Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:42 am BST

PDB ID	:	5KLS
Title	:	Structure of CavAb in complex with Br-dihydropyridine derivative UK-59811
Authors	:	Tang, L.; Gamal EL-Din, T.M.; Swanson, T.M.; Pryde, D.C.; Scheuer, T.; Zheng, N.; Catterall, W.A.
Deposited on	:	2016-06-25
Resolution	:	3.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

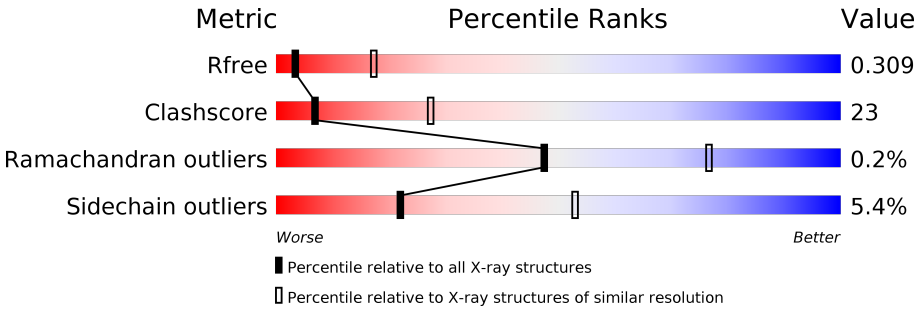
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 on 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	285	43% 32% • 23%
1	B	285	40% 34% • 23%
1	C	285	45% 30% • 23%
1	D	285	46% 28% • 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	6UC	C	1304	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7401 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1800	1227	269	294	10			
1	B	219	Total	C	N	O	S	0	0	0
			1800	1227	269	294	10			
1	C	219	Total	C	N	O	S	0	0	0
			1800	1227	269	294	10			
1	D	219	Total	C	N	O	S	0	0	0
			1800	1227	269	294	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	initiating methionine	UNP A8EVM5
A	984	ASP	-	expression tag	UNP A8EVM5
A	985	TYR	-	expression tag	UNP A8EVM5
A	986	LYS	-	expression tag	UNP A8EVM5
A	987	ASP	-	expression tag	UNP A8EVM5
A	988	ASP	-	expression tag	UNP A8EVM5
A	989	ASP	-	expression tag	UNP A8EVM5
A	990	ASP	-	expression tag	UNP A8EVM5
A	991	LYS	-	expression tag	UNP A8EVM5
A	992	GLY	-	expression tag	UNP A8EVM5
A	993	SER	-	expression tag	UNP A8EVM5
A	994	LEU	-	expression tag	UNP A8EVM5
A	995	VAL	-	expression tag	UNP A8EVM5
A	996	PRO	-	expression tag	UNP A8EVM5
A	997	ARG	-	expression tag	UNP A8EVM5
A	998	GLY	-	expression tag	UNP A8EVM5
A	999	SER	-	expression tag	UNP A8EVM5
A	1000	HIS	-	expression tag	UNP A8EVM5
A	1177	ASP	GLU	conflict	UNP A8EVM5
A	1178	ASP	SER	conflict	UNP A8EVM5
A	1181	ASN	MET	conflict	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	983	MET	-	initiating methionine	UNP A8EVM5
B	984	ASP	-	expression tag	UNP A8EVM5
B	985	TYR	-	expression tag	UNP A8EVM5
B	986	LYS	-	expression tag	UNP A8EVM5
B	987	ASP	-	expression tag	UNP A8EVM5
B	988	ASP	-	expression tag	UNP A8EVM5
B	989	ASP	-	expression tag	UNP A8EVM5
B	990	ASP	-	expression tag	UNP A8EVM5
B	991	LYS	-	expression tag	UNP A8EVM5
B	992	GLY	-	expression tag	UNP A8EVM5
B	993	SER	-	expression tag	UNP A8EVM5
B	994	LEU	-	expression tag	UNP A8EVM5
B	995	VAL	-	expression tag	UNP A8EVM5
B	996	PRO	-	expression tag	UNP A8EVM5
B	997	ARG	-	expression tag	UNP A8EVM5
B	998	GLY	-	expression tag	UNP A8EVM5
B	999	SER	-	expression tag	UNP A8EVM5
B	1000	HIS	-	expression tag	UNP A8EVM5
B	1177	ASP	GLU	conflict	UNP A8EVM5
B	1178	ASP	SER	conflict	UNP A8EVM5
B	1181	ASN	MET	conflict	UNP A8EVM5
C	983	MET	-	initiating methionine	UNP A8EVM5
C	984	ASP	-	expression tag	UNP A8EVM5
C	985	TYR	-	expression tag	UNP A8EVM5
C	986	LYS	-	expression tag	UNP A8EVM5
C	987	ASP	-	expression tag	UNP A8EVM5
C	988	ASP	-	expression tag	UNP A8EVM5
C	989	ASP	-	expression tag	UNP A8EVM5
C	990	ASP	-	expression tag	UNP A8EVM5
C	991	LYS	-	expression tag	UNP A8EVM5
C	992	GLY	-	expression tag	UNP A8EVM5
C	993	SER	-	expression tag	UNP A8EVM5
C	994	LEU	-	expression tag	UNP A8EVM5
C	995	VAL	-	expression tag	UNP A8EVM5
C	996	PRO	-	expression tag	UNP A8EVM5
C	997	ARG	-	expression tag	UNP A8EVM5
C	998	GLY	-	expression tag	UNP A8EVM5
C	999	SER	-	expression tag	UNP A8EVM5
C	1000	HIS	-	expression tag	UNP A8EVM5
C	1177	ASP	GLU	conflict	UNP A8EVM5
C	1178	ASP	SER	conflict	UNP A8EVM5
C	1181	ASN	MET	conflict	UNP A8EVM5

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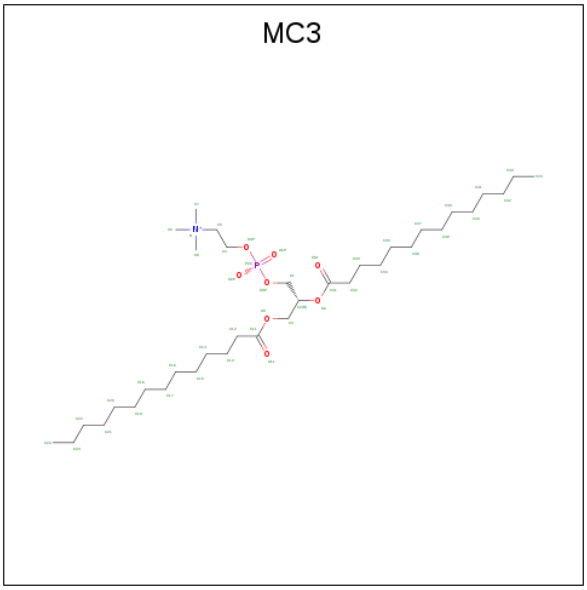
Chain	Residue	Modelled	Actual	Comment	Reference
D	983	MET	-	initiating methionine	UNP A8EVM5
D	984	ASP	-	expression tag	UNP A8EVM5
D	985	TYR	-	expression tag	UNP A8EVM5
D	986	LYS	-	expression tag	UNP A8EVM5
D	987	ASP	-	expression tag	UNP A8EVM5
D	988	ASP	-	expression tag	UNP A8EVM5
D	989	ASP	-	expression tag	UNP A8EVM5
D	990	ASP	-	expression tag	UNP A8EVM5
D	991	LYS	-	expression tag	UNP A8EVM5
D	992	GLY	-	expression tag	UNP A8EVM5
D	993	SER	-	expression tag	UNP A8EVM5
D	994	LEU	-	expression tag	UNP A8EVM5
D	995	VAL	-	expression tag	UNP A8EVM5
D	996	PRO	-	expression tag	UNP A8EVM5
D	997	ARG	-	expression tag	UNP A8EVM5
D	998	GLY	-	expression tag	UNP A8EVM5
D	999	SER	-	expression tag	UNP A8EVM5
D	1000	HIS	-	expression tag	UNP A8EVM5
D	1177	ASP	GLU	conflict	UNP A8EVM5
D	1178	ASP	SER	conflict	UNP A8EVM5
D	1181	ASN	MET	conflict	UNP A8EVM5

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula: $C_{36}H_{72}NO_8P$).

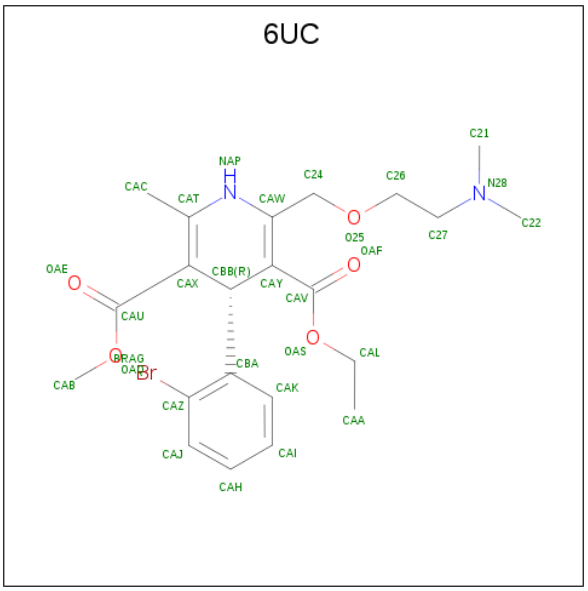


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 21 13 7 1	0	0
2	A	1	Total C O P 21 13 7 1	0	0
2	A	1	Total C O P 10 3 6 1	0	0
2	A	1	Total C O P 10 3 6 1	0	0
2	B	1	Total C O P 10 3 6 1	0	0
2	B	1	Total C O P 10 3 6 1	0	0
2	B	1	Total C 6 6	0	0
2	C	1	Total C O P 10 3 6 1	0	0
2	C	1	Total C O P 10 3 6 1	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	D	1	Total C O P 21 13 7 1	0	0
2	D	1	Total C O P 10 3 6 1	0	0
2	D	1	Total C O P 10 3 6 1	0	0
2	D	1	Total C 6 6	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is O3-ethyl O5-methyl (4R)-4-(2-bromophenyl)-2-[2-(dimethylamino)ethoxymethyl]-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate (three-letter code: 6UC) (formula: $C_{22}H_{29}BrN_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	Br	C	N	O	0	0
			30	1	22	2	5		

- Molecule 5 is water.

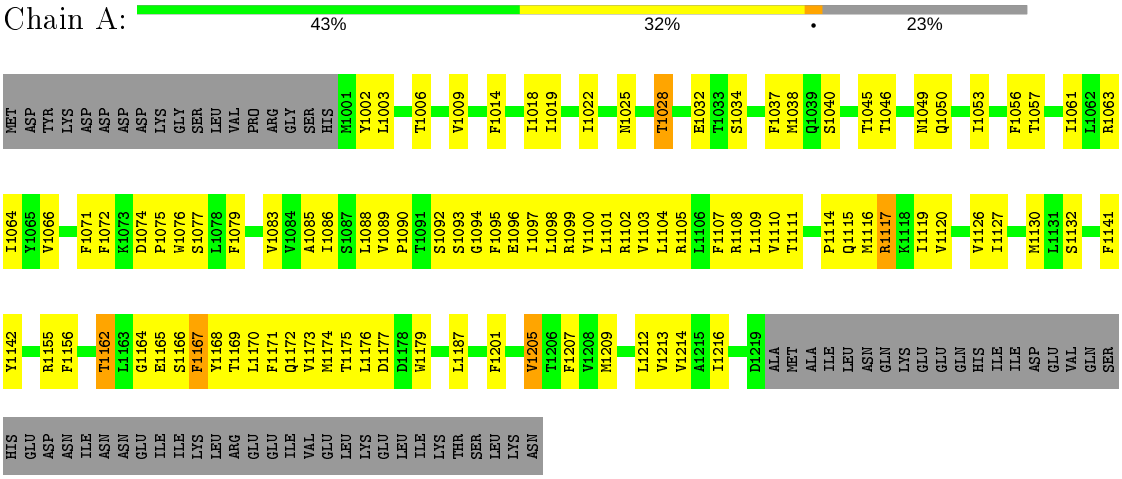
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

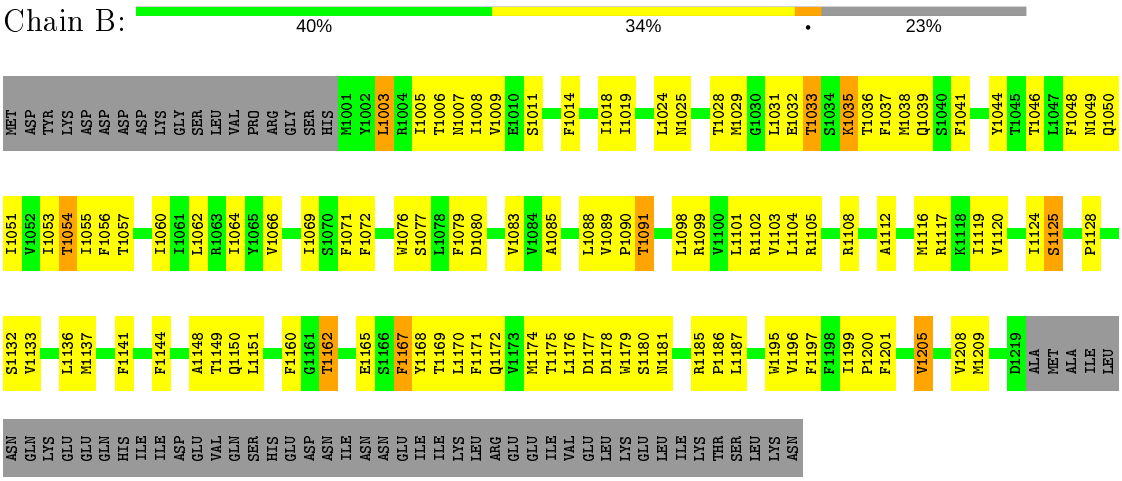
- Molecule 1: Ion transport protein

Chain A:



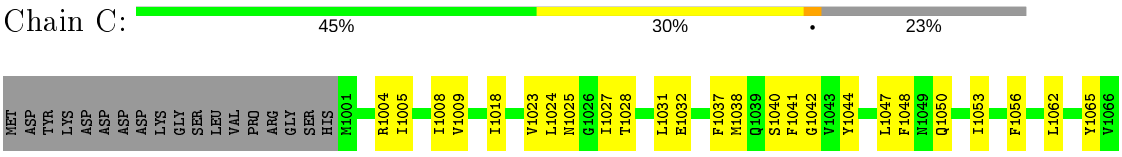
- Molecule 1: Ion transport protein

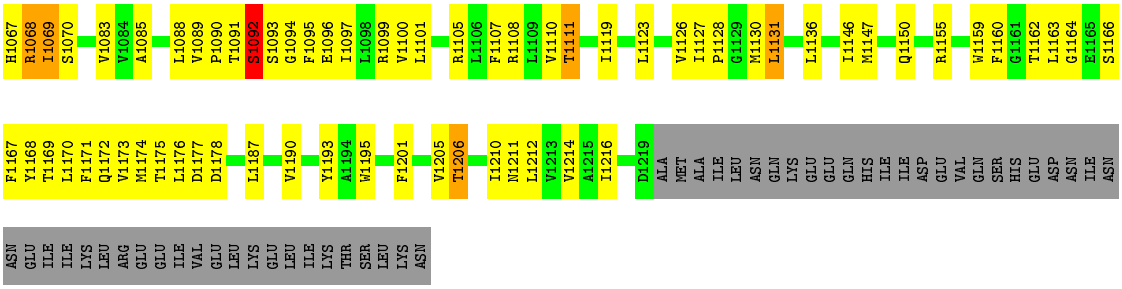
Chain B:



- Molecule 1: Ion transport protein

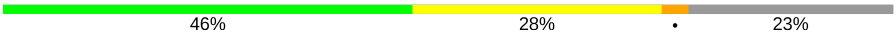
Chain C:

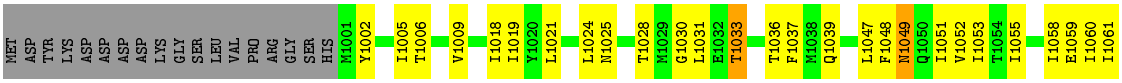


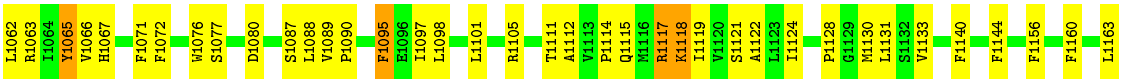


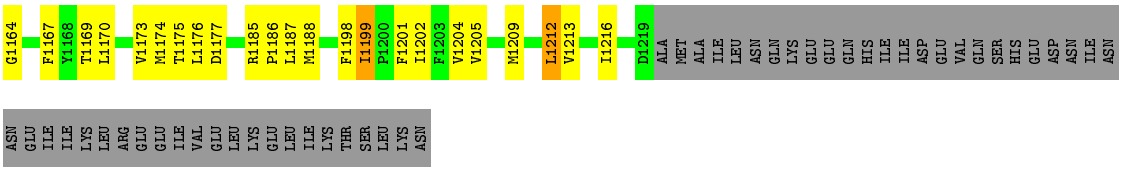
- Molecule 1: Ion transport protein

Chain D:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	125.47Å 125.87Å 191.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 3.30 29.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.0 (29.81-3.30) 90.9 (29.81-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 3.31Å)	Xtriage
Refinement program	PHENIX dev_1839	Depositor
R, R_{free}	0.274 , 0.300 0.280 , 0.309	Depositor DCC
R_{free} test set	2162 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	90.2	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 77.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.449 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7401	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.25% 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: CA, MC3, 6UC

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	0.66	0/1851	0.86	0/2520
1	B	0.68	0/1851	0.85	0/2520
1	C	0.66	0/1851	0.87	1/2520 (0.0%)
1	D	0.68	0/1851	0.90	0/2520
All	All	0.67	0/7404	0.87	1/10080 (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	C	1131	LEU	CA-CB-CG	6.21	129.58	115.30

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	1800	0	1869	100	0
1	B	1800	0	1869	108	0
1	C	1800	0	1869	83	0
1	D	1800	0	1869	82	0
2	A	62	0	48	7	0
2	B	26	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	32	0	26	0	0
2	D	47	0	37	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	30	0	0	2	0
5	A	2	0	0	0	0
All	All	7401	0	7605	347	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 23.

