wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 05:01 am GMT

PDB ID	:	4A51
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

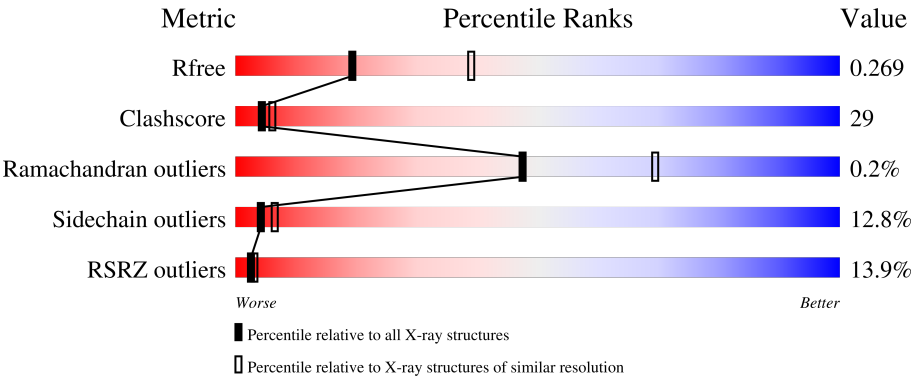
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	368	10% 50% 33% · 12%
1	B	368	11% 59% 24% 5% 12%
1	C	368	6% 55% 28% 5% 12%
1	D	368	7% 57% 29% · 12%
1	E	368	14% 46% 36% 5% 13%

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Mol	Chain	Length	Quality of chain
1	F	368	16% 36% 42% 10% 13%
1	G	368	20% 35% 39% 13% 14%

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)

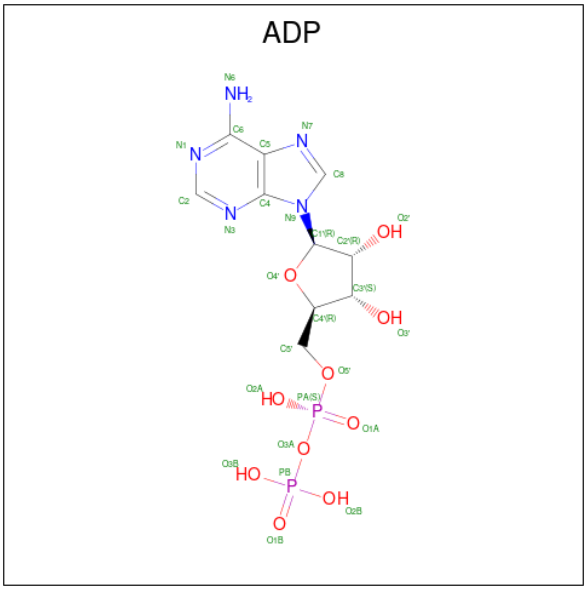
There are 7 unique types of molecules in this entry. The entry contains 18210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

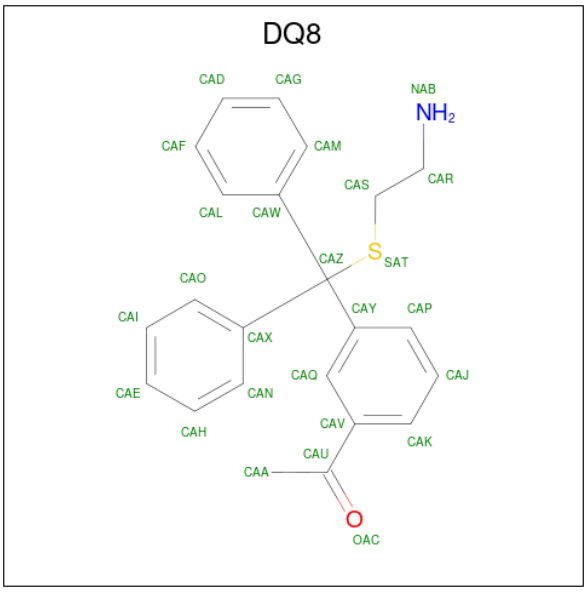


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G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

- Molecule 3 is MAGNESIUM ION (three-letter code: 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 (three-letter code: DQ8) (formula: $C_{23}H_{23}NOS$).



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 (three-letter code: 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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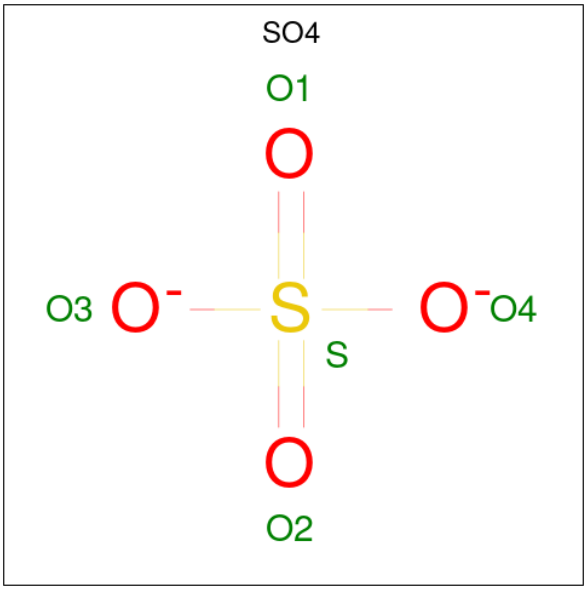
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is water.

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

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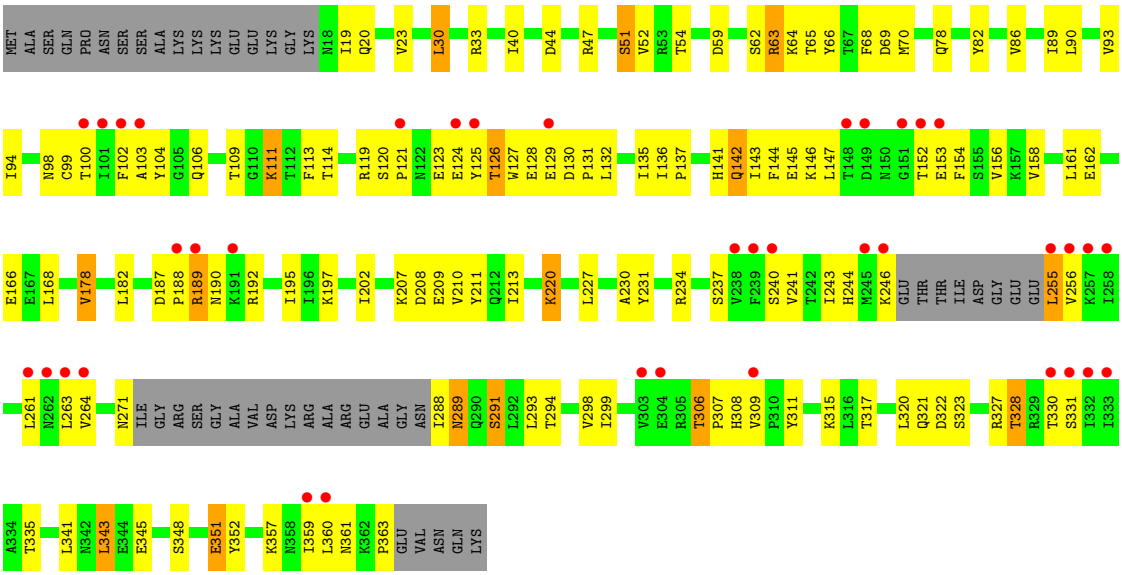
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	19	Total 19	O 19	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

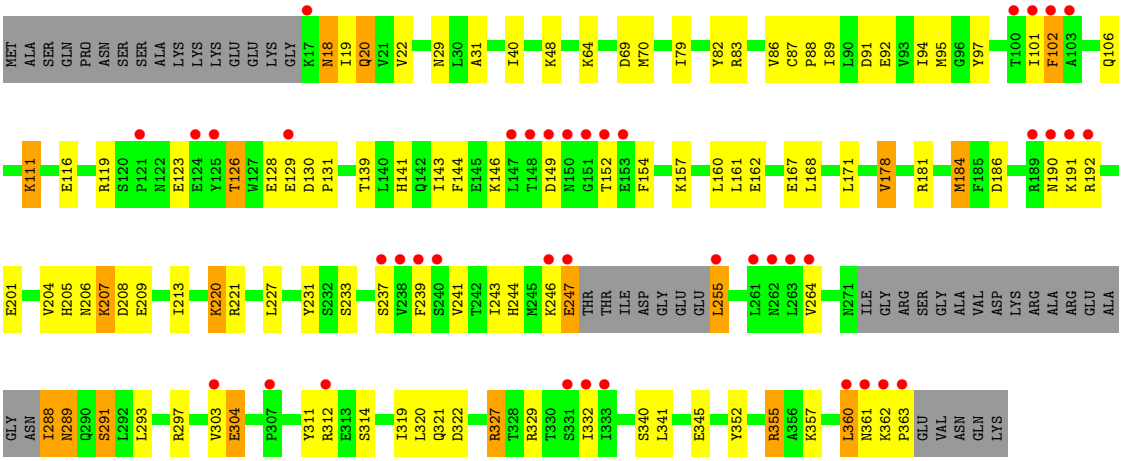
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain A:



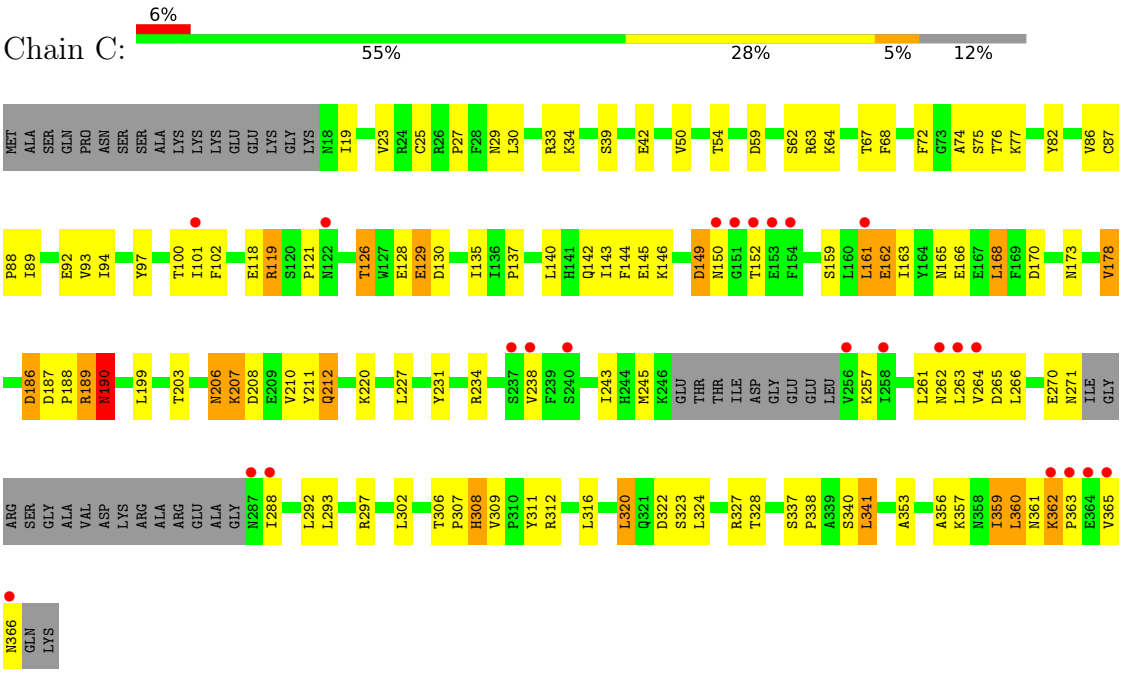
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain B:



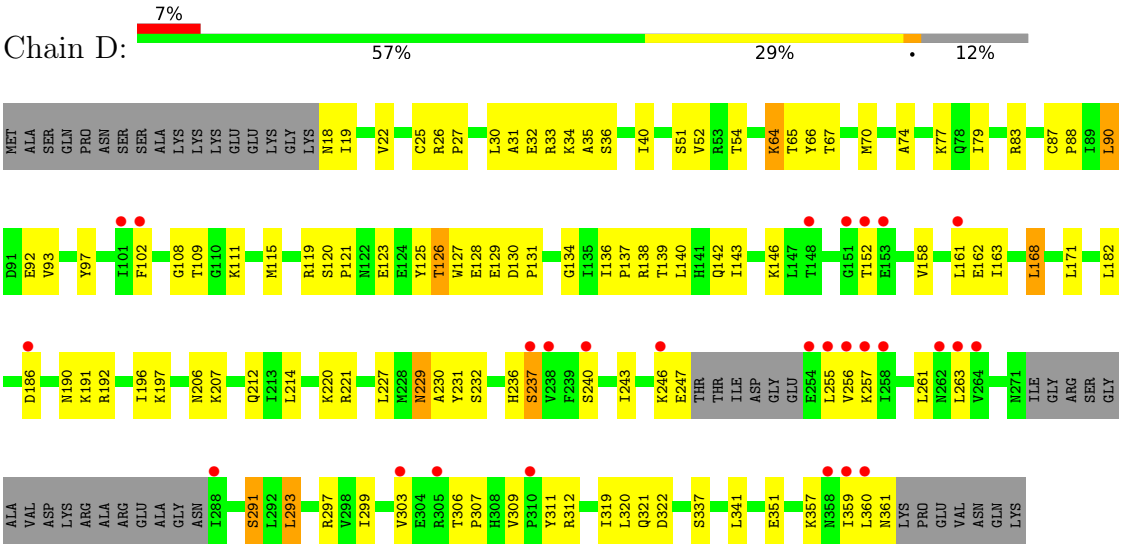
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain C:



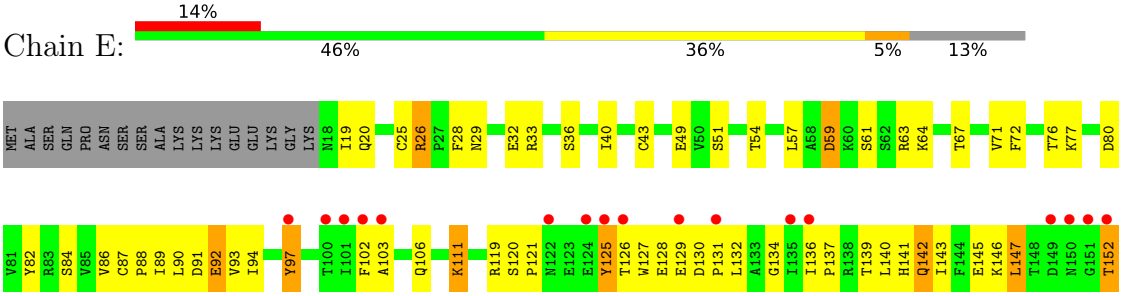
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

