Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 03:34 AM EDT

PDB ID	:	7K15
Title	:	Crystal structure of the Human Leukotriene B4 Receptor 1 in Complex with Selective Antagonist MK-D-046
Authors	:	Michaelian, N.; Han, G.W.; Cherezov, V.
Deposited on	:	2020-09-07
Resolution	:	2.88 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

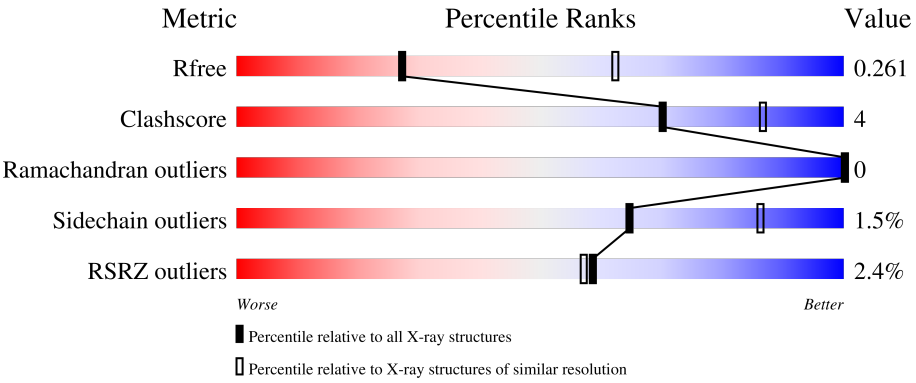
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	490	2% 83% 10% 7%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 3624 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 Leukotriene B4 receptor 1,Flavodoxin,Leukotriene B4 receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	455	3439	2229	589	607	14	0	1	0

There are 44 discrepancies between the modelled and reference sequences:

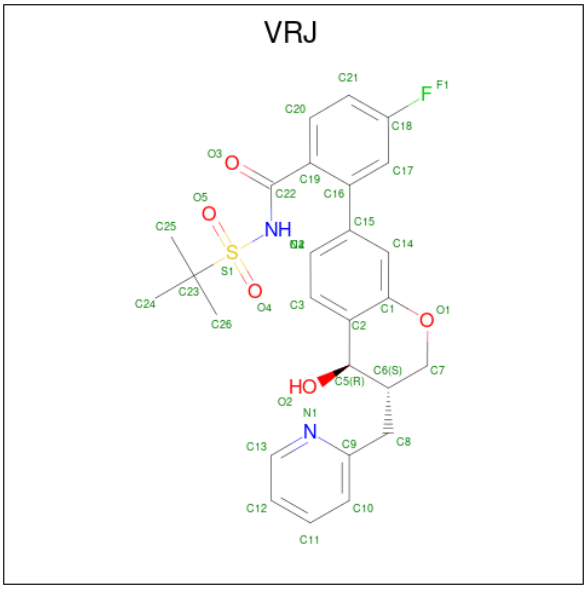
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q15722
A	-21	LYS	-	expression tag	UNP Q15722
A	-20	THR	-	expression tag	UNP Q15722
A	-19	ILE	-	expression tag	UNP Q15722
A	-18	ILE	-	expression tag	UNP Q15722
A	-17	ALA	-	expression tag	UNP Q15722
A	-16	LEU	-	expression tag	UNP Q15722
A	-15	SER	-	expression tag	UNP Q15722
A	-14	TYR	-	expression tag	UNP Q15722
A	-13	ILE	-	expression tag	UNP Q15722
A	-12	PHE	-	expression tag	UNP Q15722
A	-11	CYS	-	expression tag	UNP Q15722
A	-10	LEU	-	expression tag	UNP Q15722
A	-9	VAL	-	expression tag	UNP Q15722
A	-8	PHE	-	expression tag	UNP Q15722
A	-7	ALA	-	expression tag	UNP Q15722
A	-6	ASP	-	expression tag	UNP Q15722
A	-5	TYR	-	expression tag	UNP Q15722
A	-4	LYS	-	expression tag	UNP Q15722
A	-3	ASP	-	expression tag	UNP Q15722
A	-2	ASP	-	expression tag	UNP Q15722
A	-1	ASP	-	expression tag	UNP Q15722
A	0	ASP	-	expression tag	UNP Q15722
A	1	ALA	-	expression tag	UNP Q15722
A	2	GLY	-	expression tag	UNP Q15722
A	3	ARG	-	expression tag	UNP Q15722

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ALA	-	expression tag	UNP Q15722
A	106	TRP	LEU	engineered mutation	UNP Q15722
A	116	TYR	SER	engineered mutation	UNP Q15722
A	196	ILE	ALA	engineered mutation	UNP Q15722
A	1002	ALA	PRO	engineered mutation	UNP P00323
A	1098	TRP	TYR	engineered mutation	UNP P00323
A	1149	ARG	-	linker	UNP P00323
A	1150	ARG	-	linker	UNP P00323
A	287	PHE	CYS	engineered mutation	UNP Q15722
A	310	ALA	SER	engineered mutation	UNP Q15722
A	311	GLU	-	expression tag	UNP Q15722
A	312	PHE	-	expression tag	UNP Q15722
A	313	LEU	-	expression tag	UNP Q15722
A	314	GLU	-	expression tag	UNP Q15722
A	315	VAL	-	expression tag	UNP Q15722
A	316	LEU	-	expression tag	UNP Q15722
A	317	PHE	-	expression tag	UNP Q15722
A	318	GLN	-	expression tag	UNP Q15722

- Molecule 2 is N-(tert-butylsulfonyl)-4-fluoro-2-{(3S,4R)-4-hydroxy-3-[(pyridin-2-yl)methyl]-3,4-dihydro-2H-1-benzopyran-7-yl}benzamide (three-letter code: VRJ) (formula: $C_{26}H_{27}FN_2O_5S$) (labeled as "Ligand of Interest" by depositor).

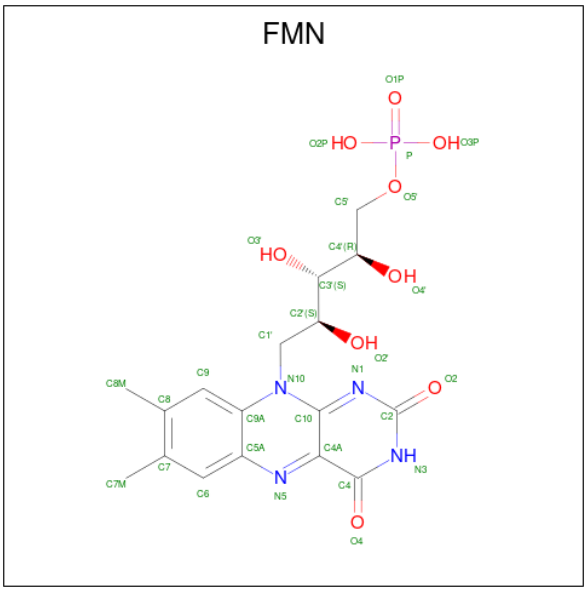


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			35	26	1	2	5	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

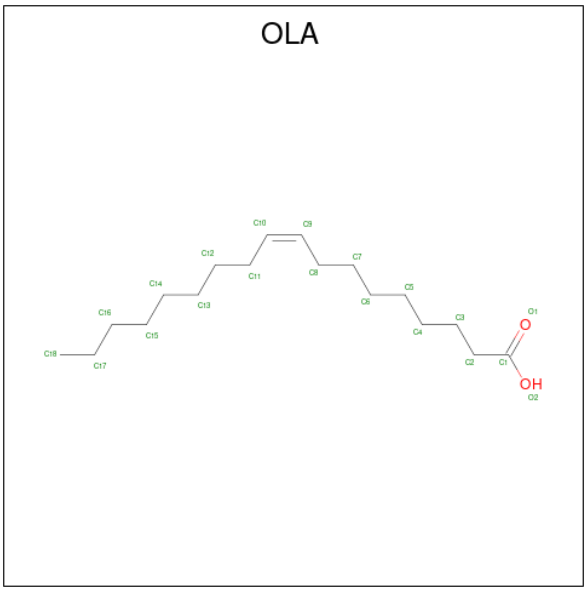
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



