Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 11:22 am BST

PDB ID	:	6HXK
Title	:	Structure of the citryl-CoA lyase core module of human ATP citrate lyase in complex with citrate
Authors	:	Verstraete, K.; Verschueren, K.
Deposited on	:	2018-10-17
Resolution	:	1.85 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 (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:

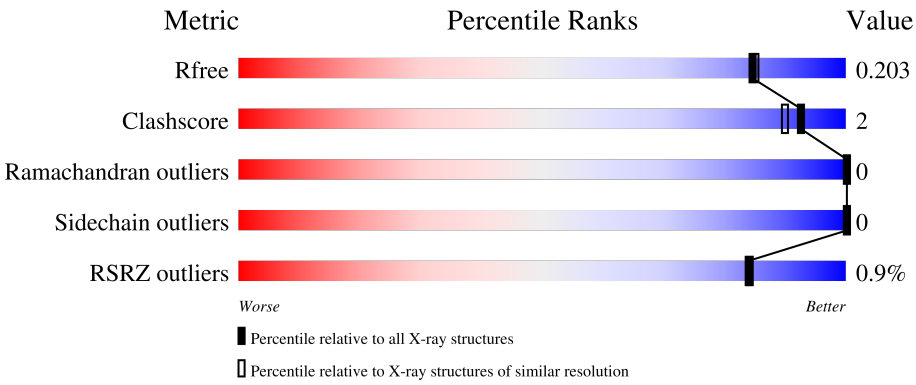
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	270	93%
1	B	270	3%, 93%
1	C	270	92%
1	D	270	93%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17644 atoms, of which 8569 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.

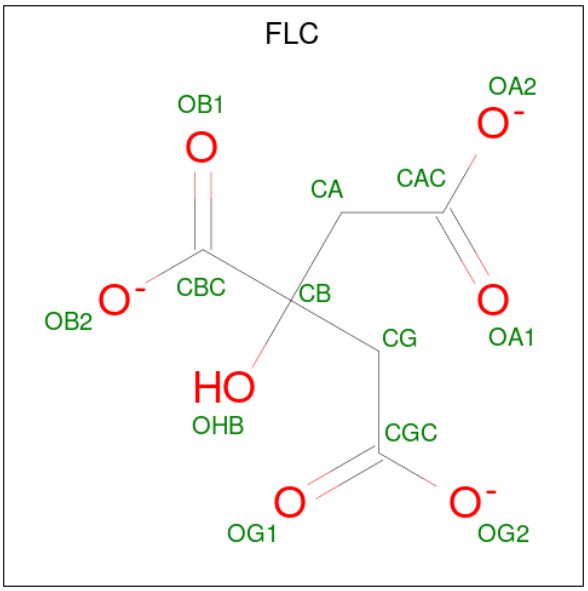
- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	262	4210	1342	2114	354	379	21	0	8	0
1	B	261	4229	1344	2127	354	382	22	0	10	0
1	C	260	4190	1331	2111	350	377	21	0	8	0
1	D	260	4181	1328	2109	349	374	21	11	7	0

There are 16 discrepancies between the modelled and reference sequences:

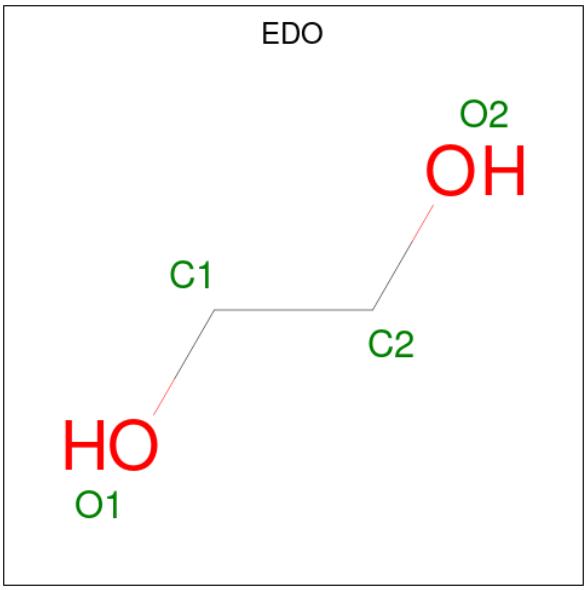
Chain	Residue	Modelled	Actual	Comment	Reference
A	832	GLY	-	expression tag	UNP P53396
A	833	SER	-	expression tag	UNP P53396
A	834	HIS	-	expression tag	UNP P53396
A	835	MET	-	expression tag	UNP P53396
B	832	GLY	-	expression tag	UNP P53396
B	833	SER	-	expression tag	UNP P53396
B	834	HIS	-	expression tag	UNP P53396
B	835	MET	-	expression tag	UNP P53396
C	832	GLY	-	expression tag	UNP P53396
C	833	SER	-	expression tag	UNP P53396
C	834	HIS	-	expression tag	UNP P53396
C	835	MET	-	expression tag	UNP P53396
D	832	GLY	-	expression tag	UNP P53396
D	833	SER	-	expression tag	UNP P53396
D	834	HIS	-	expression tag	UNP P53396
D	835	MET	-	expression tag	UNP P53396

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$) (labeled as "Ligand of Interest" by depositor).



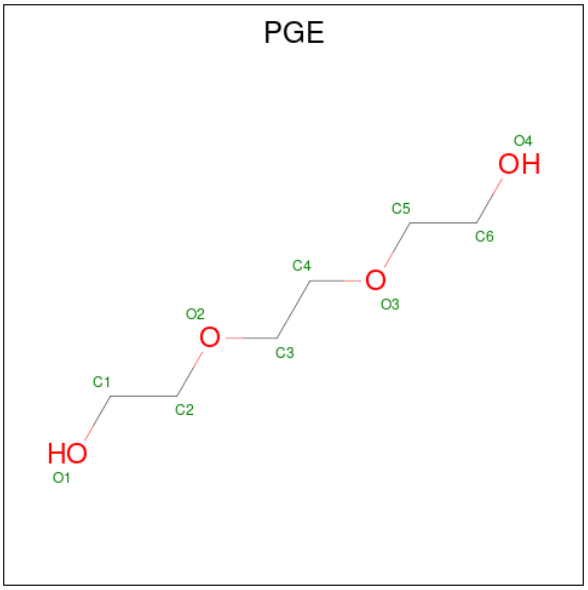
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	36	12	10	14	0	1
			Total	C	H	O		
2	B	1	18	6	5	7	0	0
			Total	C	H	O		
2	C	1	18	6	5	7	0	0
			Total	C	H	O		
2	D	1	36	12	10	14	0	1

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



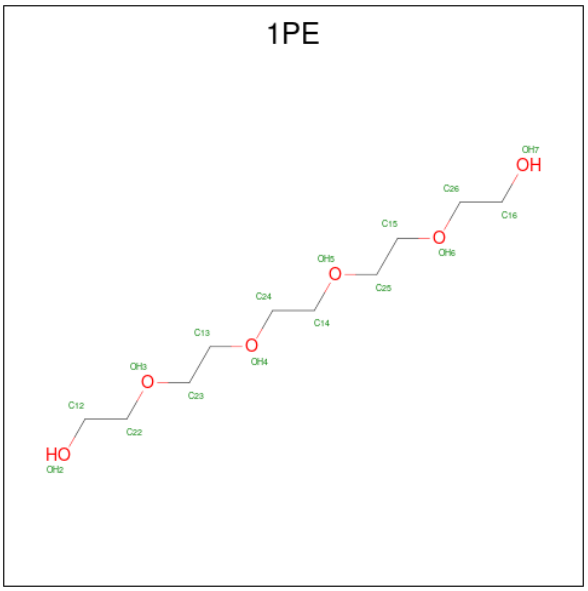
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	A	1	Total 10	C 2	H 6	O 2	0	0
3	D	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



