wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 06:31 AM EDT

PDB ID	:	2B99
Title	:	Crystal Structure of an archaeal pentameric riboflavin synthase Complex with a Substrate analog inhibitor
Authors	:	Ramsperger, A.; Augustin, M.; Schott, A.K.; Gerhardt, S.; Krojer, T.; Eisenreich, W.; Illarionov, B.; Cushman, M.; Bacher, A.; Huber, R.; Fischer, M.
Deposited on	:	2005-10-11
Resolution	:	2.22 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:

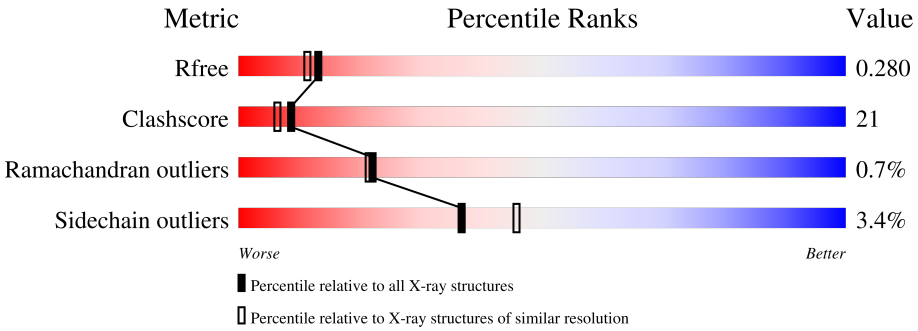
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)

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%

Mol	Chain	Length	Quality of chain
1	A	156	67% 22% • 6%
1	B	156	63% 26% • • 8%
1	C	156	66% 27% • •
1	D	156	62% 26% • 10%
1	E	156	69% 26% • •

2 Entry composition (i)

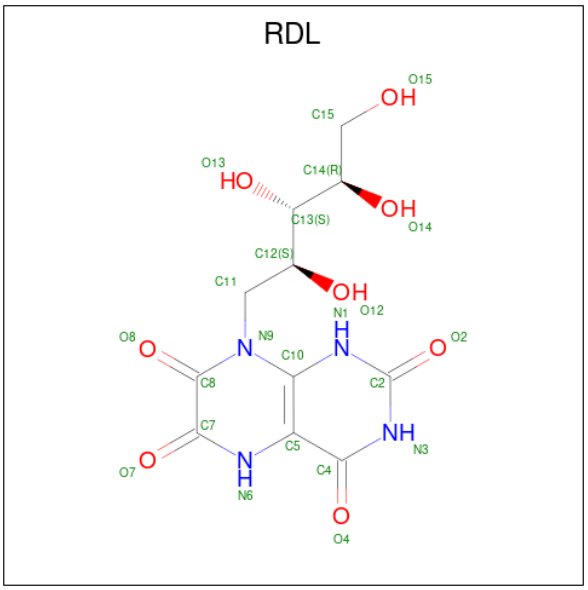
There are 3 unique types of molecules in this entry. The entry contains 6187 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Riboflavin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	65	0	0
			1145	730	197	209	9			
1	B	143	Total	C	N	O	S	67	0	0
			1121	717	190	205	9			
1	C	152	Total	C	N	O	S	50	0	0
			1189	758	203	219	9			
1	D	141	Total	C	N	O	S	51	0	0
			1106	707	188	202	9			
1	E	152	Total	C	N	O	S	53	0	0
			1189	758	203	219	9			

- Molecule 2 is 6,7-DIOXO-5H-8-RIBITYLAMINOLUMAZINE (three-letter code: RDL) (formula: $C_{11}H_{14}N_4O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	11	4	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	11	4	8		
2	B	1	Total	C	N	O	23	0
			23	11	4	8		
2	B	1	Total	C	N	O	0	0
			23	11	4	8		
2	B	1	Total	C	N	O	0	0
			23	11	4	8		
2	C	1	Total	C	N	O	0	0
			23	11	4	8		
2	C	1	Total	C	N	O	0	0
			23	11	4	8		
2	D	1	Total	C	N	O	0	0
			23	11	4	8		
2	E	1	Total	C	N	O	0	0
			23	11	4	8		
2	E	1	Total	C	N	O	0	0
			23	11	4	8		

- Molecule 3 is water.

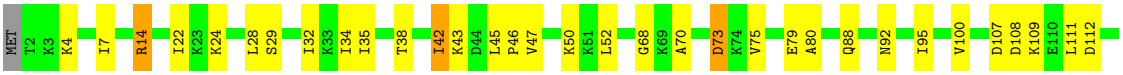
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	44	Total	O	0	0
			44	44		
3	C	50	Total	O	0	0
			50	50		
3	D	33	Total	O	0	0
			33	33		
3	E	41	Total	O	0	0
			41	41		

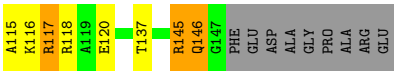
3 Residue-property plots (i)

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. 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. 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: Riboflavin synthase

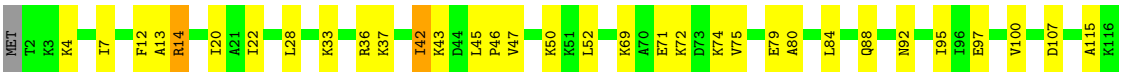
Chain A:





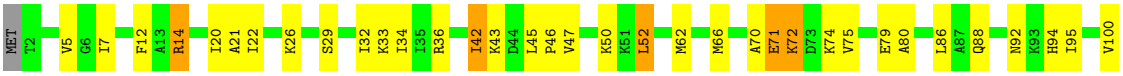
• Molecule 1: Riboflavin synthase

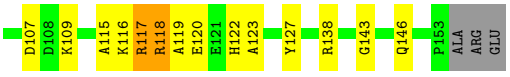
Chain B:



• Molecule 1: Riboflavin synthase

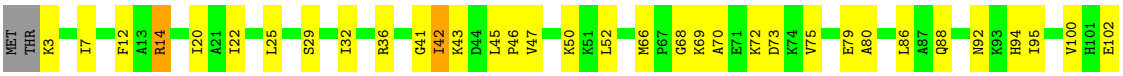
Chain C:

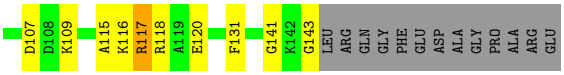




• Molecule 1: Riboflavin synthase

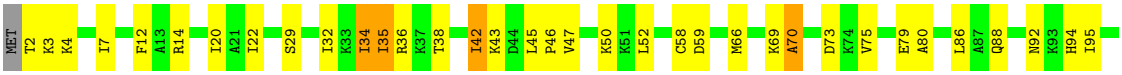
Chain D:





• Molecule 1: Riboflavin synthase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.94Å 72.91Å 72.78Å 68.50° 74.39° 74.53°	Depositor
Resolution (Å)	19.92 – 2.22 19.92 – 2.22	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.92-2.22) 92.8 (19.92-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.258 , 0.296 0.245 , 0.280	Depositor DCC
R_{free} test set	1831 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 24.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.077 for h,h-k,h-l 0.208 for -h,-l,-k 0.075 for -h,-h+l,-h+k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6187	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.96% 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: RDL

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	0.38	0/1161	0.97	8/1556 (0.5%)
1	B	0.37	0/1137	1.22	11/1525 (0.7%)
1	C	0.38	0/1207	0.92	9/1619 (0.6%)
1	D	0.36	0/1122	0.96	7/1504 (0.5%)
1	E	0.37	0/1207	0.85	6/1619 (0.4%)
All	All	0.37	0/5834	0.99	41/7823 (0.5%)

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	ARG	NE-CZ-NH1	18.05	129.33	120.30
1	B	138	ARG	NE-CZ-NH2	-17.82	111.39	120.30
1	B	14	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	C	14	ARG	NE-CZ-NH2	-14.28	113.16	120.30
1	B	14	ARG	NE-CZ-NH1	14.25	127.42	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1145	0	1204	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1121	0	1180	53	0
1	C	1189	0	1238	60	0
1	D	1106	0	1162	52	0
1	E	1189	0	1238	56	0
2	A	46	0	28	1	0
2	B	69	0	42	3	0
2	C	46	0	28	2	0
2	D	23	0	14	6	0
2	E	46	0	28	2	0
3	A	39	0	0	3	0
3	B	44	0	0	5	0
3	C	50	0	0	10	0
3	D	33	0	0	5	0
3	E	41	0	0	2	0
All	All	6187	0	6162	233	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 21.