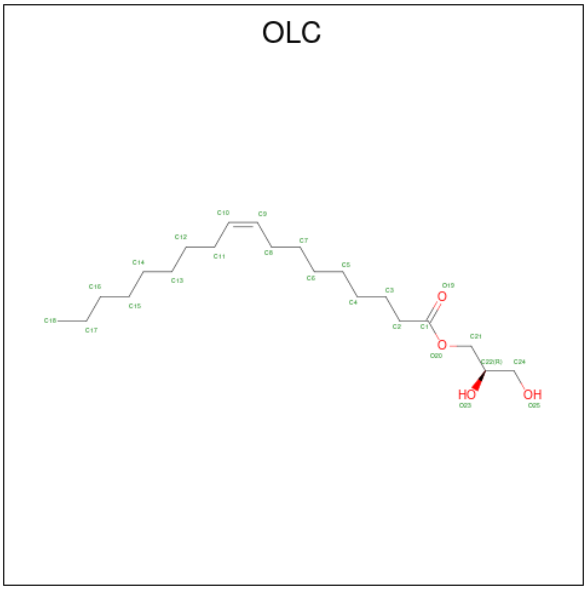
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



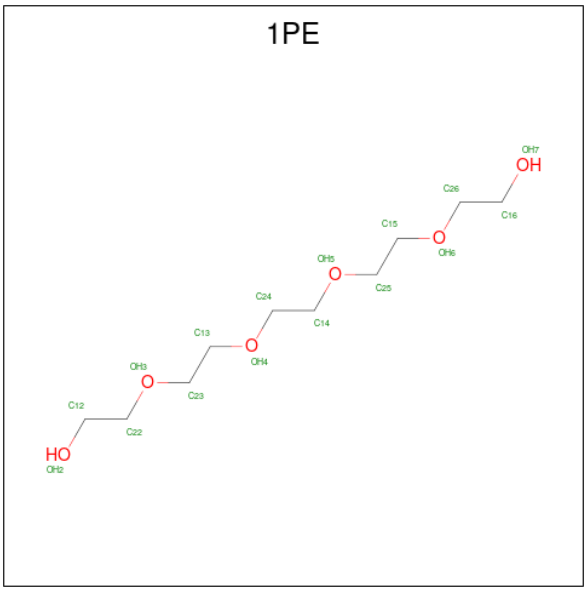
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 12 10 2	0	0

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



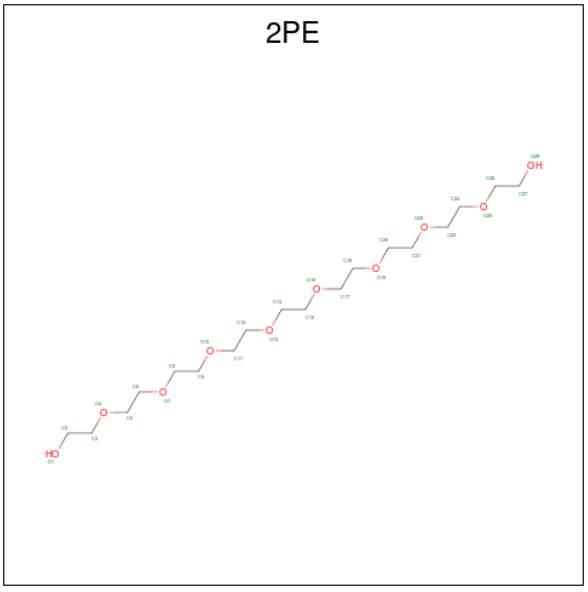
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 9 4	0	0
6	A	1	Total C O 25 21 4	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



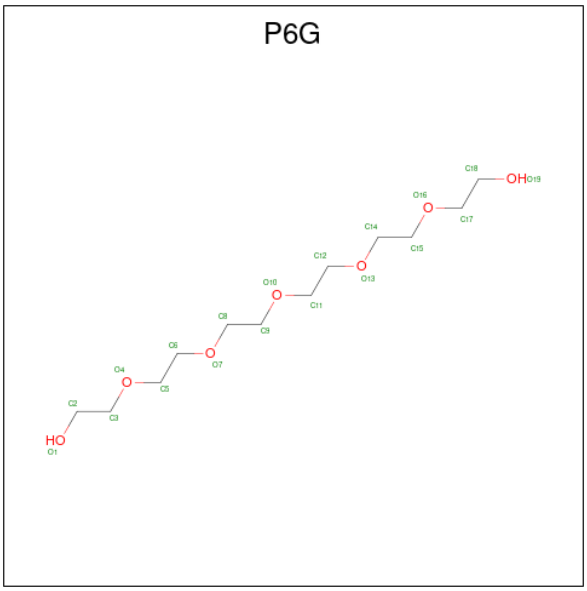
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			28	18	10		

- Molecule 9 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 19 12 7	0	0

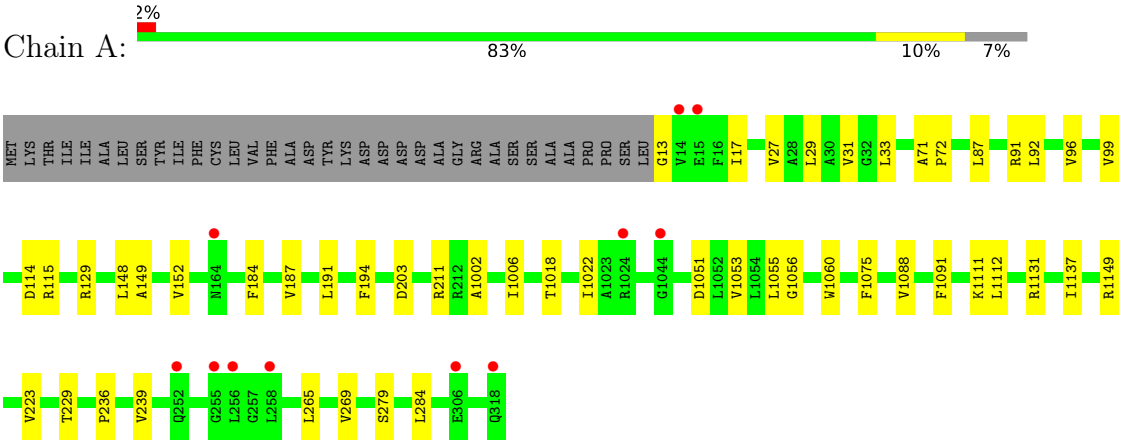
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	5	Total O 5 5	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: Leukotriene B4 receptor 1,Flavodoxin,Leukotriene B4 receptor 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	70.77Å 82.67Å 127.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.37 – 2.88 34.37 – 2.88	Depositor EDS
% Data completeness (in resolution range)	78.8 (34.37-2.88) 78.8 (34.37-2.88)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.212 , 0.261 0.212 , 0.261	Depositor DCC
R_{free} test set	714 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	65.7	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3624	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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: OLC, 2PE, VRJ, OLA, NA, 1PE, FMN, P6G

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	0.26	0/3515	0.42	0/4779

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3439	0	3458	26	0
2	A	35	0	0	0	0
3	A	1	0	0	0	0
4	A	31	0	19	1	0
5	A	12	0	15	0	0
6	A	38	0	55	0	0
7	A	16	0	22	1	0
8	A	28	0	38	0	0
9	A	19	0	26	1	0
10	A	5	0	0	0	0
All	All	3624	0	3633	26	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 4.