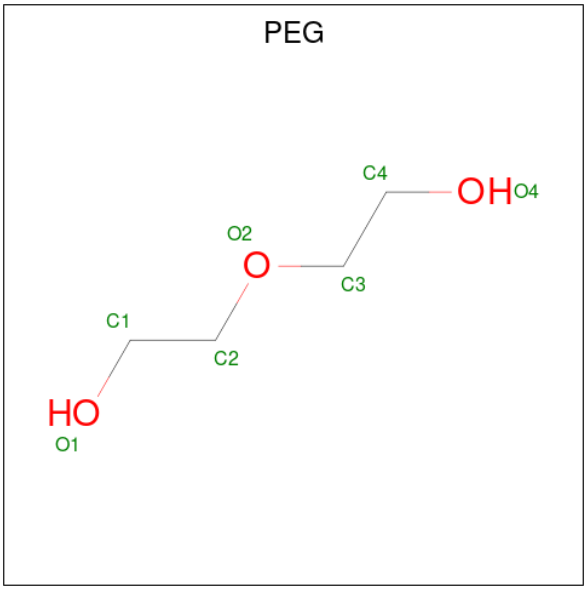
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 24	C 6	H 14	O 4	0	0
4	D	1	Total 24	C 6	H 14	O 4	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	C	1	38	10	22	6	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	C	1	17	4	10	3	0	0

- Molecule 7 is water.

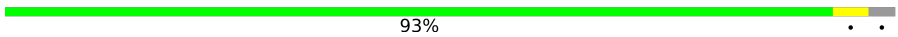
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	156	156	156	0	0
			Total	O		
7	B	129	129	129	0	0
			Total	O		
7	C	154	154	154	0	0
			Total	O		
7	D	154	154	154	0	0

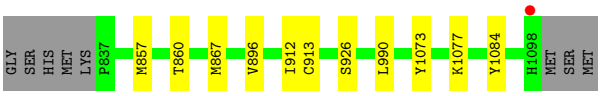
3 Residue-property plots (i)

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: ATP-citrate synthase

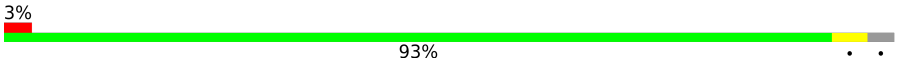
Chain A:

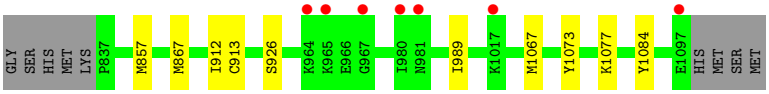




- Molecule 1: ATP-citrate synthase

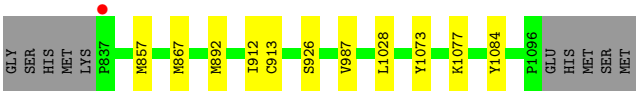
Chain B:





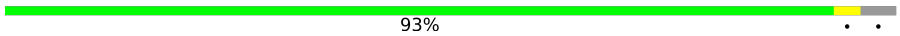
- Molecule 1: ATP-citrate synthase

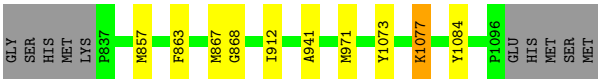
Chain C:



- Molecule 1: ATP-citrate synthase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.34Å 123.89Å 139.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.94 – 1.85 61.95 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (61.94-1.85) 99.8 (61.95-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 1.86Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.165 , 0.193 0.178 , 0.203	Depositor DCC
R_{free} test set	4982 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17644	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, FLC, 1PE, EDO, PGE

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	0.50	0/2138	0.61	0/2878
1	B	0.50	0/2143	0.59	0/2883
1	C	0.50	0/2120	0.61	0/2853
1	D	0.50	0/2113	0.60	1/2843 (0.0%)
All	All	0.50	0/8514	0.60	1/11457 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1077	LYS	CD-CE-NZ	5.21	123.69	111.70

There are no chirality outliers.

There are no planarity outliers.

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	2096	2114	2119	7	0
1	B	2102	2127	2123	7	0
1	C	2079	2111	2103	7	0
1	D	2072	2109	2102	6	0
2	A	26	10	10	0	0
2	B	13	5	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	5	5	0	0
2	D	26	10	10	0	0
3	A	8	12	12	0	0
3	D	4	6	6	0	0
4	B	10	14	14	0	0
4	D	10	14	14	0	0
5	C	16	22	22	3	0
6	C	7	10	10	0	0
7	A	156	0	0	0	0
7	B	129	0	0	1	0
7	C	154	0	0	0	0
7	D	154	0	0	0	0
All	All	9075	8569	8555	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 2.

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:B:1067[B]:MET:SD	7:B:1317:HOH:O	2.56	0.62
1:A:857:MET:SD	1:A:867[B]:MET:SD	2.99	0.60
1:C:857:MET:SD	1:C:867[B]:MET:SD	3.01	0.58
1:B:857:MET:SD	1:B:867[B]:MET:SD	3.02	0.58
1:D:1073:TYR:CE1	1:D:1077:LYS:HE3	2.43	0.54
1:B:1073:TYR:CE1	1:B:1077:LYS:HE3	2.45	0.52
1:C:1073:TYR:CE1	1:C:1077:LYS:HE3	2.46	0.51
1:A:1073:TYR:CE1	1:A:1077:LYS:HE3	2.46	0.50
1:C:987:VAL:HG13	1:C:1028:LEU:HD13	1.93	0.49
1:C:913[B]:CYS:SG	1:C:926:SER:CB	3.02	0.47
1:A:913[B]:CYS:SG	1:A:926:SER:CB	3.04	0.46
1:B:913[B]:CYS:SG	1:B:926:SER:CB	3.04	0.45
1:A:1073:TYR:CZ	1:A:1077:LYS:HE3	2.52	0.45
1:C:1073:TYR:CZ	1:C:1077:LYS:HE3	2.52	0.45
1:A:896:VAL:HG21	1:A:990:LEU:HD11	1.98	0.44
1:B:1073:TYR:CZ	1:B:1077:LYS:HE3	2.52	0.44
5:C:1201:1PE:H162	1:D:863:PHE:HB3	1.99	0.44
1:B:912:ILE:HD12	1:B:1084:TYR:CD2	2.54	0.43
5:C:1201:1PE:H232	1:D:868:GLY:HA2	2.00	0.43
1:D:857:MET:SD	1:D:867[B]:MET:SD	3.17	0.43
1:C:912:ILE:HD12	1:C:1084:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:THR:HG22	1:B:989:ILE:HD11	2.01	0.41
1:A:912:ILE:HD12	1:A:1084:TYR:CD2	2.55	0.41
1:D:941:ALA:HB1	1:D:971:MET:HG3	2.03	0.41
1:D:912:ILE:HD12	1:D:1084:TYR:CD2	2.56	0.41
1:C:892[A]:MET:SD	5:C:1201:1PE:H142	2.61	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	268/270 (99%)	263 (98%)	5 (2%)	0	100	100
1	B	269/270 (100%)	264 (98%)	5 (2%)	0	100	100
1	C	266/270 (98%)	262 (98%)	4 (2%)	0	100	100
1	D	265/270 (98%)	261 (98%)	4 (2%)	0	100	100
All	All	1068/1080 (99%)	1050 (98%)	18 (2%)	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	227/226 (100%)	227 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	228/226 (101%)	228 (100%)	0	100	100
1	C	225/226 (100%)	225 (100%)	0	100	100
1	D	224/226 (99%)	224 (100%)	0	100	100
All	All	904/904 (100%)	904 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	888	GLN

