Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 06:20 PM JST

PDB ID	:	8H5A
Title	:	Crystal structure of YhaJ effector binding domain (ligand-bound)
Authors	:	Kim, M.; Ryu, S.E.
Deposited on	:	2022-10-12
Resolution	:	2.80 Å(reported)

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

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

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

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

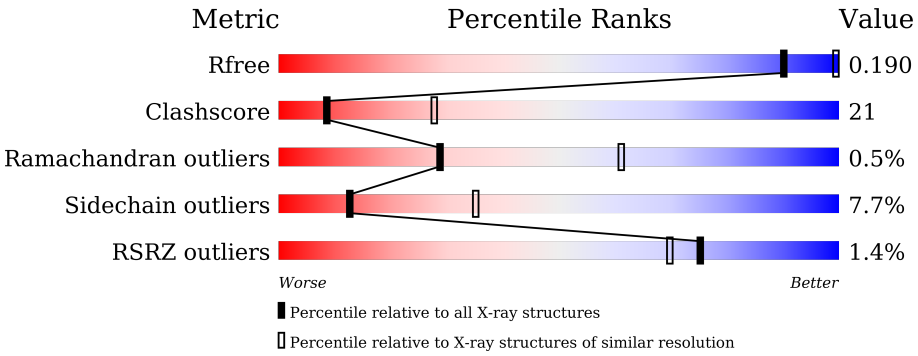
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	207	2% 57% 34% 5%
1	B	207	59% 36%
1	C	207	71% 24%
1	D	207	59% 32% 5%
1	E	207	64% 28%
1	F	207	58% 35% 6%

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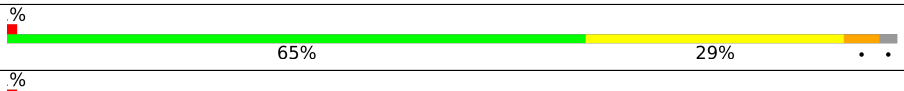
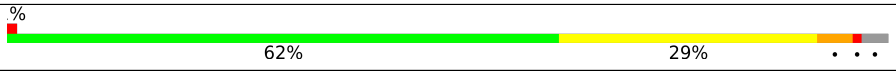
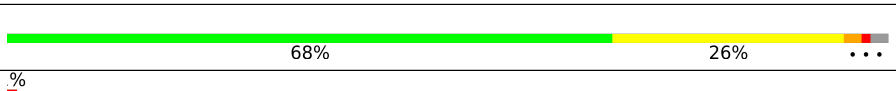
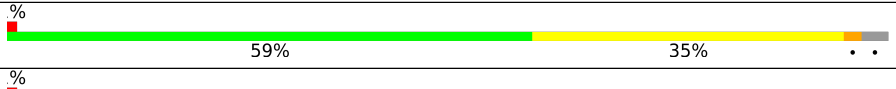
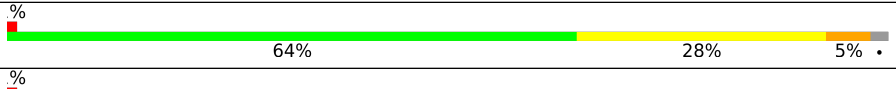
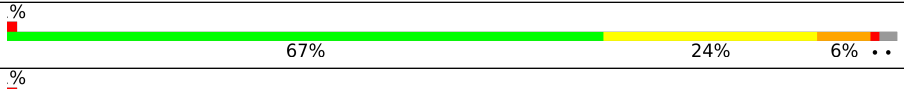
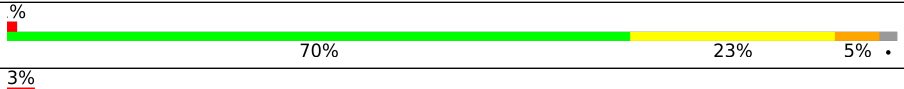
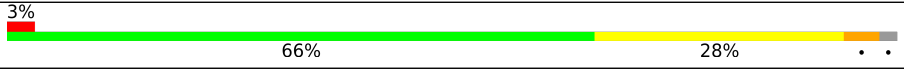
Mol	Chain	Length	Quality of chain
1	G	207	
1	H	207	
1	I	207	
1	J	207	
1	K	207	
1	L	207	
1	M	207	
1	N	207	
1	O	207	
1	P	207	

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
2	7DV	A	301	-	-	X	-
2	7DV	B	302	-	-	X	-
2	7DV	C	301	-	-	X	-
2	7DV	E	301	-	-	X	-
2	7DV	F	301	-	-	X	-
2	7DV	H	303	-	-	X	-
2	7DV	I	301	-	-	X	-
2	7DV	J	301	-	-	X	-
2	7DV	M	301	-	-	X	-
2	7DV	N	301	-	-	X	-
2	7DV	N	302	-	-	X	-
2	7DV	P	301	-	-	X	-
2	7DV	P	302	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25837 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 HTH-type transcriptional regulator YhaJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	B	202	Total	C	N	O	S	0	0	0
			1584	1005	276	295	8			
1	C	202	Total	C	N	O	S	0	0	0
			1580	1004	278	291	7			
1	D	203	Total	C	N	O	S	0	0	0
			1570	996	272	294	8			
1	E	202	Total	C	N	O	S	0	0	0
			1581	1003	278	293	7			
1	F	204	Total	C	N	O	S	0	0	0
			1597	1013	279	297	8			
1	G	202	Total	C	N	O	S	0	0	0
			1580	1003	277	293	7			
1	H	203	Total	C	N	O	S	0	0	0
			1588	1007	277	296	8			
1	I	202	Total	C	N	O	S	0	0	0
			1581	1005	277	292	7			
1	J	200	Total	C	N	O	S	0	0	0
			1569	995	273	293	8			
1	K	202	Total	C	N	O	S	0	0	0
			1580	1003	277	293	7			
1	L	201	Total	C	N	O	S	0	0	0
			1574	998	274	294	8			
1	M	202	Total	C	N	O	S	0	0	0
			1580	1003	277	293	7			
1	N	203	Total	C	N	O	S	0	0	0
			1584	1005	277	294	8			
1	O	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	P	203	Total	C	N	O	S	0	0	0
			1584	1004	276	296	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLY	-	expression tag	UNP P67661
A	93	SER	-	expression tag	UNP P67661
A	94	HIS	-	expression tag	UNP P67661
A	95	MET	-	expression tag	UNP P67661
B	92	GLY	-	expression tag	UNP P67661
B	93	SER	-	expression tag	UNP P67661
B	94	HIS	-	expression tag	UNP P67661
B	95	MET	-	expression tag	UNP P67661
C	92	GLY	-	expression tag	UNP P67661
C	93	SER	-	expression tag	UNP P67661
C	94	HIS	-	expression tag	UNP P67661
C	95	MET	-	expression tag	UNP P67661
D	92	GLY	-	expression tag	UNP P67661
D	93	SER	-	expression tag	UNP P67661
D	94	HIS	-	expression tag	UNP P67661
D	95	MET	-	expression tag	UNP P67661
E	92	GLY	-	expression tag	UNP P67661
E	93	SER	-	expression tag	UNP P67661
E	94	HIS	-	expression tag	UNP P67661
E	95	MET	-	expression tag	UNP P67661
F	92	GLY	-	expression tag	UNP P67661
F	93	SER	-	expression tag	UNP P67661
F	94	HIS	-	expression tag	UNP P67661
F	95	MET	-	expression tag	UNP P67661
G	92	GLY	-	expression tag	UNP P67661
G	93	SER	-	expression tag	UNP P67661
G	94	HIS	-	expression tag	UNP P67661
G	95	MET	-	expression tag	UNP P67661
H	92	GLY	-	expression tag	UNP P67661
H	93	SER	-	expression tag	UNP P67661
H	94	HIS	-	expression tag	UNP P67661
H	95	MET	-	expression tag	UNP P67661
I	92	GLY	-	expression tag	UNP P67661
I	93	SER	-	expression tag	UNP P67661
I	94	HIS	-	expression tag	UNP P67661
I	95	MET	-	expression tag	UNP P67661
J	92	GLY	-	expression tag	UNP P67661
J	93	SER	-	expression tag	UNP P67661
J	94	HIS	-	expression tag	UNP P67661
J	95	MET	-	expression tag	UNP P67661
K	92	GLY	-	expression tag	UNP P67661
K	93	SER	-	expression tag	UNP P67661

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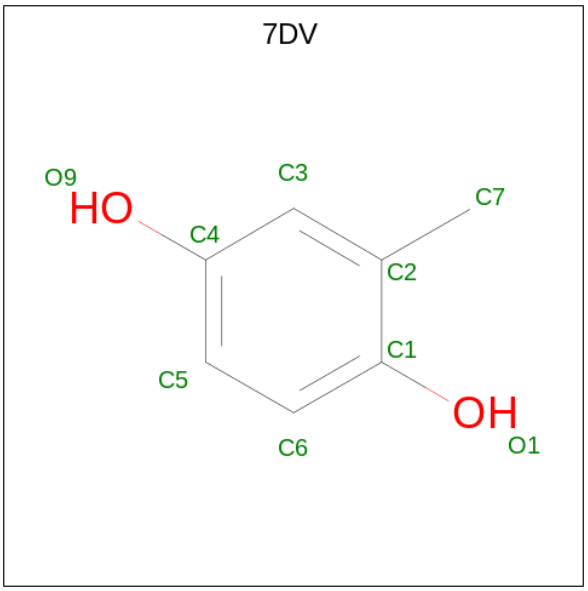
Chain	Residue	Modelled	Actual	Comment	Reference
K	94	HIS	-	expression tag	UNP P67661
K	95	MET	-	expression tag	UNP P67661
L	92	GLY	-	expression tag	UNP P67661
L	93	SER	-	expression tag	UNP P67661
L	94	HIS	-	expression tag	UNP P67661
L	95	MET	-	expression tag	UNP P67661
M	92	GLY	-	expression tag	UNP P67661
M	93	SER	-	expression tag	UNP P67661
M	94	HIS	-	expression tag	UNP P67661
M	95	MET	-	expression tag	UNP P67661
N	92	GLY	-	expression tag	UNP P67661
N	93	SER	-	expression tag	UNP P67661
N	94	HIS	-	expression tag	UNP P67661
N	95	MET	-	expression tag	UNP P67661
O	92	GLY	-	expression tag	UNP P67661
O	93	SER	-	expression tag	UNP P67661
O	94	HIS	-	expression tag	UNP P67661
O	95	MET	-	expression tag	UNP P67661
P	92	GLY	-	expression tag	UNP P67661
P	93	SER	-	expression tag	UNP P67661
P	94	HIS	-	expression tag	UNP P67661
P	95	MET	-	expression tag	UNP P67661

- Molecule 2 is 2-methylbenzene-1,4-diol (three-letter code: 7DV) (formula: $C_7H_8O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 7 2	0	0
2	A	1	Total C O 9 7 2	0	0
2	A	1	Total C O 9 7 2	0	0
2	B	1	Total C O 9 7 2	0	0
2	B	1	Total C O 9 7 2	0	0
2	B	1	Total C O 9 7 2	0	0
2	C	1	Total C O 9 7 2	0	0
2	C	1	Total C O 9 7 2	0	0
2	C	1	Total C O 9 7 2	0	0
2	D	1	Total C O 9 7 2	0	0
2	D	1	Total C O 9 7 2	0	0
2	D	1	Total C O 9 7 2	0	0
2	D	1	Total C O 9 7 2	0	0
2	E	1	Total C O 9 7 2	0	0
2	E	1	Total C O 9 7 2	0	0
2	E	1	Total C O 9 7 2	0	0
2	F	1	Total C O 9 7 2	0	0
2	F	1	Total C O 9 7 2	0	0
2	F	1	Total C O 9 7 2	0	0
2	G	1	Total C O 9 7 2	0	0
2	G	1	Total C O 9 7 2	0	0
2	G	1	Total C O 9 7 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C O 9 7 2	0	0
2	H	1	Total C O 9 7 2	0	0
2	H	1	Total C O 9 7 2	0	0
2	I	1	Total C O 9 7 2	0	0
2	I	1	Total C O 9 7 2	0	0
2	I	1	Total C O 9 7 2	0	0
2	J	1	Total C O 9 7 2	0	0
2	J	1	Total C O 9 7 2	0	0
2	J	1	Total C O 9 7 2	0	0
2	K	1	Total C O 9 7 2	0	0
2	K	1	Total C O 9 7 2	0	0
2	K	1	Total C O 9 7 2	0	0
2	L	1	Total C O 9 7 2	0	0
2	L	1	Total C O 9 7 2	0	0
2	L	1	Total C O 9 7 2	0	0
2	L	1	Total C O 9 7 2	0	0
2	M	1	Total C O 9 7 2	0	0
2	M	1	Total C O 9 7 2	0	0
2	M	1	Total C O 9 7 2	0	0
2	N	1	Total C O 9 7 2	0	0
2	N	1	Total C O 9 7 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	N	1	Total C O 9 7 2	0	0
2	O	1	Total C O 9 7 2	0	0
2	O	1	Total C O 9 7 2	0	0
2	O	1	Total C O 9 7 2	0	0
2	P	1	Total C O 9 7 2	0	0
2	P	1	Total C O 9 7 2	0	0
2	P	1	Total C O 9 7 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0
3	I	2	Total Na 2 2	0	0
3	K	1	Total Na 1 1	0	0
3	L	1	Total Na 1 1	0	0
3	N	2	Total Na 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total Na 1 1	0	0
3	P	1	Total Na 1 1	0	0

- Molecule 4 is water.

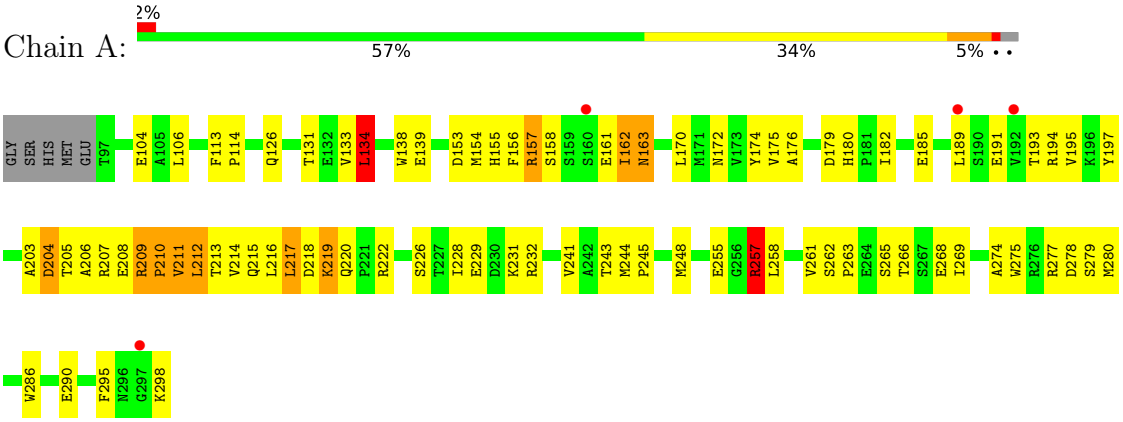
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	4	Total O 4 4	0	0
4	C	5	Total O 5 5	0	0
4	D	3	Total O 3 3	0	0
4	E	3	Total O 3 3	0	0
4	F	5	Total O 5 5	0	0
4	G	1	Total O 1 1	0	0
4	H	6	Total O 6 6	0	0
4	I	6	Total O 6 6	0	0
4	J	4	Total O 4 4	0	0
4	K	1	Total O 1 1	0	0
4	L	4	Total O 4 4	0	0
4	M	9	Total O 9 9	0	0
4	N	4	Total O 4 4	0	0
4	O	11	Total O 11 11	0	0
4	P	3	Total O 3 3	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.

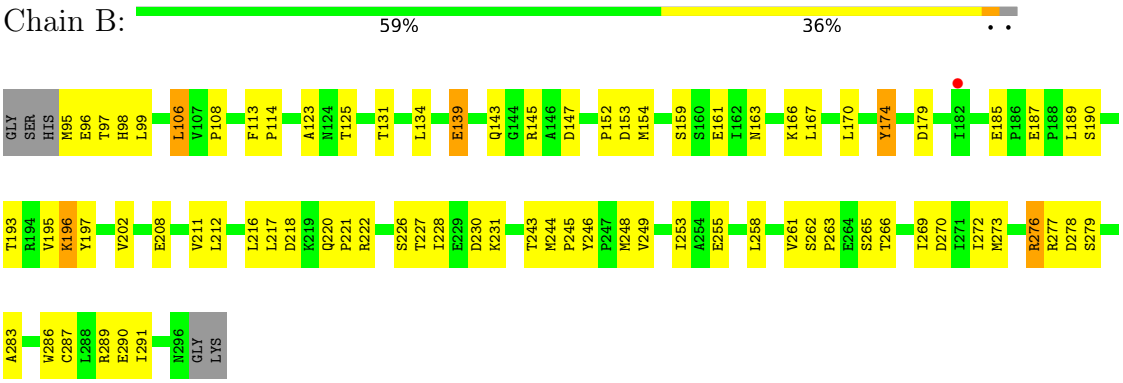
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain A:



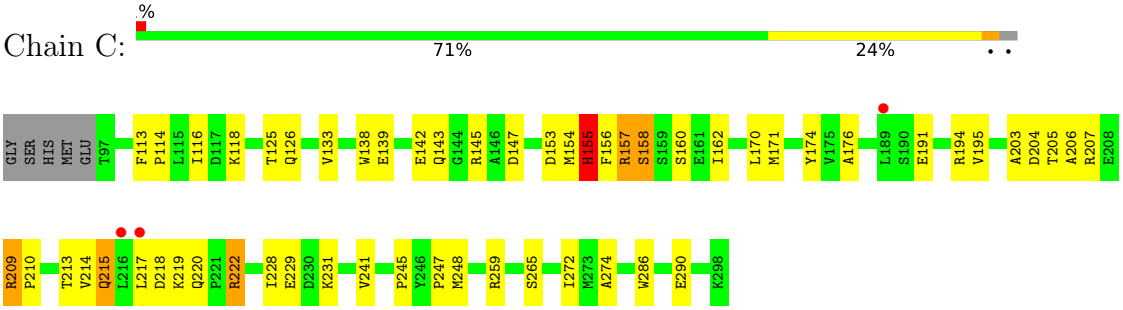
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain B:



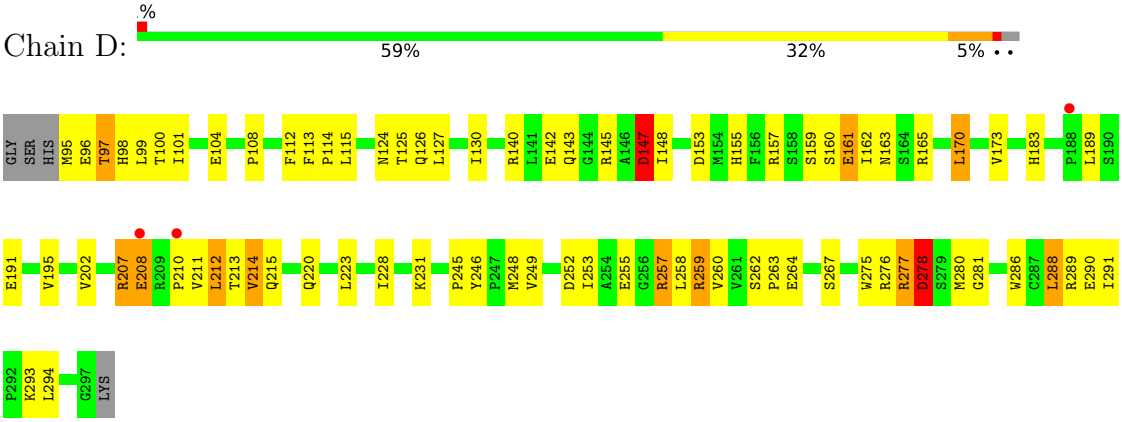
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain C:



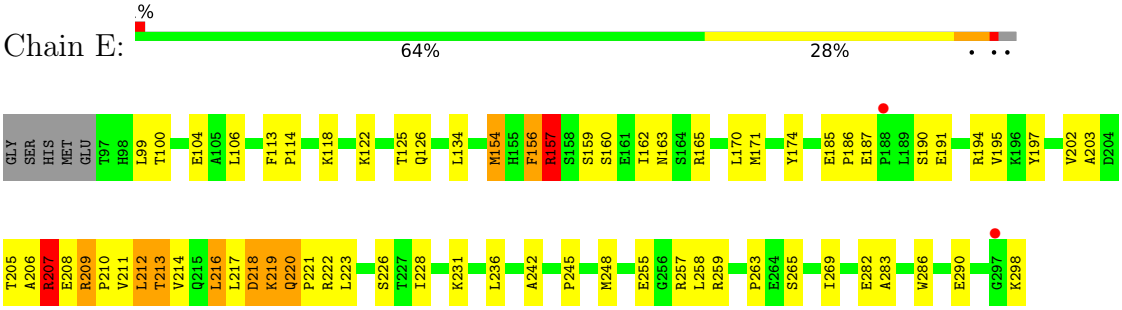
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain D:



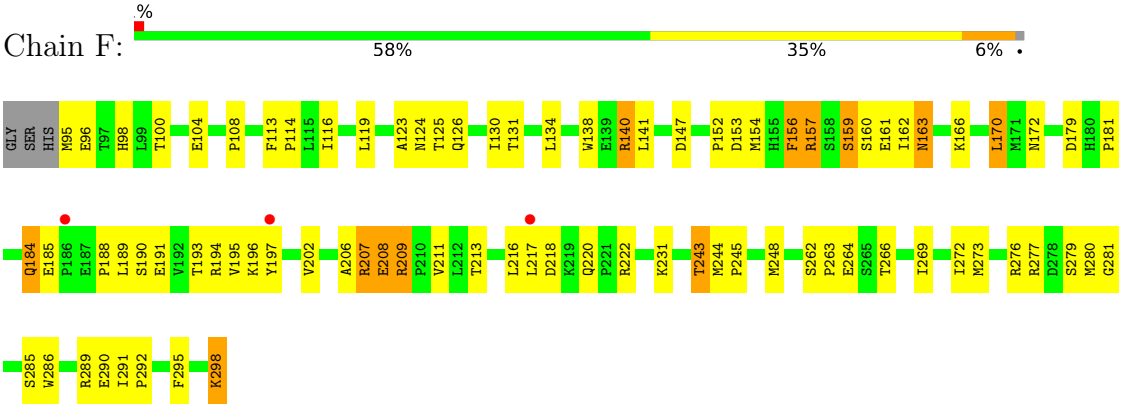
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain E:



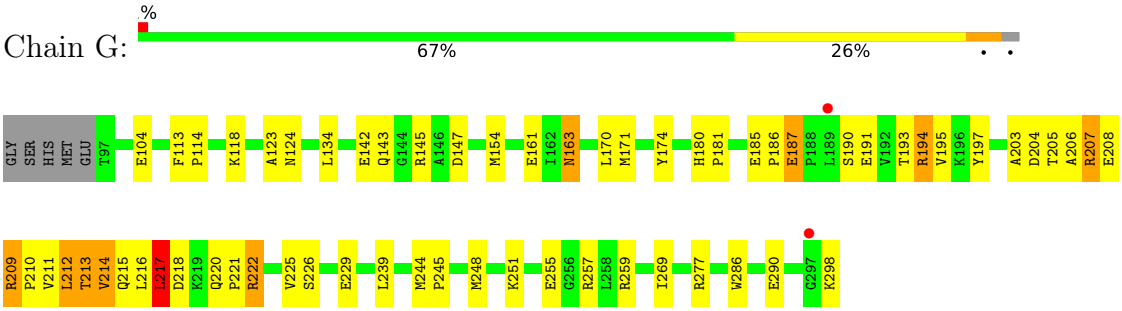
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain F:



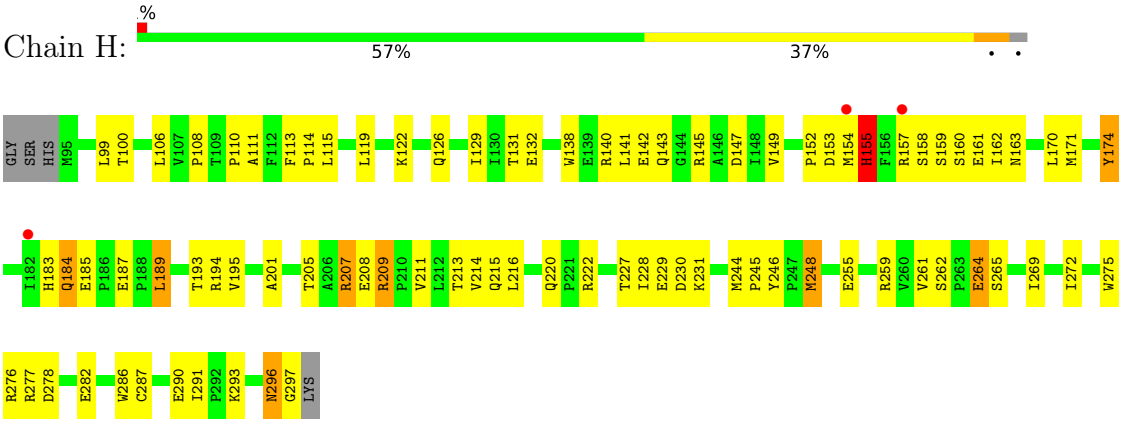
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain G:



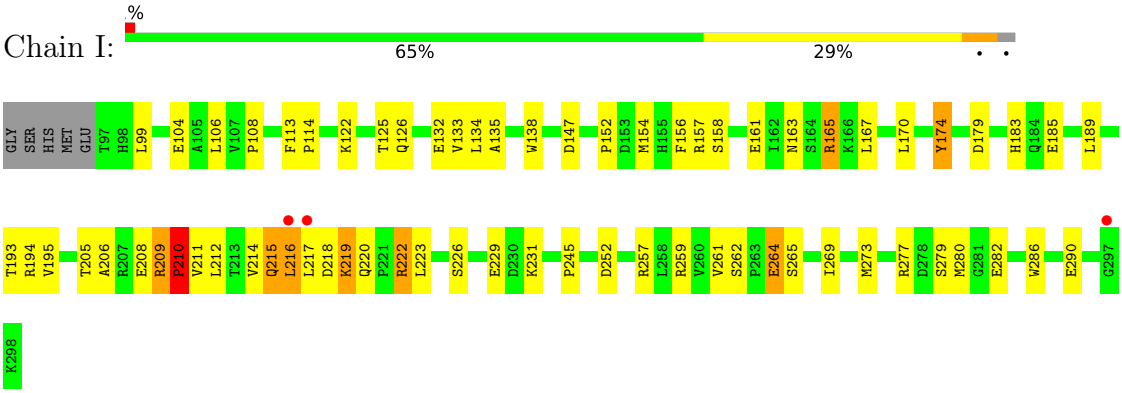
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain H:



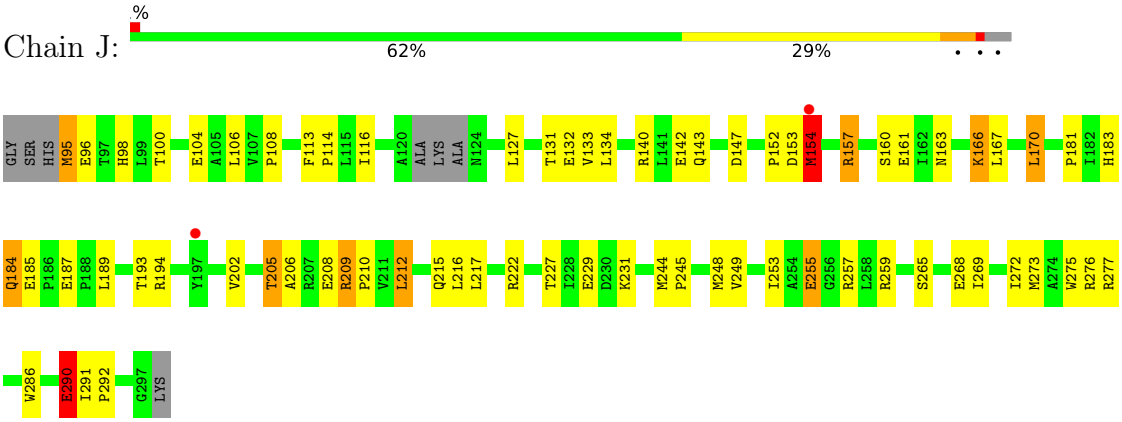
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain I:



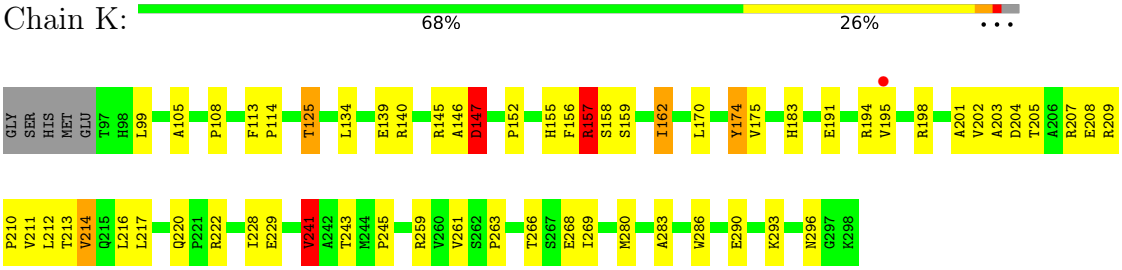
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain J:



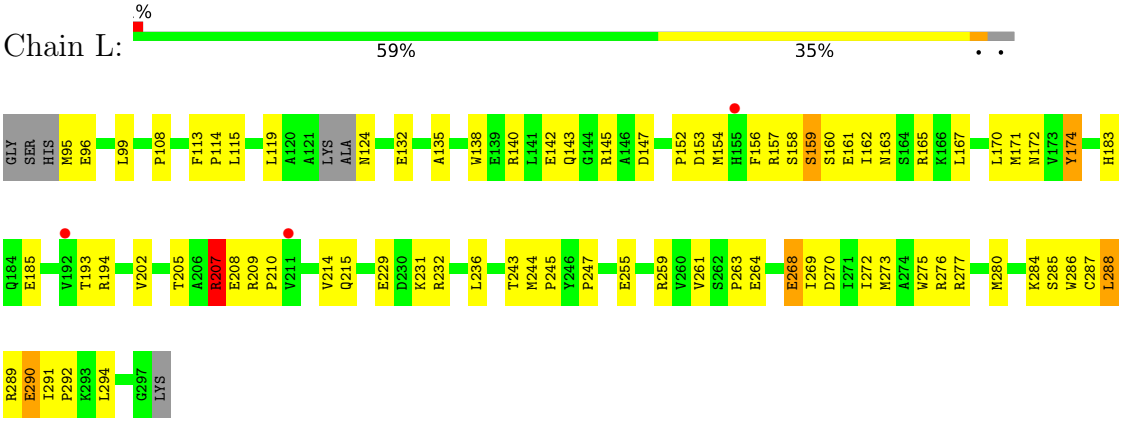
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain K:



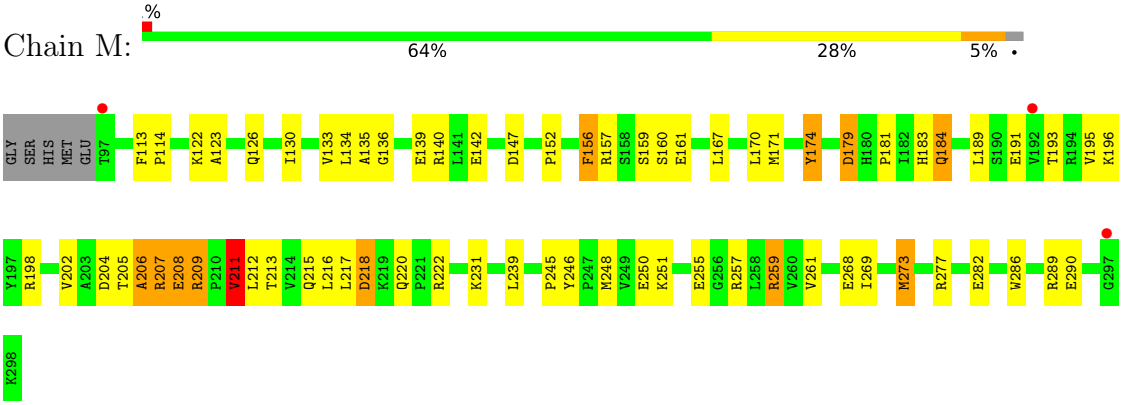
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain L:



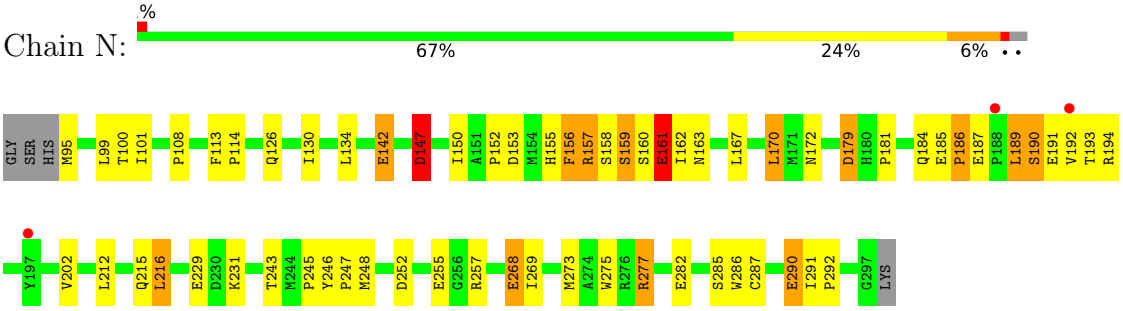
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain M:



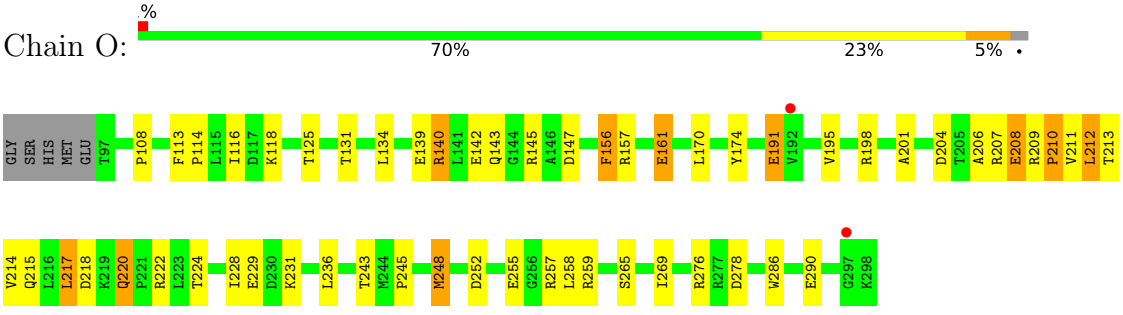
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain N:



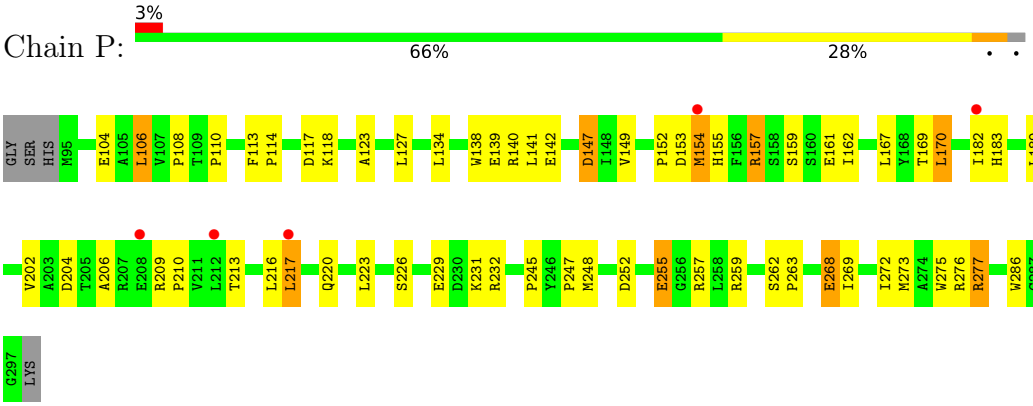
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain O:



• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain P:


3%
66%
28%
GLY SER HIS M95 E104 A105 L106 V107 P108 T109 P110 F113 P114 D117 K118 A123 L127 L134 W138 E139 R140 L141 E142 D147 T148 V149 P152 D153 M154 H155 F156 R157 S158 S159 S160 E161 I162 L167 Y168 T169 L170 I182 H183 L189 V192 V195
V202 A203 D204 T205 A206 R207 E208 R209 P210 V211 L212 T213 L216 L217 Q220 L223 S226 E229 D230 K231 R232 P245 Y246 P247 M248 D252 E255 G256 R257 L258 R259 S262 P263 E268 I269 I272 M273 A274 W275 R276 R277 W286 C287 L288 R289 E290
G297 LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	215.75Å 215.75Å 264.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 2.80 35.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (35.00-2.80) 99.9 (35.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.232 0.156 , 0.190	Depositor DCC
R_{free} test set	5969 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.170 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.175 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.176 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.176 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.176 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.176 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.197 for h,-h-k,-l	Xtriage

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[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.

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Property	Value	Source
Reported twinning fraction	0.122 for H, K, L 0.125 for K, H, -L 0.128 for -K, -1/3H+1/3K-2/3L, 4/3H+2/3K-1/3L 0.120 for -1/3H-2/3K-2/3L, -2/3H-1/3K+2/3L, -2/3H+2/3K-1/3L 0.128 for -1/3H+1/3K-2/3L, -K, -4/3H-2/3K+1/3L 0.130 for -H, 1/3H-1/3K+2/3L, 2/3H+4/3K+1/3L 0.125 for 1/3H-1/3K+2/3L, -H, -2/3H-4/3K-1/3L 0.122 for -2/3H-1/3K+2/3L, -1/3H-2/3K-2/3L, 2/3H-2/3K+1/3L	Depositor
Outliers	0 of 112445 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25837	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7DV, NA

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	0.56	1/1615 (0.1%)	0.88	3/2196 (0.1%)
1	B	0.52	0/1615	0.82	4/2198 (0.2%)
1	C	0.51	0/1611	0.80	0/2191
1	D	0.55	1/1601 (0.1%)	0.89	7/2183 (0.3%)
1	E	0.55	0/1612	0.85	2/2192 (0.1%)
1	F	0.52	0/1628	0.93	3/2214 (0.1%)
1	G	0.55	2/1611 (0.1%)	0.86	2/2192 (0.1%)
1	H	0.53	0/1619	0.82	1/2203 (0.0%)
1	I	0.53	0/1612	0.82	2/2192 (0.1%)
1	J	0.66	3/1599 (0.2%)	0.93	5/2175 (0.2%)
1	K	0.58	0/1611	0.92	8/2192 (0.4%)
1	L	0.63	2/1604 (0.1%)	0.92	4/2182 (0.2%)
1	M	0.54	0/1611	0.86	2/2192 (0.1%)
1	N	0.58	3/1615 (0.2%)	0.83	3/2198 (0.1%)
1	O	0.57	0/1615	0.88	4/2196 (0.2%)
1	P	0.56	1/1615 (0.1%)	0.92	6/2199 (0.3%)
All	All	0.56	13/25794 (0.1%)	0.87	56/35095 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	2
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
1	N	0	2
1	P	0	1
All	All	0	12

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	290	GLU	CD-OE2	-12.04	1.12	1.25
1	L	290	GLU	CD-OE1	-8.71	1.16	1.25
1	D	255	GLU	CD-OE1	-6.71	1.18	1.25
1	J	132	GLU	CD-OE1	-6.70	1.18	1.25
1	J	268	GLU	CD-OE2	6.67	1.32	1.25
1	P	255	GLU	CD-OE2	5.82	1.32	1.25
1	A	268	GLU	CD-OE2	-5.80	1.19	1.25
1	N	290	GLU	CD-OE1	5.79	1.32	1.25
1	L	268	GLU	CD-OE1	5.55	1.31	1.25
1	G	142	GLU	CD-OE1	5.52	1.31	1.25
1	N	142	GLU	CD-OE2	5.32	1.31	1.25
1	N	268	GLU	CD-OE2	5.02	1.31	1.25
1	G	187	GLU	CD-OE1	5.01	1.31	1.25

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	157	ARG	CB-CG-CD	12.33	143.66	111.60
1	K	174	TYR	CB-CG-CD1	-12.09	113.75	121.00
1	O	191	GLU	CB-CA-C	10.65	131.69	110.40
1	P	147	ASP	CB-CG-OD1	9.06	126.45	118.30
1	K	174	TYR	CB-CG-CD2	8.83	126.30	121.00
1	P	123	ALA	N-CA-CB	8.12	121.47	110.10
1	O	140	ARG	CB-CG-CD	7.84	131.98	111.60
1	I	165	ARG	CG-CD-NE	7.76	128.10	111.80
1	D	278	ASP	N-CA-CB	7.68	124.42	110.60
1	P	147	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	J	290	GLU	CG-CD-OE2	-7.60	103.10	118.30
1	K	241	VAL	CA-CB-CG1	7.44	122.06	110.90
1	L	165	ARG	CG-CD-NE	7.35	127.24	111.80
1	N	161	GLU	CB-CA-C	-7.20	96.01	110.40
1	J	290	GLU	CG-CD-OE1	6.98	132.25	118.30
1	K	174	TYR	CE1-CZ-OH	-6.97	101.28	120.10
1	P	277	ARG	CB-CG-CD	-6.90	93.66	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	289	ARG	CG-CD-NE	-6.77	97.58	111.80
1	J	290	GLU	N-CA-CB	-6.76	98.43	110.60
1	K	147	ASP	CB-CG-OD1	6.72	124.35	118.30
1	D	278	ASP	CA-C-N	-6.61	102.66	117.20
1	D	147	ASP	CB-CG-OD1	6.55	124.20	118.30
1	K	174	TYR	OH-CZ-CE2	6.30	137.11	120.10
1	L	207	ARG	CG-CD-NE	6.27	124.97	111.80
1	A	134	LEU	CB-CG-CD2	6.16	121.48	111.00
1	G	217	LEU	CA-CB-CG	6.14	129.41	115.30
1	D	278	ASP	CA-C-O	6.13	132.97	120.10
1	A	257	ARG	CG-CD-NE	6.12	124.65	111.80
1	D	278	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	L	157	ARG	CG-CD-NE	6.02	124.45	111.80
1	K	174	TYR	CA-CB-CG	-5.99	102.02	113.40
1	M	184	GLN	N-CA-CB	5.98	121.36	110.60
1	P	259	ARG	CB-CG-CD	5.96	127.11	111.60
1	G	217	LEU	CB-CG-CD1	5.88	121.00	111.00
1	B	246	TYR	CB-CG-CD2	-5.84	117.50	121.00
1	A	232	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	B	246	TYR	CB-CG-CD1	5.81	124.49	121.00
1	J	257	ARG	CG-CD-NE	-5.75	99.74	111.80
1	H	159	SER	CB-CA-C	5.66	120.86	110.10
1	O	191	GLU	CA-CB-CG	-5.65	100.97	113.40
1	K	241	VAL	CA-CB-CG2	5.56	119.24	110.90
1	D	259	ARG	CB-CG-CD	5.47	125.81	111.60
1	F	157	ARG	CA-CB-CG	5.39	125.26	113.40
1	B	106	LEU	CB-CG-CD2	5.38	120.14	111.00
1	D	288	LEU	CA-CB-CG	-5.29	103.12	115.30
1	B	276	ARG	CB-CG-CD	-5.29	97.86	111.60
1	E	207	ARG	CB-CA-C	5.25	120.90	110.40
1	P	106	LEU	CB-CG-CD2	5.21	119.85	111.00
1	I	210	PRO	CB-CA-C	-5.20	98.99	112.00
1	O	191	GLU	N-CA-CB	-5.19	101.26	110.60
1	F	140	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	J	248	MET	CA-CB-CG	5.04	121.86	113.30
1	N	229	GLU	CB-CG-CD	5.03	127.79	114.20
1	N	147	ASP	CB-CG-OD1	5.03	122.83	118.30
1	M	208	GLU	CA-CB-CG	5.02	124.45	113.40
1	E	218	ASP	N-CA-CB	-5.01	101.58	110.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ALA	Mainchain
1	D	278	ASP	Peptide
1	E	156	PHE	Peptide
1	F	156	PHE	Peptide
1	G	214	VAL	Peptide
1	H	155	HIS	Peptide
1	H	158	SER	Peptide
1	J	154	MET	Peptide
1	M	206	ALA	Peptide
1	N	179	ASP	Sidechain
1	N	186	PRO	Mainchain
1	P	183	HIS	Sidechain