All (347) 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:1071:PHE:CD2	1:B:1072:PHE:HE2	1.46	1.33
1:B:1071:PHE:CD2	1:B:1072:PHE:CE2	2.23	1.26
1:B:1031:LEU:HD13	1:B:1037:PHE:CE1	1.73	1.22
1:B:1071:PHE:CE1	1:B:1077:SER:HB3	1.84	1.12
1:B:1071:PHE:HD2	1:B:1072:PHE:CE2	1.63	1.09
1:B:1119:ILE:HD11	1:D:1133:VAL:HG22	1.38	1.05
1:B:1091:THR:HG22	1:B:1099:ARG:HG3	1.41	1.01
1:A:1089:VAL:CG1	1:A:1090:PRO:HD2	2.01	0.91
1:B:1171:PHE:CE2	1:D:1199:ILE:HD13	2.07	0.89
1:D:1076:TRP:HB3	1:D:1111:THR:HG23	1.55	0.87
1:B:1071:PHE:HE1	1:B:1077:SER:HB3	1.39	0.83
1:A:1089:VAL:HG13	1:A:1090:PRO:HD2	1.58	0.83
1:C:1089:VAL:HG12	1:C:1090:PRO:HD2	1.61	0.82
1:B:1071:PHE:HD2	1:B:1072:PHE:HE2	0.83	0.79
1:D:1053:ILE:HD12	1:D:1088:LEU:HD23	1.65	0.79
1:A:1116:MET:HA	1:A:1119:ILE:HD12	1.66	0.78
1:C:1089:VAL:CG1	1:C:1090:PRO:HD2	2.15	0.77
1:B:1174:MET:HG3	1:B:1205:VAL:HG13	1.67	0.76
1:B:1071:PHE:CD2	1:B:1072:PHE:CD2	2.73	0.76
1:B:1003:LEU:HA	1:B:1006:THR:HB	1.67	0.76
1:B:1171:PHE:CD2	1:D:1199:ILE:HD13	2.19	0.76
1:B:1162:THR:HG22	1:B:1165:GLU:H	1.50	0.76
1:A:1114:PRO:HA	1:A:1117:ARG:HD2	1.67	0.75
1:D:1061:ILE:HG22	1:D:1065:TYR:CE1	2.22	0.74
1:D:1062:LEU:HA	1:D:1065:TYR:CE2	2.23	0.74
1:B:1119:ILE:HD11	1:D:1133:VAL:CG2	2.16	0.74
1:C:1031:LEU:HB3	1:C:1037:PHE:CZ	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1064:ILE:HG12	1:B:1071:PHE:CD2	2.23	0.73
1:B:1019:ILE:HD11	1:B:1112:ALA:HB3	1.71	0.72
1:D:1066:VAL:HG23	1:D:1067:HIS:ND1	2.05	0.72
1:C:1174:MET:HG3	1:C:1205:VAL:HG11	1.72	0.71
1:C:1040:SER:C	1:C:1041:PHE:HD2	1.95	0.70
1:A:1170:LEU:HD22	1:A:1201:PHE:CZ	2.26	0.70
1:B:1171:PHE:CD2	1:D:1199:ILE:CD1	2.74	0.70
1:B:1174:MET:HG3	1:B:1205:VAL:CG1	2.21	0.70
1:B:1071:PHE:CE2	1:B:1072:PHE:CE2	2.79	0.69
1:B:1003:LEU:O	1:B:1007:ASN:N	2.23	0.69
1:B:1071:PHE:CE2	1:B:1072:PHE:HE2	2.08	0.69
1:A:1116:MET:O	1:A:1120:VAL:HG13	1.93	0.69
1:D:1025:ASN:OD1	1:D:1105:ARG:HD2	1.93	0.68
2:A:1304:MC3:O3P	2:A:1304:MC3:O3	2.10	0.68
1:B:1085:ALA:O	1:B:1088:LEU:HB2	1.91	0.68
1:B:1031:LEU:HD13	1:B:1037:PHE:HE1	1.51	0.68
1:A:1100:VAL:O	1:A:1103:VAL:HG12	1.94	0.68
1:C:1047:LEU:HD12	1:C:1048:PHE:N	2.09	0.68
1:C:1174:MET:HG3	1:C:1205:VAL:CG1	2.24	0.68
1:A:1089:VAL:HG12	1:A:1090:PRO:HD2	1.76	0.67
1:A:1092:SER:O	1:A:1093:SER:HB2	1.92	0.67
1:D:1009:VAL:HG11	1:D:1066:VAL:HG21	1.76	0.67
1:D:1061:ILE:HG22	1:D:1065:TYR:HE1	1.56	0.67
1:A:1094:GLY:C	1:A:1095:PHE:HD1	1.98	0.67
1:D:1212:LEU:C	1:D:1212:LEU:HD12	2.16	0.66
1:C:1027:ILE:O	1:C:1031:LEU:HG	1.96	0.65
1:A:1132:SER:HB2	1:D:1119:ILE:HD11	1.78	0.65
1:B:1176:LEU:HD13	1:C:1175:THR:CG2	2.27	0.65
1:D:1062:LEU:HA	1:D:1065:TYR:CZ	2.31	0.65
1:B:1170:LEU:HD21	1:B:1197:PHE:HE1	1.61	0.64
1:B:1014:PHE:CZ	1:B:1062:LEU:HD12	2.32	0.64
1:A:1095:PHE:HB3	1:A:1097:ILE:HG22	1.80	0.64
1:B:1071:PHE:CD1	1:B:1077:SER:HB3	2.30	0.63
1:C:1094:GLY:O	1:C:1095:PHE:CD1	2.51	0.63
1:B:1064:ILE:HG12	1:B:1071:PHE:HD2	1.61	0.63
1:B:1031:LEU:HD13	1:B:1037:PHE:CZ	2.31	0.63
1:B:1080:ASP:OD1	1:B:1108:ARG:HG2	1.99	0.63
1:B:1049:ASN:O	1:B:1053:ILE:HG23	1.98	0.63
1:A:1141:PHE:HB3	1:A:1167:PHE:CE1	2.34	0.62
1:D:1115:GLN:N	1:D:1115:GLN:OE1	2.30	0.62
1:A:1174:MET:HG3	1:A:1205:VAL:CG1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1064:ILE:CG1	1:B:1071:PHE:CD2	2.82	0.61
1:C:1025:ASN:OD1	1:C:1105:ARG:NH1	2.31	0.61
1:D:1114:PRO:HA	1:D:1117:ARG:CG	2.31	0.61
1:C:1053:ILE:HD13	1:C:1105:ARG:NH2	2.16	0.61
1:B:1101:LEU:O	1:B:1104:LEU:HB2	2.01	0.61
1:A:1117:ARG:O	1:A:1120:VAL:HG22	2.00	0.61
1:D:1144:PHE:CD2	1:D:1201:PHE:HD1	2.19	0.61
1:A:1098:LEU:HD23	1:A:1101:LEU:HD12	1.83	0.60
1:A:1170:LEU:HD22	1:A:1201:PHE:CE1	2.37	0.60
1:A:1130:MET:HG2	1:A:1212:LEU:HD11	1.83	0.60
1:A:1006:THR:HG23	1:A:1066:VAL:HG13	1.83	0.60
1:D:1198:PHE:O	1:D:1202:ILE:HG13	2.01	0.60
1:D:1160:PHE:CZ	1:D:1169:THR:HG21	2.37	0.59
1:A:1110:VAL:HG22	1:A:1116:MET:HG2	1.84	0.59
1:B:1079:PHE:CZ	1:B:1083:VAL:HG21	2.38	0.59
1:D:1049:ASN:O	1:D:1053:ILE:HG23	2.02	0.59
1:A:1079:PHE:CZ	1:A:1083:VAL:HG21	2.38	0.59
1:D:1114:PRO:HA	1:D:1117:ARG:HG3	1.84	0.59
1:B:1076:TRP:CD2	1:B:1117:ARG:HD3	2.37	0.58
1:B:1076:TRP:CG	1:B:1117:ARG:HD3	2.38	0.58
1:C:1005:ILE:HA	1:C:1008:ILE:HD12	1.85	0.58
1:A:1105:ARG:HB3	1:A:1105:ARG:NH1	2.19	0.58
1:A:1127:ILE:HA	1:A:1130:MET:HE2	1.85	0.58
1:A:1006:THR:HA	1:A:1066:VAL:HG22	1.85	0.58
1:C:1131:LEU:O	1:C:1131:LEU:HD23	2.04	0.58
1:B:1028:THR:HG21	1:B:1048:PHE:CD1	2.39	0.57
1:D:1005:ILE:HD12	1:D:1065:TYR:CD2	2.40	0.57
1:B:1062:LEU:O	1:B:1066:VAL:HG23	2.04	0.57
1:A:1174:MET:HG3	1:A:1205:VAL:HG11	1.86	0.57
1:D:1071:PHE:HD2	1:D:1072:PHE:CD2	2.23	0.57
1:B:1025:ASN:OD1	1:B:1105:ARG:NE	2.31	0.57
1:D:1062:LEU:HD23	1:D:1065:TYR:OH	2.05	0.57
1:D:1089:VAL:CG1	1:D:1090:PRO:HD2	2.35	0.56
1:D:1036:THR:O	1:D:1039:GLN:HG2	2.05	0.56
1:B:1172:GLN:HG3	1:B:1177:ASP:HB3	1.88	0.56
1:B:1036:THR:O	1:B:1039:GLN:HB2	2.05	0.56
1:B:1079:PHE:CE2	1:B:1083:VAL:HG21	2.40	0.56
1:B:1175:THR:HB	1:D:1176:LEU:HD13	1.88	0.56
1:C:1041:PHE:N	1:C:1041:PHE:HD2	2.04	0.56
1:C:1038:MET:O	1:C:1042:GLY:N	2.38	0.56
1:C:1085:ALA:O	1:C:1088:LEU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:PRO:HA	1:A:1117:ARG:CD	2.36	0.56
1:C:1123:LEU:O	1:C:1126:VAL:HG22	2.05	0.56
1:D:1071:PHE:CE1	1:D:1077:SER:HB3	2.40	0.56
2:A:1303:MC3:H2	1:C:1162:THR:HB	1.89	0.55
1:C:1041:PHE:N	1:C:1041:PHE:CD2	2.74	0.55
1:A:1002:TYR:CD2	1:A:1003:LEU:HD23	2.42	0.55
1:A:1102:ARG:O	1:A:1105:ARG:HB2	2.07	0.55
1:D:1030:GLY:O	1:D:1033:THR:HB	2.07	0.55
1:A:1032:GLU:HA	1:A:1038:MET:HE3	1.89	0.55
1:B:1098:LEU:HD23	1:B:1101:LEU:HD12	1.89	0.55
1:C:1108:ARG:HA	1:C:1111:THR:HB	1.89	0.55
1:A:1214:VAL:HG11	1:D:1216:ILE:HG22	1.89	0.54
1:C:1031:LEU:HB3	1:C:1037:PHE:CE2	2.42	0.54
1:C:1193:TYR:HA	1:C:1195:TRP:NE1	2.20	0.54
1:B:1179:TRP:HE1	1:C:1175:THR:HG21	1.73	0.54
1:A:1032:GLU:HG2	1:A:1045:THR:HG21	1.88	0.54
1:A:1095:PHE:N	1:A:1095:PHE:CD1	2.76	0.54
1:D:1130:MET:CE	1:D:1216:ILE:HD11	2.37	0.54
1:A:1009:VAL:HG11	1:A:1063:ARG:HG2	1.90	0.54
1:B:1144:PHE:CD2	1:B:1201:PHE:HD2	2.25	0.54
1:A:1162:THR:HG22	1:A:1165:GLU:H	1.72	0.54
1:D:1095:PHE:CD2	1:D:1095:PHE:N	2.75	0.54
1:B:1176:LEU:HD13	1:C:1175:THR:HG23	1.89	0.53
1:B:1116:MET:O	1:B:1119:ILE:HG22	2.08	0.53
1:D:1173:VAL:O	1:D:1176:LEU:HD23	2.09	0.53
2:B:1302:MC3:H31	1:C:1097:ILE:HG13	1.91	0.53
1:C:1211:ASN:HA	1:C:1214:VAL:HB	1.91	0.53
1:A:1095:PHE:N	1:A:1095:PHE:HD1	2.06	0.53
1:D:1098:LEU:HD23	1:D:1101:LEU:HD12	1.91	0.53
1:A:1071:PHE:CE1	1:A:1077:SER:HB3	2.43	0.53
1:B:1177:ASP:O	1:B:1178:ASP:C	2.48	0.52
1:D:1024:LEU:HB3	1:D:1048:PHE:HZ	1.74	0.52
1:B:1168:TYR:CZ	1:D:1188:MET:HE1	2.44	0.52
1:B:1091:THR:HG23	1:B:1102:ARG:NH2	2.24	0.52
1:C:1170:LEU:HD22	1:C:1201:PHE:CZ	2.45	0.52
1:C:1169:THR:O	1:C:1173:VAL:HG23	2.08	0.52
1:B:1053:ILE:HG13	1:B:1054:THR:N	2.24	0.52
1:A:1142:TYR:OH	1:D:1030:GLY:HA3	2.10	0.52
1:C:1023:VAL:O	1:C:1027:ILE:HG13	2.09	0.52
1:D:1118:LYS:O	1:D:1122:ALA:N	2.27	0.52
1:D:1169:THR:O	1:D:1173:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1061:ILE:HD13	1:A:1064:ILE:HD12	1.91	0.51
1:B:1024:LEU:O	1:B:1028:THR:HG23	2.09	0.51
2:A:1301:MC3:H11	1:D:1164:GLY:HA3	1.92	0.51
1:A:1089:VAL:CG1	1:A:1090:PRO:CD	2.83	0.51
1:B:1201:PHE:O	1:B:1205:VAL:HB	2.10	0.51
1:A:1018:ILE:HG21	1:A:1108:ARG:HH22	1.76	0.51
1:C:1130:MET:HG2	1:C:1212:LEU:HD11	1.93	0.51
1:C:1130:MET:HE2	1:C:1216:ILE:HD11	1.93	0.51
1:A:1028:THR:HG23	1:A:1045:THR:HG23	1.92	0.51
1:D:1051:ILE:O	1:D:1055:ILE:HG13	2.11	0.50
1:C:1018:ILE:HG23	1:C:1056:PHE:CE1	2.47	0.50
1:C:1130:MET:CE	1:C:1216:ILE:HD11	2.42	0.50
1:B:1025:ASN:ND2	1:B:1028:THR:OG1	2.42	0.50
1:B:1019:ILE:HD11	1:B:1112:ALA:CB	2.38	0.50
1:B:1085:ALA:HA	1:B:1088:LEU:HD12	1.93	0.50
1:B:1005:ILE:O	1:B:1008:ILE:HB	2.12	0.50
1:A:1071:PHE:HD2	1:A:1072:PHE:CD1	2.30	0.50
1:A:1096:GLU:O	1:A:1099:ARG:HB3	2.12	0.50
1:A:1074:ASP:OD1	1:A:1076:TRP:HD1	1.94	0.50
1:C:1050:GLN:HA	1:C:1053:ILE:HG22	1.93	0.50
1:D:1124:ILE:O	1:D:1128:PRO:HD3	2.12	0.50
1:A:1049:ASN:OD1	1:A:1102:ARG:NH1	2.44	0.50
1:B:1089:VAL:HG11	1:B:1098:LEU:HD13	1.94	0.50
1:C:1009:VAL:CG2	1:C:1062:LEU:HB3	2.42	0.50
1:C:1096:GLU:O	1:C:1099:ARG:HB3	2.12	0.50
1:D:1006:THR:HA	1:D:1066:VAL:HG12	1.94	0.50
1:B:1199:ILE:HB	1:B:1200:PRO:HD3	1.94	0.49
1:C:1095:PHE:C	1:C:1097:ILE:N	2.64	0.49
1:B:1033:THR:HG21	1:D:1163:LEU:HB2	1.95	0.49
1:A:1037:PHE:HD2	1:A:1038:MET:HE2	1.76	0.49
1:B:1195:TRP:CZ3	1:B:1196:VAL:HG22	2.47	0.49
1:C:1095:PHE:C	1:C:1097:ILE:H	2.14	0.49
1:D:1205:VAL:O	1:D:1209:MET:HG2	2.12	0.49
1:B:1162:THR:HG22	1:B:1165:GLU:N	2.23	0.49
1:A:1002:TYR:HD2	1:A:1003:LEU:HD23	1.78	0.49
1:B:1209:MET:HA	1:B:1209:MET:CE	2.42	0.49
1:C:1053:ILE:HD13	1:C:1105:ARG:HH21	1.77	0.49
1:A:1025:ASN:OD1	1:A:1105:ARG:NH2	2.45	0.49
1:B:1050:GLN:O	1:B:1053:ILE:HG12	2.12	0.49
1:B:1151:LEU:HG	1:C:1100:VAL:HG11	1.95	0.49
1:B:1137:MET:SD	1:B:1208:VAL:HG11	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1114:PRO:HA	1:D:1117:ARG:CD	2.44	0.48
1:C:1146:ILE:HG13	1:C:1163:LEU:HD21	1.95	0.48
1:B:1018:ILE:HD11	1:B:1055:ILE:HG22	1.94	0.48
1:A:1114:PRO:HA	1:A:1117:ARG:HG3	1.96	0.48
1:B:1169:THR:O	1:B:1172:GLN:HB3	2.13	0.48
1:B:1091:THR:HG22	1:B:1099:ARG:CG	2.29	0.48
1:C:1193:TYR:HA	1:C:1195:TRP:HE1	1.77	0.48
1:A:1207:PHE:HE1	1:D:1130:MET:SD	2.37	0.48
1:C:1068:ARG:CG	1:C:1069:ILE:N	2.76	0.48
1:C:1175:THR:HG22	1:C:1175:THR:O	2.13	0.48
1:A:1075:PRO:HD2	1:A:1076:TRP:CD1	2.49	0.47
1:B:1032:GLU:HA	1:B:1038:MET:HE3	1.95	0.47
1:B:1089:VAL:CG1	1:B:1090:PRO:HD2	2.43	0.47
1:D:1089:VAL:HG12	1:D:1090:PRO:HD2	1.96	0.47
1:D:1156:PHE:CZ	1:D:1187:LEU:HA	2.50	0.47
1:A:1103:VAL:HG11	1:C:1147:MET:HG2	1.96	0.47
1:A:1050:GLN:O	1:A:1053:ILE:HG22	2.15	0.47
1:C:1108:ARG:O	1:C:1111:THR:HG22	2.15	0.47
1:A:1169:THR:O	1:A:1172:GLN:HB3	2.15	0.47
1:A:1022:ILE:HD12	1:A:1109:LEU:HA	1.96	0.47
1:B:1170:LEU:HD22	1:B:1201:PHE:CZ	2.50	0.47
1:B:1008:ILE:O	1:B:1011:SER:HB3	2.15	0.47
1:B:1035:LYS:O	1:B:1039:GLN:HG3	2.15	0.47
1:C:1160:PHE:CZ	1:C:1169:THR:HG21	2.49	0.46
1:D:1089:VAL:HG13	1:D:1090:PRO:HD2	1.97	0.46
1:B:1029:MET:HE2	1:B:1103:VAL:HG12	1.96	0.46
1:A:1173:VAL:O	1:A:1176:LEU:HD23	2.16	0.46
1:B:1185:ARG:HB2	1:B:1186:PRO:HD3	1.98	0.46
1:D:1060:ILE:HD11	1:D:1080:ASP:HB3	1.98	0.46
1:A:1028:THR:O	1:A:1032:GLU:HG3	2.15	0.46
1:B:1057:THR:O	1:B:1060:ILE:HG12	2.16	0.46
1:B:1174:MET:C	1:B:1176:LEU:H	2.18	0.46
1:D:1063:ARG:HA	1:D:1066:VAL:HG22	1.98	0.46
1:B:1072:PHE:N	1:B:1072:PHE:HD2	2.14	0.46
1:B:1195:TRP:CZ3	4:C:1304:6UC:CAC	2.99	0.46
1:B:1150:GLN:HE21	1:C:1100:VAL:HG13	1.81	0.46
1:A:1177:ASP:OD1	1:C:1178:ASP:HA	2.16	0.46
1:B:1149:THR:HA	1:B:1160:PHE:O	2.16	0.45
1:C:1041:PHE:O	1:C:1044:TYR:HB3	2.16	0.45
1:C:1005:ILE:HD12	1:C:1065:TYR:CE2	2.51	0.45
1:A:1116:MET:HG3	1:C:1136:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:ILE:HA	1:A:1022:ILE:HD11	1.97	0.45
1:A:1114:PRO:HA	1:A:1117:ARG:CG	2.46	0.45
1:A:1216:ILE:CG2	1:C:1214:VAL:HG21	2.47	0.45
1:D:1019:ILE:HD11	1:D:1112:ALA:O	2.16	0.45
1:A:1018:ILE:O	1:A:1022:ILE:HG12	2.16	0.45
1:B:1072:PHE:N	1:B:1072:PHE:CD2	2.84	0.45
1:D:1071:PHE:CD2	1:D:1072:PHE:CD2	3.04	0.45
1:D:1140:PHE:CZ	1:D:1204:VAL:HG11	2.51	0.45
1:C:1101:LEU:HA	1:C:1101:LEU:HD23	1.68	0.45
1:C:1095:PHE:HB3	1:C:1097:ILE:HG12	1.98	0.45
1:C:1171:PHE:O	1:C:1174:MET:HB3	2.16	0.45
1:A:1071:PHE:CZ	1:A:1077:SER:HB3	2.51	0.45
1:A:1168:TYR:HA	2:A:1302:MC3:H121	1.99	0.45
1:C:1004:ARG:O	1:C:1008:ILE:HG13	2.17	0.45
1:C:1212:LEU:O	1:C:1216:ILE:HG13	2.17	0.45
1:A:1071:PHE:HD2	1:A:1072:PHE:HD1	1.64	0.45
1:C:1067:HIS:ND1	1:C:1070:SER:OG	2.46	0.45
1:D:1087:SER:HB3	1:D:1105:ARG:HH21	1.81	0.45
1:A:1141:PHE:HB3	1:A:1167:PHE:CZ	2.52	0.45
1:B:1133:VAL:O	1:B:1136:LEU:HB3	2.16	0.44
1:B:1149:THR:HG23	1:B:1160:PHE:O	2.17	0.44
1:A:1216:ILE:HG22	1:C:1214:VAL:HG21	1.99	0.44
1:A:1179:TRP:N	1:D:1177:ASP:OD2	2.49	0.44
1:A:1171:PHE:O	1:A:1175:THR:HG23	2.17	0.44
1:B:1089:VAL:HG12	1:B:1090:PRO:HD2	2.00	0.44
2:B:1301:MC3:H32	1:D:1163:LEU:HD23	2.00	0.44
1:D:1174:MET:C	1:D:1176:LEU:H	2.20	0.44
1:D:1058:ILE:O	1:D:1062:LEU:HG	2.18	0.44
1:D:1212:LEU:HD12	1:D:1213:VAL:N	2.32	0.44
1:A:1115:GLN:O	1:A:1119:ILE:HG13	2.17	0.44
1:B:1180:SER:HB3	1:C:1177:ASP:OD2	2.18	0.44
1:C:1094:GLY:O	1:C:1095:PHE:CG	2.71	0.44
1:D:1047:LEU:HD12	1:D:1048:PHE:N	2.32	0.43
1:D:1051:ILE:HG13	1:D:1052:VAL:N	2.30	0.43
1:B:1005:ILE:HA	1:B:1008:ILE:HD12	2.00	0.43
1:C:1107:PHE:O	1:C:1110:VAL:HB	2.19	0.43
1:C:1169:THR:O	1:C:1172:GLN:HB3	2.18	0.43
1:A:1094:GLY:C	1:A:1095:PHE:CD1	2.86	0.43
1:D:1024:LEU:HB3	1:D:1048:PHE:CZ	2.52	0.43
1:D:1058:ILE:HA	1:D:1061:ILE:HD12	2.00	0.43
1:D:1031:LEU:HA	1:D:1031:LEU:HD23	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:THR:HG23	1:A:1164:GLY:H	1.84	0.43
1:A:1009:VAL:HA	1:A:1014:PHE:CD2	2.54	0.43
1:A:1101:LEU:HA	1:A:1101:LEU:HD23	1.76	0.43
1:D:1087:SER:CB	1:D:1105:ARG:HH21	2.32	0.43
1:D:1185:ARG:HB2	1:D:1186:PRO:HD3	2.01	0.43
1:A:1022:ILE:HG23	1:A:1056:PHE:CZ	2.54	0.43
1:C:1068:ARG:HG3	1:C:1069:ILE:N	2.34	0.43
1:B:1132:SER:HB2	1:C:1119:ILE:HG13	2.01	0.43
1:A:1057:THR:O	1:A:1061:ILE:HG12	2.19	0.43
1:C:1168:TYR:CD1	1:C:1168:TYR:C	2.92	0.42
1:D:1009:VAL:HB	1:D:1066:VAL:HG11	2.01	0.42
1:A:1098:LEU:HA	1:A:1101:LEU:HD12	2.00	0.42
1:B:1003:LEU:HG	1:B:1003:LEU:H	1.48	0.42
1:B:1181:ASN:HA	1:B:1185:ARG:HD2	2.00	0.42
1:C:1032:GLU:HG2	1:C:1038:MET:HE1	2.00	0.42
1:A:1032:GLU:HG2	1:A:1038:MET:HE3	2.01	0.42
1:A:1156:PHE:CE1	1:A:1187:LEU:HD12	2.55	0.42
1:B:1019:ILE:HD12	1:B:1019:ILE:HG23	1.69	0.42
1:A:1079:PHE:CE1	1:A:1083:VAL:HG21	2.54	0.42
1:A:1126:VAL:HG21	1:A:1216:ILE:HG23	2.00	0.42
1:B:1018:ILE:HD12	1:B:1056:PHE:CD1	2.54	0.42
1:C:1028:THR:HG21	1:C:1048:PHE:CD2	2.55	0.42
1:D:1170:LEU:HD23	1:D:1170:LEU:HA	1.90	0.42
1:D:1199:ILE:HA	1:D:1202:ILE:HD12	2.02	0.42
1:A:1105:ARG:HB3	1:A:1105:ARG:HH11	1.83	0.42
1:B:1179:TRP:NE1	1:C:1175:THR:HG21	2.34	0.42
1:C:1173:VAL:O	1:C:1176:LEU:HD23	2.19	0.42
1:B:1041:PHE:O	1:B:1044:TYR:HB2	2.20	0.42
1:B:1120:VAL:O	1:B:1124:ILE:HG13	2.20	0.42
1:D:1021:LEU:HA	1:D:1021:LEU:HD23	1.70	0.42
1:B:1009:VAL:HG21	1:B:1062:LEU:HB3	2.02	0.42
1:C:1024:LEU:HB3	1:C:1048:PHE:CZ	2.55	0.42
1:A:1103:VAL:CG1	1:C:1147:MET:HG2	2.50	0.42
1:D:1031:LEU:HB3	1:D:1037:PHE:CE2	2.54	0.42
1:D:1018:ILE:HG13	1:D:1059:GLU:CD	2.40	0.42
1:C:1155:ARG:HD2	1:C:1190:VAL:HG11	2.02	0.41
1:D:1199:ILE:O	1:D:1202:ILE:HB	2.19	0.41
1:A:1096:GLU:HB3	1:A:1099:ARG:HH21	1.83	0.41
1:A:1107:PHE:O	1:A:1110:VAL:HB	2.20	0.41
1:A:1034:SER:HA	2:A:1303:MC3:O4P	2.20	0.41
1:B:1125:SER:O	1:B:1128:PRO:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1159:TRP:O	1:C:1169:THR:OG1	2.25	0.41
1:A:1162:THR:HG23	1:A:1164:GLY:N	2.36	0.41
1:C:1127:ILE:HB	1:C:1128:PRO:HD3	2.02	0.41
1:A:1019:ILE:O	1:A:1022:ILE:HG13	2.20	0.41
1:A:1079:PHE:O	1:A:1083:VAL:HG23	2.21	0.41
1:B:1148:ALA:HB2	1:B:1197:PHE:CZ	2.55	0.41
1:B:1141:PHE:HB3	1:B:1167:PHE:CE2	2.56	0.41
1:C:1090:PRO:O	1:C:1092:SER:N	2.49	0.41
1:A:1155:ARG:HH11	1:A:1155:ARG:HD3	1.77	0.41
1:C:1031:LEU:HD13	1:C:1037:PHE:CZ	2.56	0.41
1:A:1025:ASN:HA	1:A:1028:THR:HB	2.03	0.41
1:A:1166:SER:O	1:A:1170:LEU:HB2	2.21	0.41
1:A:1167:PHE:HD1	2:A:1302:MC3:C13	2.33	0.41
1:A:1104:LEU:HA	1:A:1104:LEU:HD23	1.83	0.41
1:B:1174:MET:C	1:B:1176:LEU:N	2.74	0.41
1:D:1062:LEU:HA	1:D:1065:TYR:CD2	2.55	0.41
1:B:1049:ASN:HB2	1:B:1105:ARG:HH22	1.86	0.40
1:B:1046:THR:O	1:B:1050:GLN:HG3	2.20	0.40
1:B:1091:THR:HG23	1:B:1102:ARG:HH21	1.85	0.40
1:C:1041:PHE:O	1:C:1044:TYR:N	2.55	0.40
1:C:1164:GLY:HA2	4:C:1304:6UC:CBB	2.51	0.40
1:D:1118:LYS:HA	1:D:1121:SER:OG	2.20	0.40
1:D:1144:PHE:CD2	1:D:1201:PHE:CD1	3.04	0.40
1:B:1057:THR:HA	1:B:1060:ILE:HG12	2.02	0.40
1:C:1206:THR:O	1:C:1210:ILE:HG13	2.21	0.40
1:D:1131:LEU:HD23	1:D:1131:LEU:HA	1.82	0.40
1:A:1061:ILE:HD13	1:A:1061:ILE:HA	1.94	0.40
1:A:1083:VAL:HA	1:A:1086:ILE:HD12	2.03	0.40
1:A:1209:MET:O	1:A:1213:VAL:HG23	2.21	0.40
1:A:1085:ALA:O	1:A:1088:LEU:HB2	2.22	0.40
1:C:1089:VAL:HG12	1:C:1090:PRO:CD	2.42	0.40
1:A:1167:PHE:HB3	2:A:1302:MC3:H131	2.04	0.40
1:D:1173:VAL:O	1:D:1176:LEU:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/285 (76%)	213 (98%)	4 (2%)	0	100	100
1	B	217/285 (76%)	209 (96%)	8 (4%)	0	100	100
1	C	217/285 (76%)	207 (95%)	9 (4%)	1 (0%)	29	61
1	D	217/285 (76%)	206 (95%)	10 (5%)	1 (0%)	29	61
All	All	868/1140 (76%)	835 (96%)	31 (4%)	2 (0%)	47	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1092	SER
1	D	1002	TYR