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)

13 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	FLC	C	1202	-	12,12,12	0.99	0	17,17,17	1.53	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FLC	A	1200[A]	-	12,12,12	1.04	0	17,17,17	1.54	3 (17%)
4	PGE	B	1202	-	9,9,9	0.13	0	8,8,8	0.30	0
2	FLC	D	1200[B]	-	12,12,12	1.05	0	17,17,17	1.27	2 (11%)
5	1PE	C	1201	-	15,15,15	0.24	0	14,14,14	0.30	0
2	FLC	A	1200[B]	-	12,12,12	1.09	0	17,17,17	1.48	3 (17%)
3	EDO	D	1202	-	3,3,3	0.51	0	2,2,2	0.17	0
4	PGE	D	1201	-	9,9,9	0.15	0	8,8,8	0.20	0
6	PEG	C	1203	-	6,6,6	0.16	0	5,5,5	0.26	0
3	EDO	A	1201	-	3,3,3	0.58	0	2,2,2	0.10	0
3	EDO	A	1202	-	3,3,3	0.60	0	2,2,2	0.38	0
2	FLC	B	1201	-	12,12,12	1.02	1 (8%)	17,17,17	1.29	3 (17%)
2	FLC	D	1200[A]	-	12,12,12	1.23	1 (8%)	17,17,17	1.89	5 (29%)

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	FLC	C	1202	-	-	3/16/16/16	-
2	FLC	A	1200[A]	-	-	1/16/16/16	-
4	PGE	B	1202	-	-	2/7/7/7	-
2	FLC	D	1200[B]	-	-	0/16/16/16	-
5	1PE	C	1201	-	-	5/13/13/13	-
2	FLC	A	1200[B]	-	-	0/16/16/16	-
3	EDO	D	1202	-	-	0/1/1/1	-
4	PGE	D	1201	-	-	0/7/7/7	-
6	PEG	C	1203	-	-	1/4/4/4	-
3	EDO	A	1201	-	-	1/1/1/1	-
3	EDO	A	1202	-	-	0/1/1/1	-
2	FLC	B	1201	-	-	4/16/16/16	-
2	FLC	D	1200[A]	-	-	7/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1200[A]	FLC	OG2-CGC	-2.33	1.22	1.30
2	B	1201	FLC	OB2-CBC	-2.04	1.22	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1202	FLC	OB1-CBC-CB	-3.85	116.80	122.25
2	A	1200[A]	FLC	OB1-CBC-CB	-3.72	116.99	122.25
2	A	1200[B]	FLC	OB1-CBC-CB	-3.70	117.01	122.25
2	C	1202	FLC	OB2-CBC-CB	3.51	119.15	113.05
2	D	1200[A]	FLC	OB1-CBC-CB	-3.49	117.31	122.25
2	D	1200[A]	FLC	CG-CB-CBC	-3.45	102.69	110.11
2	D	1200[A]	FLC	CB-CA-CAC	3.25	121.69	113.81
2	D	1200[B]	FLC	OB1-CBC-CB	-3.20	117.73	122.25
2	A	1200[A]	FLC	OB2-CBC-CB	2.93	118.14	113.05
2	D	1200[A]	FLC	OB2-CBC-CB	2.79	117.89	113.05
2	A	1200[B]	FLC	OB2-CBC-CB	2.74	117.81	113.05
2	B	1201	FLC	OB2-CBC-CB	2.51	117.41	113.05
2	D	1200[B]	FLC	OB2-CBC-CB	2.37	117.17	113.05
2	B	1201	FLC	OB1-CBC-CB	-2.19	119.16	122.25
2	C	1202	FLC	OA1-CAC-CA	-2.16	116.64	122.94
2	A	1200[A]	FLC	CB-CA-CAC	2.14	119.00	113.81
2	B	1201	FLC	OA1-CAC-CA	-2.13	116.70	122.94
2	D	1200[A]	FLC	CA-CB-CBC	2.05	114.51	110.11
2	A	1200[B]	FLC	CB-CA-CAC	2.01	118.67	113.81

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1201	1PE	OH4-C13-C23-OH3
4	B	1202	PGE	O1-C1-C2-O2
5	C	1201	1PE	OH6-C15-C25-OH5
2	D	1200[A]	FLC	CA-CB-CBC-OB1
3	A	1201	EDO	O1-C1-C2-O2
5	C	1201	1PE	OH5-C14-C24-OH4
2	D	1200[A]	FLC	CA-CB-CBC-OB2
2	D	1200[A]	FLC	CG-CB-CBC-OB2
2	A	1200[A]	FLC	CAC-CA-CB-OHB
2	B	1201	FLC	CBC-CB-CG-CGC
2	C	1202	FLC	CBC-CB-CG-CGC
2	D	1200[A]	FLC	CB-CA-CAC-OA1
2	B	1201	FLC	CA-CB-CG-CGC
6	C	1203	PEG	C1-C2-O2-C3
2	B	1201	FLC	CG-CB-CBC-OB1
2	D	1200[A]	FLC	CB-CA-CAC-OA2
4	B	1202	PGE	O3-C5-C6-O4
5	C	1201	1PE	OH7-C16-C26-OH6
2	B	1201	FLC	OHB-CB-CG-CGC

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Mol	Chain	Res	Type	Atoms
2	C	1202	FLC	CA-CB-CG-CGC
2	C	1202	FLC	OHB-CB-CG-CGC
2	D	1200[A]	FLC	OHB-CB-CBC-OB1
2	D	1200[A]	FLC	CG-CB-CBC-OB1
5	C	1201	1PE	C25-C15-OH6-C26

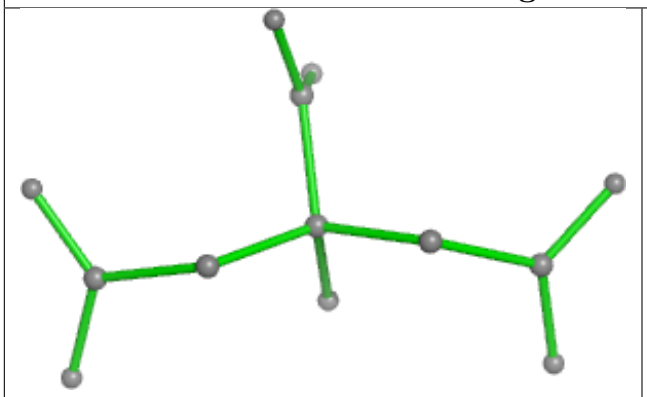
There are no ring outliers.