The worst 5 of 233 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:C:47:VAL:HG21	1:E:88:GLN:HB3	1.23	1.16
1:A:47:VAL:HG21	1:B:88:GLN:HB3	1.25	1.15
1:B:47:VAL:HG21	1:D:88:GLN:HB3	1.25	1.14
1:A:88:GLN:HB3	1:E:47:VAL:HG21	1.29	1.13
1:C:88:GLN:HB3	1:D:47:VAL:HG21	1.26	1.10

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	144/156 (92%)	137 (95%)	6 (4%)	1 (1%)	22	21
1	B	141/156 (90%)	133 (94%)	7 (5%)	1 (1%)	22	21
1	C	150/156 (96%)	145 (97%)	4 (3%)	1 (1%)	22	21
1	D	139/156 (89%)	135 (97%)	3 (2%)	1 (1%)	22	21
1	E	150/156 (96%)	143 (95%)	6 (4%)	1 (1%)	22	21
All	All	724/780 (93%)	693 (96%)	26 (4%)	5 (1%)	22	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	70	ALA
1	C	70	ALA
1	B	142	LYS
1	A	145	ARG
1	D	70	ALA

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	123/130 (95%)	118 (96%)	5 (4%)	30	37
1	B	121/130 (93%)	117 (97%)	4 (3%)	38	47
1	C	127/130 (98%)	122 (96%)	5 (4%)	32	40
1	D	119/130 (92%)	116 (98%)	3 (2%)	47	58
1	E	127/130 (98%)	123 (97%)	4 (3%)	40	50
All	All	617/650 (95%)	596 (97%)	21 (3%)	37	46

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	42	ILE
1	E	34	ILE
1	E	52	LEU

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Mol	Chain	Res	Type
1	E	35	ILE
1	D	72	LYS

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

Mol	Chain	Res	Type
1	D	88	GLN
1	D	92	ASN
1	E	92	ASN
1	E	88	GLN
1	B	92	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)

10 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	RDL	A	1208	-	22,24,24	2.50	6 (27%)	20,35,35	2.58	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	RDL	D	1203	-	22,24,24	2.62	5 (22%)	20,35,35	2.99	7 (35%)
2	RDL	E	1207	-	22,24,24	2.64	7 (31%)	20,35,35	2.73	6 (30%)
2	RDL	B	1209	-	22,24,24	2.59	6 (27%)	20,35,35	2.64	6 (30%)
2	RDL	C	1201	-	22,24,24	2.53	6 (27%)	20,35,35	2.63	6 (30%)
2	RDL	A	1205	-	22,24,24	2.55	6 (27%)	20,35,35	2.65	6 (30%)
2	RDL	E	1202	-	22,24,24	2.40	4 (18%)	20,35,35	2.65	7 (35%)
2	RDL	B	1206	-	22,24,24	2.53	6 (27%)	20,35,35	2.74	7 (35%)
2	RDL	C	1204	-	22,24,24	2.57	6 (27%)	20,35,35	2.60	7 (35%)
2	RDL	B	1210	-	22,24,24	2.64	7 (31%)	20,35,35	2.75	6 (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
2	RDL	A	1208	-	-	3/14/14/14	0/2/2/2
2	RDL	D	1203	-	-	4/14/14/14	0/2/2/2
2	RDL	E	1207	-	-	0/14/14/14	0/2/2/2
2	RDL	B	1209	-	-	6/14/14/14	0/2/2/2
2	RDL	C	1201	-	-	0/14/14/14	0/2/2/2
2	RDL	A	1205	-	-	1/14/14/14	0/2/2/2
2	RDL	E	1202	-	-	2/14/14/14	0/2/2/2
2	RDL	B	1206	-	-	3/14/14/14	0/2/2/2
2	RDL	C	1204	-	-	0/14/14/14	0/2/2/2
2	RDL	B	1210	-	-	0/14/14/14	0/2/2/2

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1203	RDL	C5-C10	9.91	1.48	1.38
2	B	1209	RDL	C5-C10	9.83	1.48	1.38
2	B	1210	RDL	C5-C10	9.72	1.48	1.38
2	C	1201	RDL	C5-C10	9.61	1.48	1.38
2	C	1204	RDL	C5-C10	9.39	1.48	1.38

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1207	RDL	C2-N3-C4	8.81	122.53	115.09
2	B	1210	RDL	C2-N3-C4	8.71	122.44	115.09
2	B	1209	RDL	C2-N3-C4	8.52	122.28	115.09
2	B	1206	RDL	C2-N3-C4	8.47	122.24	115.09
2	D	1203	RDL	C2-N3-C4	8.45	122.22	115.09

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1208	RDL	N9-C11-C12-C13
2	A	1208	RDL	N9-C11-C12-O12
2	A	1208	RDL	C12-C11-N9-C10
2	B	1206	RDL	C12-C11-N9-C8
2	B	1206	RDL	C12-C11-N9-C10

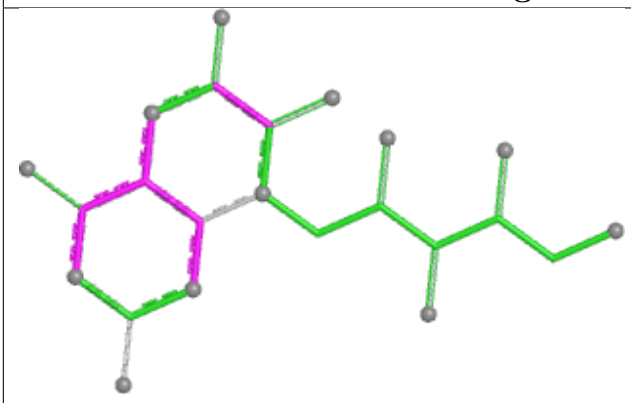
There are no ring outliers.

8 monomers are involved in 14 short contacts:

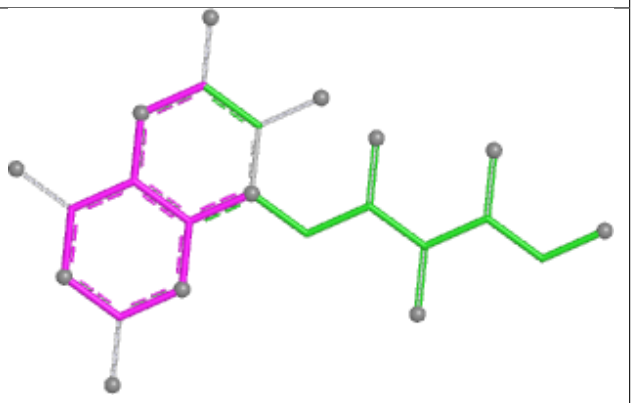
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1208	RDL	1	0
2	D	1203	RDL	6	0
2	E	1207	RDL	1	0
2	B	1209	RDL	2	0
2	C	1201	RDL	1	0
2	E	1202	RDL	1	0
2	C	1204	RDL	1	0
2	B	1210	RDL	1	0