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/264 (76%)	194 (96%)	8 (4%)	31	61
1	B	202/264 (76%)	190 (94%)	12 (6%)	19	49
1	C	202/264 (76%)	190 (94%)	12 (6%)	19	49
1	D	202/264 (76%)	190 (94%)	12 (6%)	19	49
All	All	808/1056 (76%)	764 (95%)	44 (5%)	22	53

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1028	THR
1	A	1040	SER
1	A	1046	THR
1	A	1111	THR
1	A	1117	ARG
1	A	1162	THR
1	A	1167	PHE
1	A	1205	VAL
1	B	1003	LEU
1	B	1033	THR
1	B	1035	LYS
1	B	1051	ILE
1	B	1054	THR
1	B	1069	ILE
1	B	1091	THR
1	B	1125	SER
1	B	1162	THR
1	B	1167	PHE
1	B	1187	LEU
1	B	1205	VAL
1	C	1068	ARG
1	C	1069	ILE
1	C	1083	VAL
1	C	1091	THR
1	C	1092	SER
1	C	1093	SER
1	C	1111	THR
1	C	1150	GLN
1	C	1166	SER
1	C	1167	PHE
1	C	1187	LEU
1	C	1206	THR
1	D	1028	THR
1	D	1033	THR
1	D	1049	ASN
1	D	1065	TYR
1	D	1095	PHE
1	D	1097	ILE
1	D	1117	ARG
1	D	1118	LYS
1	D	1167	PHE
1	D	1175	THR
1	D	1199	ILE

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Mol	Chain	Res	Type
1	D	1212	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1007	ASN
1	B	1150	GLN
1	D	1007	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
2	MC3	C	1302	-	9,9,45	1.10	1 (11%)	11,12,53	1.10	0
2	MC3	A	1301	-	20,20,45	1.36	2 (10%)	22,24,53	1.18	3 (13%)
2	MC3	D	1302	-	20,20,45	1.32	3 (15%)	22,24,53	1.41	2 (9%)
2	MC3	C	1306	-	5,5,45	0.35	0	4,4,53	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MC3	B	1303	-	5,5,45	0.52	0	4,4,53	0.19	0
2	MC3	D	1304	-	9,9,45	0.95	0	11,12,53	0.83	0
2	MC3	D	1303	-	9,9,45	1.09	1 (11%)	11,12,53	1.12	1 (9%)
2	MC3	C	1305	-	5,5,45	0.56	0	4,4,53	0.16	0
4	6UC	C	1304	-	31,31,31	4.14	13 (41%)	39,42,42	5.50	25 (64%)
2	MC3	C	1303	-	9,9,45	0.90	0	11,12,53	0.97	1 (9%)
2	MC3	A	1304	-	9,9,45	0.92	0	11,12,53	0.94	1 (9%)
2	MC3	B	1301	-	9,9,45	1.31	1 (11%)	11,12,53	1.45	2 (18%)
2	MC3	A	1303	-	9,9,45	1.02	1 (11%)	11,12,53	1.12	0
2	MC3	D	1305	-	5,5,45	0.59	0	4,4,53	0.36	0
2	MC3	B	1302	-	9,9,45	0.96	1 (11%)	11,12,53	0.74	0
2	MC3	A	1302	-	20,20,45	1.12	3 (15%)	22,24,53	1.08	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
2	MC3	C	1302	-	-	8/8/8/49	-
2	MC3	A	1301	-	-	15/22/22/49	-
2	MC3	D	1302	-	-	8/22/22/49	-
2	MC3	C	1306	-	-	2/3/3/49	-
2	MC3	B	1303	-	-	1/3/3/49	-
2	MC3	D	1304	-	-	5/8/8/49	-
2	MC3	D	1303	-	-	4/8/8/49	-
2	MC3	C	1305	-	-	2/3/3/49	-
4	6UC	C	1304	-	-	21/24/44/44	0/2/2/2
2	MC3	C	1303	-	-	2/8/8/49	-
2	MC3	A	1304	-	-	2/8/8/49	-
2	MC3	B	1301	-	-	1/8/8/49	-
2	MC3	A	1303	-	-	4/8/8/49	-
2	MC3	D	1305	-	-	2/3/3/49	-
2	MC3	B	1302	-	-	2/8/8/49	-
2	MC3	A	1302	-	-	12/22/22/49	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1304	6UC	CAW-NAP	11.70	1.56	1.37
4	C	1304	6UC	CAU-CAX	11.38	1.68	1.47
4	C	1304	6UC	CBA-CBB	9.69	1.67	1.53
4	C	1304	6UC	CAT-NAP	6.53	1.47	1.38
4	C	1304	6UC	OAS-CAV	5.30	1.43	1.33
4	C	1304	6UC	OAQ-CAU	4.89	1.44	1.33
4	C	1304	6UC	CAV-CAY	4.62	1.56	1.47
2	D	1302	MC3	O3-C11	3.20	1.42	1.33
2	A	1301	MC3	O3-C11	3.13	1.42	1.33
4	C	1304	6UC	CAC-CAT	3.09	1.55	1.49
2	A	1301	MC3	P-O4P	3.05	1.70	1.59
2	A	1302	MC3	O3-C11	2.93	1.41	1.33
2	D	1302	MC3	P-O4P	2.81	1.69	1.59
2	B	1301	MC3	P-O3P	2.75	1.69	1.60
2	C	1302	MC3	P-O3P	2.62	1.68	1.60
4	C	1304	6UC	CAK-CBA	2.56	1.43	1.39
2	A	1302	MC3	P-O4P	2.52	1.68	1.59
4	C	1304	6UC	CAT-CAX	-2.40	1.32	1.35
4	C	1304	6UC	CBB-CAX	2.26	1.55	1.52
2	D	1303	MC3	P-O3P	2.25	1.67	1.60
4	C	1304	6UC	O25-C24	2.08	1.47	1.42
2	A	1303	MC3	P-O3P	2.04	1.66	1.60
4	C	1304	6UC	OAE-CAU	-2.04	1.17	1.21
2	D	1302	MC3	P-O3P	2.02	1.67	1.59
2	A	1302	MC3	P-O3P	2.00	1.67	1.59
2	B	1302	MC3	P-O3P	2.00	1.66	1.60

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1304	6UC	CAT-NAP-CAW	-26.15	100.66	122.43
4	C	1304	6UC	CBA-CBB-CAX	7.23	125.93	111.05
4	C	1304	6UC	CAC-CAT-CAX	-6.86	120.76	127.62
4	C	1304	6UC	OAS-CAV-CAY	5.89	122.81	112.31
4	C	1304	6UC	CAY-CAW-NAP	-5.86	114.31	120.55
4	C	1304	6UC	CAU-CAX-CAT	-5.74	109.27	122.40
4	C	1304	6UC	BRAG-CAZ-CAJ	-5.07	107.93	117.81
4	C	1304	6UC	C24-CAW-NAP	5.00	123.37	115.49
2	D	1302	MC3	O3-C11-C12	4.87	127.20	111.91
4	C	1304	6UC	CBB-CAX-CAT	-4.57	115.55	120.85
4	C	1304	6UC	CAB-OAQ-CAU	4.53	124.44	115.86
4	C	1304	6UC	OAQ-CAU-CAX	4.51	120.33	112.30
4	C	1304	6UC	BRAG-CAZ-CBA	4.38	128.76	120.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1304	6UC	CBB-CAX-CAU	4.08	127.05	117.15
4	C	1304	6UC	OAF-CAV-CAY	-4.05	116.82	125.20
4	C	1304	6UC	CAK-CBA-CAZ	-4.04	111.65	116.79
4	C	1304	6UC	CBA-CBB-CAY	-3.95	102.90	111.05
4	C	1304	6UC	CAX-CAT-NAP	-3.95	115.99	119.27
2	B	1301	MC3	O3P-P-O1P	3.66	116.75	106.47
4	C	1304	6UC	CBB-CAY-CAW	-3.54	116.84	121.53
4	C	1304	6UC	CAI-CAK-CBA	3.51	125.47	121.01
2	A	1302	MC3	O3-C11-C12	3.32	122.31	111.91
4	C	1304	6UC	CAC-CAT-NAP	3.11	117.14	113.45
2	A	1301	MC3	O3-C11-C12	3.00	121.31	111.91
2	D	1302	MC3	O3-C11-O11	-2.88	116.32	123.59
4	C	1304	6UC	CAL-OAS-CAV	2.79	121.44	116.50
2	A	1301	MC3	O3-C11-O11	-2.56	117.14	123.59
4	C	1304	6UC	OAQ-CAU-OAE	-2.54	118.64	123.53
4	C	1304	6UC	CAK-CBA-CBB	-2.42	114.89	119.44
4	C	1304	6UC	CBB-CAY-CAV	2.31	122.77	117.15
2	A	1301	MC3	O3P-P-O1P	-2.29	100.11	109.07
2	A	1304	MC3	O2P-P-O3P	2.22	112.63	106.73
2	D	1303	MC3	O3-C3-C2	2.21	120.81	110.20
2	C	1303	MC3	O2P-P-O3P	2.19	112.55	106.73
4	C	1304	6UC	OAE-CAU-CAX	-2.13	120.79	125.20
2	B	1301	MC3	P-O3P-C1	2.08	124.02	118.30