1 monomer is involved in 3 short contacts:

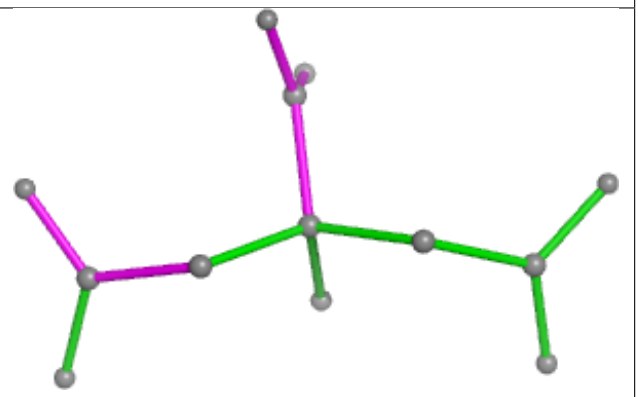
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1201	1PE	3	0

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.

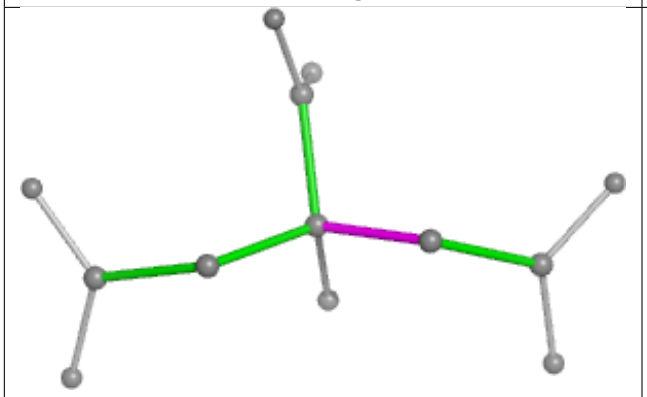
Ligand FLC C 1202



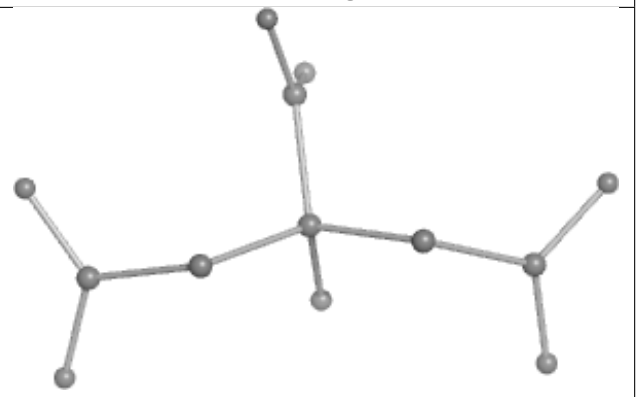
Bond lengths