All (26) 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:A:31:VAL:HG13	1:A:279:SER:HB2	1.82	0.61
1:A:115:ARG:HH21	1:A:223:VAL:HG21	1.72	0.54
1:A:114:ASP:OD2	1:A:129:ARG:NH1	2.43	0.52
1:A:1055:LEU:HD12	1:A:1112:LEU:HD11	1.91	0.51
1:A:29:LEU:HD11	1:A:72:PRO:HD3	1.92	0.51
1:A:87:LEU:HD21	1:A:91:ARG:HH11	1.74	0.51
1:A:187:VAL:HA	1:A:191:LEU:HB2	1.94	0.50
1:A:1056:GLY:HA2	1:A:1091:PHE:O	2.12	0.49
1:A:27:VAL:O	1:A:31:VAL:HG12	2.13	0.48
1:A:1006:ILE:HD13	1:A:1022:ILE:HG13	1.95	0.48
1:A:229:THR:HG21	1:A:284:LEU:HD11	1.95	0.48
1:A:1060:TRP:CZ3	4:A:2103:FMN:HM83	2.50	0.47
1:A:1149:ARG:O	7:A:2107:1PE:H241	2.15	0.46
1:A:149:ALA:O	1:A:152:VAL:HG12	2.16	0.46
1:A:17:ILE:HG13	1:A:265:LEU:HD12	2.00	0.44
1:A:13:GLY:O	1:A:17:ILE:HG12	2.18	0.43
1:A:71:ALA:N	1:A:72:PRO:HD2	2.34	0.42
1:A:1075:PHE:CZ	1:A:1111:LYS:HD2	2.54	0.42
1:A:96:VAL:HA	1:A:99:VAL:HG22	2.01	0.42
1:A:211:ARG:NH2	1:A:1051:ASP:OD2	2.52	0.42
1:A:1002:ALA:HB2	9:A:2109:P6G:H82	2.02	0.42
1:A:1053:VAL:HB	1:A:1088:VAL:HG12	2.00	0.41
1:A:17:ILE:HG23	1:A:269:VAL:HG22	2.01	0.41
1:A:148:LEU:HD22	1:A:184:PHE:HZ	1.85	0.41
1:A:1018:THR:HG22	1:A:1137:ILE:HD13	2.03	0.41
1:A:236:PRO:HA	1:A:239:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	454/490 (93%)	440 (97%)	14 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	344/384 (90%)	339 (98%)	5 (2%)	65 86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	92	LEU
1	A	194	PHE
1	A	203	ASP
1	A	1131	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
6	OLC	A	2105	-	12,12,24	0.89	0	13,13,25	0.96	1 (7%)
8	2PE	A	2108	-	27,27,27	0.55	0	26,26,26	0.20	0
9	P6G	A	2109	-	18,18,18	0.44	0	17,17,17	0.48	0
2	VRJ	A	2101	-	38,38,38	1.59	3 (7%)	53,57,57	1.15	4 (7%)
7	1PE	A	2107	-	15,15,15	0.45	0	14,14,14	0.50	0
5	OLA	A	2104	-	11,11,19	0.74	0	11,11,19	1.09	1 (9%)
4	FMN	A	2103	-	33,33,33	1.07	2 (6%)	48,50,50	1.27	8 (16%)
6	OLC	A	2106	-	24,24,24	0.60	0	25,25,25	0.92	1 (4%)

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
6	OLC	A	2105	-	-	8/12/12/24	-
8	2PE	A	2108	-	-	9/25/25/25	-
9	P6G	A	2109	-	-	4/16/16/16	-
2	VRJ	A	2101	-	-	10/26/39/39	0/4/4/4
7	1PE	A	2107	-	-	7/13/13/13	-
5	OLA	A	2104	-	-	4/9/9/17	-
4	FMN	A	2103	-	-	3/18/18/18	0/3/3/3
6	OLC	A	2106	-	-	8/24/24/24	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2101	VRJ	S1-N2	7.21	1.71	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2103	FMN	C4A-N5	3.86	1.38	1.30
2	A	2101	VRJ	C22-N2	3.63	1.43	1.39
2	A	2101	VRJ	O1-C1	2.82	1.40	1.37
4	A	2103	FMN	C10-N1	2.58	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2101	VRJ	O1-C7-C6	3.35	116.14	112.25
4	A	2103	FMN	C4-N3-C2	-3.15	119.83	125.64
4	A	2103	FMN	O4-C4-C4A	-2.95	118.79	126.60
4	A	2103	FMN	C4A-C4-N3	2.68	119.99	113.19
4	A	2103	FMN	C9A-C5A-N5	-2.51	119.71	122.43
2	A	2101	VRJ	C26-C23-S1	2.24	111.14	107.86
2	A	2101	VRJ	C19-C16-C15	2.23	126.37	123.08
4	A	2103	FMN	C4A-C10-N10	2.23	119.74	116.48
4	A	2103	FMN	C5A-C9A-N10	2.21	120.23	117.95
2	A	2101	VRJ	C16-C17-C18	2.15	122.10	119.26
5	A	2104	OLA	O2-C1-C2	2.08	120.70	114.03
4	A	2103	FMN	C10-C4A-N5	-2.07	120.46	124.86
6	A	2106	OLC	C3-C2-C1	-2.03	106.23	113.62
4	A	2103	FMN	C4A-C10-N1	-2.03	120.03	124.73
6	A	2105	OLC	O20-C1-O19	-2.02	118.50	123.59

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2101	VRJ	C6-C8-C9-N1
2	A	2101	VRJ	C22-N2-S1-C23
4	A	2103	FMN	C5'-O5'-P-O1P
4	A	2103	FMN	C5'-O5'-P-O2P
4	A	2103	FMN	C5'-O5'-P-O3P
6	A	2105	OLC	C21-C22-C24-O25
6	A	2105	OLC	O19-C1-O20-C21
6	A	2105	OLC	C2-C1-O20-C21
8	A	2108	2PE	O4-C5-C6-O7
8	A	2108	2PE	O13-C14-C15-O16
2	A	2101	VRJ	C25-C23-S1-O4
8	A	2108	2PE	O16-C17-C18-O19
9	A	2109	P6G	O4-C5-C6-O7
6	A	2105	OLC	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