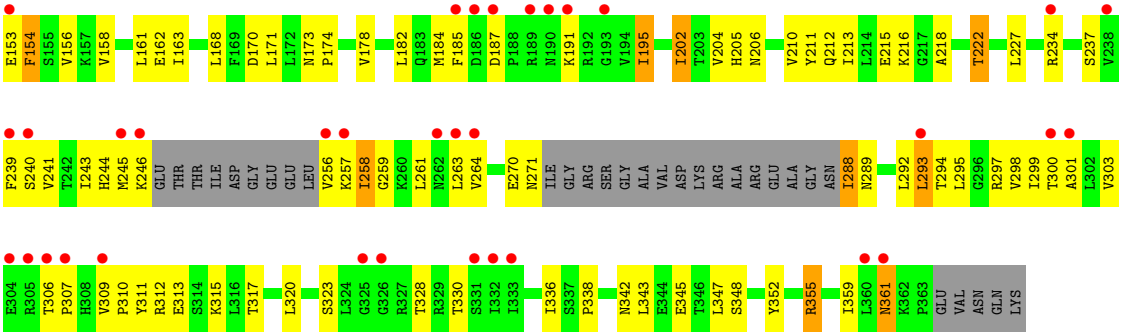
Chain D:



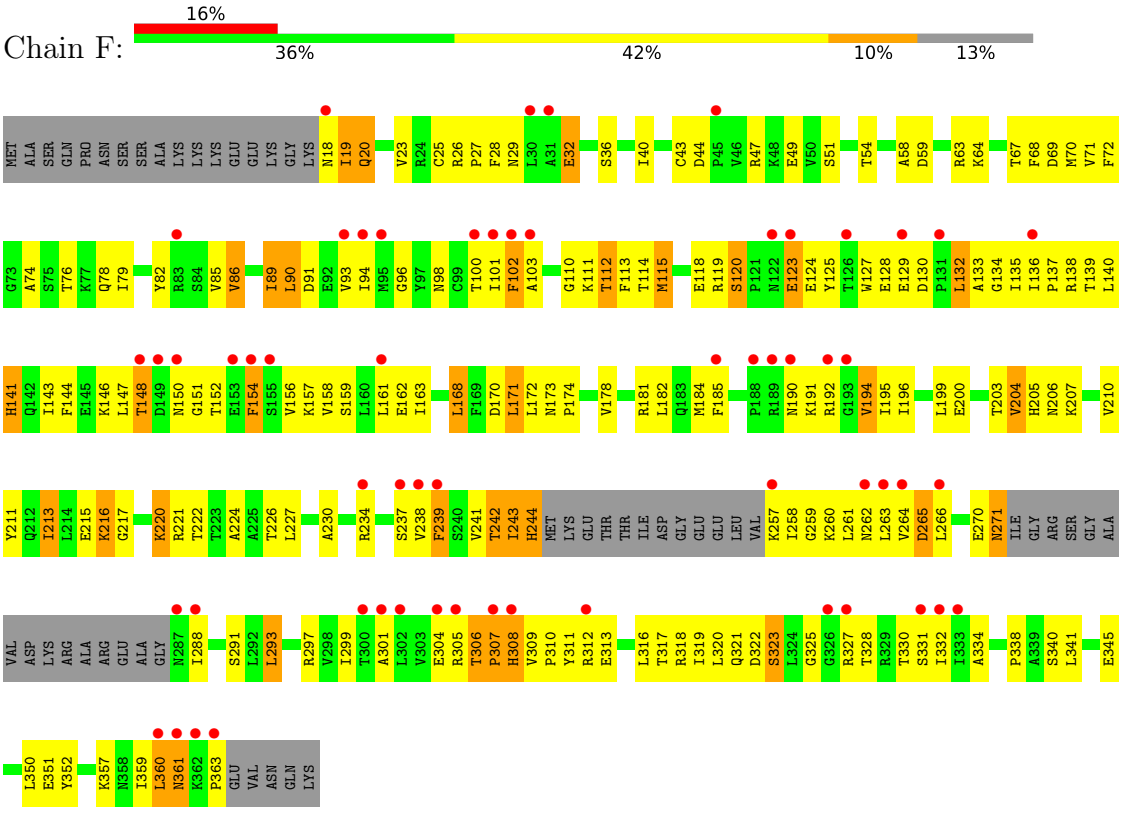
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain E:

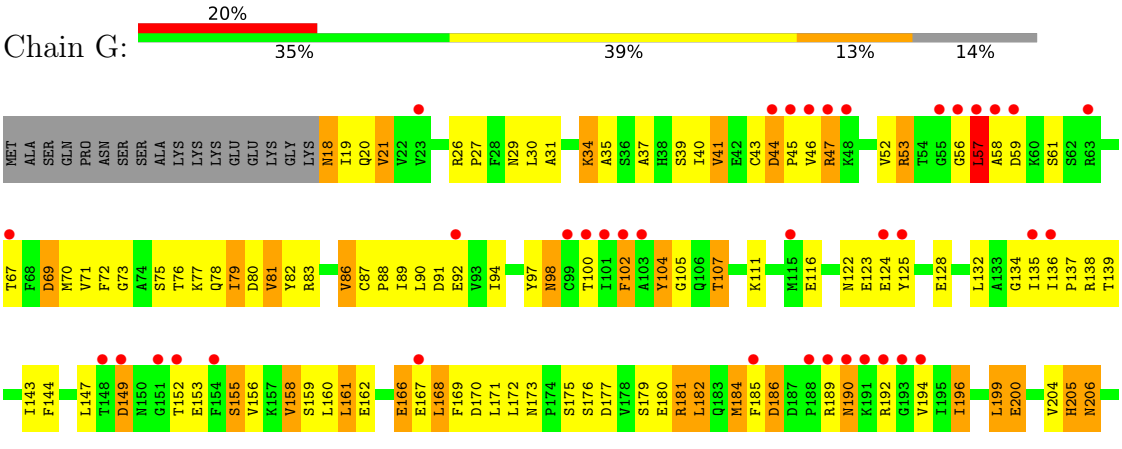


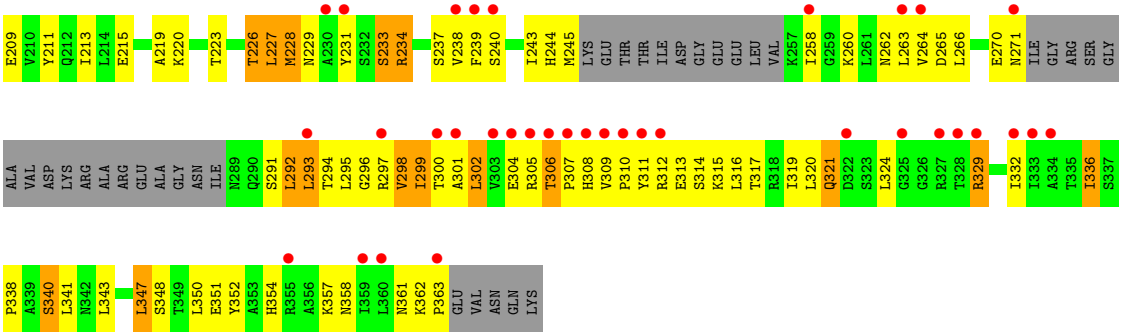


• Molecule 1: KINESIN-LIKE PROTEIN KIF11



• Molecule 1: KINESIN-LIKE PROTEIN KIF11




E209 V210 Y211 Q212 I213 L214 E215 A219 K220 T223 T226 L227 M228 N229 A230 Y231 S232 S233 R234 S237 V238 F239 S240 I243 H244 M245 LYS GLU THR THR ILE ASP GLY GLU GLU LEU VAL K257 I258 G259 K260 L261 N262 L263 V264 D265 L266 E270 N271 ILE GLY ARG SER GLY
ALA VAL ASP LYS ARG ALA ARG GLU ALA GLY ASN ILE N289 Q290 S291 L292 L293 T294 L295 G296 R297 V298 I299 T300 A301 L302 V303 E304 R305 T306 P307 H308 V309 P310 Y311 R312 E313 S314 K315 L316 T317 R318 I319 L320 Q321 D322 S323 L324 G325 G326 R327 T328 R329 I332 I333 A334 T335 I336 S337
P338 A339 S340 L341 N342 L343 L347 S348 T349 L350 E351 Y352 A353 H354 R355 A356 K357 N358 I359 L360 N361 K362 P363 GLU VAL ASN GLN LYS

4 Data and refinement statistics (i)

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) 97.4 (29.99-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.280 0.213 , 0.269	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)	0.34 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, CL, SO4, 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	0.68	0/2563	0.83	0/3467
1	B	0.65	0/2593	0.80	1/3505 (0.0%)
1	C	0.66	0/2589	0.83	1/3503 (0.0%)
1	D	0.67	0/2566	0.80	1/3471 (0.0%)
1	E	0.53	0/2542	0.71	0/3440
1	F	0.54	0/2527	0.78	0/3421
1	G	0.52	0/2483	0.75	2/3364 (0.1%)
All	All	0.61	0/17863	0.79	5/24171 (0.0%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	190	ASN	N-CA-C	-6.89	92.40	111.00
1	G	57	LEU	CA-CB-CG	6.63	130.54	115.30
1	D	263	LEU	CA-CB-CG	-5.99	101.53	115.30
1	B	241	VAL	CB-CA-C	-5.68	100.60	111.40
1	G	57	LEU	N-CA-C	5.36	125.47	111.00

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 (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	2522	0	2550	138	0
1	B	2552	0	2584	78	0
1	C	2551	0	2563	117	0
1	D	2526	0	2539	88	0
1	E	2504	0	2520	139	0
1	F	2487	0	2494	222	0
1	G	2446	0	2442	232	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1040	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 29.

The worst 5 of 1040 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 (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	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%)	41	60
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%)	41	60
1	G	312/368 (85%)	277 (89%)	33 (11%)	2 (1%)	25	42
All	All	2214/2576 (86%)	2076 (94%)	134 (6%)	4 (0%)	47	69

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/322 (88%)	256 (90%)	28 (10%)	8	13
1	B	288/322 (89%)	260 (90%)	28 (10%)	8	14
1	C	287/322 (89%)	255 (89%)	32 (11%)	6	10
1	D	284/322 (88%)	262 (92%)	22 (8%)	13	22
1	E	281/322 (87%)	248 (88%)	33 (12%)	5	8
1	F	279/322 (87%)	233 (84%)	46 (16%)	2	3
1	G	269/322 (84%)	206 (77%)	63 (23%)	1	1
All	All	1972/2254 (88%)	1720 (87%)	252 (13%)	4	6

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	59	ASP
1	G	185	PHE
1	F	19	ILE
1	G	182	LEU
1	G	243	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	20	GLN
1	G	18	ASN
1	G	262	ASN
1	G	354	HIS
1	G	358	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	E	801	-	28,28,28	0.69	1 (3%)	38,38,38	1.07	4 (10%)
6	SO4	D	1362	-	4,4,4	0.21	0	6,6,6	0.38	0
4	DQ8	D	801	-	28,28,28	0.99	2 (7%)	38,38,38	1.32	5 (13%)
2	ADP	F	601	3	24,29,29	1.05	1 (4%)	29,45,45	1.58	6 (20%)
4	DQ8	A	801	-	28,28,28	0.86	1 (3%)	38,38,38	1.08	2 (5%)
2	ADP	A	601	3	24,29,29	1.12	2 (8%)	29,45,45	1.58	6 (20%)
2	ADP	G	601	3	24,29,29	1.12	3 (12%)	29,45,45	1.73	5 (17%)
4	DQ8	C	801	-	28,28,28	0.77	0	38,38,38	1.26	6 (15%)
4	DQ8	F	801	-	28,28,28	0.77	1 (3%)	38,38,38	1.08	3 (7%)
4	DQ8	G	801	-	28,28,28	0.93	2 (7%)	38,38,38	1.24	5 (13%)
2	ADP	E	601	3	24,29,29	1.07	1 (4%)	29,45,45	1.57	5 (17%)
2	ADP	D	601	3	24,29,29	1.05	1 (4%)	29,45,45	1.48	4 (13%)
2	ADP	B	601	3	24,29,29	1.07	1 (4%)	29,45,45	1.60	8 (27%)
2	ADP	C	601	3	24,29,29	1.21	2 (8%)	29,45,45	1.83	9 (31%)
4	DQ8	B	801	-	28,28,28	0.66	0	38,38,38	1.02	2 (5%)

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	E	801	-	-	1/27/27/27	0/3/3/3
4	DQ8	D	801	-	-	2/27/27/27	0/3/3/3
2	ADP	F	601	3	-	1/12/32/32	0/3/3/3
4	DQ8	A	801	-	-	0/27/27/27	0/3/3/3
2	ADP	A	601	3	-	2/12/32/32	0/3/3/3
2	ADP	G	601	3	-	1/12/32/32	0/3/3/3
4	DQ8	C	801	-	-	2/27/27/27	0/3/3/3
4	DQ8	F	801	-	-	0/27/27/27	0/3/3/3
4	DQ8	G	801	-	-	2/27/27/27	0/3/3/3
2	ADP	E	601	3	-	5/12/32/32	0/3/3/3
2	ADP	D	601	3	-	2/12/32/32	0/3/3/3
2	ADP	B	601	3	-	2/12/32/32	0/3/3/3
2	ADP	C	601	3	-	3/12/32/32	0/3/3/3
4	DQ8	B	801	-	-	2/27/27/27	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ADP	C2'-C1'	-3.04	1.49	1.53
2	A	601	ADP	C2'-C1'	-2.84	1.49	1.53
2	G	601	ADP	C5-C4	2.75	1.48	1.40
2	F	601	ADP	C5-C4	2.72	1.48	1.40
2	C	601	ADP	C5-C4	2.56	1.47	1.40

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	601	ADP	PA-O3A-PB	-4.61	117.02	132.83
2	G	601	ADP	C5'-C4'-C3'	-4.52	98.25	115.18
2	C	601	ADP	PA-O3A-PB	-3.83	119.67	132.83
2	E	601	ADP	N3-C2-N1	-3.67	122.94	128.68
2	A	601	ADP	C4-C5-N7	-3.40	105.85	109.40

There are no chirality outliers.

5 of 25 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	F	601	ADP	O4'-C4'-C5'-O5'
2	B	601	ADP	PA-O3A-PB-O1B

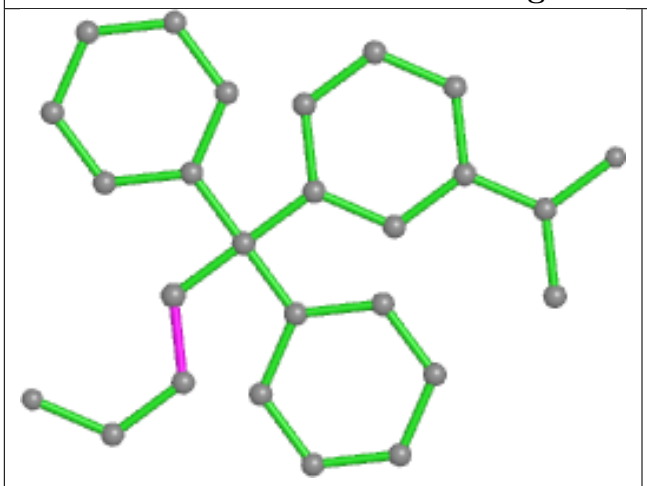
There are no ring outliers.