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1302	MC3	O3P-C1-C2-C3
2	C	1302	MC3	C1-O3P-P-O1P
2	C	1302	MC3	C1-O3P-P-O2P
2	C	1302	MC3	C1-O3P-P-O4P
2	A	1301	MC3	C1-C2-C3-O3
2	A	1301	MC3	C1-O3P-P-O1P
2	A	1301	MC3	C1-O3P-P-O2P
2	A	1301	MC3	C1-O3P-P-O4P
2	D	1304	MC3	C1-O3P-P-O2P
2	D	1304	MC3	C1-O3P-P-O4P
2	D	1303	MC3	C1-C2-C3-O3
4	C	1304	6UC	OAF-CAV-CAY-CAW
4	C	1304	6UC	O25-C24-CAW-CAY
4	C	1304	6UC	O25-C24-CAW-NAP

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Mol	Chain	Res	Type	Atoms
4	C	1304	6UC	C26-C27-N28-C21
2	C	1303	MC3	C1-C2-C3-O3
2	C	1303	MC3	O2-C2-C3-O3
2	B	1301	MC3	C2-C1-O3P-P
2	A	1303	MC3	C1-C2-C3-O3
2	B	1302	MC3	O3P-C1-C2-O2
2	A	1302	MC3	C1-O3P-P-O1P
2	A	1302	MC3	C1-O3P-P-O4P
4	C	1304	6UC	CAX-CAU-OAQ-CAB
4	C	1304	6UC	CAY-CAV-OAS-CAL
4	C	1304	6UC	OAS-CAV-CAY-CAW
2	A	1301	MC3	O11-C11-O3-C3
4	C	1304	6UC	OAE-CAU-OAQ-CAB
4	C	1304	6UC	OAF-CAV-OAS-CAL
2	A	1301	MC3	C12-C11-O3-C3
2	C	1302	MC3	O3P-C1-C2-O2
2	A	1301	MC3	O2-C2-C3-O3
2	C	1306	MC3	C32-C33-C34-C35
2	A	1304	MC3	O3P-C1-C2-C3
2	A	1302	MC3	C12-C11-O3-C3
4	C	1304	6UC	C26-C27-N28-C22
2	A	1304	MC3	O3P-C1-C2-O2
2	A	1302	MC3	O3P-C1-C2-O2
2	A	1301	MC3	C11-C12-C13-C14
2	A	1302	MC3	O11-C11-O3-C3
2	D	1304	MC3	O3P-C1-C2-O2
4	C	1304	6UC	CAK-CBA-CBB-CAY
2	D	1304	MC3	O3P-C1-C2-C3
2	A	1301	MC3	C12-C13-C14-C15
2	D	1302	MC3	O3P-C1-C2-O2
2	D	1302	MC3	C13-C14-C15-C16
2	C	1302	MC3	C1-C2-C3-O3
2	D	1302	MC3	C15-C16-C17-C18
2	A	1301	MC3	C14-C15-C16-C17
4	C	1304	6UC	CAW-C24-O25-C26
4	C	1304	6UC	OAF-CAV-CAY-CBB
4	C	1304	6UC	CAZ-CBA-CBB-CAX
2	B	1303	MC3	C32-C33-C34-C35
2	D	1303	MC3	O2-C2-C3-O3
2	B	1302	MC3	O3P-C1-C2-C3
4	C	1304	6UC	OAS-CAV-CAY-CBB
2	A	1302	MC3	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
2	D	1305	MC3	C33-C34-C35-C36
2	C	1302	MC3	O2-C2-C3-O3
2	A	1303	MC3	O2-C2-C3-O3
2	A	1301	MC3	C16-C17-C18-C19
2	D	1304	MC3	C1-O3P-P-O1P
2	D	1305	MC3	C32-C33-C34-C35
2	C	1306	MC3	C33-C34-C35-C36
2	A	1301	MC3	C4-O4P-P-O1P
2	A	1302	MC3	C4-O4P-P-O1P
2	D	1302	MC3	O3P-C1-C2-C3
4	C	1304	6UC	CAZ-CBA-CBB-CAY
2	A	1303	MC3	O3P-C1-C2-O2
4	C	1304	6UC	CAK-CBA-CBB-CAX
2	C	1305	MC3	C31-C32-C33-C34
2	D	1302	MC3	C4-O4P-P-O1P
4	C	1304	6UC	OAE-CAU-CAX-CBB
2	A	1302	MC3	C12-C13-C14-C15
2	C	1302	MC3	C2-C1-O3P-P
4	C	1304	6UC	OAQ-CAU-CAX-CBB
2	C	1305	MC3	C32-C33-C34-C35
2	D	1303	MC3	C1-O3P-P-O1P
2	A	1301	MC3	C13-C14-C15-C16
2	D	1302	MC3	C11-C12-C13-C14
2	A	1302	MC3	C14-C15-C16-C17
2	A	1302	MC3	C16-C17-C18-C19
2	D	1302	MC3	C14-C15-C16-C17
4	C	1304	6UC	CAA-CAL-OAS-CAV
2	A	1302	MC3	O3P-C1-C2-C3
2	D	1303	MC3	C1-O3P-P-O2P
2	A	1303	MC3	C1-O3P-P-O4P
2	A	1301	MC3	O3-C11-C12-C13
2	A	1301	MC3	O11-C11-C12-C13
2	D	1302	MC3	C1-O3P-P-O1P
2	A	1302	MC3	C11-C12-C13-C14
4	C	1304	6UC	OAQ-CAU-CAX-CAT

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	MC3	1	0
4	C	1304	6UC	2	0

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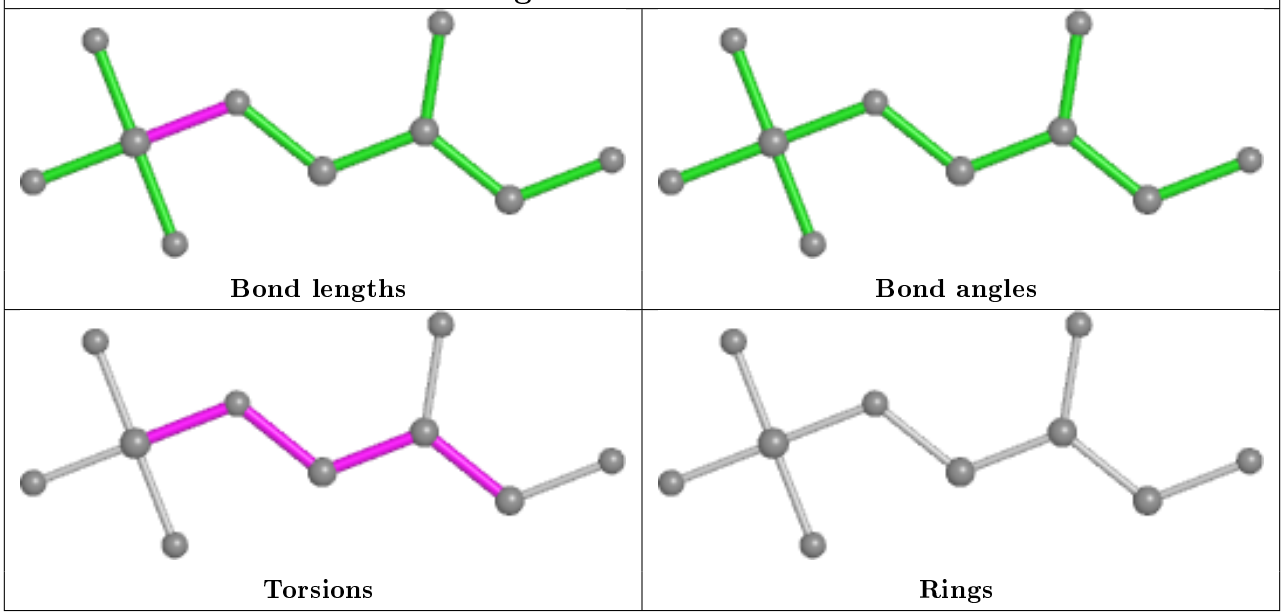
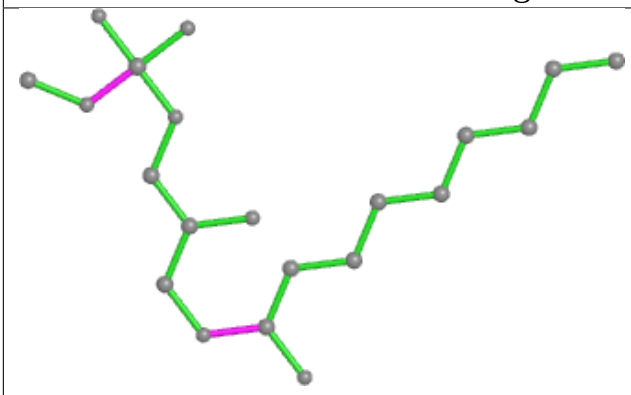
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1304	MC3	1	0
2	B	1301	MC3	1	0
2	A	1303	MC3	2	0
2	B	1302	MC3	1	0
2	A	1302	MC3	3	0

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.