Bond angles

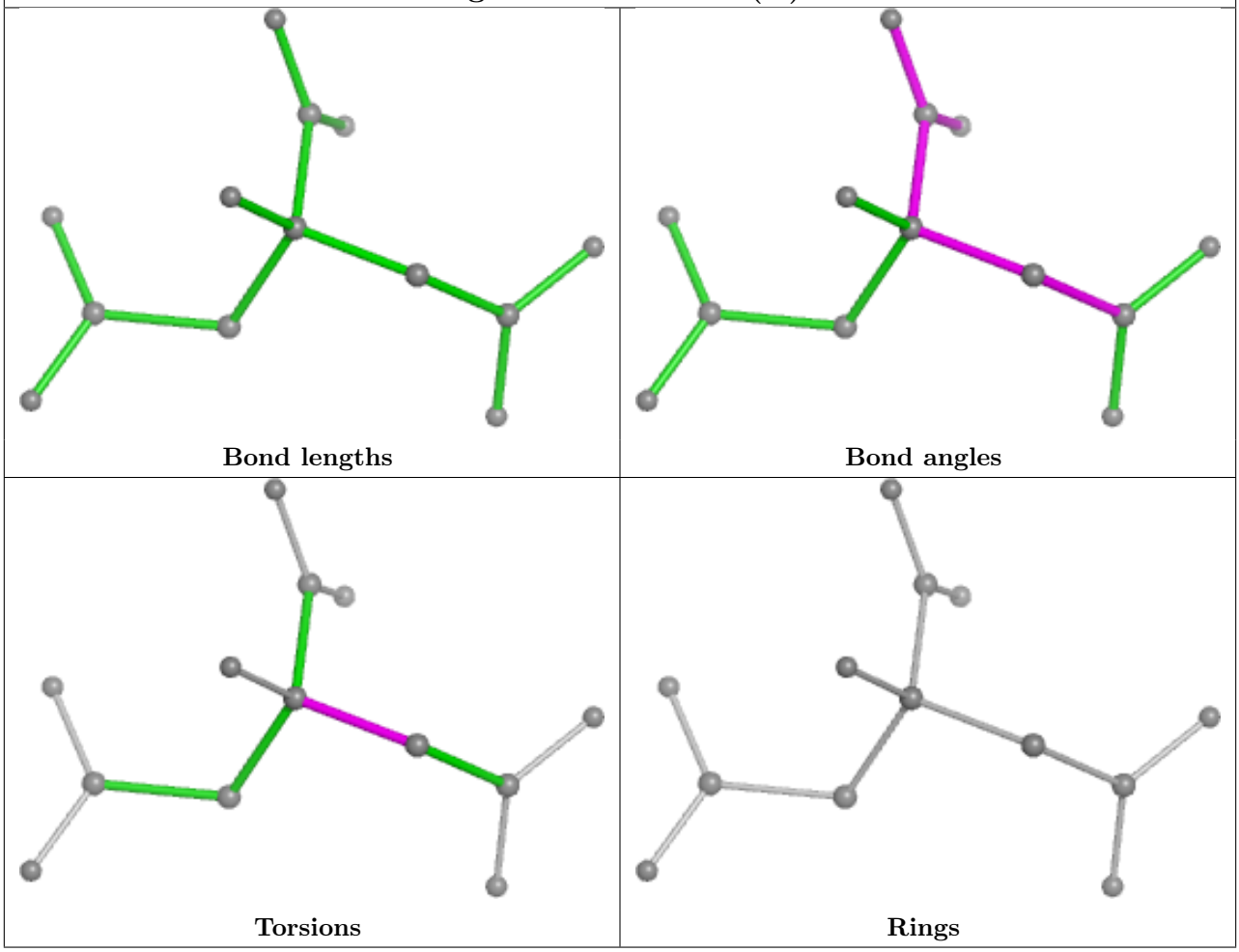


Torsions

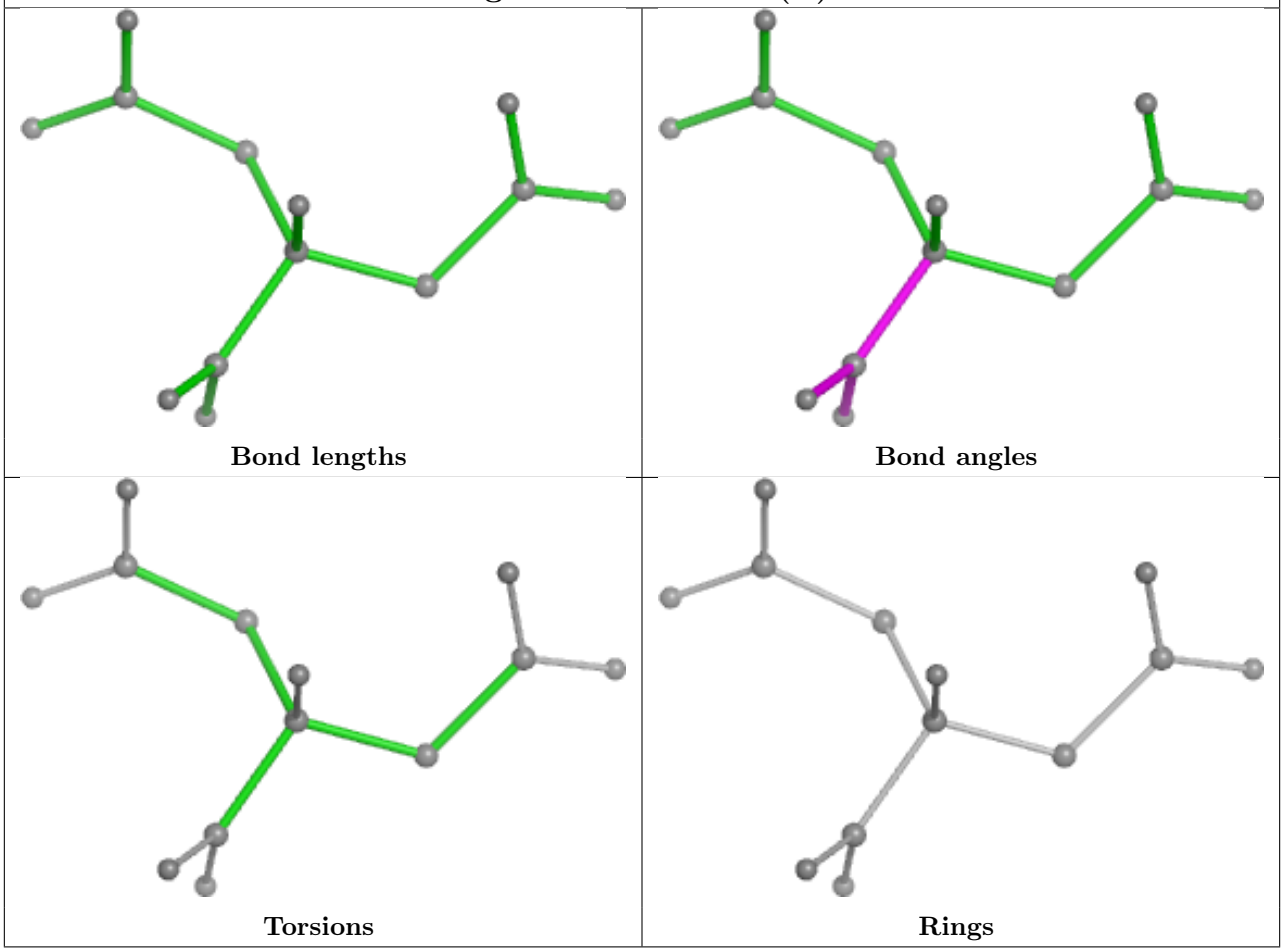


Rings

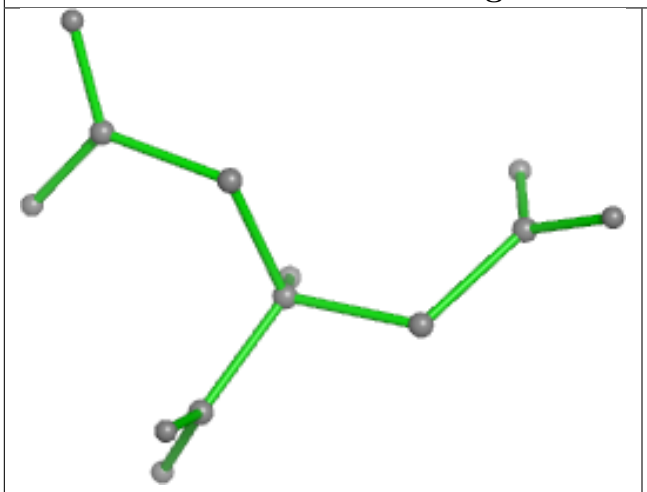
Ligand FLC A 1200 (A)



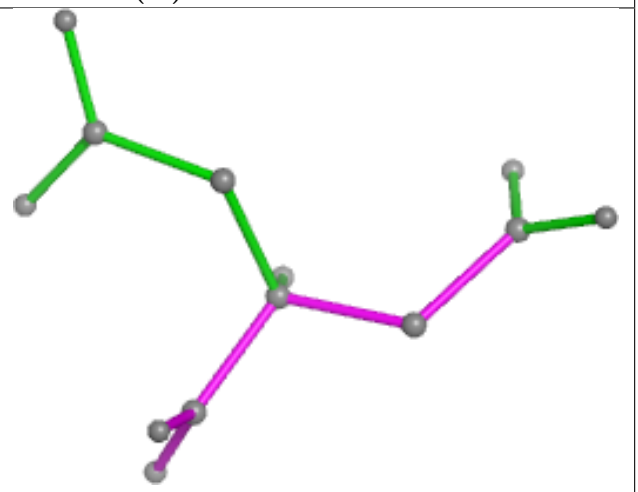
Ligand FLC D 1200 (B)



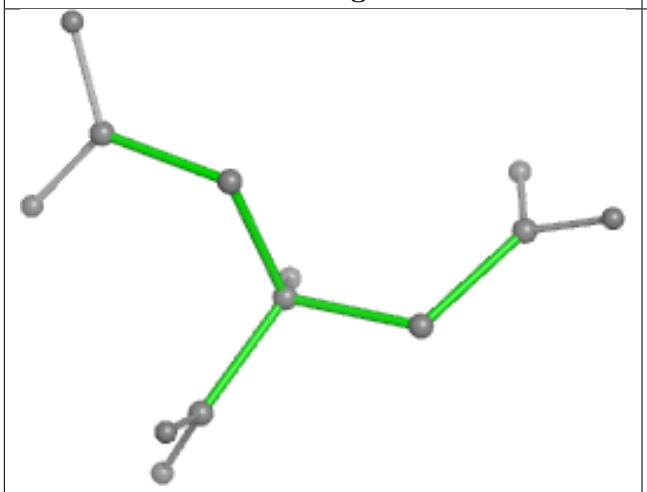
Ligand FLC A 1200 (B)