12 monomers are involved in 63 short contacts:

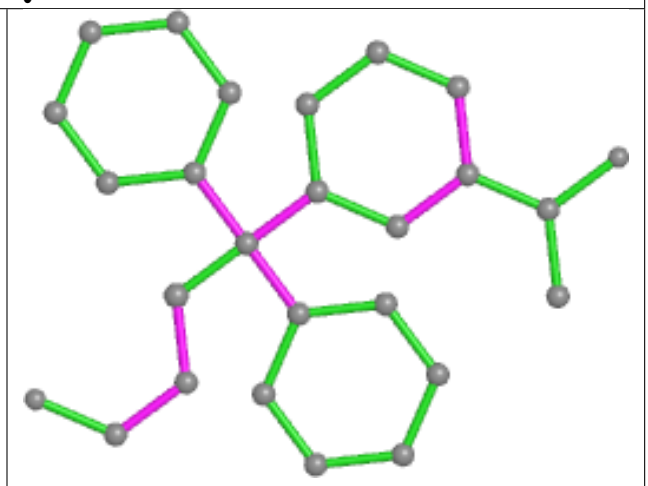
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	801	DQ8	9	0
4	D	801	DQ8	4	0
2	F	601	ADP	3	0
4	A	801	DQ8	7	0
2	G	601	ADP	2	0
4	C	801	DQ8	2	0
4	F	801	DQ8	7	0
4	G	801	DQ8	7	0
2	E	601	ADP	5	0
2	D	601	ADP	5	0
2	C	601	ADP	4	0
4	B	801	DQ8	8	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

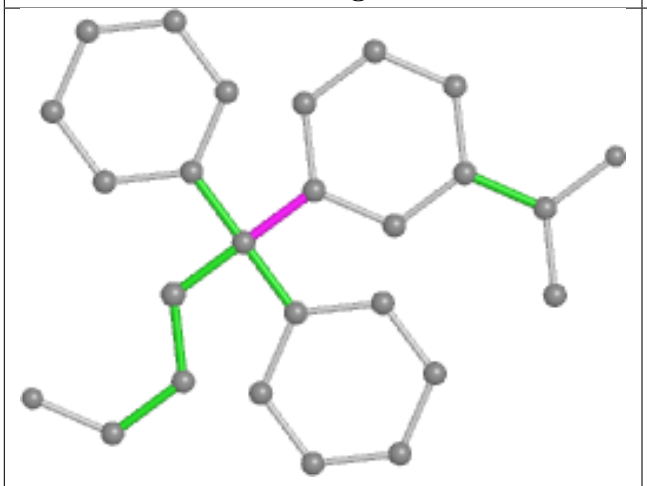
Ligand DQ8 E 801



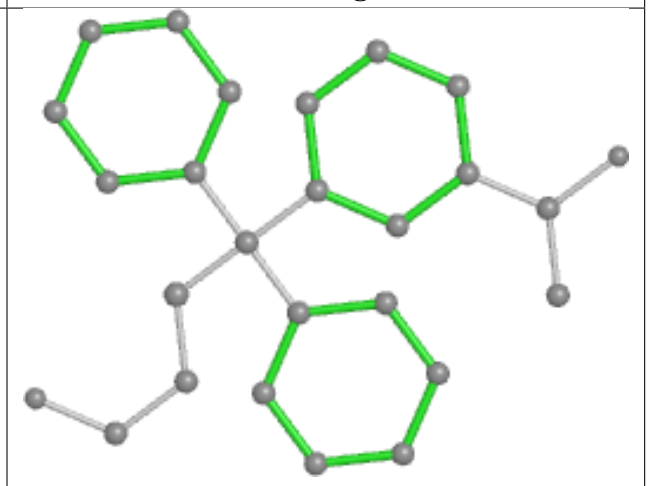
Bond lengths



Bond angles

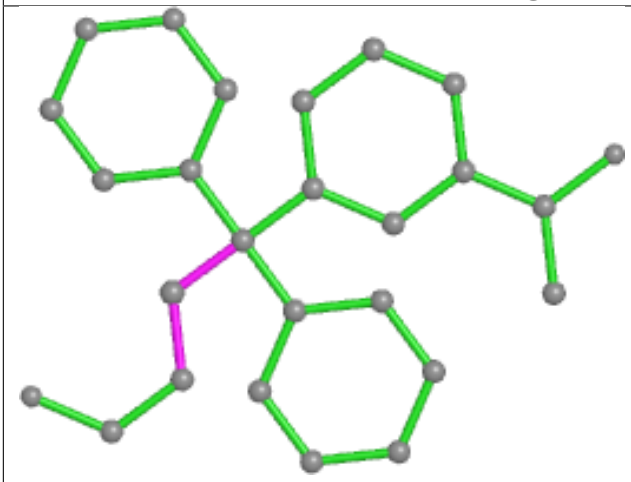


Torsions



Rings

Ligand DQ8 D 801



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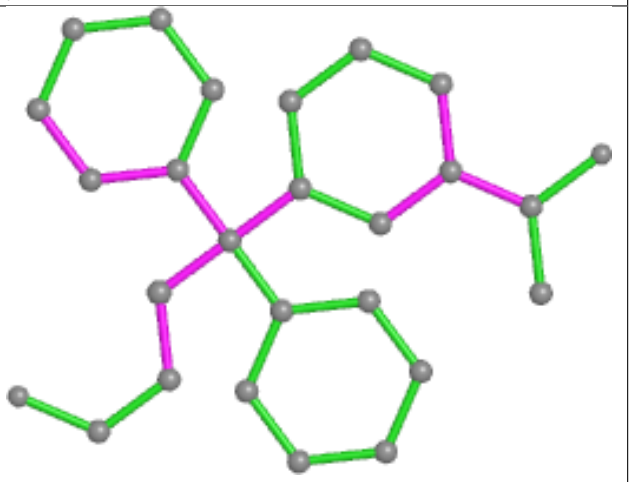

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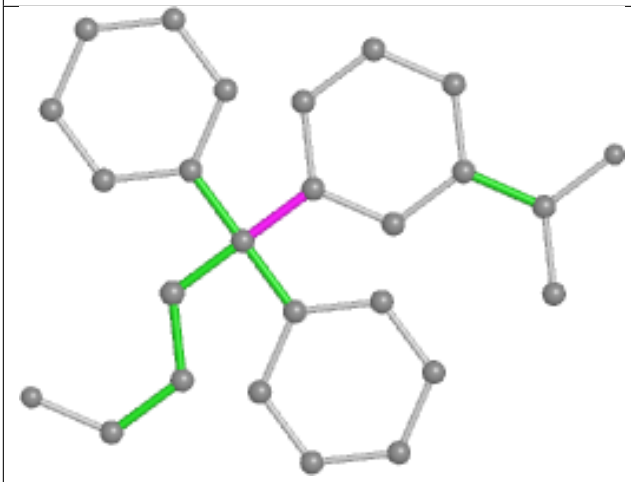

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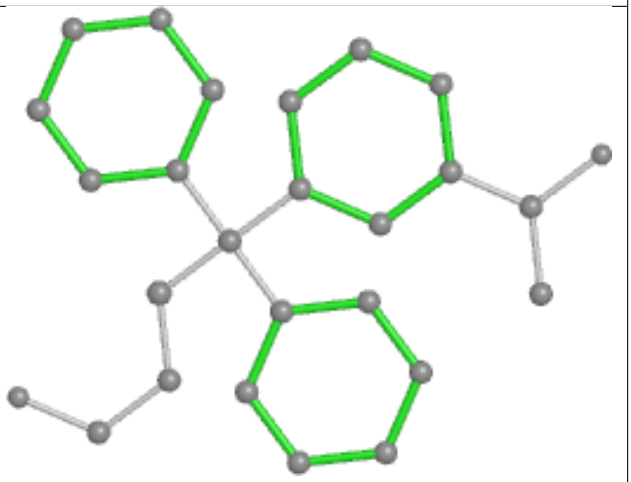
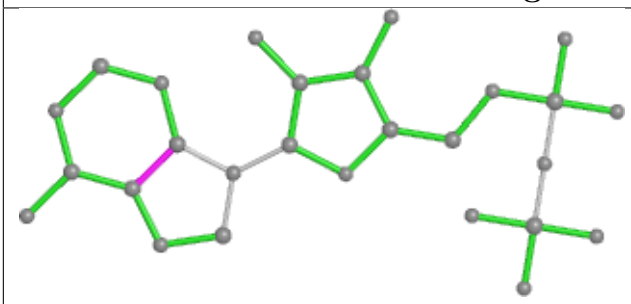


Rings

Ligand ADP F 601



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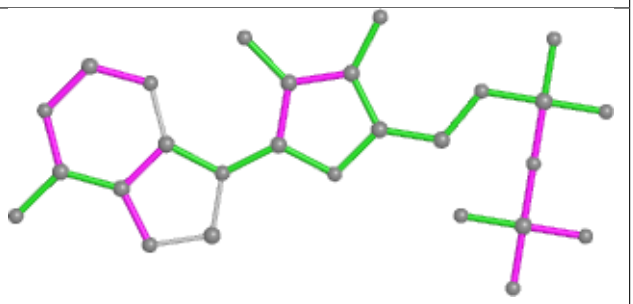
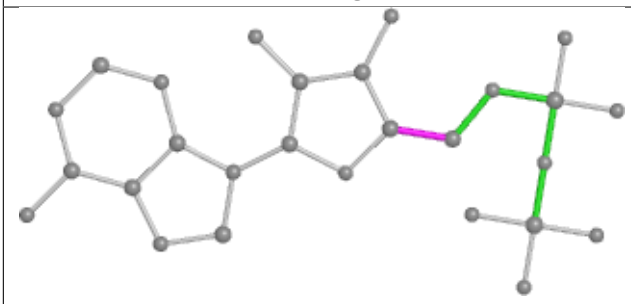


Bond angles



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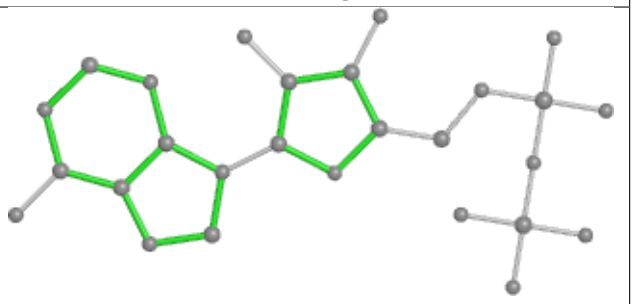
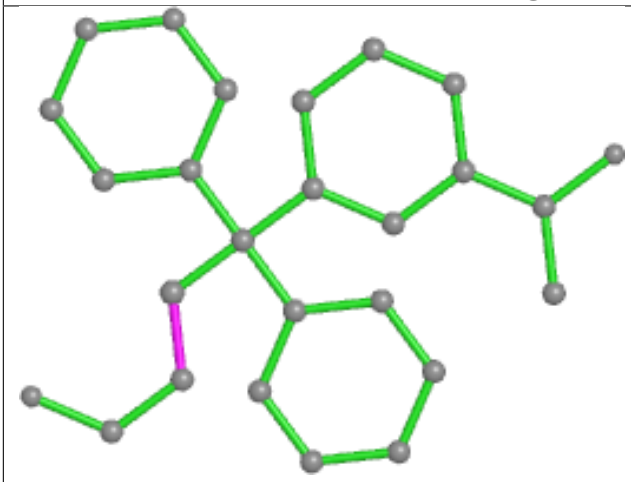


Rings

Ligand DQ8 A 801



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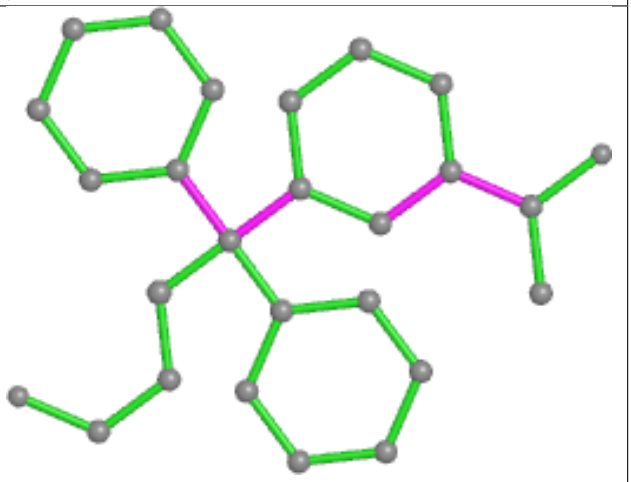

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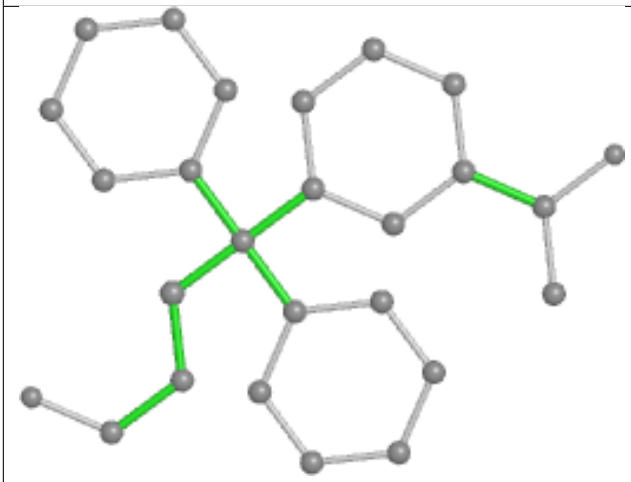

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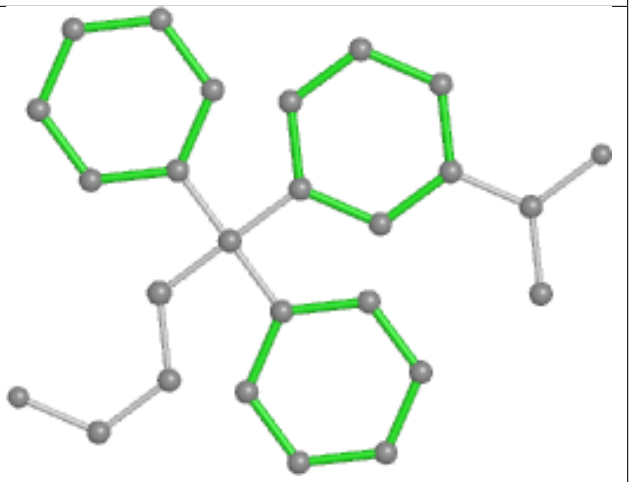
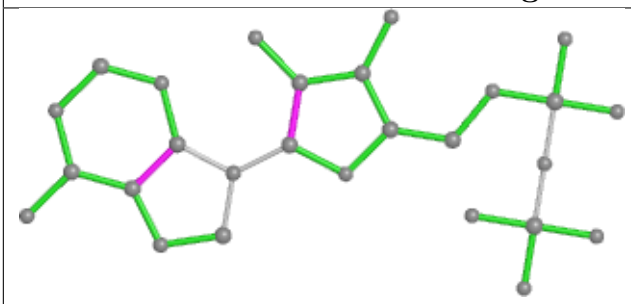