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	1584	0	1629	108	0
1	B	1584	0	1617	85	1
1	C	1580	0	1625	74	0
1	D	1570	0	1583	83	0
1	E	1581	0	1621	79	0
1	F	1597	0	1633	82	1
1	G	1580	0	1618	61	0
1	H	1588	0	1620	89	0
1	I	1581	0	1626	92	0
1	J	1569	0	1596	60	1
1	K	1580	0	1619	75	0
1	L	1574	0	1600	73	1
1	M	1580	0	1619	66	0
1	N	1584	0	1615	54	2
1	O	1584	0	1628	63	0
1	P	1584	0	1610	57	0
2	A	27	0	0	6	0
2	B	27	0	0	8	0
2	C	27	0	0	7	0
2	D	36	0	0	5	0
2	E	27	0	0	8	0
2	F	27	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	27	0	0	1	0
2	H	27	0	0	8	0
2	I	27	0	0	8	0
2	J	27	0	0	7	0
2	K	27	0	0	2	0
2	L	36	0	0	2	0
2	M	27	0	0	5	0
2	N	27	0	0	10	0
2	O	27	0	0	5	0
2	P	27	0	0	15	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	N	2	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	2	0	0	0	0
4	B	4	0	0	0	0
4	C	5	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	5	0	0	0	0
4	G	1	0	0	0	0
4	H	6	0	0	5	0
4	I	6	0	0	0	0
4	J	4	0	0	1	0
4	K	1	0	0	0	0
4	L	4	0	0	0	0
4	M	9	0	0	2	0
4	N	4	0	0	0	0
4	O	11	0	0	1	0
4	P	3	0	0	0	0
All	All	25837	0	25859	1070	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1070) 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:L:275:TRP:CZ3	1:L:280:MET:CE	2.08	1.36
1:L:275:TRP:CZ3	1:L:280:MET:HE2	1.60	1.33
1:I:134:LEU:CD1	2:I:301:7DV:O9	1.80	1.29
1:L:275:TRP:HZ3	1:L:280:MET:CE	1.43	1.29
1:K:174:TYR:OH	1:K:241:VAL:HG12	1.19	1.26
1:A:263:PRO:O	1:A:266:THR:HG22	1.35	1.24
1:K:174:TYR:OH	1:K:241:VAL:CG1	1.86	1.22
1:M:136:GLY:HA2	1:M:206:ALA:HB3	1.23	1.16
1:D:101:ILE:HD11	1:D:127:LEU:HD11	1.15	1.14
1:M:136:GLY:HA2	1:M:206:ALA:CB	1.78	1.12
1:O:204:ASP:HB3	1:O:210:PRO:HG2	1.32	1.11
1:H:155:HIS:HA	1:H:157:ARG:HH12	1.07	1.11
1:I:134:LEU:HD11	2:I:301:7DV:O9	1.38	1.11
1:I:154:MET:O	1:K:157:ARG:N	1.82	1.10
1:J:106:LEU:HD11	2:J:301:7DV:O9	1.51	1.09
1:E:134:LEU:CD1	2:E:301:7DV:O9	2.01	1.07
1:J:106:LEU:CD1	2:J:301:7DV:O9	2.02	1.07
1:I:219:LYS:HD2	1:L:207:ARG:HD2	1.37	1.06
1:A:106:LEU:HD21	2:A:301:7DV:C6	1.85	1.05
1:P:167:LEU:HD11	1:P:273:MET:HB2	1.40	1.04
1:D:101:ILE:CD1	1:D:127:LEU:HD11	1.87	1.02
1:I:135:ALA:HB2	1:I:210:PRO:HG3	1.41	1.01
1:M:136:GLY:CA	1:M:206:ALA:HB3	1.89	1.01
1:H:155:HIS:HA	1:H:157:ARG:NH1	1.74	1.01
1:G:212:LEU:HD21	1:G:216:LEU:O	1.61	1.00
1:I:216:LEU:HD12	1:I:217:LEU:H	1.28	0.97
1:J:106:LEU:HD11	2:J:301:7DV:C4	1.94	0.96
1:D:143:GLN:OE1	1:D:145:ARG:NH1	1.98	0.96
1:B:143:GLN:HA	1:D:96:GLU:HG3	1.47	0.95
1:F:108:PRO:HD3	2:F:302:7DV:C5	1.96	0.95
1:A:255:GLU:HB2	1:A:257:ARG:HH12	1.32	0.94
1:G:222:ARG:N	1:H:126:GLN:OE1	1.98	0.94
1:M:152:PRO:HB3	1:M:269:ILE:HD11	1.48	0.93
1:M:135:ALA:HB2	1:M:209:ARG:HG2	1.49	0.92
1:J:142:GLU:HG2	1:L:95:MET:SD	2.10	0.92
1:A:154:MET:HG2	1:A:211:VAL:HG11	1.50	0.91
1:C:174:TYR:OH	1:C:214:VAL:HG11	1.70	0.90
1:L:275:TRP:CZ3	1:L:280:MET:HE1	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:140:ARG:HG2	1:K:146:ALA:HB2	1.53	0.90
1:L:275:TRP:HZ3	1:L:280:MET:HE2	0.73	0.90
1:B:95:MET:CE	1:D:161:GLU:HG2	2.01	0.90
1:A:208:GLU:HB3	1:A:209:ARG:HH21	1.37	0.89
1:E:134:LEU:HD11	2:E:301:7DV:O9	1.71	0.89
1:I:217:LEU:O	1:I:222:ARG:NH2	2.07	0.88
1:C:213:THR:HG22	1:C:214:VAL:HG23	1.56	0.88
1:J:133:VAL:HB	1:J:205:THR:CG2	2.04	0.88
1:K:174:TYR:CZ	1:K:241:VAL:HG12	2.08	0.88
1:O:143:GLN:OE1	1:O:145:ARG:NH1	2.07	0.87
1:M:134:LEU:HD23	2:M:301:7DV:O9	1.72	0.87
1:I:211:VAL:HB	1:K:156:PHE:CE2	2.11	0.86
1:I:134:LEU:HD12	2:I:301:7DV:O9	1.75	0.86
1:C:204:ASP:HB3	1:C:210:PRO:CG	2.06	0.86
1:G:217:LEU:HD12	1:G:218:ASP:H	1.41	0.86
1:A:138:TRP:HB3	1:A:157:ARG:HB2	1.57	0.85
1:H:138:TRP:HE1	1:H:154:MET:HG3	1.41	0.85
1:L:183:HIS:HE1	1:L:259:ARG:HB3	1.37	0.85
1:K:174:TYR:CD1	1:K:174:TYR:C	2.48	0.85
1:H:211:VAL:HG23	1:H:213:THR:HG23	1.59	0.85
1:B:145:ARG:HH12	1:C:222:ARG:HH22	1.25	0.84
1:L:115:LEU:HD11	1:L:294:LEU:HD11	1.59	0.84
1:B:95:MET:CE	1:D:276:ARG:HD2	2.07	0.84
1:P:138:TRP:HE1	1:P:154:MET:HG3	1.41	0.84
1:H:194:ARG:HB3	1:H:216:LEU:HD21	1.59	0.83
1:K:201:ALA:HB1	1:K:211:VAL:HG21	1.59	0.83
1:I:209:ARG:NH1	1:K:205:THR:OG1	2.11	0.83
1:L:153:ASP:HB3	1:L:272:ILE:HD11	1.58	0.83
1:N:159:SER:HB2	1:N:161:GLU:OE1	1.79	0.83
1:I:154:MET:HG3	1:K:156:PHE:CE1	2.14	0.82
1:D:246:TYR:CD2	1:P:263:PRO:HG2	2.14	0.82
1:G:163:ASN:OD1	1:G:277:ARG:NE	2.12	0.81
1:N:108:PRO:HD3	2:N:302:7DV:C5	2.10	0.81
1:L:138:TRP:HE1	1:L:154:MET:HG3	1.45	0.81
1:I:134:LEU:HD11	2:I:301:7DV:C4	2.10	0.81
1:B:95:MET:HE1	1:D:161:GLU:HG2	1.63	0.80
1:I:229:GLU:HG2	1:J:229:GLU:HG2	1.62	0.80
1:J:185:GLU:OE2	1:J:193:THR:HG21	1.82	0.80
1:J:133:VAL:HB	1:J:205:THR:HG22	1.63	0.80
1:J:108:PRO:HD3	2:J:302:7DV:C5	2.12	0.79
1:C:204:ASP:HB3	1:C:210:PRO:HG2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:THR:HG23	2:C:301:7DV:C7	2.13	0.79
1:F:119:LEU:HD22	1:F:125:THR:HG21	1.63	0.79
1:H:108:PRO:HD3	2:H:302:7DV:O9	1.82	0.79
1:B:123:ALA:HB3	1:B:125:THR:HG23	1.64	0.79
1:I:209:ARG:HG3	1:I:212:LEU:CD2	2.13	0.79
1:I:210:PRO:HD2	1:I:212:LEU:HB3	1.63	0.79
1:K:191:GLU:HB2	1:K:217:LEU:HD21	1.63	0.79
1:M:134:LEU:CD2	2:M:301:7DV:O9	2.30	0.79
1:A:255:GLU:HB2	1:A:257:ARG:NH1	1.97	0.78
1:I:185:GLU:HG2	1:I:193:THR:HG21	1.65	0.78
1:I:209:ARG:HG3	1:I:212:LEU:HD21	1.64	0.78
1:I:108:PRO:HD3	2:I:302:7DV:C5	2.13	0.78
1:A:295:PHE:HA	1:A:298:LYS:HD3	1.66	0.78
1:I:189:LEU:HD21	1:I:265:SER:HB3	1.66	0.78
1:A:210:PRO:HG3	1:C:138:TRP:HB2	1.66	0.78
1:C:138:TRP:HE1	1:C:153:ASP:HB2	1.47	0.78
1:K:198:ARG:O	1:K:241:VAL:HG23	1.83	0.77
1:N:161:GLU:H	1:N:161:GLU:CD	1.86	0.77
1:L:286:TRP:CZ2	1:L:290:GLU:HG3	2.20	0.77
1:J:194:ARG:HD3	1:J:216:LEU:HB2	1.66	0.77
1:N:172:ASN:HD22	1:N:243:THR:HG22	1.48	0.77
1:G:214:VAL:HG12	1:G:215:GLN:H	1.50	0.77
1:J:106:LEU:HD12	2:J:301:7DV:O9	1.86	0.76
1:G:206:ALA:O	1:G:207:ARG:HG2	1.85	0.76
1:I:209:ARG:HA	1:I:212:LEU:HD22	1.66	0.76
1:J:95:MET:CE	1:L:276:ARG:HE	1.98	0.76
1:O:108:PRO:HD3	2:O:302:7DV:O9	1.85	0.76
1:A:182:ILE:HD13	1:A:241:VAL:HG11	1.68	0.76
1:A:155:HIS:HE1	1:A:211:VAL:HB	1.50	0.75
1:B:145:ARG:HH22	1:C:222:ARG:HH12	1.32	0.75
1:F:104:GLU:OE2	2:F:301:7DV:O9	2.04	0.75
1:G:203:ALA:HA	1:G:210:PRO:HD3	1.67	0.75
1:H:189:LEU:HD22	1:H:265:SER:OG	1.87	0.75
1:M:134:LEU:HD22	1:M:211:VAL:HG11	1.69	0.75
1:I:212:LEU:H	1:I:212:LEU:HD23	1.52	0.74
1:O:143:GLN:HG3	1:O:145:ARG:HD3	1.69	0.74
1:G:161:GLU:HB3	1:G:277:ARG:HD2	1.69	0.74
1:A:218:ASP:HB2	1:D:207:ARG:HD2	1.68	0.74
1:H:264:GLU:HA	1:L:171:MET:CE	2.17	0.74
1:J:133:VAL:H	1:J:205:THR:HG23	1.51	0.74
1:K:213:THR:HG23	1:K:214:VAL:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:95:MET:HE1	1:L:276:ARG:HE	1.52	0.74
1:M:133:VAL:HG12	1:M:134:LEU:HG	1.70	0.74
1:G:143:GLN:HE21	1:G:145:ARG:HH11	1.35	0.73
1:C:138:TRP:NE1	1:C:153:ASP:HB2	2.02	0.73
1:H:264:GLU:HA	1:L:171:MET:HE1	1.69	0.73
1:M:136:GLY:HA2	1:M:206:ALA:HB2	1.70	0.73
1:K:207:ARG:HB2	1:L:132:GLU:OE2	1.89	0.73
1:M:135:ALA:CB	1:M:209:ARG:HG2	2.19	0.72
1:E:218:ASP:CG	1:E:219:LYS:H	1.93	0.72
1:E:134:LEU:HD12	2:E:301:7DV:O9	1.89	0.72
1:O:142:GLU:HG2	1:O:156:PHE:HE2	1.55	0.72
1:L:232:ARG:HE	1:L:236:LEU:HD11	1.53	0.72
1:E:282:GLU:HG2	1:E:283:ALA:N	2.04	0.72
1:G:212:LEU:CD2	1:G:216:LEU:O	2.37	0.72
1:N:181:PRO:O	1:N:184:GLN:HG3	1.89	0.72
1:N:273:MET:HE1	1:N:292:PRO:HD3	1.72	0.72
1:C:153:ASP:O	1:C:272:ILE:HD11	1.89	0.71
1:F:170:LEU:HD23	1:F:172:ASN:OD1	1.90	0.71
1:G:229:GLU:HG2	1:H:229:GLU:HG3	1.70	0.71
1:E:174:TYR:CD2	1:E:265:SER:HB2	2.26	0.71
1:B:96:GLU:HG3	1:D:143:GLN:HA	1.71	0.71
1:O:139:GLU:OE1	1:O:206:ALA:HB1	1.89	0.71
1:D:96:GLU:OE2	1:D:98:HIS:NE2	2.24	0.71
1:P:167:LEU:HD11	1:P:273:MET:CB	2.20	0.71
1:A:263:PRO:O	1:A:266:THR:CG2	2.27	0.71
1:K:157:ARG:NH1	1:K:162:ILE:HD13	2.06	0.70
1:L:273:MET:HE1	1:L:292:PRO:HD3	1.73	0.70
1:B:95:MET:HE3	1:D:276:ARG:HD2	1.72	0.70
1:F:231:LYS:NZ	2:F:301:7DV:O1	2.24	0.70
1:B:143:GLN:HA	1:D:96:GLU:CG	2.21	0.70
1:D:115:LEU:HD11	1:D:291:ILE:CD1	2.22	0.70
1:G:197:TYR:O	1:G:220:GLN:NE2	2.25	0.70
1:N:252:ASP:OD1	1:N:257:ARG:NH2	2.25	0.70
1:H:108:PRO:HD3	2:H:302:7DV:C4	2.21	0.70
1:A:106:LEU:HD21	2:A:301:7DV:C5	2.21	0.70
1:J:189:LEU:HD21	1:J:265:SER:HB3	1.74	0.70
1:K:204:ASP:HB3	1:K:210:PRO:HG2	1.74	0.70
1:A:161:GLU:HB3	1:A:277:ARG:HD2	1.74	0.70
1:E:171:MET:HE3	1:G:118:LYS:HE2	1.73	0.70
1:L:171:MET:SD	1:L:268:GLU:HG2	2.32	0.70
1:O:134:LEU:CD2	2:O:301:7DV:O9	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:GLU:HA	1:D:124:ASN:HB3	1.74	0.70
1:H:160:SER:HB2	1:H:162:ILE:HG12	1.74	0.69
1:N:167:LEU:HD21	1:N:273:MET:HE3	1.74	0.69
1:A:155:HIS:CE1	1:A:211:VAL:HB	2.26	0.69
1:E:171:MET:CE	1:G:118:LYS:HE2	2.23	0.69
1:O:229:GLU:HG3	1:P:229:GLU:HG2	1.75	0.69
1:B:189:LEU:HD11	1:B:265:SER:HB3	1.74	0.69
1:B:276:ARG:HD3	1:D:95:MET:CE	2.23	0.69
1:P:134:LEU:HB2	1:P:204:ASP:OD1	1.92	0.69
1:J:167:LEU:HD21	1:J:273:MET:HE3	1.73	0.68
1:N:189:LEU:HD22	1:N:189:LEU:H	1.58	0.68
1:M:136:GLY:N	1:M:206:ALA:HB3	2.08	0.68
1:D:108:PRO:HD3	2:D:302:7DV:C5	2.24	0.68
1:F:153:ASP:HA	1:F:156:PHE:CZ	2.28	0.68
1:O:174:TYR:CD2	1:O:265:SER:HB2	2.28	0.68
1:O:228:ILE:HG12	1:O:248:MET:HE1	1.76	0.68
1:J:154:MET:SD	1:J:212:LEU:HD21	2.34	0.68
1:A:210:PRO:HG3	1:C:138:TRP:CB	2.23	0.68
1:A:212:LEU:HD23	1:A:214:VAL:H	1.58	0.68
1:I:135:ALA:HB2	1:I:210:PRO:CG	2.22	0.68
1:I:220:GLN:O	1:I:222:ARG:NH1	2.28	0.67
1:E:203:ALA:CB	1:E:209:ARG:HG3	2.24	0.67
1:A:210:PRO:CG	1:C:138:TRP:HB2	2.24	0.67
1:D:98:HIS:HD2	1:D:126:GLN:HB2	1.60	0.67
1:J:206:ALA:HB1	1:J:210:PRO:HD2	1.77	0.67
1:B:167:LEU:HD21	1:B:273:MET:HB2	1.75	0.66
1:K:229:GLU:HG2	1:L:229:GLU:HG2	1.78	0.66
1:J:273:MET:HE1	1:J:292:PRO:HD3	1.76	0.66
1:C:174:TYR:CD2	1:C:265:SER:HB2	2.31	0.66
1:H:115:LEU:HB3	1:H:119:LEU:HD23	1.77	0.66
1:J:133:VAL:H	1:J:205:THR:CG2	2.08	0.66
1:H:138:TRP:NE1	1:H:154:MET:HG3	2.10	0.66
1:A:157:ARG:O	1:A:157:ARG:HG2	1.95	0.66
1:E:211:VAL:HG12	1:E:212:LEU:HB3	1.78	0.66
1:D:163:ASN:HB2	1:D:275:TRP:CE2	2.31	0.65
1:K:174:TYR:OH	1:K:241:VAL:CB	2.43	0.65
1:I:134:LEU:CD1	2:I:301:7DV:C4	2.70	0.65
1:M:134:LEU:HD12	1:M:204:ASP:HB2	1.77	0.65
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.62	0.65
1:I:194:ARG:CZ	1:I:216:LEU:HD13	2.25	0.65
1:I:220:GLN:HB3	1:I:222:ARG:NH2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:263:PRO:HB2	1:M:123:ALA:HA	1.77	0.65
1:B:134:LEU:HD13	1:B:211:VAL:CG1	2.27	0.65
1:D:140:ARG:HG2	1:D:145:ARG:NH2	2.11	0.65
1:F:298:LYS:H	1:F:298:LYS:HD3	1.62	0.64
1:L:153:ASP:HB3	1:L:272:ILE:CD1	2.27	0.64
1:G:195:VAL:HG13	1:G:217:LEU:HD23	1.79	0.64
1:P:139:GLU:OE1	1:P:206:ALA:HA	1.98	0.64
1:E:159:SER:HB2	1:E:162:ILE:HD11	1.77	0.64
1:J:286:TRP:O	1:J:290:GLU:HB2	1.97	0.64
1:D:263:PRO:HB3	2:D:304:7DV:C7	2.28	0.64
1:I:211:VAL:HG13	1:K:139:GLU:HA	1.78	0.64
1:L:185:GLU:HG2	1:L:193:THR:HG21	1.80	0.64
1:O:134:LEU:HD21	2:O:301:7DV:O9	1.96	0.64
1:P:138:TRP:NE1	1:P:154:MET:HG3	2.12	0.64
1:A:210:PRO:CB	1:C:138:TRP:HB2	2.28	0.63
1:N:255:GLU:O	1:N:255:GLU:HG3	1.98	0.63
1:O:140:ARG:HD2	1:O:145:ARG:CZ	2.28	0.63
1:C:203:ALA:HB1	1:C:207:ARG:O	1.98	0.63
1:F:119:LEU:HD22	1:F:125:THR:CG2	2.28	0.63
1:A:155:HIS:O	1:C:155:HIS:HA	1.98	0.63
1:I:133:VAL:H	1:I:205:THR:CG2	2.12	0.63
1:A:206:ALA:HB1	1:C:210:PRO:HA	1.79	0.63
1:C:206:ALA:O	1:C:207:ARG:HG3	1.99	0.63
1:M:206:ALA:HA	1:M:207:ARG:HB2	1.80	0.63
1:L:231:LYS:HE2	1:L:244:MET:HE3	1.81	0.63
1:E:210:PRO:HD3	1:F:140:ARG:NH2	2.14	0.63
1:E:208:GLU:HB2	1:E:211:VAL:HG21	1.81	0.62
1:H:184:GLN:HG2	1:H:184:GLN:O	1.97	0.62
1:N:248:MET:HE2	2:N:302:7DV:O1	1.99	0.62
1:P:108:PRO:HD3	2:P:302:7DV:C5	2.29	0.62
1:D:159:SER:O	1:D:162:ILE:N	2.30	0.62
1:A:154:MET:CG	1:A:211:VAL:HG11	2.26	0.62
1:F:100:THR:HG23	1:F:130:ILE:HD13	1.82	0.62
1:O:195:VAL:HA	1:O:220:GLN:HB3	1.81	0.62
1:A:154:MET:CE	1:A:211:VAL:HG13	2.29	0.62
1:H:161:GLU:HB3	1:H:277:ARG:H	1.64	0.62
1:A:139:GLU:HA	1:A:139:GLU:OE1	2.00	0.62
1:B:249:VAL:HG22	1:B:249:VAL:O	2.00	0.62
1:J:133:VAL:CB	1:J:205:THR:CG2	2.76	0.62
1:C:204:ASP:CB	1:C:210:PRO:HG2	2.29	0.61
1:O:139:GLU:O	1:O:143:GLN:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:ARG:NH1	1:F:126:GLN:OE1	2.33	0.61
1:C:156:PHE:O	1:C:157:ARG:HG3	2.00	0.61
1:A:174:TYR:HE1	1:A:215:GLN:HB2	1.65	0.61
1:A:182:ILE:HD13	1:A:241:VAL:CG1	2.30	0.61
1:L:286:TRP:CH2	1:L:290:GLU:HG3	2.34	0.61
1:E:209:ARG:HB2	1:F:140:ARG:HH12	1.65	0.61
1:N:172:ASN:HD22	1:N:243:THR:CG2	2.14	0.61
1:M:216:LEU:O	1:M:222:ARG:NH1	2.34	0.61
1:A:154:MET:HE2	1:A:211:VAL:HG13	1.82	0.60
1:D:115:LEU:HD11	1:D:291:ILE:HD11	1.83	0.60
1:K:174:TYR:CD1	1:K:261:VAL:HG22	2.37	0.60
1:B:123:ALA:CB	1:B:125:THR:HG23	2.30	0.60
1:H:208:GLU:O	1:H:209:ARG:NE	2.34	0.60
1:J:133:VAL:HB	1:J:205:THR:HG23	1.81	0.60
1:O:252:ASP:HB3	1:O:258:LEU:HD13	1.83	0.60
1:F:295:PHE:HA	1:F:298:LYS:HD2	1.83	0.60
1:H:108:PRO:HB3	2:H:302:7DV:C3	2.32	0.60
1:E:185:GLU:OE2	1:E:197:TYR:OH	2.20	0.60
1:A:154:MET:HE2	1:A:211:VAL:CG1	2.31	0.60
1:B:95:MET:SD	1:D:276:ARG:CD	2.90	0.60
1:D:246:TYR:CE2	1:P:263:PRO:HG2	2.37	0.60
1:F:263:PRO:HG2	1:N:246:TYR:CG	2.36	0.60
1:B:108:PRO:HD3	2:B:302:7DV:C4	2.32	0.60
1:D:163:ASN:HB2	1:D:275:TRP:CZ2	2.37	0.60
1:D:246:TYR:CE2	1:P:263:PRO:CG	2.85	0.60
1:D:252:ASP:HB3	1:D:257:ARG:HG3	1.84	0.60
1:H:185:GLU:HG2	1:H:193:THR:HG21	1.84	0.60
1:H:171:MET:CG	1:L:264:GLU:OE2	2.50	0.59
1:D:101:ILE:CD1	1:D:127:LEU:CD1	2.72	0.59
1:E:203:ALA:CB	1:E:209:ARG:HD2	2.32	0.59
1:B:161:GLU:HA	1:B:277:ARG:HE	1.68	0.59
1:I:231:LYS:NZ	2:I:301:7DV:O1	2.31	0.59
1:L:159:SER:O	1:L:162:ILE:N	2.34	0.59
1:C:204:ASP:HB3	1:C:210:PRO:HG3	1.83	0.59
1:H:155:HIS:CA	1:H:157:ARG:HH12	1.99	0.59
1:J:275:TRP:HZ3	1:J:277:ARG:HA	1.68	0.59
1:H:155:HIS:HB3	1:H:157:ARG:HH22	1.67	0.59
1:P:247:PRO:HB2	2:P:302:7DV:C3	2.33	0.59
1:A:155:HIS:HB3	1:C:155:HIS:CE1	2.38	0.58
1:D:130:ILE:HG21	1:D:140:ARG:NH1	2.18	0.58
1:L:174:TYR:O	1:L:261:VAL:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:248:MET:CG	2:P:302:7DV:O1	2.51	0.58
1:F:185:GLU:OE2	1:F:193:THR:HG21	2.03	0.58
1:P:209:ARG:HG2	1:P:210:PRO:HD2	1.84	0.58
1:N:167:LEU:HD21	1:N:273:MET:CE	2.32	0.58
1:I:104:GLU:OE2	1:I:134:LEU:HD12	2.04	0.58
1:H:154:MET:O	1:H:157:ARG:NH1	2.37	0.58
1:I:132:GLU:OE1	1:I:205:THR:HG21	2.03	0.58
1:M:135:ALA:HB3	1:M:206:ALA:C	2.24	0.58
1:A:161:GLU:HB2	1:A:278:ASP:OD1	2.04	0.58
1:B:255:GLU:HG3	1:B:255:GLU:O	2.03	0.58
1:L:138:TRP:NE1	1:L:154:MET:HG3	2.18	0.58
1:A:161:GLU:HB3	1:A:277:ARG:HB2	1.85	0.58
1:B:161:GLU:OE1	1:B:277:ARG:NH2	2.36	0.58
1:F:141:LEU:HD23	1:F:162:ILE:HD11	1.85	0.58
1:A:206:ALA:HB1	1:C:210:PRO:CA	2.33	0.58
1:E:134:LEU:HD11	2:E:301:7DV:C4	2.33	0.58
1:E:205:THR:C	1:E:207:ARG:H	2.06	0.58
1:G:194:ARG:HH12	1:G:216:LEU:HA	1.68	0.58
1:H:227:THR:HG23	1:H:230:ASP:H	1.69	0.58
1:A:245:PRO:HG2	1:A:248:MET:HE2	1.86	0.57
1:G:221:PRO:HA	1:H:126:GLN:OE1	2.03	0.57
1:N:248:MET:CE	2:N:302:7DV:O1	2.51	0.57
1:A:172:ASN:OD1	2:A:301:7DV:O1	2.21	0.57
1:B:174:TYR:CD2	1:B:261:VAL:HG21	2.39	0.57
1:F:119:LEU:HB3	1:F:125:THR:HG23	1.86	0.57
1:O:140:ARG:HD2	1:O:145:ARG:NH1	2.19	0.57
1:A:156:PHE:HB3	1:A:209:ARG:HG3	1.86	0.57
1:J:153:ASP:HB2	1:J:272:ILE:CD1	2.34	0.57
1:P:275:TRP:CD2	1:P:288:LEU:HD11	2.38	0.57
1:G:143:GLN:HE21	1:G:145:ARG:NH1	2.02	0.57
1:K:174:TYR:C	1:K:174:TYR:HD1	2.07	0.57
1:A:189:LEU:HD21	1:A:265:SER:OG	2.04	0.57
1:B:139:GLU:OE1	1:B:208:GLU:HB2	2.05	0.57
1:D:130:ILE:HG21	1:D:140:ARG:HH11	1.70	0.57
1:D:277:ARG:HG2	1:D:278:ASP:OD1	2.05	0.57
1:F:273:MET:HE1	1:F:291:ILE:HB	1.87	0.57
1:L:167:LEU:HD21	1:L:273:MET:HE3	1.86	0.57
1:P:161:GLU:O	1:P:276:ARG:HA	2.04	0.57
1:F:206:ALA:HB3	1:F:209:ARG:HB3	1.87	0.57
1:F:153:ASP:HA	1:F:156:PHE:HZ	1.69	0.57
1:J:104:GLU:OE1	1:J:106:LEU:HD12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:154:MET:HG3	1:K:156:PHE:HE1	1.65	0.57
1:A:180:HIS:ND1	1:A:182:ILE:HG12	2.20	0.57
1:O:198:ARG:NH2	1:P:117:ASP:OD1	2.38	0.56
1:A:138:TRP:CE3	1:A:157:ARG:HG3	2.40	0.56
1:C:126:GLN:HA	1:C:126:GLN:NE2	2.21	0.56
1:E:154:MET:HB3	1:E:156:PHE:CE2	2.40	0.56
1:E:157:ARG:HE	1:E:160:SER:HA	1.69	0.56
1:F:244:MET:HE1	1:F:248:MET:CE	2.36	0.56
1:G:174:TYR:OH	1:G:215:GLN:HB3	2.05	0.56
1:G:214:VAL:HG13	2:G:301:7DV:C7	2.36	0.56
1:H:255:GLU:O	1:H:255:GLU:HG3	2.05	0.56
1:I:210:PRO:HB2	1:K:156:PHE:CG	2.41	0.56
1:K:208:GLU:HA	1:L:140:ARG:HH12	1.70	0.56
1:N:161:GLU:CD	1:N:161:GLU:N	2.57	0.56
1:O:212:LEU:HG	1:O:213:THR:N	2.18	0.56
1:C:142:GLU:OE1	1:C:142:GLU:HA	2.03	0.56
1:F:166:LYS:N	1:F:166:LYS:HD3	2.20	0.56
1:O:142:GLU:HG2	1:O:156:PHE:CE2	2.39	0.56
1:O:208:GLU:HG2	1:O:209:ARG:HG2	1.88	0.56
1:P:134:LEU:HD21	2:P:301:7DV:C4	2.35	0.56
1:K:268:GLU:OE2	1:M:286:TRP:HD1	1.88	0.56
1:B:95:MET:SD	1:D:276:ARG:HD2	2.45	0.56
1:B:196:LYS:HD3	1:B:197:TYR:CZ	2.41	0.56
1:D:115:LEU:HD11	1:D:291:ILE:HD13	1.86	0.56
1:F:262:SER:OG	1:F:264:GLU:HG3	2.05	0.56
1:M:268:GLU:OE2	1:O:286:TRP:HD1	1.88	0.56
1:J:143:GLN:NE2	1:J:208:GLU:OE2	2.38	0.56
1:J:183:HIS:HB3	1:J:259:ARG:HH21	1.70	0.56
1:B:273:MET:HE1	1:B:291:ILE:HB	1.88	0.56
1:D:104:GLU:OE2	2:D:301:7DV:O9	2.23	0.56
1:O:174:TYR:CE2	1:O:265:SER:HB2	2.40	0.56
1:P:248:MET:HB2	2:P:302:7DV:C1	2.36	0.56
1:F:231:LYS:HE3	1:F:244:MET:SD	2.46	0.56
1:F:248:MET:SD	2:F:302:7DV:O1	2.64	0.56
1:O:174:TYR:HD2	1:O:265:SER:HB2	1.70	0.56
1:A:185:GLU:HG2	1:A:193:THR:HG21	1.88	0.56
1:E:210:PRO:HD3	1:F:140:ARG:HH22	1.71	0.56
1:K:214:VAL:HG13	1:K:243:THR:HG23	1.86	0.56
1:P:248:MET:SD	2:P:302:7DV:O1	2.63	0.56
1:E:228:ILE:HG12	1:E:248:MET:HE1	1.89	0.55
1:E:282:GLU:CG	1:E:283:ALA:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:204:ASP:HB3	1:O:210:PRO:CG	2.22	0.55
1:H:214:VAL:CG2	4:H:403:HOH:O	2.53	0.55
1:H:214:VAL:HG21	4:H:403:HOH:O	2.06	0.55
1:B:95:MET:SD	1:D:276:ARG:HD3	2.47	0.55
1:C:191:GLU:HA	1:C:194:ARG:HG2	1.89	0.55
1:E:220:GLN:HG2	1:E:221:PRO:HD2	1.89	0.55
1:G:239:LEU:HD11	1:H:113:PHE:HB3	1.87	0.55
1:A:218:ASP:O	1:A:219:LYS:HD3	2.07	0.55
1:G:181:PRO:HB2	1:G:197:TYR:HE2	1.70	0.55
1:C:228:ILE:HD12	2:C:301:7DV:C6	2.37	0.55
1:E:174:TYR:CE2	1:E:265:SER:HB2	2.41	0.55
1:E:217:LEU:O	1:E:218:ASP:HB3	2.06	0.55
1:L:96:GLU:HA	1:L:124:ASN:HB3	1.88	0.55
1:O:218:ASP:HA	1:O:222:ARG:HH22	1.72	0.55
1:A:206:ALA:HB1	1:C:210:PRO:CB	2.37	0.55
1:C:248:MET:HE2	2:C:302:7DV:C6	2.36	0.55
1:J:206:ALA:CB	1:J:210:PRO:HD2	2.37	0.55
1:N:160:SER:O	1:N:277:ARG:NH1	2.40	0.55
1:B:212:LEU:HA	1:B:216:LEU:HD13	1.89	0.54
1:A:170:LEU:HD23	1:A:269:ILE:HD11	1.89	0.54
1:N:134:LEU:CD2	2:N:301:7DV:O9	2.55	0.54
1:O:195:VAL:CG1	1:O:217:LEU:HD11	2.37	0.54
1:H:115:LEU:HB3	1:H:119:LEU:CD2	2.38	0.54
1:O:245:PRO:HG2	1:O:248:MET:HE2	1.88	0.54
1:H:262:SER:OG	1:H:264:GLU:HG2	2.08	0.54
1:K:266:THR:HG21	1:M:122:LYS:HA	1.89	0.54
1:M:174:TYR:HB3	1:M:261:VAL:HG22	1.90	0.54
1:P:157:ARG:O	1:P:162:ILE:HD11	2.07	0.54
1:B:95:MET:HE2	1:D:161:GLU:HG2	1.88	0.54
1:F:195:VAL:HG12	1:F:217:LEU:HD11	1.89	0.54
1:L:115:LEU:HD21	1:L:291:ILE:CD1	2.38	0.54
1:N:157:ARG:NH2	1:N:158:SER:HB3	2.22	0.54
1:J:133:VAL:N	1:J:205:THR:CG2	2.69	0.54
1:J:231:LYS:HE2	1:J:244:MET:HE3	1.91	0.54
1:A:126:GLN:OE1	1:B:222:ARG:O	2.26	0.53
1:A:155:HIS:ND1	1:A:211:VAL:HG12	2.22	0.53
1:A:175:VAL:HG22	1:A:176:ALA:H	1.74	0.53
1:A:180:HIS:CE1	1:A:182:ILE:HG23	2.43	0.53
1:E:157:ARG:O	1:E:157:ARG:NE	2.41	0.53
1:E:207:ARG:O	1:E:207:ARG:HG2	2.08	0.53
1:A:106:LEU:CD2	2:A:301:7DV:C5	2.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:THR:N	1:B:226:SER:OG	2.32	0.53
1:A:194:ARG:NH2	1:A:217:LEU:HG	2.24	0.53
1:G:194:ARG:NH1	1:G:216:LEU:HA	2.23	0.53
1:H:228:ILE:HG12	1:H:248:MET:HE1	1.91	0.53
1:N:215:GLN:O	1:N:216:LEU:HB3	2.06	0.53
1:I:138:TRP:NE1	1:I:154:MET:HB3	2.23	0.53
1:J:133:VAL:N	1:J:205:THR:HG23	2.19	0.53
1:O:211:VAL:HG12	1:O:214:VAL:HG13	1.90	0.53
1:N:134:LEU:HD21	2:N:301:7DV:C4	2.38	0.53
1:M:171:MET:HE2	1:O:286:TRP:HE1	1.73	0.53
1:H:264:GLU:HB3	1:L:171:MET:HE3	1.90	0.53
1:I:122:LYS:NZ	1:I:282:GLU:HG2	2.24	0.53
1:L:115:LEU:HD21	1:L:291:ILE:HD11	1.89	0.53
1:O:161:GLU:OE2	1:O:276:ARG:NE	2.42	0.53
1:B:108:PRO:HB3	2:B:302:7DV:C2	2.39	0.53
1:B:278:ASP:O	1:D:281:GLY:HA2	2.08	0.53
1:C:214:VAL:HG12	1:C:215:GLN:N	2.24	0.53
1:N:158:SER:OG	1:N:159:SER:N	2.42	0.53
1:L:284:LYS:O	1:L:288:LEU:HD12	2.07	0.53
1:A:161:GLU:CB	1:A:277:ARG:HD2	2.40	0.52
1:A:175:VAL:CG2	1:A:258:LEU:HB3	2.38	0.52
1:K:174:TYR:CD1	1:K:175:VAL:N	2.77	0.52
1:N:231:LYS:NZ	2:N:301:7DV:O1	2.43	0.52
1:G:204:ASP:H	1:G:210:PRO:HD3	1.75	0.52
1:H:264:GLU:N	1:H:264:GLU:OE1	2.39	0.52
1:I:99:LEU:HD12	1:I:147:ASP:OD2	2.10	0.52
1:J:95:MET:SD	1:L:276:ARG:NH2	2.82	0.52
1:O:286:TRP:CZ2	1:O:290:GLU:HG3	2.44	0.52
1:E:174:TYR:HD2	1:E:265:SER:HB2	1.74	0.52
1:F:194:ARG:HH22	1:F:216:LEU:HA	1.73	0.52
1:L:161:GLU:O	1:L:276:ARG:HA	2.09	0.52
1:D:97:THR:OG1	1:D:125:THR:HG23	2.10	0.52
1:D:249:VAL:O	1:D:249:VAL:HG12	2.09	0.52
1:L:275:TRP:CD2	1:L:288:LEU:HD21	2.44	0.52
1:M:206:ALA:HA	1:M:207:ARG:HD2	1.91	0.52
1:P:104:GLU:OE2	2:P:301:7DV:O9	2.28	0.52
1:O:161:GLU:CD	1:O:161:GLU:H	2.13	0.52
1:A:207:ARG:HG3	1:C:209:ARG:HH21	1.75	0.52
1:I:264:GLU:OE1	1:I:265:SER:N	2.42	0.52
1:A:104:GLU:OE2	1:A:134:LEU:HD22	2.09	0.52
1:M:216:LEU:HD23	1:M:218:ASP:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:THR:HG22	1:E:209:ARG:CZ	2.40	0.52
1:D:286:TRP:O	1:D:289:ARG:HG2	2.10	0.52
1:F:181:PRO:HB2	1:F:197:TYR:HE2	1.75	0.52
1:B:106:LEU:HD21	2:B:301:7DV:C4	2.39	0.52
1:F:194:ARG:NH2	1:F:216:LEU:HA	2.24	0.52
1:F:244:MET:CE	1:F:248:MET:CE	2.88	0.52
1:H:246:TYR:CG	1:L:263:PRO:HG2	2.45	0.52
1:I:185:GLU:HG2	1:I:193:THR:CG2	2.37	0.52
1:O:170:LEU:HD21	1:O:245:PRO:HB3	1.92	0.52
1:I:210:PRO:HB2	1:K:156:PHE:CD1	2.45	0.51
1:K:140:ARG:HG3	1:K:145:ARG:HB3	1.91	0.51
1:D:100:THR:HG23	1:D:130:ILE:HD13	1.90	0.51
1:N:150:ILE:N	1:N:150:ILE:HD12	2.24	0.51
1:B:145:ARG:NH1	1:C:222:ARG:HH22	2.03	0.51
1:C:231:LYS:NZ	2:C:301:7DV:O1	2.40	0.51
1:G:209:ARG:HD3	4:H:401:HOH:O	2.10	0.51
1:H:264:GLU:HA	1:L:171:MET:HE3	1.92	0.51
1:I:211:VAL:CG1	1:K:139:GLU:HA	2.41	0.51
1:L:183:HIS:CE1	1:L:259:ARG:HB3	2.29	0.51
1:A:279:SER:O	1:A:280:MET:SD	2.68	0.51
1:I:158:SER:HB2	1:K:155:HIS:CE1	2.46	0.51
1:I:195:VAL:HG11	1:I:219:LYS:HE2	1.93	0.51
1:L:142:GLU:CD	1:L:156:PHE:HZ	2.13	0.51
1:M:134:LEU:HD21	2:M:301:7DV:O9	2.10	0.51
1:B:108:PRO:HD3	2:B:302:7DV:C5	2.40	0.51
1:E:205:THR:HG22	1:E:209:ARG:NH2	2.25	0.51
1:G:286:TRP:CZ2	1:G:290:GLU:HG3	2.46	0.51
1:I:126:GLN:HA	1:I:126:GLN:NE2	2.25	0.51
1:A:138:TRP:HB3	1:A:157:ARG:CB	2.35	0.51
1:K:99:LEU:HD12	1:K:147:ASP:OD2	2.11	0.51
1:M:179:ASP:OD1	1:M:179:ASP:N	2.44	0.51
1:B:228:ILE:HG12	1:B:248:MET:HE1	1.92	0.51
1:E:104:GLU:OE2	2:E:301:7DV:O9	2.27	0.51
1:E:213:THR:HG23	1:E:216:LEU:HA	1.93	0.51
1:F:141:LEU:CD2	1:F:162:ILE:HD11	2.41	0.51
1:I:154:MET:HG3	1:K:156:PHE:CD1	2.46	0.51
1:M:215:GLN:HE22	1:M:222:ARG:HD3	1.74	0.51
1:P:106:LEU:HD21	2:P:301:7DV:C5	2.40	0.51
1:B:153:ASP:HB3	1:B:272:ILE:HD11	1.92	0.51
1:B:249:VAL:HG23	1:B:258:LEU:HD12	1.92	0.51
1:C:170:LEU:HD21	1:C:245:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:156:PHE:O	1:M:157:ARG:HG3	2.11	0.51
1:O:245:PRO:HG2	1:O:248:MET:CE	2.41	0.51
1:B:263:PRO:O	1:B:266:THR:HG22	2.11	0.50
1:K:208:GLU:C	1:K:210:PRO:HD3	2.32	0.50
1:L:247:PRO:HB2	2:L:302:7DV:O9	2.11	0.50
1:M:170:LEU:HB3	1:M:269:ILE:HG23	1.92	0.50
1:N:100:THR:HG23	1:N:130:ILE:HD13	1.91	0.50
1:H:99:LEU:HD13	1:H:100:THR:N	2.26	0.50
1:H:110:PRO:HB2	2:H:303:7DV:C7	2.40	0.50
1:O:220:GLN:H	1:O:222:ARG:HH21	1.59	0.50
1:B:153:ASP:HB3	1:B:272:ILE:CD1	2.41	0.50
1:L:170:LEU:HD23	1:L:172:ASN:ND2	2.27	0.50
1:B:125:THR:HG21	1:B:283:ALA:HB2	1.94	0.50
1:H:174:TYR:CD2	1:H:261:VAL:HG21	2.46	0.50
1:H:287:CYS:O	1:H:291:ILE:HG12	2.11	0.50
1:L:143:GLN:OE1	1:L:145:ARG:NH1	2.44	0.50
1:A:138:TRP:HB2	1:A:209:ARG:HD3	1.94	0.50
1:B:279:SER:HA	1:D:280:MET:O	2.12	0.50
1:D:262:SER:OG	1:D:264:GLU:HG2	2.11	0.50
1:F:185:GLU:OE1	1:F:188:PRO:HA	2.12	0.50
1:K:170:LEU:HD21	1:K:245:PRO:HB3	1.93	0.50
1:A:175:VAL:HG22	1:A:176:ALA:N	2.26	0.50
1:C:154:MET:O	1:C:155:HIS:HB2	2.11	0.50
1:M:171:MET:CE	1:O:118:LYS:HE2	2.41	0.50
1:A:170:LEU:HD21	1:A:245:PRO:HB3	1.94	0.50
1:D:246:TYR:CG	1:P:263:PRO:HG2	2.46	0.50
1:E:170:LEU:HD21	1:E:245:PRO:HB3	1.93	0.50
1:E:203:ALA:HB3	1:E:209:ARG:HD2	1.93	0.50
1:I:252:ASP:OD1	1:I:257:ARG:NH2	2.45	0.50
1:J:215:GLN:HE21	1:J:217:LEU:HD21	1.77	0.50
1:B:106:LEU:HD21	2:B:301:7DV:C5	2.42	0.50
1:F:159:SER:O	1:F:162:ILE:HG22	2.11	0.50
1:O:116:ILE:HD13	1:P:223:LEU:HD22	1.94	0.50
1:P:113:PHE:N	1:P:114:PRO:CD	2.75	0.50
1:A:286:TRP:CZ2	1:A:290:GLU:HG3	2.47	0.50
1:G:113:PHE:N	1:G:114:PRO:CD	2.75	0.50
1:J:113:PHE:N	1:J:114:PRO:CD	2.75	0.50
1:N:161:GLU:OE2	1:N:162:ILE:HG12	2.12	0.50
1:P:134:LEU:CD2	2:P:301:7DV:C4	2.90	0.50
1:I:167:LEU:HD21	1:I:273:MET:CE	2.42	0.49
1:C:113:PHE:N	1:C:114:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:174:TYR:OH	1:K:241:VAL:CA	2.60	0.49
1:C:203:ALA:HB1	1:C:207:ARG:H	1.75	0.49
1:F:207:ARG:HA	1:F:207:ARG:NE	2.27	0.49
1:B:113:PHE:N	1:B:114:PRO:CD	2.75	0.49
1:G:209:ARG:CD	4:H:401:HOH:O	2.60	0.49
1:I:217:LEU:HD23	1:I:219:LYS:NZ	2.28	0.49
1:N:113:PHE:N	1:N:114:PRO:CD	2.75	0.49
1:N:286:TRP:CE2	1:N:290:GLU:HG3	2.47	0.49
1:O:207:ARG:O	1:O:208:GLU:CB	2.60	0.49
1:D:173:VAL:HG11	1:D:260:VAL:HG22	1.95	0.49
1:E:187:GLU:O	1:E:187:GLU:HG2	2.12	0.49
1:E:286:TRP:CZ2	1:E:290:GLU:HG3	2.47	0.49
1:G:170:LEU:HB3	1:G:269:ILE:HG23	1.95	0.49
1:I:154:MET:O	1:K:156:PHE:C	2.49	0.49
1:N:286:TRP:CZ2	1:N:290:GLU:HG3	2.48	0.49
1:A:175:VAL:HG21	1:A:258:LEU:HB3	1.95	0.49
1:A:210:PRO:HG3	1:C:138:TRP:CD1	2.48	0.49
1:B:167:LEU:N	1:B:167:LEU:HD22	2.28	0.49
1:F:113:PHE:N	1:F:114:PRO:CD	2.75	0.49
1:I:286:TRP:CZ2	1:I:290:GLU:HG3	2.48	0.49
1:M:193:THR:HA	1:M:196:LYS:HD2	1.94	0.49
1:M:205:THR:HG22	4:M:407:HOH:O	2.12	0.49
1:I:212:LEU:CD2	1:I:212:LEU:H	2.22	0.49
1:L:287:CYS:O	1:L:291:ILE:HG12	2.11	0.49
1:A:210:PRO:HG3	1:C:138:TRP:CG	2.48	0.49
1:B:145:ARG:NH2	1:C:222:ARG:HH12	2.05	0.49
1:B:170:LEU:HD21	1:B:245:PRO:HB3	1.95	0.49
1:B:249:VAL:HG22	1:B:253:ILE:HG13	1.94	0.49
1:H:110:PRO:HB2	2:H:303:7DV:C3	2.42	0.49
1:K:113:PHE:N	1:K:114:PRO:CD	2.75	0.49
1:K:214:VAL:HG12	1:K:214:VAL:O	2.13	0.49
1:M:286:TRP:CZ2	1:M:290:GLU:HG3	2.48	0.49
1:E:122:LYS:HD2	1:E:286:TRP:CG	2.48	0.49
1:H:140:ARG:HD3	1:H:143:GLN:NE2	2.28	0.49
1:M:159:SER:C	1:M:161:GLU:H	2.15	0.49
1:E:113:PHE:N	1:E:114:PRO:CD	2.75	0.49
1:F:273:MET:HE1	1:F:292:PRO:HD3	1.95	0.49
1:L:194:ARG:NH1	1:L:215:GLN:HG3	2.28	0.49
1:A:208:GLU:HB3	1:A:209:ARG:NH2	2.17	0.48
1:E:187:GLU:HG2	1:E:190:SER:HB2	1.94	0.48
1:F:209:ARG:H	1:F:209:ARG:HD3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:PHE:N	1:I:114:PRO:CD	2.76	0.48
1:I:156:PHE:CD2	1:I:157:ARG:HG3	2.47	0.48
1:L:135:ALA:CB	1:L:210:PRO:HG3	2.43	0.48
1:P:153:ASP:HB3	1:P:272:ILE:HD11	1.95	0.48
1:H:246:TYR:CD2	1:L:263:PRO:HG2	2.48	0.48
1:K:286:TRP:CZ2	1:K:290:GLU:HG3	2.48	0.48
1:M:113:PHE:N	1:M:114:PRO:CD	2.76	0.48
1:C:219:LYS:O	1:C:219:LYS:HG3	2.13	0.48
1:E:209:ARG:NH1	1:E:226:SER:OG	2.46	0.48
1:G:214:VAL:HG12	1:G:215:GLN:N	2.24	0.48
1:I:218:ASP:O	1:I:219:LYS:HD3	2.13	0.48
1:A:217:LEU:HD13	1:A:218:ASP:O	2.12	0.48
1:B:243:THR:OG1	2:B:301:7DV:C7	2.62	0.48
1:H:201:ALA:HB2	1:H:222:ARG:HH11	1.78	0.48
1:L:113:PHE:N	1:L:114:PRO:CD	2.75	0.48
1:N:202:VAL:HG23	1:N:231:LYS:HD2	1.95	0.48
1:O:113:PHE:N	1:O:114:PRO:CD	2.76	0.48
1:D:113:PHE:N	1:D:114:PRO:CD	2.76	0.48
1:F:216:LEU:HD12	1:F:222:ARG:HH21	1.77	0.48
1:H:113:PHE:N	1:H:114:PRO:CD	2.75	0.48
1:M:231:LYS:NZ	2:M:301:7DV:O1	2.41	0.48
1:H:132:GLU:OE1	1:H:205:THR:OG1	2.14	0.48
1:I:205:THR:OG1	1:I:206:ALA:N	2.45	0.48
1:C:174:TYR:HD2	1:C:265:SER:HB2	1.78	0.48
1:C:207:ARG:HA	1:D:140:ARG:HH12	1.77	0.48
1:F:134:LEU:HD21	2:F:301:7DV:C4	2.43	0.48
1:J:170:LEU:HD21	1:J:245:PRO:HB3	1.96	0.48
1:K:134:LEU:HD21	2:K:301:7DV:C3	2.44	0.48
1:A:113:PHE:N	1:A:114:PRO:CD	2.76	0.48
1:A:218:ASP:CB	1:D:207:ARG:HD2	2.40	0.48
1:A:222:ARG:NH2	1:B:98:HIS:CE1	2.81	0.48
1:H:111:ALA:HA	2:H:303:7DV:O1	2.14	0.48
1:M:135:ALA:C	1:M:206:ALA:HB3	2.34	0.48
1:C:220:GLN:O	1:C:222:ARG:CD	2.62	0.48
1:I:138:TRP:HE1	1:I:154:MET:HB3	1.78	0.48
1:I:212:LEU:HD23	1:I:212:LEU:N	2.26	0.48
1:J:167:LEU:HD21	1:J:273:MET:CE	2.42	0.48
1:G:212:LEU:HG	1:G:218:ASP:OD2	2.14	0.48
1:H:115:LEU:HD11	1:H:291:ILE:CD1	2.44	0.48
1:H:170:LEU:HD21	1:H:245:PRO:HB3	1.96	0.48
1:M:170:LEU:HD21	1:M:245:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:174:TYR:CE1	1:O:243:THR:HG23	2.48	0.48
1:C:220:GLN:O	1:C:222:ARG:HD2	2.14	0.47
1:D:286:TRP:CZ2	1:D:290:GLU:HG3	2.49	0.47
1:F:138:TRP:CE2	1:F:156:PHE:HE1	2.31	0.47
1:F:170:LEU:HD21	1:F:245:PRO:HB3	1.96	0.47
1:G:134:LEU:HA	1:G:154:MET:HE1	1.96	0.47
1:I:219:LYS:O	1:I:219:LYS:HG2	2.14	0.47
1:E:203:ALA:HB1	1:E:209:ARG:HD2	1.96	0.47
1:H:152:PRO:HB3	1:H:269:ILE:CG2	2.44	0.47
1:I:158:SER:CB	1:K:155:HIS:CE1	2.97	0.47
1:I:215:GLN:HG2	1:I:216:LEU:N	2.20	0.47
1:N:134:LEU:HD21	2:N:301:7DV:O9	2.14	0.47
1:E:219:LYS:O	1:E:220:GLN:HB2	2.14	0.47
1:G:180:HIS:HE1	1:G:197:TYR:CD2	2.32	0.47
1:J:273:MET:HE1	1:J:291:ILE:HB	1.95	0.47
1:O:174:TYR:HD2	1:O:265:SER:CB	2.27	0.47
1:E:187:GLU:CG	1:E:190:SER:HB2	2.44	0.47
1:F:211:VAL:HG12	1:F:213:THR:HG23	1.96	0.47
1:K:203:ALA:HB1	1:K:209:ARG:H	1.79	0.47
1:A:138:TRP:CZ3	1:A:274:ALA:HB3	2.49	0.47
1:D:202:VAL:HG23	1:D:231:LYS:HD2	1.97	0.47
1:I:194:ARG:HH12	1:I:216:LEU:HA	1.78	0.47
1:A:228:ILE:HD12	1:A:229:GLU:N	2.29	0.47
1:B:249:VAL:HG23	1:B:258:LEU:CD1	2.44	0.47
1:G:211:VAL:O	1:G:212:LEU:CB	2.62	0.47
1:G:255:GLU:OE1	1:G:257:ARG:NH2	2.48	0.47
1:H:189:LEU:CD2	1:H:265:SER:OG	2.62	0.47
1:L:167:LEU:HD21	1:L:273:MET:CE	2.44	0.47
1:M:195:VAL:HA	1:M:220:GLN:HG3	1.95	0.47
1:B:152:PRO:HB3	1:B:269:ILE:HG21	1.97	0.47
1:B:153:ASP:OD1	1:B:153:ASP:N	2.46	0.47
1:C:259:ARG:NH1	1:F:196:LYS:HE3	2.29	0.47
1:C:286:TRP:CZ2	1:C:290:GLU:HG3	2.50	0.47
1:F:195:VAL:HA	1:F:220:GLN:HG3	1.95	0.47
1:G:185:GLU:CD	1:G:193:THR:HG21	2.35	0.47
1:H:189:LEU:HD22	1:H:265:SER:HG	1.78	0.47
1:J:255:GLU:CG	1:J:255:GLU:O	2.62	0.47
1:K:212:LEU:N	1:K:212:LEU:HD23	2.30	0.47
1:L:162:ILE:HD13	1:L:276:ARG:HG2	1.96	0.47
1:N:99:LEU:HD12	1:N:147:ASP:OD2	2.15	0.47
1:O:142:GLU:CG	1:O:156:PHE:HE2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HB3	1:A:269:ILE:HG13	1.96	0.47
1:B:167:LEU:HD21	1:B:273:MET:CB	2.44	0.47
1:C:133:VAL:HG13	2:C:301:7DV:O9	2.15	0.47
1:E:211:VAL:HG12	1:E:212:LEU:N	2.30	0.47
1:I:174:TYR:CD2	1:I:261:VAL:HG21	2.50	0.47
1:M:134:LEU:HD21	2:M:301:7DV:C4	2.45	0.47
1:B:174:TYR:HD2	1:B:261:VAL:HG21	1.80	0.47
1:E:263:PRO:HG2	1:G:124:ASN:OD1	2.15	0.47
1:L:160:SER:O	1:L:163:ASN:ND2	2.43	0.47
1:A:133:VAL:CG1	1:A:134:LEU:HD23	2.45	0.47
1:I:170:LEU:HD21	1:I:245:PRO:HB3	1.97	0.47
1:O:195:VAL:HG13	1:O:217:LEU:HD11	1.96	0.47
1:B:217:LEU:HB3	1:B:220:GLN:OE1	2.15	0.46
1:B:227:THR:HG23	1:B:230:ASP:H	1.80	0.46
1:E:226:SER:HB2	1:F:131:THR:H	1.79	0.46
1:J:209:ARG:N	1:J:210:PRO:HD3	2.30	0.46
1:N:248:MET:HE2	1:N:248:MET:HB2	1.79	0.46
1:O:276:ARG:HD3	1:O:278:ASP:OD2	2.15	0.46
1:E:219:LYS:O	1:E:219:LYS:CG	2.63	0.46
1:E:236:LEU:HD23	1:E:258:LEU:HD11	1.96	0.46
1:E:282:GLU:OE1	1:E:282:GLU:N	2.48	0.46
1:H:215:GLN:HG3	1:H:216:LEU:H	1.80	0.46
1:J:108:PRO:HD3	2:J:302:7DV:C4	2.44	0.46
1:L:99:LEU:HD12	1:L:147:ASP:OD2	2.15	0.46
1:N:190:SER:O	1:N:194:ARG:HG3	2.15	0.46
1:D:155:HIS:HB3	1:D:157:ARG:HD2	1.97	0.46
1:F:123:ALA:HB3	1:F:125:THR:HG22	1.98	0.46
1:I:156:PHE:O	1:I:157:ARG:HG2	2.16	0.46
1:I:179:ASP:OD1	1:I:179:ASP:N	2.44	0.46
1:E:191:GLU:HA	1:E:194:ARG:HH11	1.80	0.46
1:D:228:ILE:HG12	1:D:248:MET:HE1	1.98	0.46
1:F:280:MET:HE1	1:F:285:SER:HB3	1.98	0.46
1:G:251:LYS:NZ	1:G:255:GLU:OE2	2.46	0.46
1:H:161:GLU:HG2	1:H:278:ASP:HB3	1.97	0.46
1:H:183:HIS:CE1	1:H:259:ARG:HD2	2.51	0.46
1:J:215:GLN:H	1:J:215:GLN:CD	2.17	0.46
1:K:293:LYS:HA	1:K:296:ASN:OD1	2.16	0.46
1:B:95:MET:HB2	1:D:142:GLU:CA	2.46	0.46
1:F:161:GLU:O	1:F:276:ARG:HA	2.15	0.46
1:F:244:MET:CE	1:F:245:PRO:HD2	2.45	0.46
1:H:286:TRP:CE2	1:H:290:GLU:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:227:THR:HG22	1:J:229:GLU:H	1.80	0.46
1:N:170:LEU:HD23	1:N:172:ASN:OD1	2.15	0.46
1:B:286:TRP:CZ2	1:B:290:GLU:HG3	2.50	0.46
1:H:162:ILE:HA	1:H:275:TRP:O	2.16	0.46
1:J:202:VAL:HG23	1:J:231:LYS:HD2	1.97	0.46
1:C:171:MET:CE	1:E:118:LYS:HE2	2.45	0.46
1:D:252:ASP:CB	1:D:257:ARG:HG3	2.45	0.46
1:H:211:VAL:CG2	1:H:213:THR:HG23	2.38	0.46
1:K:268:GLU:OE2	1:M:289:ARG:NH2	2.48	0.46
1:L:115:LEU:HB3	1:L:119:LEU:HD12	1.96	0.46
1:O:207:ARG:HB2	1:O:210:PRO:HG3	1.98	0.46
1:C:116:ILE:HD13	1:D:223:LEU:HD22	1.97	0.46
1:C:286:TRP:CE2	1:C:290:GLU:HG3	2.51	0.46
1:L:115:LEU:CD1	1:L:294:LEU:HD11	2.39	0.46
1:M:134:LEU:HD22	1:M:211:VAL:CG1	2.43	0.46
1:O:209:ARG:HH12	1:O:224:THR:HG21	1.81	0.46
1:O:236:LEU:HD23	1:O:258:LEU:CD1	2.46	0.46
1:F:119:LEU:CD2	1:F:125:THR:HG21	2.40	0.46
1:H:171:MET:HG2	1:L:264:GLU:OE2	2.15	0.46
1:K:174:TYR:CD1	1:K:261:VAL:CG2	2.99	0.46
1:O:257:ARG:C	1:O:258:LEU:HD12	2.36	0.46
1:B:108:PRO:HB3	2:B:302:7DV:C3	2.47	0.45
1:F:195:VAL:CG1	1:F:217:LEU:HD21	2.46	0.45
1:F:244:MET:CE	1:F:248:MET:HE2	2.46	0.45
1:M:286:TRP:CE2	1:M:290:GLU:HG3	2.51	0.45
1:P:169:THR:HG21	1:P:268:GLU:OE1	2.16	0.45
1:P:189:LEU:HD21	1:P:262:SER:CB	2.46	0.45
1:A:162:ILE:HD12	1:A:275:TRP:O	2.17	0.45
1:D:195:VAL:HA	1:D:220:GLN:HG3	1.98	0.45
1:I:135:ALA:CB	1:I:208:GLU:OE1	2.64	0.45
1:I:154:MET:CE	1:K:156:PHE:CE1	2.99	0.45
1:K:174:TYR:HH	1:K:241:VAL:CG1	2.17	0.45
1:P:142:GLU:OE2	1:P:209:ARG:NH1	2.49	0.45
1:C:194:ARG:CZ	1:C:217:LEU:HD22	2.46	0.45
1:D:170:LEU:HD21	1:D:245:PRO:HB3	1.98	0.45
1:H:143:GLN:HE21	1:H:145:ARG:HB2	1.82	0.45
1:M:209:ARG:HH21	1:M:211:VAL:CG1	2.30	0.45
1:N:179:ASP:OD1	1:N:179:ASP:N	2.42	0.45
1:P:195:VAL:HA	1:P:220:GLN:HG3	1.97	0.45
1:D:246:TYR:CZ	1:P:263:PRO:CG	3.00	0.45
1:K:214:VAL:HB	1:K:216:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:209:ARG:N	1:O:210:PRO:HD3	2.31	0.45
1:A:174:TYR:HD2	1:A:265:SER:HB2	1.81	0.45
1:D:108:PRO:HB3	2:D:302:7DV:C1	2.47	0.45
1:I:167:LEU:HD21	1:I:273:MET:HE2	1.98	0.45
1:I:183:HIS:CE1	1:I:259:ARG:HD3	2.52	0.45
1:A:106:LEU:CD2	2:A:301:7DV:C6	2.77	0.45
1:D:286:TRP:CE2	1:D:290:GLU:HG3	2.51	0.45
1:F:244:MET:HE3	1:F:244:MET:HB3	1.66	0.45
1:F:248:MET:HE2	1:F:248:MET:HB3	1.85	0.45
1:M:161:GLU:HG2	1:M:277:ARG:CD	2.46	0.45
1:P:286:TRP:CH2	1:P:290:GLU:HG2	2.51	0.45
1:A:194:ARG:HH12	1:A:217:LEU:HD23	1.81	0.45
1:E:231:LYS:HE3	1:E:242:ALA:HB1	1.98	0.45
1:I:134:LEU:HD23	1:I:212:LEU:HB2	1.98	0.45
1:I:208:GLU:O	1:I:209:ARG:HB3	2.16	0.45
1:I:286:TRP:CE2	1:I:290:GLU:HG3	2.52	0.45
1:C:247:PRO:HB2	2:C:302:7DV:O9	2.17	0.45
1:D:101:ILE:HD11	1:D:127:LEU:CD1	2.11	0.45
1:B:195:VAL:HA	1:B:220:GLN:HG3	1.99	0.45
1:D:99:LEU:HD12	1:D:147:ASP:OD2	2.17	0.45
1:E:263:PRO:HB2	1:G:123:ALA:HA	1.99	0.45
1:F:134:LEU:HD21	2:F:301:7DV:C3	2.47	0.45
1:G:185:GLU:OE2	1:G:193:THR:HG21	2.17	0.45
1:G:216:LEU:HB3	1:G:220:GLN:OE1	2.16	0.45
1:H:215:GLN:CG	1:H:216:LEU:H	2.29	0.45
1:H:286:TRP:CZ2	1:H:290:GLU:HG3	2.51	0.45
1:N:170:LEU:HD21	1:N:245:PRO:HB3	1.99	0.45
1:O:201:ALA:HB2	1:O:214:VAL:HG11	1.98	0.45
1:O:236:LEU:HD23	1:O:258:LEU:HD11	1.99	0.45
1:P:202:VAL:HG23	1:P:231:LYS:HD2	1.99	0.45
1:A:126:GLN:NE2	1:B:221:PRO:HA	2.32	0.44
1:B:208:GLU:OE2	1:C:219:LYS:NZ	2.41	0.44
1:C:219:LYS:O	1:C:219:LYS:CG	2.65	0.44
1:C:248:MET:HE2	1:C:248:MET:HB2	1.78	0.44
1:G:209:ARG:O	1:G:211:VAL:HG23	2.17	0.44
1:G:225:VAL:HA	1:H:129:ILE:O	2.17	0.44
1:I:216:LEU:HG	1:I:220:GLN:OE1	2.17	0.44
1:I:219:LYS:HD2	1:L:207:ARG:CD	2.27	0.44
1:N:247:PRO:HB2	2:N:302:7DV:C4	2.47	0.44
1:D:112:PHE:CD2	1:D:291:ILE:HD12	2.52	0.44
1:G:206:ALA:O	1:G:208:GLU:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:HIS:HA	1:H:157:ARG:CZ	2.41	0.44
1:I:220:GLN:OE1	1:I:222:ARG:NH2	2.50	0.44
1:J:134:LEU:HD21	2:J:301:7DV:C3	2.47	0.44
1:J:255:GLU:O	1:J:255:GLU:CD	2.55	0.44
1:M:126:GLN:HA	4:M:402:HOH:O	2.17	0.44
1:P:152:PRO:HB3	1:P:269:ILE:HG21	1.99	0.44
1:A:217:LEU:CD1	1:A:220:GLN:HB2	2.47	0.44
1:I:154:MET:CE	1:K:156:PHE:HE1	2.31	0.44
1:M:239:LEU:HD11	1:N:113:PHE:HB3	1.99	0.44
1:P:189:LEU:HD22	1:P:189:LEU:N	2.33	0.44
1:A:133:VAL:HG13	1:A:134:LEU:HD23	2.00	0.44
1:C:142:GLU:OE2	1:C:162:ILE:HD11	2.17	0.44
1:F:162:ILE:O	1:F:162:ILE:CG2	2.65	0.44
1:F:181:PRO:O	1:F:184:GLN:HG3	2.17	0.44
1:G:170:LEU:HD21	1:G:245:PRO:HB3	1.99	0.44
1:N:134:LEU:HD23	2:N:301:7DV:O9	2.17	0.44
1:P:170:LEU:HD21	1:P:245:PRO:HB3	2.00	0.44
1:B:276:ARG:HH12	1:D:97:THR:HG22	1.82	0.44
1:I:174:TYR:HB3	1:I:261:VAL:HG22	1.99	0.44
1:P:108:PRO:HD3	2:P:302:7DV:C4	2.46	0.44
1:A:286:TRP:CE2	1:A:290:GLU:HG3	2.52	0.44
1:E:202:VAL:O	1:E:212:LEU:HD21	2.18	0.44
1:I:161:GLU:OE1	1:I:277:ARG:HB2	2.17	0.44
1:M:136:GLY:CA	1:M:206:ALA:CB	2.64	0.44
1:N:142:GLU:CD	1:N:156:PHE:HZ	2.21	0.44
1:P:134:LEU:HD23	2:P:301:7DV:O9	2.16	0.44
1:P:140:ARG:HD2	1:P:140:ARG:HA	1.85	0.44
1:F:134:LEU:CD2	2:F:301:7DV:O9	2.65	0.44
1:I:217:LEU:HD23	1:I:219:LYS:HZ2	1.83	0.44
1:A:219:LYS:O	1:A:219:LYS:HG2	2.18	0.44
1:E:286:TRP:CE2	1:E:290:GLU:HG3	2.53	0.44
1:G:191:GLU:HA	1:G:194:ARG:HG2	1.99	0.44
1:K:183:HIS:CE1	1:K:259:ARG:HG2	2.53	0.44
1:K:202:VAL:HG21	1:K:228:ILE:HD13	2.00	0.44
1:A:106:LEU:HD11	2:A:301:7DV:C3	2.48	0.43
1:C:133:VAL:O	1:C:204:ASP:OD1	2.35	0.43
1:D:160:SER:C	1:D:161:GLU:CD	2.77	0.43
1:E:104:GLU:OE2	1:E:134:LEU:HD12	2.17	0.43
1:E:106:LEU:HG	2:E:301:7DV:C5	2.48	0.43
1:E:218:ASP:CG	1:E:219:LYS:N	2.67	0.43
1:E:236:LEU:HD23	1:E:258:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:VAL:HG23	1:F:231:LYS:HD3	1.99	0.43
1:H:143:GLN:NE2	1:H:145:ARG:HB2	2.33	0.43
1:L:277:ARG:O	1:L:277:ARG:HG2	2.18	0.43
1:M:181:PRO:HA	1:M:184:GLN:OE1	2.18	0.43
1:N:157:ARG:CZ	1:N:158:SER:HB3	2.47	0.43
1:B:202:VAL:HG23	1:B:231:LYS:HD2	2.00	0.43
1:F:195:VAL:HG13	1:F:217:LEU:HD21	1.99	0.43
1:F:286:TRP:CZ2	1:F:290:GLU:HG3	2.54	0.43
1:H:140:ARG:HD3	1:H:143:GLN:HE21	1.83	0.43
1:H:162:ILE:HD13	1:H:276:ARG:HG2	1.99	0.43
1:O:217:LEU:C	1:O:220:GLN:HE21	2.22	0.43
1:P:248:MET:HG3	2:P:302:7DV:O1	2.17	0.43
1:P:255:GLU:OE1	1:P:257:ARG:NH2	2.51	0.43
1:A:231:LYS:HD3	1:A:244:MET:HE1	2.00	0.43
1:C:209:ARG:NH2	1:C:210:PRO:HG3	2.33	0.43
1:D:208:GLU:HB3	1:D:210:PRO:HD2	1.99	0.43
1:E:106:LEU:O	2:E:302:7DV:C5	2.66	0.43
1:E:203:ALA:HB1	1:E:209:ARG:HG3	1.99	0.43
1:F:273:MET:CE	1:F:291:ILE:HB	2.48	0.43
1:C:194:ARG:NE	1:C:217:LEU:HD22	2.33	0.43
1:E:99:LEU:HD13	1:E:100:THR:N	2.33	0.43
1:A:155:HIS:CD2	1:C:158:SER:HB3	2.53	0.43
1:A:156:PHE:HD2	1:A:208:GLU:O	2.02	0.43
1:C:155:HIS:HA	1:C:155:HIS:HD1	1.77	0.43
1:D:148:ILE:HD13	1:D:288:LEU:HD12	2.00	0.43
1:F:138:TRP:CE2	1:F:156:PHE:CE1	3.06	0.43
1:F:280:MET:HE3	1:F:281:GLY:H	1.83	0.43
1:J:157:ARG:HA	1:J:157:ARG:HD3	1.75	0.43
1:K:286:TRP:CE2	1:K:290:GLU:HG3	2.53	0.43
1:N:172:ASN:HB3	1:N:243:THR:CG2	2.48	0.43
1:O:208:GLU:C	1:O:210:PRO:HD3	2.39	0.43
1:D:208:GLU:OE1	1:D:208:GLU:HA	2.18	0.43
1:F:190:SER:O	1:F:193:THR:OG1	2.33	0.43
1:G:195:VAL:CG1	1:G:217:LEU:HD23	2.46	0.43
1:G:286:TRP:CE2	1:G:290:GLU:HG3	2.54	0.43
1:I:219:LYS:CD	1:L:207:ARG:HD2	2.28	0.43
1:I:223:LEU:HD22	1:J:116:ILE:HD13	2.00	0.43
1:J:163:ASN:ND2	1:J:275:TRP:CH2	2.87	0.43
1:K:105:ALA:HB1	1:K:228:ILE:HG12	2.00	0.43
1:C:248:MET:CE	2:C:302:7DV:C6	2.96	0.43
1:D:246:TYR:CZ	1:P:263:PRO:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:THR:C	1:G:207:ARG:H	2.22	0.43
1:H:119:LEU:HD22	1:H:286:TRP:CZ3	2.53	0.43
1:H:195:VAL:HA	1:H:220:GLN:HG3	2.00	0.43
1:K:198:ARG:O	1:K:241:VAL:CG2	2.62	0.43
1:L:170:LEU:HD21	1:L:245:PRO:HB3	2.01	0.43
1:A:174:TYR:CE1	1:A:243:THR:HG23	2.54	0.43
1:M:130:ILE:HG21	1:M:140:ARG:HH21	1.84	0.43
1:D:183:HIS:HB3	1:D:259:ARG:NH2	2.33	0.43
1:D:211:VAL:HG23	1:D:212:LEU:HD23	2.01	0.43
1:L:194:ARG:HH12	1:L:215:GLN:HG3	1.84	0.43
1:M:251:LYS:NZ	1:M:255:GLU:OE2	2.51	0.43
1:B:152:PRO:HB3	1:B:269:ILE:CG2	2.49	0.43
1:C:204:ASP:H	1:C:210:PRO:HG2	1.83	0.43
1:D:231:LYS:NZ	2:D:301:7DV:O1	2.51	0.43
1:F:95:MET:O	1:F:124:ASN:HB2	2.18	0.43
1:H:122:LYS:NZ	1:H:282:GLU:OE1	2.52	0.43
1:P:110:PRO:HB2	2:P:303:7DV:C2	2.48	0.43
1:B:97:THR:HB	1:B:125:THR:HG22	2.01	0.42
1:B:106:LEU:O	2:B:302:7DV:C5	2.67	0.42
1:B:166:LYS:HE3	1:B:270:ASP:OD1	2.19	0.42
1:E:219:LYS:O	1:E:219:LYS:HD3	2.18	0.42
1:H:140:ARG:NH2	4:H:401:HOH:O	2.52	0.42
1:H:142:GLU:HG2	1:H:143:GLN:N	2.34	0.42
1:H:296:ASN:OD1	1:H:296:ASN:N	2.51	0.42
1:J:209:ARG:HD2	4:J:402:HOH:O	2.18	0.42
1:K:174:TYR:HE1	1:K:261:VAL:HG11	1.83	0.42
1:A:126:GLN:CD	1:B:222:ARG:H	2.19	0.42
1:E:245:PRO:HG2	1:E:248:MET:HE2	2.01	0.42
1:G:185:GLU:OE1	1:G:187:GLU:N	2.52	0.42
1:H:152:PRO:HB3	1:H:269:ILE:HG21	2.01	0.42
1:J:134:LEU:HB3	1:J:212:LEU:HD23	2.00	0.42
1:B:286:TRP:CH2	1:B:290:GLU:HG3	2.54	0.42
1:H:189:LEU:H	1:H:189:LEU:HG	1.64	0.42
1:N:152:PRO:HB3	1:N:269:ILE:CG2	2.50	0.42
1:O:108:PRO:HB3	2:O:302:7DV:C4	2.49	0.42
1:O:157:ARG:NH1	4:O:401:HOH:O	2.52	0.42
1:A:156:PHE:O	1:A:157:ARG:NE	2.52	0.42
1:A:204:ASP:CG	1:A:205:THR:N	2.72	0.42
1:A:257:ARG:HH11	1:A:257:ARG:CG	2.31	0.42
1:F:152:PRO:HB3	1:F:269:ILE:CG2	2.49	0.42
1:M:171:MET:HE1	1:O:118:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:170:LEU:HB3	1:O:269:ILE:HG23	2.02	0.42
1:A:138:TRP:HE3	1:A:157:ARG:HG3	1.85	0.42
1:B:161:GLU:HA	1:B:277:ARG:HH21	1.85	0.42
1:B:190:SER:O	1:B:193:THR:OG1	2.30	0.42
1:B:261:VAL:HG23	1:B:262:SER:N	2.35	0.42
1:D:189:LEU:HD21	1:D:262:SER:HB3	2.01	0.42
1:H:153:ASP:HB2	1:H:272:ILE:HD11	2.01	0.42
1:H:189:LEU:HD11	1:H:264:GLU:HG2	2.01	0.42
1:J:98:HIS:CE1	1:J:100:THR:OG1	2.73	0.42
1:J:181:PRO:O	1:J:184:GLN:HG3	2.19	0.42
1:K:152:PRO:HB3	1:K:269:ILE:CG2	2.49	0.42
1:M:139:GLU:HB3	1:M:206:ALA:HB1	2.01	0.42
1:M:202:VAL:HG23	1:M:231:LYS:HD2	2.01	0.42
1:O:131:THR:H	1:P:226:SER:HB2	1.83	0.42
1:B:249:VAL:O	1:B:249:VAL:CG2	2.67	0.42
1:G:221:PRO:HA	1:H:126:GLN:CD	2.40	0.42
1:I:226:SER:HB2	1:J:131:THR:H	1.84	0.42
1:K:183:HIS:CE1	1:K:259:ARG:HB3	2.55	0.42
1:M:209:ARG:HH21	1:M:211:VAL:HG13	1.85	0.42
1:C:204:ASP:N	1:C:210:PRO:HG2	2.35	0.42
1:D:246:TYR:CE2	1:P:263:PRO:CD	3.03	0.42
1:E:134:LEU:CD1	2:E:301:7DV:C4	2.92	0.42
1:F:189:LEU:HD23	1:F:189:LEU:HA	1.88	0.42
1:J:161:GLU:O	1:J:276:ARG:HA	2.20	0.42
1:L:135:ALA:HA	1:L:154:MET:HE1	2.00	0.42
1:O:231:LYS:NZ	2:O:301:7DV:O1	2.50	0.42
1:B:185:GLU:OE1	1:B:187:GLU:N	2.53	0.42
1:E:186:PRO:O	1:E:187:GLU:C	2.58	0.42
1:G:248:MET:HB2	1:G:248:MET:HE2	1.96	0.42
1:L:140:ARG:HD3	1:L:145:ARG:HH21	1.84	0.42
1:P:141:LEU:HB2	1:P:149:VAL:HG21	2.02	0.42
1:C:118:LYS:HE2	1:G:171:MET:CE	2.50	0.42
1:E:195:VAL:HA	1:E:220:GLN:HG3	2.01	0.42
1:E:209:ARG:HD3	1:E:209:ARG:HA	1.75	0.42
1:E:282:GLU:CG	1:E:283:ALA:H	2.33	0.42
1:G:185:GLU:CD	1:G:186:PRO:HD2	2.40	0.42
1:G:212:LEU:HD13	1:G:212:LEU:O	2.20	0.42
1:H:231:LYS:HD3	1:H:244:MET:HE3	2.01	0.42
1:I:220:GLN:H	1:I:222:ARG:HH12	1.67	0.42
1:J:255:GLU:O	1:J:255:GLU:OE1	2.37	0.42
1:L:152:PRO:HB3	1:L:269:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:255:GLU:OE1	1:M:257:ARG:NH2	2.52	0.42
1:A:134:LEU:HD13	1:A:154:MET:SD	2.60	0.42
1:B:179:ASP:OD1	1:B:179:ASP:N	2.43	0.42
1:B:196:LYS:HE2	1:B:197:TYR:CE1	2.55	0.42
1:F:138:TRP:CZ2	1:F:156:PHE:CE1	3.08	0.42
1:F:208:GLU:H	1:F:208:GLU:HG3	1.74	0.42
1:F:172:ASN:HB3	1:F:243:THR:CG2	2.49	0.41
1:F:286:TRP:CE2	1:F:290:GLU:HG3	2.55	0.41
1:H:132:GLU:CD	1:H:207:ARG:HH22	2.22	0.41
1:J:152:PRO:HB3	1:J:269:ILE:CG2	2.50	0.41
1:M:135:ALA:HA	1:M:209:ARG:HD3	2.01	0.41
1:N:101:ILE:HG23	1:N:150:ILE:CD1	2.50	0.41
1:O:131:THR:H	1:P:226:SER:CB	2.33	0.41
1:A:195:VAL:HA	1:A:220:GLN:HG3	2.02	0.41
1:B:276:ARG:HD3	1:D:95:MET:HE3	1.99	0.41
1:D:214:VAL:O	1:D:215:GLN:HB3	2.20	0.41
1:E:219:LYS:O	1:E:219:LYS:HG3	2.20	0.41
1:G:205:THR:HG22	1:G:205:THR:O	2.19	0.41
1:J:166:LYS:HD3	1:J:166:LYS:N	2.36	0.41
1:K:156:PHE:CG	1:K:157:ARG:N	2.87	0.41
1:L:153:ASP:OD1	1:L:270:ASP:O	2.38	0.41
1:N:248:MET:HG3	2:N:302:7DV:C7	2.50	0.41
1:O:207:ARG:O	1:O:208:GLU:HB3	2.20	0.41
1:B:231:LYS:HD3	1:B:244:MET:HE3	2.02	0.41
1:B:287:CYS:O	1:B:291:ILE:HG13	2.21	0.41
1:C:138:TRP:HZ3	1:C:274:ALA:HB3	1.85	0.41
1:E:255:GLU:OE1	1:E:257:ARG:NH2	2.54	0.41
1:F:95:MET:HB3	1:F:96:GLU:H	1.64	0.41
1:N:273:MET:HE1	1:N:291:ILE:HB	2.01	0.41
1:A:154:MET:CE	1:A:211:VAL:CG1	2.95	0.41
1:A:182:ILE:HG22	1:A:197:TYR:CD2	2.55	0.41
1:A:231:LYS:HD3	1:A:244:MET:CE	2.51	0.41
1:C:113:PHE:N	1:C:114:PRO:HD2	2.36	0.41
1:C:171:MET:HE3	1:E:118:LYS:HE2	2.00	0.41
1:C:176:ALA:HB2	1:C:241:VAL:HG12	2.01	0.41
1:I:106:LEU:HG	2:I:301:7DV:C5	2.50	0.41
1:I:152:PRO:HB3	1:I:269:ILE:CG2	2.50	0.41
1:I:209:ARG:HH12	1:K:205:THR:HG1	1.60	0.41
1:N:190:SER:OG	1:N:193:THR:HG23	2.19	0.41
1:P:217:LEU:HD22	1:P:217:LEU:HA	1.89	0.41
1:A:174:TYR:CD2	1:A:265:SER:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:SER:HB2	1:B:131:THR:H	1.85	0.41
1:E:222:ARG:NH1	1:F:98:HIS:NE2	2.69	0.41
1:G:190:SER:O	1:G:193:THR:OG1	2.31	0.41
1:I:208:GLU:O	1:I:209:ARG:CB	2.68	0.41
1:K:108:PRO:HD3	2:K:302:7DV:C5	2.50	0.41
1:K:195:VAL:HA	1:K:220:GLN:HG3	2.01	0.41
1:L:108:PRO:HB3	2:L:302:7DV:C2	2.51	0.41
1:M:167:LEU:HD21	1:M:273:MET:HE2	2.01	0.41
1:M:183:HIS:HB3	1:M:259:ARG:HH21	1.86	0.41
1:M:189:LEU:HD23	1:M:189:LEU:HA	1.94	0.41
1:A:207:ARG:O	1:A:208:GLU:HB2	2.20	0.41
1:D:249:VAL:HG12	1:D:253:ILE:HG13	2.03	0.41
1:F:179:ASP:OD1	1:F:179:ASP:N	2.43	0.41
1:G:195:VAL:HA	1:G:220:GLN:HB2	2.00	0.41
1:H:171:MET:HG3	1:L:264:GLU:OE2	2.19	0.41
1:D:115:LEU:HD21	1:D:294:LEU:HD11	2.02	0.41
1:F:152:PRO:HB3	1:F:269:ILE:HG21	2.02	0.41
1:H:141:LEU:HB2	1:H:149:VAL:HG21	2.03	0.41
1:O:286:TRP:CE2	1:O:290:GLU:HG3	2.55	0.41
1:A:155:HIS:CE1	1:A:211:VAL:CB	2.99	0.41
1:A:163:ASN:HD22	1:A:163:ASN:HA	1.70	0.41
1:A:261:VAL:HG23	1:A:262:SER:N	2.36	0.41
1:H:106:LEU:HG	2:H:301:7DV:C4	2.51	0.41
1:J:249:VAL:HG23	1:J:253:ILE:HD11	2.03	0.41
1:K:202:VAL:HG21	1:K:228:ILE:CD1	2.51	0.41
1:M:135:ALA:CA	1:M:209:ARG:HG2	2.50	0.41
1:P:189:LEU:HD22	1:P:189:LEU:H	1.86	0.41
1:A:243:THR:O	1:A:244:MET:HG2	2.21	0.41
1:D:161:GLU:O	1:D:276:ARG:HA	2.21	0.41
1:D:248:MET:HB2	1:D:248:MET:HE2	1.98	0.41
1:E:170:LEU:HB3	1:E:269:ILE:HG23	2.03	0.41
1:E:223:LEU:HD22	1:F:116:ILE:HD13	2.02	0.41
1:F:153:ASP:HB2	1:F:272:ILE:HD11	2.02	0.41
1:M:135:ALA:HB3	1:M:207:ARG:N	2.36	0.41
1:M:159:SER:O	1:M:161:GLU:N	2.54	0.41
1:M:248:MET:HB2	1:M:248:MET:HE2	1.82	0.41
1:N:186:PRO:O	1:N:187:GLU:C	2.58	0.41
1:P:108:PRO:CB	2:P:303:7DV:O9	2.69	0.41
1:P:182:ILE:HA	1:P:182:ILE:HD12	1.86	0.41
1:A:194:ARG:HH22	1:A:217:LEU:HB3	1.86	0.41
1:C:195:VAL:HA	1:C:220:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:SER:CB	1:H:131:THR:H	2.34	0.41
1:I:154:MET:CG	1:K:156:PHE:CD1	3.03	0.41
1:K:157:ARG:HG2	1:K:158:SER:N	2.35	0.41
1:K:280:MET:HE3	1:K:280:MET:HA	2.02	0.41
1:N:160:SER:HB3	1:N:277:ARG:HH12	1.86	0.41
1:N:287:CYS:O	1:N:291:ILE:HG13	2.20	0.41
1:O:255:GLU:OE1	1:O:257:ARG:NH2	2.54	0.41
1:A:191:GLU:HA	1:A:194:ARG:HH11	1.86	0.40
1:B:95:MET:O	1:B:95:MET:HG3	2.21	0.40
1:C:139:GLU:HG2	1:C:143:GLN:OE1	2.21	0.40
1:E:208:GLU:HB2	1:E:211:VAL:CG2	2.50	0.40
1:H:110:PRO:HB2	2:H:303:7DV:C2	2.51	0.40
1:I:261:VAL:HG23	1:I:262:SER:N	2.36	0.40
1:J:127:LEU:HD12	1:J:127:LEU:HA	1.92	0.40
1:L:152:PRO:HB3	1:L:269:ILE:HG21	2.03	0.40
1:L:202:VAL:HG23	1:L:231:LYS:HD2	2.02	0.40
1:M:211:VAL:HB	1:M:212:LEU:H	1.70	0.40
1:N:162:ILE:HA	1:N:275:TRP:O	2.21	0.40
1:P:206:ALA:HB1	1:P:209:ARG:HB3	2.03	0.40
1:P:247:PRO:HB2	2:P:302:7DV:C4	2.51	0.40
1:D:249:VAL:HG13	1:D:258:LEU:CD1	2.51	0.40
1:E:126:GLN:NE2	1:E:126:GLN:HA	2.35	0.40
1:F:244:MET:HE1	1:F:245:PRO:HD2	2.03	0.40
1:G:210:PRO:HB2	1:G:213:THR:HG22	2.03	0.40
1:G:226:SER:HB2	1:H:131:THR:H	1.86	0.40
1:K:125:THR:HG21	1:K:283:ALA:CB	2.52	0.40
1:K:174:TYR:HD1	1:K:261:VAL:HG22	1.84	0.40
1:K:174:TYR:CE1	1:K:261:VAL:HG11	2.57	0.40
1:P:155:HIS:O	1:P:155:HIS:CD2	2.74	0.40
1:B:99:LEU:HD12	1:B:147:ASP:OD2	2.22	0.40
1:H:293:LYS:HA	1:H:297:GLY:HA3	2.03	0.40
1:I:208:GLU:OE1	1:I:210:PRO:CD	2.69	0.40
1:I:216:LEU:CD1	1:I:217:LEU:H	2.16	0.40
1:K:174:TYR:HE1	1:K:261:VAL:CG1	2.35	0.40
1:N:159:SER:HB2	1:N:161:GLU:CD	2.40	0.40
1:F:166:LYS:N	1:F:166:LYS:CD	2.84	0.40
1:F:263:PRO:HD3	1:N:246:TYR:CZ	2.57	0.40
1:H:113:PHE:N	1:H:114:PRO:HD2	2.37	0.40
1:L:275:TRP:CH2	1:L:280:MET:CE	2.91	0.40
1:A:206:ALA:CB	1:C:210:PRO:HA	2.46	0.40
1:D:155:HIS:HA	1:D:157:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:194:ARG:NH2	1:I:216:LEU:HD13	2.37	0.40
1:I:220:GLN:HB3	1:I:222:ARG:HH22	1.86	0.40
1:K:157:ARG:HH11	1:K:162:ILE:HG21	1.87	0.40
1:K:194:ARG:HB2	1:K:217:LEU:CD1	2.52	0.40
1:L:174:TYR:CD2	1:L:261:VAL:HG11	2.57	0.40
1:M:246:TYR:CE1	1:M:250:GLU:HB2	2.56	0.40
1:P:232:ARG:NH1	1:P:252:ASP:OD2	2.55	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:285:SER:OG	1:N:282:GLU:OE1[8_544]	1.91	0.29
1:B:163:ASN:OD1	1:F:163:ASN:ND2[6_555]	2.05	0.15
1:J:277:ARG:NH1	1:N:285:SER:OG[8_544]	2.09	0.11