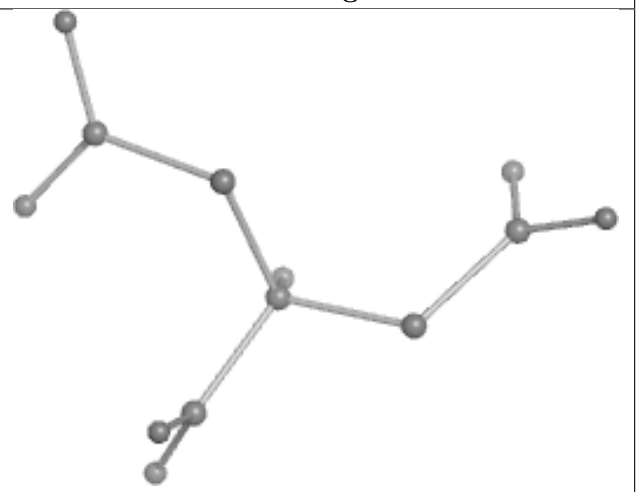
Bond lengths



Bond angles

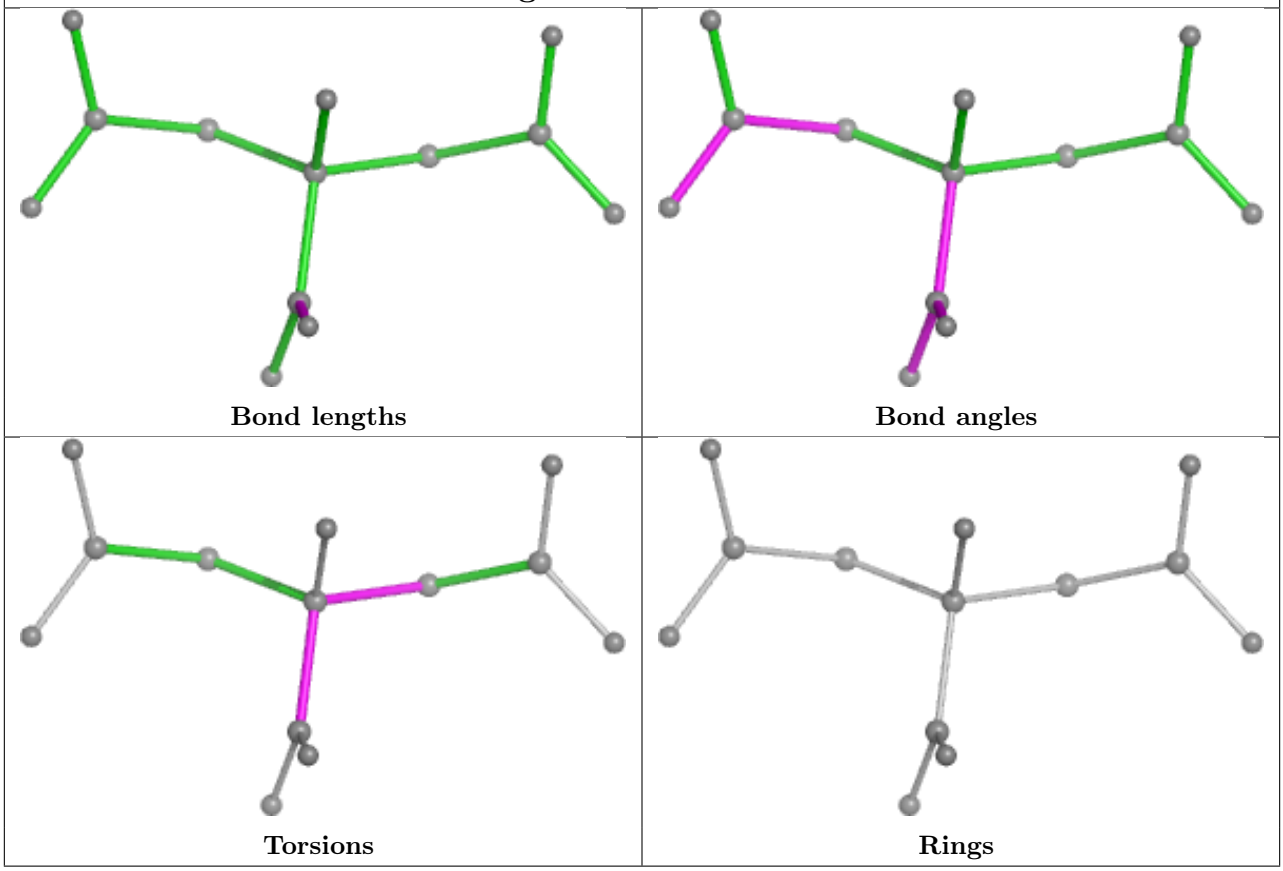


Torsions

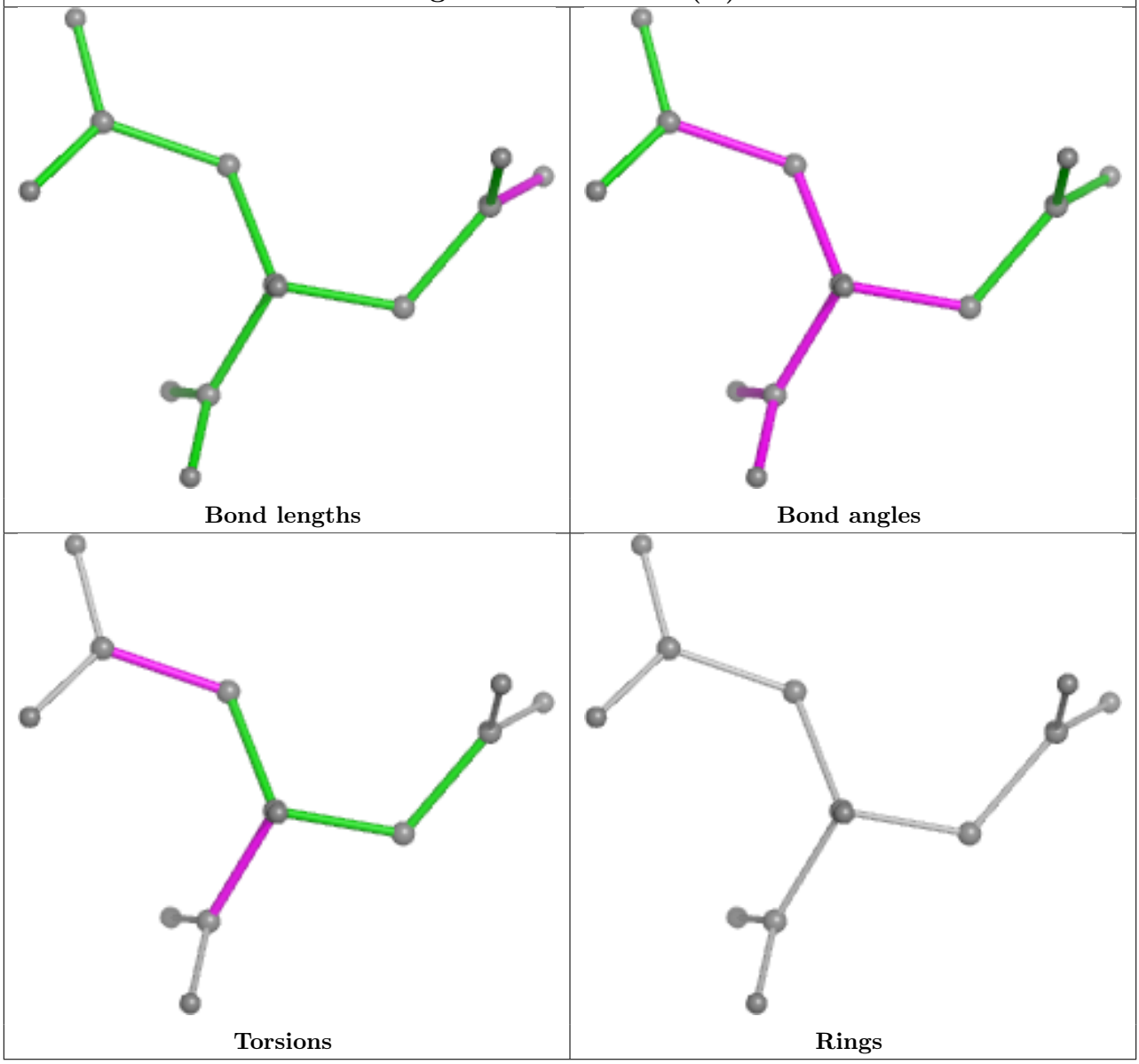


Rings

Ligand FLC B 1201



Ligand FLC D 1200 (A)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	262/270 (97%)	-0.23	1 (0%)	92	92	17, 25, 46, 69	0
1	B	261/270 (96%)	-0.14	7 (2%)	54	53	17, 26, 54, 90	0
1	C	260/270 (96%)	-0.31	1 (0%)	92	92	16, 24, 52, 80	0
1	D	260/270 (96%)	-0.21	0	100	100	16, 25, 50, 80	0
All	All	1043/1080 (96%)	-0.22	9 (0%)	84	84	16, 25, 51, 90	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	980	ILE	4.0
1	A	1098	HIS	2.7
1	B	981	ASN	2.4
1	B	964	LYS	2.3
1	B	965	LYS	2.2
1	B	1017	LYS	2.1
1	C	837	PRO	2.1
1	B	967	GLY	2.1
1	B	1097	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