Rings

Ligand ADP A 601



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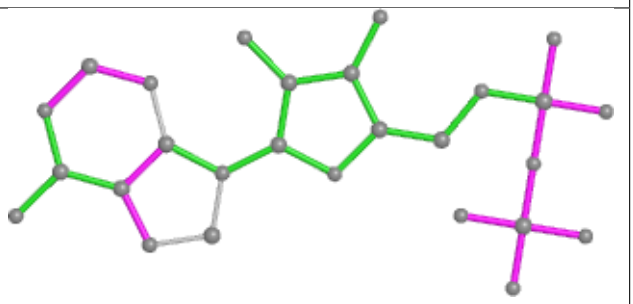
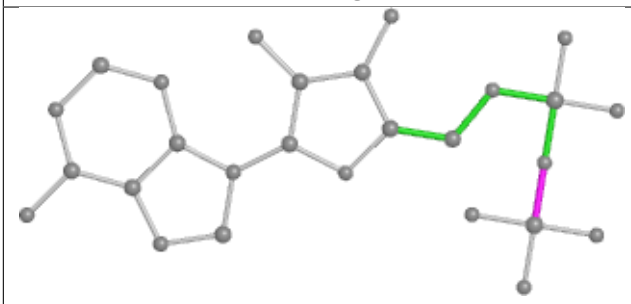


Bond angles



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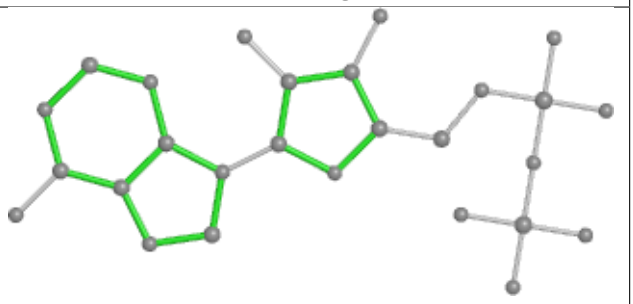
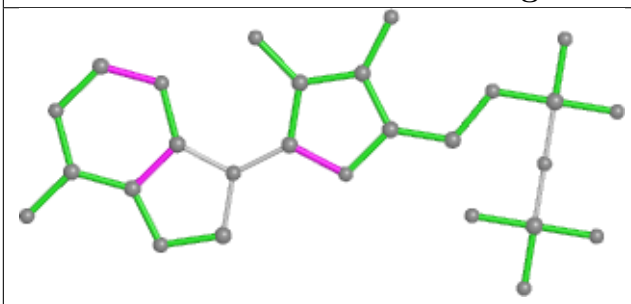


Rings

Ligand ADP G 601



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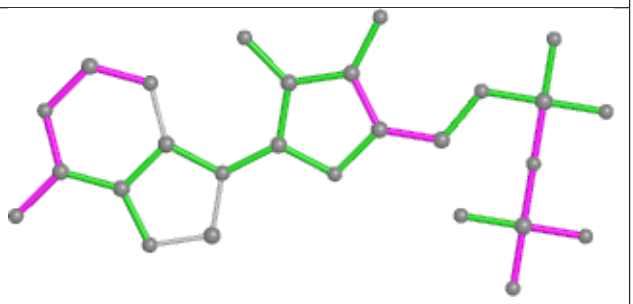

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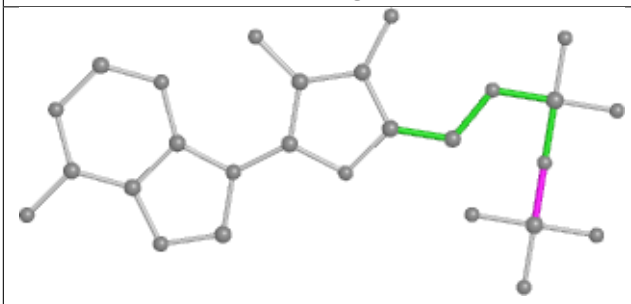

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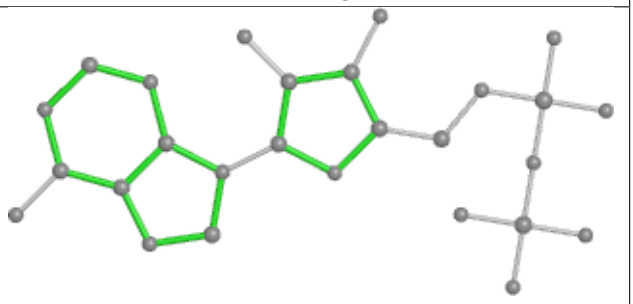
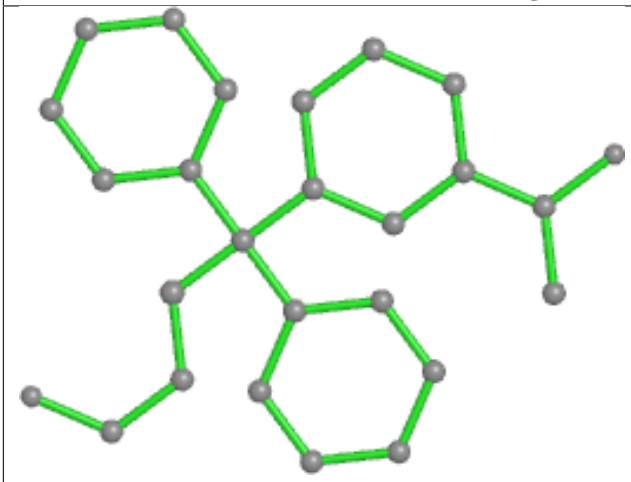


Rings

Ligand DQ8 C 801



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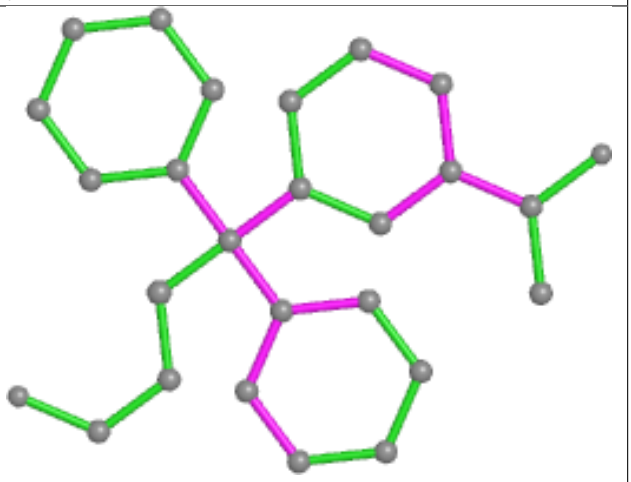
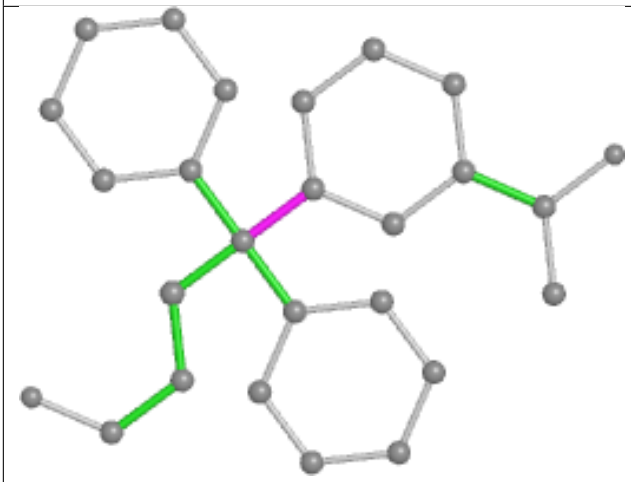


Bond angles



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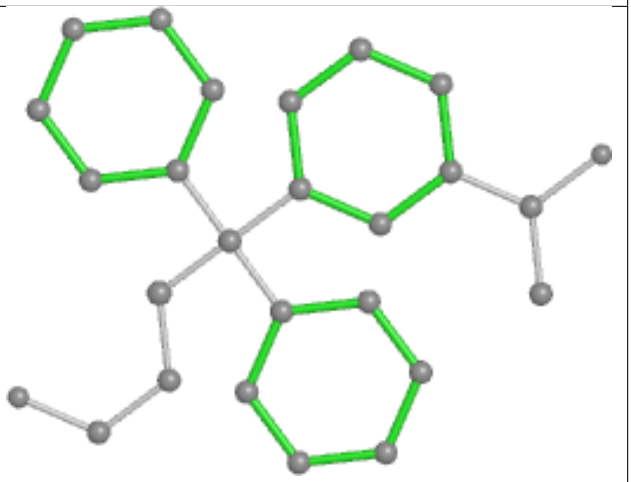
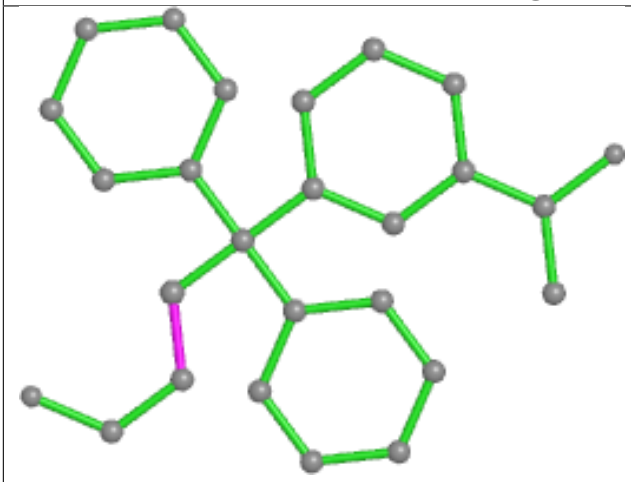
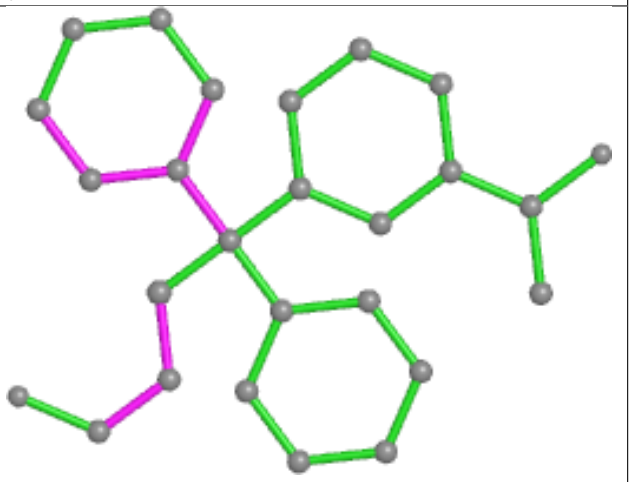