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	200/207 (97%)	185 (92%)	14 (7%)	1 (0%)	29 61
1	B	200/207 (97%)	193 (96%)	7 (4%)	0	100 100
1	C	200/207 (97%)	186 (93%)	11 (6%)	3 (2%)	10 33
1	D	201/207 (97%)	189 (94%)	12 (6%)	0	100 100
1	E	200/207 (97%)	186 (93%)	10 (5%)	4 (2%)	7 24
1	F	202/207 (98%)	192 (95%)	10 (5%)	0	100 100
1	G	200/207 (97%)	187 (94%)	12 (6%)	1 (0%)	29 61
1	H	201/207 (97%)	189 (94%)	12 (6%)	0	100 100
1	I	200/207 (97%)	188 (94%)	10 (5%)	2 (1%)	15 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	196/207 (95%)	187 (95%)	9 (5%)	0	100 100
1	K	200/207 (97%)	189 (94%)	9 (4%)	2 (1%)	15 44
1	L	197/207 (95%)	188 (95%)	9 (5%)	0	100 100
1	M	200/207 (97%)	191 (96%)	7 (4%)	2 (1%)	15 44
1	N	201/207 (97%)	191 (95%)	10 (5%)	0	100 100
1	O	200/207 (97%)	189 (94%)	9 (4%)	2 (1%)	15 44
1	P	201/207 (97%)	192 (96%)	9 (4%)	0	100 100
All	All	3199/3312 (97%)	3022 (94%)	160 (5%)	17 (0%)	29 61