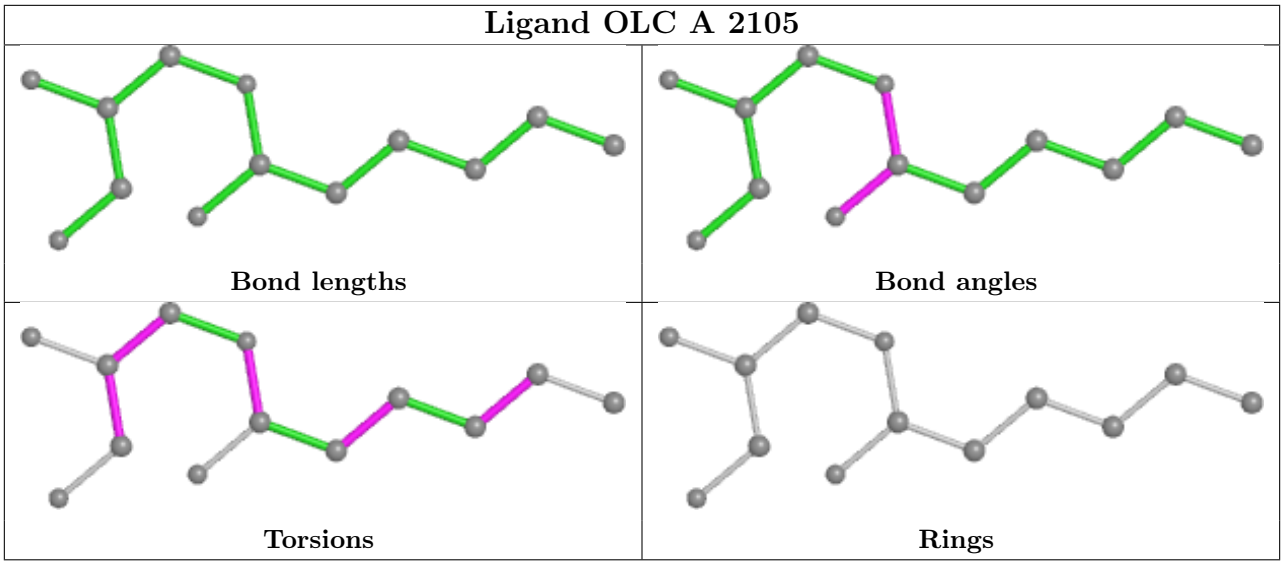
Mol	Chain	Res	Type	Atoms
8	A	2108	2PE	O19-C20-C21-O22
6	A	2106	OLC	O20-C21-C22-O23
7	A	2107	1PE	OH2-C12-C22-OH3
6	A	2106	OLC	C2-C1-O20-C21
6	A	2106	OLC	O20-C21-C22-C24
2	A	2101	VRJ	C24-C23-S1-O4
6	A	2106	OLC	O19-C1-O20-C21
8	A	2108	2PE	O10-C11-C12-O13
6	A	2105	OLC	O20-C21-C22-O23
6	A	2105	OLC	O23-C22-C24-O25
6	A	2106	OLC	C12-C13-C14-C15
7	A	2107	1PE	OH5-C14-C24-OH4
9	A	2109	P6G	O1-C2-C3-O4
5	A	2104	OLA	C2-C3-C4-C5
5	A	2104	OLA	C1-C2-C3-C4
6	A	2105	OLC	O20-C21-C22-C24
2	A	2101	VRJ	C26-C23-S1-O4
6	A	2106	OLC	C14-C15-C16-C17
8	A	2108	2PE	C21-C20-O19-C18
7	A	2107	1PE	C13-C23-OH3-C22
8	A	2108	2PE	C27-C26-O25-C24
9	A	2109	P6G	C14-C15-O16-C17
9	A	2109	P6G	C18-C17-O16-C15
8	A	2108	2PE	C11-C12-O13-C14
2	A	2101	VRJ	C5-C6-C8-C9
6	A	2106	OLC	C15-C16-C17-C18
2	A	2101	VRJ	C22-N2-S1-O5
7	A	2107	1PE	OH7-C16-C26-OH6
5	A	2104	OLA	C7-C8-C9-C10
7	A	2107	1PE	C24-C14-OH5-C25
2	A	2101	VRJ	C25-C23-S1-N2
7	A	2107	1PE	OH6-C15-C25-OH5
5	A	2104	OLA	C4-C5-C6-C7
2	A	2101	VRJ	C24-C23-S1-N2
6	A	2106	OLC	C9-C10-C11-C12
8	A	2108	2PE	O22-C23-C24-O25
6	A	2105	OLC	C3-C4-C5-C6
2	A	2101	VRJ	C20-C19-C22-O3
7	A	2107	1PE	C23-C13-OH4-C24

There are no ring outliers.

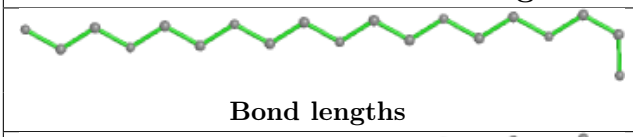
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2109	P6G	1	0
7	A	2107	1PE	1	0
4	A	2103	FMN	1	0

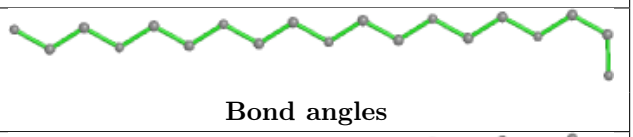
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