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

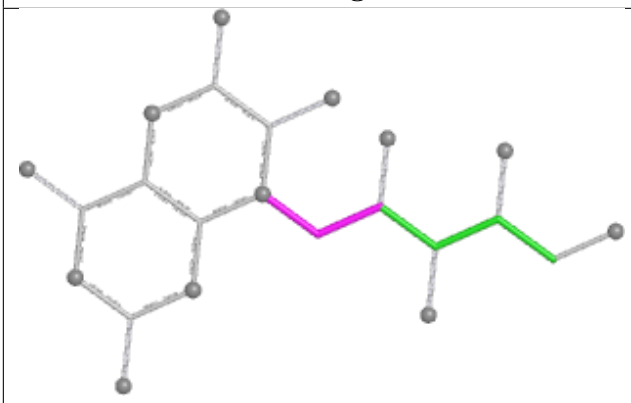
Ligand RDL A 1208



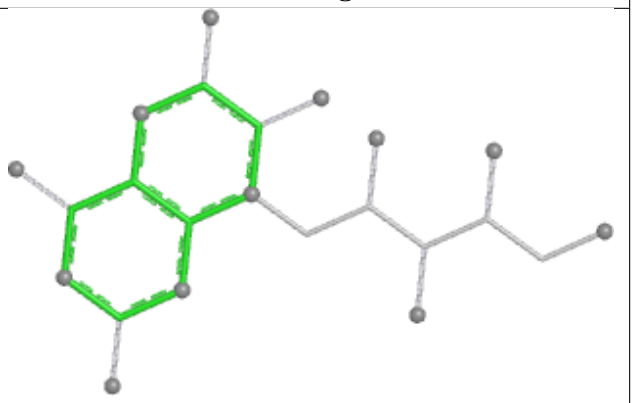
Bond lengths



Bond angles

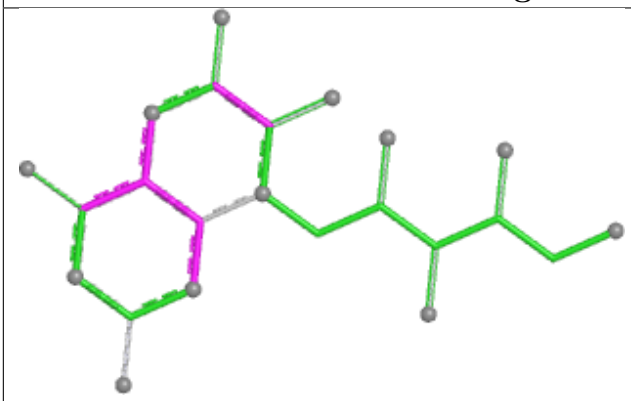


Torsions

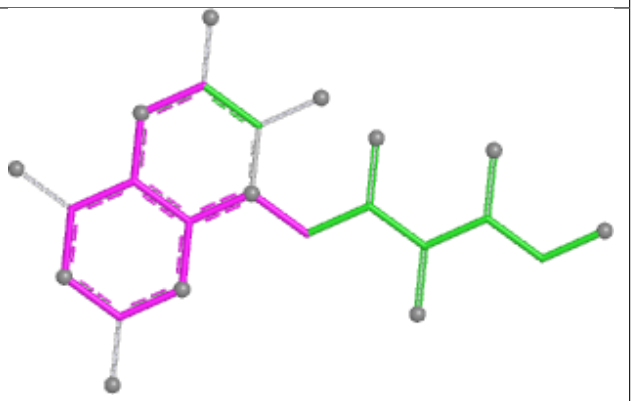


Rings

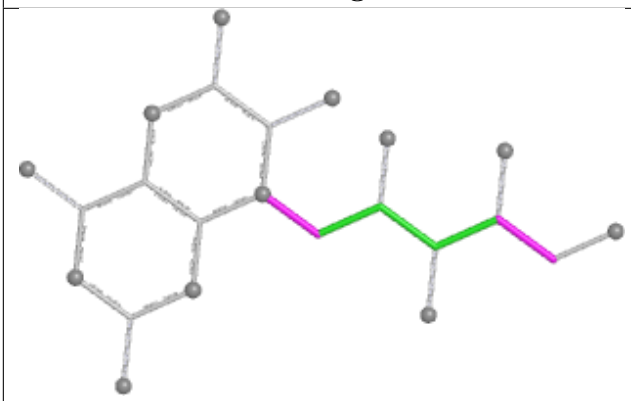
Ligand RDL D 1203



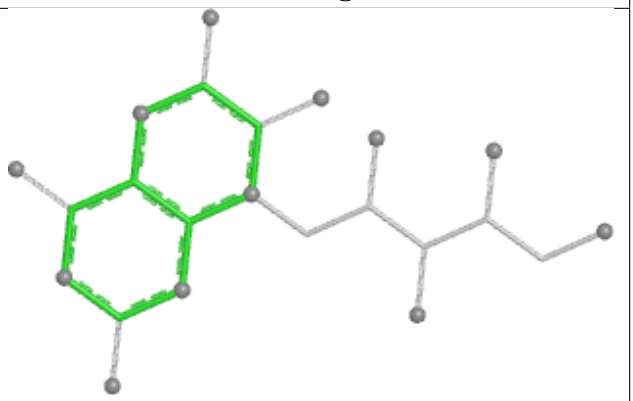
Bond lengths



Bond angles

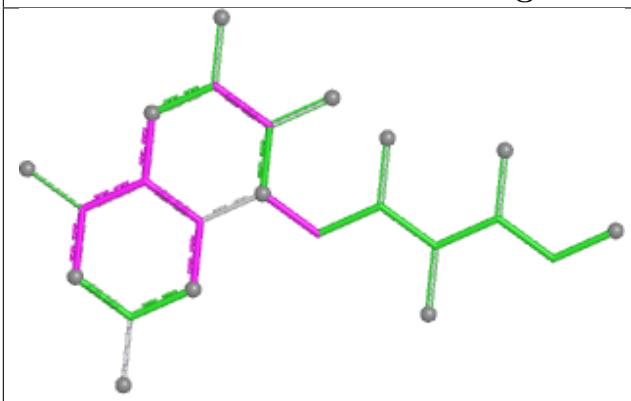


Torsions

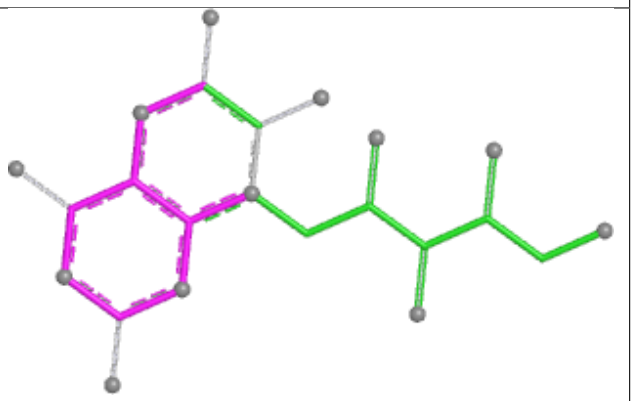


Rings

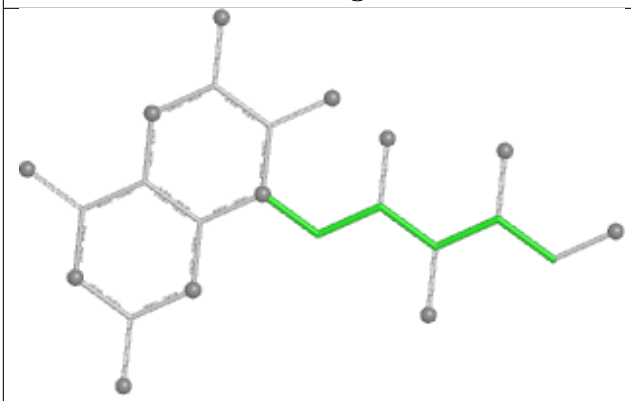
Ligand RDL E 1207



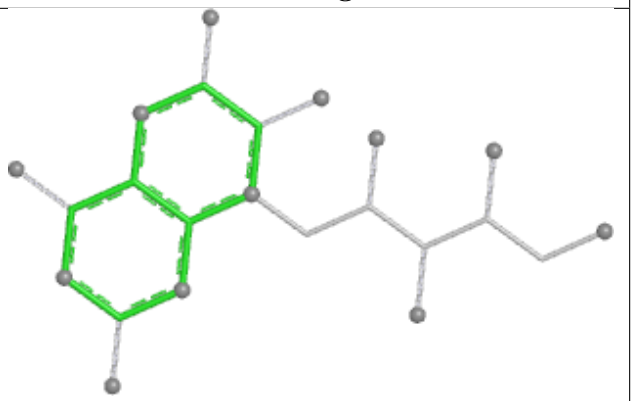
Bond lengths