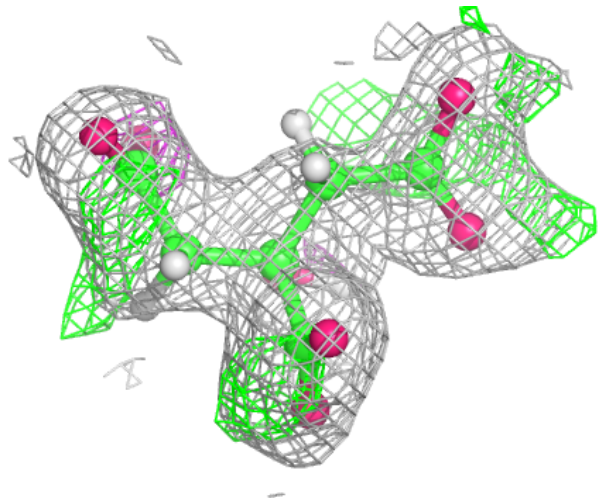
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

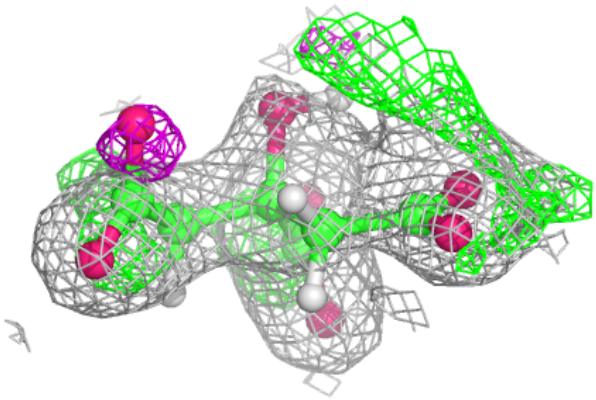
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FLC	D	1200[A]	13/13	0.75	0.27	8,19,26,37	18
2	FLC	D	1200[B]	13/13	0.75	0.27	114,119,124,125	18
3	EDO	A	1202	4/4	0.76	0.19	57,58,60,60	0
3	EDO	A	1201	4/4	0.81	0.12	61,61,64,64	0
2	FLC	B	1201	13/13	0.82	0.20	32,45,49,54	0
3	EDO	D	1202	4/4	0.83	0.11	49,50,54,54	0
6	PEG	C	1203	7/7	0.84	0.17	50,53,56,57	0
4	PGE	B	1202	10/10	0.88	0.15	47,54,59,64	0
5	1PE	C	1201	16/16	0.89	0.16	30,41,52,55	0
2	FLC	C	1202	13/13	0.90	0.17	30,44,50,51	0
2	FLC	A	1200[B]	13/13	0.90	0.15	4,20,26,26	18
2	FLC	A	1200[A]	13/13	0.90	0.15	40,58,62,65	18
4	PGE	D	1201	10/10	0.93	0.12	35,42,47,52	0

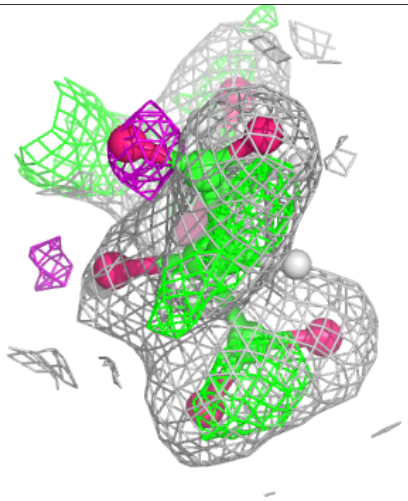
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FLC D 1200 (A):

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

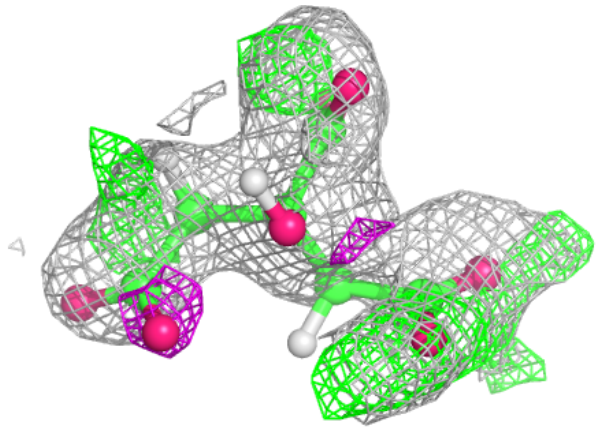


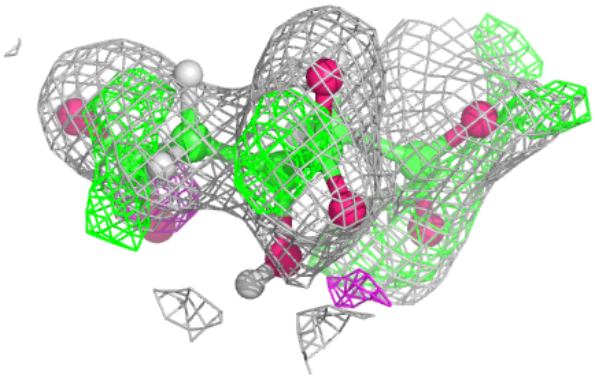


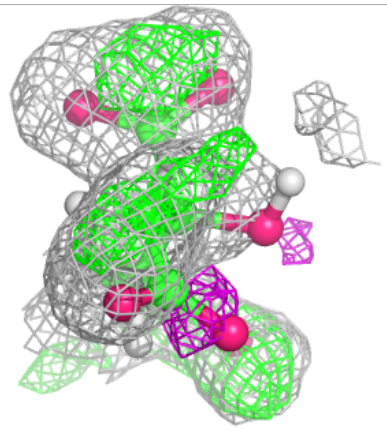


Electron density around FLC D 1200 (B):