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	157	ARG
1	O	208	GLU
1	O	210	PRO
1	C	215	GLN
1	E	206	ALA
1	E	214	VAL
1	M	211	VAL
1	G	207	ARG
1	I	210	PRO
1	K	214	VAL
1	M	160	SER
1	C	158	SER
1	E	157	ARG
1	C	155	HIS
1	I	209	ARG
1	A	210	PRO
1	E	220	GLN

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	173/177 (98%)	157 (91%)	16 (9%)	9 27
1	B	173/177 (98%)	166 (96%)	7 (4%)	31 65
1	C	172/177 (97%)	161 (94%)	11 (6%)	17 45
1	D	169/177 (96%)	153 (90%)	16 (10%)	8 25
1	E	172/177 (97%)	159 (92%)	13 (8%)	13 36
1	F	174/177 (98%)	155 (89%)	19 (11%)	6 19
1	G	172/177 (97%)	160 (93%)	12 (7%)	15 40
1	H	173/177 (98%)	161 (93%)	12 (7%)	15 41
1	I	172/177 (97%)	160 (93%)	12 (7%)	15 40
1	J	172/177 (97%)	155 (90%)	17 (10%)	8 23
1	K	172/177 (97%)	165 (96%)	7 (4%)	30 64
1	L	172/177 (97%)	161 (94%)	11 (6%)	17 45
1	M	172/177 (97%)	155 (90%)	17 (10%)	8 23
1	N	172/177 (97%)	152 (88%)	20 (12%)	5 17
1	O	173/177 (98%)	162 (94%)	11 (6%)	17 45
1	P	172/177 (97%)	160 (93%)	12 (7%)	15 40
All	All	2755/2832 (97%)	2542 (92%)	213 (8%)	13 35

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	LEU
1	A	153	ASP
1	A	157	ARG
1	A	158	SER
1	A	162	ILE
1	A	163	ASN
1	A	179	ASP
1	A	204	ASP
1	A	209	ARG
1	A	211	VAL
1	A	212	LEU
1	A	213	THR
1	A	216	LEU
1	A	217	LEU
1	A	219	LYS
1	A	257	ARG

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Mol	Chain	Res	Type
1	B	139	GLU
1	B	154	MET
1	B	159	SER
1	B	174	TYR
1	B	196	LYS
1	B	218	ASP
1	B	289	ARG
1	C	125	THR
1	C	145	ARG
1	C	147	ASP
1	C	155	HIS
1	C	157	ARG
1	C	160	SER
1	C	205	THR
1	C	209	ARG
1	C	218	ASP
1	C	222	ARG
1	C	229	GLU
1	D	97	THR
1	D	147	ASP
1	D	153	ASP
1	D	161	GLU
1	D	165	ARG
1	D	170	LEU
1	D	191	GLU
1	D	207	ARG
1	D	208	GLU
1	D	212	LEU
1	D	213	THR
1	D	214	VAL
1	D	257	ARG
1	D	267	SER
1	D	277	ARG
1	D	293	LYS
1	E	125	THR
1	E	154	MET
1	E	157	ARG
1	E	163	ASN
1	E	165	ARG
1	E	207	ARG
1	E	209	ARG
1	E	212	LEU

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Mol	Chain	Res	Type
1	E	213	THR
1	E	216	LEU
1	E	219	LYS
1	E	259	ARG
1	E	298	LYS
1	F	147	ASP
1	F	154	MET
1	F	157	ARG
1	F	159	SER
1	F	160	SER
1	F	163	ASN
1	F	170	LEU
1	F	184	GLN
1	F	191	GLU
1	F	207	ARG
1	F	208	GLU
1	F	209	ARG
1	F	218	ASP
1	F	243	THR
1	F	266	THR
1	F	277	ARG
1	F	279	SER
1	F	289	ARG
1	F	298	LYS
1	G	104	GLU
1	G	147	ASP
1	G	163	ASN
1	G	194	ARG
1	G	209	ARG
1	G	212	LEU
1	G	213	THR
1	G	217	LEU
1	G	222	ARG
1	G	244	MET
1	G	259	ARG
1	G	298	LYS
1	H	147	ASP
1	H	155	HIS
1	H	163	ASN
1	H	174	TYR
1	H	184	GLN
1	H	187	GLU

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Mol	Chain	Res	Type
1	H	189	LEU
1	H	207	ARG
1	H	209	ARG
1	H	248	MET
1	H	264	GLU
1	H	296	ASN
1	I	125	THR
1	I	163	ASN
1	I	165	ARG
1	I	174	TYR
1	I	214	VAL
1	I	215	GLN
1	I	216	LEU
1	I	219	LYS
1	I	222	ARG
1	I	264	GLU
1	I	279	SER
1	I	280	MET
1	J	95	MET
1	J	96	GLU
1	J	140	ARG
1	J	147	ASP
1	J	154	MET
1	J	157	ARG
1	J	160	SER
1	J	166	LYS
1	J	170	LEU
1	J	184	GLN
1	J	187	GLU
1	J	205	THR
1	J	209	ARG
1	J	212	LEU
1	J	222	ARG
1	J	255	GLU
1	J	290	GLU
1	K	125	THR
1	K	147	ASP
1	K	157	ARG
1	K	159	SER
1	K	162	ILE
1	K	222	ARG
1	K	241	VAL

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Mol	Chain	Res	Type
1	L	158	SER
1	L	159	SER
1	L	174	TYR
1	L	205	THR
1	L	207	ARG
1	L	208	GLU
1	L	209	ARG
1	L	214	VAL
1	L	243	THR
1	L	255	GLU
1	L	288	LEU
1	M	142	GLU
1	M	147	ASP
1	M	156	PHE
1	M	174	TYR
1	M	179	ASP
1	M	191	GLU
1	M	198	ARG
1	M	207	ARG
1	M	208	GLU
1	M	209	ARG
1	M	211	VAL
1	M	213	THR
1	M	217	LEU
1	M	218	ASP
1	M	259	ARG
1	M	273	MET
1	M	282	GLU
1	N	95	MET
1	N	126	GLN
1	N	147	ASP
1	N	153	ASP
1	N	155	HIS
1	N	156	PHE
1	N	157	ARG
1	N	159	SER
1	N	161	GLU
1	N	163	ASN
1	N	170	LEU
1	N	185	GLU
1	N	189	LEU
1	N	190	SER

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Mol	Chain	Res	Type
1	N	191	GLU
1	N	192	VAL
1	N	212	LEU
1	N	216	LEU
1	N	268	GLU
1	N	277	ARG
1	O	125	THR
1	O	147	ASP
1	O	156	PHE
1	O	161	GLU
1	O	191	GLU
1	O	212	LEU
1	O	215	GLN
1	O	217	LEU
1	O	220	GLN
1	O	248	MET
1	O	259	ARG
1	P	118	LYS
1	P	127	LEU
1	P	147	ASP
1	P	154	MET
1	P	157	ARG
1	P	159	SER
1	P	170	LEU
1	P	213	THR
1	P	216	LEU
1	P	217	LEU
1	P	268	GLU
1	P	277	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	163	ASN
1	C	124	ASN
1	C	126	GLN
1	D	155	HIS
1	E	180	HIS
1	G	143	GLN
1	G	296	ASN
1	H	143	GLN

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Mol	Chain	Res	Type
1	I	126	GLN
1	J	98	HIS
1	J	126	GLN
1	J	215	GLN
1	K	155	HIS
1	K	183	HIS
1	K	215	GLN
1	K	233	GLN
1	L	172	ASN
1	L	183	HIS
1	L	233	GLN
1	M	215	GLN
1	N	124	ASN
1	N	172	ASN
1	O	215	GLN
1	P	155	HIS
1	P	220	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 66 ligands modelled in this entry, 16 are monoatomic - leaving 50 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	7DV	D	303	-	9,9,9	0.82	0	12,12,12	0.86	1 (8%)
2	7DV	D	301	-	9,9,9	1.16	0	12,12,12	1.62	3 (25%)
2	7DV	A	302	-	9,9,9	1.05	0	12,12,12	1.09	1 (8%)
2	7DV	C	301	-	9,9,9	1.03	0	12,12,12	1.54	3 (25%)
2	7DV	C	303	-	9,9,9	1.11	1 (11%)	12,12,12	2.22	4 (33%)
2	7DV	G	303	-	9,9,9	0.96	0	12,12,12	1.60	3 (25%)
2	7DV	J	302	-	9,9,9	0.84	0	12,12,12	1.14	1 (8%)
2	7DV	K	303	-	9,9,9	1.30	2 (22%)	12,12,12	0.84	0
2	7DV	A	301	-	9,9,9	0.87	0	12,12,12	1.38	3 (25%)
2	7DV	D	304	-	9,9,9	1.09	1 (11%)	12,12,12	1.67	2 (16%)
2	7DV	L	301	-	9,9,9	0.92	0	12,12,12	1.06	1 (8%)
2	7DV	L	303	-	9,9,9	1.13	1 (11%)	12,12,12	1.06	1 (8%)
2	7DV	N	301	-	9,9,9	1.43	1 (11%)	12,12,12	1.18	1 (8%)
2	7DV	K	302	-	9,9,9	1.59	2 (22%)	12,12,12	1.23	1 (8%)
2	7DV	F	303	-	9,9,9	0.77	0	12,12,12	0.83	0
2	7DV	N	302	-	9,9,9	1.10	0	12,12,12	1.41	1 (8%)
2	7DV	D	302	-	9,9,9	1.06	1 (11%)	12,12,12	1.13	1 (8%)
2	7DV	I	301	-	9,9,9	1.26	2 (22%)	12,12,12	1.83	2 (16%)
2	7DV	I	303	-	9,9,9	0.90	0	12,12,12	1.19	1 (8%)
2	7DV	E	301	-	9,9,9	1.44	2 (22%)	12,12,12	2.03	3 (25%)
2	7DV	P	303	-	9,9,9	1.06	0	12,12,12	1.62	4 (33%)
2	7DV	B	303	-	9,9,9	1.14	1 (11%)	12,12,12	1.40	1 (8%)
2	7DV	B	301	-	9,9,9	1.35	2 (22%)	12,12,12	1.38	1 (8%)
2	7DV	M	303	-	9,9,9	1.00	0	12,12,12	1.49	3 (25%)
2	7DV	B	302	-	9,9,9	0.89	0	12,12,12	0.64	0
2	7DV	A	303	-	9,9,9	0.99	0	12,12,12	1.30	3 (25%)
2	7DV	C	302	-	9,9,9	0.92	0	12,12,12	0.82	0
2	7DV	K	301	-	9,9,9	1.09	1 (11%)	12,12,12	0.89	0
2	7DV	H	301	-	9,9,9	0.98	1 (11%)	12,12,12	1.28	1 (8%)
2	7DV	E	302	-	9,9,9	1.48	1 (11%)	12,12,12	1.35	2 (16%)
2	7DV	I	302	-	9,9,9	1.01	0	12,12,12	1.02	1 (8%)
2	7DV	M	301	-	9,9,9	1.77	3 (33%)	12,12,12	2.49	4 (33%)
2	7DV	M	302	-	9,9,9	1.83	3 (33%)	12,12,12	1.24	2 (16%)
2	7DV	G	301	-	9,9,9	1.43	1 (11%)	12,12,12	2.18	3 (25%)
2	7DV	N	303	-	9,9,9	1.04	1 (11%)	12,12,12	1.47	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	7DV	J	301	-	9,9,9	1.21	0	12,12,12	1.27	1 (8%)
2	7DV	F	301	-	9,9,9	1.66	3 (33%)	12,12,12	1.45	2 (16%)
2	7DV	G	302	-	9,9,9	1.01	0	12,12,12	0.96	1 (8%)
2	7DV	J	303	-	9,9,9	1.02	0	12,12,12	1.64	3 (25%)
2	7DV	H	302	-	9,9,9	0.96	0	12,12,12	1.18	0
2	7DV	P	302	-	9,9,9	0.84	0	12,12,12	2.10	4 (33%)
2	7DV	O	301	-	9,9,9	1.63	2 (22%)	12,12,12	2.54	4 (33%)
2	7DV	O	303	-	9,9,9	0.99	0	12,12,12	1.48	2 (16%)
2	7DV	L	304	-	9,9,9	1.11	0	12,12,12	1.51	3 (25%)
2	7DV	O	302	-	9,9,9	1.22	0	12,12,12	1.73	2 (16%)
2	7DV	E	303	-	9,9,9	1.13	1 (11%)	12,12,12	1.42	2 (16%)
2	7DV	H	303	-	9,9,9	1.03	0	12,12,12	0.99	0
2	7DV	P	301	-	9,9,9	1.01	0	12,12,12	0.97	0
2	7DV	L	302	-	9,9,9	1.13	0	12,12,12	0.99	0
2	7DV	F	302	-	9,9,9	1.11	0	12,12,12	1.56	2 (16%)

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	7DV	D	303	-	-	-	0/1/1/1
2	7DV	D	301	-	-	-	0/1/1/1
2	7DV	A	302	-	-	-	0/1/1/1
2	7DV	C	301	-	-	-	0/1/1/1
2	7DV	C	303	-	-	-	0/1/1/1
2	7DV	G	303	-	-	-	0/1/1/1
2	7DV	J	302	-	-	-	0/1/1/1
2	7DV	K	303	-	-	-	0/1/1/1
2	7DV	A	301	-	-	-	0/1/1/1
2	7DV	D	304	-	-	-	0/1/1/1
2	7DV	L	301	-	-	-	0/1/1/1
2	7DV	L	303	-	-	-	0/1/1/1
2	7DV	N	301	-	-	-	0/1/1/1
2	7DV	K	302	-	-	-	0/1/1/1
2	7DV	F	303	-	-	-	0/1/1/1
2	7DV	N	302	-	-	-	0/1/1/1
2	7DV	D	302	-	-	-	0/1/1/1
2	7DV	I	301	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	7DV	I	303	-	-	-	0/1/1/1
2	7DV	E	301	-	-	-	0/1/1/1
2	7DV	P	303	-	-	-	0/1/1/1
2	7DV	B	303	-	-	-	0/1/1/1
2	7DV	B	301	-	-	-	0/1/1/1
2	7DV	M	303	-	-	-	0/1/1/1
2	7DV	B	302	-	-	-	0/1/1/1
2	7DV	A	303	-	-	-	0/1/1/1
2	7DV	C	302	-	-	-	0/1/1/1
2	7DV	K	301	-	-	-	0/1/1/1
2	7DV	H	301	-	-	-	0/1/1/1
2	7DV	E	302	-	-	-	0/1/1/1
2	7DV	I	302	-	-	-	0/1/1/1
2	7DV	M	301	-	-	-	0/1/1/1
2	7DV	M	302	-	-	-	0/1/1/1
2	7DV	G	301	-	-	-	0/1/1/1
2	7DV	N	303	-	-	-	0/1/1/1
2	7DV	J	301	-	-	-	0/1/1/1
2	7DV	F	301	-	-	-	0/1/1/1
2	7DV	G	302	-	-	-	0/1/1/1
2	7DV	J	303	-	-	-	0/1/1/1
2	7DV	H	302	-	-	-	0/1/1/1
2	7DV	P	302	-	-	-	0/1/1/1
2	7DV	O	301	-	-	-	0/1/1/1
2	7DV	O	303	-	-	-	0/1/1/1
2	7DV	L	304	-	-	-	0/1/1/1
2	7DV	O	302	-	-	-	0/1/1/1
2	7DV	E	303	-	-	-	0/1/1/1
2	7DV	H	303	-	-	-	0/1/1/1
2	7DV	P	301	-	-	-	0/1/1/1
2	7DV	L	302	-	-	-	0/1/1/1
2	7DV	F	302	-	-	-	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	302	7DV	O1-C1	3.55	1.43	1.36
2	K	302	7DV	O1-C1	3.47	1.43	1.36
2	E	302	7DV	O1-C1	3.26	1.43	1.36
2	M	301	7DV	O1-C1	3.21	1.42	1.36
2	O	301	7DV	O1-C1	3.19	1.42	1.36
2	F	301	7DV	C1-C2	3.17	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	7DV	O1-C1	3.12	1.42	1.36
2	O	301	7DV	C1-C2	2.83	1.43	1.40
2	E	301	7DV	O1-C1	2.81	1.42	1.36
2	F	301	7DV	O1-C1	2.69	1.41	1.36
2	B	303	7DV	O1-C1	2.64	1.41	1.36
2	L	303	7DV	O1-C1	2.60	1.41	1.36
2	I	301	7DV	O1-C1	2.50	1.41	1.36
2	M	301	7DV	C1-C2	2.46	1.43	1.40
2	N	301	7DV	O1-C1	2.46	1.41	1.36
2	M	302	7DV	C1-C2	2.44	1.43	1.40
2	M	302	7DV	O9-C4	2.44	1.42	1.37
2	K	303	7DV	C7-C2	2.41	1.55	1.51
2	M	301	7DV	C7-C2	2.39	1.55	1.51
2	K	301	7DV	O1-C1	2.38	1.41	1.36
2	B	301	7DV	C7-C2	2.28	1.55	1.51
2	N	303	7DV	O1-C1	2.27	1.41	1.36
2	E	301	7DV	C1-C2	2.21	1.43	1.40
2	B	301	7DV	O1-C1	2.18	1.40	1.36
2	F	301	7DV	C7-C2	2.17	1.55	1.51
2	I	301	7DV	C7-C2	2.15	1.55	1.51
2	E	303	7DV	O1-C1	2.13	1.40	1.36
2	K	302	7DV	C7-C2	2.13	1.55	1.51
2	C	303	7DV	O1-C1	2.06	1.40	1.36
2	D	302	7DV	O9-C4	2.04	1.41	1.37
2	D	304	7DV	O1-C1	2.04	1.40	1.36
2	K	303	7DV	O9-C4	2.03	1.41	1.37
2	H	301	7DV	O9-C4	2.02	1.41	1.37

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	301	7DV	C7-C2-C1	6.54	126.70	120.73
2	M	301	7DV	C7-C2-C1	6.00	126.21	120.73
2	C	303	7DV	C7-C2-C1	5.23	125.51	120.73
2	E	301	7DV	C7-C2-C1	5.22	125.50	120.73
2	G	301	7DV	C7-C2-C1	4.53	124.87	120.73
2	P	302	7DV	C3-C2-C1	4.22	120.93	117.56
2	N	302	7DV	C7-C2-C1	4.21	124.58	120.73
2	I	301	7DV	C7-C2-C1	4.15	124.52	120.73
2	G	301	7DV	O1-C1-C2	3.97	125.88	117.63
2	F	302	7DV	C7-C2-C1	3.82	124.22	120.73
2	O	301	7DV	O1-C1-C2	3.81	125.55	117.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	304	7DV	C7-C2-C1	-3.72	117.33	120.73
2	J	303	7DV	C3-C2-C1	3.54	120.39	117.56
2	M	301	7DV	C6-C5-C4	-3.54	116.00	119.88
2	P	302	7DV	C5-C6-C1	-3.49	116.91	120.50
2	C	303	7DV	O1-C1-C2	3.45	124.79	117.63
2	B	303	7DV	C3-C2-C1	3.44	120.30	117.56
2	O	302	7DV	C7-C2-C1	-3.42	117.60	120.73
2	O	302	7DV	C3-C2-C1	3.36	120.24	117.56
2	E	302	7DV	C7-C2-C1	3.34	123.78	120.73
2	D	304	7DV	C3-C2-C1	3.33	120.22	117.56
2	L	304	7DV	C7-C2-C1	3.13	123.59	120.73
2	P	302	7DV	C4-C3-C2	-3.06	116.81	120.70
2	F	301	7DV	C7-C2-C1	3.04	123.51	120.73
2	D	301	7DV	O1-C1-C2	3.03	123.92	117.63
2	C	301	7DV	C5-C4-C3	3.01	123.47	120.17
2	F	301	7DV	O1-C1-C2	2.98	123.82	117.63
2	O	303	7DV	C7-C2-C1	-2.97	118.02	120.73
2	M	303	7DV	C5-C4-C3	2.97	123.43	120.17
2	I	301	7DV	O1-C1-C2	2.93	123.72	117.63
2	H	301	7DV	C3-C2-C1	2.92	119.89	117.56
2	B	301	7DV	C5-C4-C3	2.90	123.35	120.17
2	P	303	7DV	C5-C4-C3	2.88	123.33	120.17
2	K	302	7DV	C3-C2-C1	2.84	119.83	117.56
2	E	303	7DV	C7-C2-C1	2.80	123.29	120.73
2	M	301	7DV	C5-C4-C3	2.78	123.22	120.17
2	D	301	7DV	C3-C2-C1	2.77	119.77	117.56
2	G	303	7DV	O1-C1-C2	2.76	123.36	117.63
2	N	303	7DV	C7-C2-C1	-2.74	118.23	120.73
2	G	303	7DV	C3-C2-C1	2.72	119.73	117.56
2	D	301	7DV	C7-C2-C1	2.69	123.19	120.73
2	L	304	7DV	C3-C2-C1	2.67	119.70	117.56
2	C	303	7DV	C5-C6-C1	2.66	123.24	120.50
2	J	302	7DV	C3-C2-C1	2.66	119.68	117.56
2	E	301	7DV	O1-C1-C2	2.61	123.05	117.63
2	I	302	7DV	C3-C2-C1	2.61	119.64	117.56
2	L	303	7DV	C3-C2-C1	2.61	119.64	117.56
2	A	302	7DV	C7-C2-C1	2.60	123.11	120.73
2	P	303	7DV	C3-C2-C1	2.60	119.63	117.56
2	M	301	7DV	O1-C1-C2	2.59	123.00	117.63
2	N	301	7DV	C5-C4-C3	2.58	123.00	120.17
2	D	303	7DV	C3-C2-C1	2.54	119.59	117.56
2	C	301	7DV	C3-C2-C1	2.52	119.58	117.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	303	7DV	C3-C2-C1	2.52	119.57	117.56
2	O	301	7DV	C7-C2-C3	-2.51	114.84	119.49
2	A	303	7DV	C5-C6-C1	-2.49	117.94	120.50
2	M	303	7DV	C3-C2-C1	2.48	119.54	117.56
2	N	303	7DV	C3-C2-C1	2.47	119.53	117.56
2	M	302	7DV	C3-C2-C1	2.46	119.53	117.56
2	A	301	7DV	C7-C2-C1	2.45	122.97	120.73
2	J	303	7DV	C4-C3-C2	-2.44	117.60	120.70
2	L	301	7DV	C3-C2-C1	2.42	119.49	117.56
2	F	302	7DV	C6-C5-C4	-2.41	117.24	119.88
2	N	303	7DV	C5-C6-C1	-2.39	118.05	120.50
2	E	302	7DV	O1-C1-C2	2.38	122.57	117.63
2	G	301	7DV	C6-C5-C4	-2.36	117.29	119.88
2	E	301	7DV	C5-C4-C3	2.35	122.75	120.17
2	I	303	7DV	O1-C1-C2	2.32	122.46	117.63
2	M	302	7DV	C5-C6-C1	-2.32	118.12	120.50
2	C	301	7DV	C6-C5-C4	-2.27	117.38	119.88
2	O	301	7DV	C5-C4-C3	2.26	122.65	120.17
2	G	303	7DV	C7-C2-C1	2.25	122.79	120.73
2	A	301	7DV	C3-C2-C1	2.24	119.35	117.56
2	P	303	7DV	C4-C3-C2	-2.23	117.87	120.70
2	L	304	7DV	O1-C1-C2	2.20	122.19	117.63
2	A	301	7DV	O1-C1-C2	2.19	122.18	117.63
2	A	303	7DV	C3-C2-C1	2.18	119.30	117.56
2	C	303	7DV	C6-C5-C4	-2.17	117.49	119.88
2	J	301	7DV	O9-C4-C5	-2.13	113.95	120.02
2	D	302	7DV	C7-C2-C1	2.13	122.67	120.73
2	A	303	7DV	C4-C3-C2	-2.12	118.00	120.70
2	M	303	7DV	C4-C3-C2	-2.11	118.01	120.70
2	E	303	7DV	O1-C1-C2	2.08	121.94	117.63
2	G	302	7DV	O1-C1-C2	2.06	121.90	117.63
2	J	303	7DV	C7-C2-C1	-2.05	118.86	120.73
2	P	302	7DV	O9-C4-C5	-2.05	114.19	120.02
2	P	303	7DV	O1-C1-C2	2.00	121.79	117.63

There are no chirality outliers.

There are no torsion outliers.

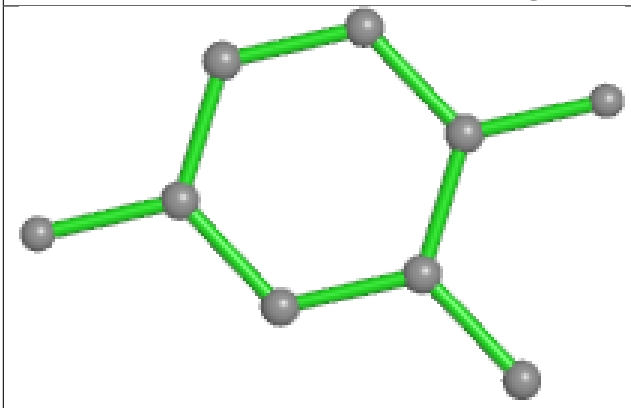
There are no ring outliers.

31 monomers are involved in 104 short contacts:

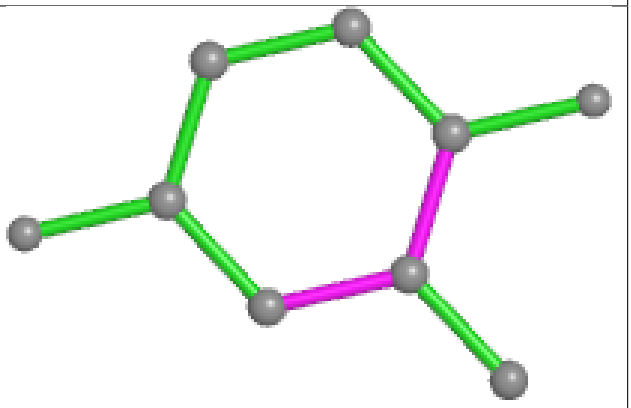
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	7DV	2	0
2	C	301	7DV	4	0
2	J	302	7DV	2	0
2	A	301	7DV	6	0
2	D	304	7DV	1	0
2	N	301	7DV	5	0
2	K	302	7DV	1	0
2	N	302	7DV	5	0
2	D	302	7DV	2	0
2	I	301	7DV	7	0
2	E	301	7DV	7	0
2	P	303	7DV	2	0
2	B	301	7DV	3	0
2	B	302	7DV	5	0
2	C	302	7DV	3	0
2	K	301	7DV	1	0
2	H	301	7DV	1	0
2	E	302	7DV	1	0
2	I	302	7DV	1	0
2	M	301	7DV	5	0
2	G	301	7DV	1	0
2	J	301	7DV	5	0
2	F	301	7DV	5	0
2	H	302	7DV	3	0
2	P	302	7DV	8	0
2	O	301	7DV	3	0
2	O	302	7DV	2	0
2	H	303	7DV	4	0
2	P	301	7DV	5	0
2	L	302	7DV	2	0
2	F	302	7DV	2	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.

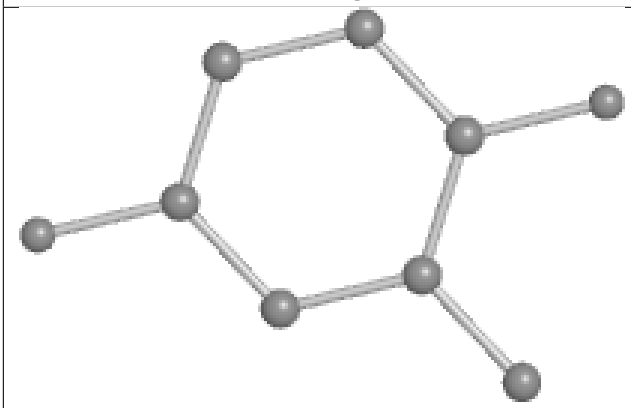
Ligand 7DV D 303



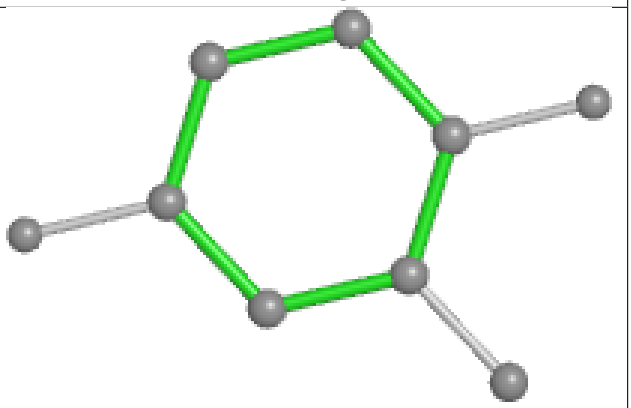
Bond lengths



Bond angles

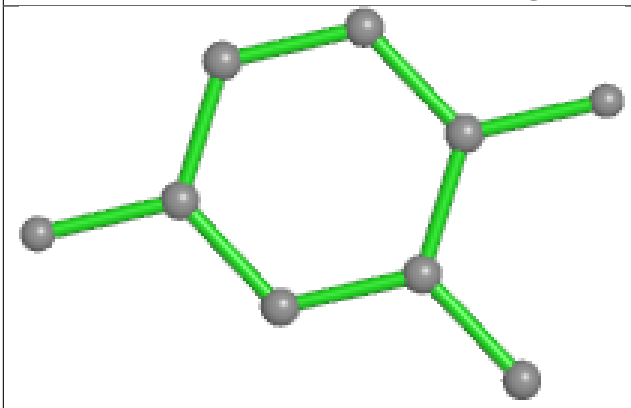


Torsions

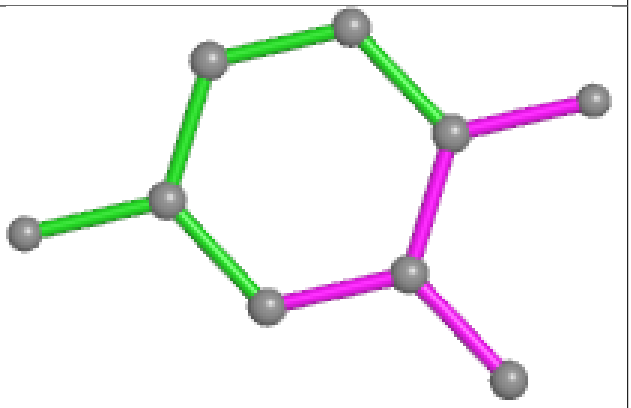


Rings

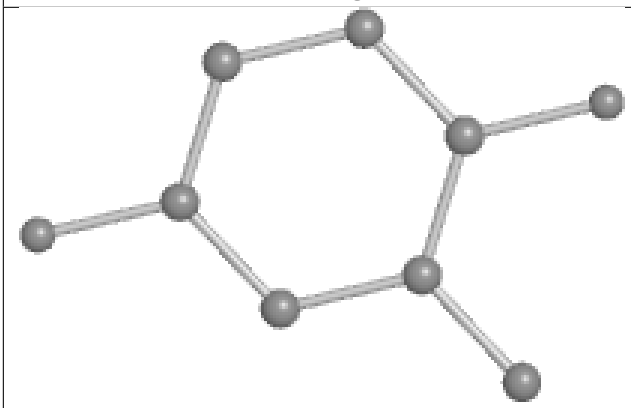
Ligand 7DV D 301



Bond lengths



Bond angles



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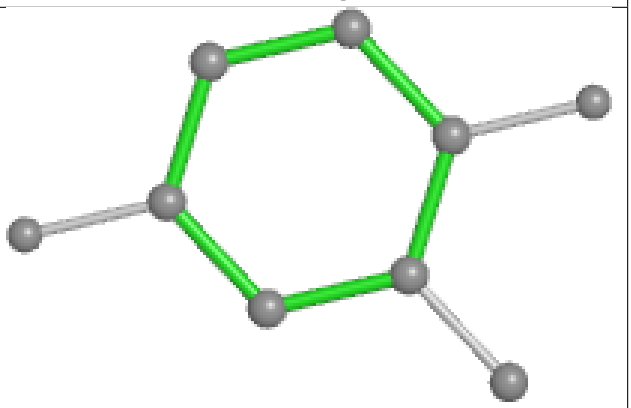
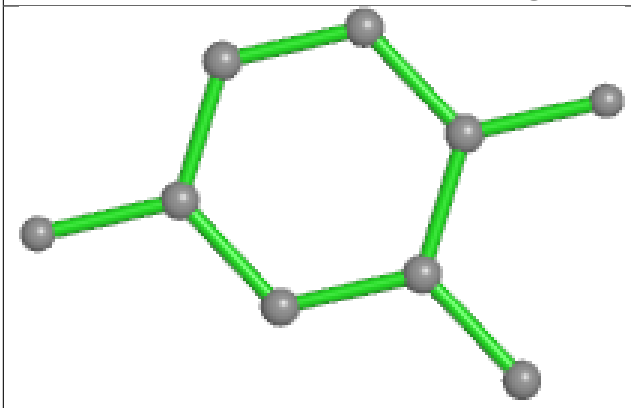
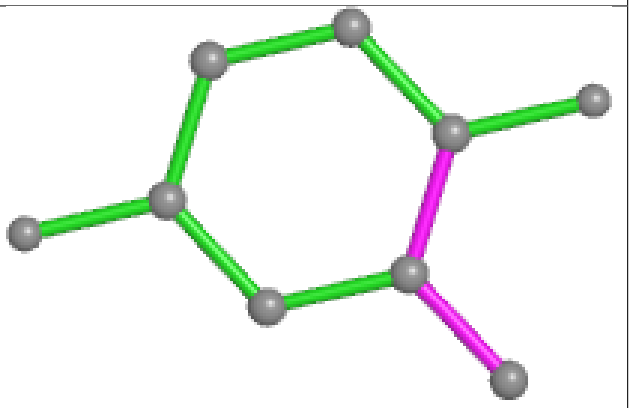


Rings

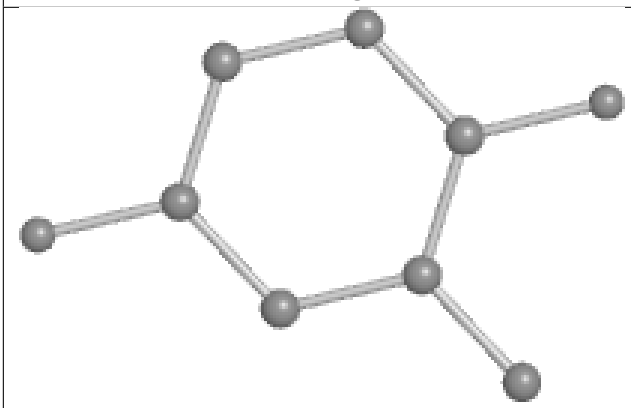
Ligand 7DV A 302



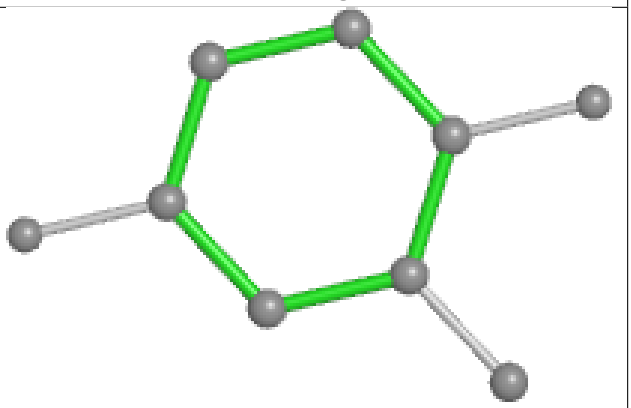
Bond lengths



Bond angles

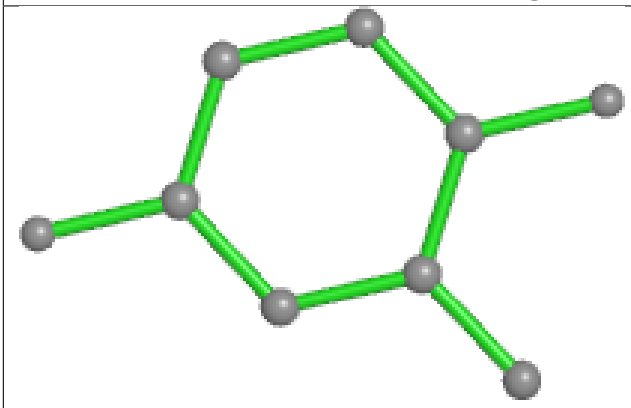


Torsions

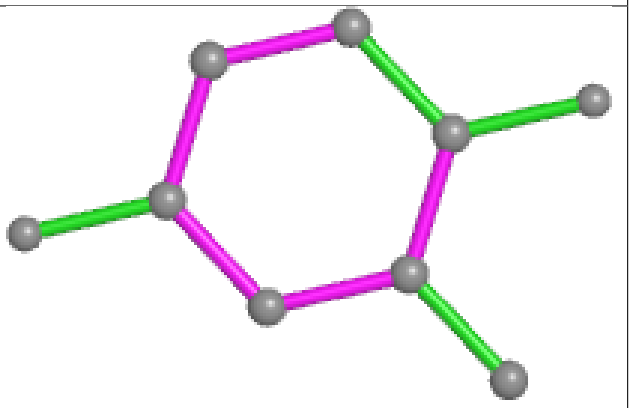


Rings

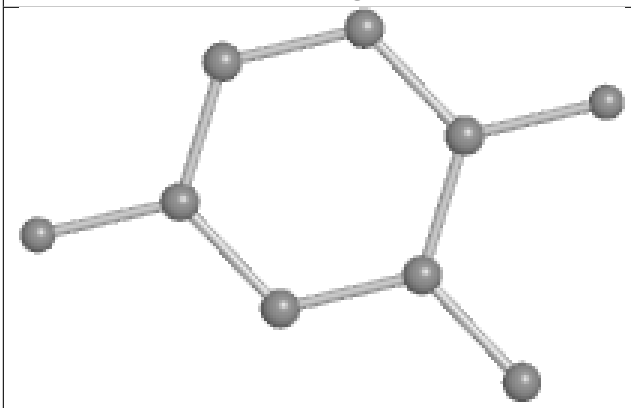
Ligand 7DV C 301



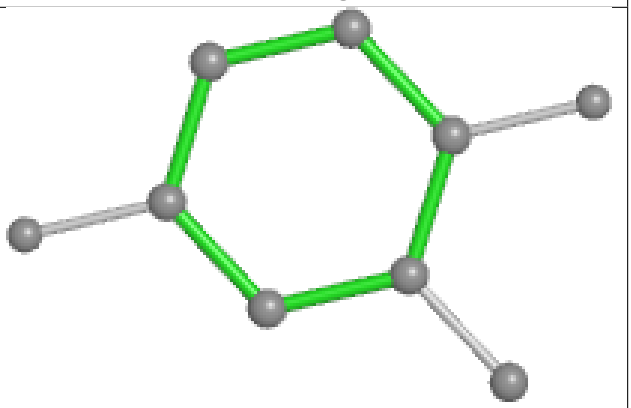
Bond lengths



Bond angles

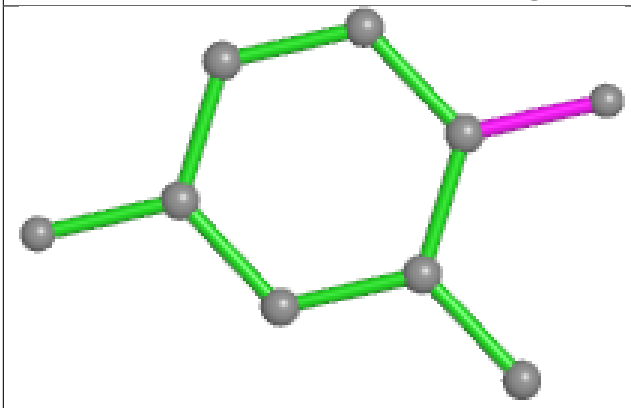


Torsions

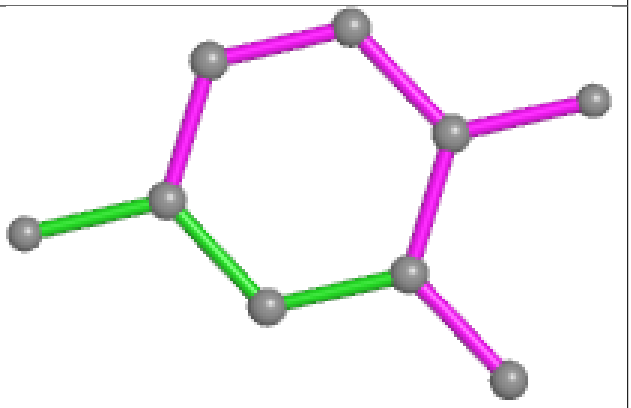


Rings

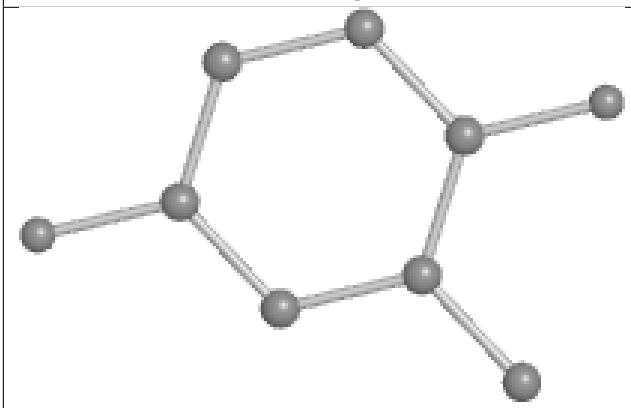
Ligand 7DV C 303



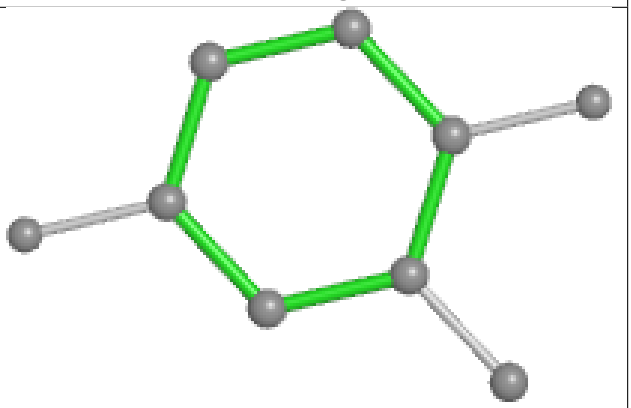
Bond lengths



Bond angles

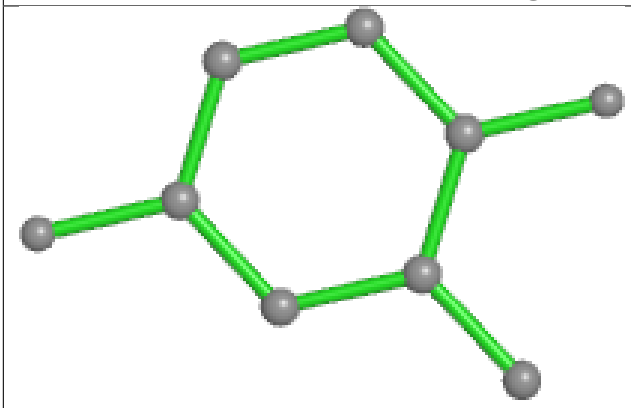


Torsions

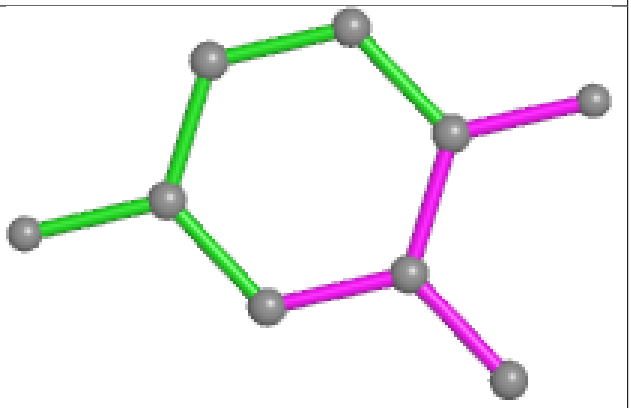


Rings

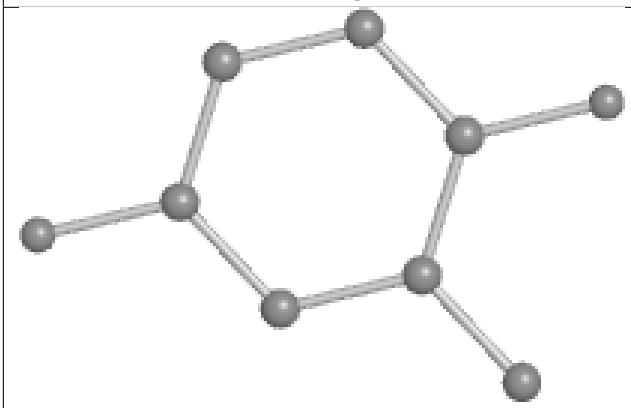
Ligand 7DV G 303



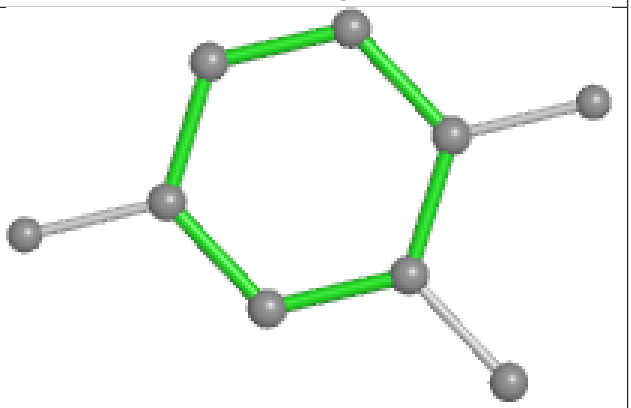
Bond lengths



Bond angles

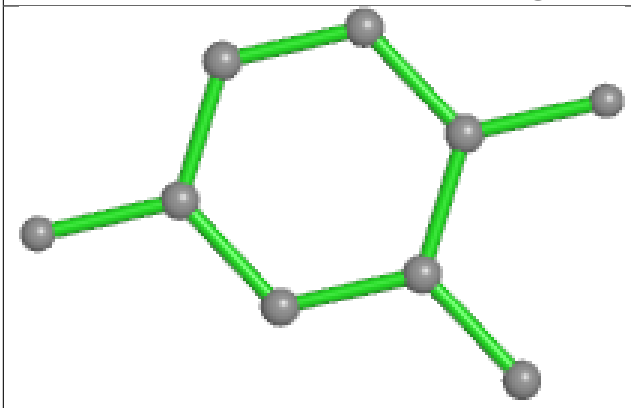


Torsions



Rings

Ligand 7DV J 302



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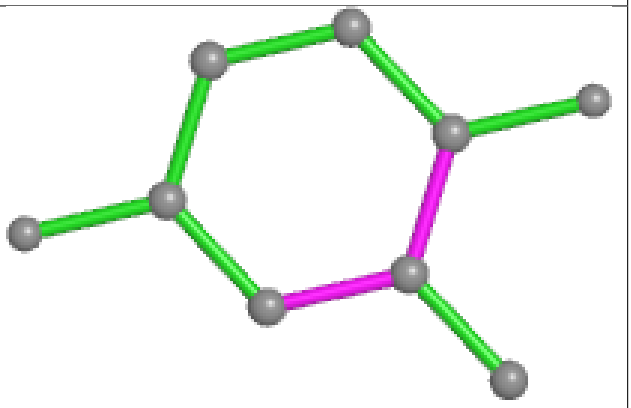
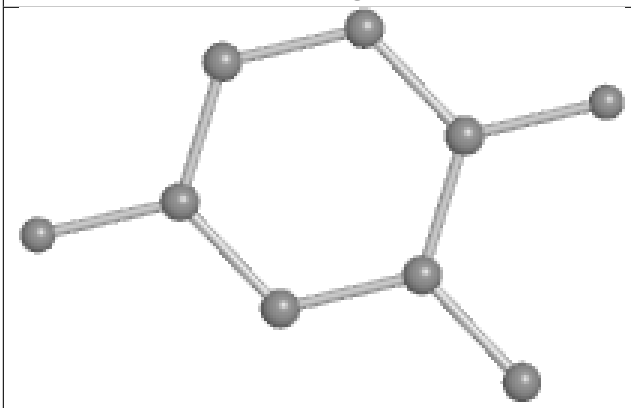
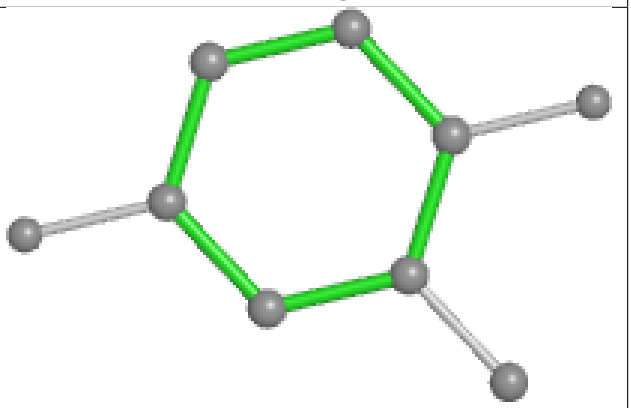