Bond angles

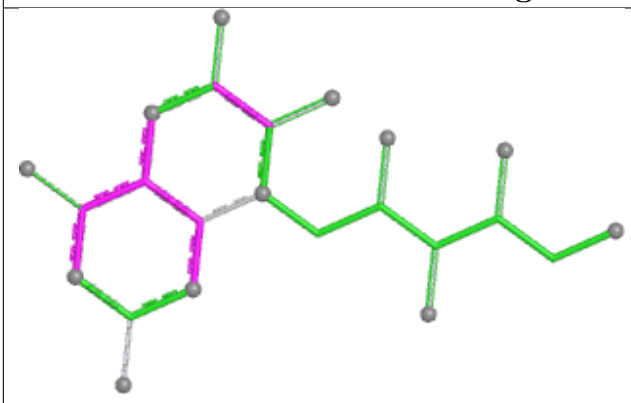


Torsions

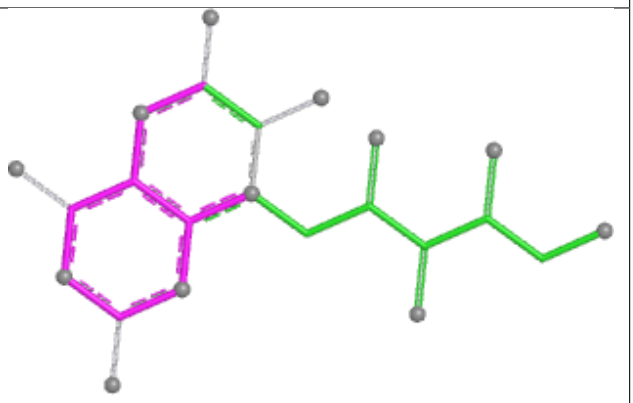


Rings

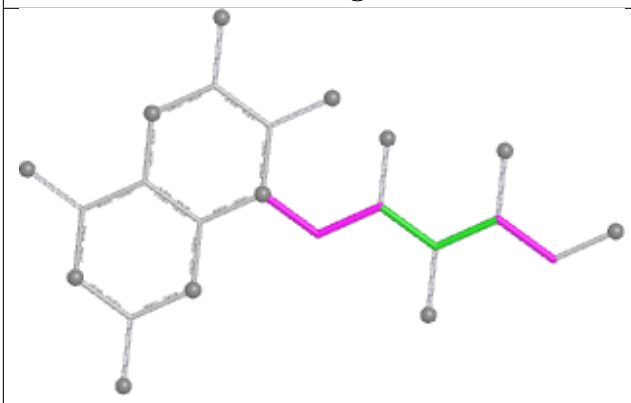
Ligand RDL B 1209



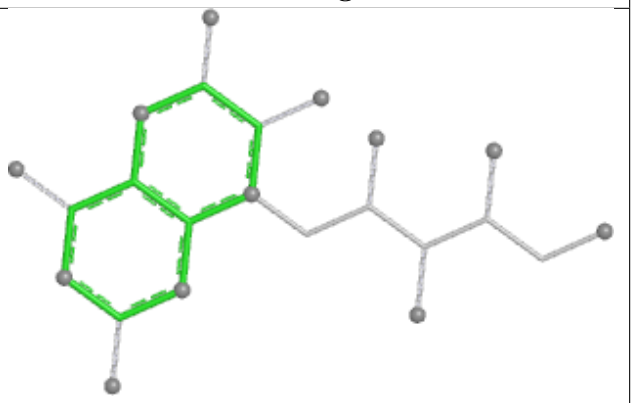
Bond lengths



Bond angles

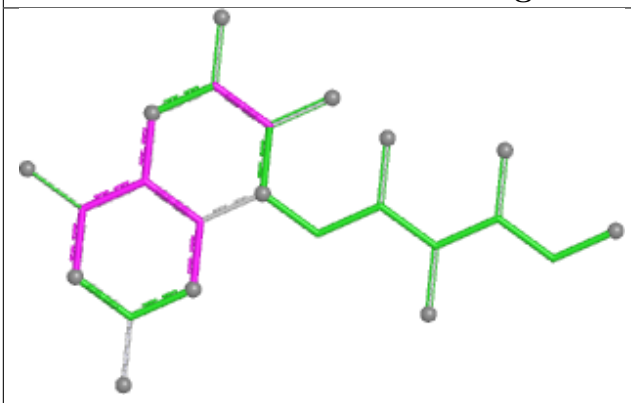


Torsions

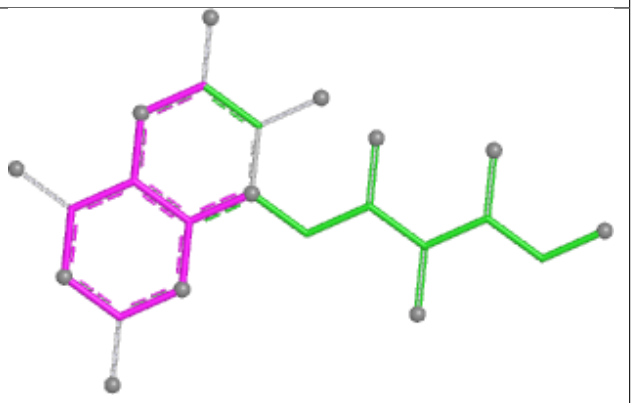


Rings

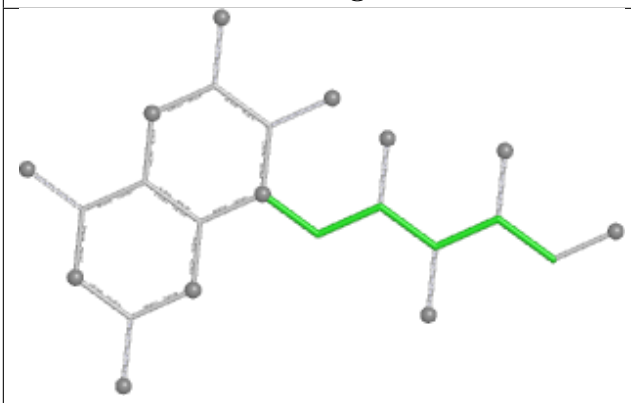
Ligand RDL C 1201



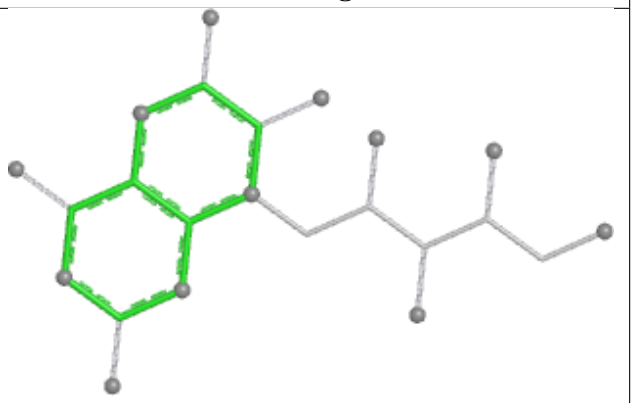
Bond lengths



Bond angles

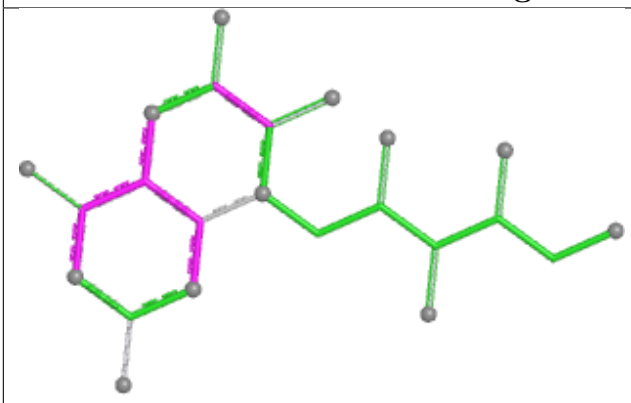


Torsions

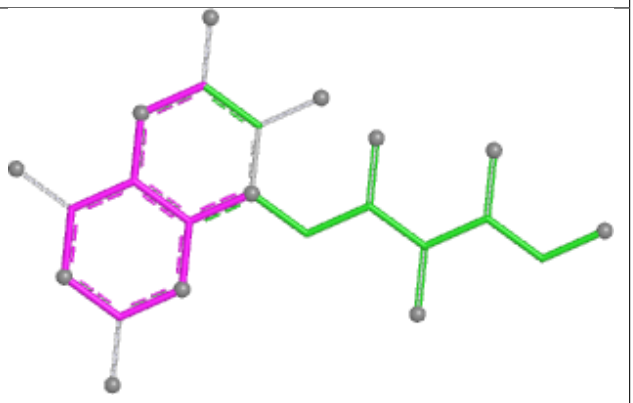


Rings

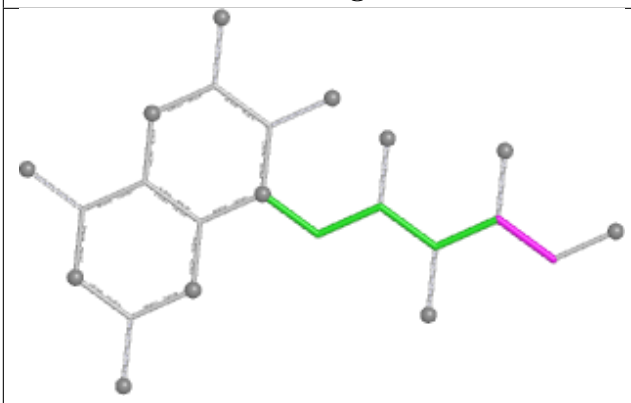