Rings

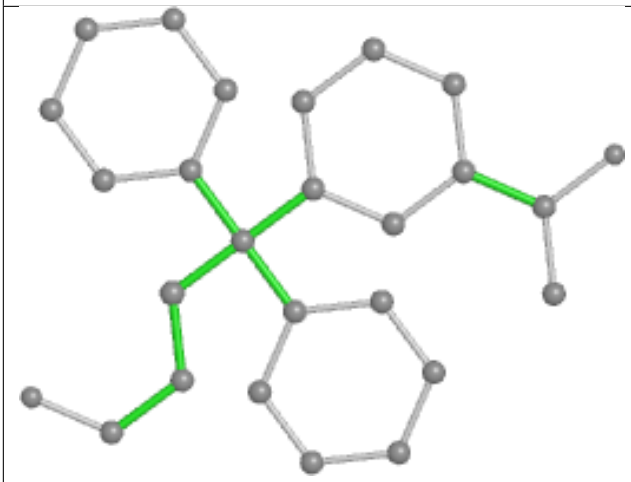
Ligand DQ8 F 801



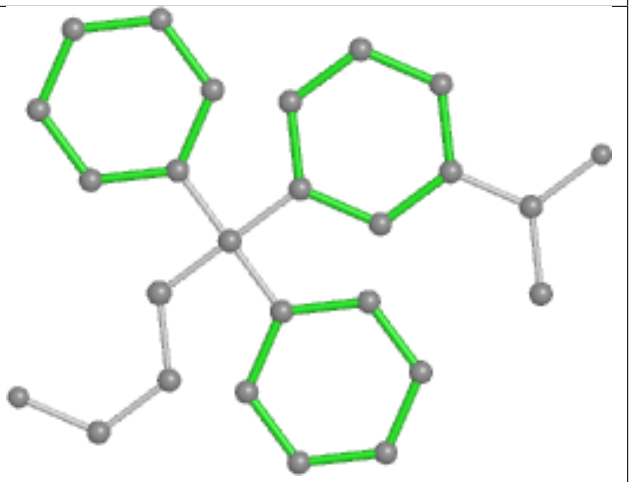
Bond lengths



Bond angles

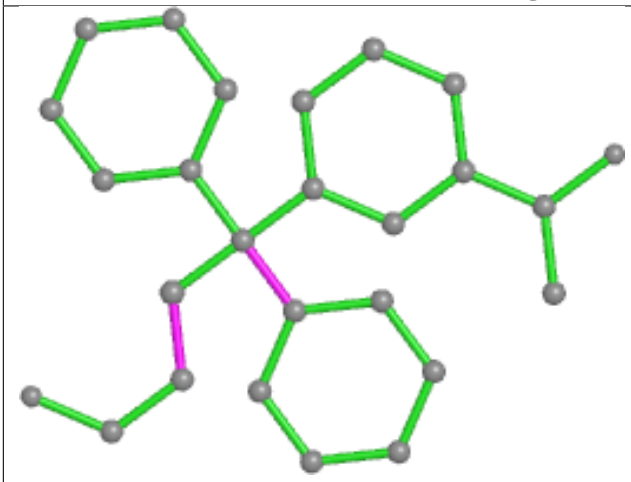


Torsions

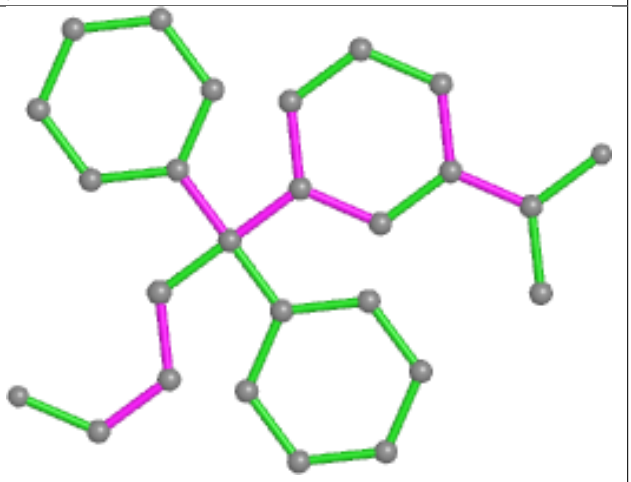


Rings

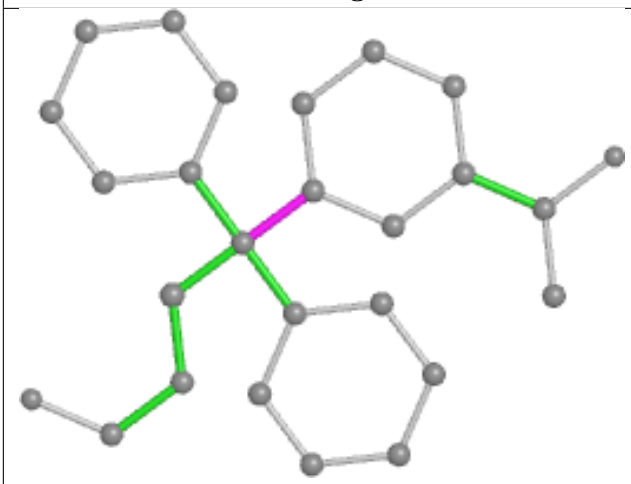
Ligand DQ8 G 801



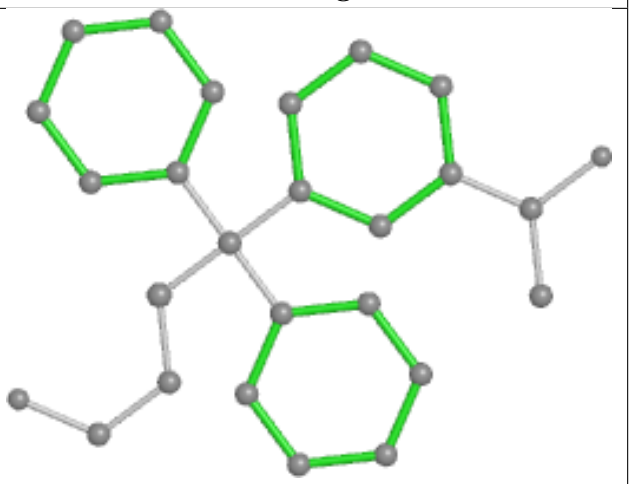
Bond lengths



Bond angles

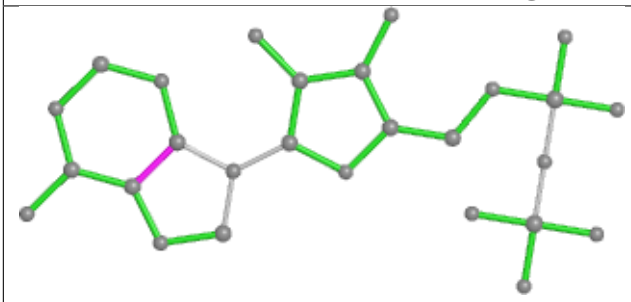


Torsions

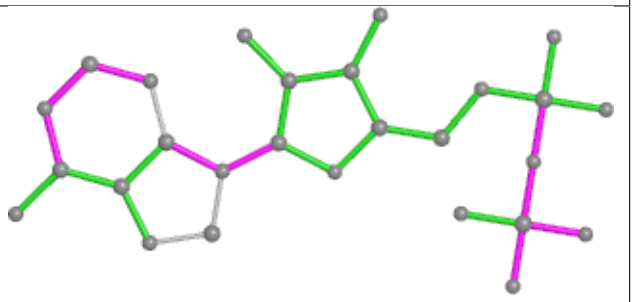


Rings

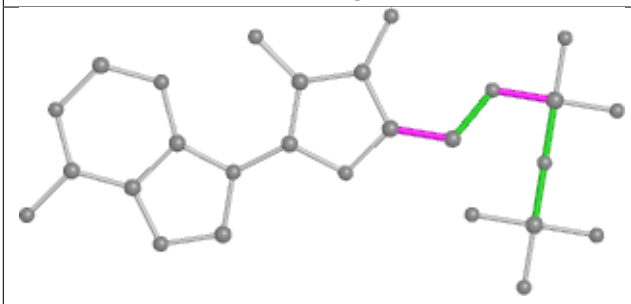
Ligand ADP E 601



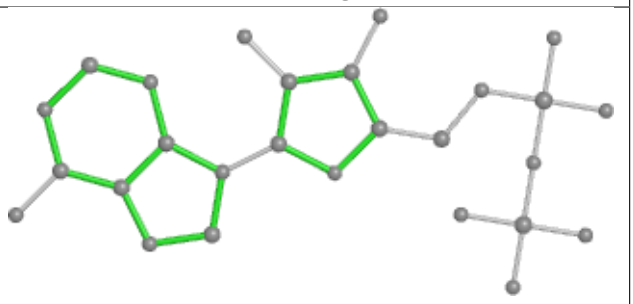
Bond lengths



Bond angles

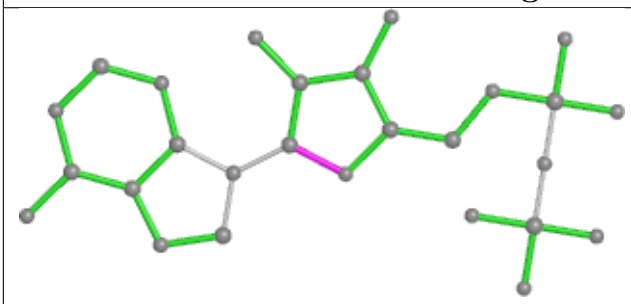


Torsions

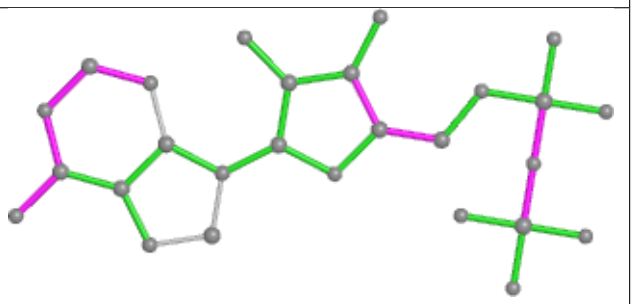


Rings

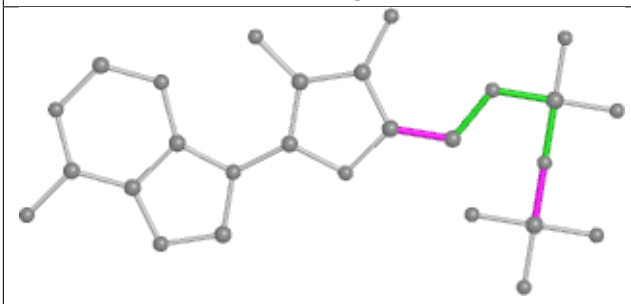
Ligand ADP D 601



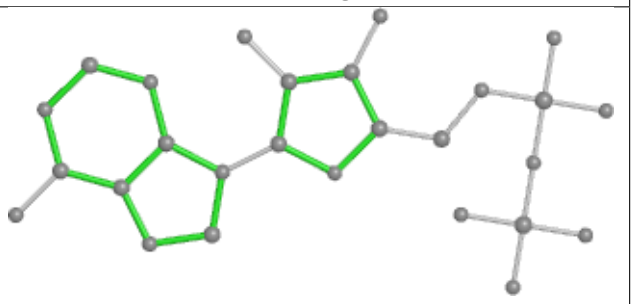
Bond lengths



Bond angles

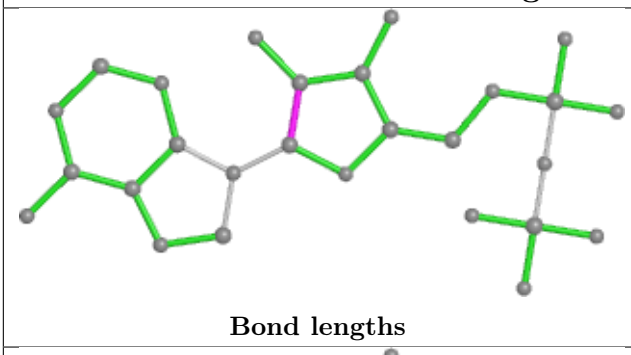


Torsions

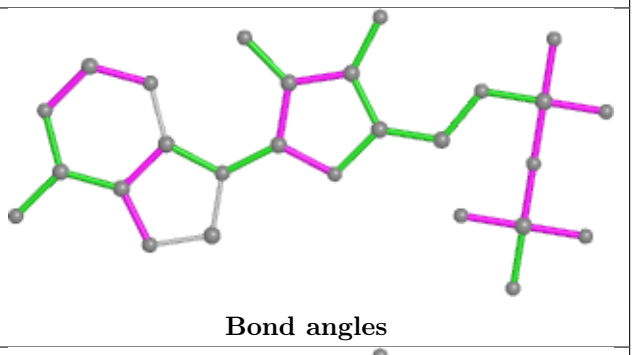


Rings

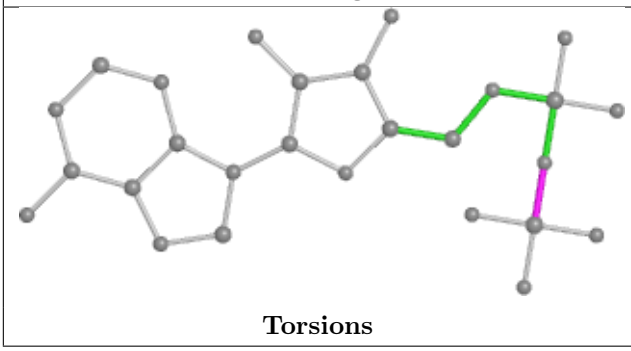
Ligand ADP B 601



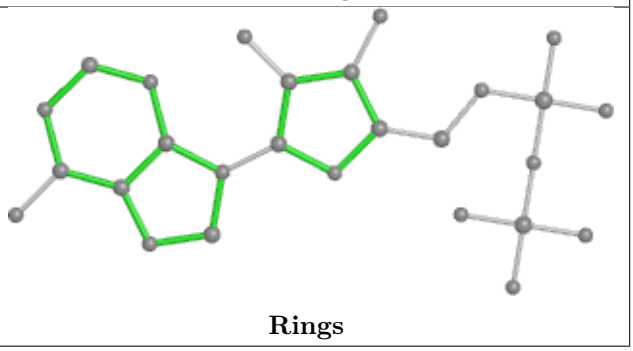
Bond lengths



Bond angles

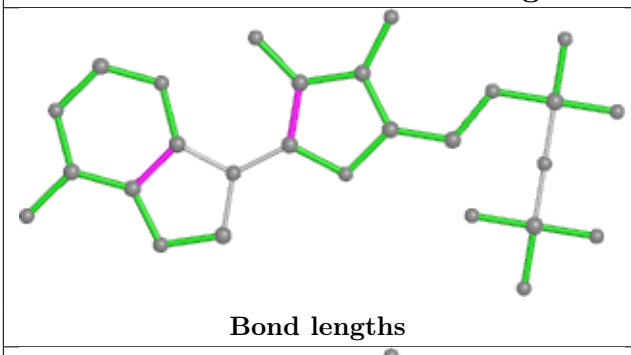


Torsions

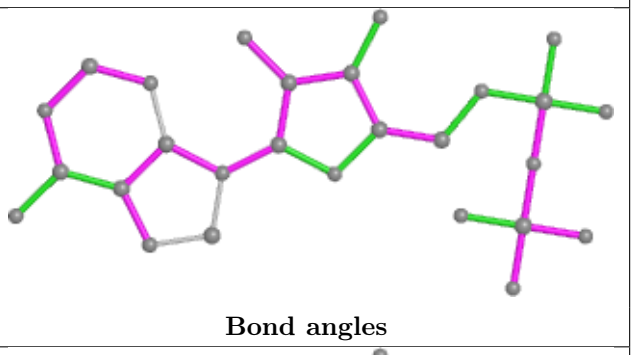


Rings

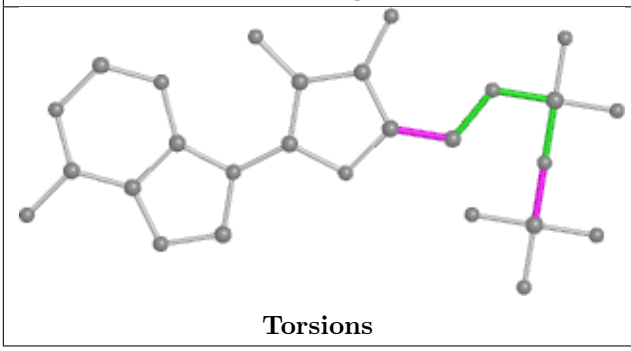
Ligand ADP C 601



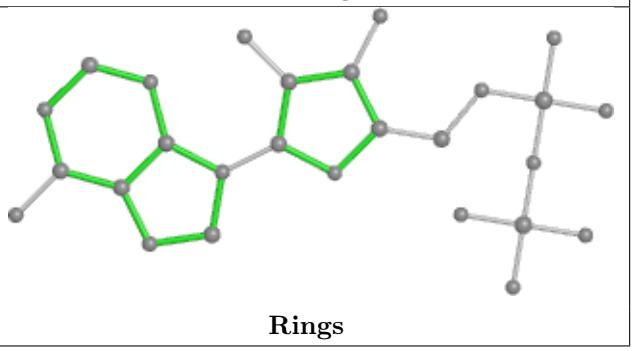
Bond lengths



Bond angles

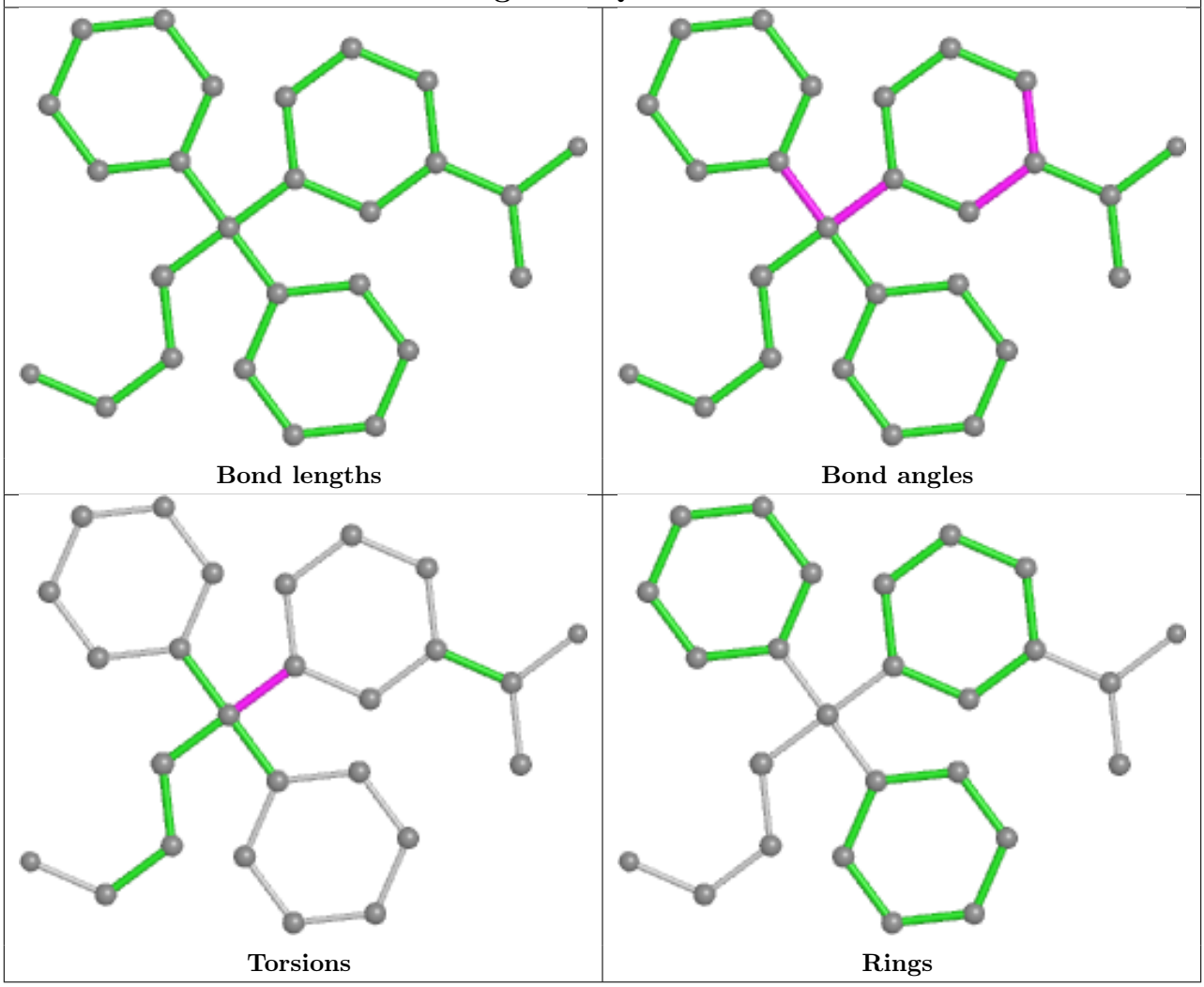


Torsions



Rings

Ligand DQ8 B 801



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	322/368 (87%)	0.50	38 (11%) 4 5	33, 54, 90, 112	0
1	B	324/368 (88%)	0.54	41 (12%) 3 4	34, 53, 92, 104	0
1	C	325/368 (88%)	0.26	23 (7%) 16 19	28, 50, 86, 113	0
1	D	322/368 (87%)	0.37	27 (8%) 11 13	28, 50, 92, 114	0
1	E	321/368 (87%)	0.70	51 (15%) 1 2	42, 67, 99, 119	0
1	F	319/368 (86%)	0.77	59 (18%) 1 1	41, 71, 106, 117	0
1	G	318/368 (86%)	1.08	73 (22%) 0 0	46, 81, 122, 140	0
All	All	2251/2576 (87%)	0.60	312 (13%) 2 3	28, 61, 105, 140	0

The worst 5 of 312 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	309	VAL	8.6
1	G	308	HIS	8.2
1	G	58	ALA	7.4
1	E	149	ASP	6.9
1	G	359	ILE	6.7

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 monosaccharides in this entry.

6.4 Ligands (i)

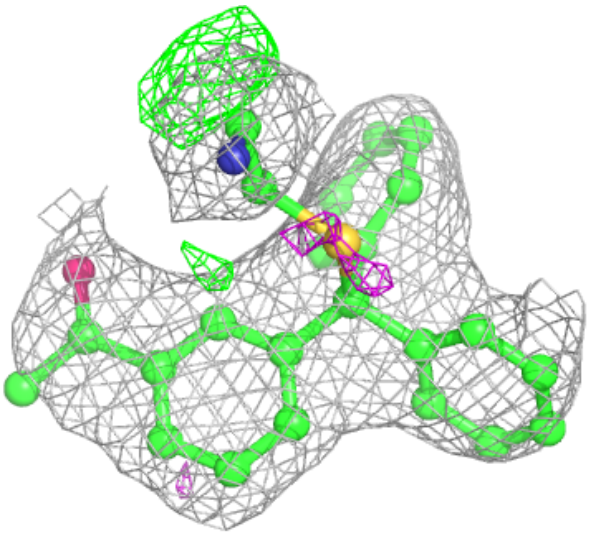