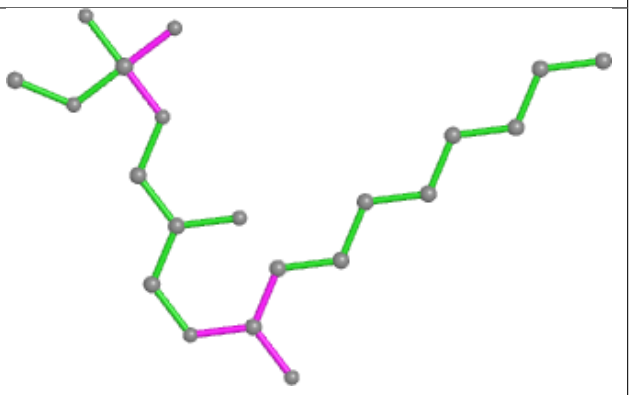
Ligand MC3 C 1302



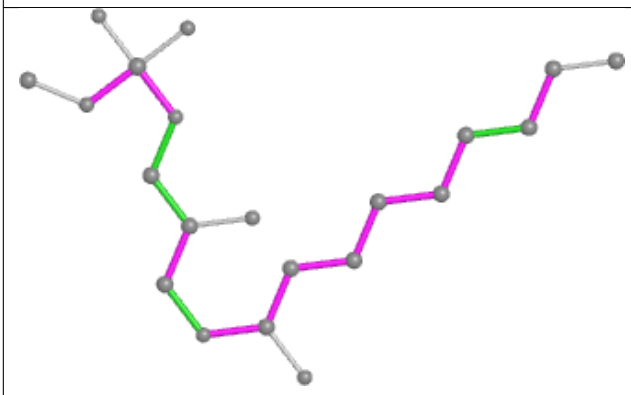
Ligand MC3 A 1301



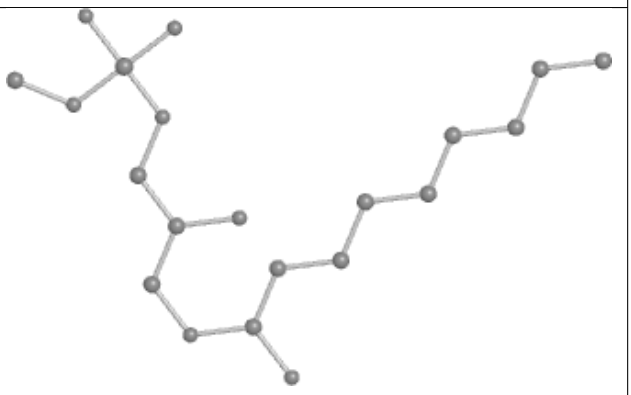
Bond lengths



Bond angles

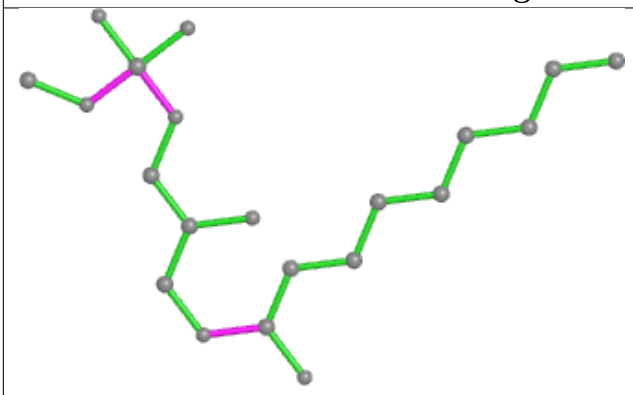


Torsions

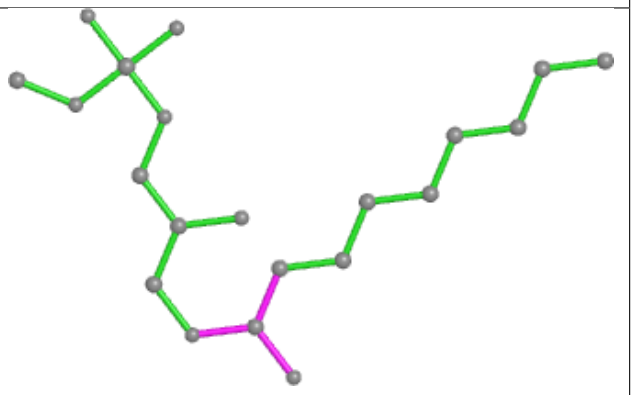


Rings

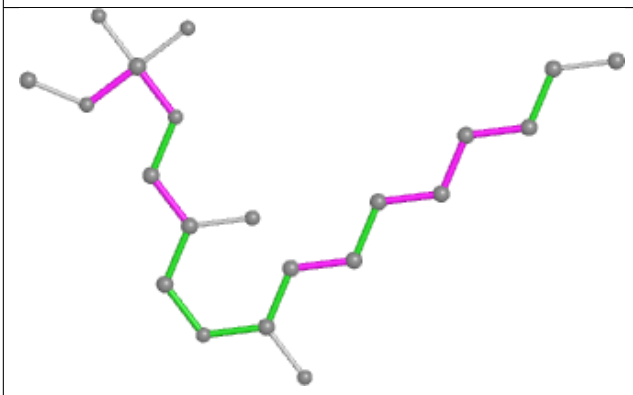
Ligand MC3 D 1302



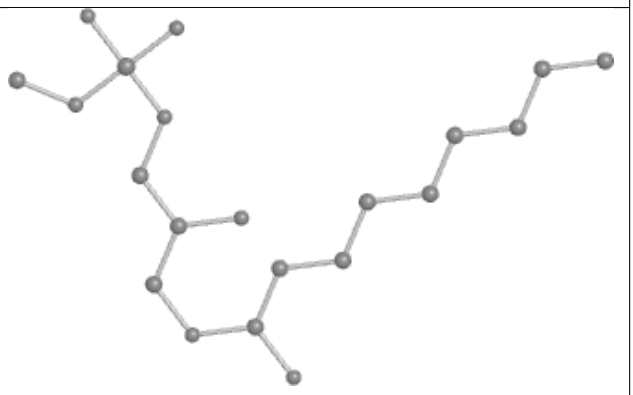
Bond lengths



Bond angles

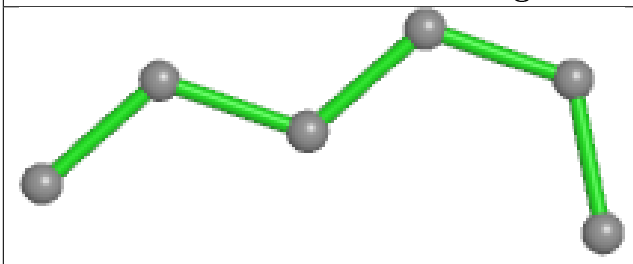


Torsions

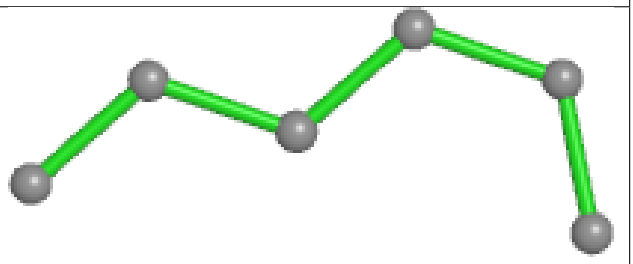


Rings

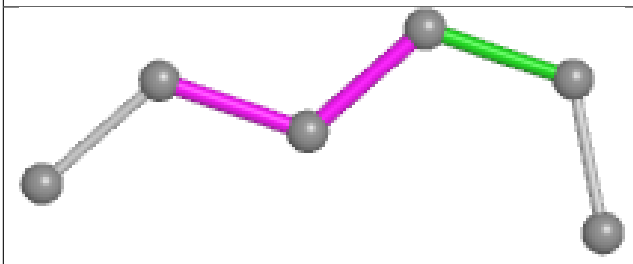
Ligand MC3 C 1306



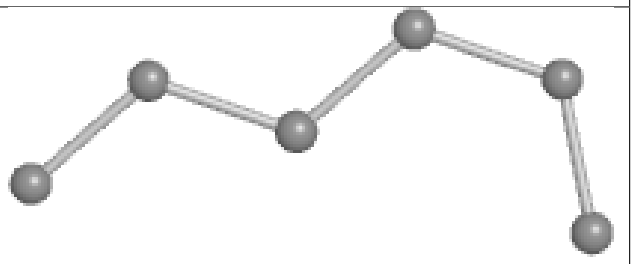
Bond lengths



Bond angles

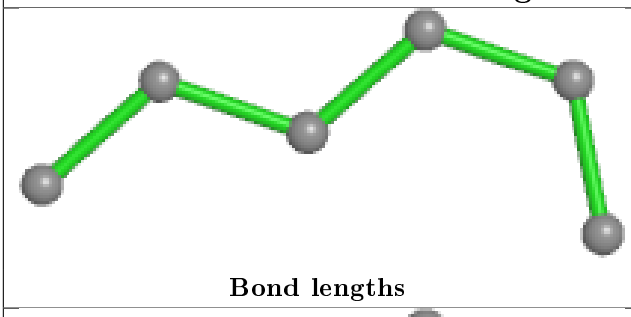


Torsions

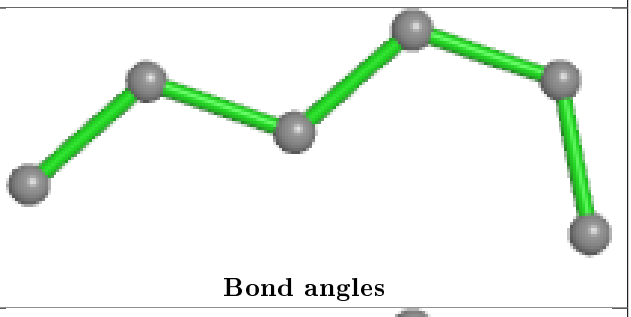


Rings

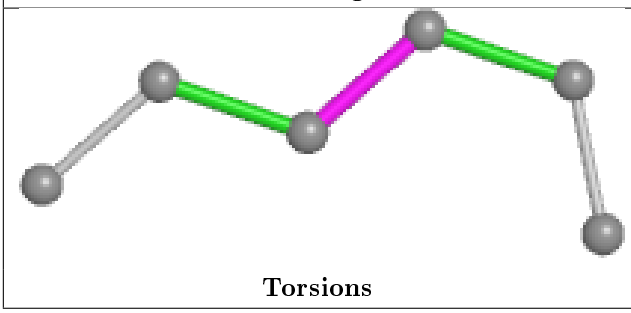
Ligand MC3 B 1303



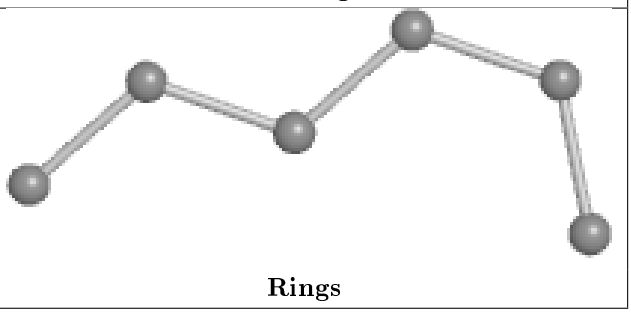
Bond lengths



Bond angles

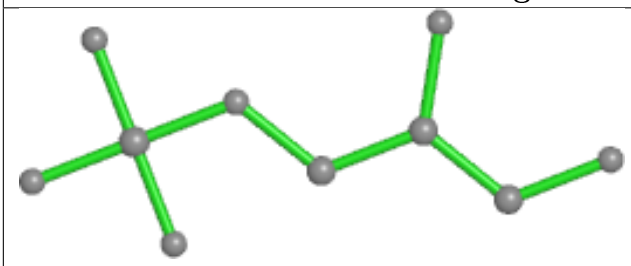


Torsions

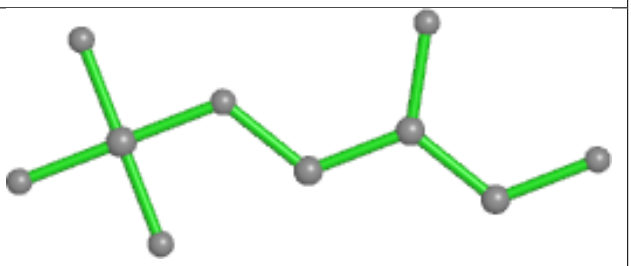


Rings

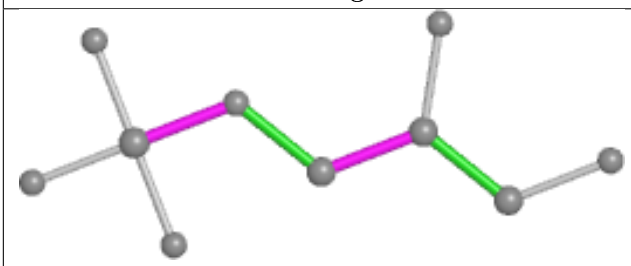
Ligand MC3 D 1304



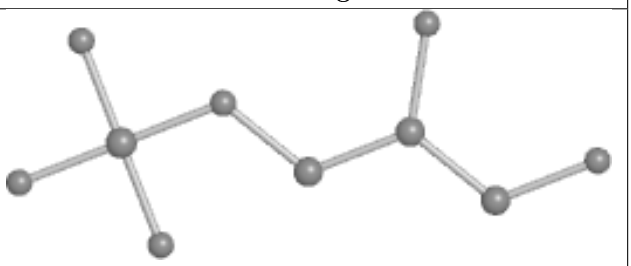
Bond lengths



Bond angles

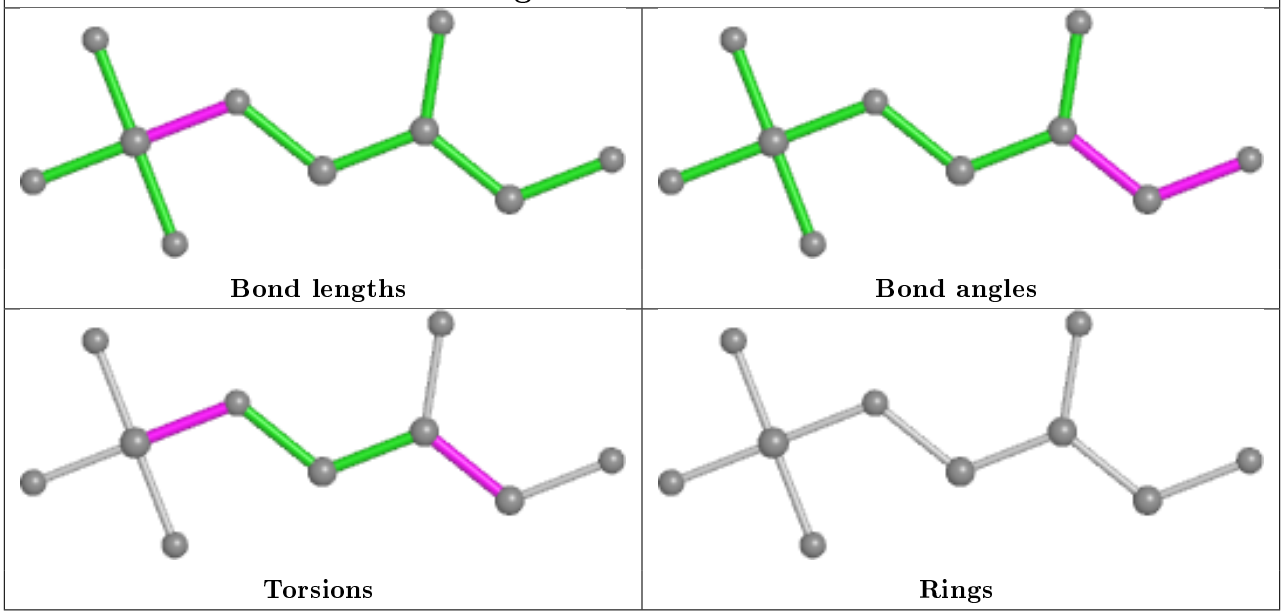


Torsions

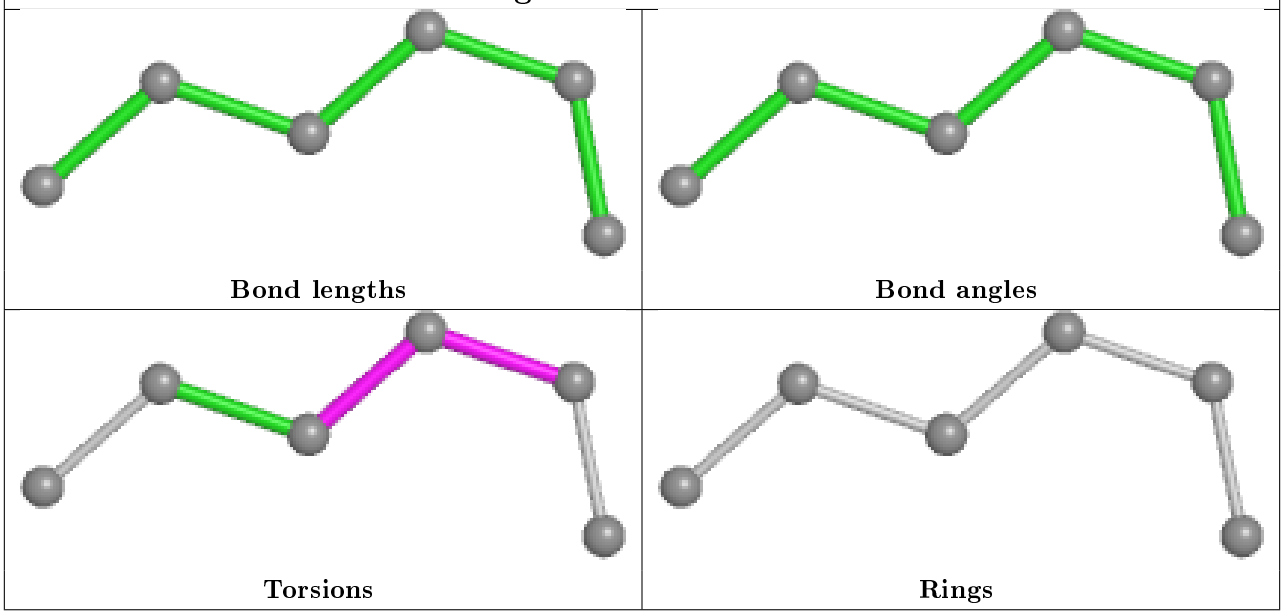


Rings

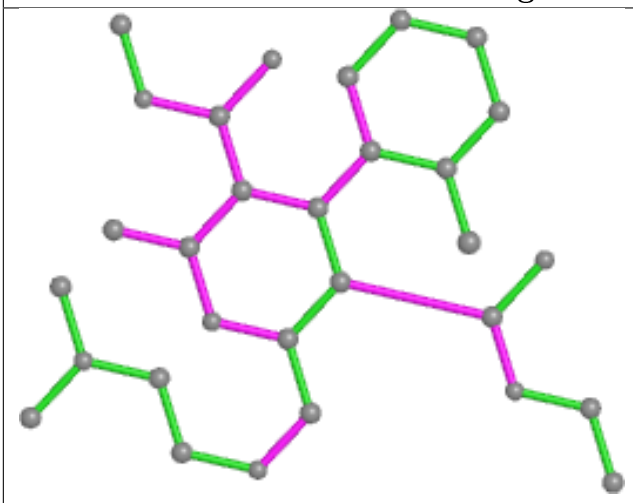
Ligand MC3 D 1303



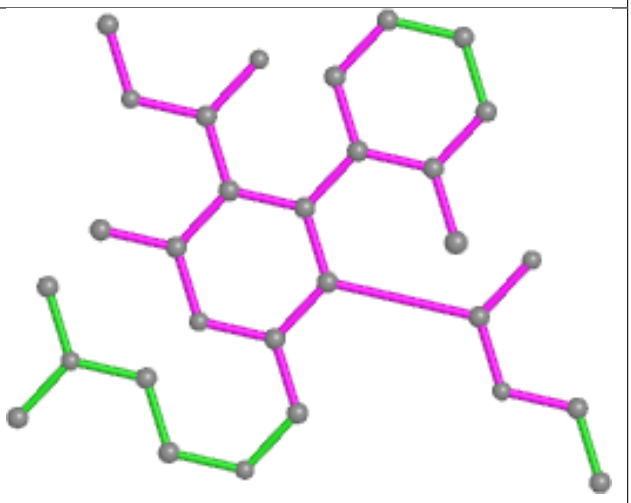
Ligand MC3 C 1305



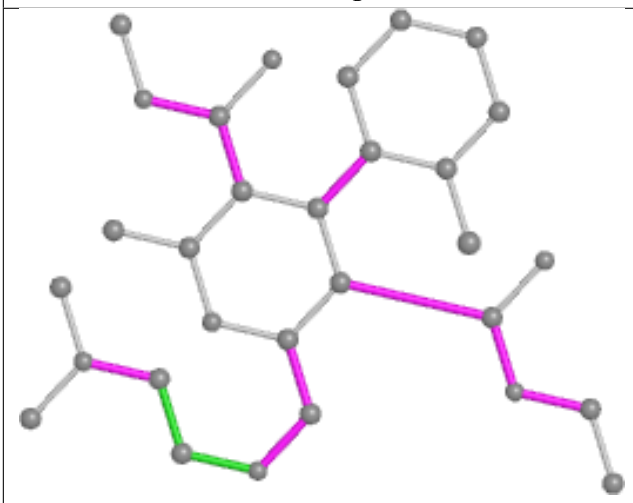
Ligand 6UC C 1304



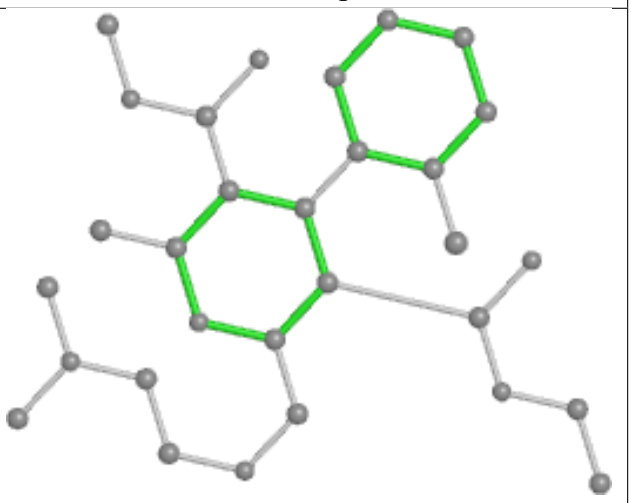