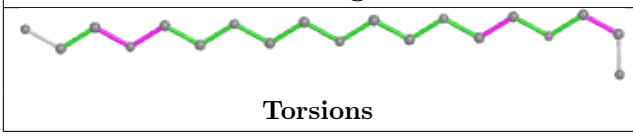
Ligand P6G A 2109



Bond lengths



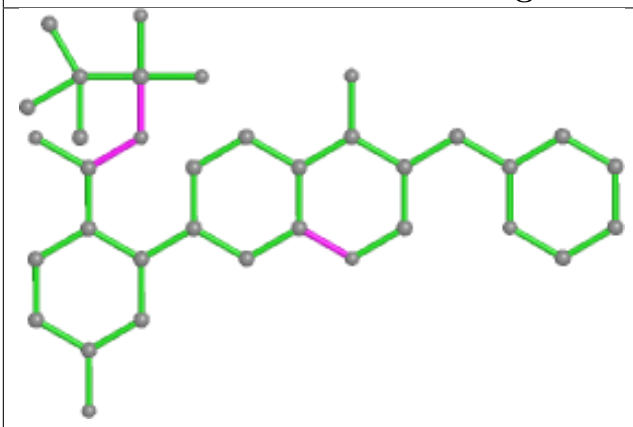
Bond angles



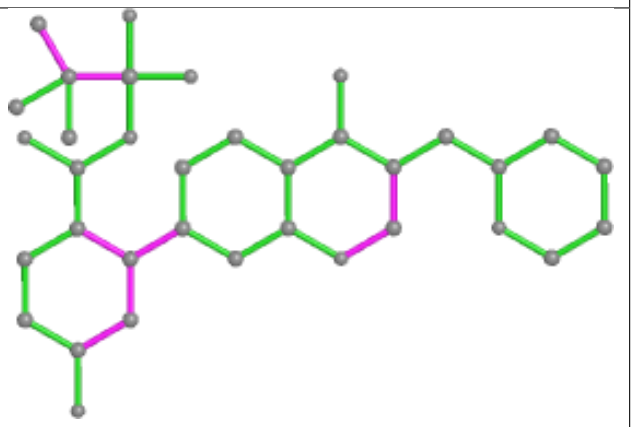
Torsions

Rings

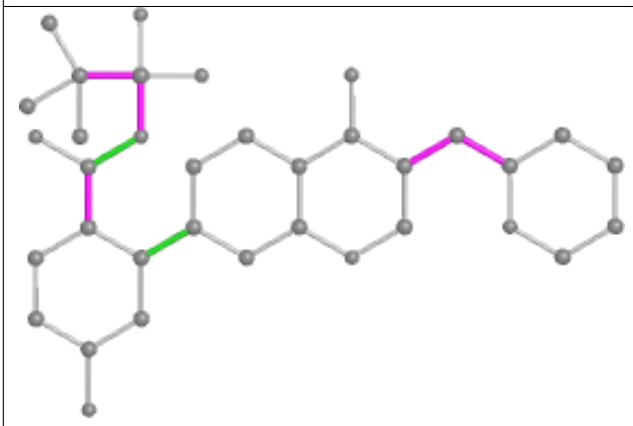
Ligand VRJ A 2101



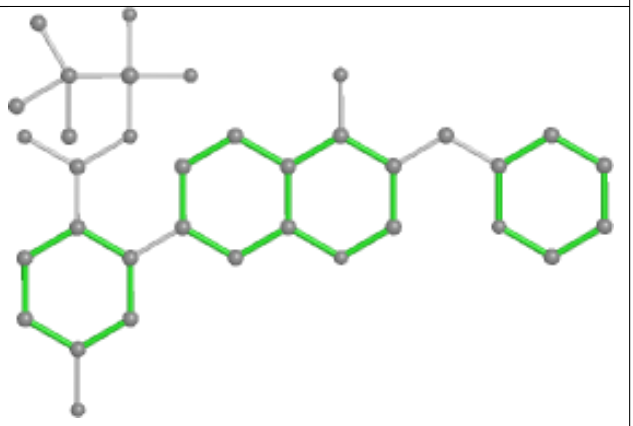
Bond lengths



Bond angles

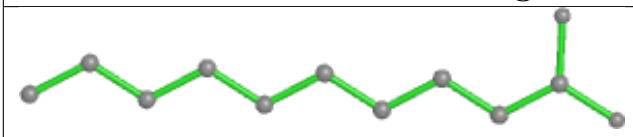


Torsions

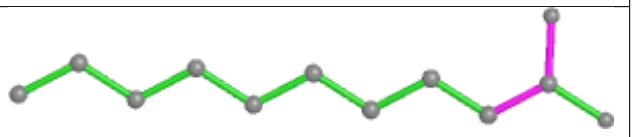


Rings

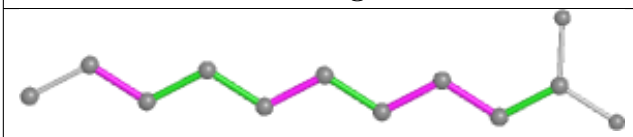
Ligand OLA A 2104



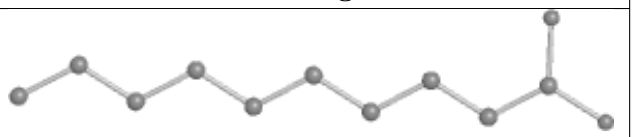
Bond lengths



Bond angles

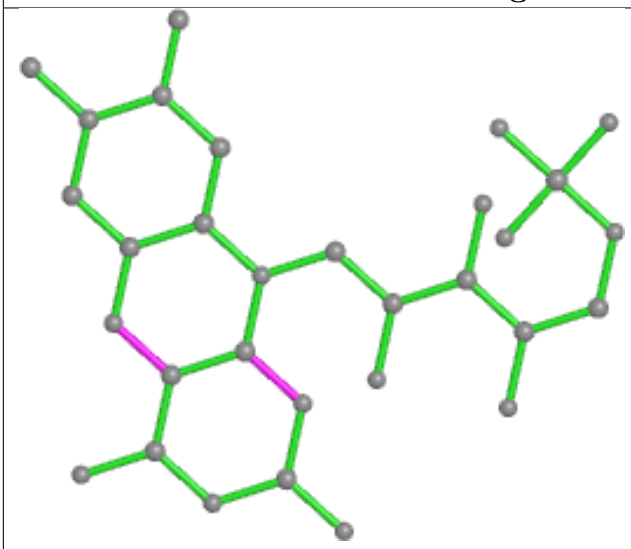


Torsions

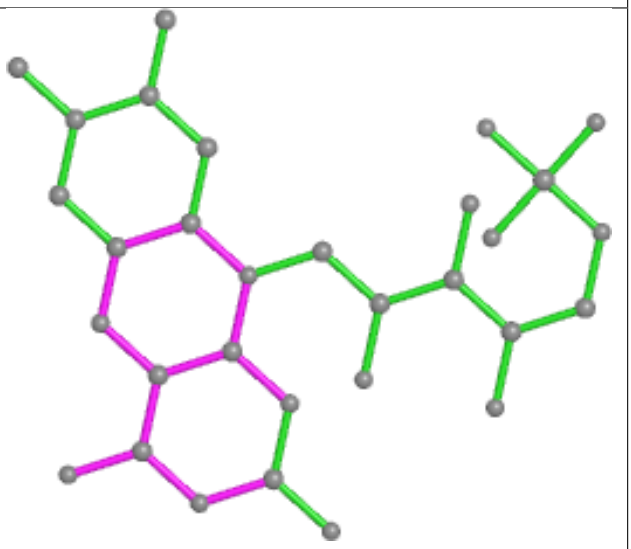


Rings

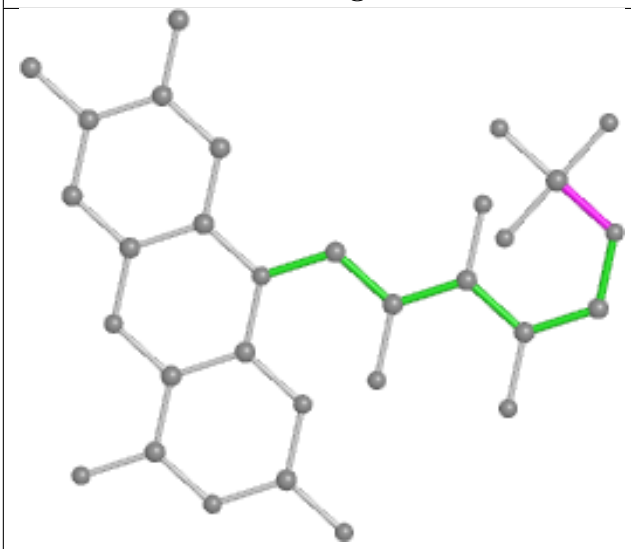
Ligand FMN A 2103



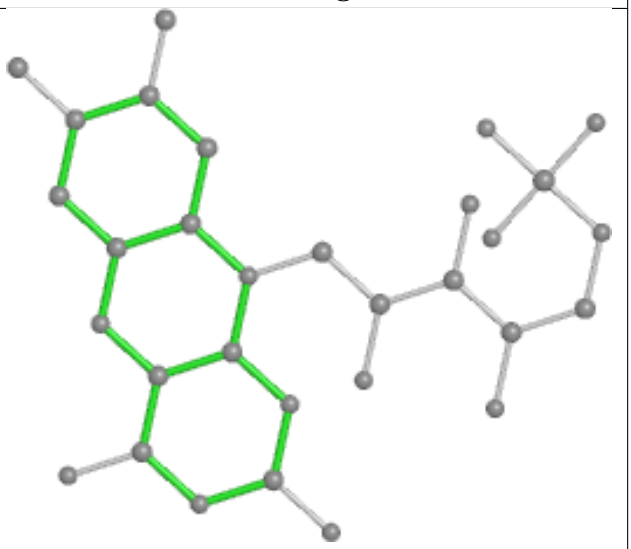
Bond lengths



Bond angles

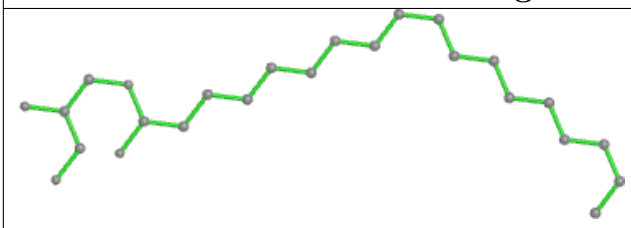


Torsions

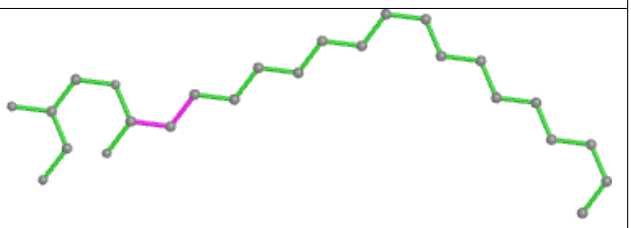


Rings

Ligand OLC A 2106



Bond lengths



Bond angles

Torsions

Rings

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	455/490 (92%)	-0.17	11 (2%) 59 57	30, 57, 112, 166	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	VAL	4.4
1	A	256	LEU	3.4
1	A	252	GLN	3.1
1	A	255	GLY	3.0
1	A	306	GLU	2.7
1	A	1044	GLY	2.5
1	A	258	LEU	2.5
1	A	164	ASN	2.3
1	A	1024	ARG	2.2
1	A	15	GLU	2.2
1	A	318	GLN	2.2

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

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,

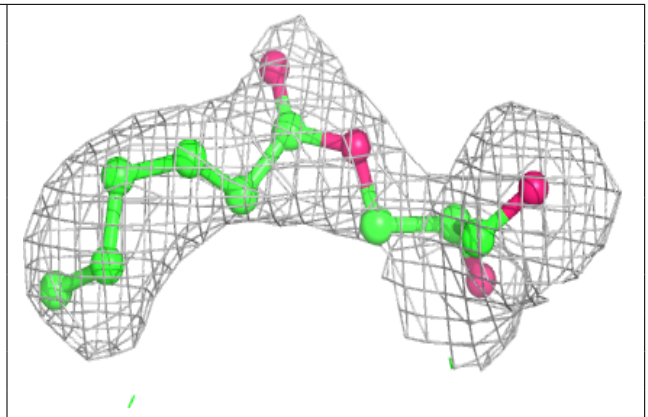
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