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

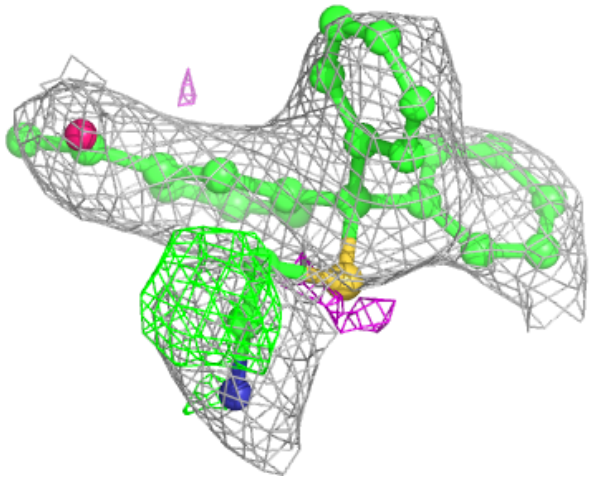
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	G	1364	1/1	0.40	0.34	106,106,106,106	0
5	CL	A	1366	1/1	0.72	0.15	89,89,89,89	0
5	CL	B	1365	1/1	0.83	0.09	78,78,78,78	0
5	CL	D	1364	1/1	0.84	0.12	77,77,77,77	0
5	CL	E	1364	1/1	0.85	0.22	90,90,90,90	0
4	DQ8	F	801	26/26	0.87	0.25	60,75,84,110	0
4	DQ8	E	801	26/26	0.88	0.22	57,67,77,98	0
5	CL	A	1364	1/1	0.89	0.08	75,75,75,75	0
4	DQ8	A	801	26/26	0.89	0.23	43,54,63,85	0
5	CL	A	1365	1/1	0.90	0.07	95,95,95,95	0
5	CL	C	1369	1/1	0.92	0.11	97,97,97,97	0
4	DQ8	C	801	26/26	0.92	0.22	39,49,61,83	0
4	DQ8	B	801	26/26	0.93	0.22	44,53,67,82	0
4	DQ8	G	801	26/26	0.93	0.22	49,57,68,85	0
3	MG	F	701	1/1	0.93	0.15	50,50,50,50	0
4	DQ8	D	801	26/26	0.93	0.21	38,47,60,79	0
3	MG	C	701	1/1	0.93	0.23	40,40,40,40	0
5	CL	F	1364	1/1	0.95	0.15	89,89,89,89	0
5	CL	A	1367	1/1	0.95	0.19	73,73,73,73	0
3	MG	B	701	1/1	0.96	0.18	37,37,37,37	0
2	ADP	E	601	27/27	0.96	0.16	45,54,61,71	0
2	ADP	F	601	27/27	0.96	0.16	45,55,70,77	0
5	CL	B	1364	1/1	0.96	0.32	80,80,80,80	0
3	MG	G	701	1/1	0.96	0.28	45,45,45,45	0
5	CL	D	1363	1/1	0.97	0.10	79,79,79,79	0
3	MG	D	701	1/1	0.97	0.18	35,35,35,35	0
5	CL	C	1367	1/1	0.97	0.29	62,62,62,62	0
5	CL	C	1368	1/1	0.97	0.09	56,56,56,56	0
3	MG	E	701	1/1	0.97	0.20	50,50,50,50	0
6	SO4	D	1362	5/5	0.97	0.12	54,54,63,68	0
2	ADP	B	601	27/27	0.98	0.16	35,42,48,58	0
2	ADP	G	601	27/27	0.98	0.14	46,54,59,64	0
2	ADP	C	601	27/27	0.98	0.16	28,38,42,48	0
2	ADP	D	601	27/27	0.98	0.14	28,40,45,51	0
2	ADP	A	601	27/27	0.98	0.13	34,41,47,50	0
3	MG	A	701	1/1	0.99	0.16	35,35,35,35	0

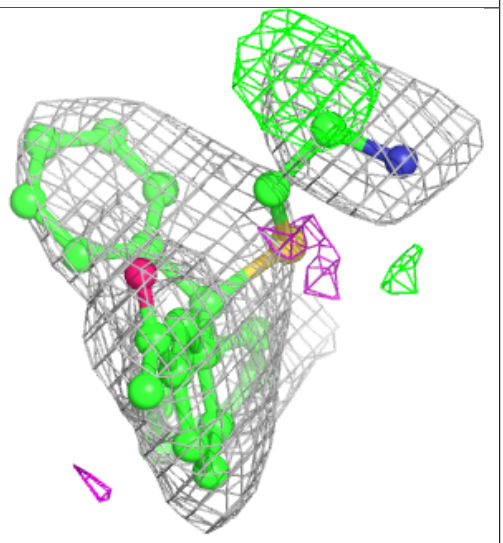
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

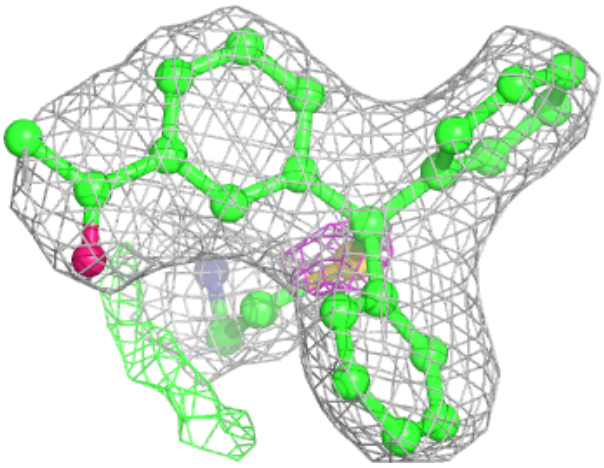


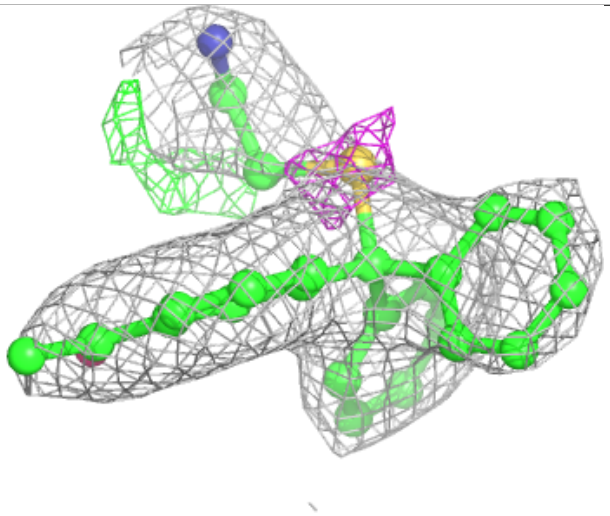


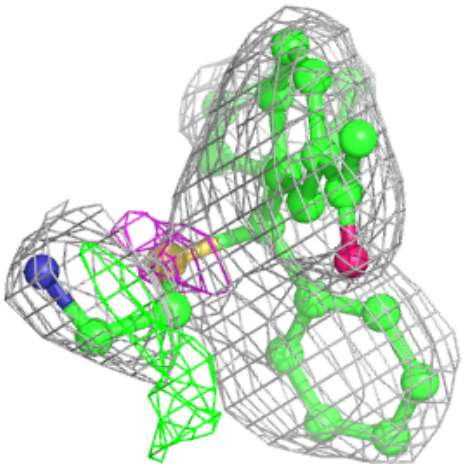


Electron density around DQ8 E 801:

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

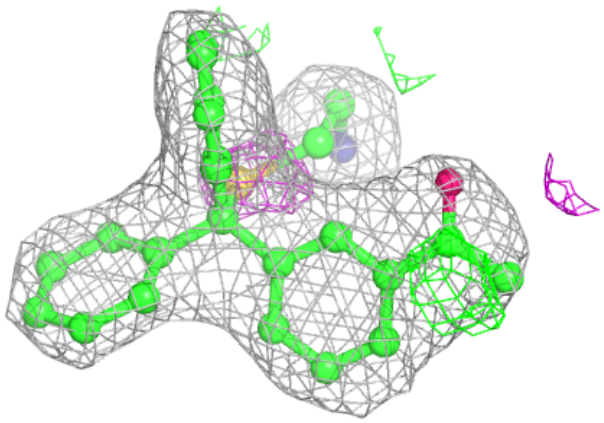


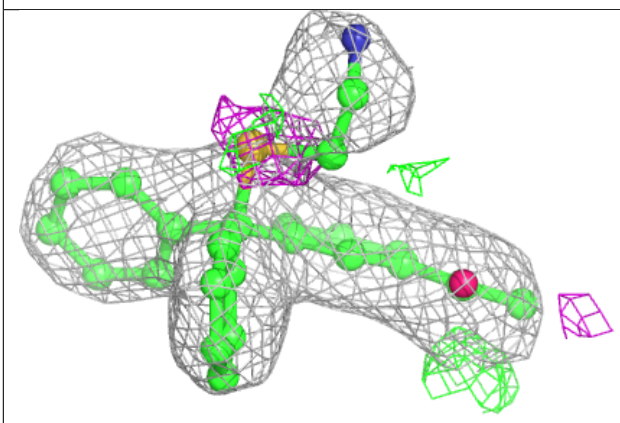


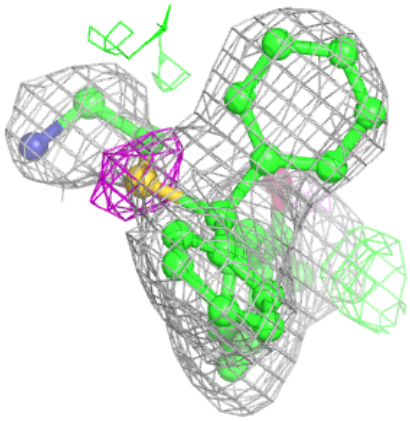


Electron density around DQ8 A 801:

$2mF_o$-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 C 801:

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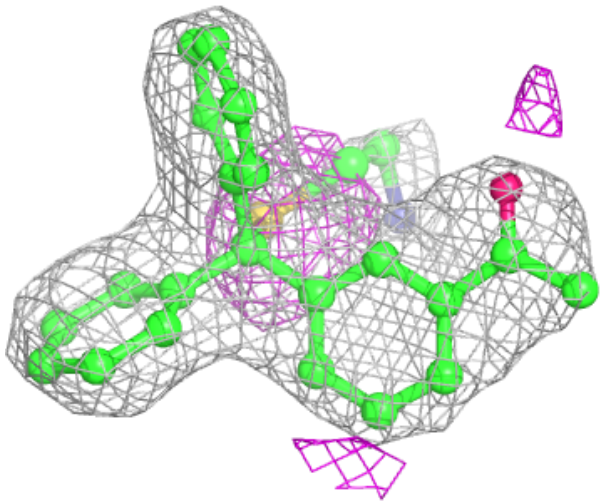
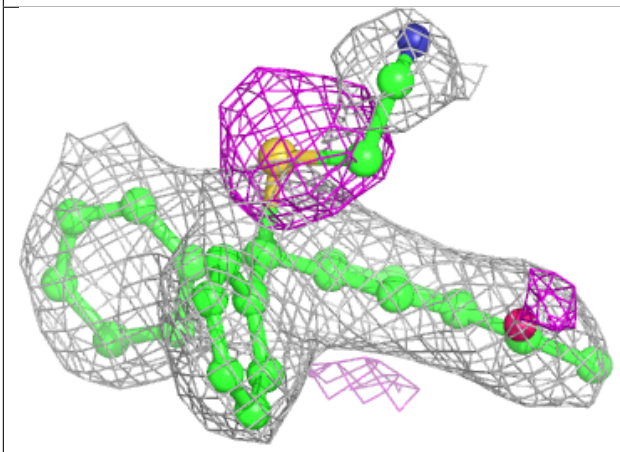
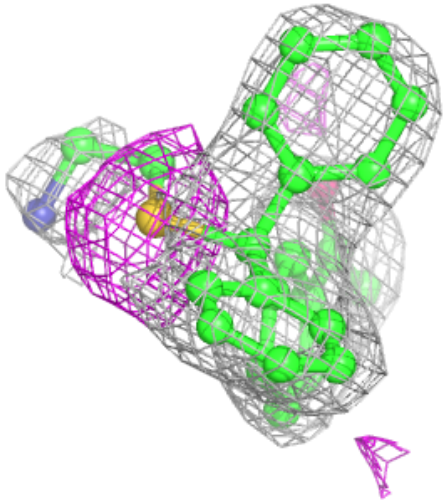
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

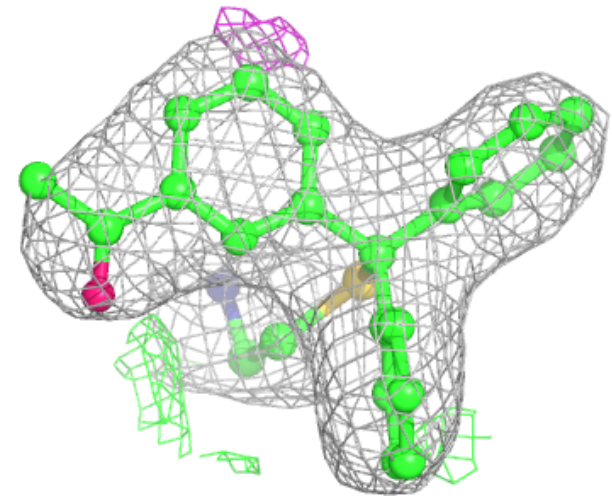


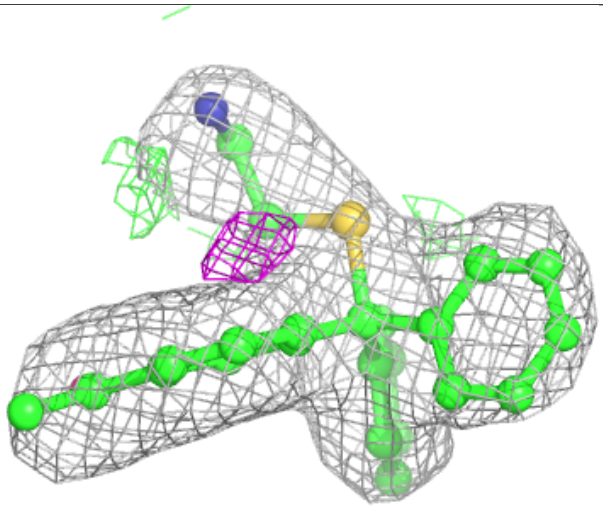


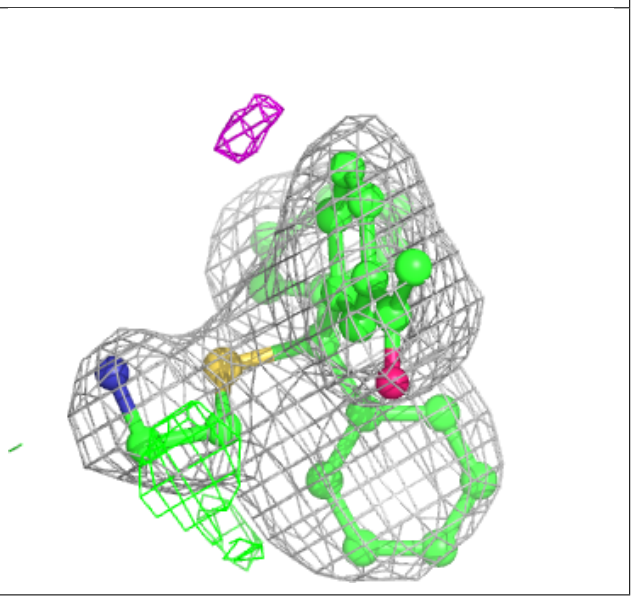


Electron density around DQ8 B 801:

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

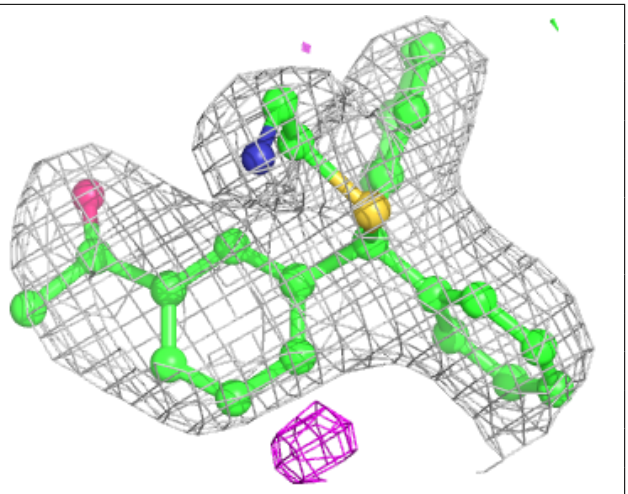


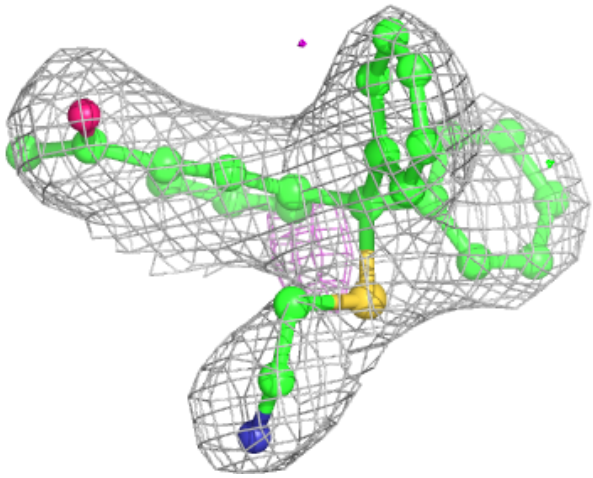


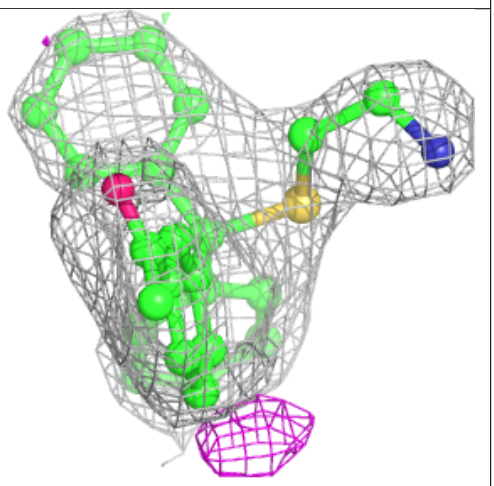


Electron density around DQ8 G 801:

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

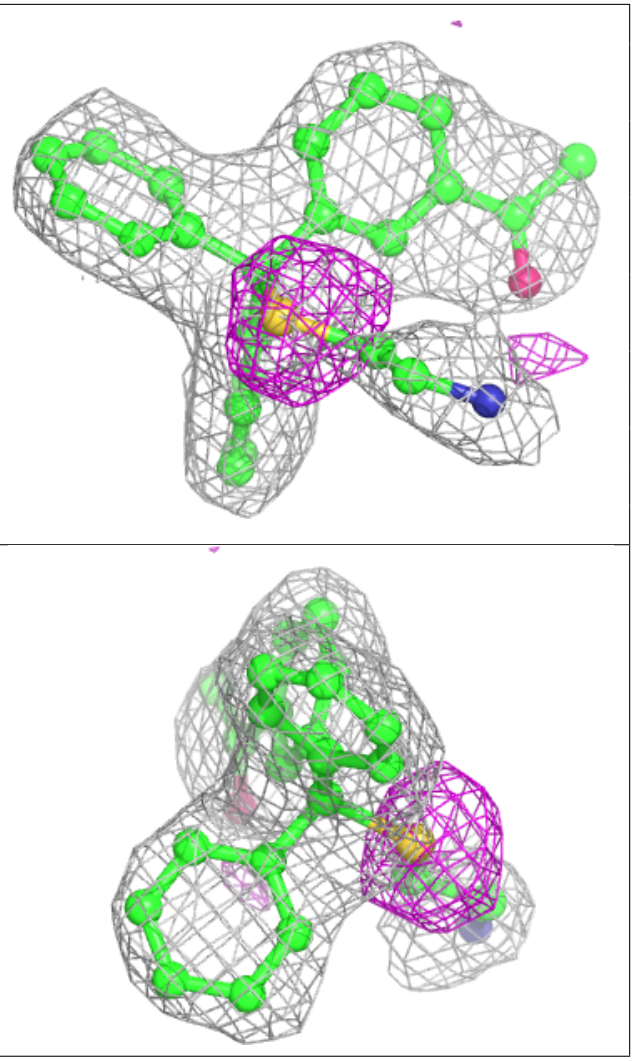






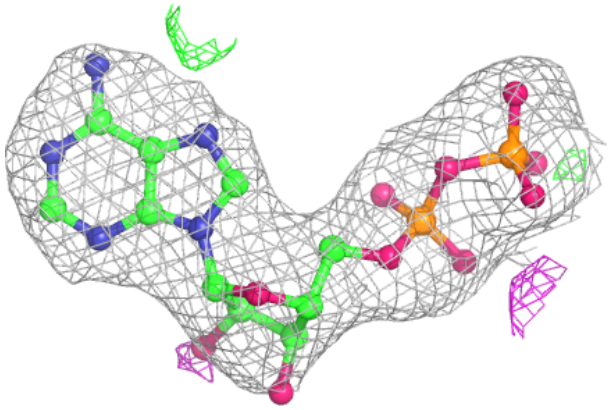
Electron density around DQ8 D 801:

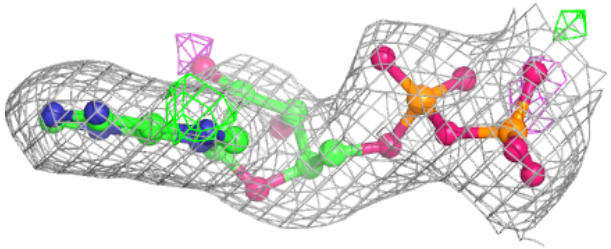
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

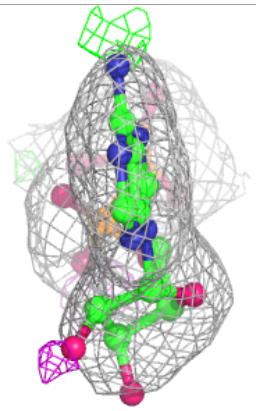


Electron density around ADP E 601:

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

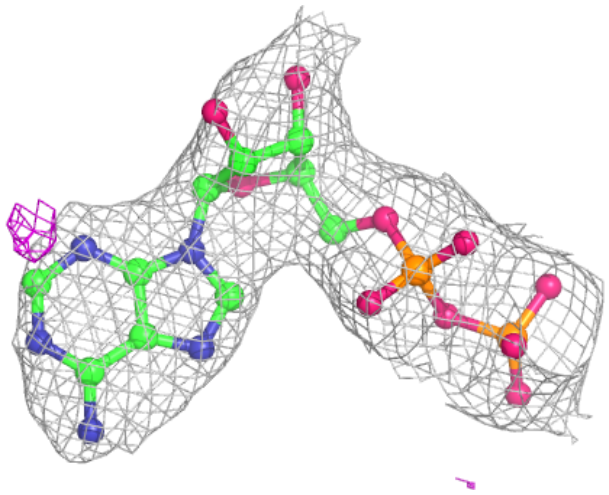


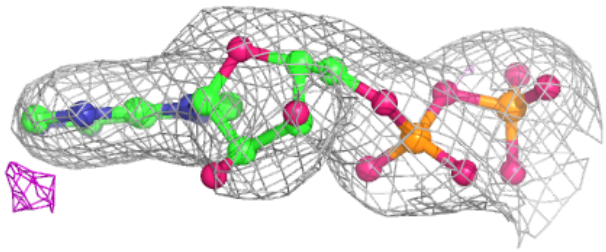


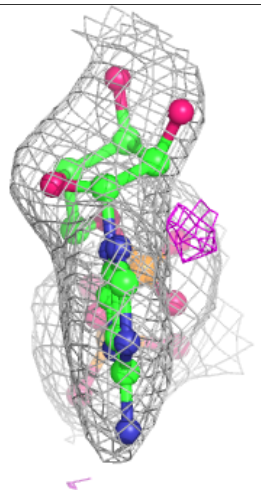


Electron density around ADP F 601:

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

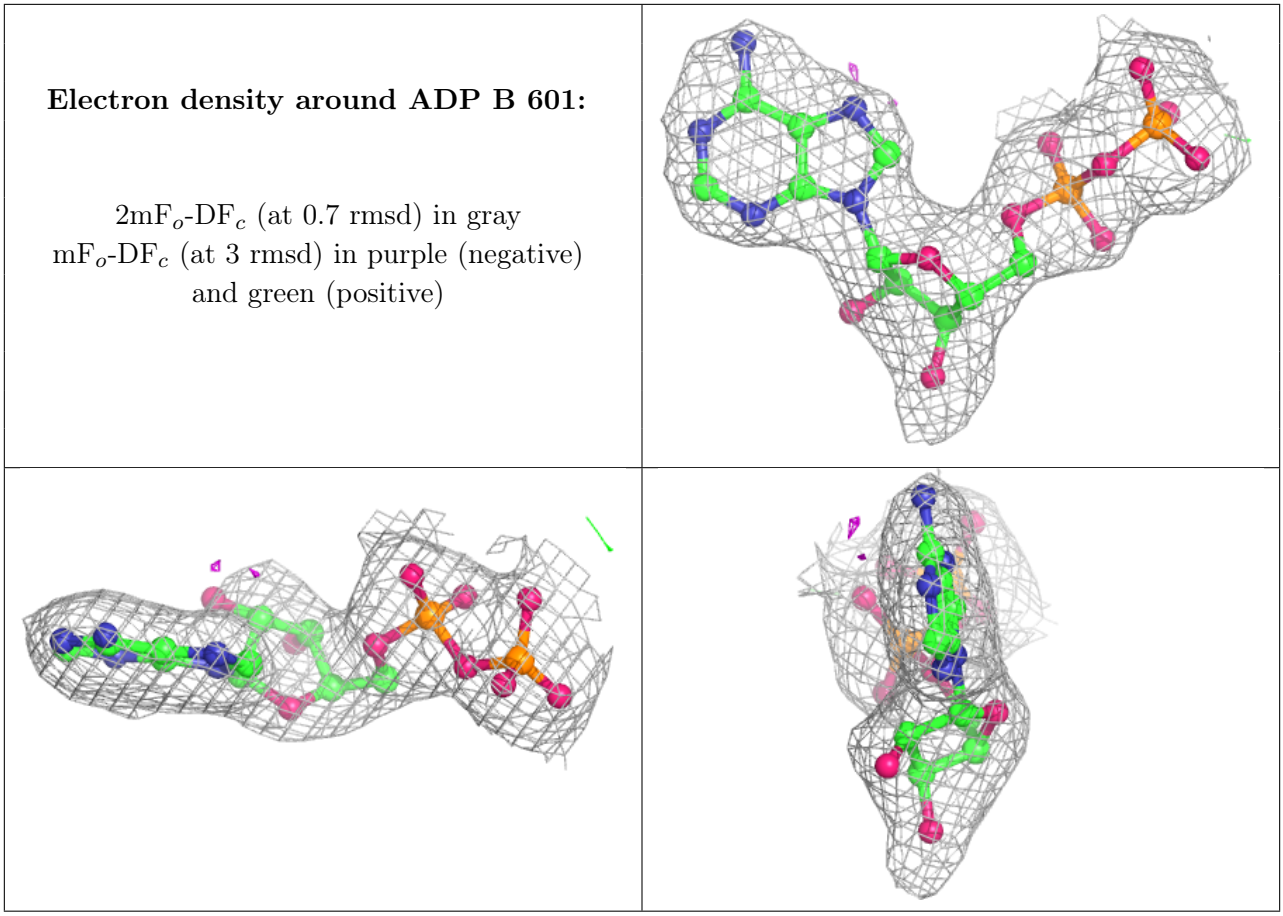






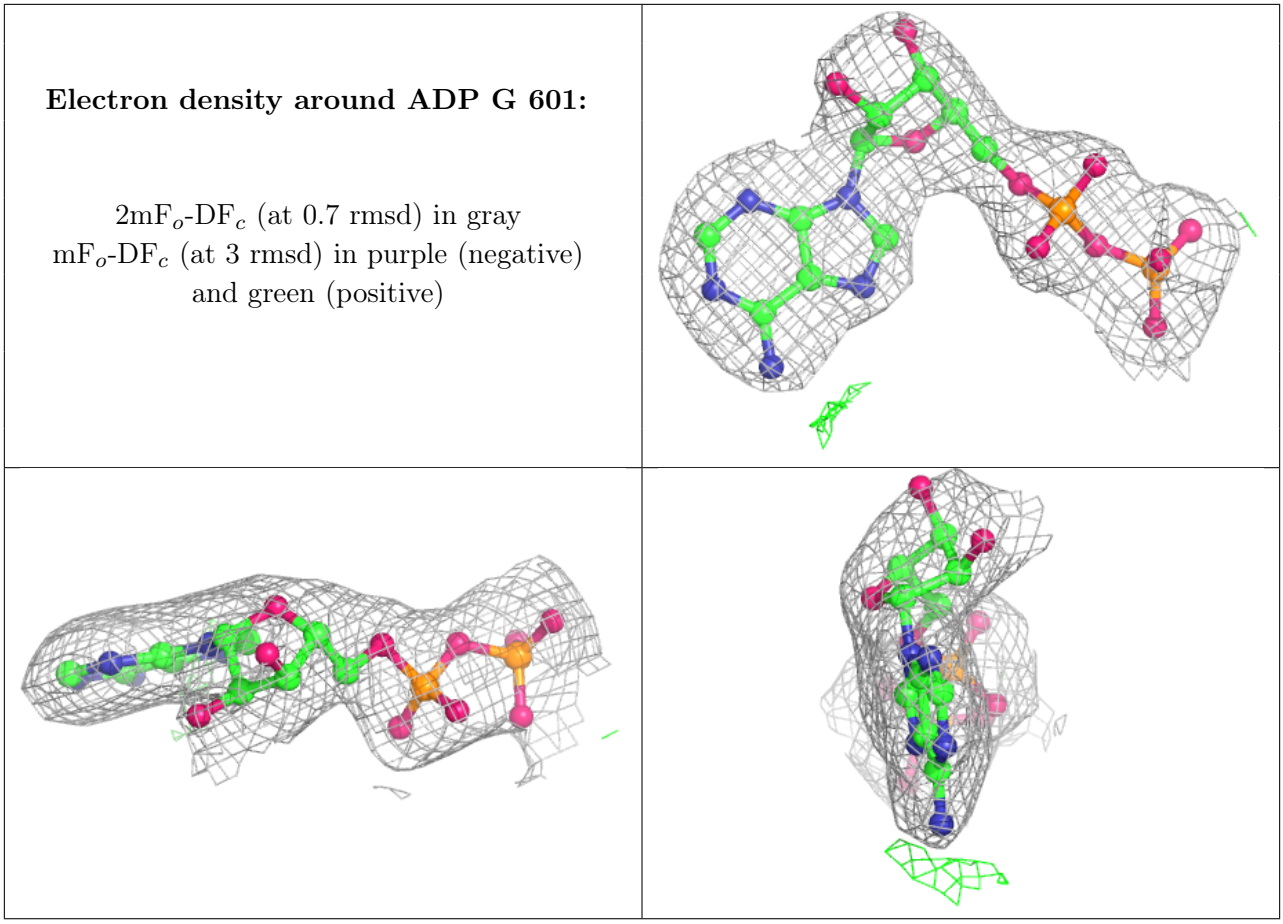
Electron density around ADP B 601:

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



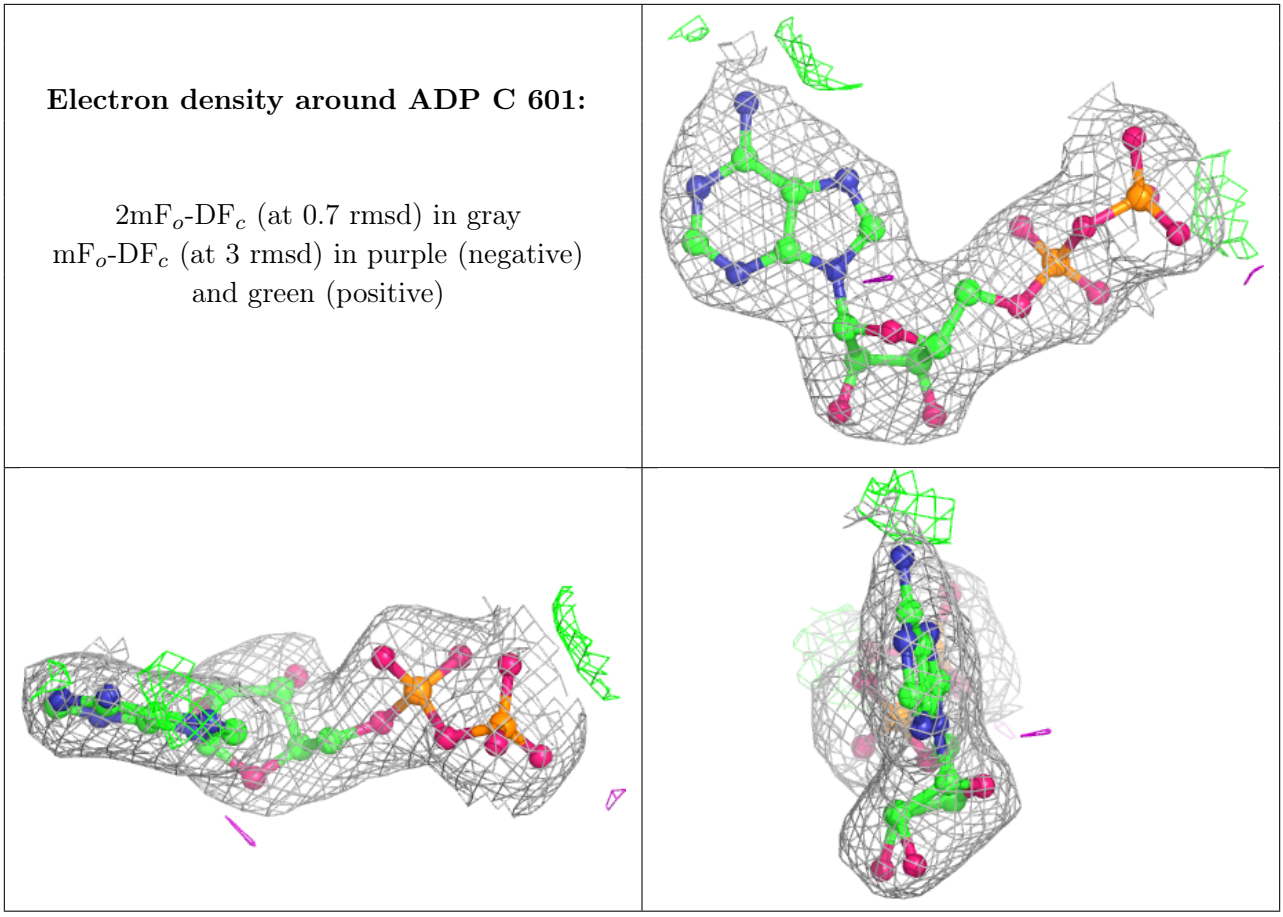
Electron density around ADP G 601:

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



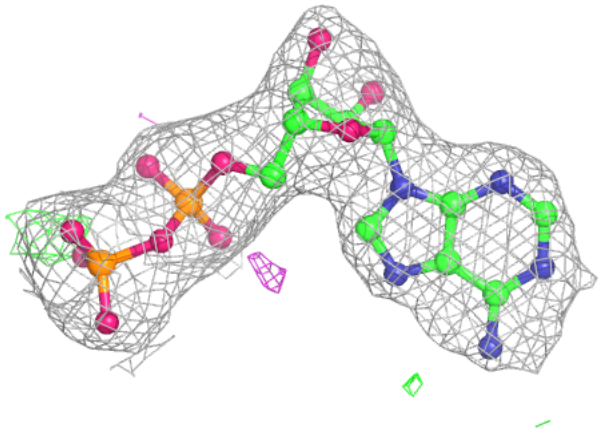
Electron density around ADP C 601:

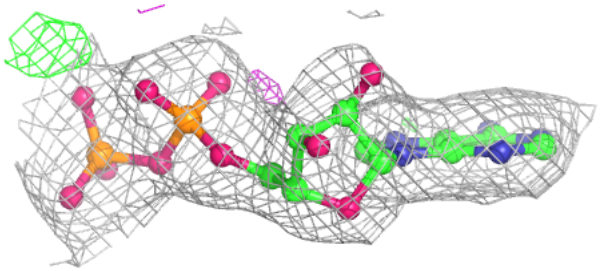
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

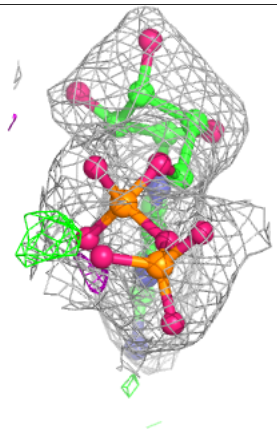


Electron density around ADP D 601:

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

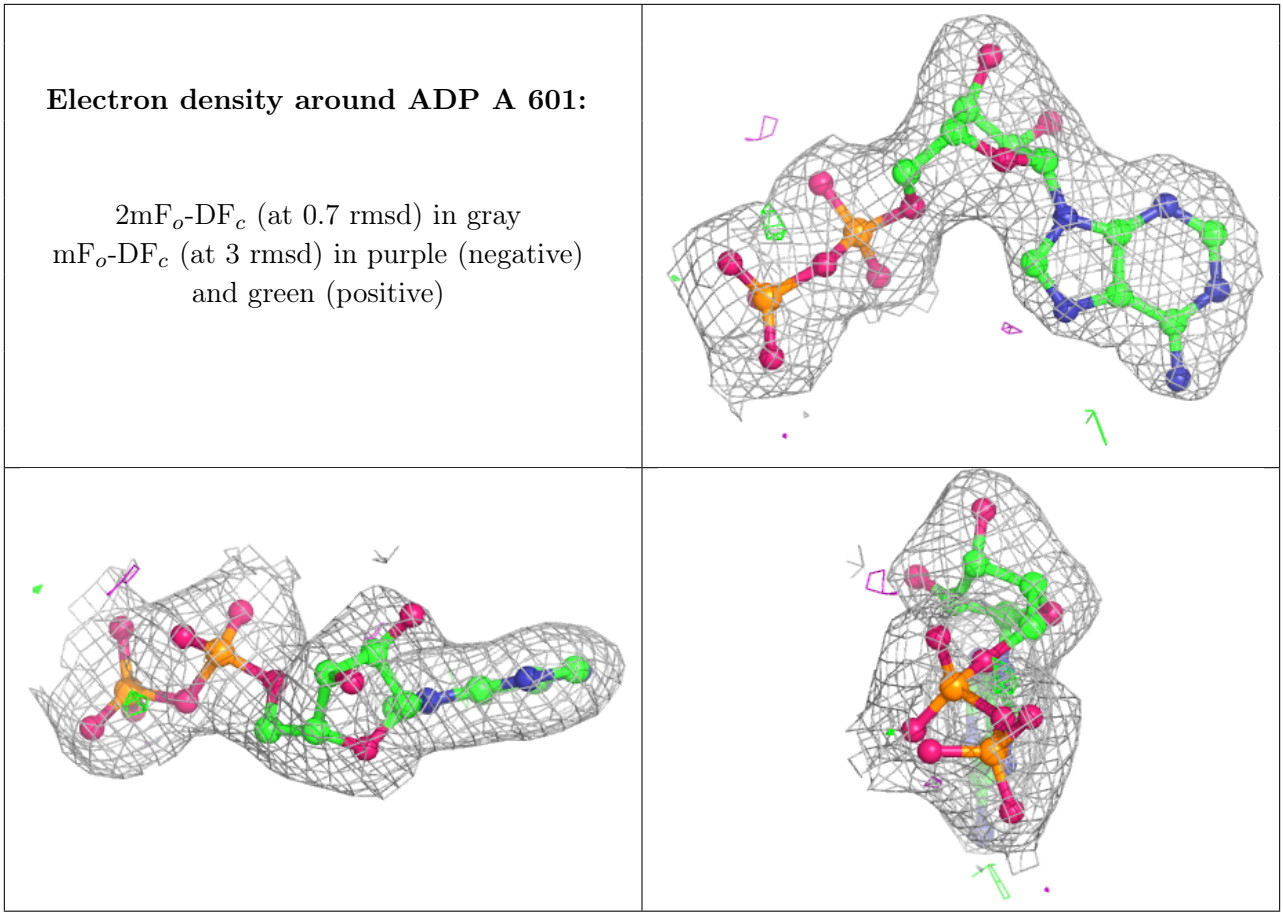






Electron density around ADP A 601:

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



6.5 Other polymers

There are no such residues in this entry.