Bond angles

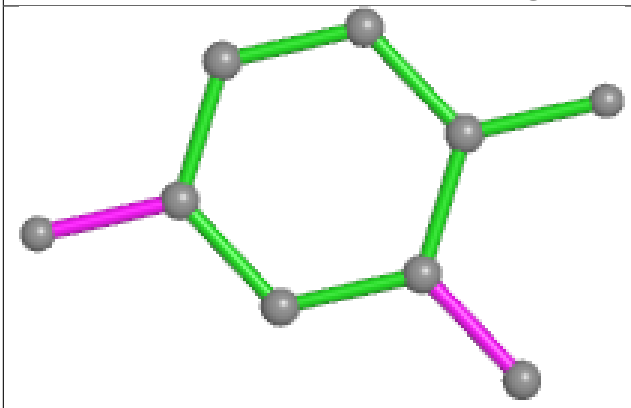


Torsions



Rings

Ligand 7DV K 303



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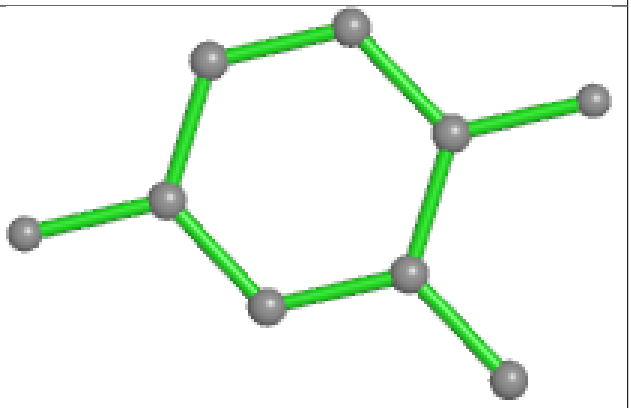

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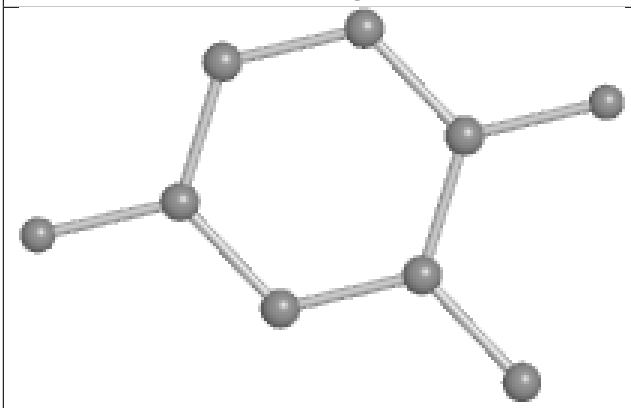

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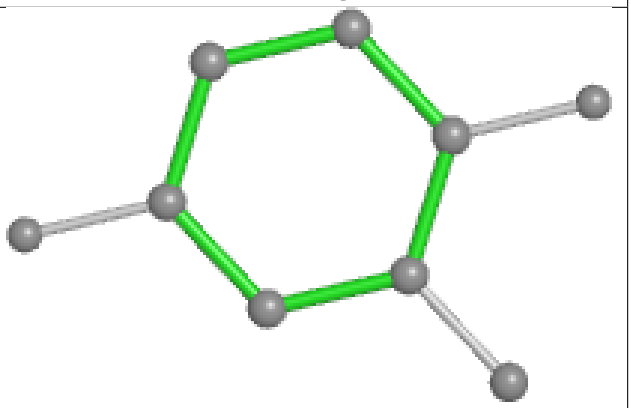
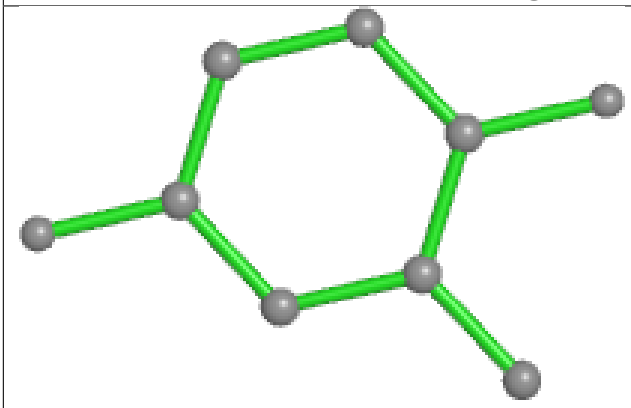


Rings

Ligand 7DV A 301



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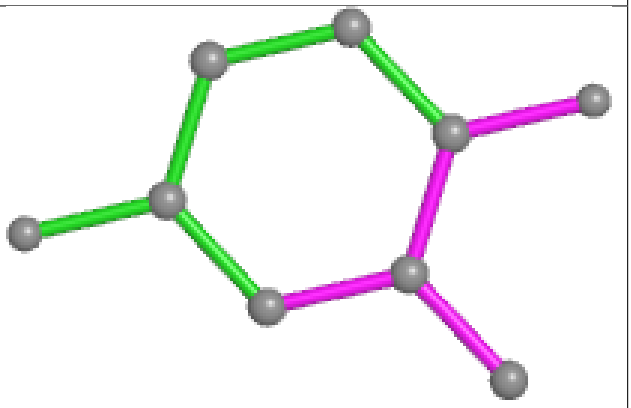

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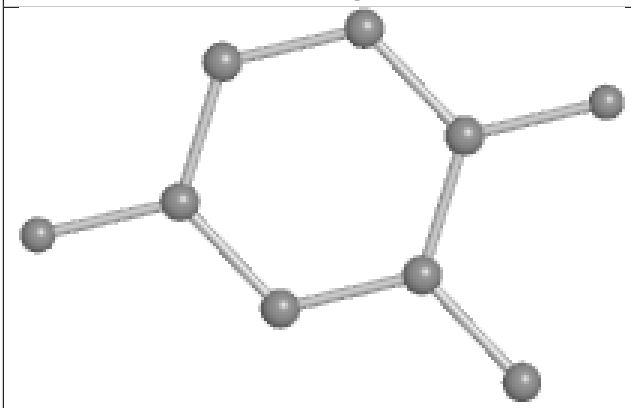

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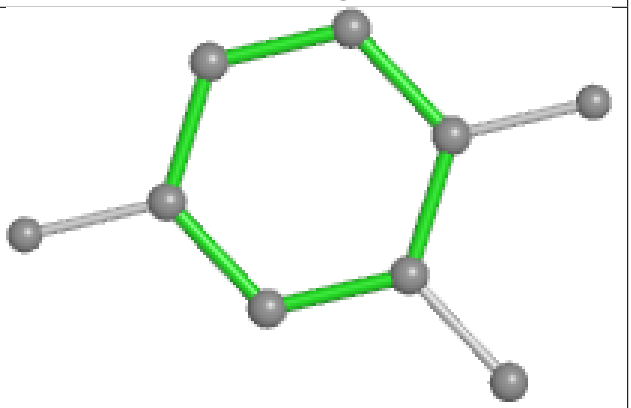
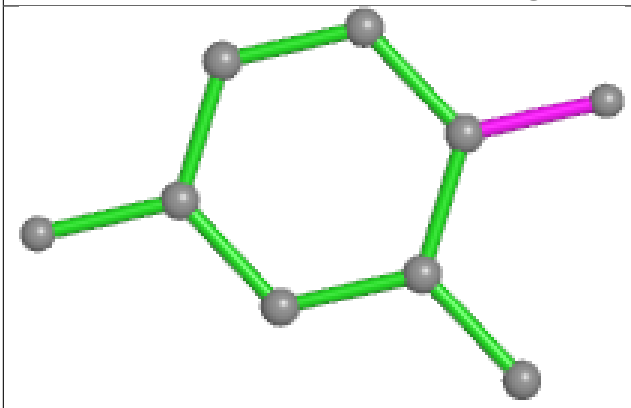


Rings

Ligand 7DV D 304



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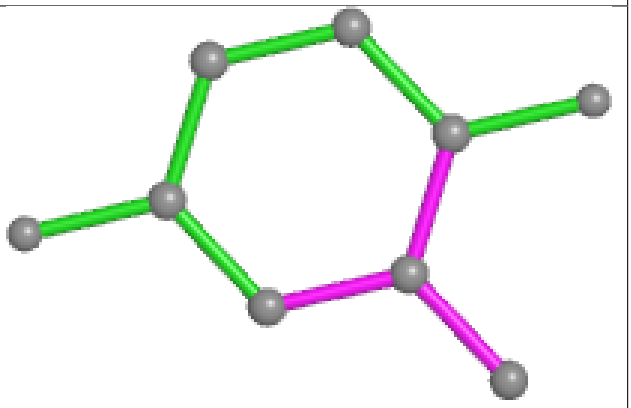

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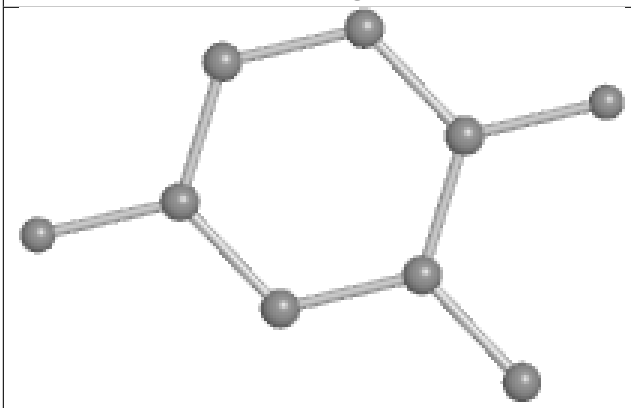

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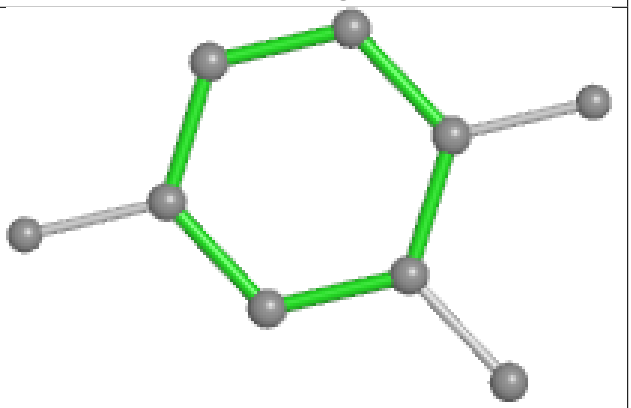
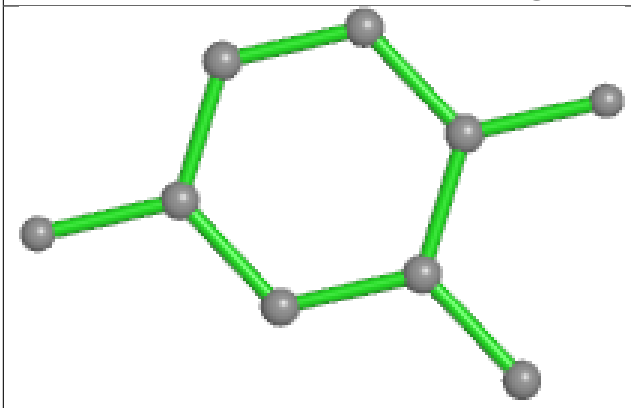


Rings

Ligand 7DV L 301



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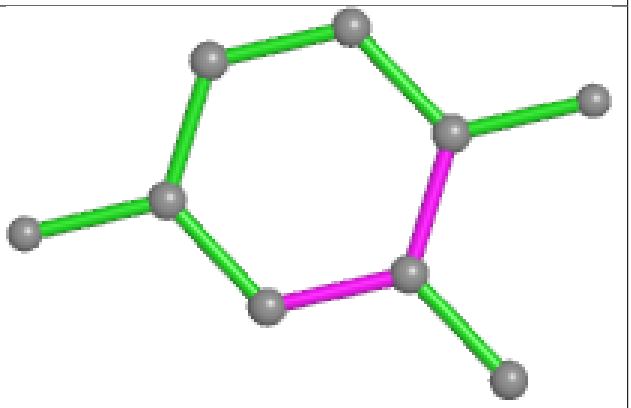

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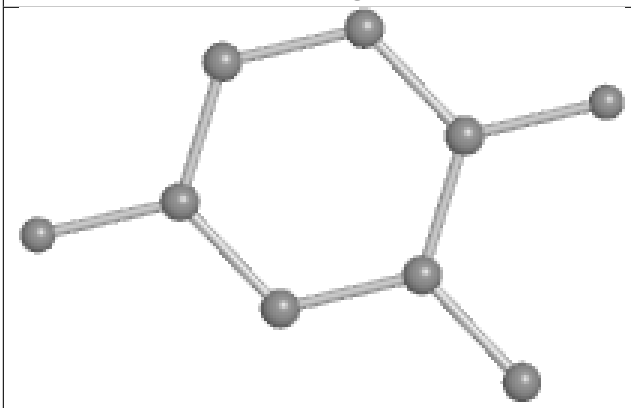

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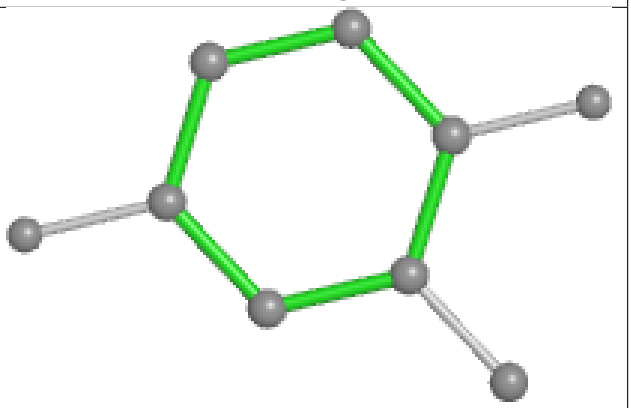
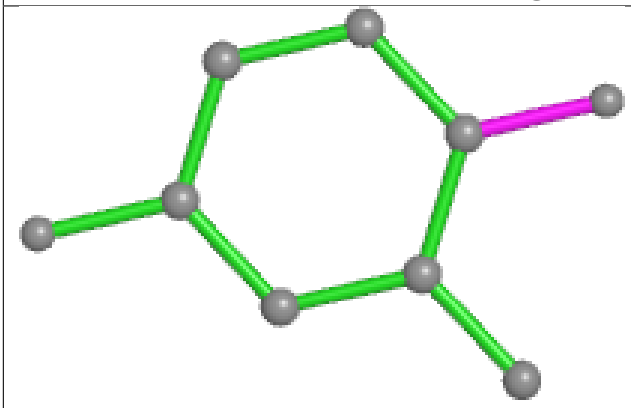


Rings

Ligand 7DV L 303



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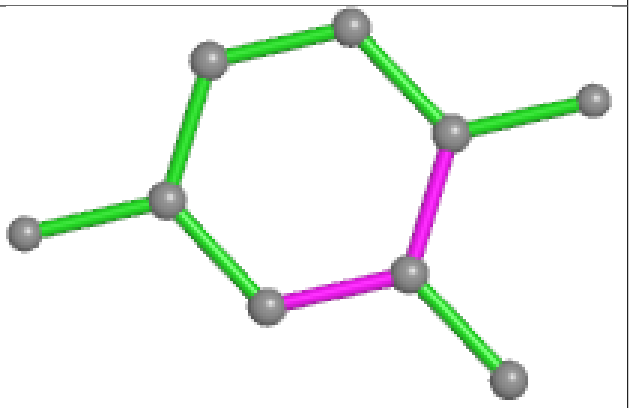

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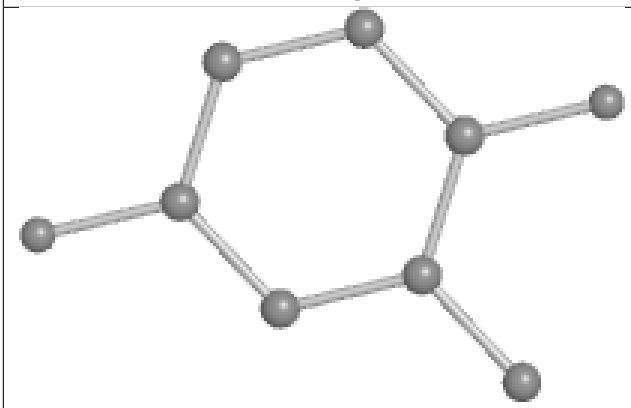

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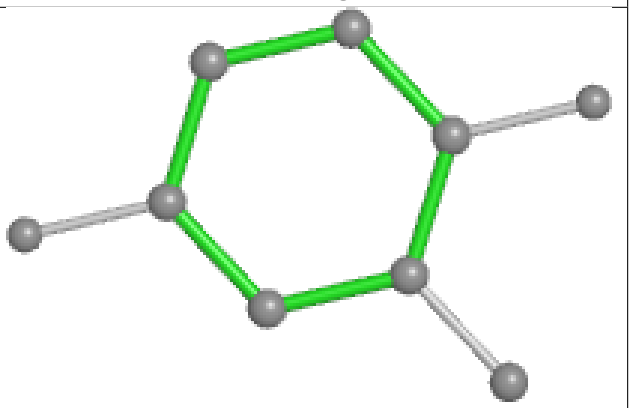
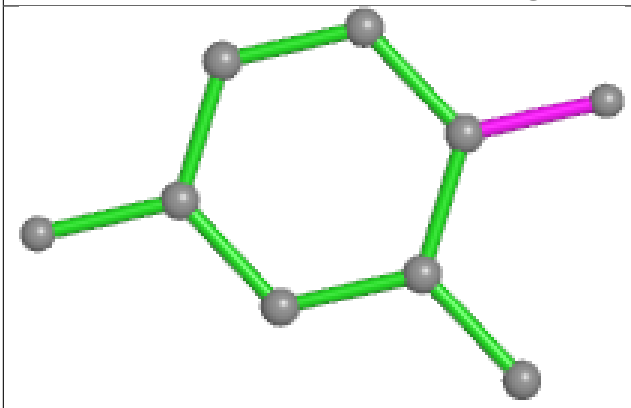


Rings

Ligand 7DV N 301



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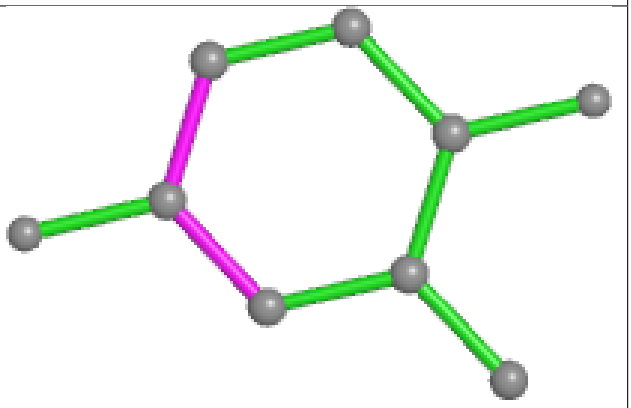

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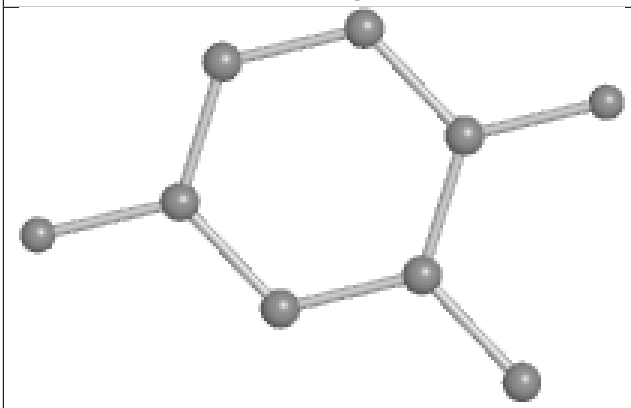

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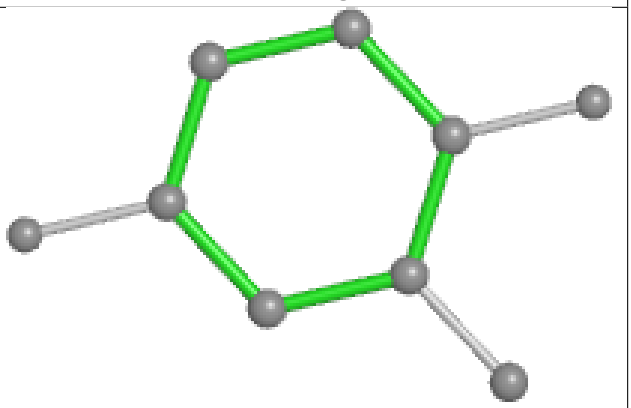
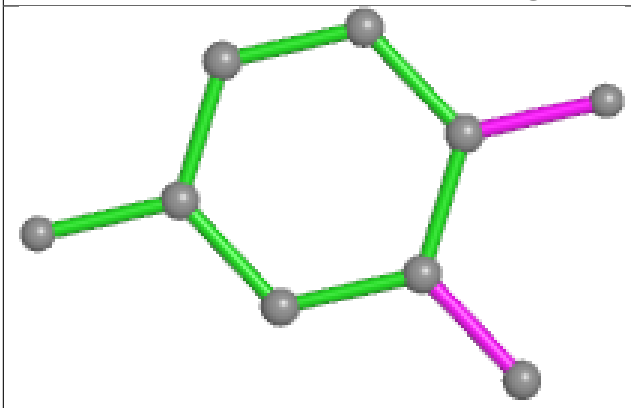


Rings

Ligand 7DV K 302



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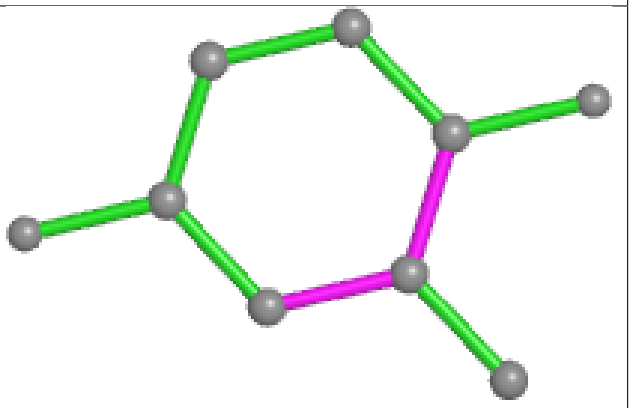
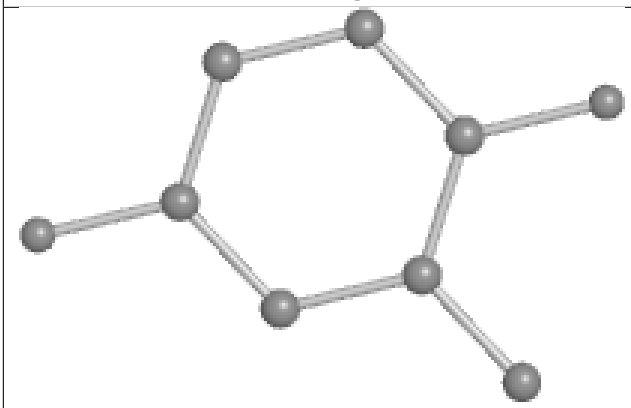


Bond angles



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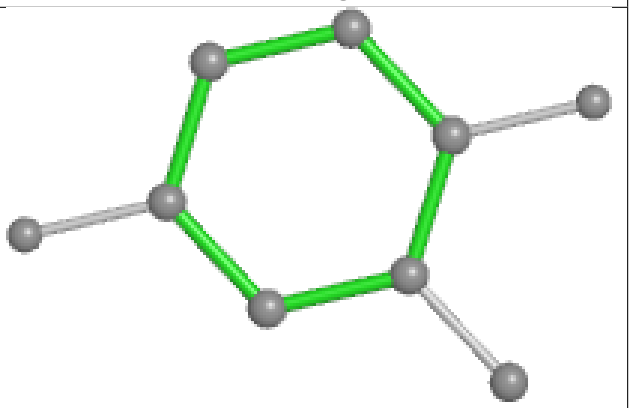
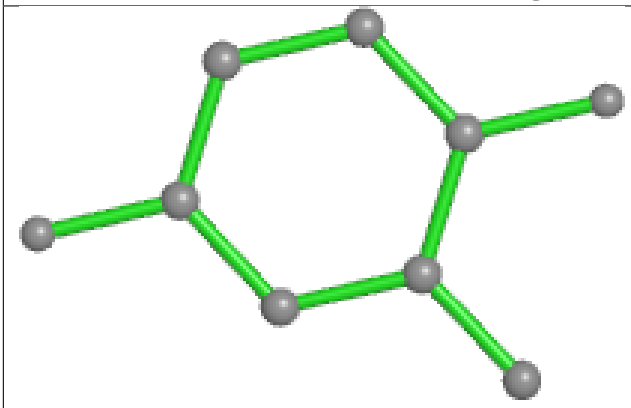


Rings

Ligand 7DV F 303



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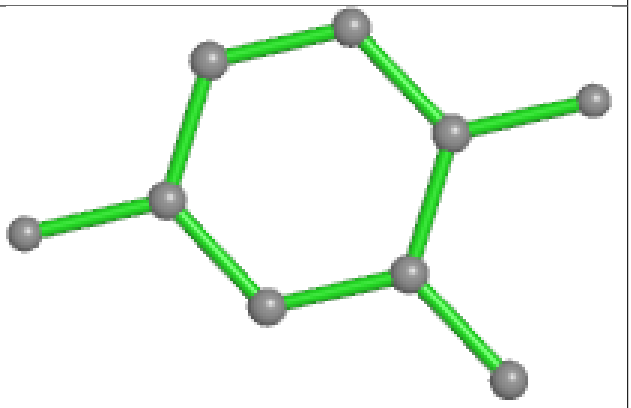
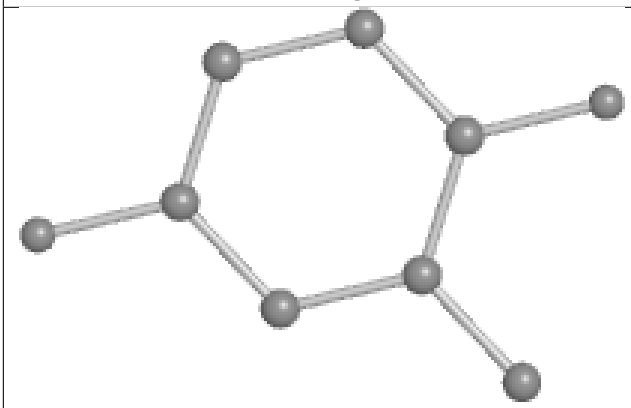


Bond angles



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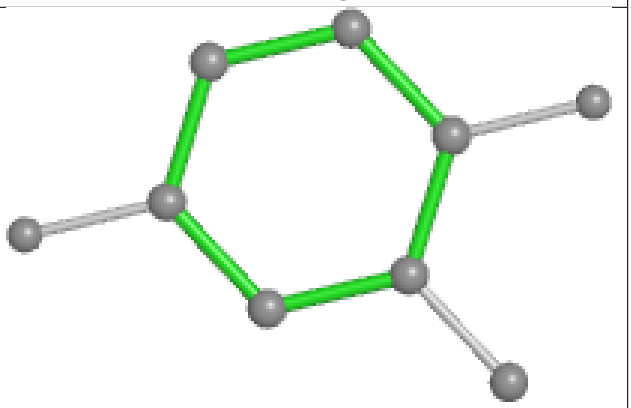
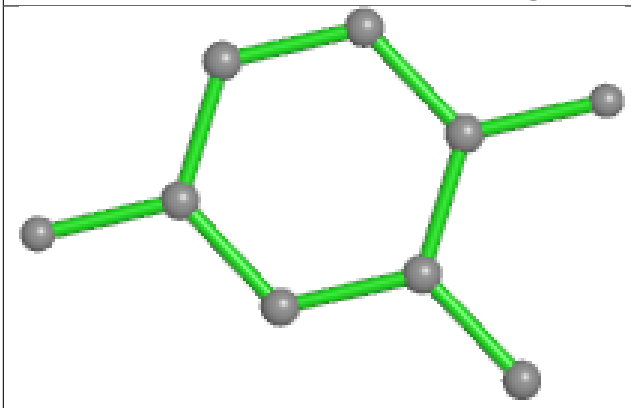


Rings

Ligand 7DV N 302



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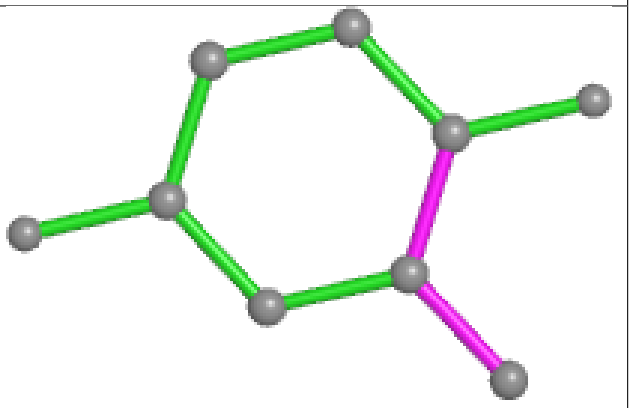

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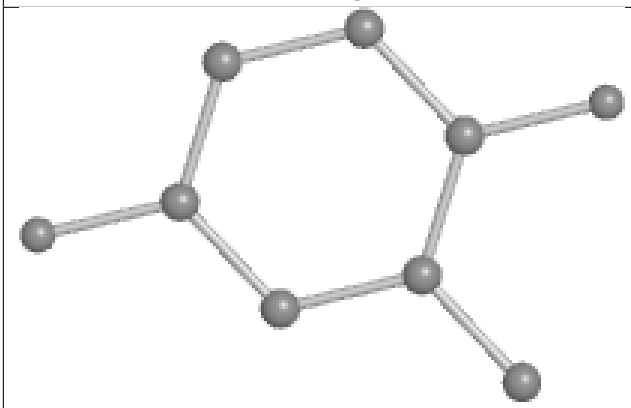

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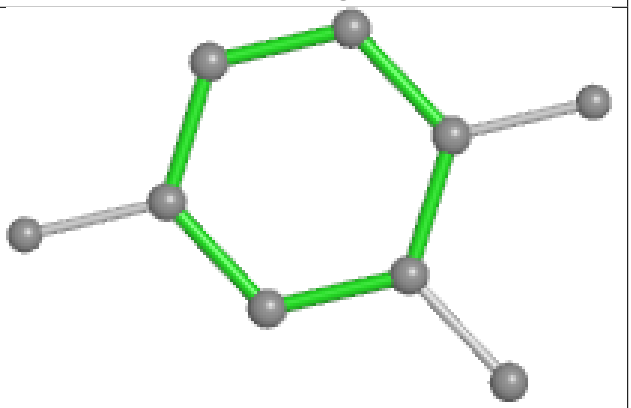
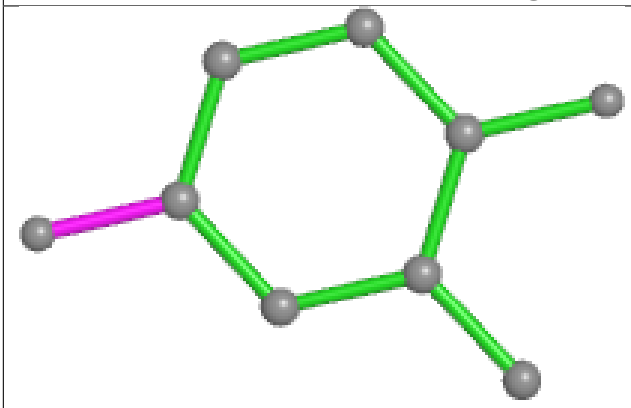


Rings

Ligand 7DV D 302



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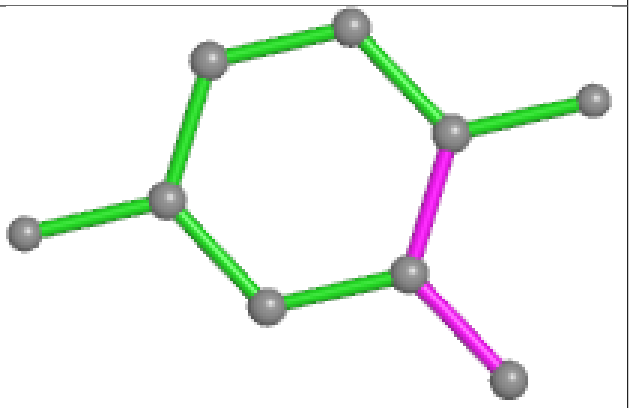

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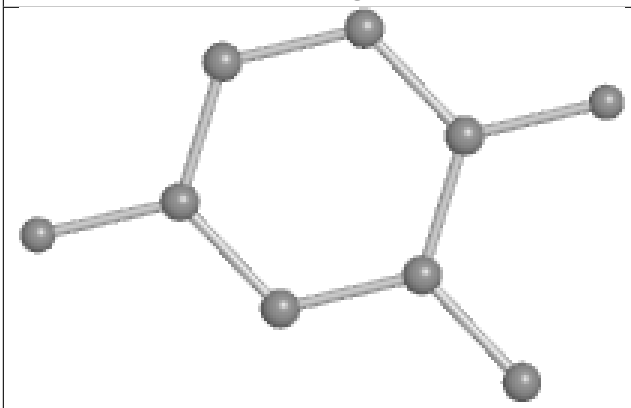

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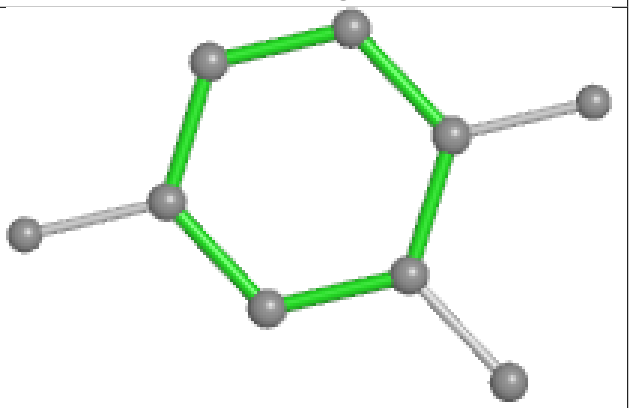
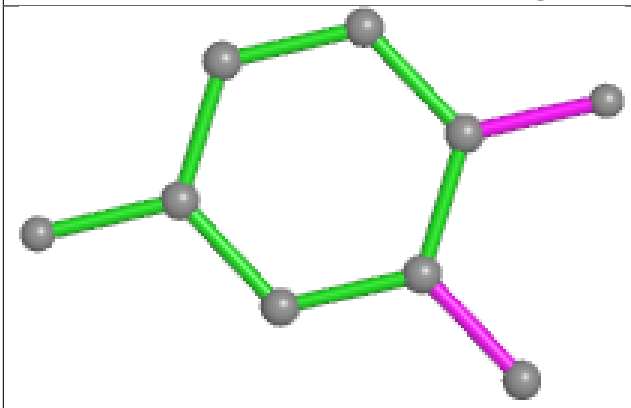


Rings

Ligand 7DV I 301



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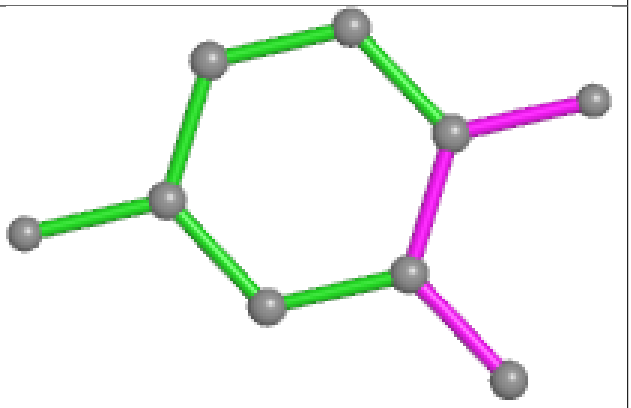

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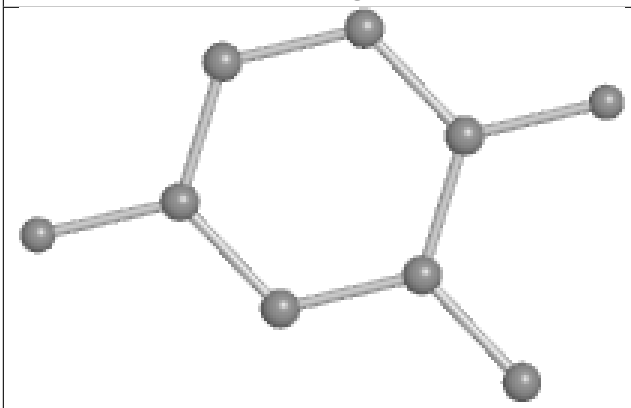
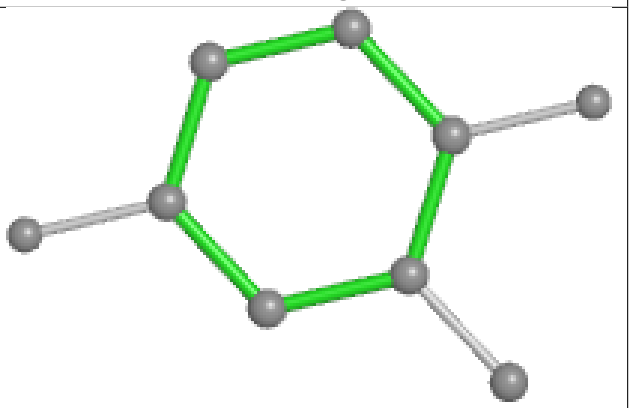
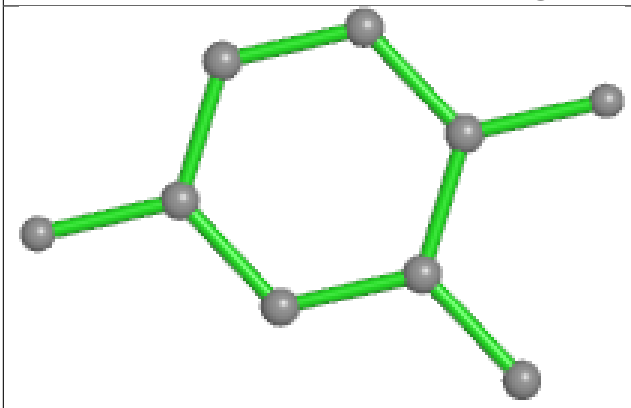


Torsions



Rings

Ligand 7DV I 303



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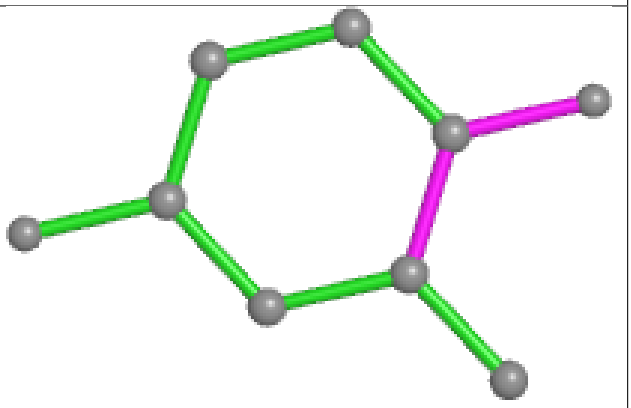

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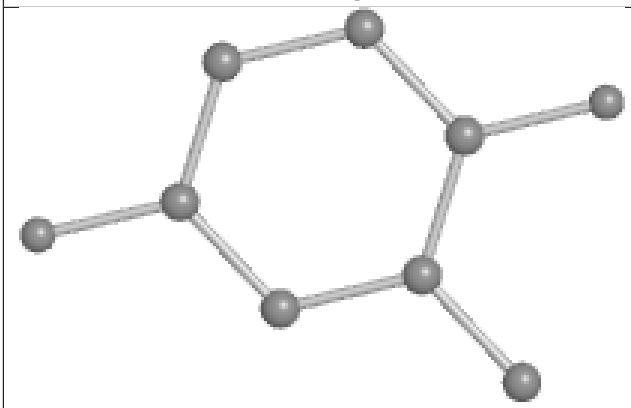