Ligand RDL A 1205



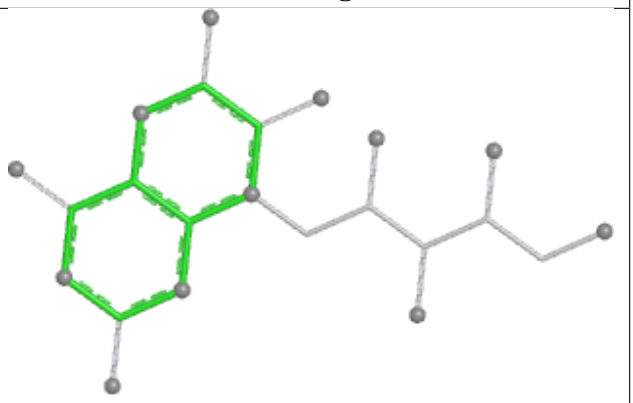
Bond lengths



Bond angles

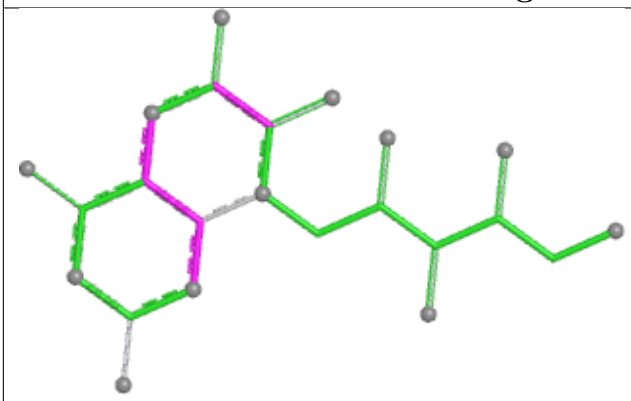


Torsions

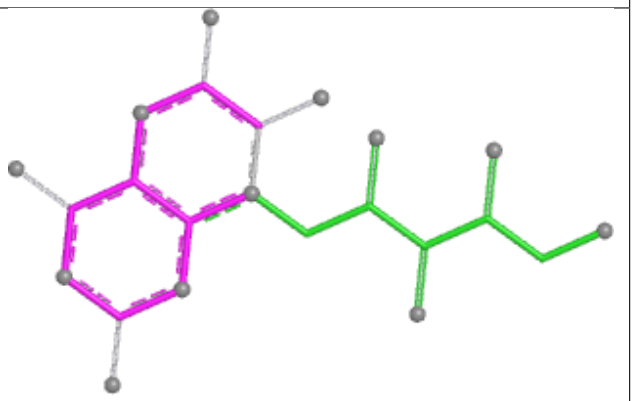


Rings

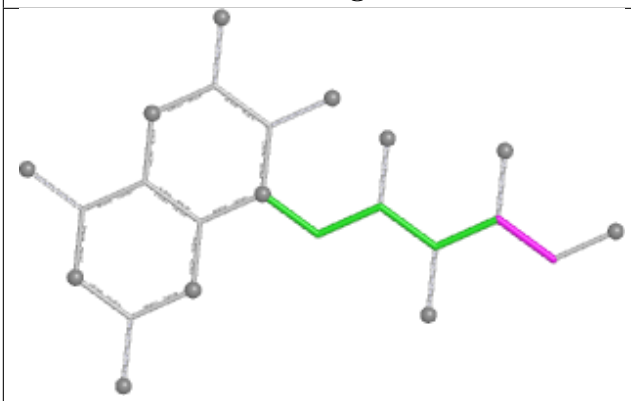
Ligand RDL E 1202



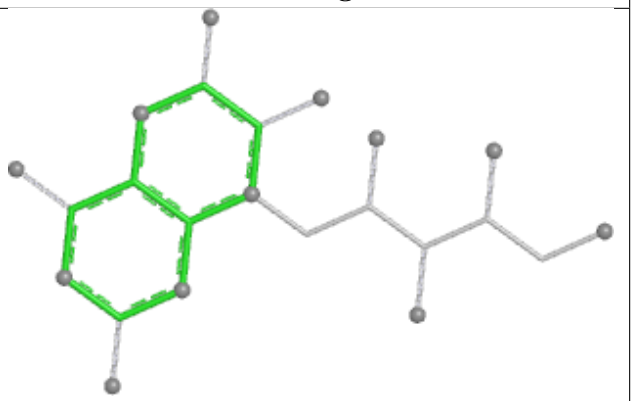
Bond lengths



Bond angles

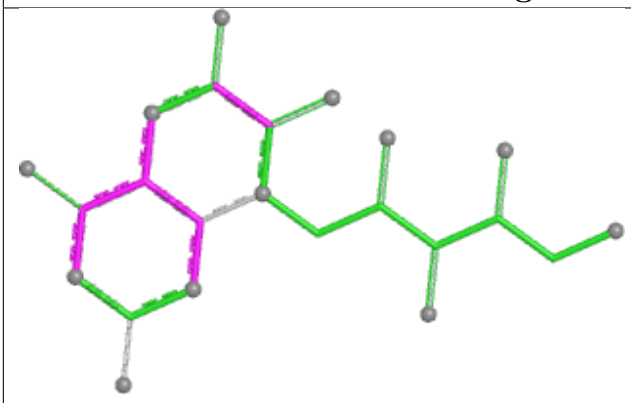


Torsions

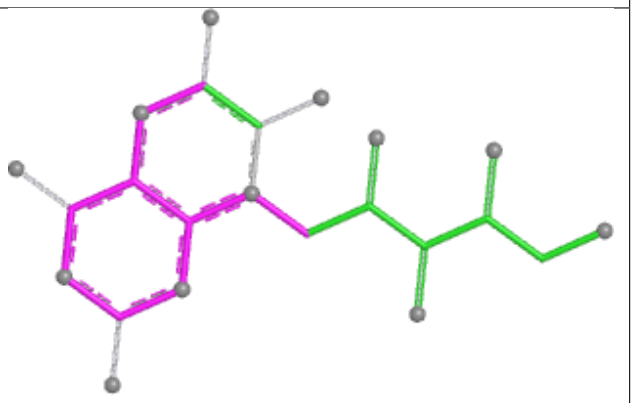


Rings

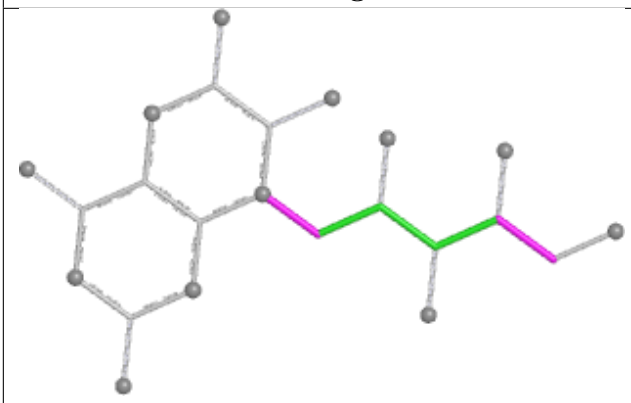
Ligand RDL B 1206



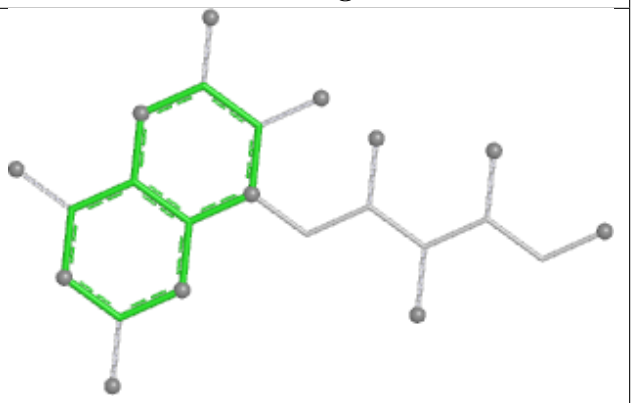
Bond lengths



Bond angles

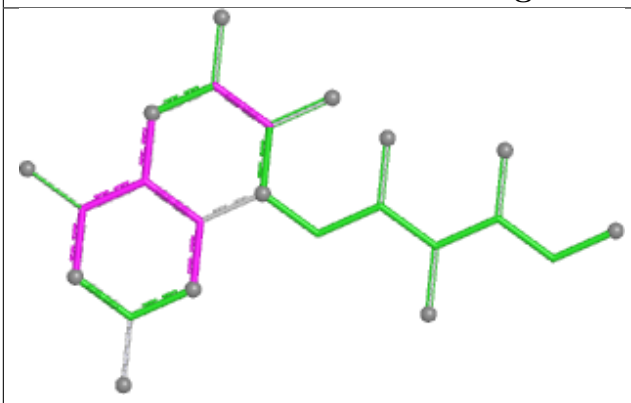


Torsions

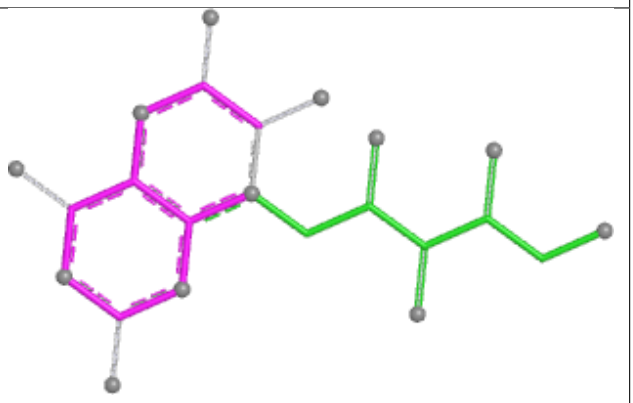