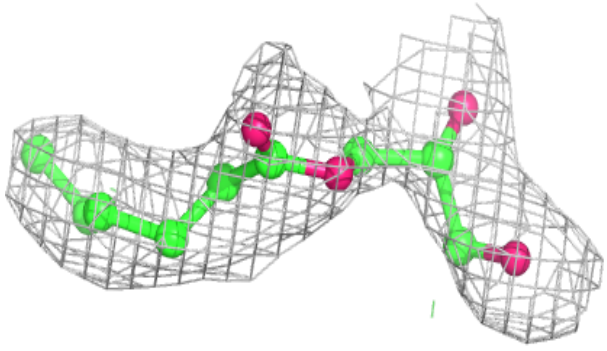
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	OLC	A	2105	13/25	0.83	0.28	29,61,99,104	0
8	2PE	A	2108	28/28	0.83	0.34	49,70,87,97	0
3	NA	A	2102	1/1	0.87	0.22	67,67,67,67	0
5	OLA	A	2104	12/20	0.88	0.35	40,57,102,103	0
7	1PE	A	2107	16/16	0.89	0.29	57,73,92,97	0
6	OLC	A	2106	25/25	0.89	0.53	36,71,92,101	0
9	P6G	A	2109	19/19	0.89	0.22	40,64,76,78	0
2	VRJ	A	2101	35/35	0.94	0.19	49,69,92,105	0
4	FMN	A	2103	31/31	0.97	0.14	34,49,62,65	0

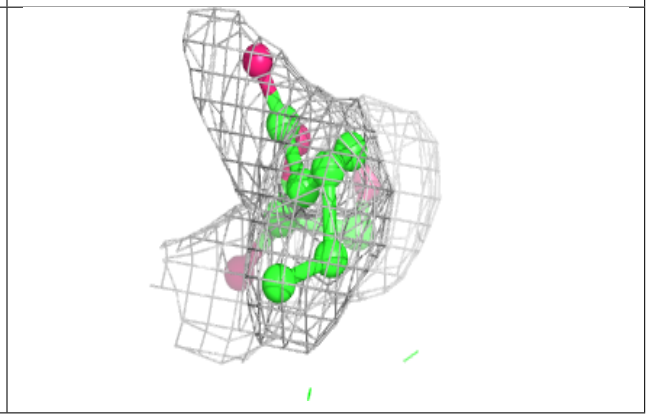
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 2105:

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

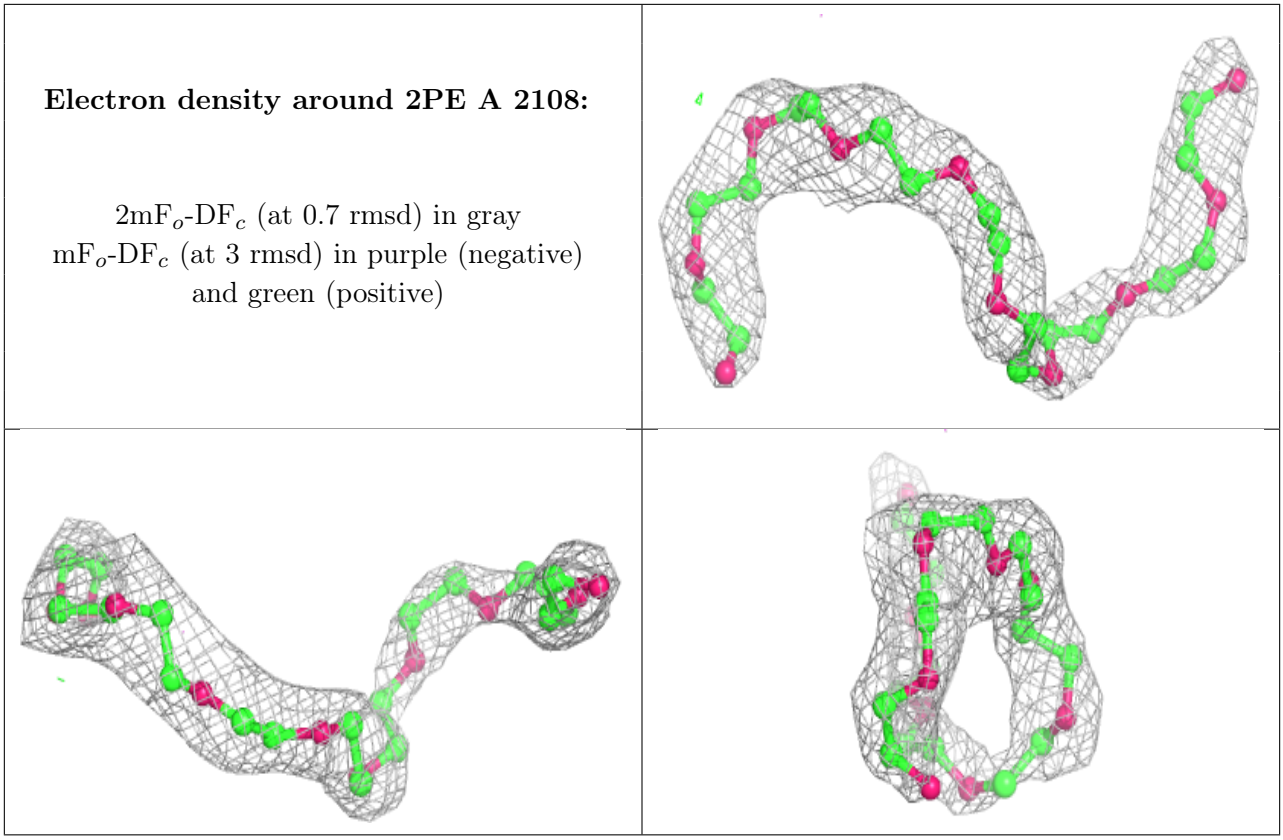






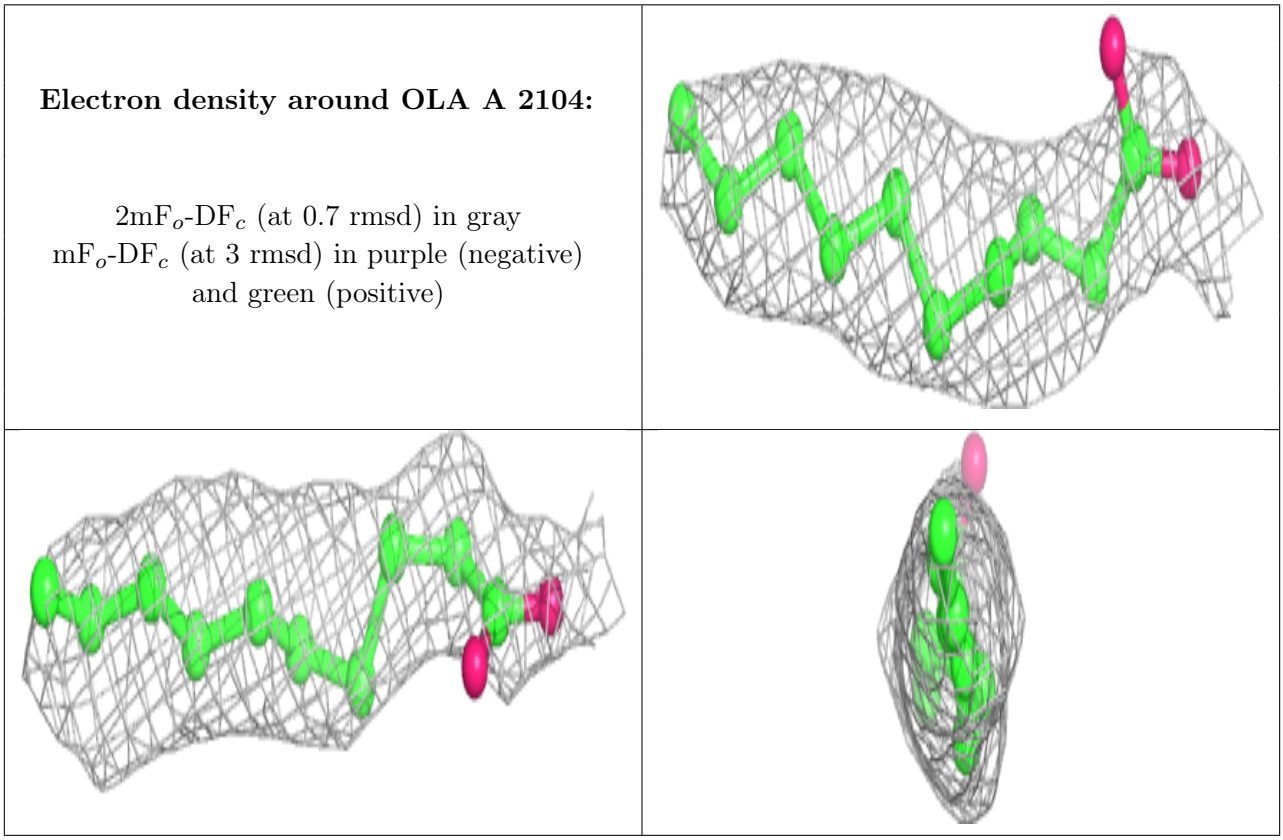
Electron density around 2PE A 2108:

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



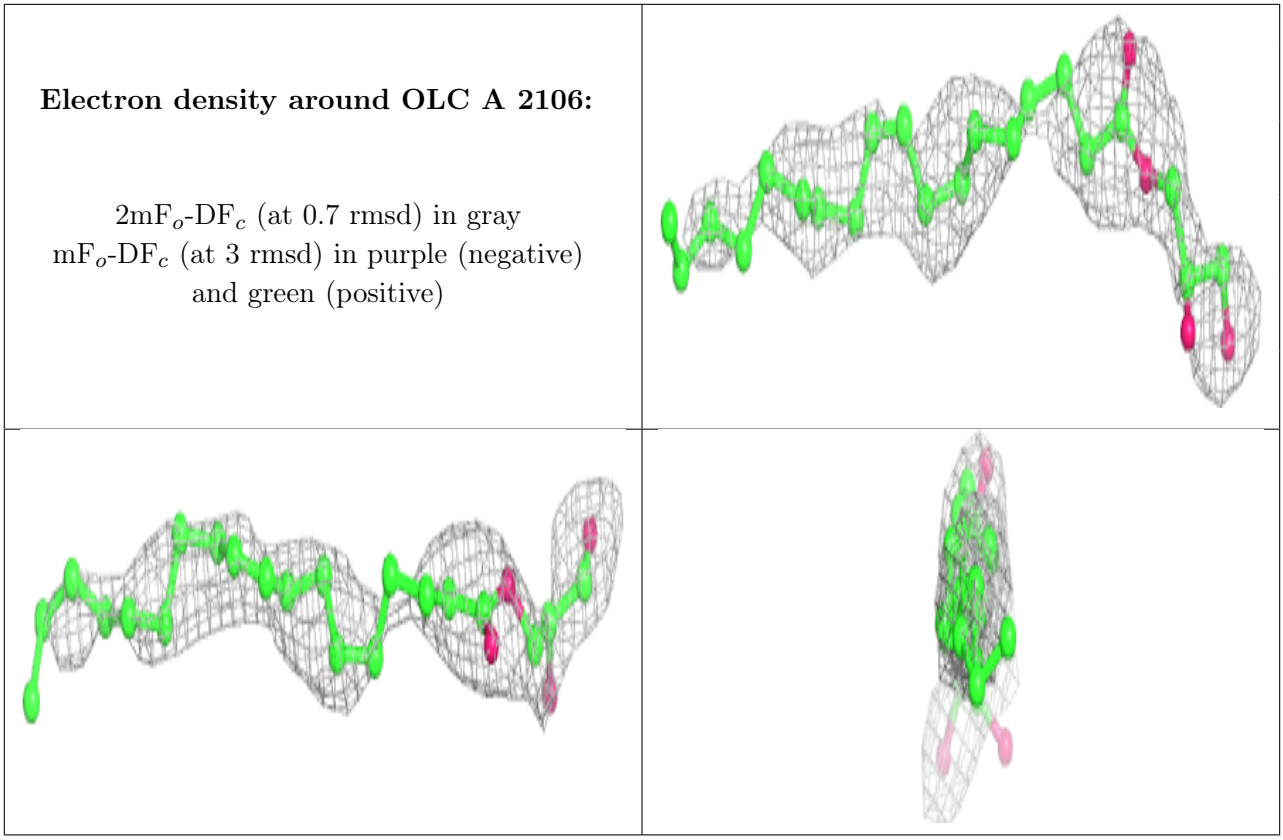
Electron density around OLA A 2104:

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



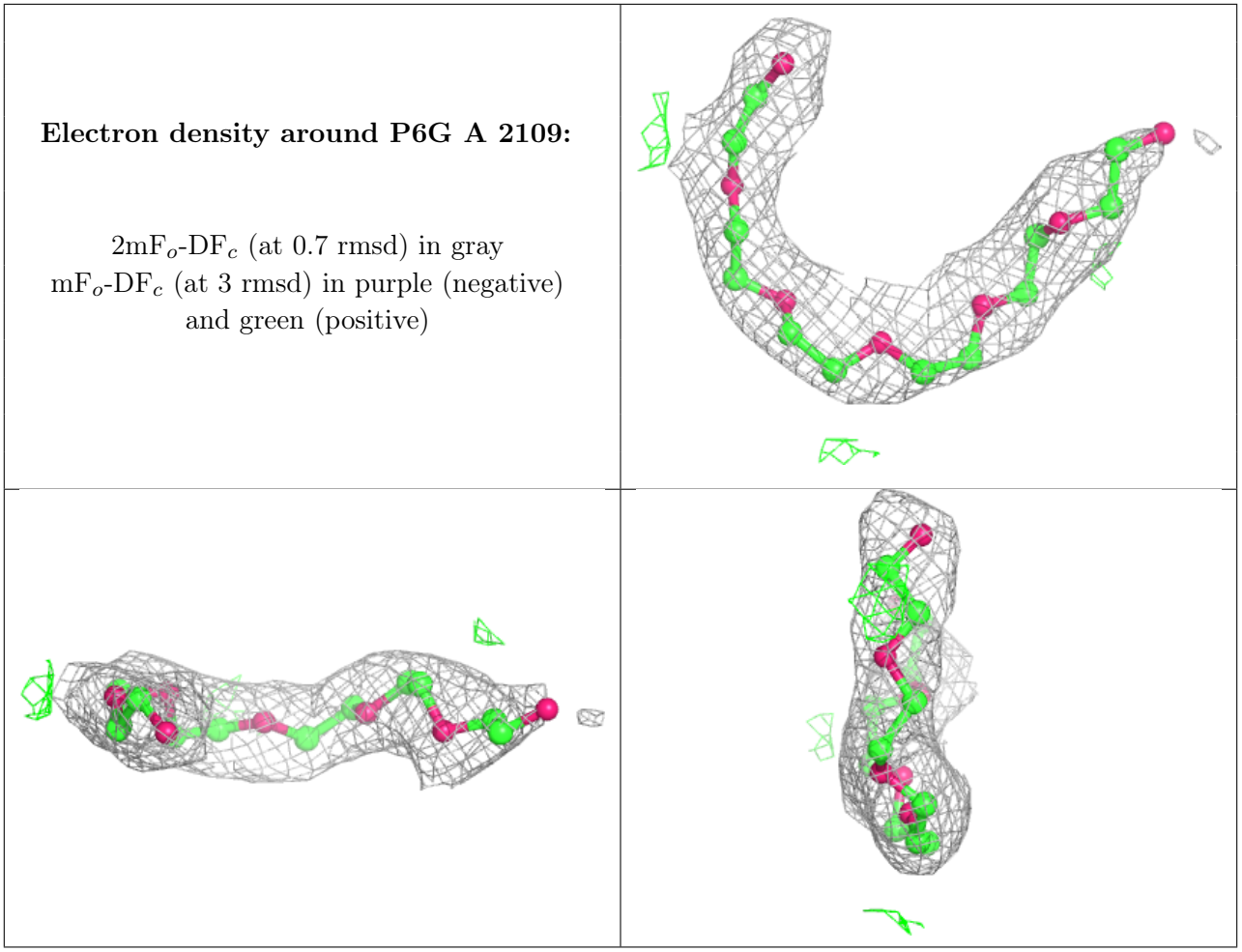
Electron density around OLC A 2106:

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



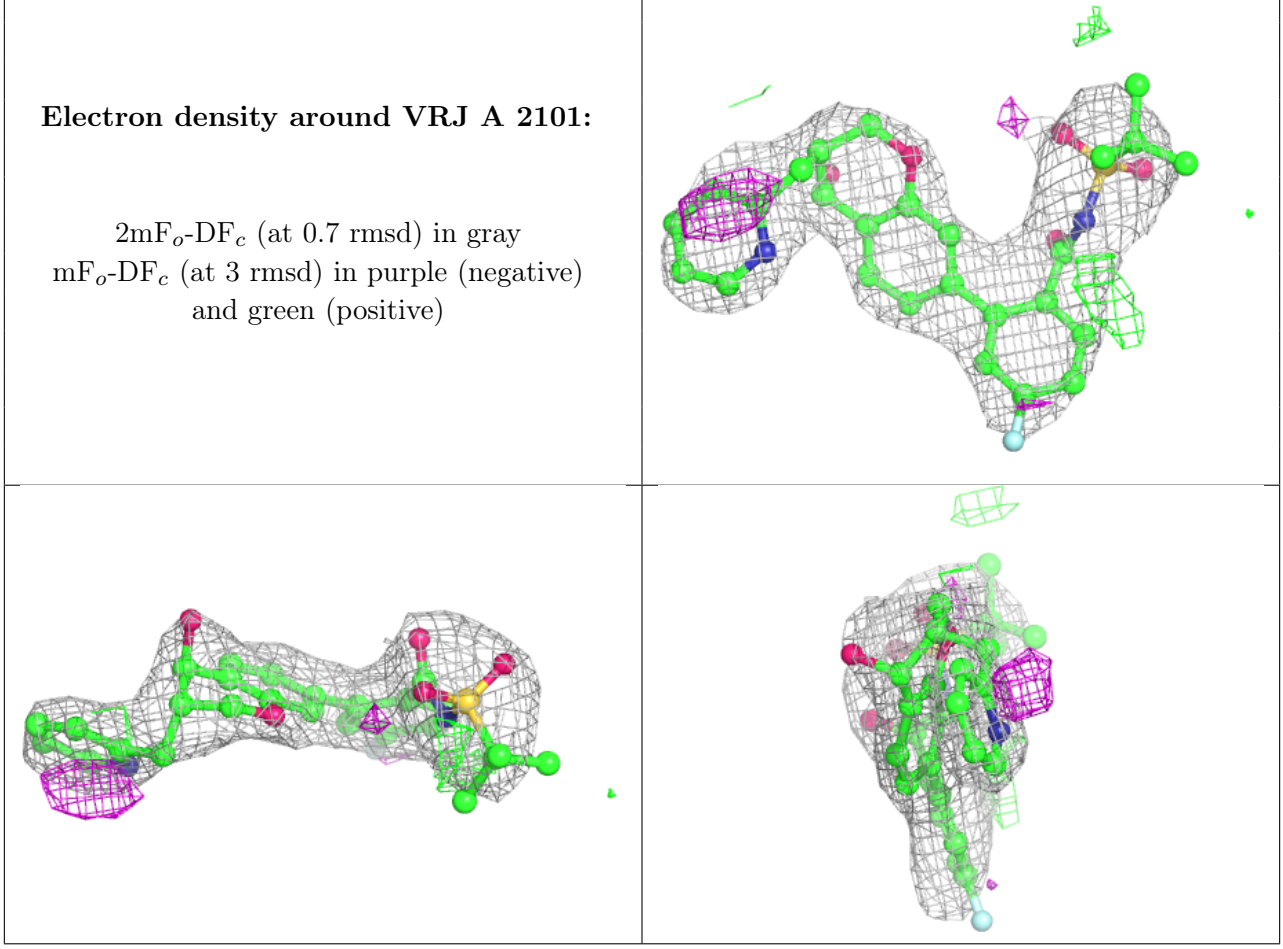
Electron density around P6G A 2109:

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



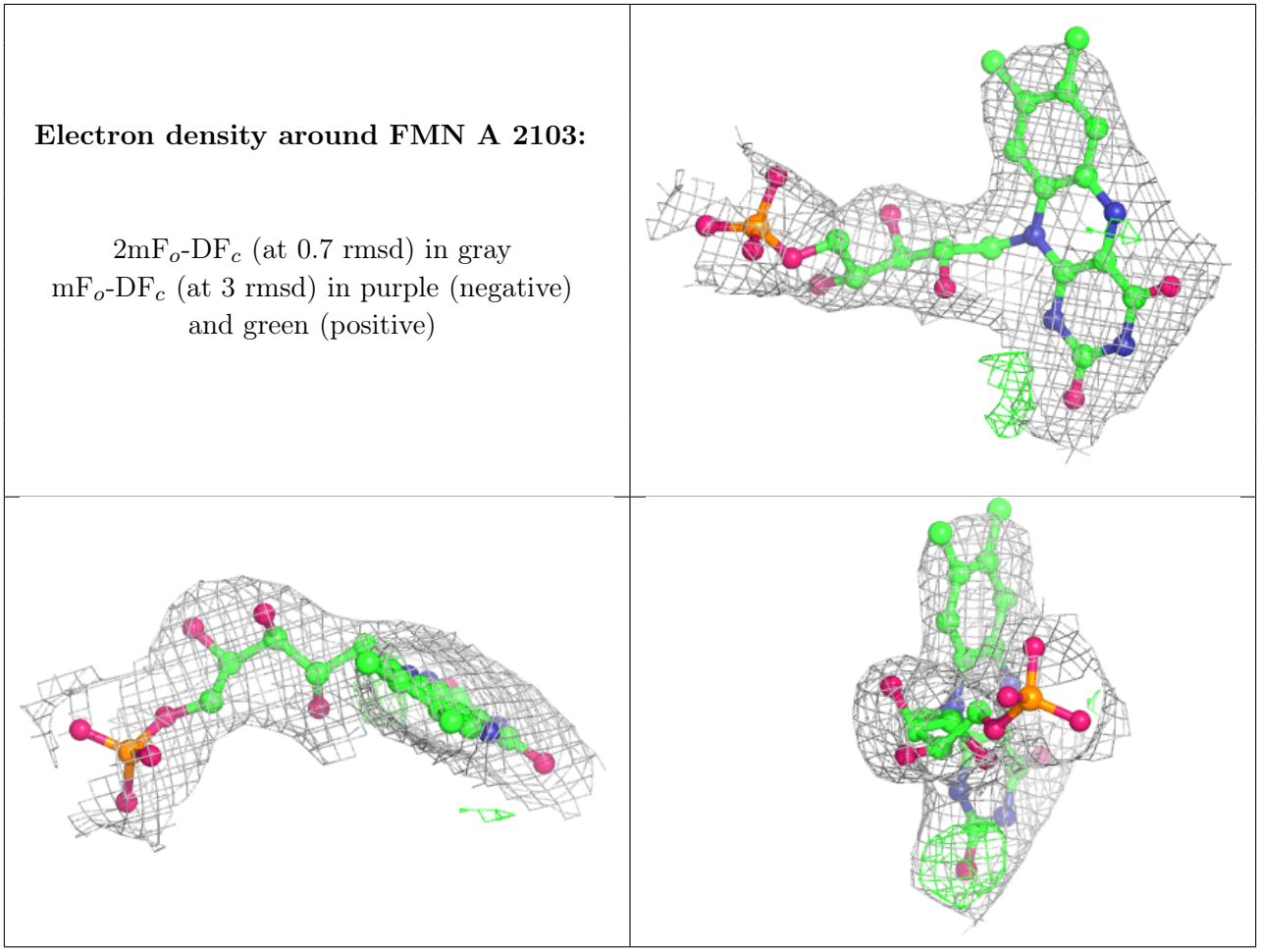
Electron density around VRJ A 2101:

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



Electron density around FMN A 2103:

$2mF_o$-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.