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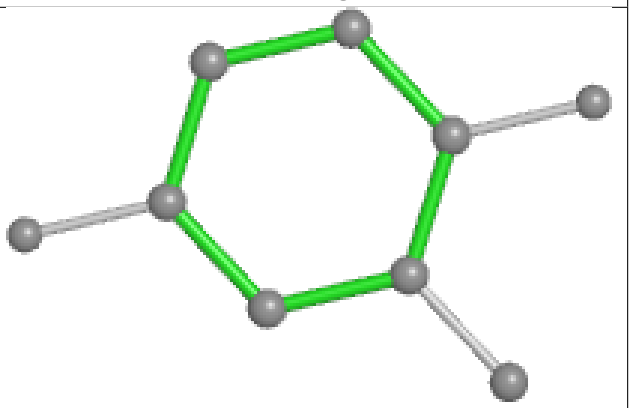
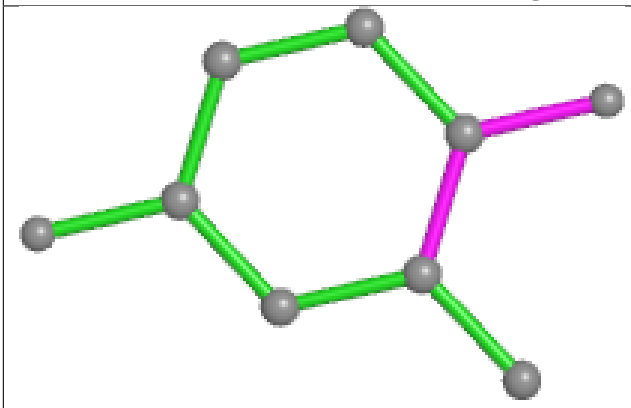


Rings

Ligand 7DV E 301



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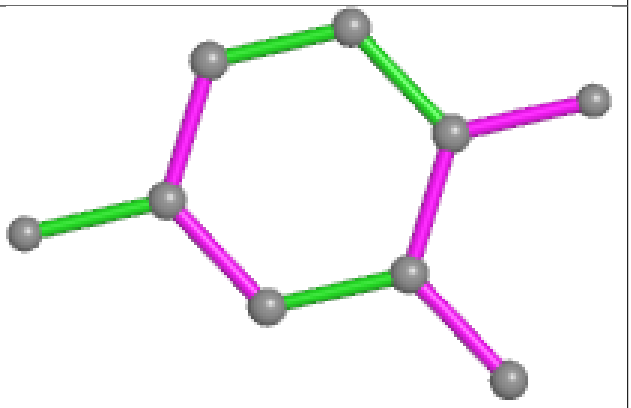
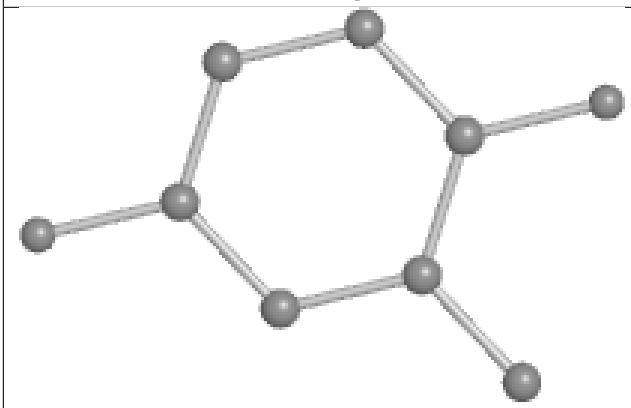


Bond angles



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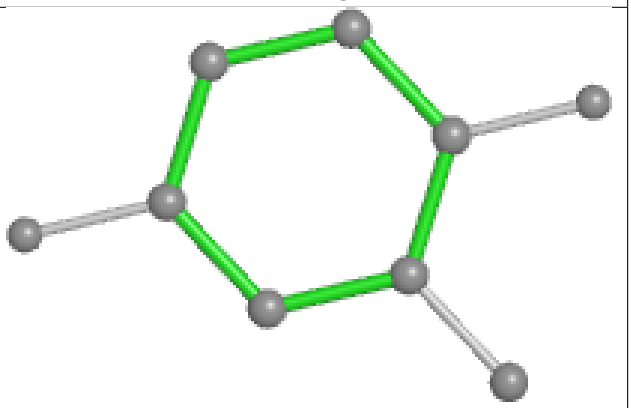
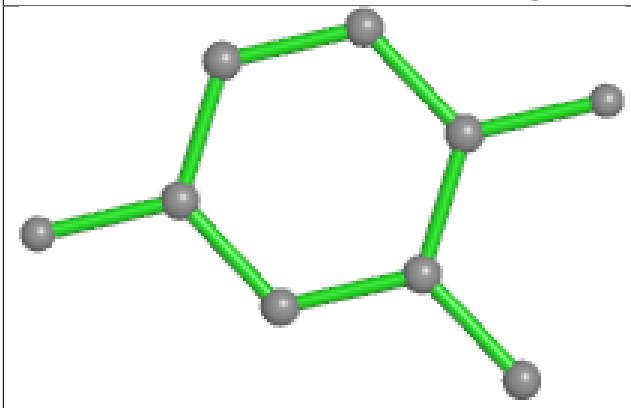
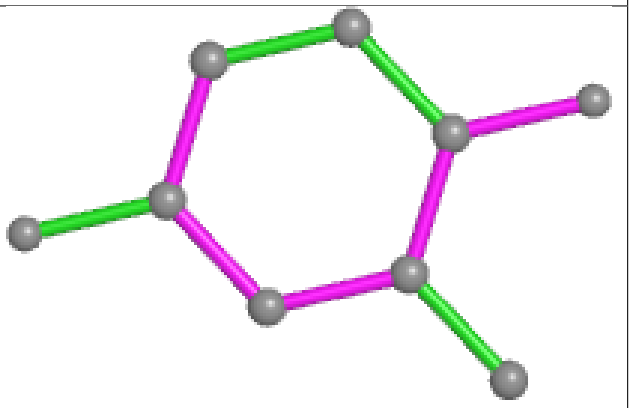


Rings

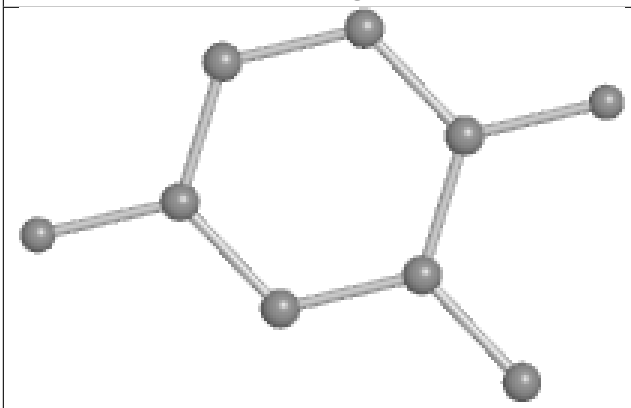
Ligand 7DV P 303



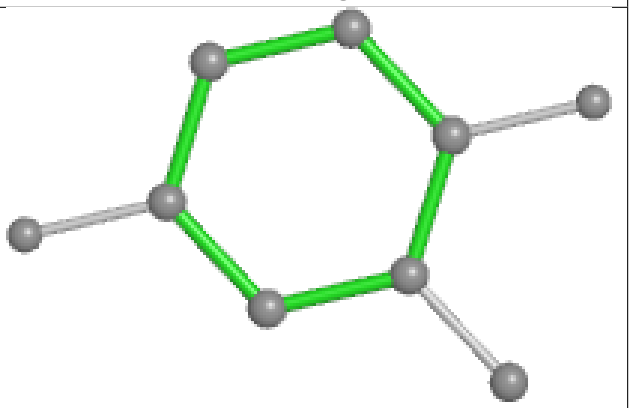
Bond lengths



Bond angles

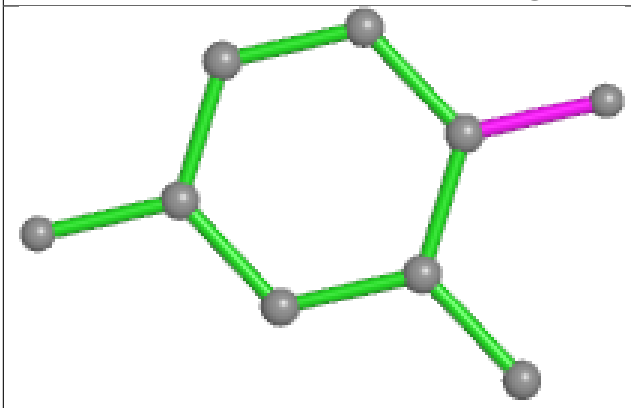


Torsions



Rings

Ligand 7DV B 303



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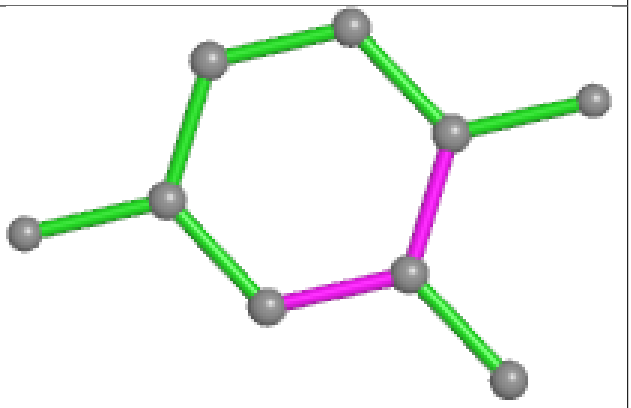

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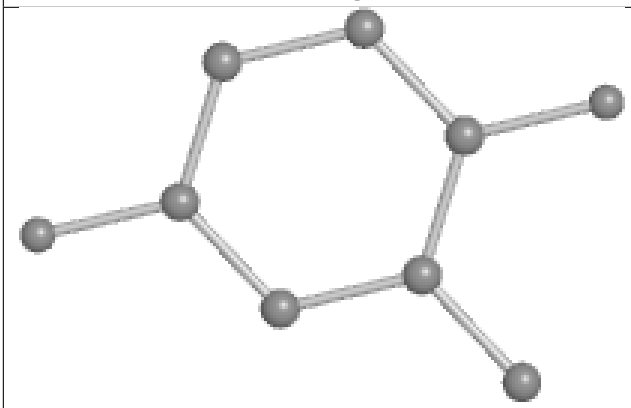

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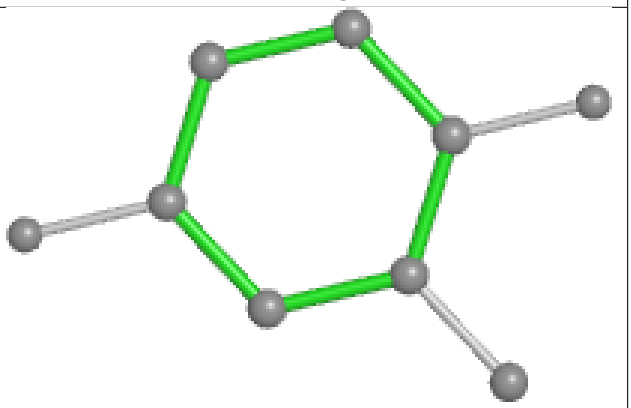
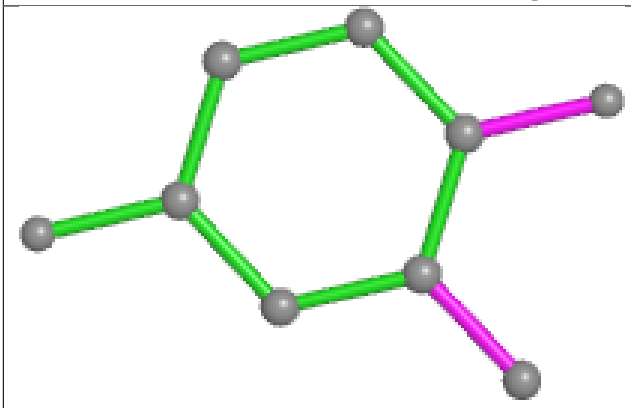


Rings

Ligand 7DV B 301



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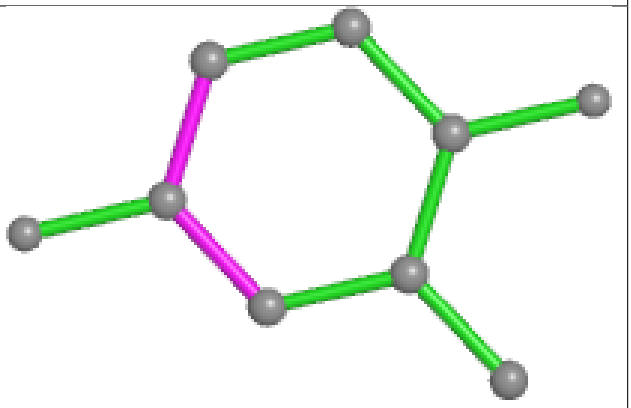

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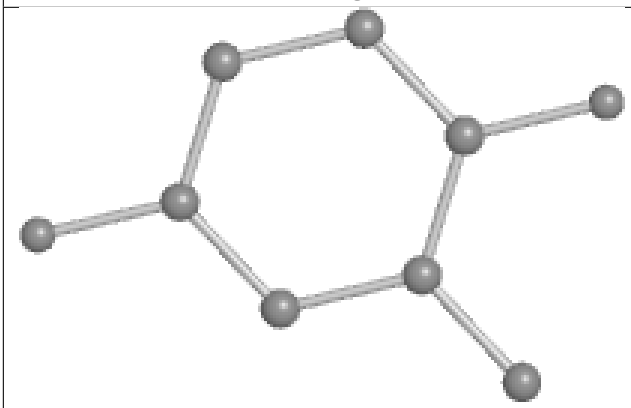

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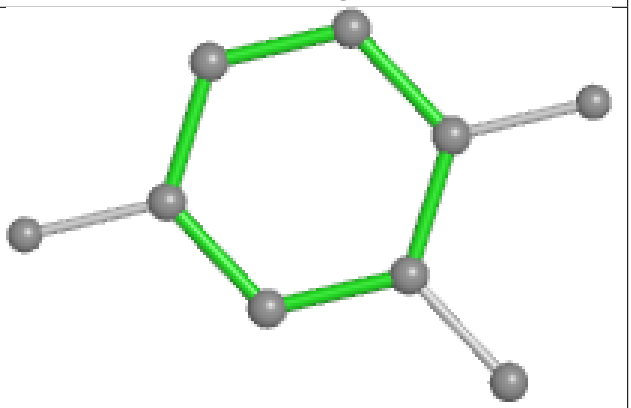
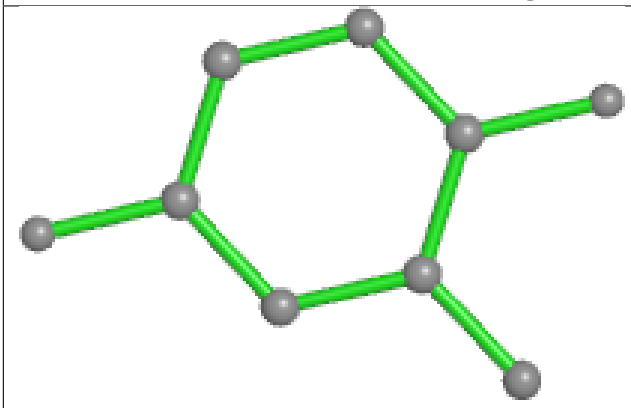


Rings

Ligand 7DV M 303



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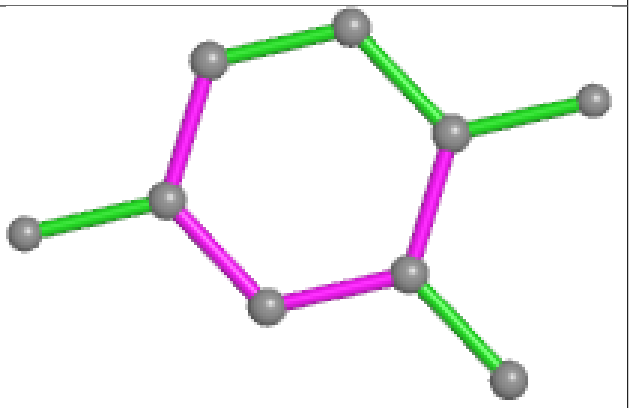
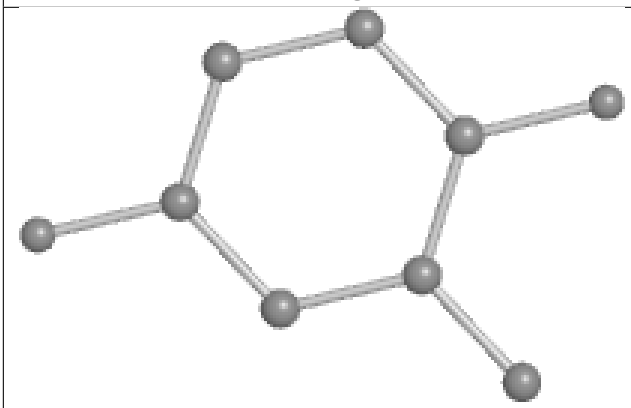


Bond angles



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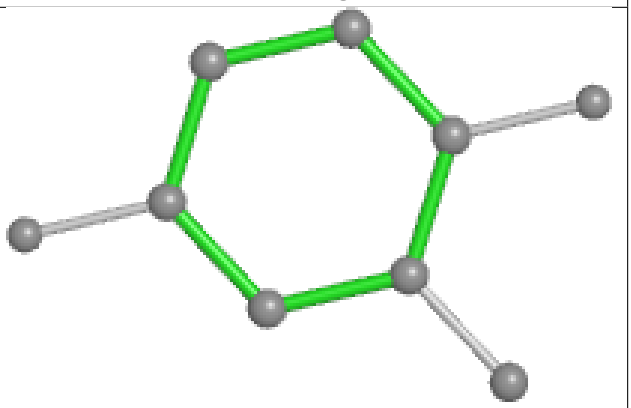
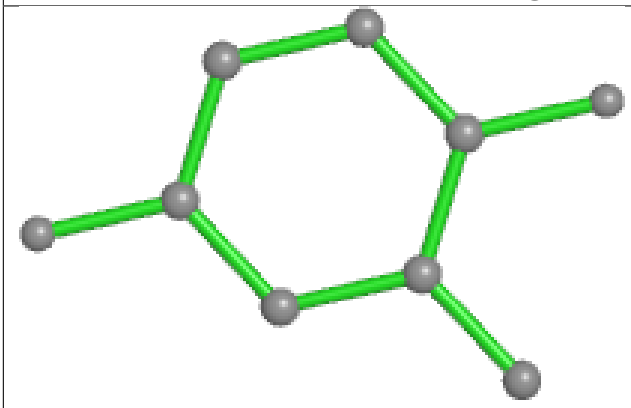


Rings

Ligand 7DV B 302



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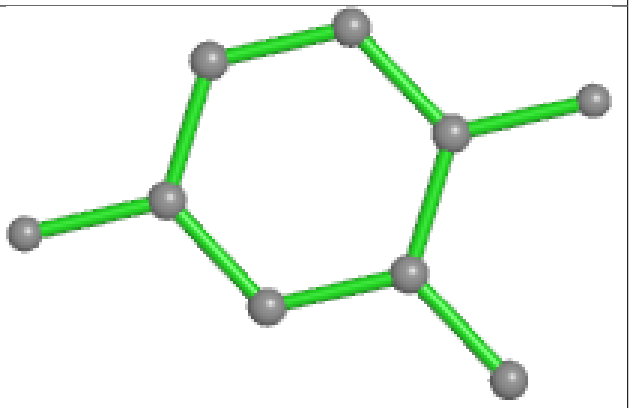

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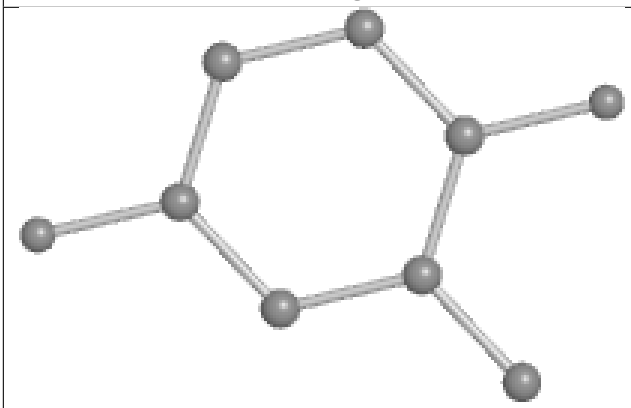

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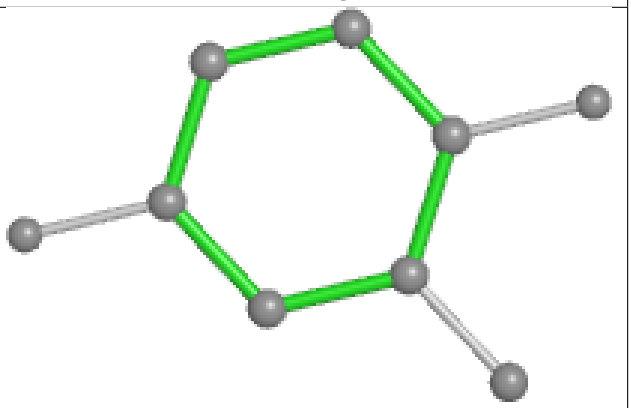
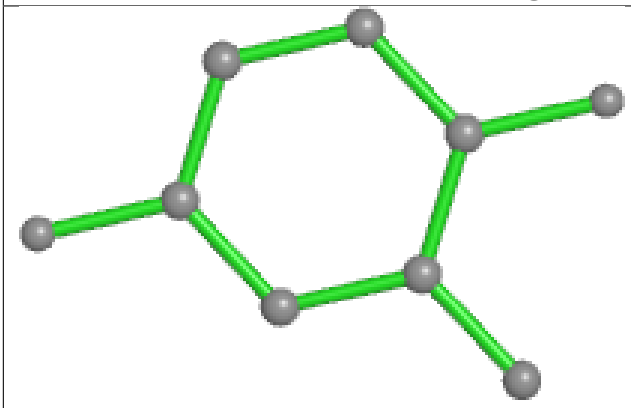


Rings

Ligand 7DV A 303



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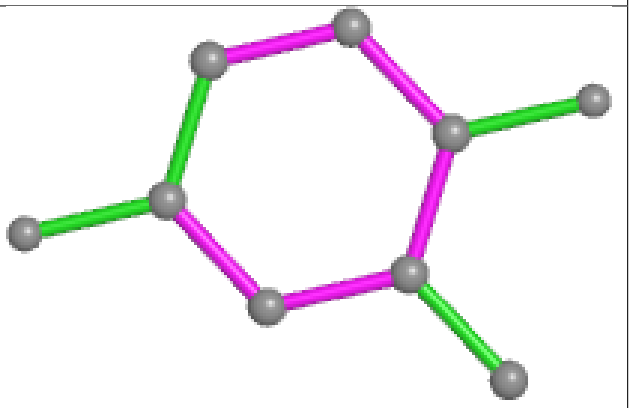

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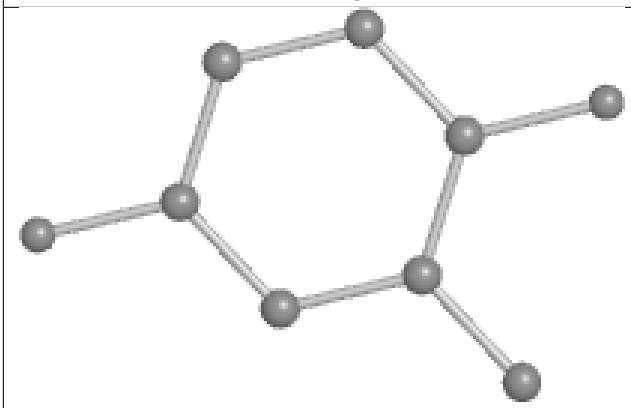

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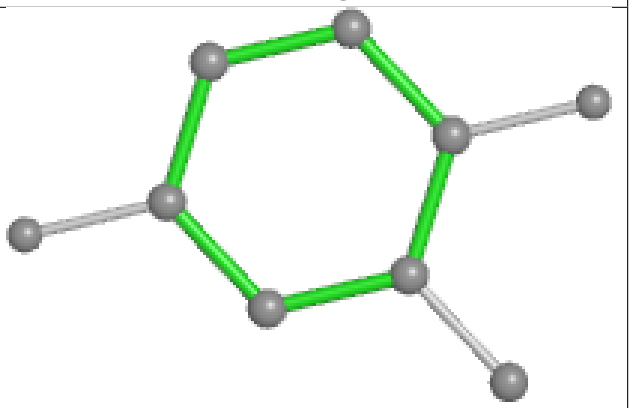
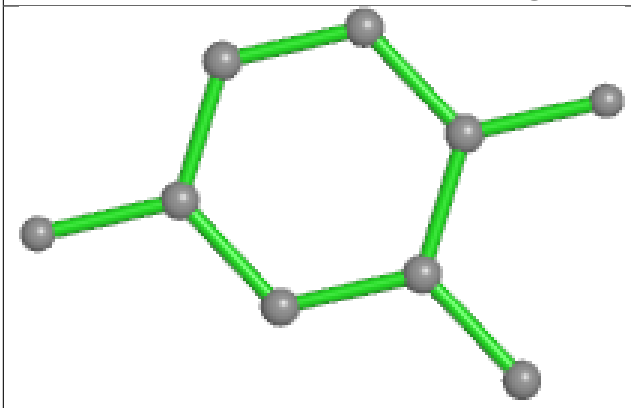


Rings

Ligand 7DV C 302



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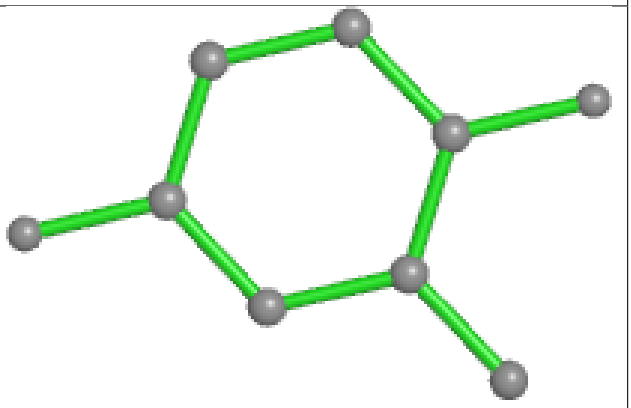

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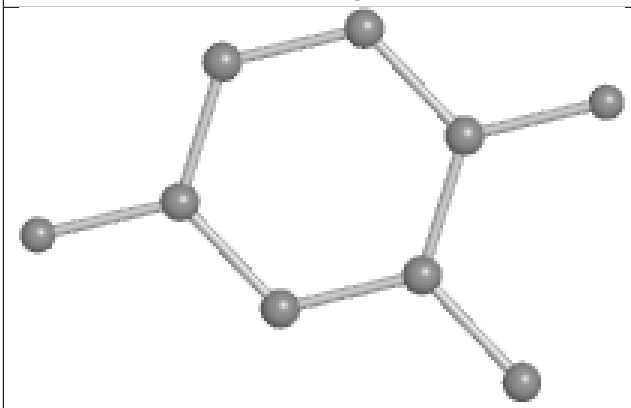

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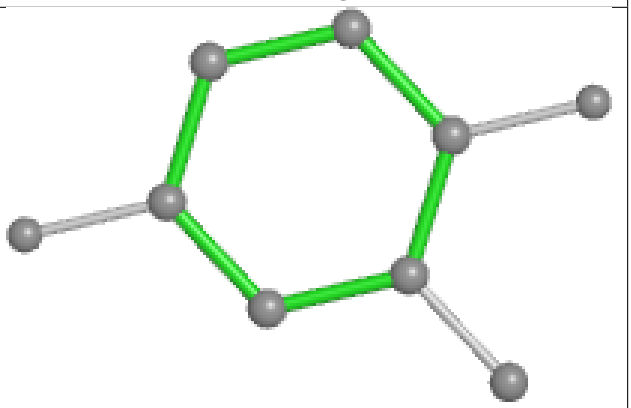
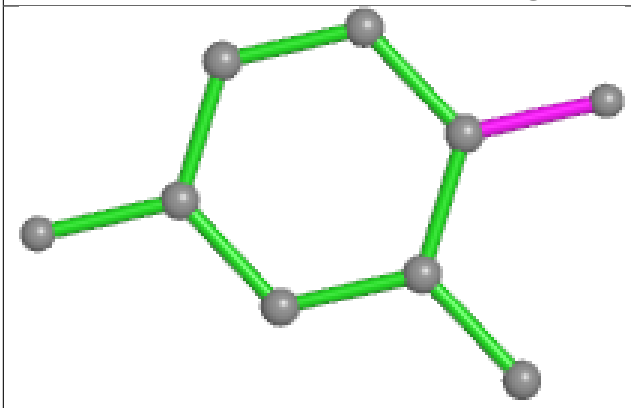


Rings

Ligand 7DV K 301



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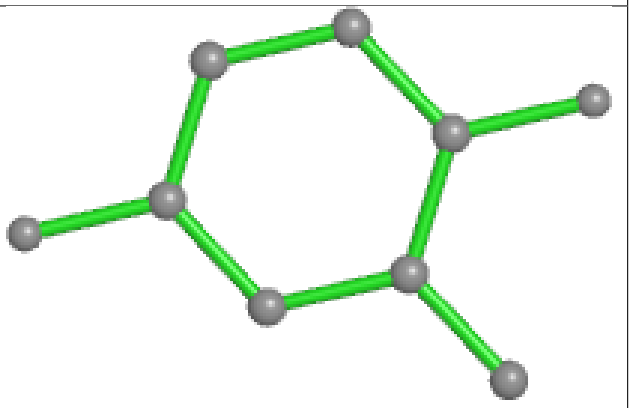

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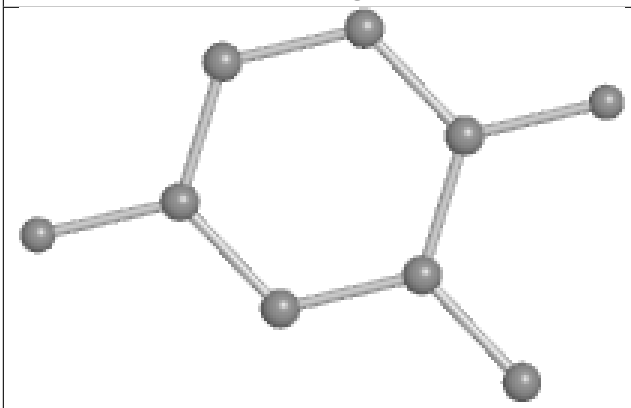

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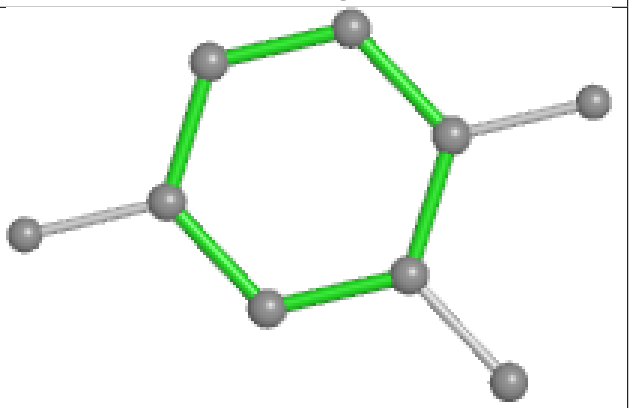
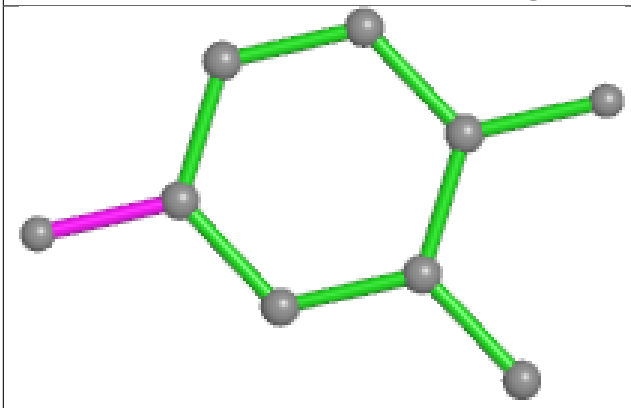


Rings

Ligand 7DV H 301



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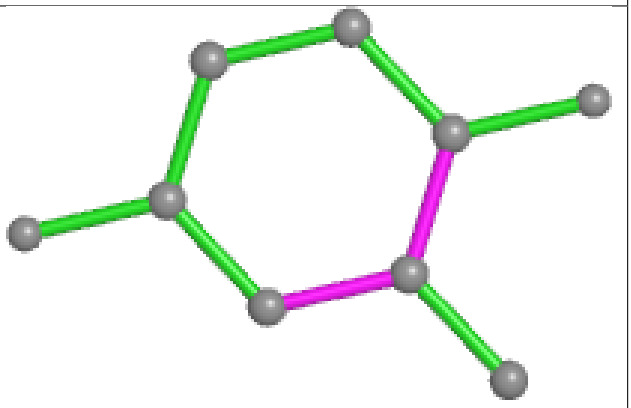
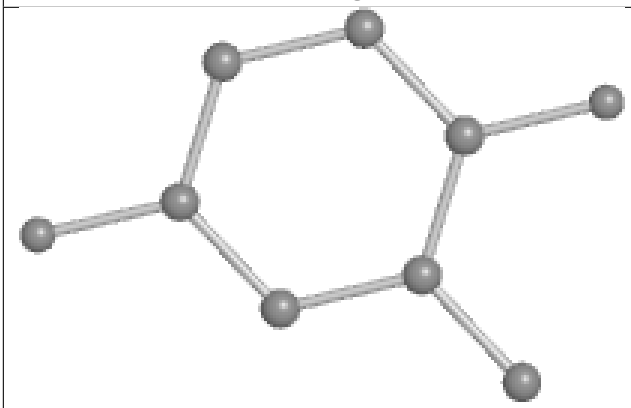


Bond angles



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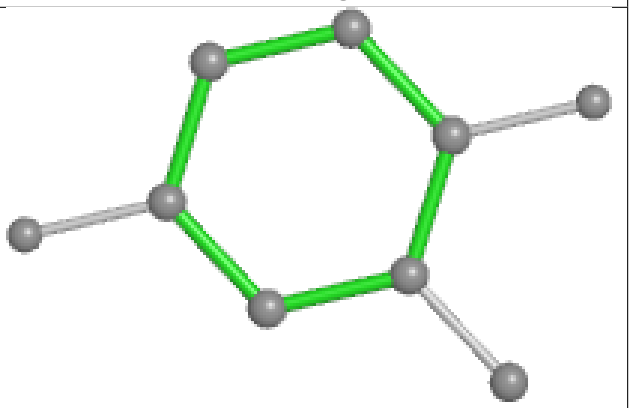
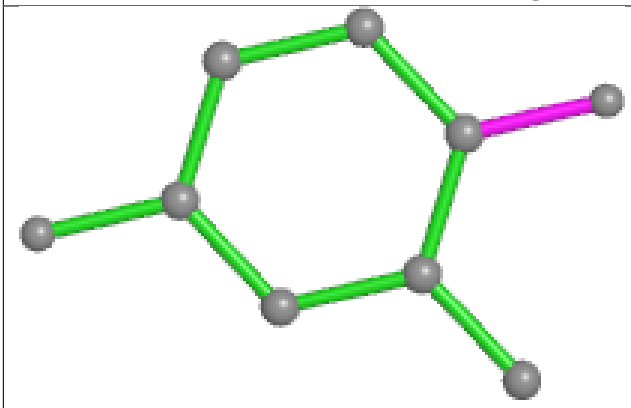


Rings

Ligand 7DV E 302



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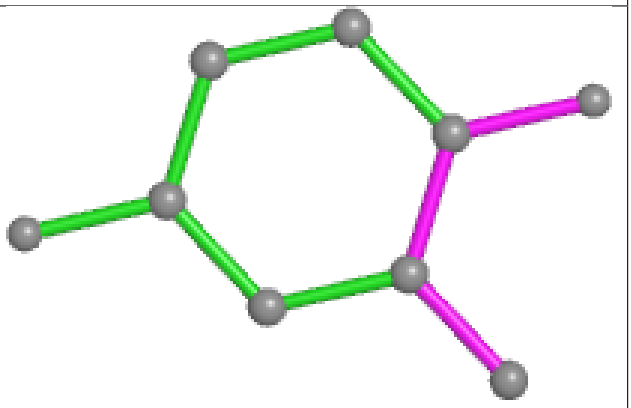

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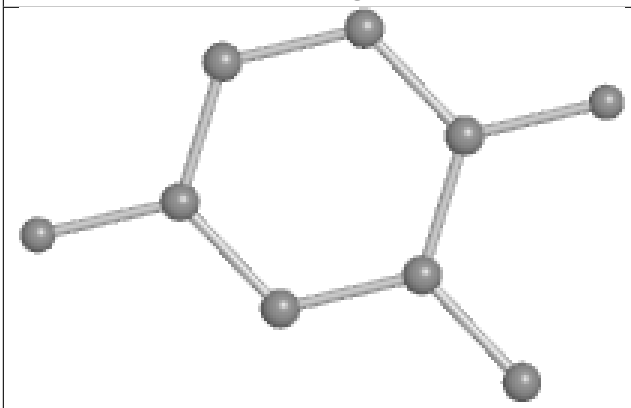

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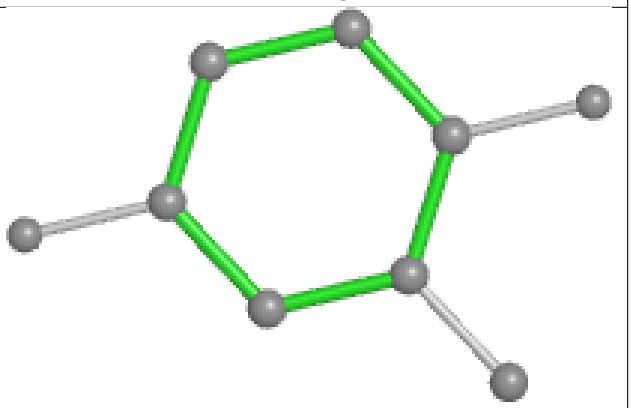
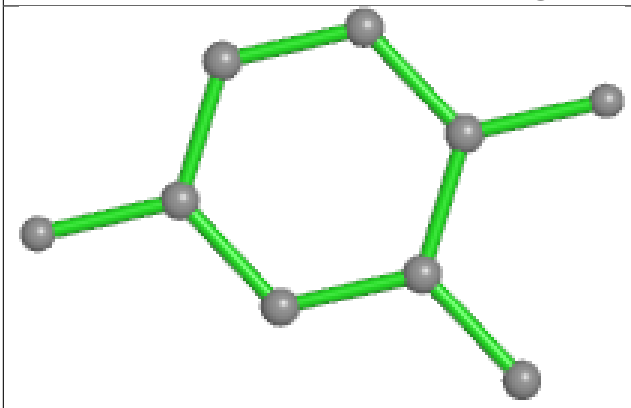


Rings

Ligand 7DV I 302



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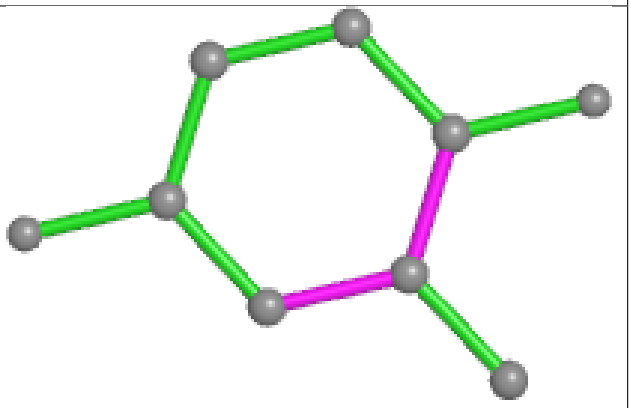

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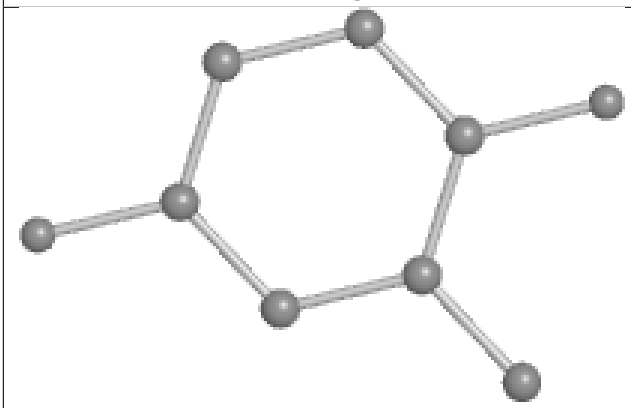

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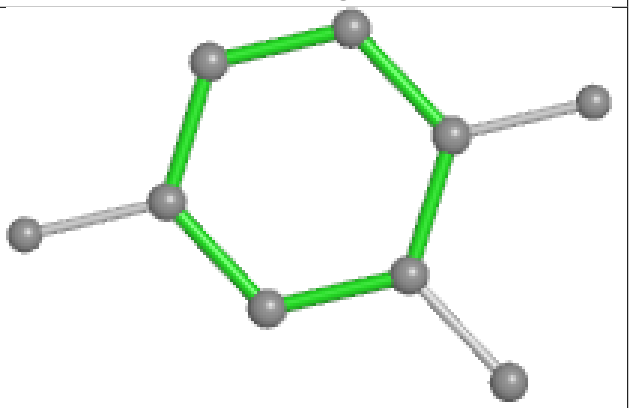
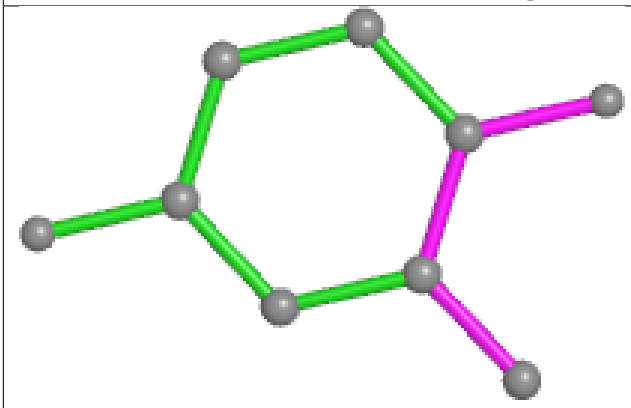


Rings

Ligand 7DV M 301



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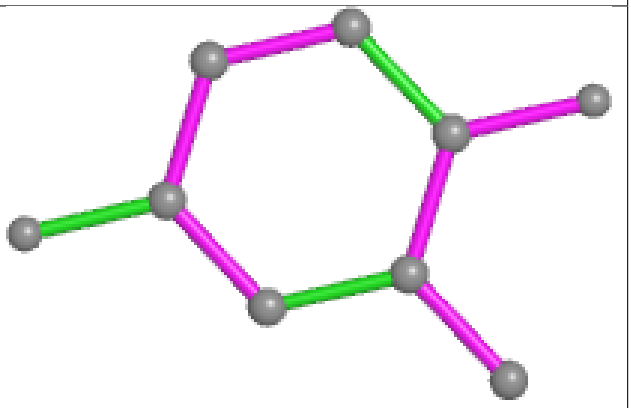

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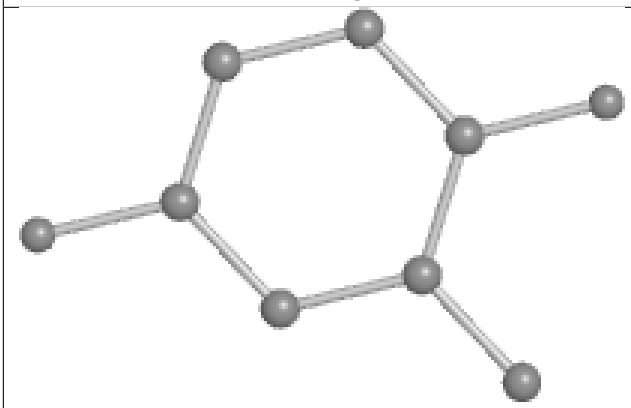

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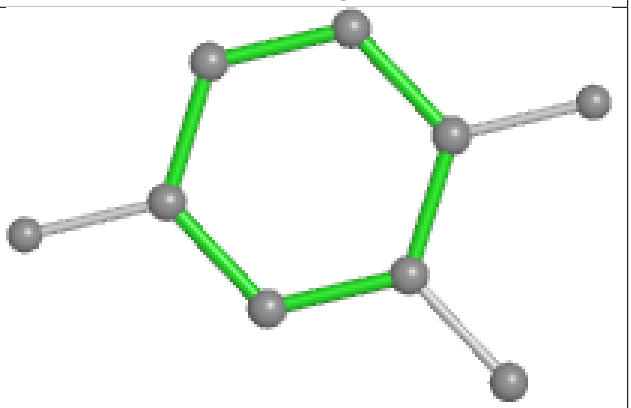
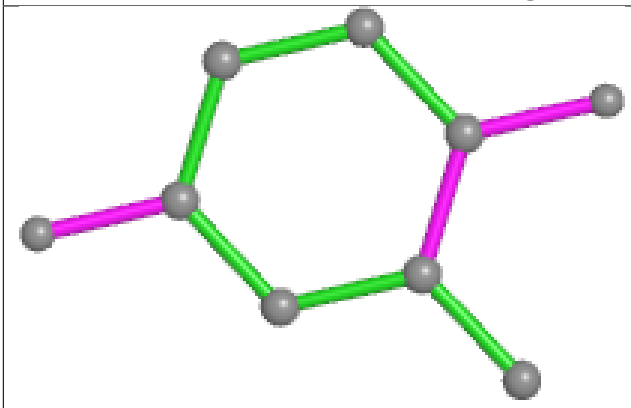