Rings

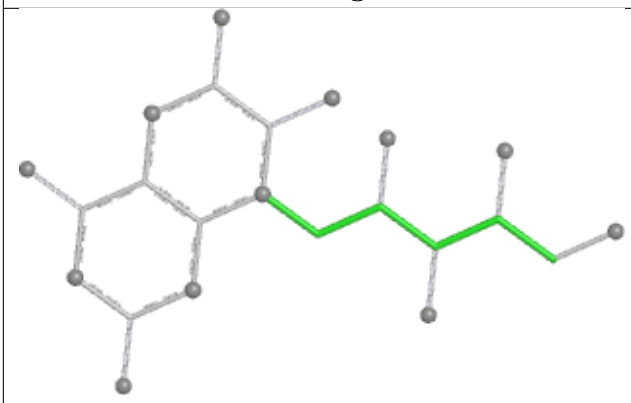
Ligand RDL C 1204



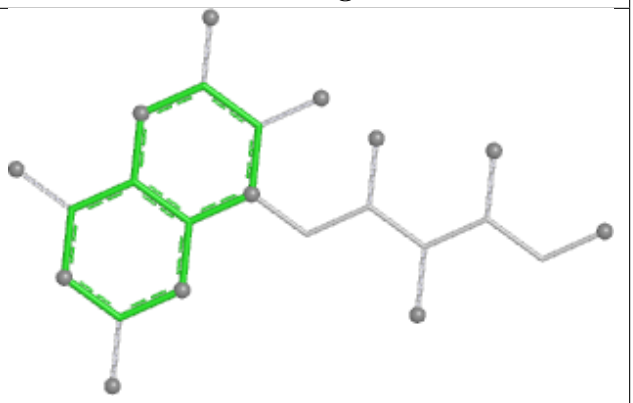
Bond lengths



Bond angles

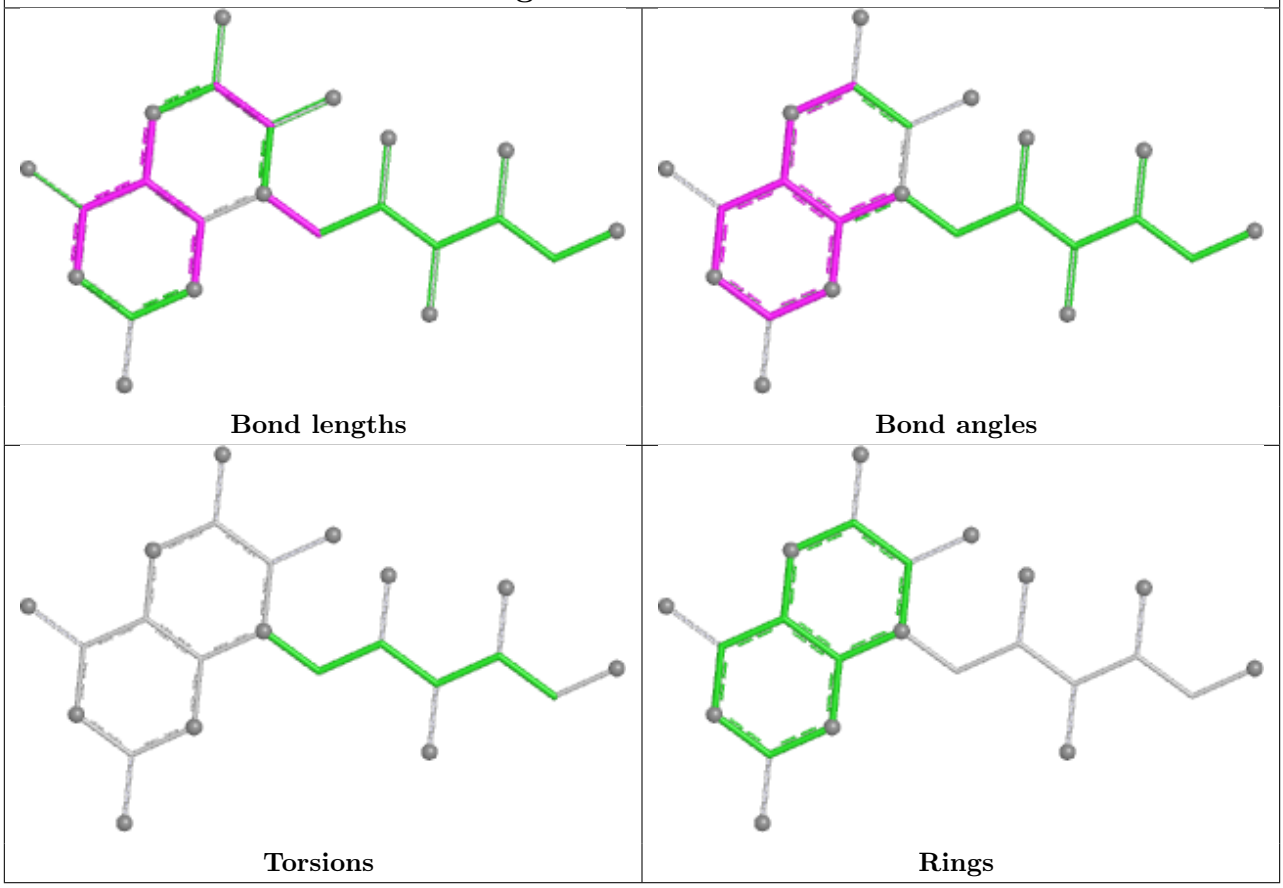


Torsions



Rings

Ligand RDL B 1210



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

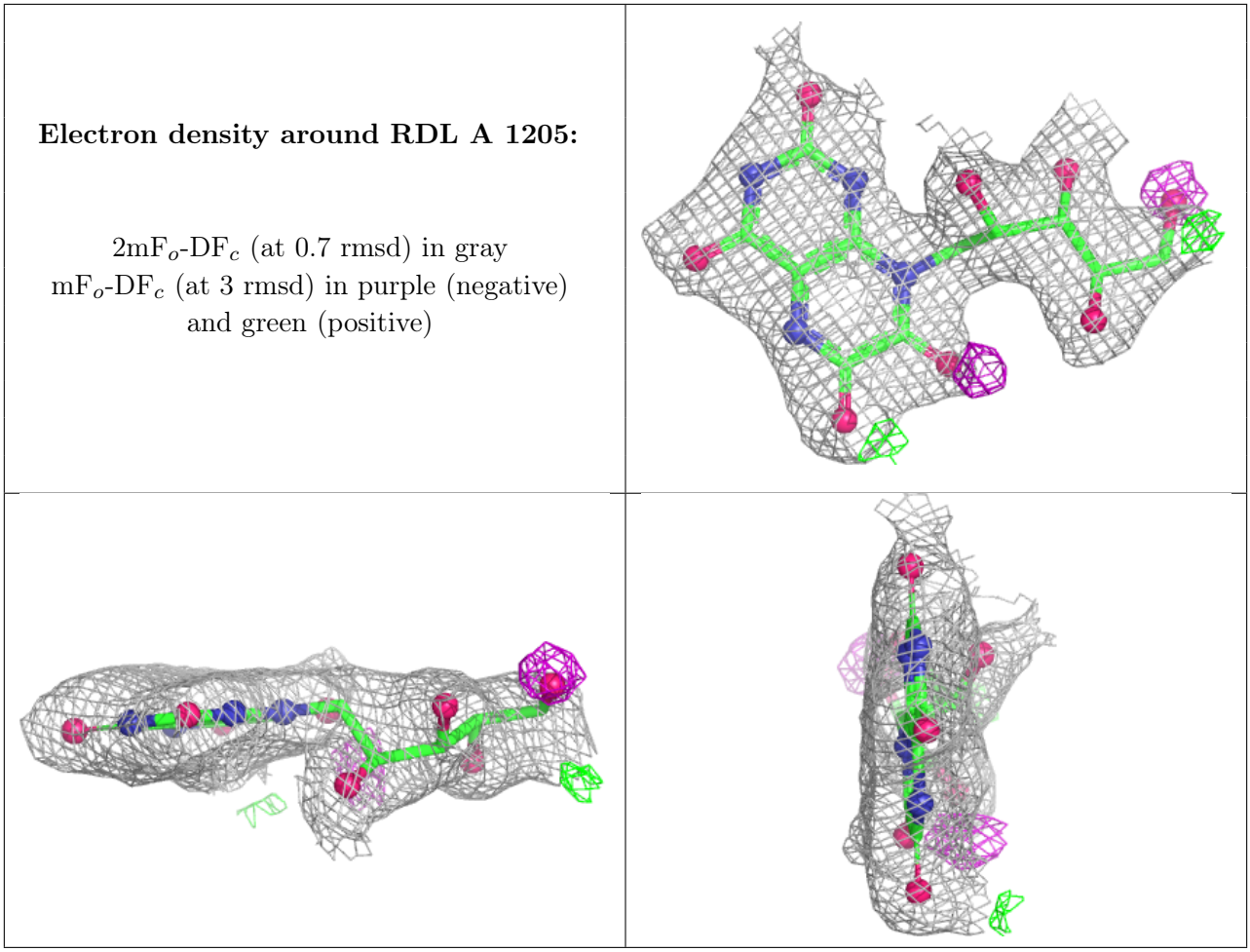
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

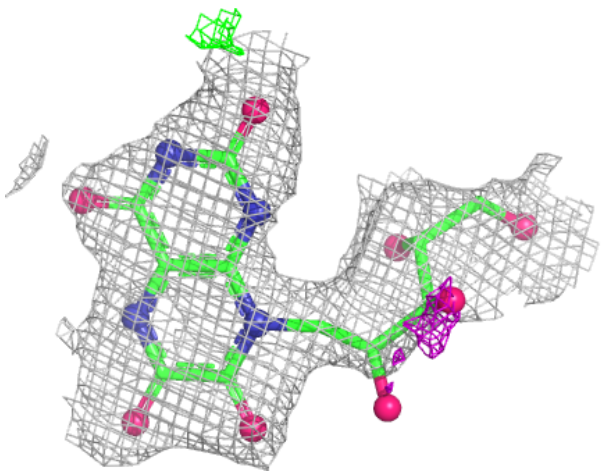
Electron density around RDL A 1205:

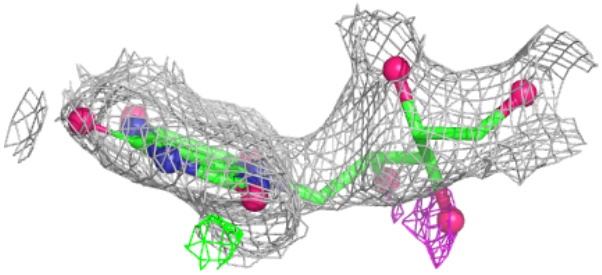
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

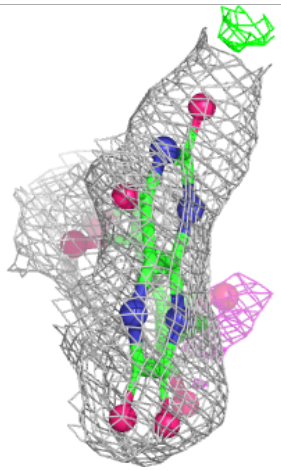


Electron density around RDL A 1208:

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

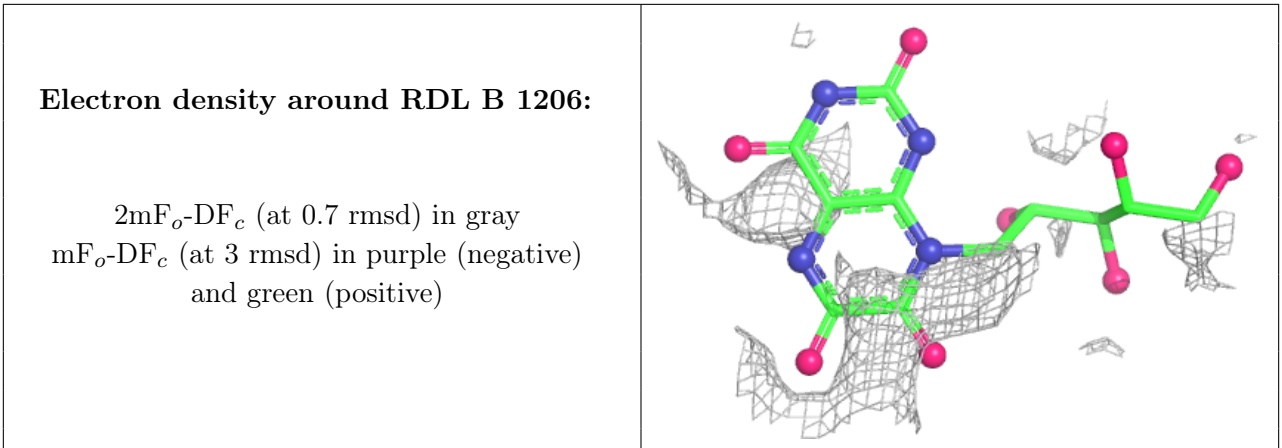






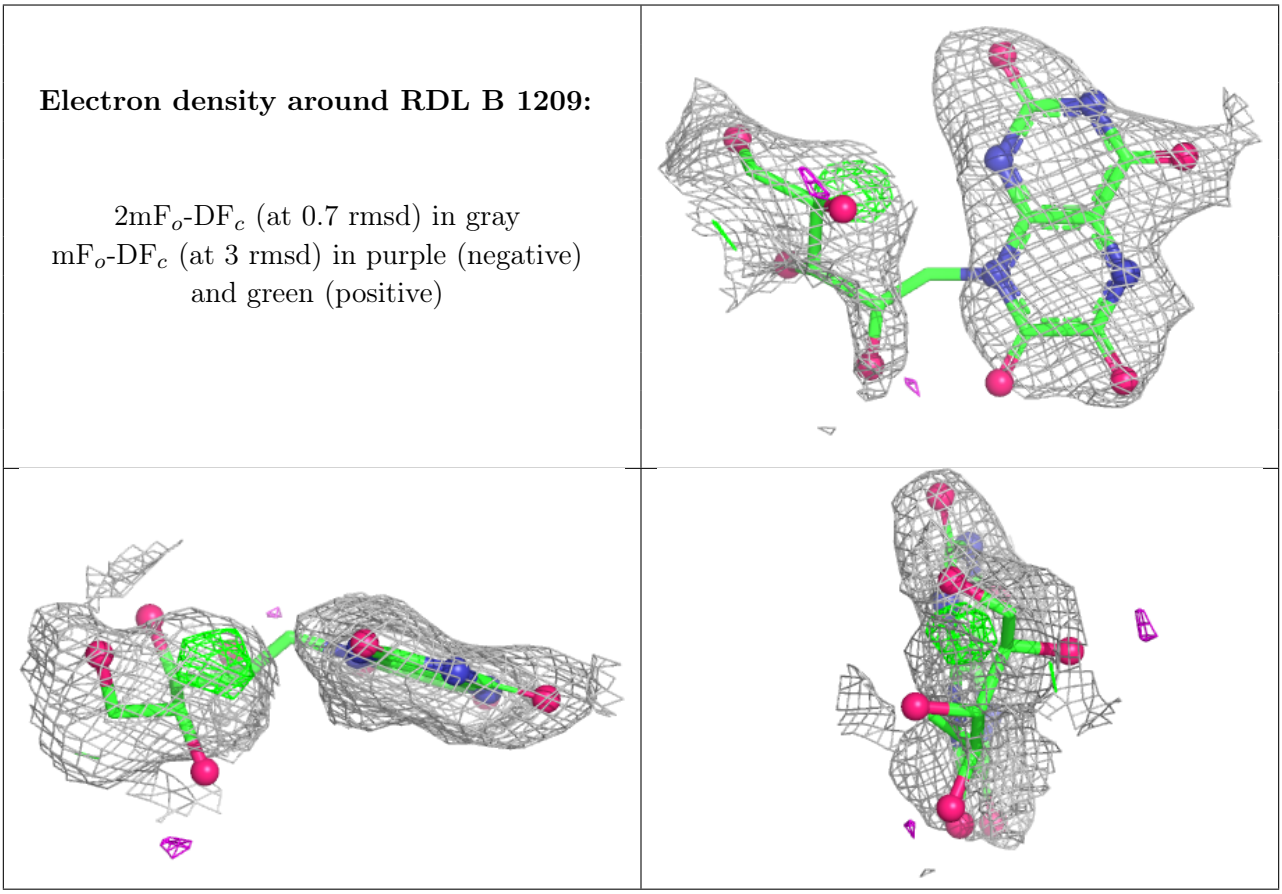
Electron density around RDL B 1206:

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



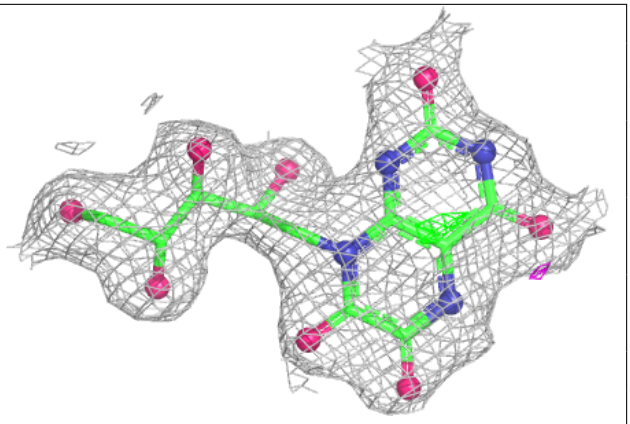
Electron density around RDL B 1209:

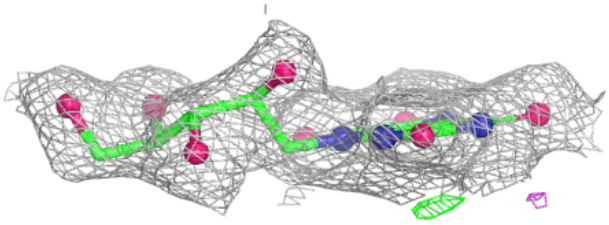
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

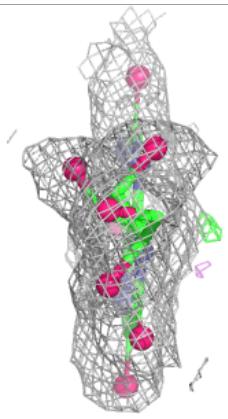


Electron density around RDL B 1210:

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

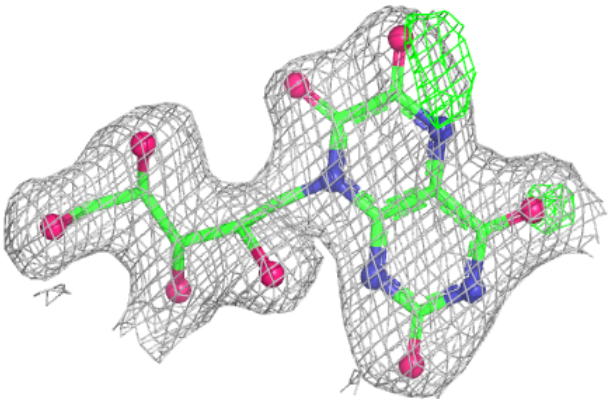


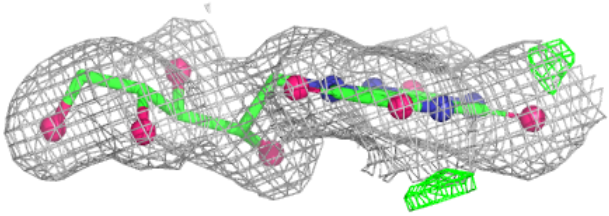


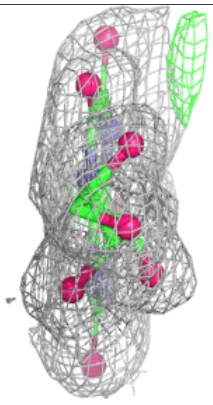


Electron density around RDL C 1201:

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

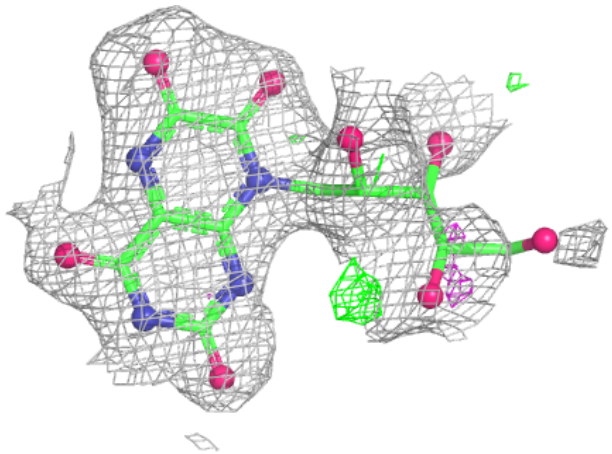


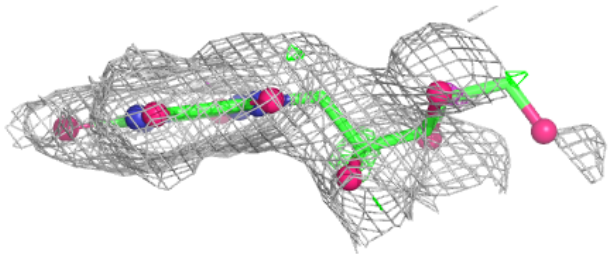


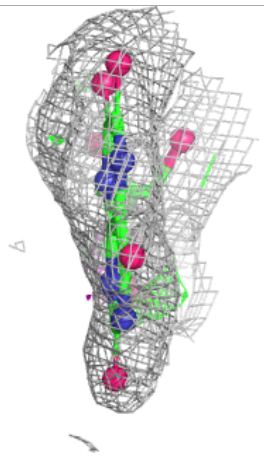


Electron density around RDL C 1204:

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

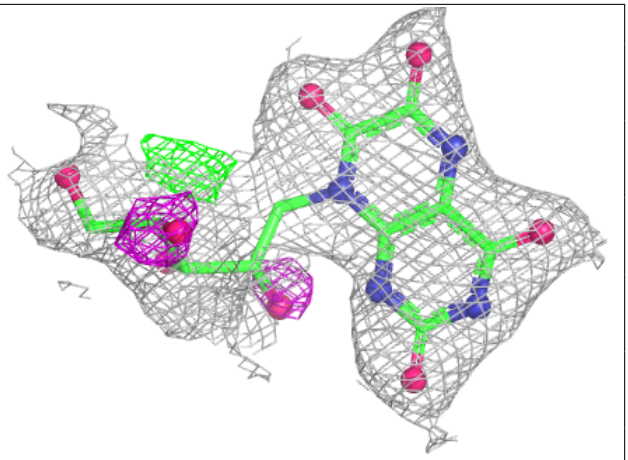


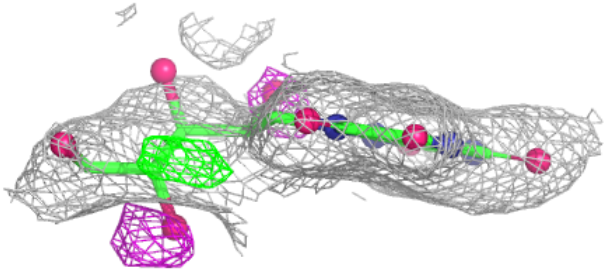


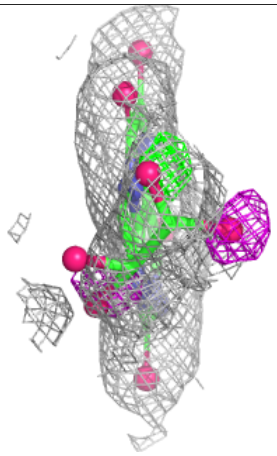


Electron density around RDL D 1203:

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

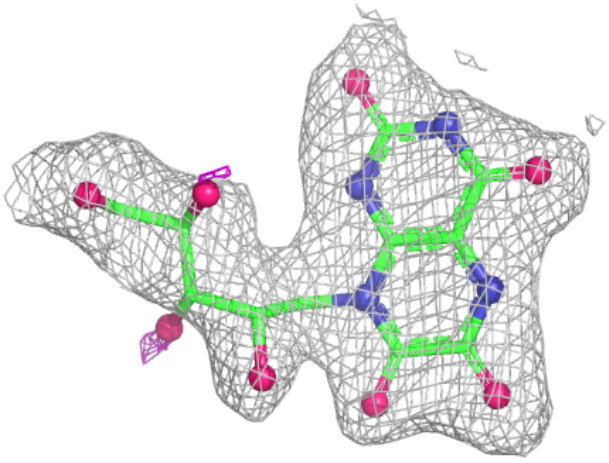


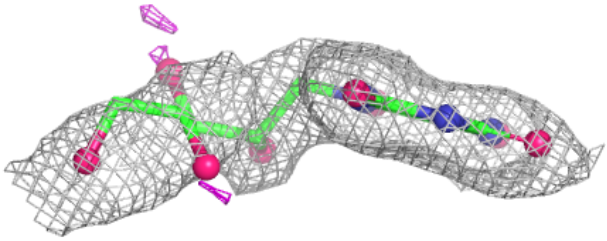


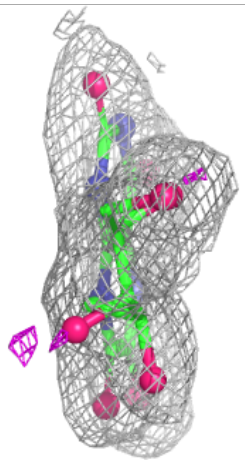


Electron density around RDL E 1202:

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

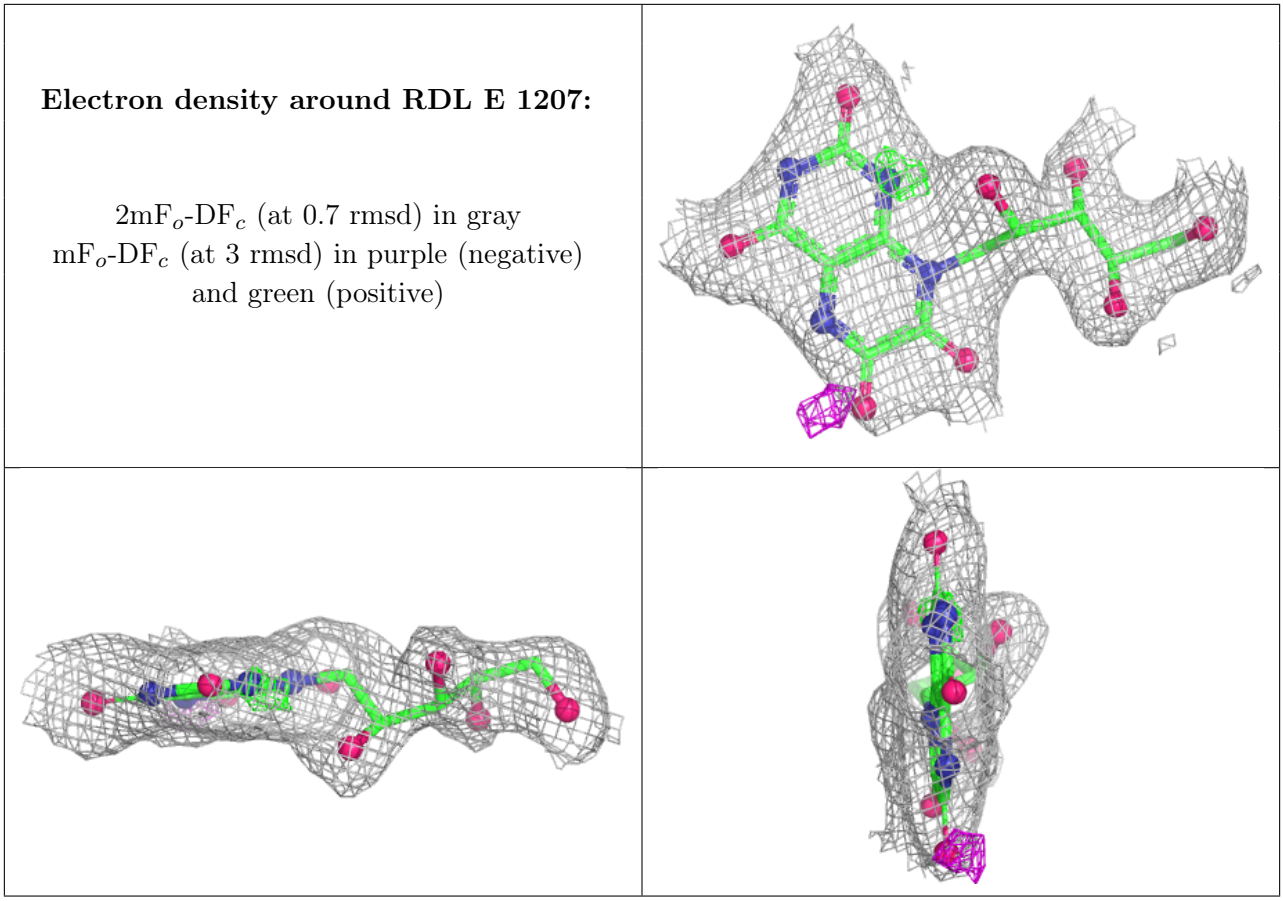






Electron density around RDL E 1207:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.