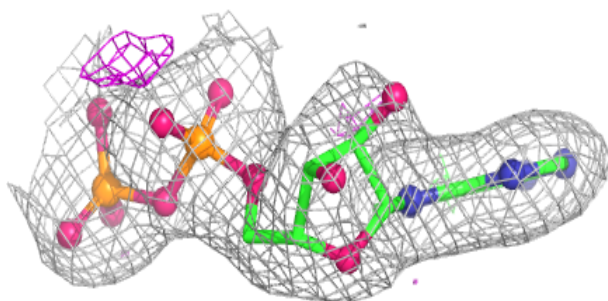
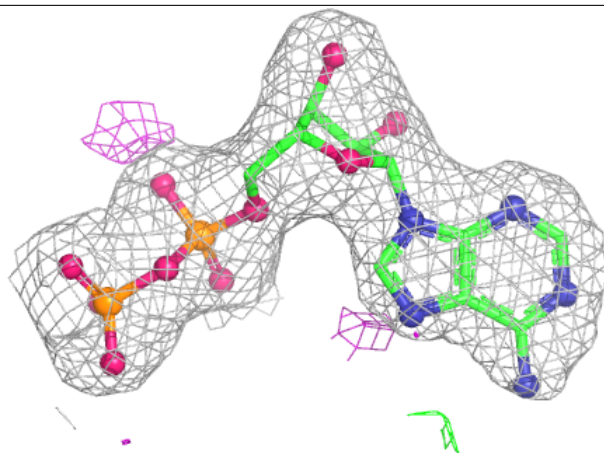
Electron density around ADP G 601:

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



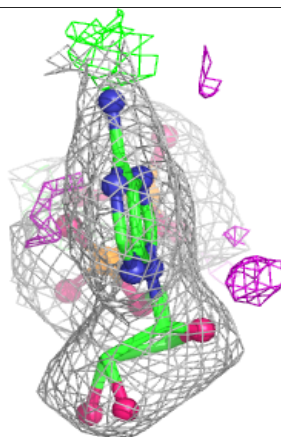
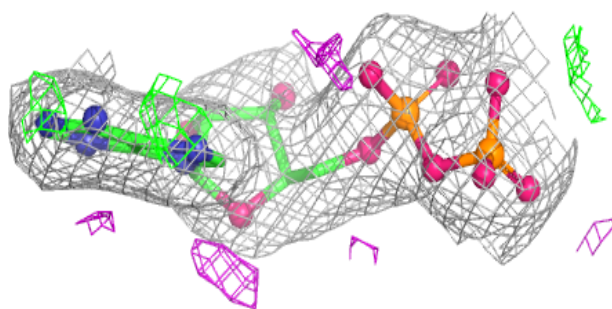
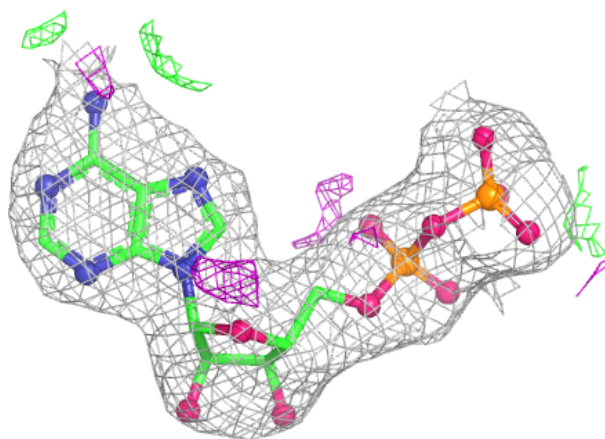
Electron density around ADP A 601:

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



Electron density around ADP C 601:

$2mF_o - DF_c$ (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.