Rings

Ligand 7DV M 302



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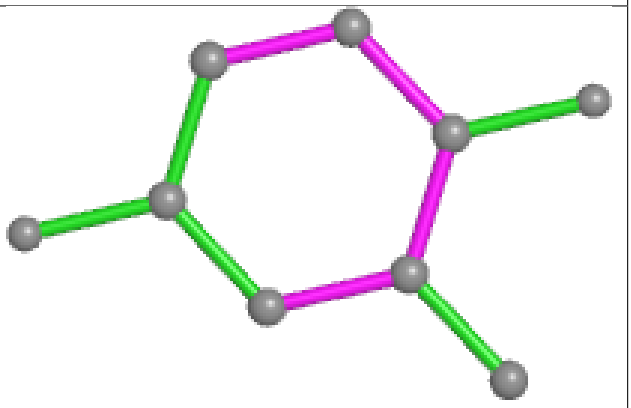

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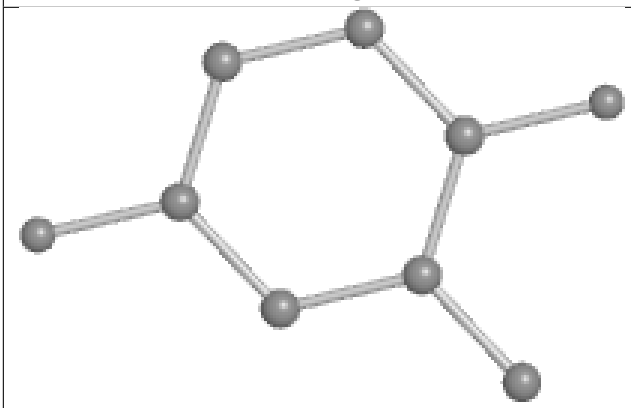

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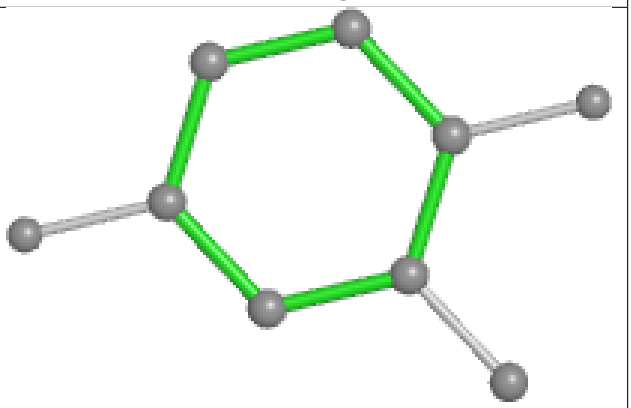
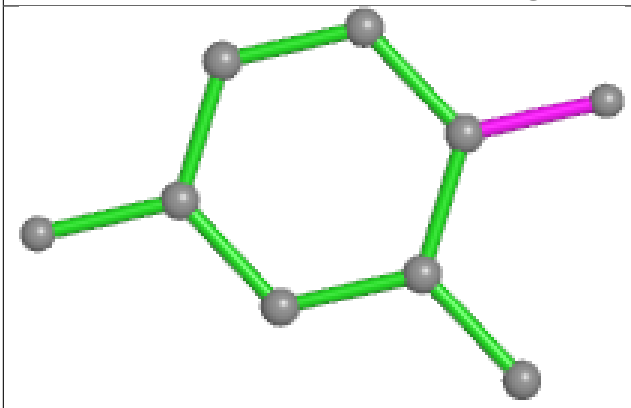


Rings

Ligand 7DV G 301



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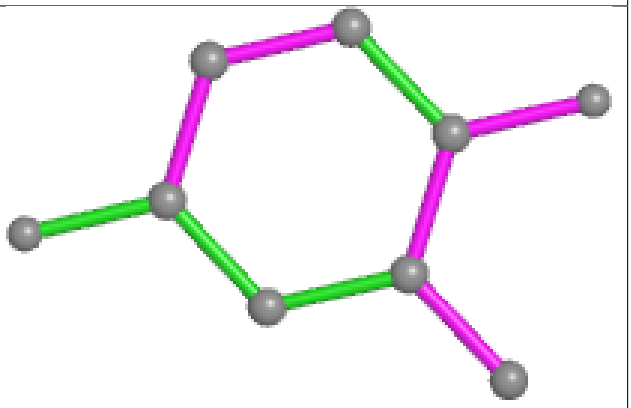
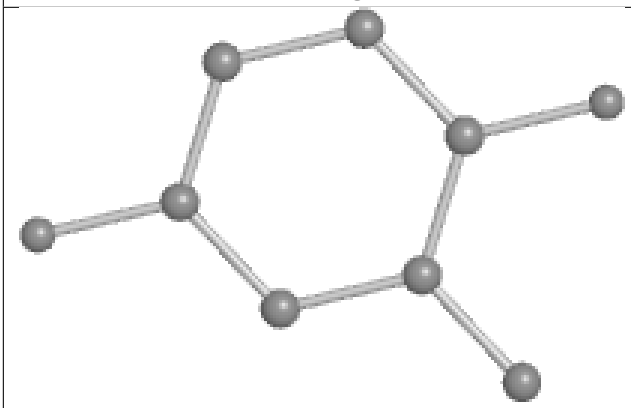


Bond angles



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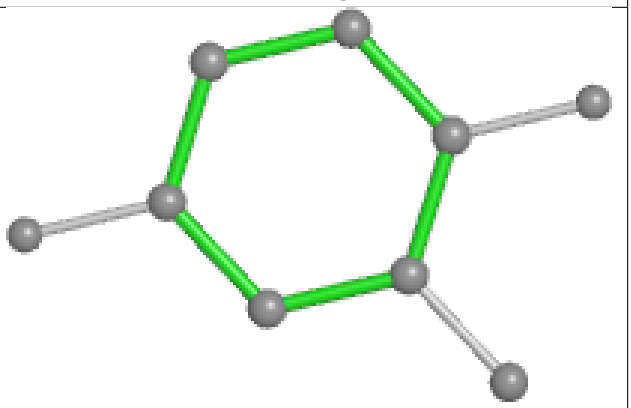
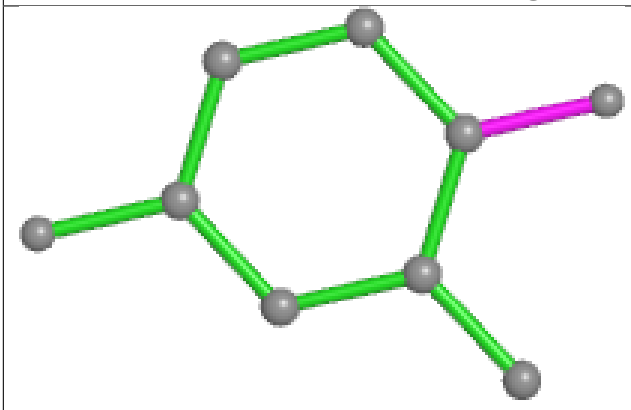


Rings

Ligand 7DV N 303



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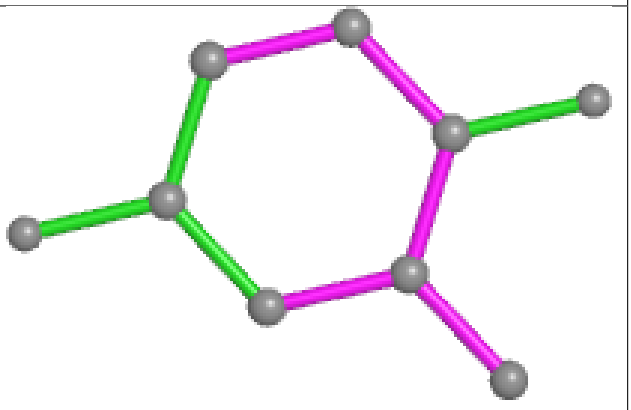

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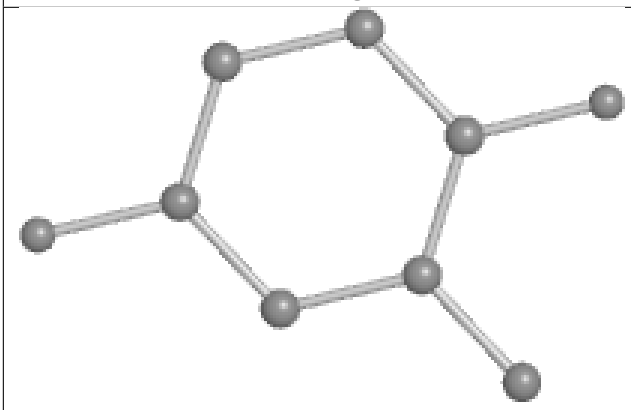
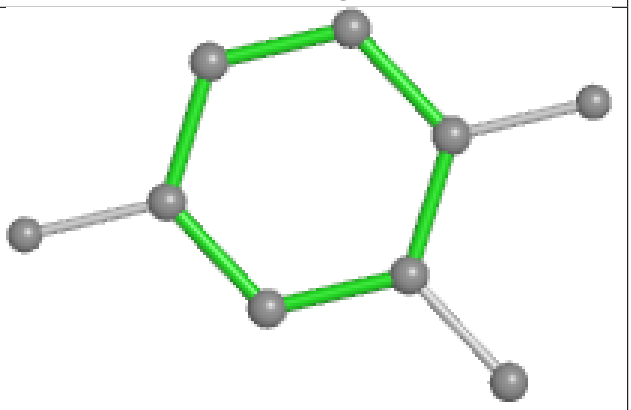
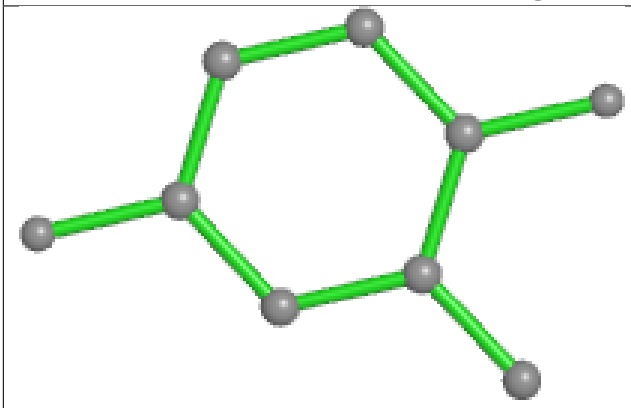


Torsions

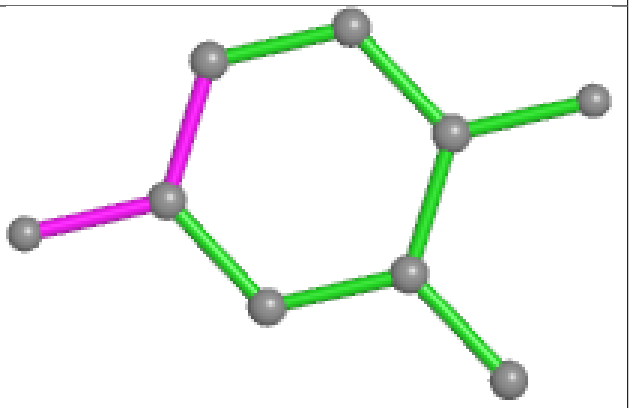


Rings

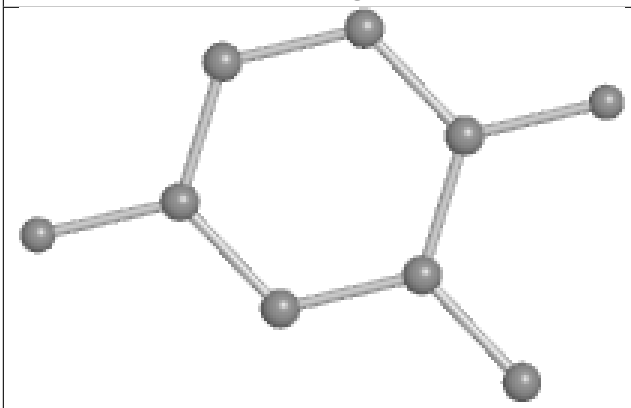
Ligand 7DV J 301



Bond lengths



Bond angles



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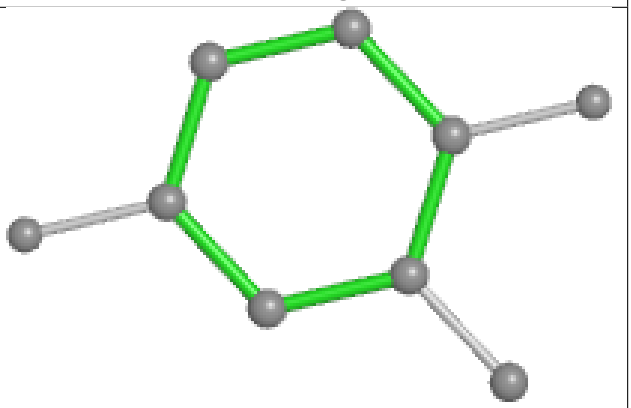
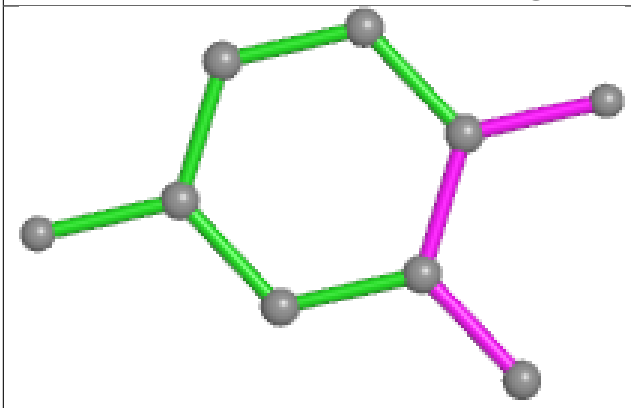


Rings

Ligand 7DV F 301



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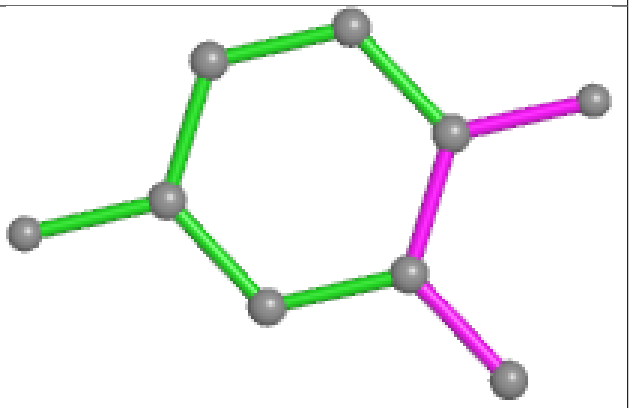

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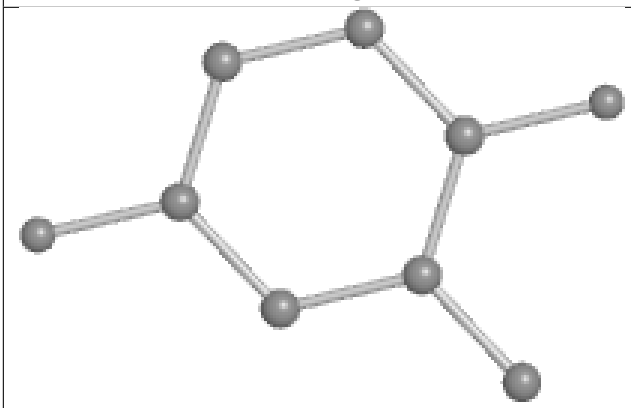

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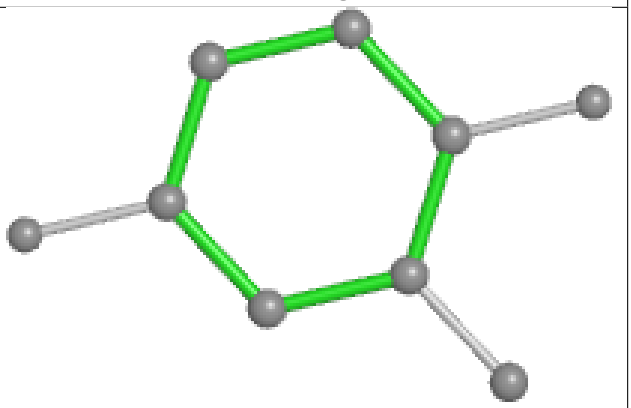
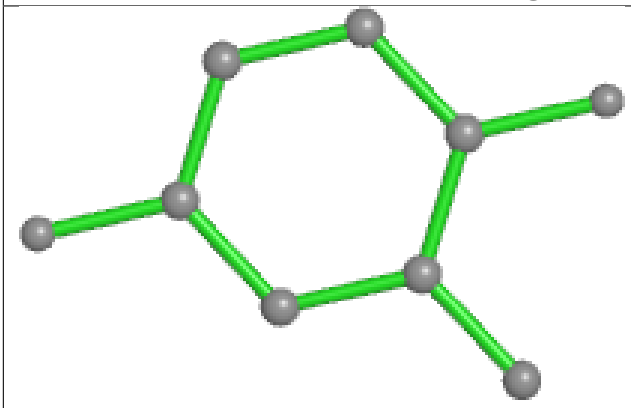


Rings

Ligand 7DV G 302



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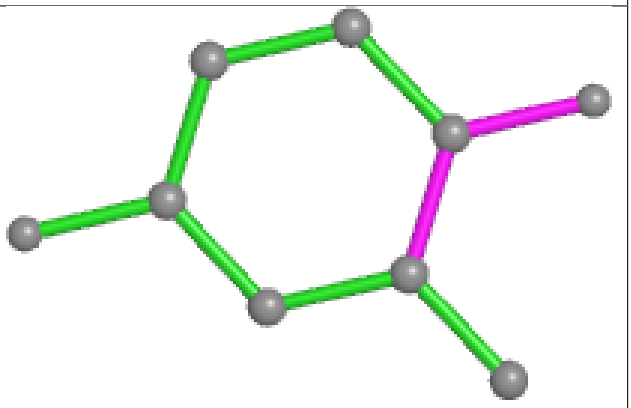

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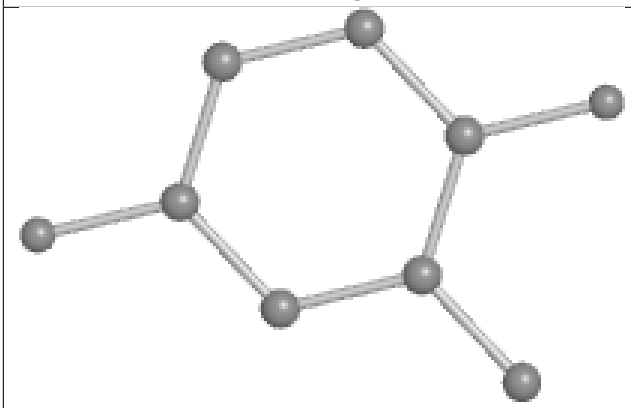

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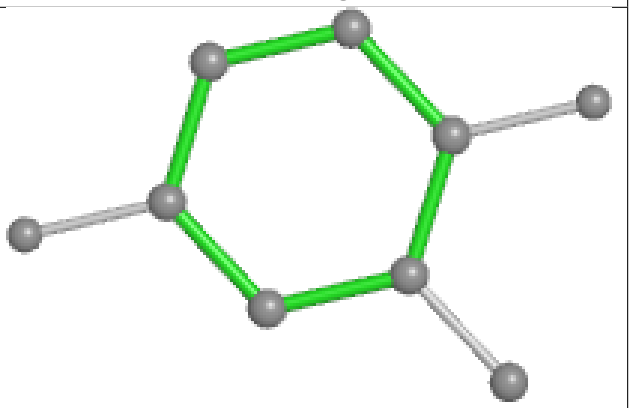
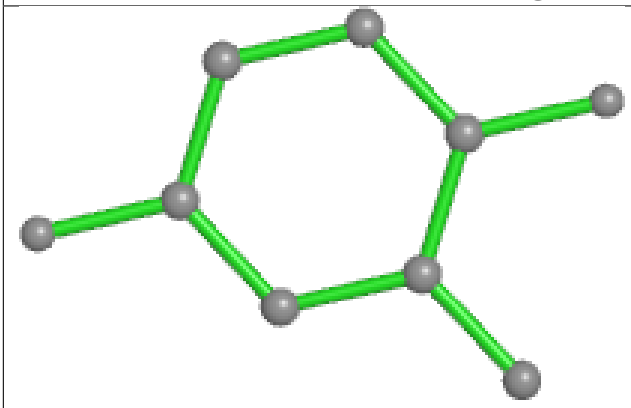


Rings

Ligand 7DV J 303



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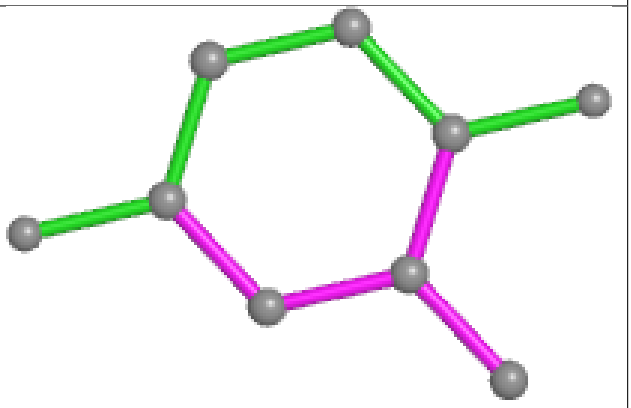

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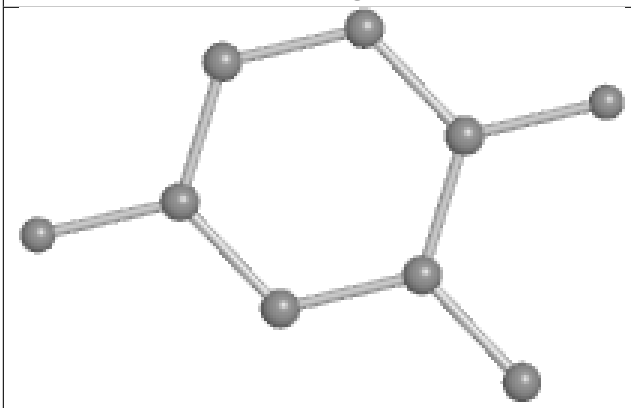

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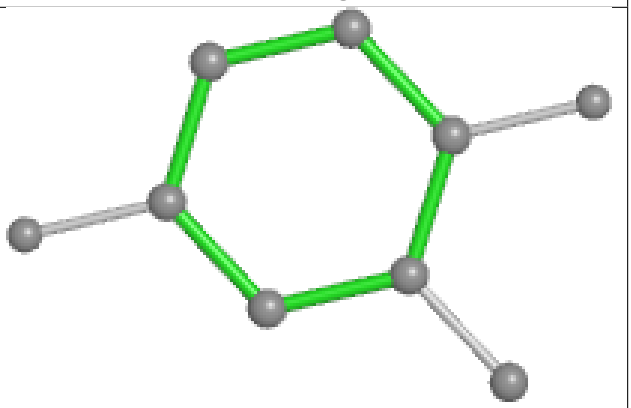
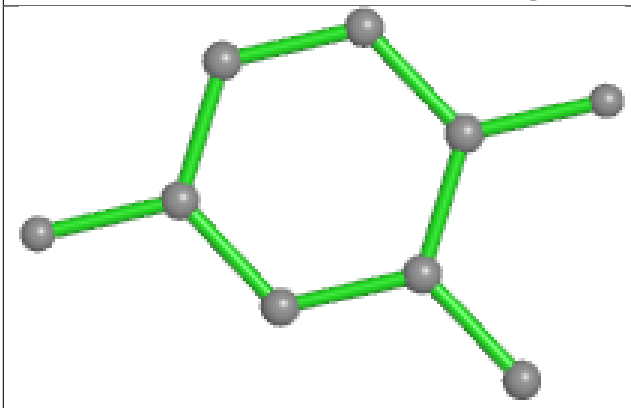


Rings

Ligand 7DV H 302



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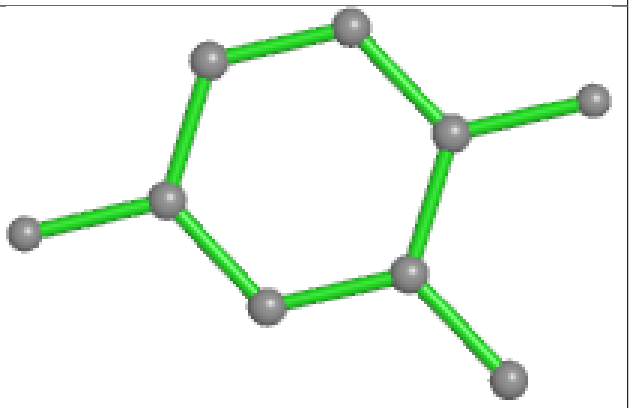
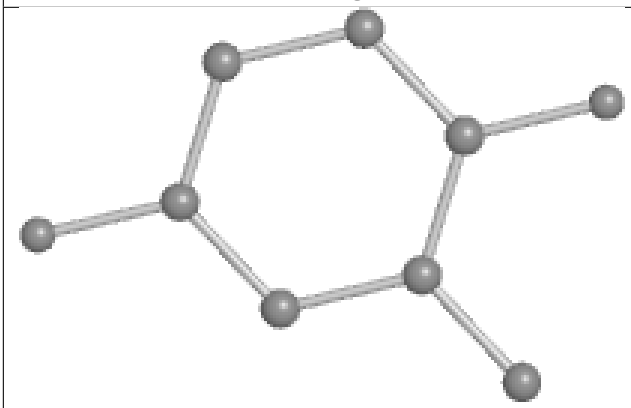


Bond angles



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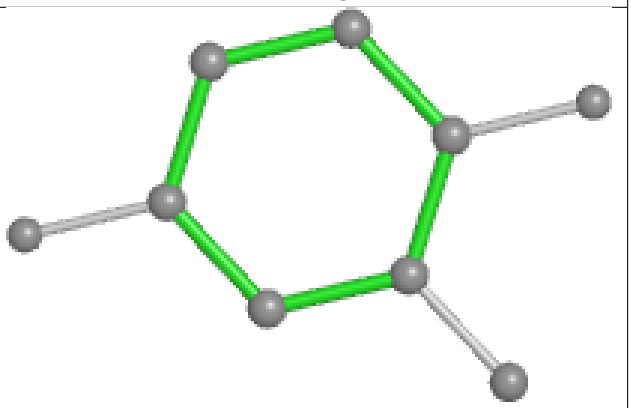
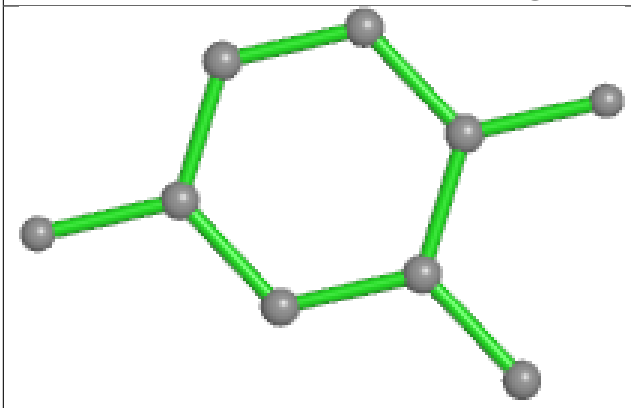


Rings

Ligand 7DV P 302



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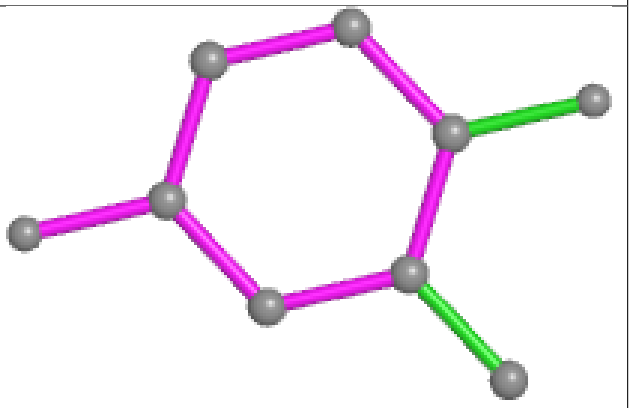

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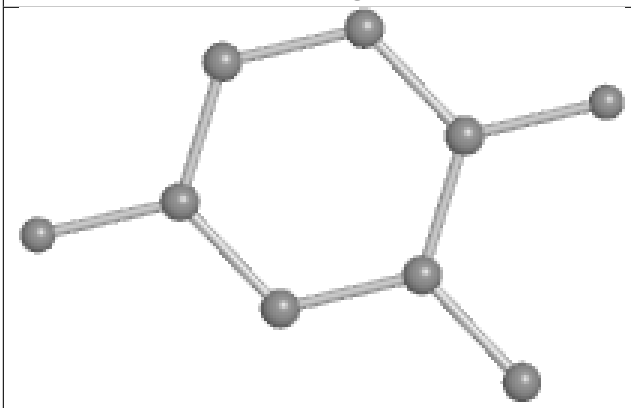

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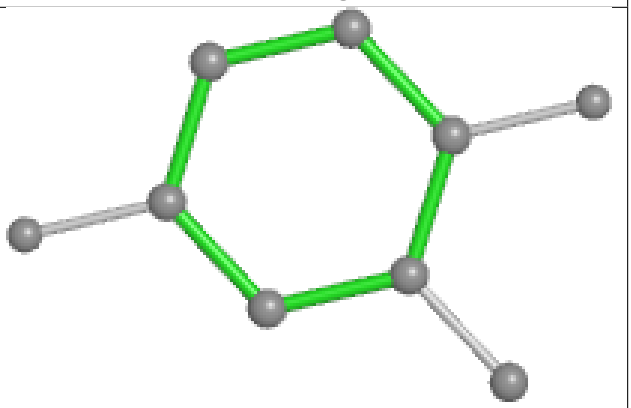
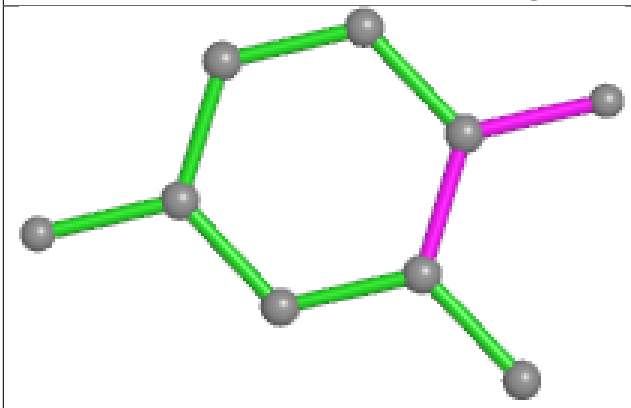


Rings

Ligand 7DV O 301



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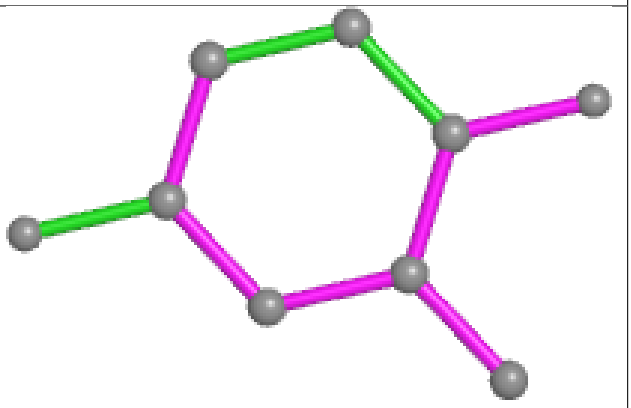

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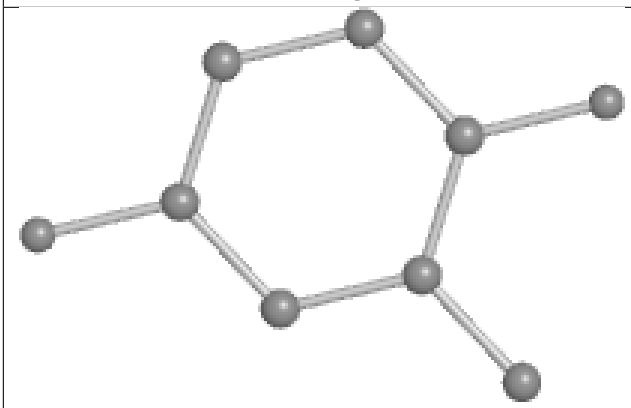

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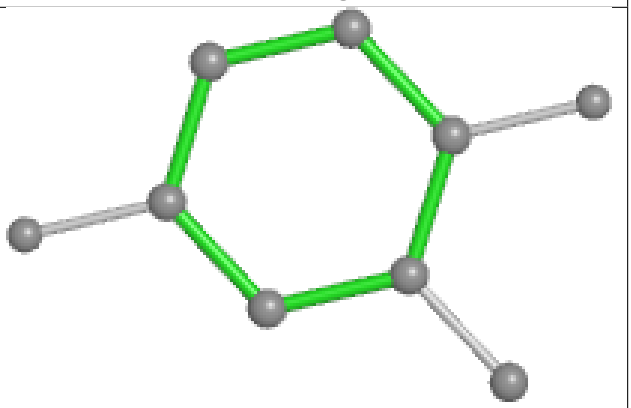
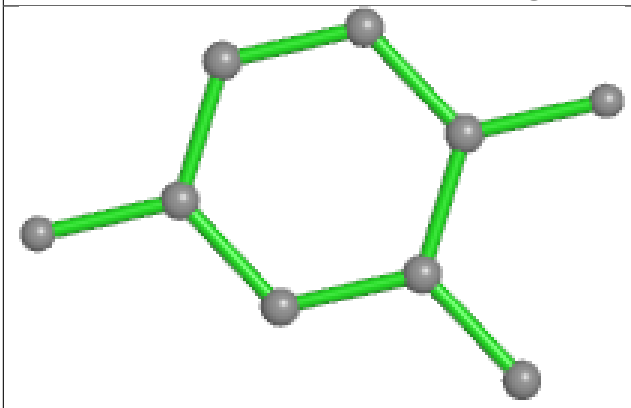


Rings

Ligand 7DV O 303



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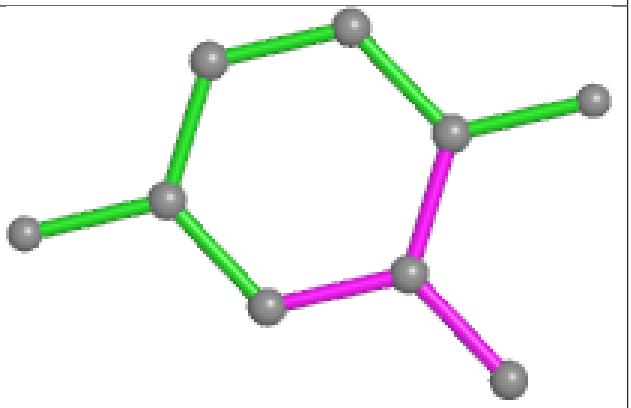
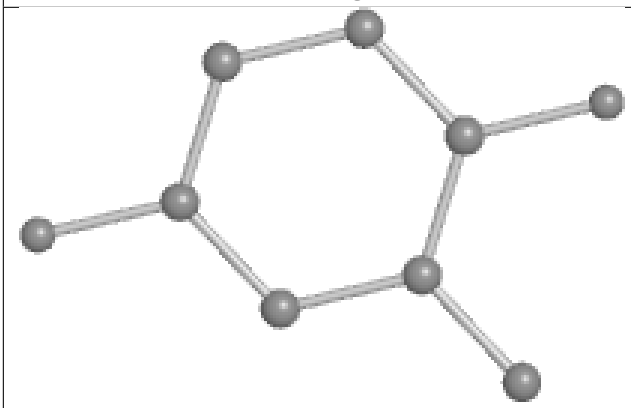


Bond angles



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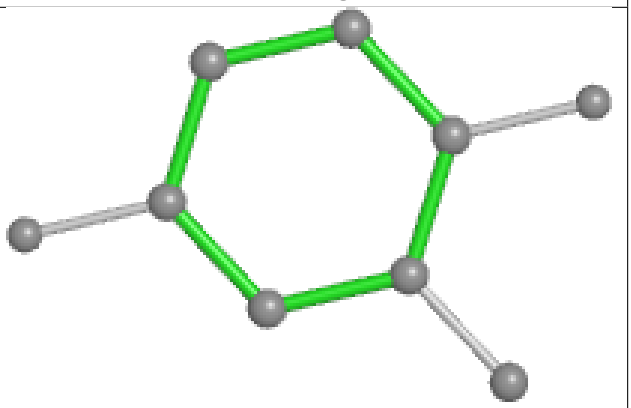
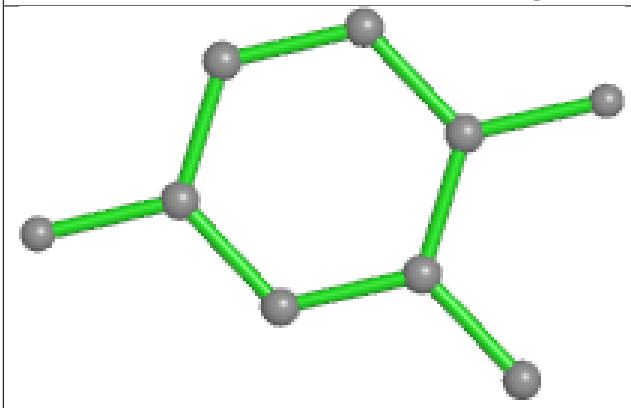


Rings

Ligand 7DV L 304



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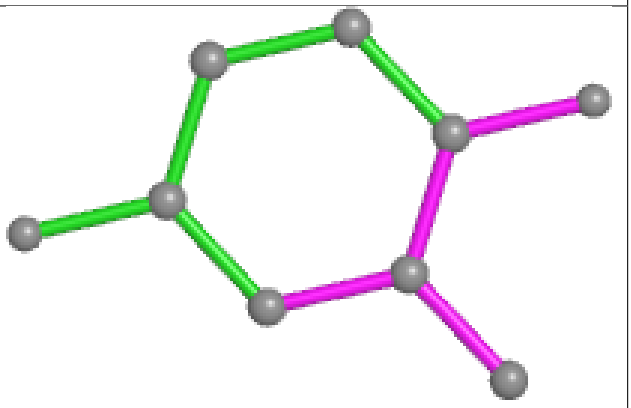
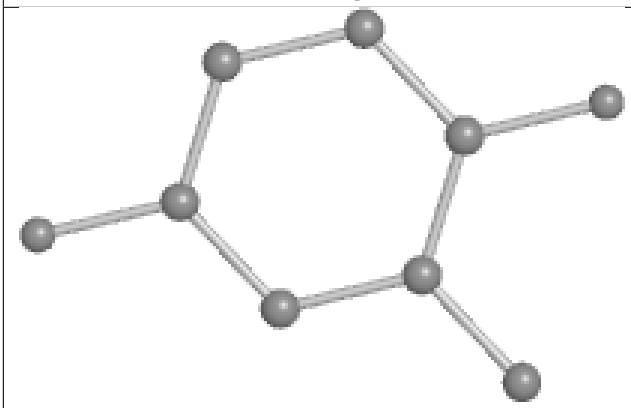
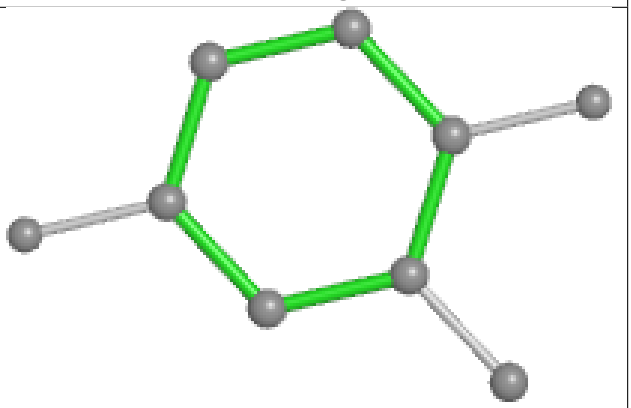


Bond angles

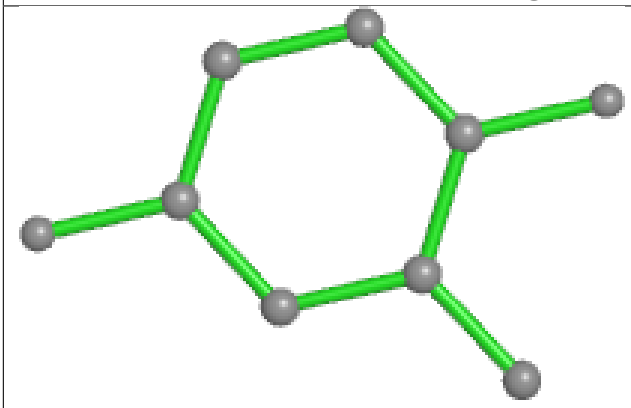


Torsions



Rings

Ligand 7DV O 302



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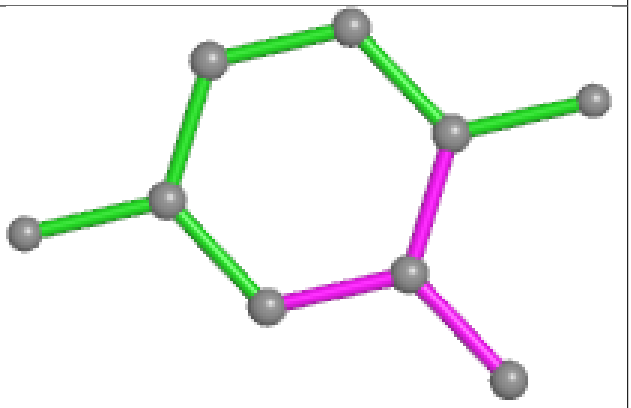

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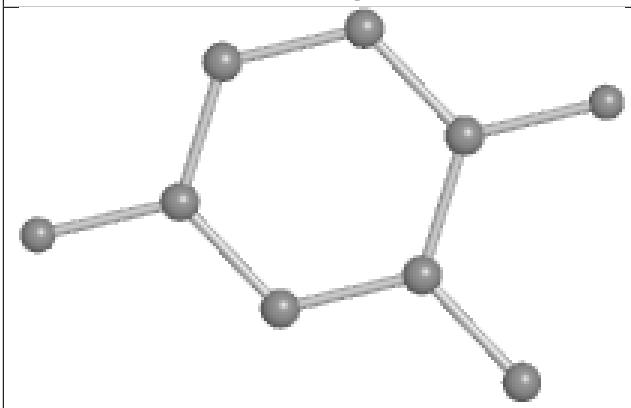

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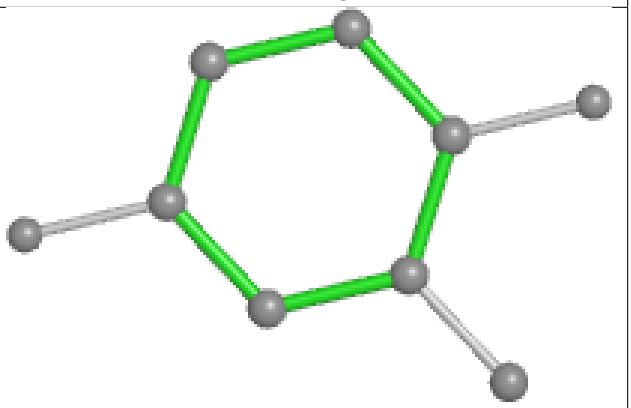
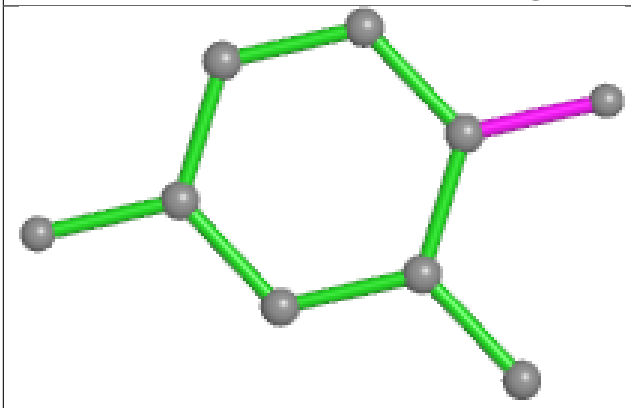