Bond lengths



Bond angles

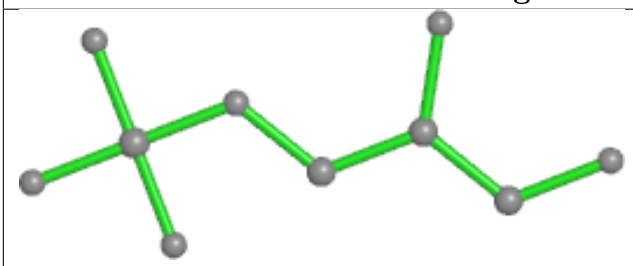


Torsions

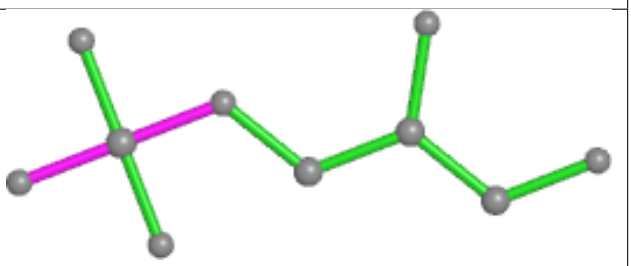


Rings

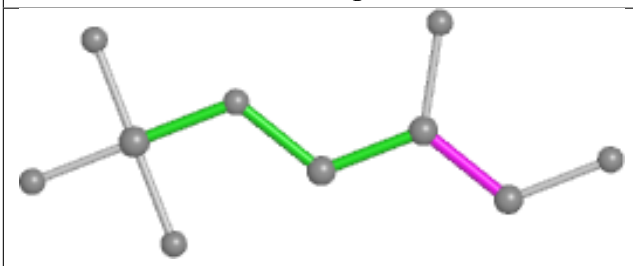
Ligand MC3 C 1303



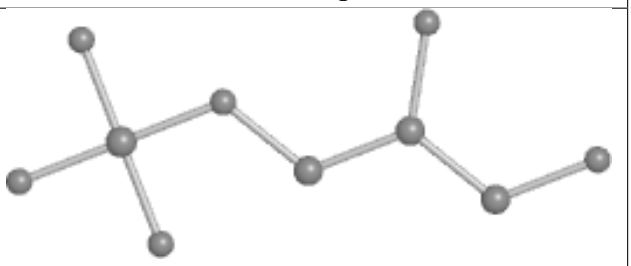
Bond lengths



Bond angles

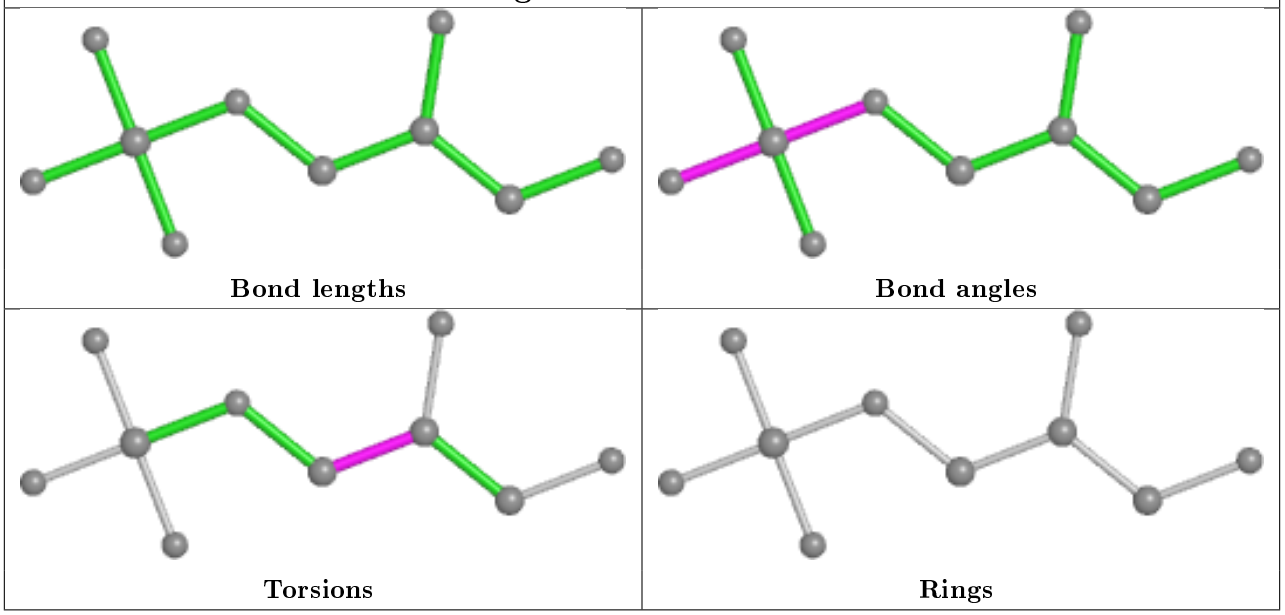


Torsions

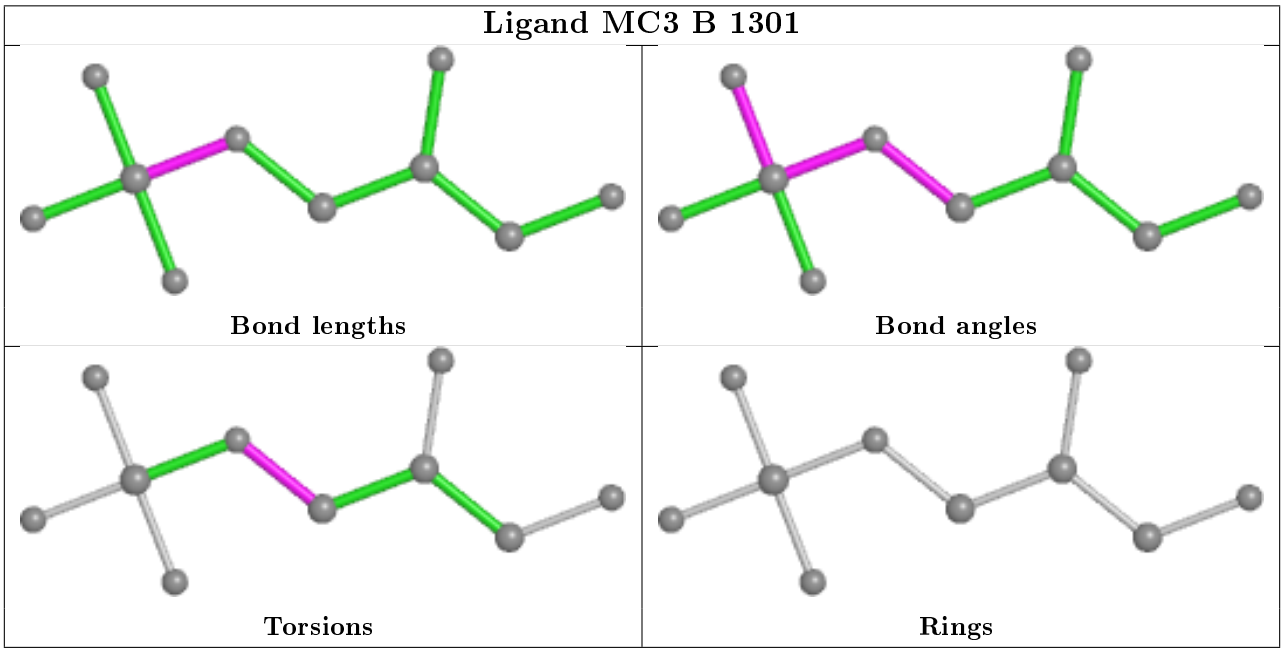


Rings

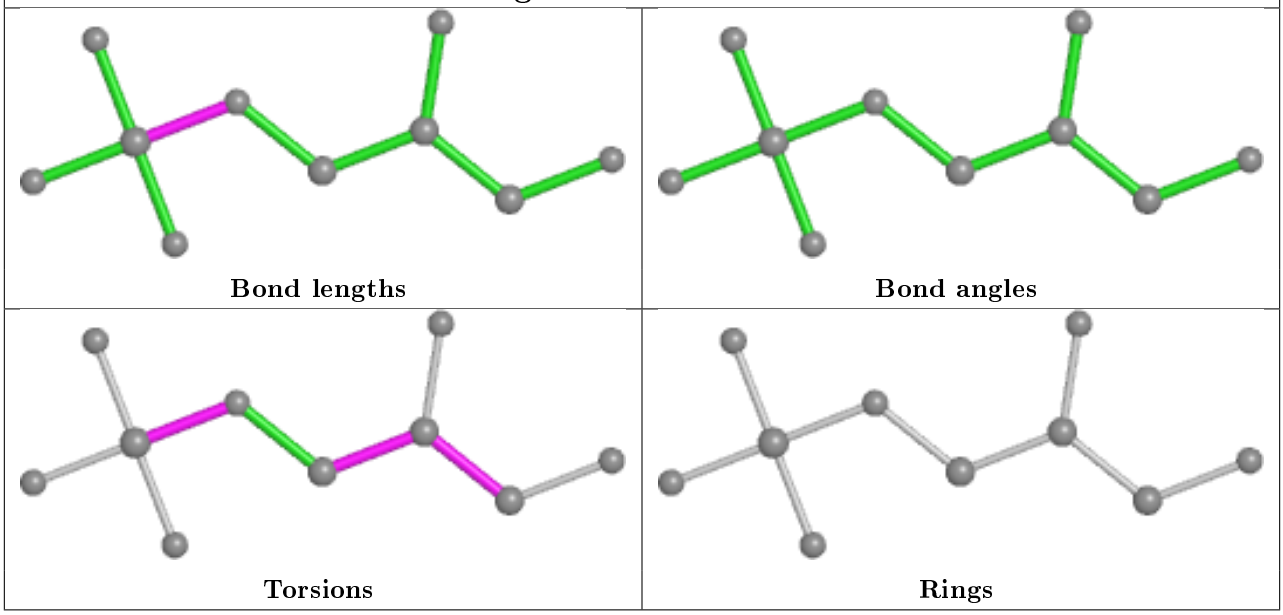
Ligand MC3 A 1304



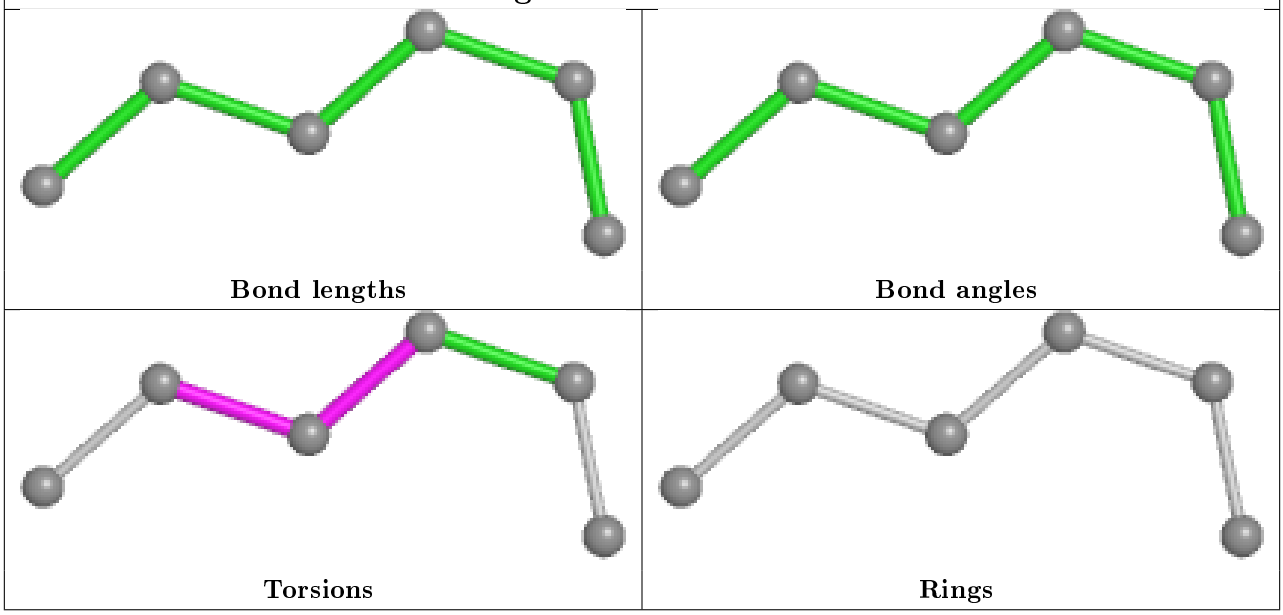
Ligand MC3 B 1301



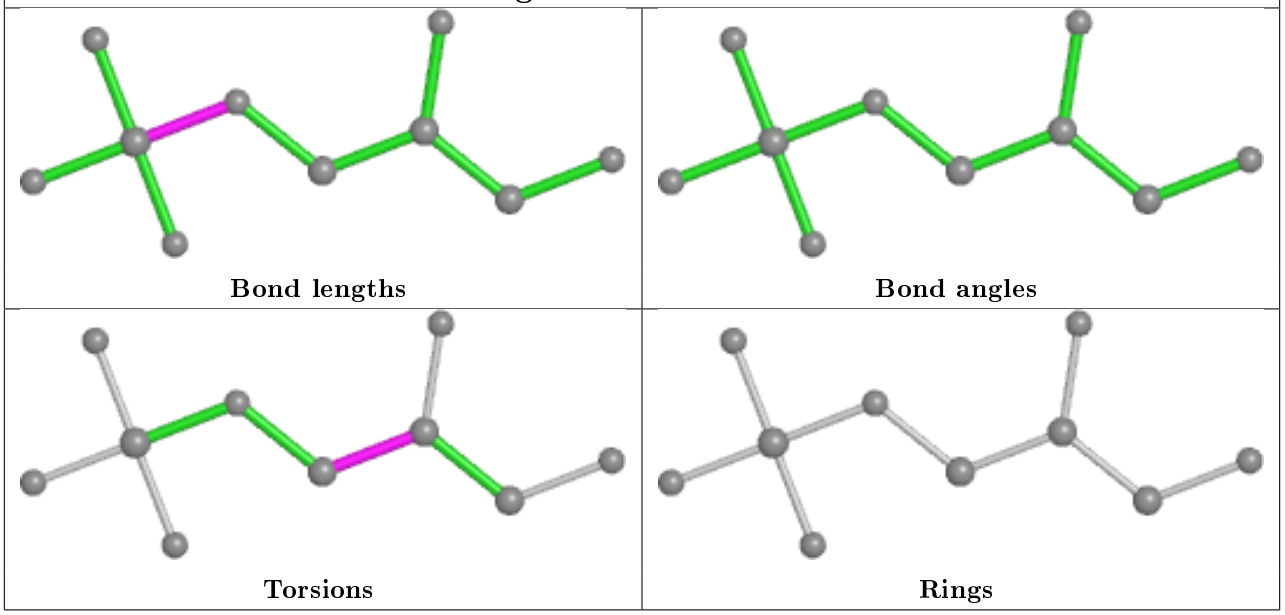
Ligand MC3 A 1303



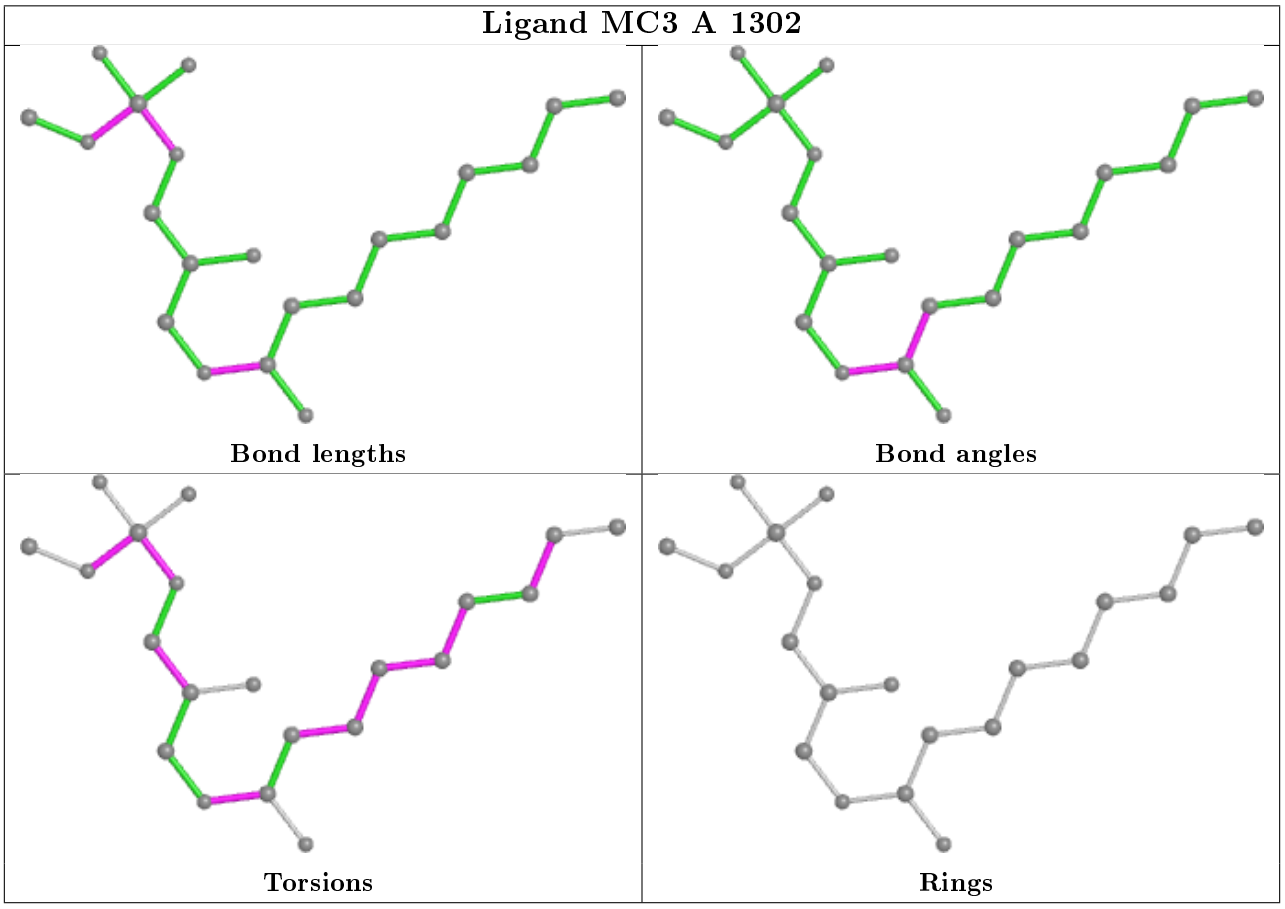
Ligand MC3 D 1305



Ligand MC3 B 1302



Ligand MC3 A 1302



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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.

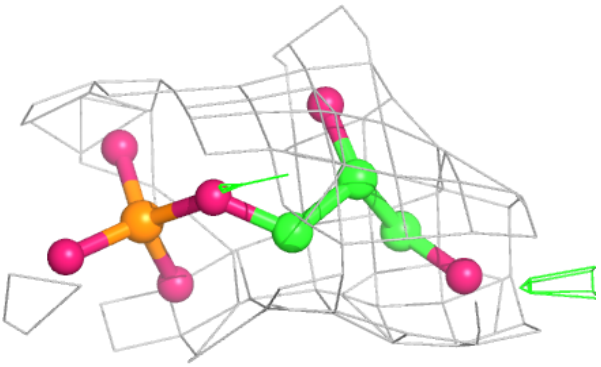
6.4 Ligands

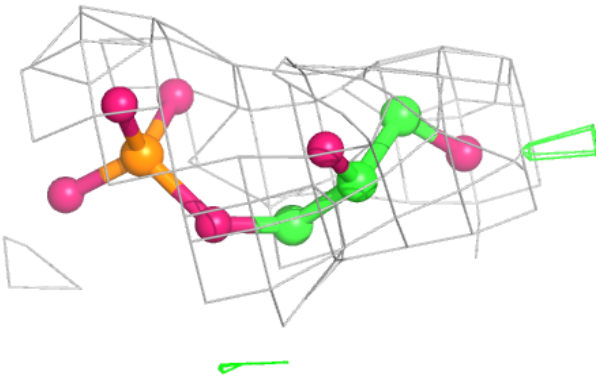
Unable to reproduce the depositors R factor - this section is therefore empty.

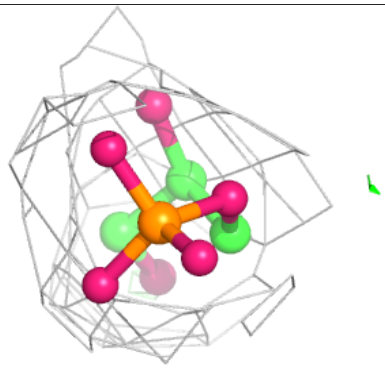
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MC3 C 1302:

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

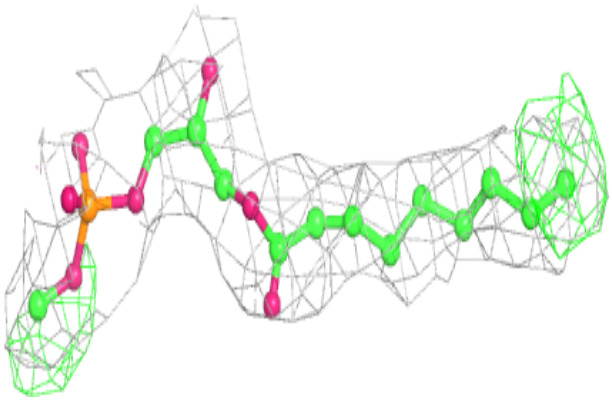


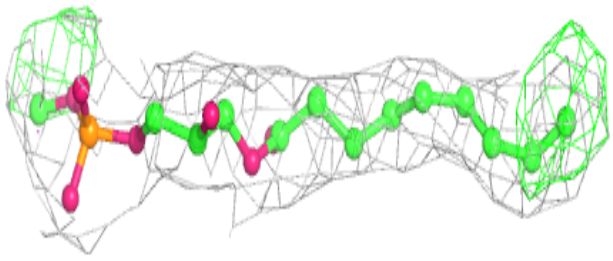


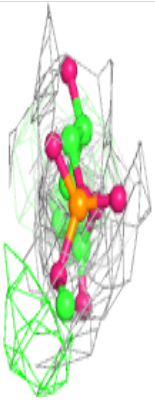


Electron density around MC3 A 1301:

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

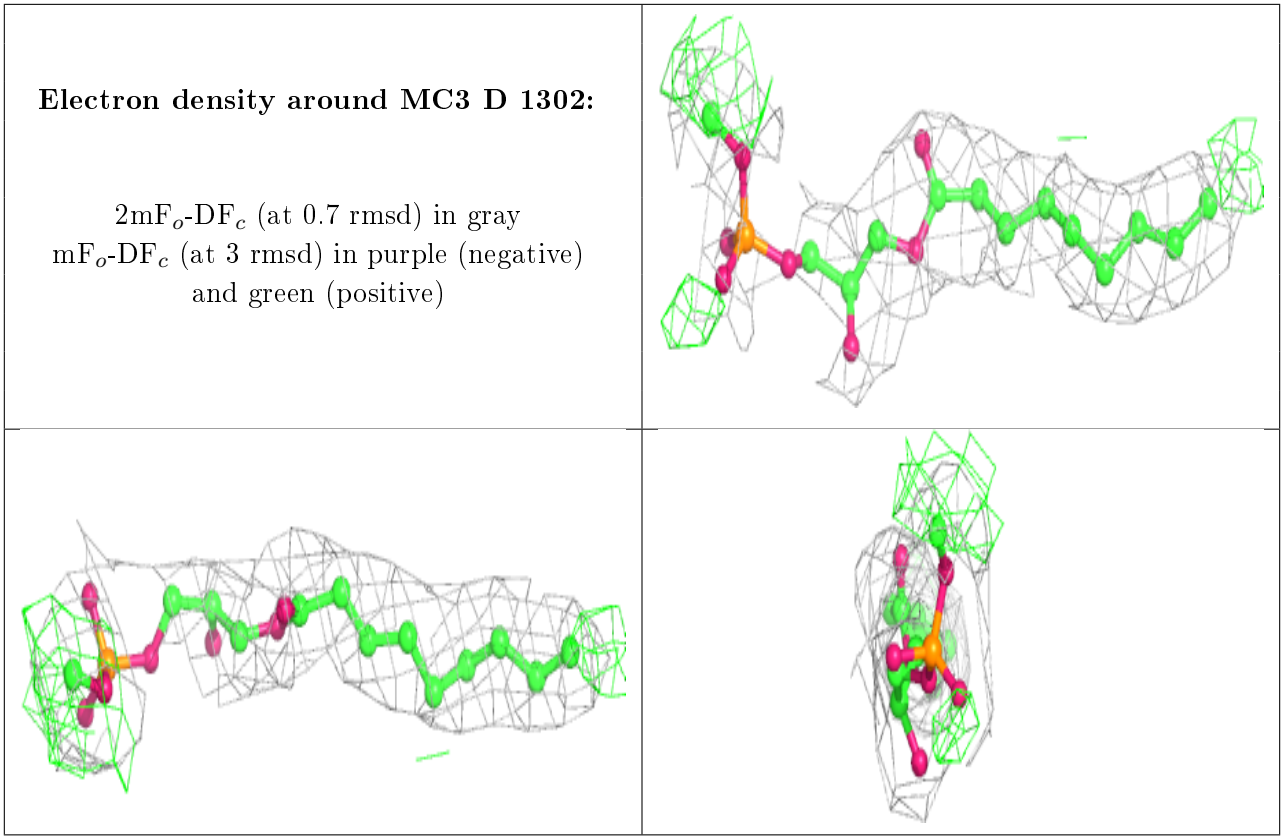






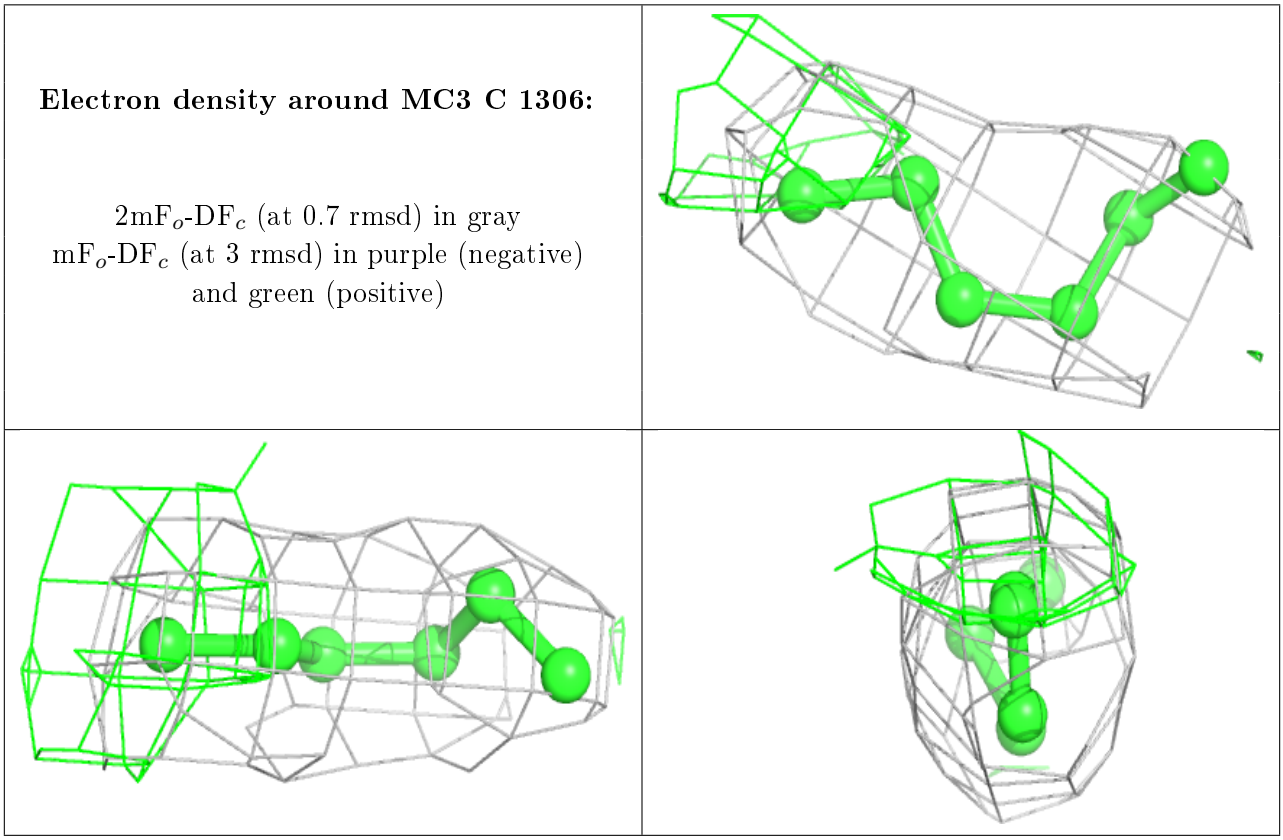
Electron density around MC3 D 1302:

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



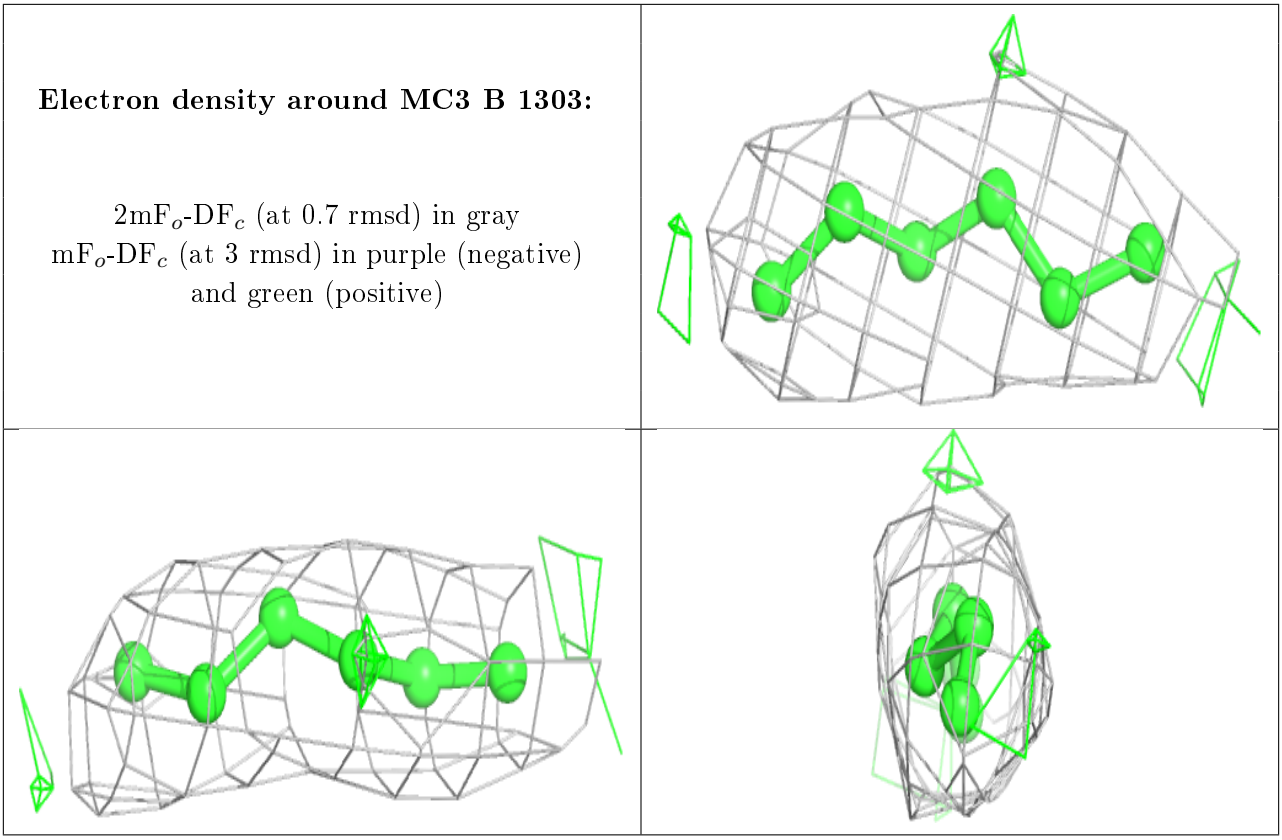
Electron density around MC3 C 1306:

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



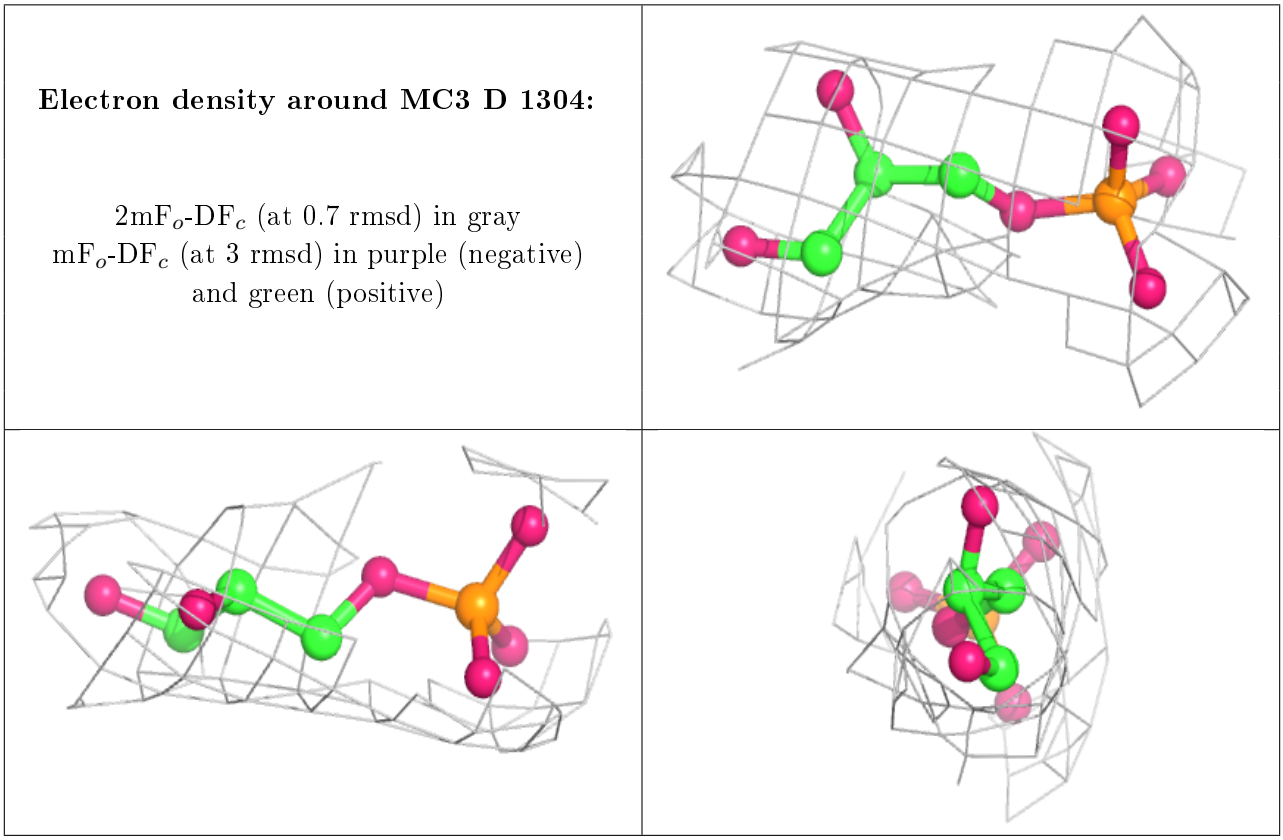
Electron density around MC3 B 1303:

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



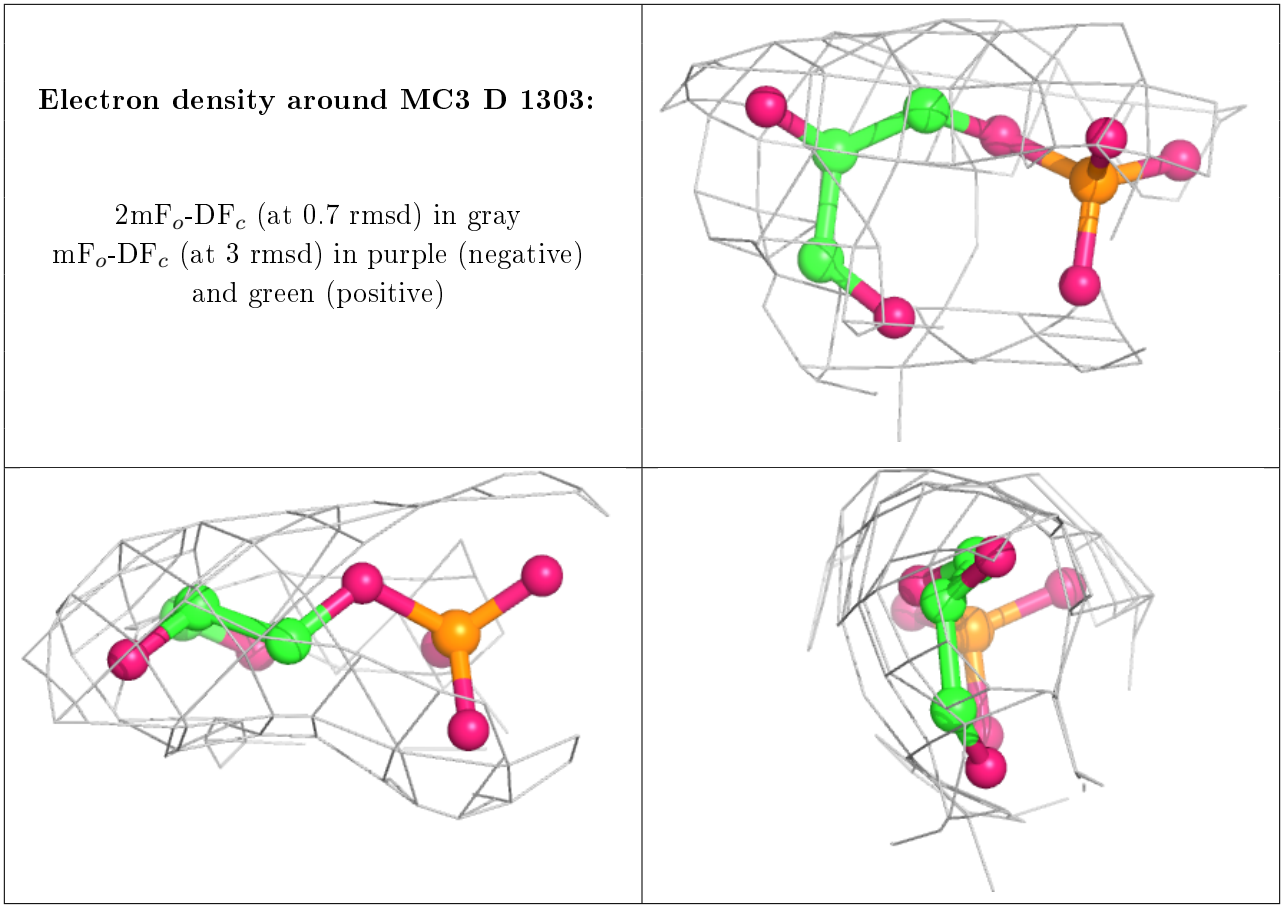
Electron density around MC3 D 1304:

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



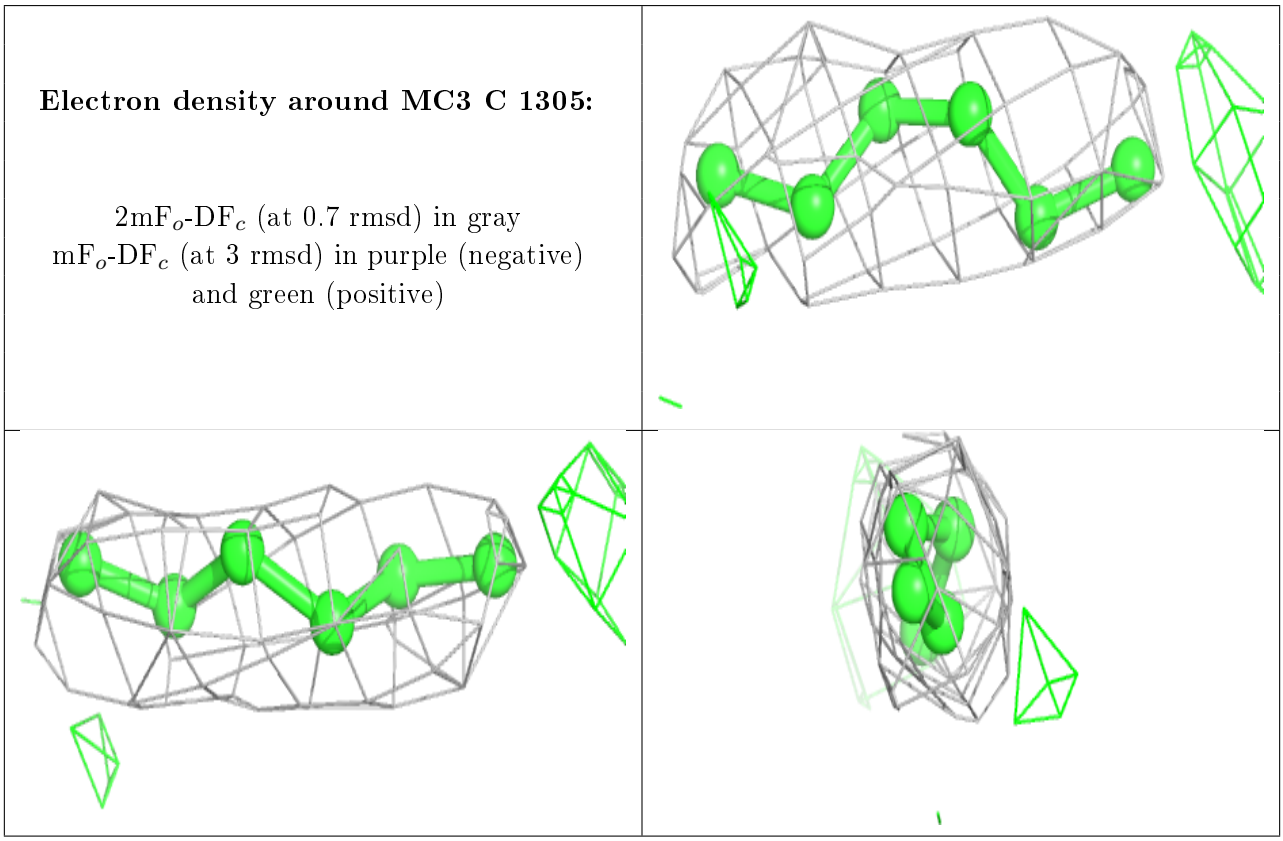
Electron density around MC3 D 1303:

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



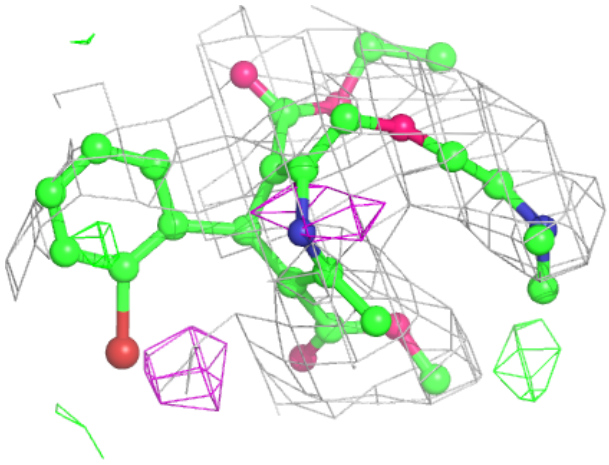
Electron density around MC3 C 1305:

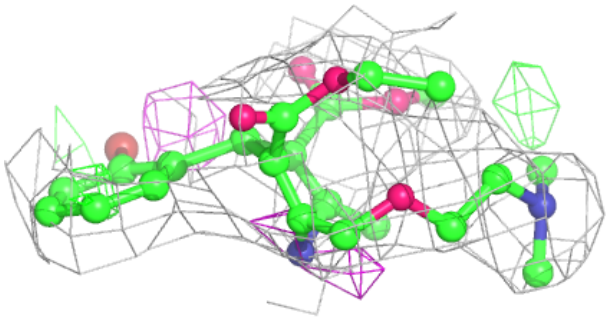
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

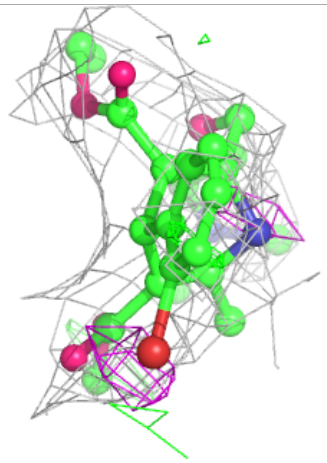


Electron density around 6UC C 1304:

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

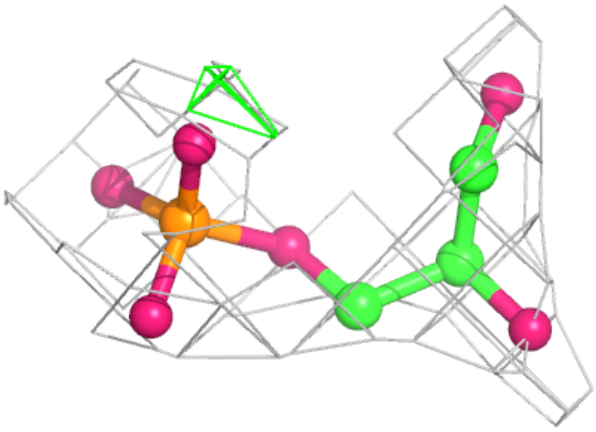


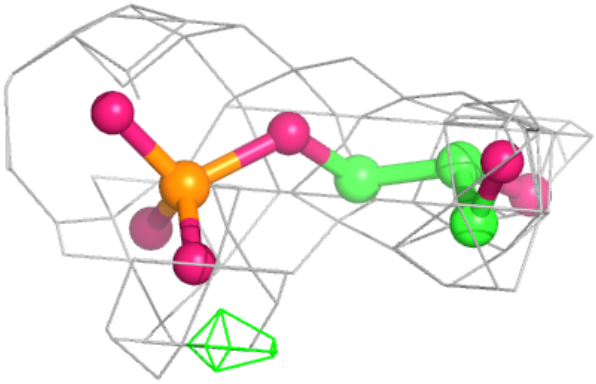


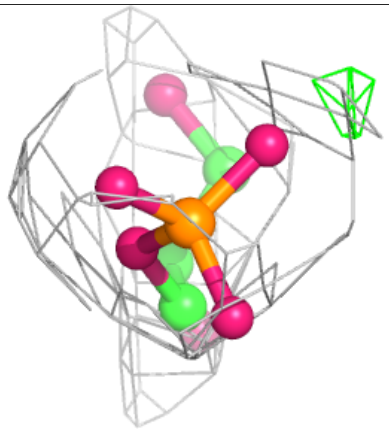


Electron density around MC3 C 1303:

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

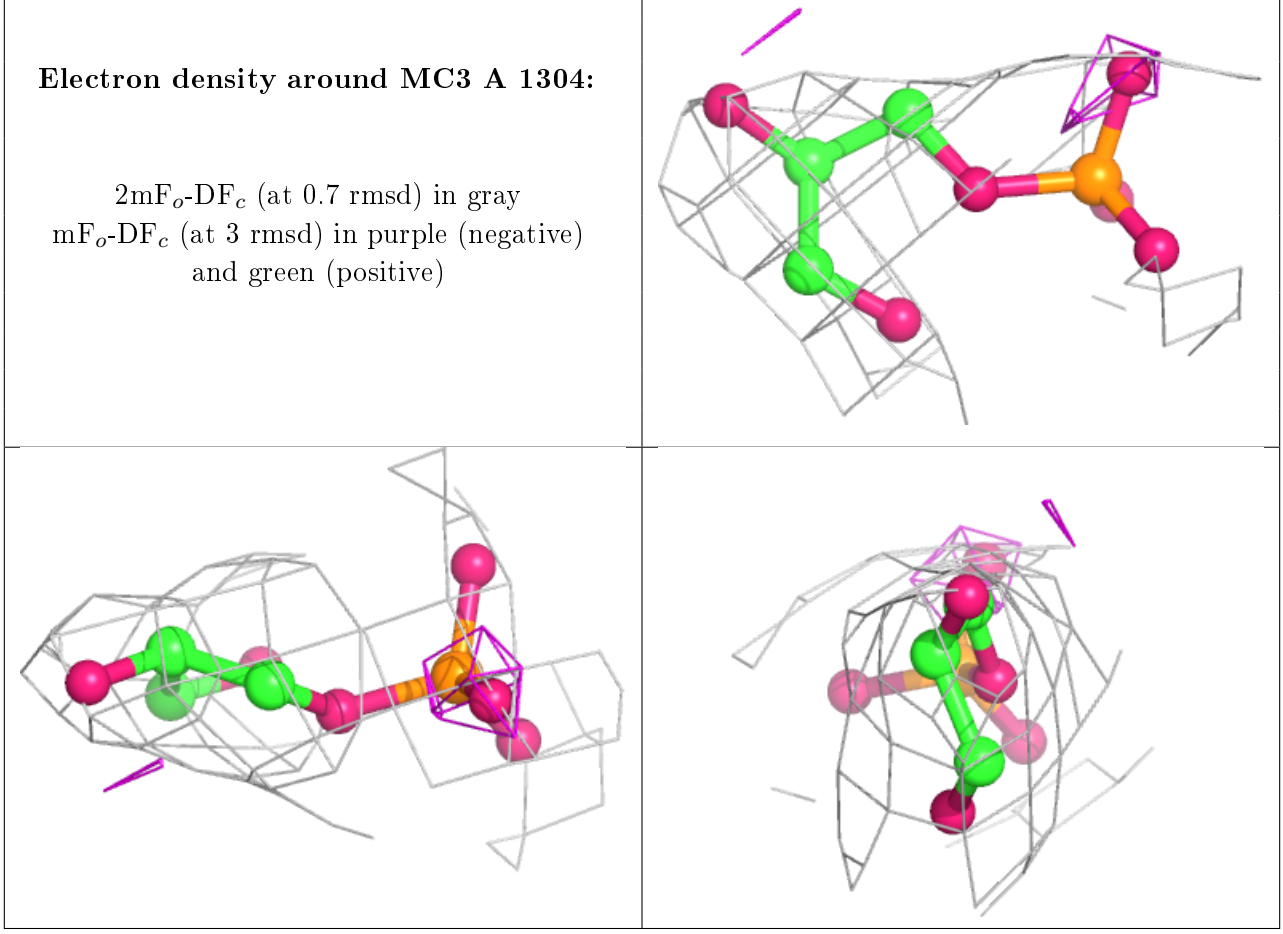






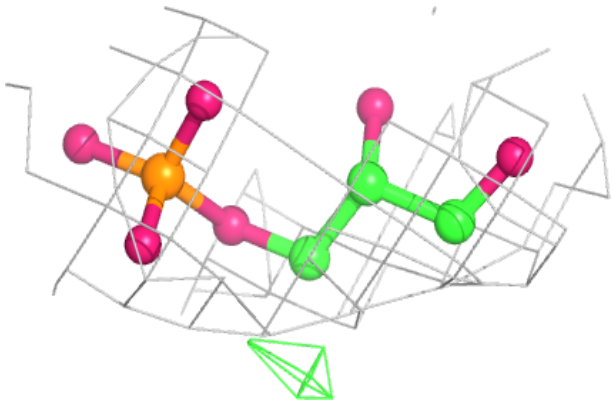
Electron density around MC3 A 1304:

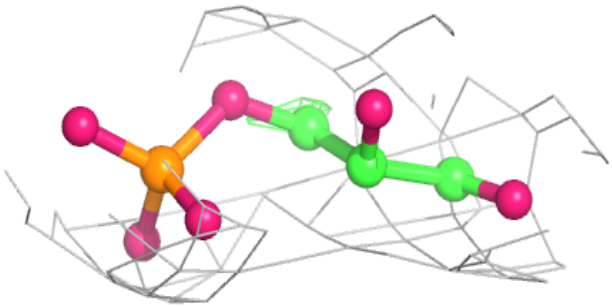
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

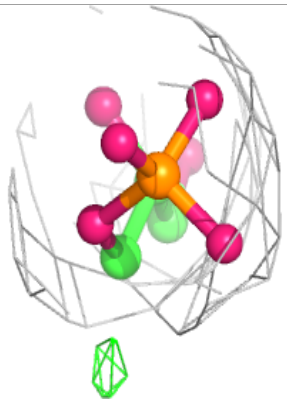


Electron density around MC3 B 1301:

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

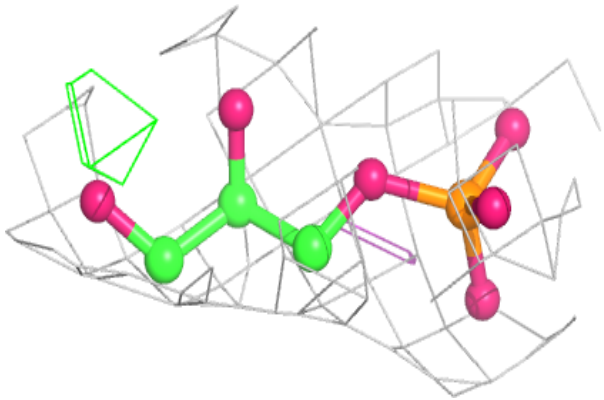


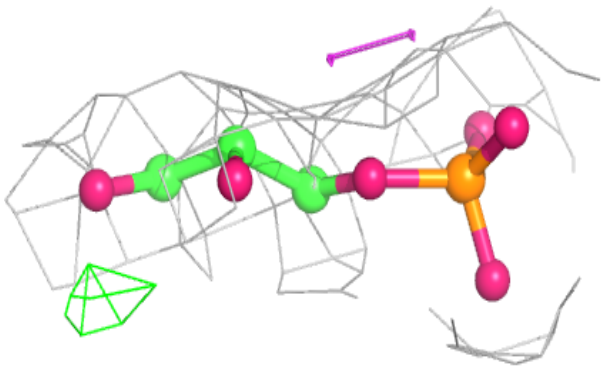


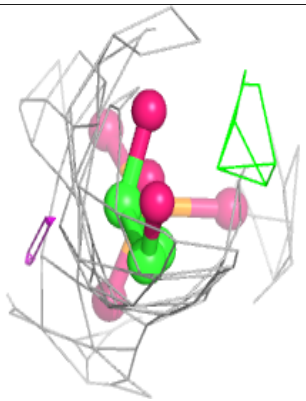


Electron density around MC3 A 1303:

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

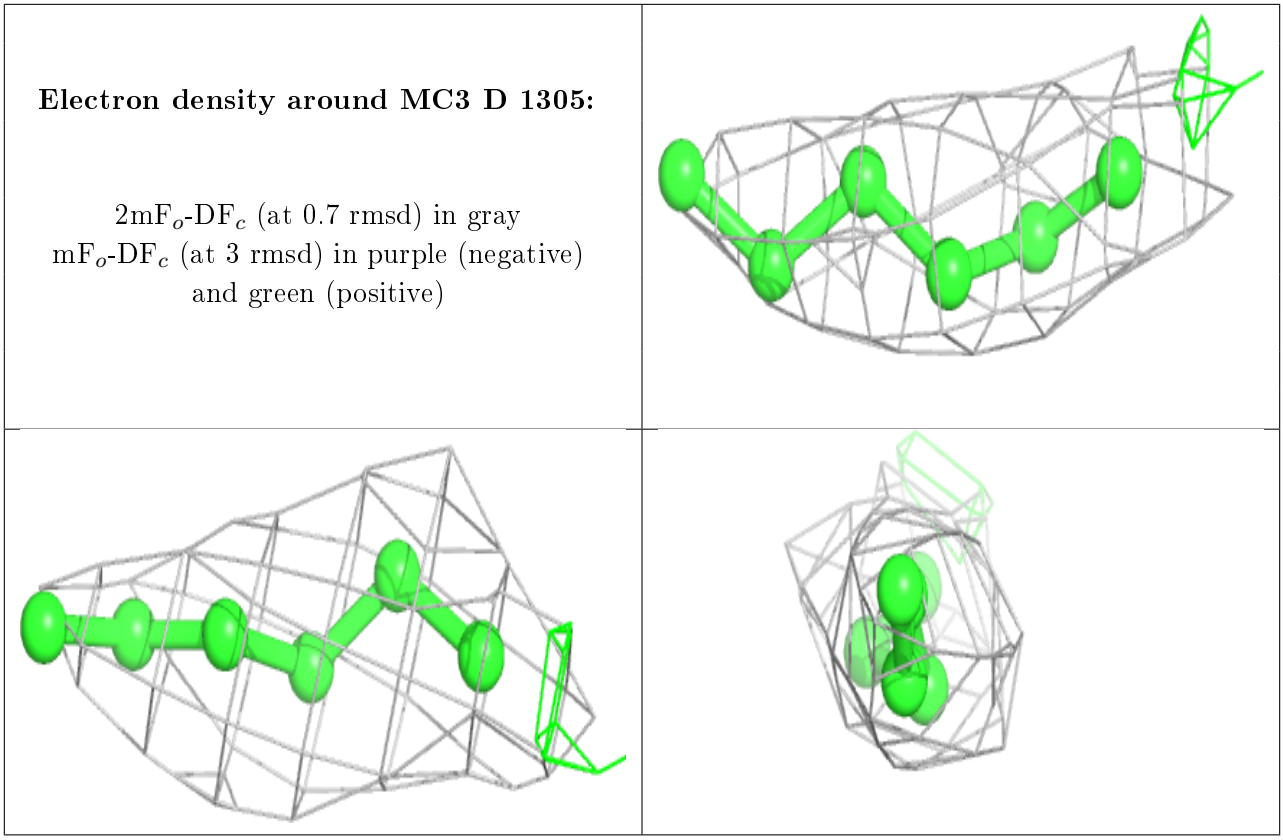






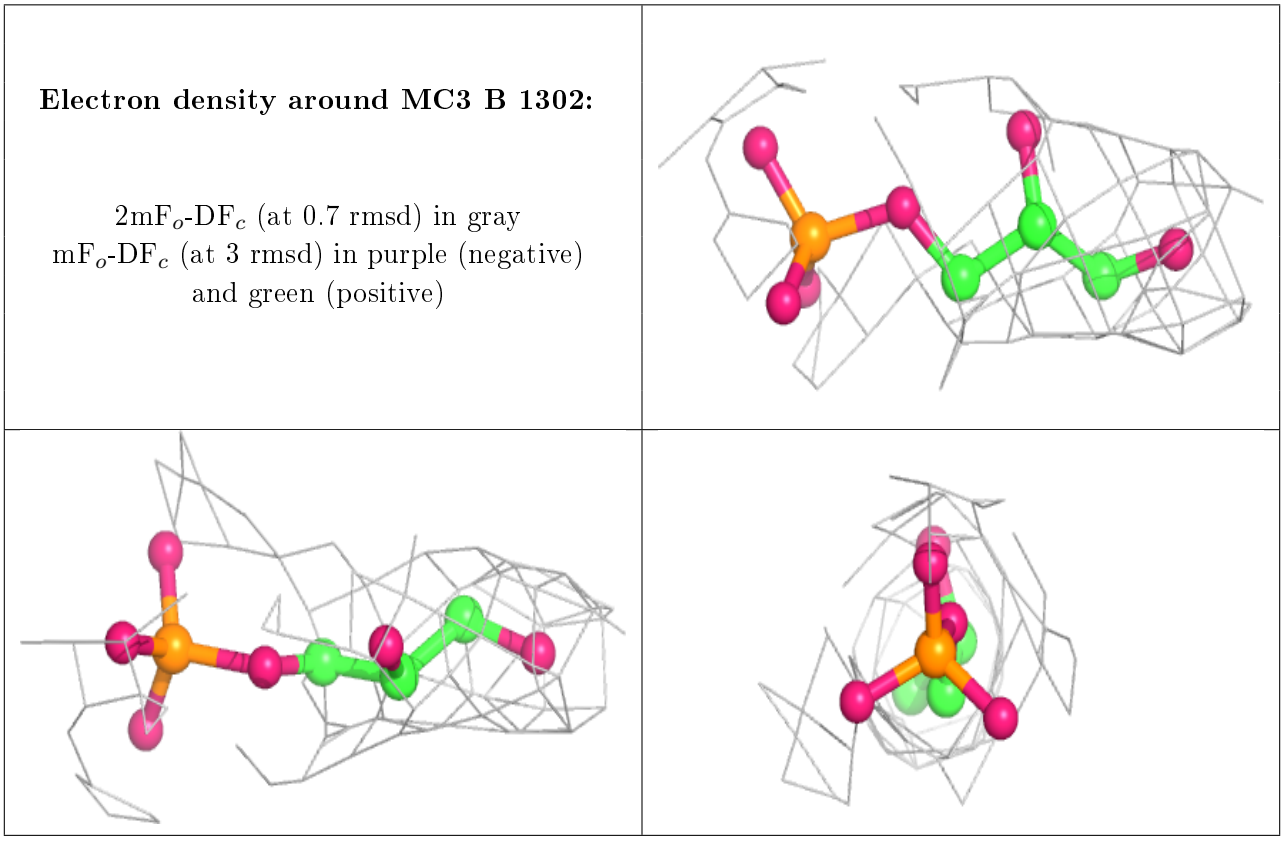
Electron density around MC3 D 1305:

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



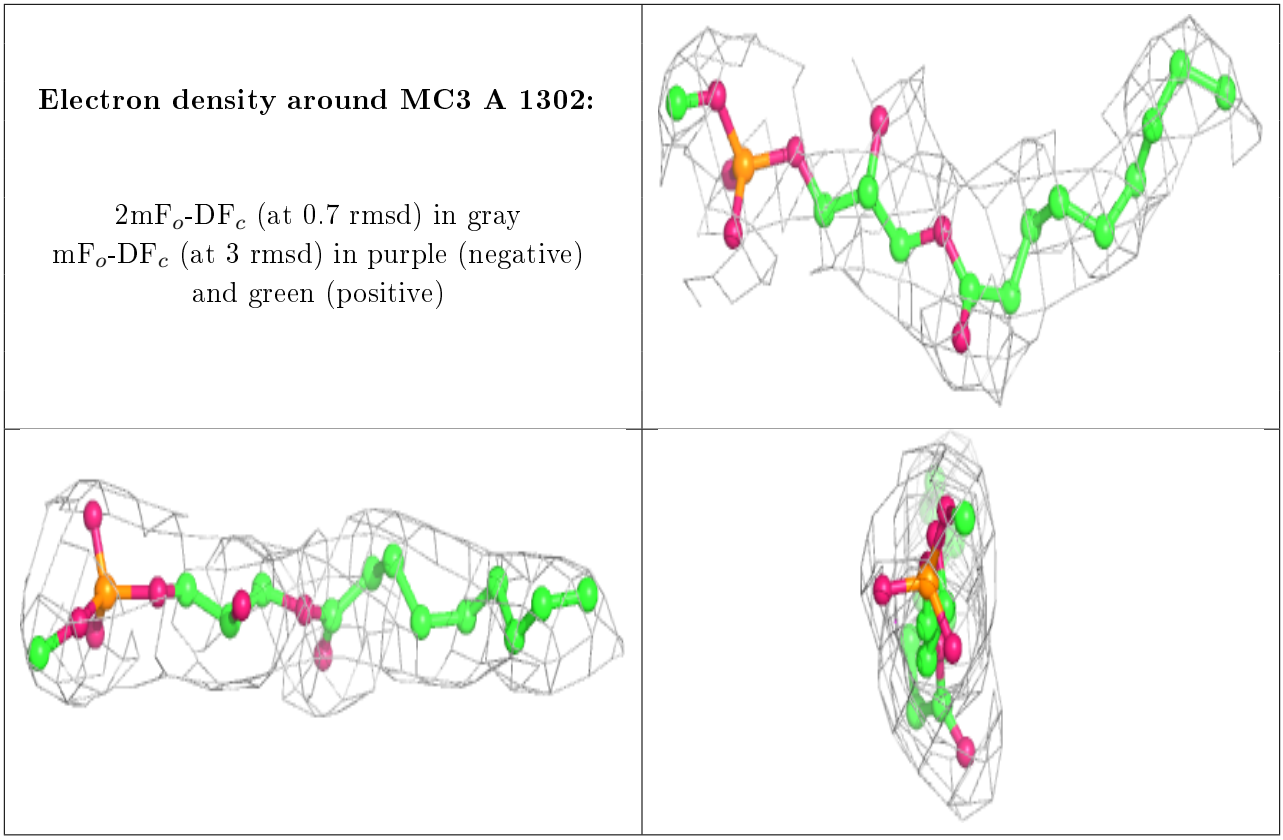
Electron density around MC3 B 1302:

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



Electron density around MC3 A 1302:

$2mF_o$-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.