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

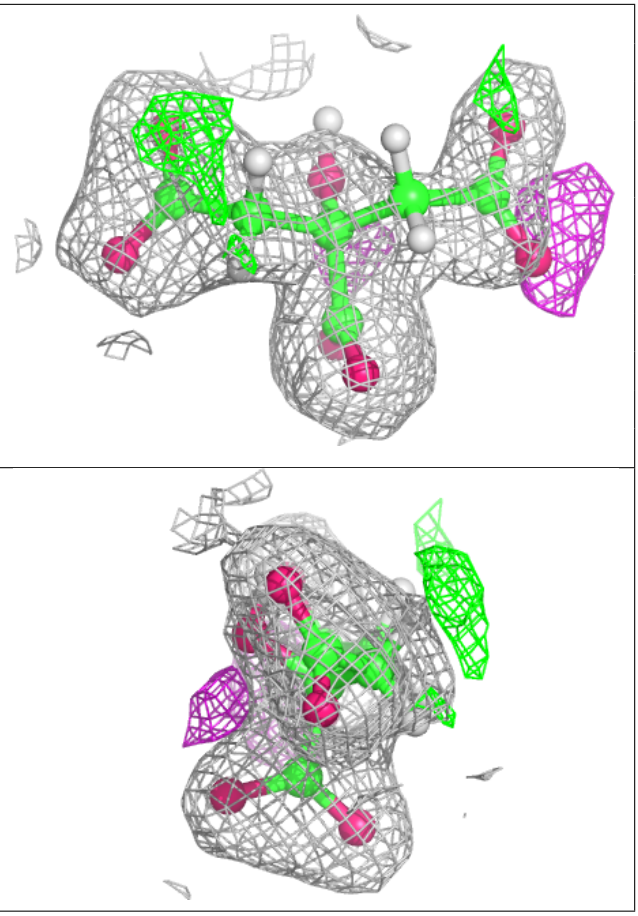






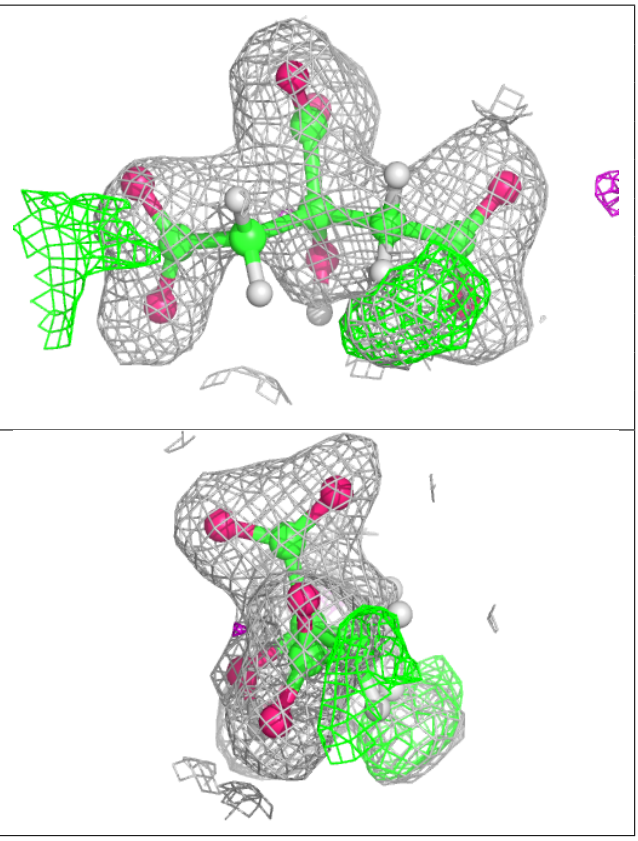
Electron density around FLC B 1201:

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



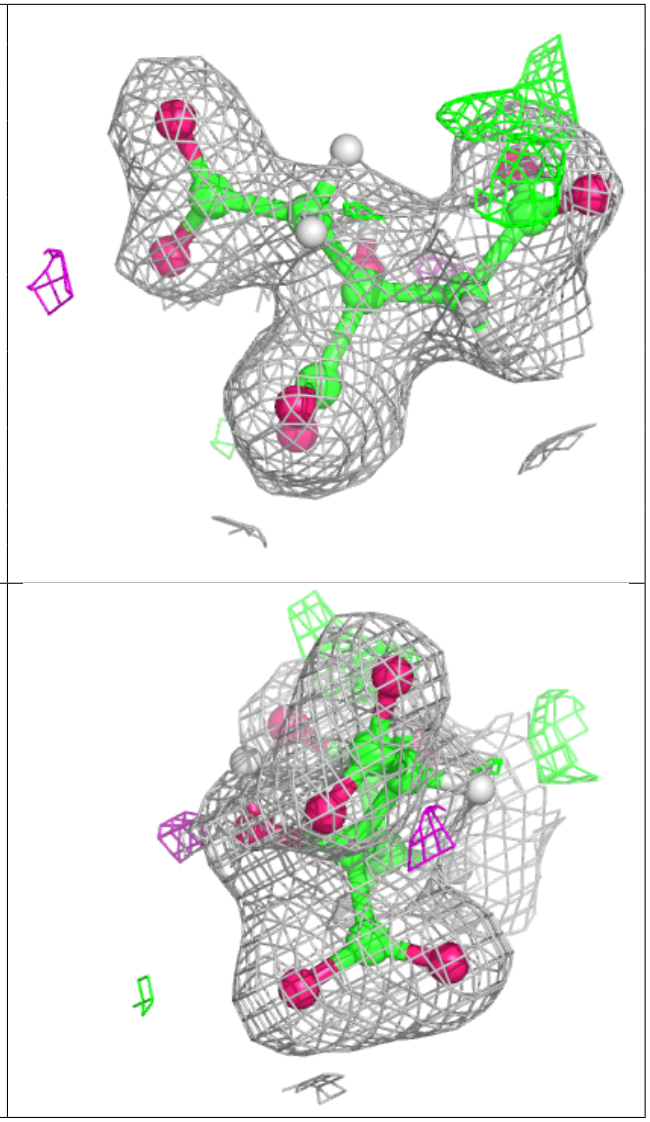
Electron density around FLC C 1202:

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



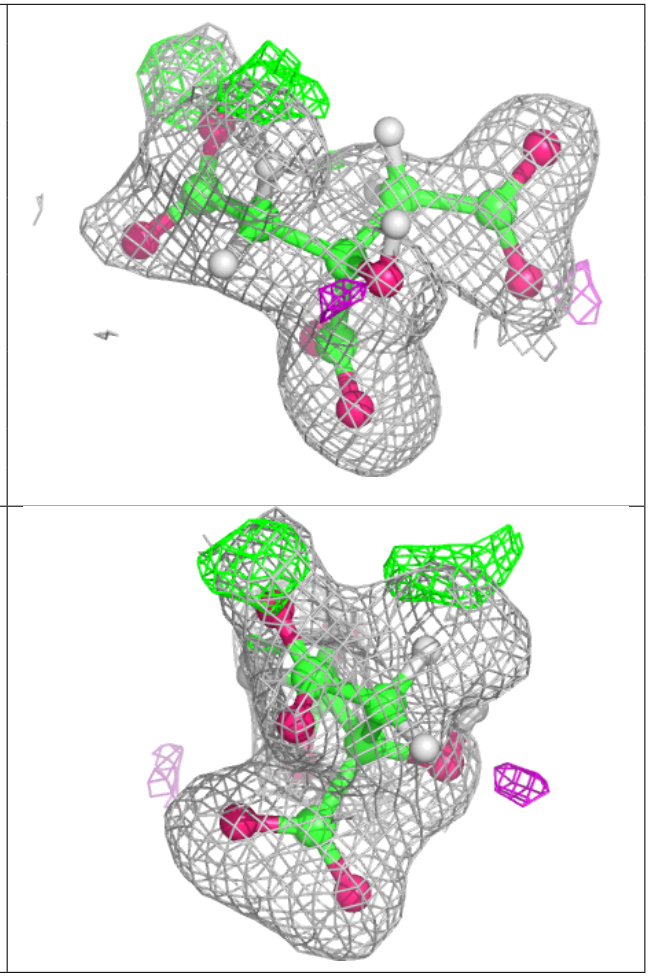
Electron density around FLC A 1200 (B):

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



Electron density around FLC A 1200 (A):

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



6.5 Other polymers (i)

There are no such residues in this entry.