Rings

Ligand 7DV E 303



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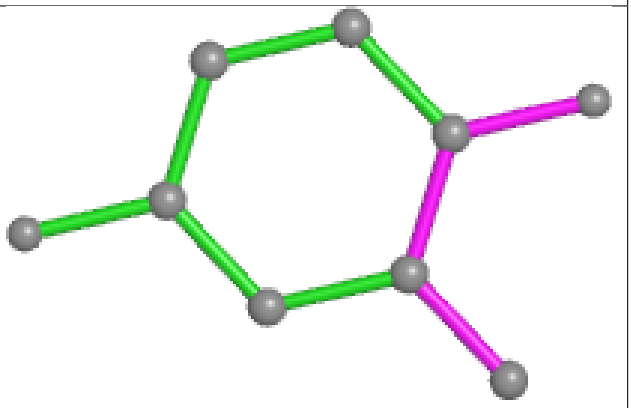

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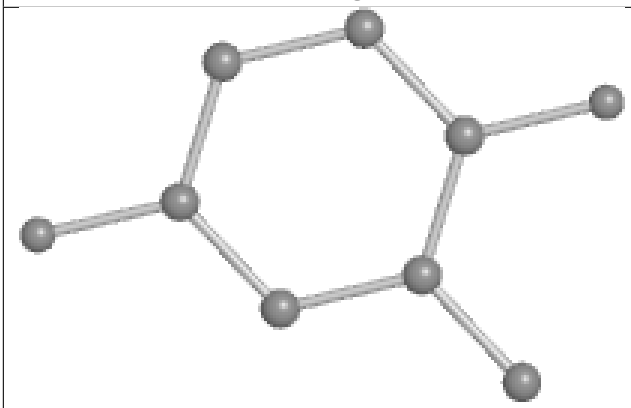

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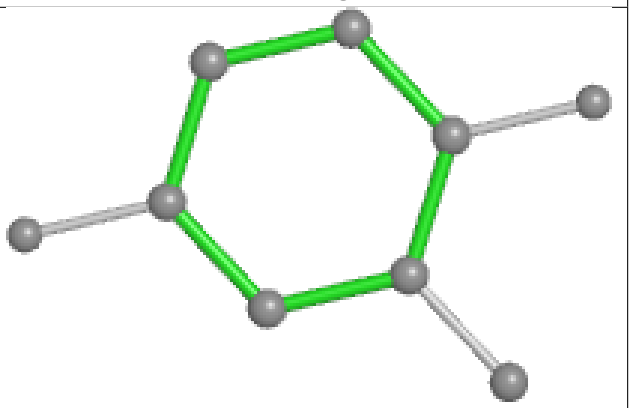
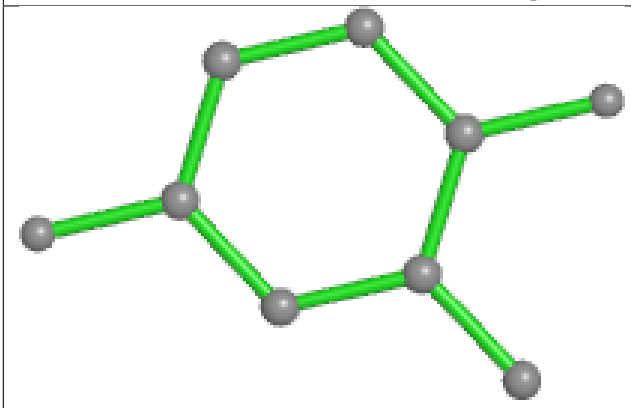


Rings

Ligand 7DV H 303



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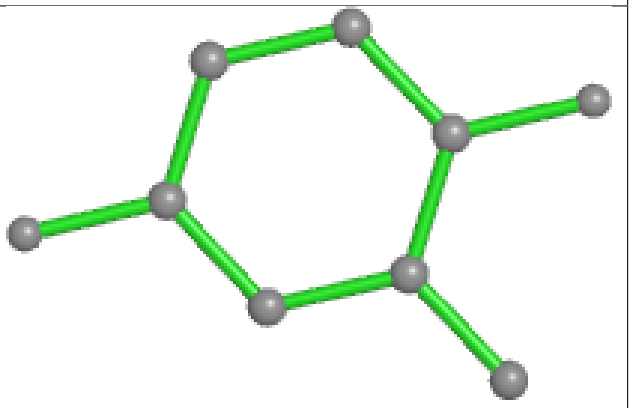
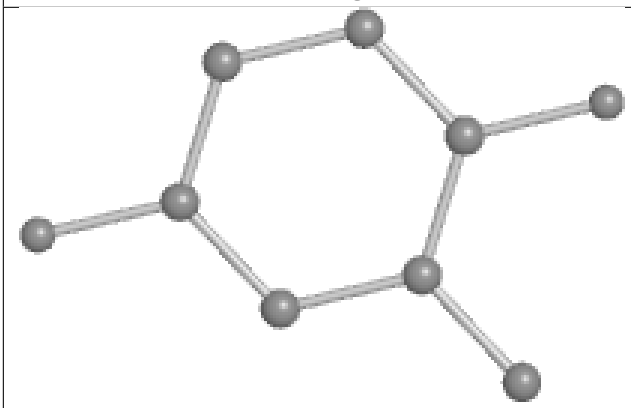
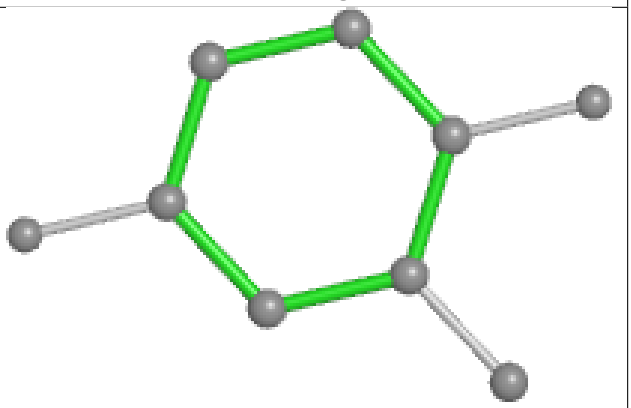


Bond angles

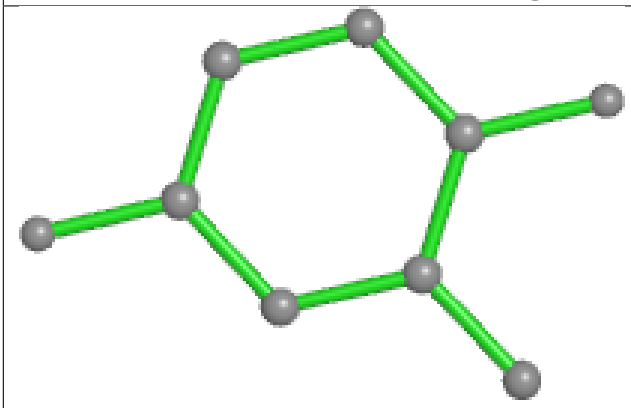


Torsions



Rings

Ligand 7DV P 301



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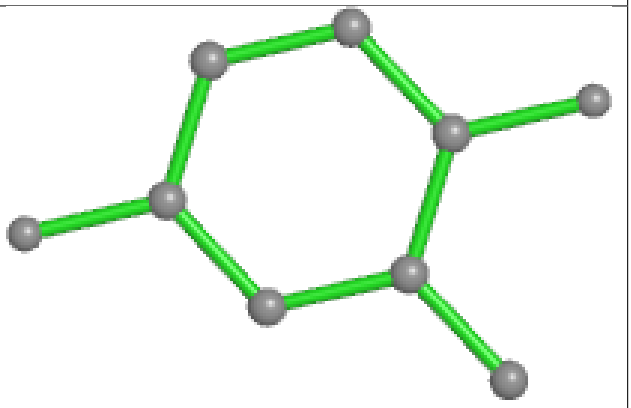
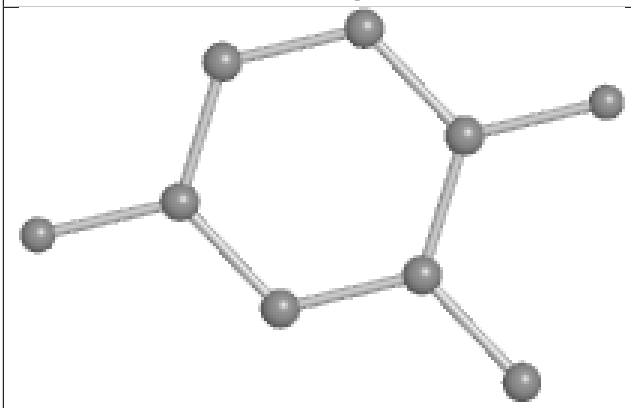


Bond angles



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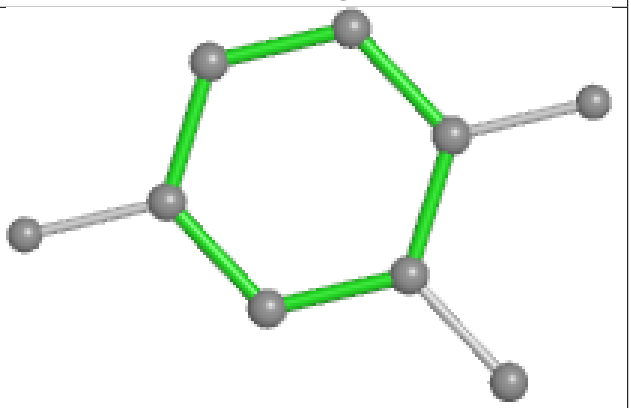
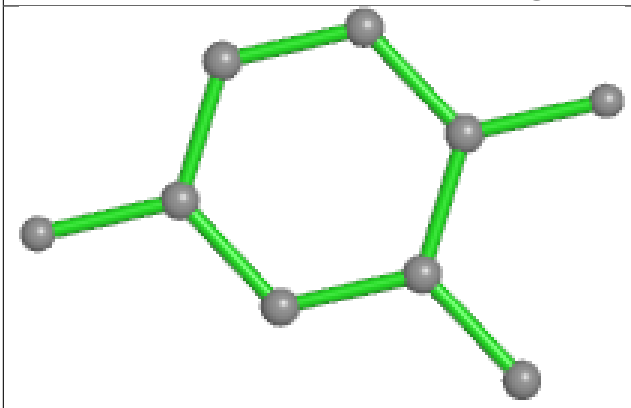
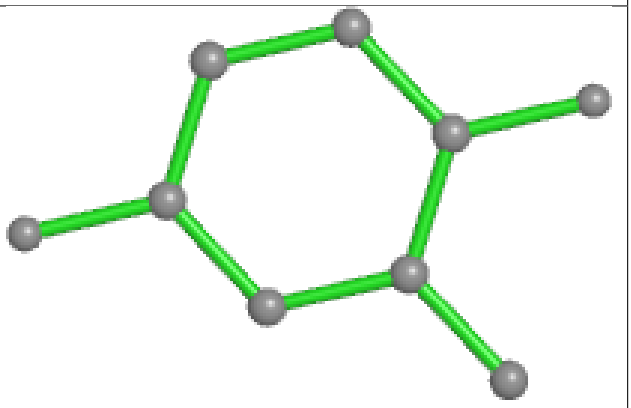


Rings

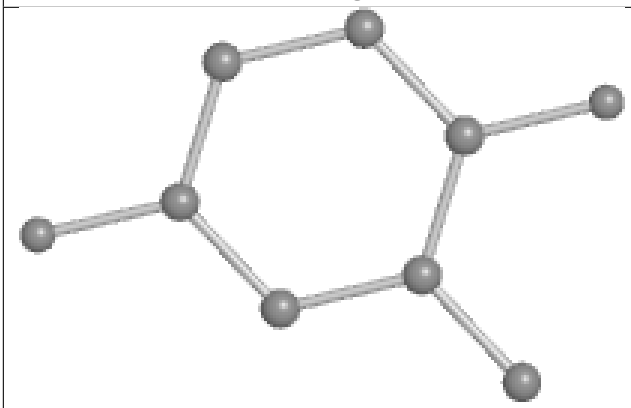
Ligand 7DV L 302



Bond lengths



Bond angles



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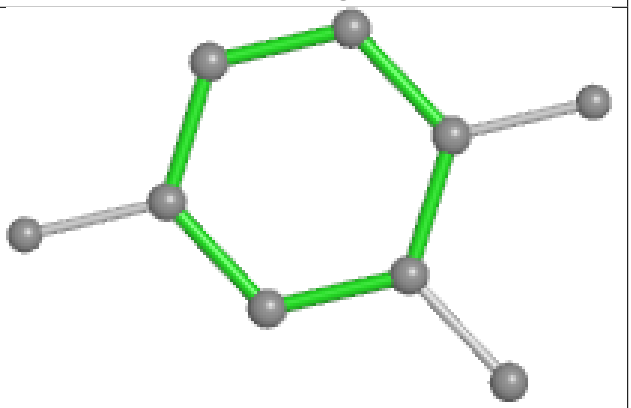
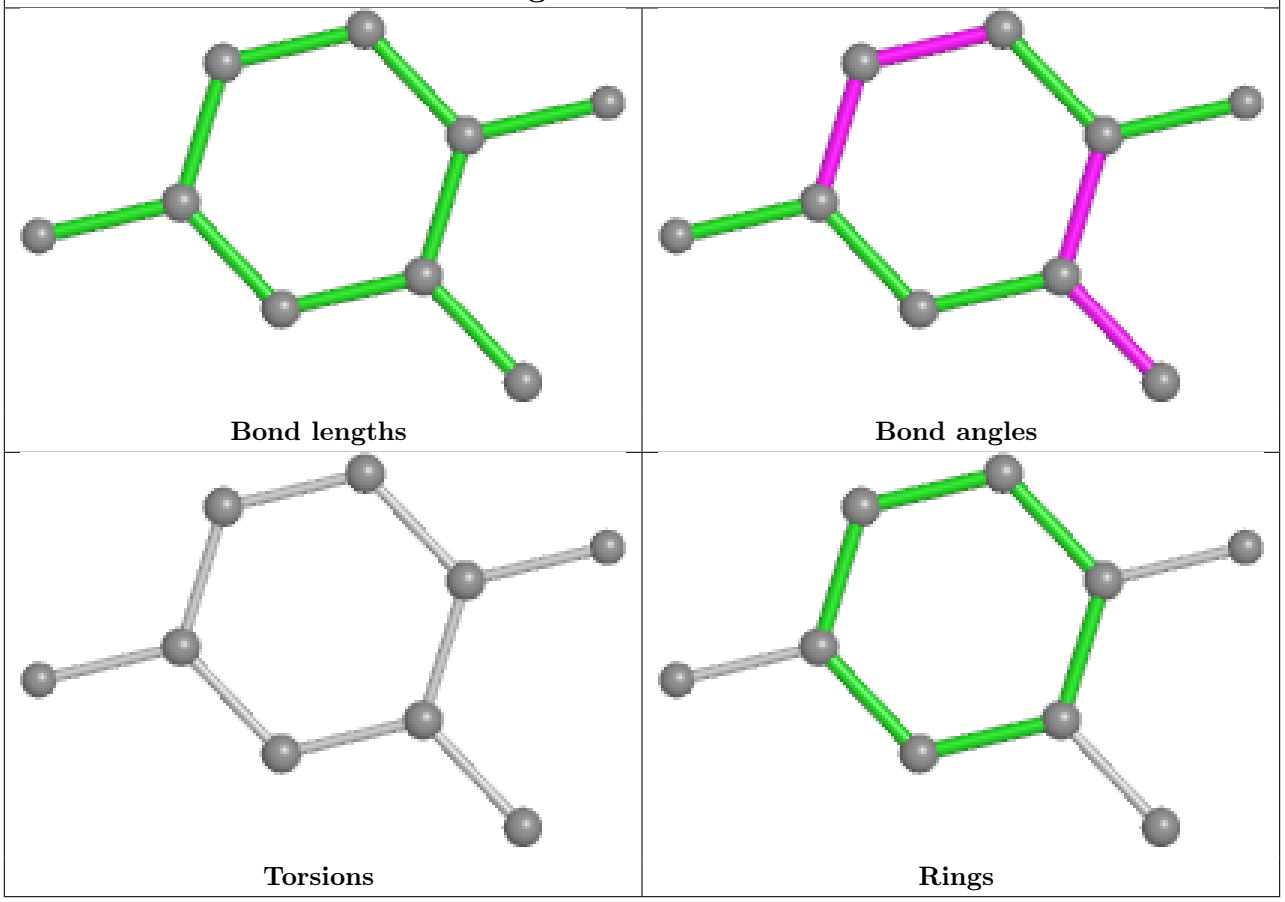


Rings

Ligand 7DV F 302



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	202/207 (97%)	-0.20	4 (1%)	65	56	45, 65, 81, 97	0
1	B	202/207 (97%)	-0.06	1 (0%)	91	88	49, 69, 85, 96	0
1	C	202/207 (97%)	-0.23	3 (1%)	73	68	45, 65, 82, 94	0
1	D	203/207 (98%)	-0.05	3 (1%)	73	68	49, 69, 83, 96	0
1	E	202/207 (97%)	-0.28	2 (0%)	82	77	43, 62, 80, 95	0
1	F	204/207 (98%)	-0.10	3 (1%)	73	68	42, 66, 83, 104	0
1	G	202/207 (97%)	-0.27	2 (0%)	82	77	44, 62, 81, 103	0
1	H	203/207 (98%)	-0.06	3 (1%)	73	68	50, 68, 84, 111	0
1	I	202/207 (97%)	-0.21	3 (1%)	73	68	44, 64, 80, 101	0
1	J	200/207 (96%)	-0.11	2 (1%)	82	77	43, 69, 84, 106	0
1	K	202/207 (97%)	-0.29	1 (0%)	91	88	42, 63, 80, 95	0
1	L	201/207 (97%)	-0.12	3 (1%)	73	68	49, 68, 79, 85	0
1	M	202/207 (97%)	-0.24	3 (1%)	73	68	45, 62, 81, 95	0
1	N	203/207 (98%)	-0.13	3 (1%)	73	68	43, 66, 81, 110	0
1	O	202/207 (97%)	-0.30	2 (0%)	82	77	44, 62, 83, 92	0
1	P	203/207 (98%)	-0.07	6 (2%)	50	40	48, 69, 82, 95	0
All	All	3235/3312 (97%)	-0.17	44 (1%)	75	70	42, 66, 83, 111	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	186	PRO	5.3
1	N	188	PRO	4.8
1	H	182	ILE	4.6
1	E	297	GLY	4.3
1	I	217	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	I	297	GLY	3.8
1	A	297	GLY	3.6
1	G	297	GLY	3.6
1	O	297	GLY	3.5
1	F	217	LEU	3.0
1	M	297	GLY	2.9
1	C	189	LEU	2.8
1	N	192	VAL	2.8
1	A	189	LEU	2.6
1	C	217	LEU	2.6
1	C	216	LEU	2.6
1	M	192	VAL	2.6
1	B	182	ILE	2.6
1	I	216	LEU	2.6
1	P	192	VAL	2.5
1	D	208	GLU	2.5
1	H	154	MET	2.5
1	J	197	TYR	2.4
1	A	160	SER	2.4
1	P	217	LEU	2.4
1	L	192	VAL	2.3
1	M	97	THR	2.3
1	L	211	VAL	2.2
1	H	157	ARG	2.2
1	K	195	VAL	2.2
1	F	197	TYR	2.2
1	D	210	PRO	2.2
1	E	188	PRO	2.2
1	D	188	PRO	2.2
1	P	154	MET	2.1
1	O	192	VAL	2.1
1	G	189	LEU	2.1
1	J	154	MET	2.1
1	P	212	LEU	2.1
1	A	192	VAL	2.1
1	N	197	TYR	2.1
1	P	208	GLU	2.0
1	L	155	HIS	2.0
1	P	182	ILE	2.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	7DV	K	301	9/9	0.85	0.26	68,84,98,100	0
2	7DV	O	301	9/9	0.86	0.27	58,88,98,107	0
3	NA	F	304	1/1	0.86	0.30	59,59,59,59	0
2	7DV	E	301	9/9	0.87	0.23	65,85,104,108	0
2	7DV	O	302	9/9	0.87	0.22	46,63,69,72	0
3	NA	D	305	1/1	0.87	0.26	45,45,45,45	0
2	7DV	N	303	9/9	0.87	0.21	48,69,87,91	0
2	7DV	E	303	9/9	0.89	0.13	41,53,70,75	0
3	NA	I	304	1/1	0.89	0.25	48,48,48,48	0
3	NA	E	304	1/1	0.90	0.46	43,43,43,43	0
2	7DV	A	303	9/9	0.90	0.16	50,70,81,86	0
2	7DV	E	302	9/9	0.90	0.19	83,89,97,101	0
2	7DV	N	301	9/9	0.91	0.19	71,80,89,96	0
2	7DV	A	301	9/9	0.91	0.22	64,74,83,85	0
2	7DV	F	301	9/9	0.91	0.17	47,56,65,70	0
2	7DV	I	302	9/9	0.91	0.17	56,67,76,77	0
2	7DV	J	301	9/9	0.91	0.17	68,72,86,87	0
2	7DV	D	301	9/9	0.91	0.16	52,60,65,65	0
2	7DV	K	303	9/9	0.91	0.15	62,70,82,82	0
2	7DV	M	301	9/9	0.91	0.24	60,72,83,83	0
2	7DV	G	301	9/9	0.92	0.22	50,64,73,80	0
2	7DV	M	302	9/9	0.92	0.17	58,67,79,82	0
2	7DV	J	303	9/9	0.92	0.16	65,78,79,87	0
2	7DV	G	303	9/9	0.92	0.15	63,65,73,78	0
2	7DV	C	301	9/9	0.92	0.23	62,67,72,87	0
3	NA	I	305	1/1	0.92	0.40	55,55,55,55	0
2	7DV	G	302	9/9	0.93	0.15	57,65,71,75	0

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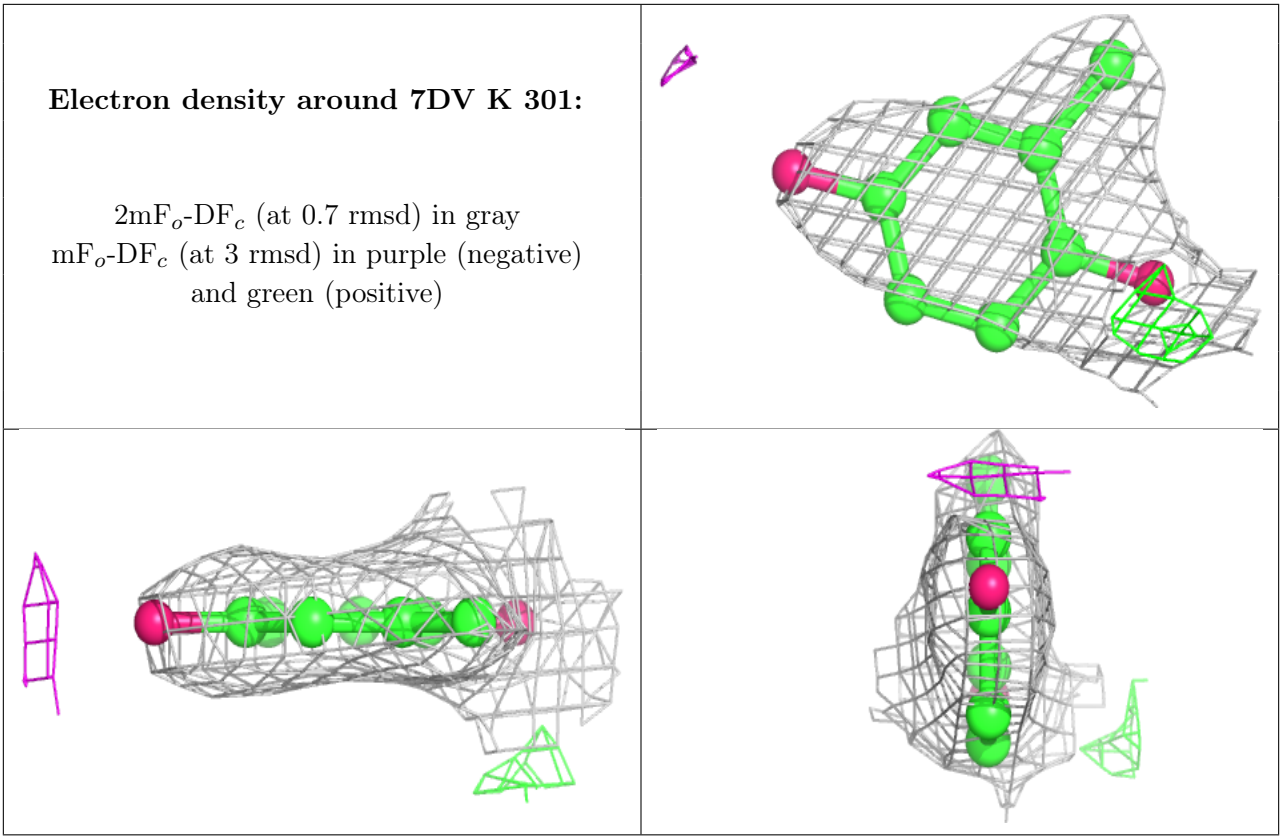
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	7DV	O	303	9/9	0.93	0.12	50,56,72,73	0
2	7DV	F	302	9/9	0.93	0.16	58,68,74,74	0
2	7DV	C	303	9/9	0.93	0.19	57,62,65,81	0
2	7DV	N	302	9/9	0.93	0.16	66,82,90,94	0
2	7DV	K	302	9/9	0.93	0.14	63,70,77,80	0
2	7DV	I	303	9/9	0.93	0.13	60,66,80,82	0
2	7DV	M	303	9/9	0.94	0.12	41,48,55,59	0
2	7DV	A	302	9/9	0.94	0.13	38,53,64,71	0
2	7DV	L	302	9/9	0.94	0.18	62,71,78,81	0
2	7DV	L	303	9/9	0.94	0.15	55,64,76,78	0
2	7DV	D	302	9/9	0.94	0.18	54,72,85,89	0
2	7DV	H	303	9/9	0.94	0.14	53,65,70,79	0
3	NA	O	304	1/1	0.94	0.38	55,55,55,55	0
2	7DV	B	303	9/9	0.95	0.15	66,71,83,88	0
2	7DV	F	303	9/9	0.95	0.11	65,73,81,84	0
3	NA	G	304	1/1	0.95	0.49	55,55,55,55	0
2	7DV	D	303	9/9	0.95	0.20	61,77,80,83	0
3	NA	B	304	1/1	0.95	0.29	44,44,44,44	0
2	7DV	J	302	9/9	0.95	0.15	63,73,77,79	0
2	7DV	B	302	9/9	0.96	0.16	67,81,94,94	0
2	7DV	H	301	9/9	0.96	0.16	65,69,75,76	0
2	7DV	P	302	9/9	0.96	0.14	42,51,58,64	0
2	7DV	L	301	9/9	0.96	0.15	49,59,64,65	0
3	NA	C	304	1/1	0.96	0.31	48,48,48,48	0
2	7DV	C	302	9/9	0.96	0.15	42,54,61,88	0
3	NA	P	304	1/1	0.96	0.41	48,48,48,48	0
2	7DV	H	302	9/9	0.97	0.14	51,57,64,65	0
3	NA	H	304	1/1	0.97	0.37	41,41,41,41	0
2	7DV	L	304	9/9	0.97	0.14	46,54,63,83	0
2	7DV	B	301	9/9	0.97	0.12	49,62,71,76	0
3	NA	L	305	1/1	0.97	0.29	54,54,54,54	0
3	NA	N	304	1/1	0.97	0.28	64,64,64,64	0
2	7DV	P	301	9/9	0.97	0.14	62,66,75,76	0
2	7DV	D	304	9/9	0.97	0.16	58,62,73,78	0
2	7DV	I	301	9/9	0.98	0.14	68,73,79,81	0
3	NA	N	305	1/1	0.98	0.43	42,42,42,42	0
3	NA	K	304	1/1	0.98	0.46	52,52,52,52	0
2	7DV	P	303	9/9	0.98	0.08	46,61,73,83	0
3	NA	A	304	1/1	0.99	0.39	59,59,59,59	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.

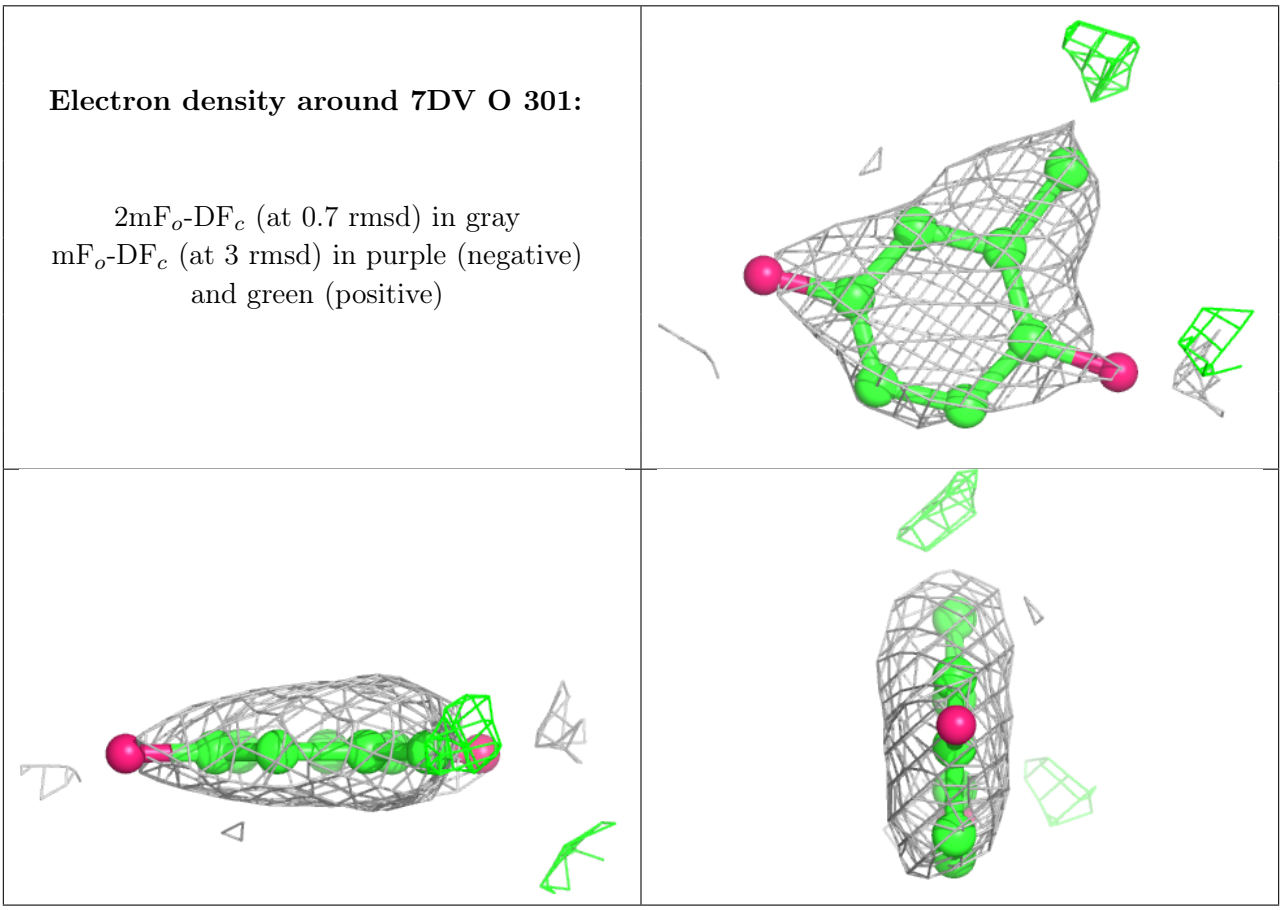
Electron density around 7DV K 301:

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



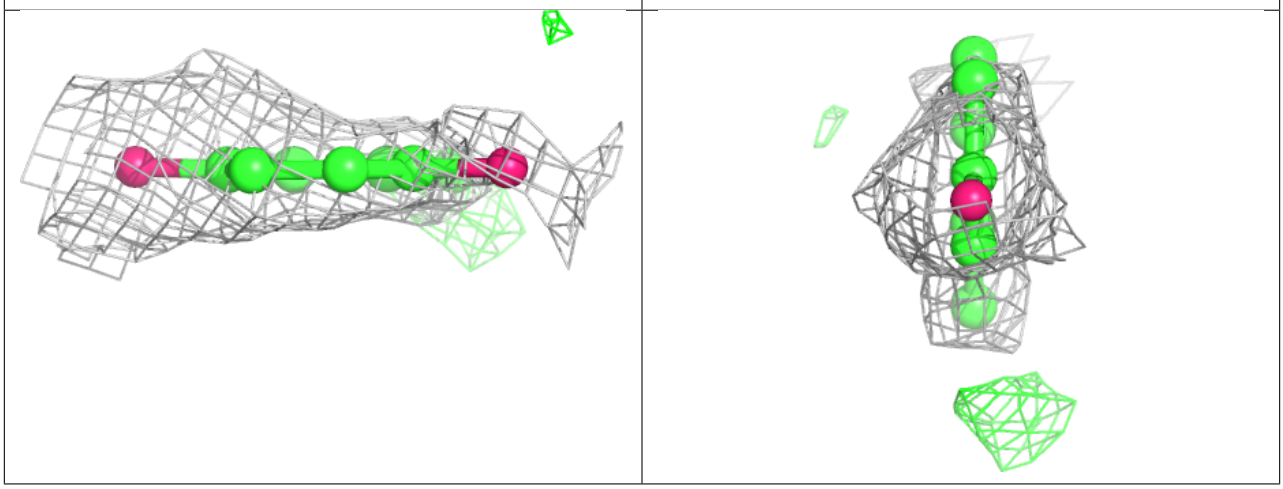
Electron density around 7DV O 301:

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



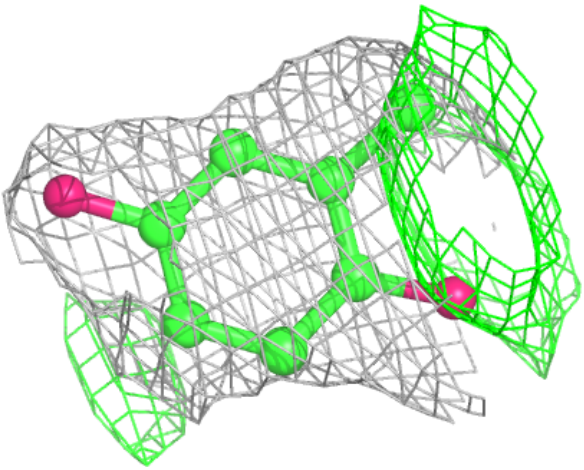
Electron density around 7DV E 301:

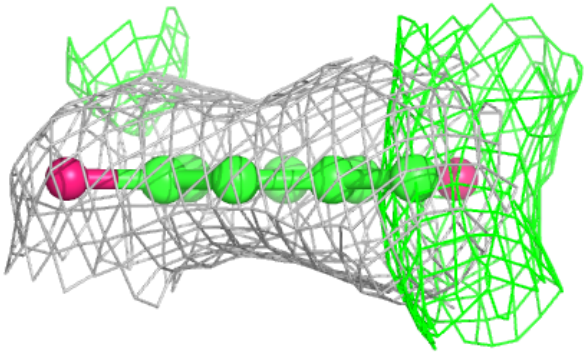
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

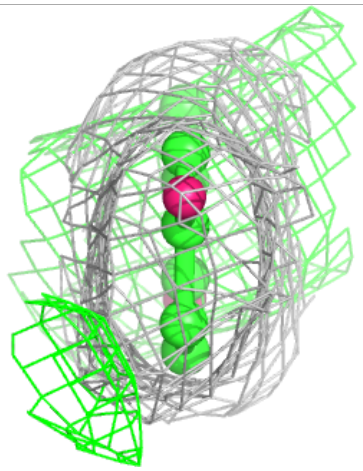


Electron density around 7DV O 302:

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

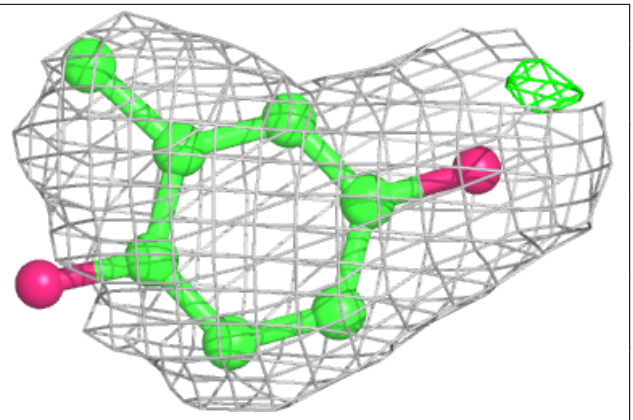


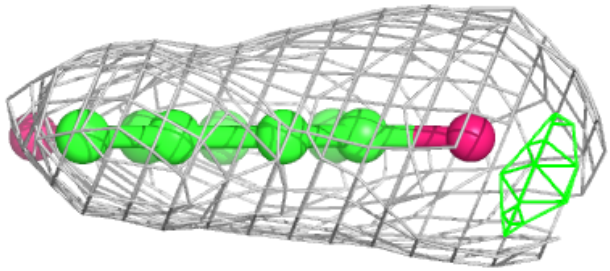


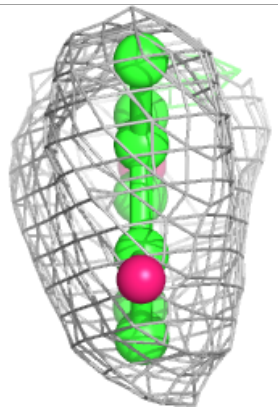


Electron density around 7DV N 303:

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

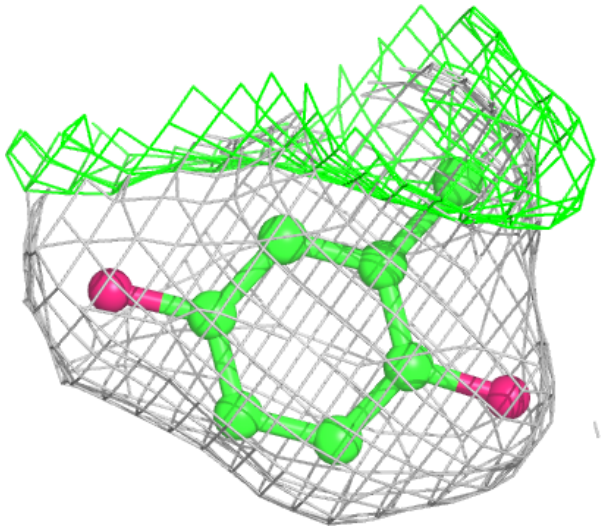


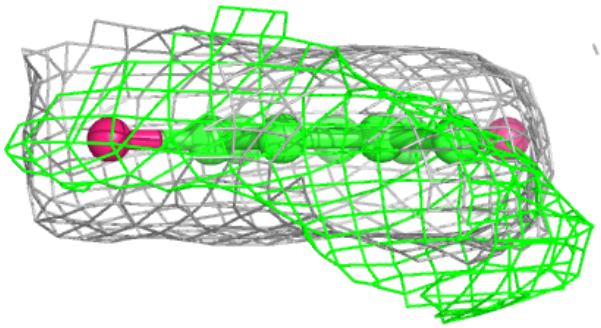


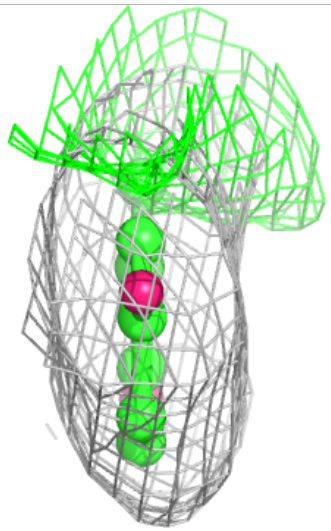


Electron density around 7DV E 303:

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

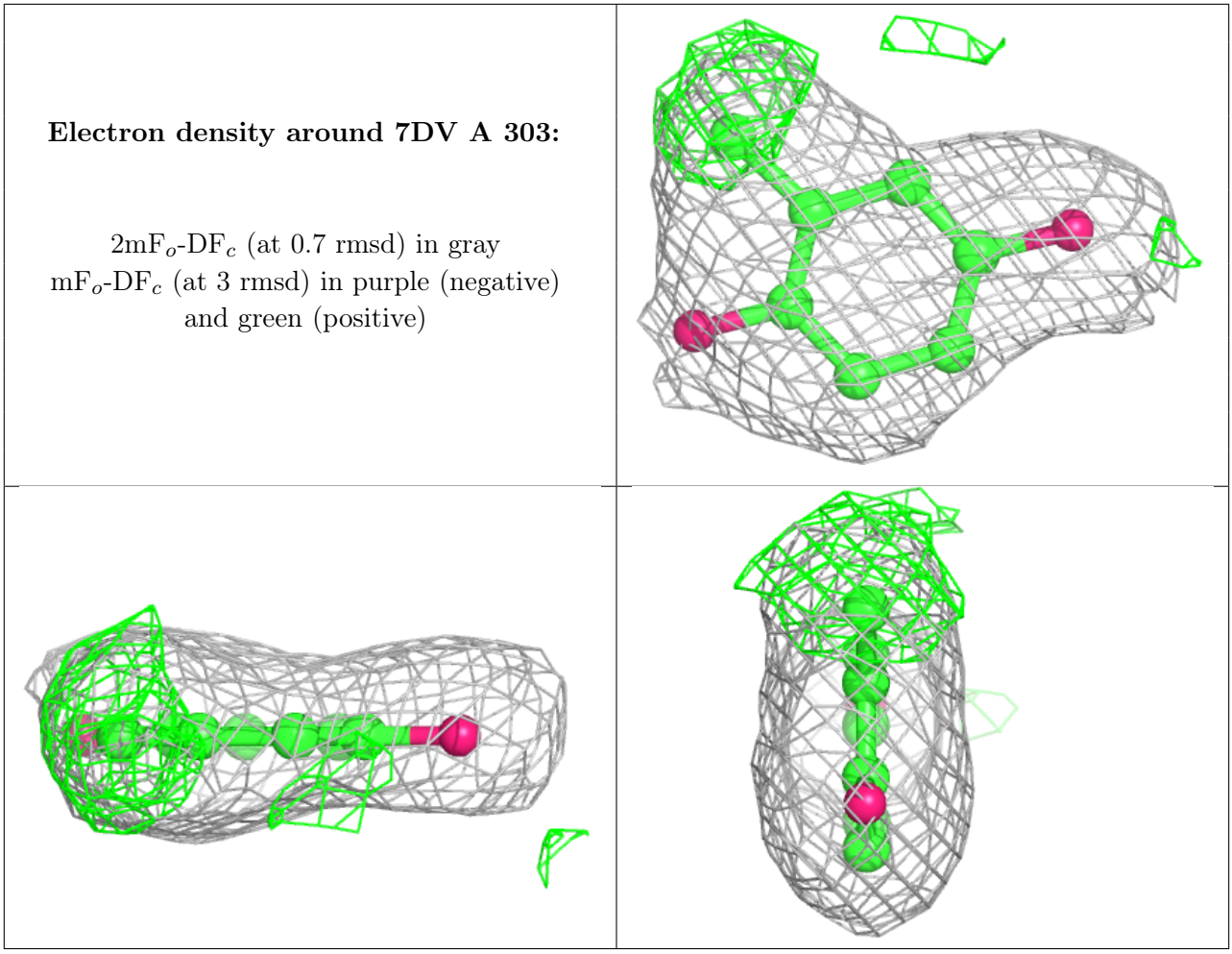






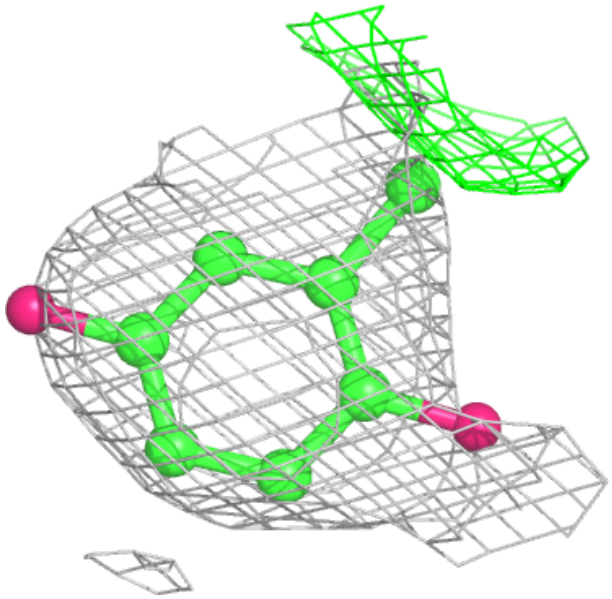
Electron density around 7DV A 303:

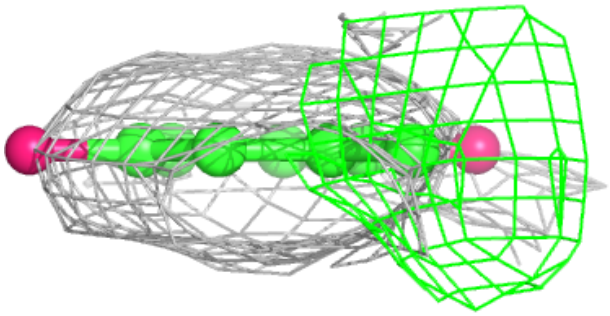
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

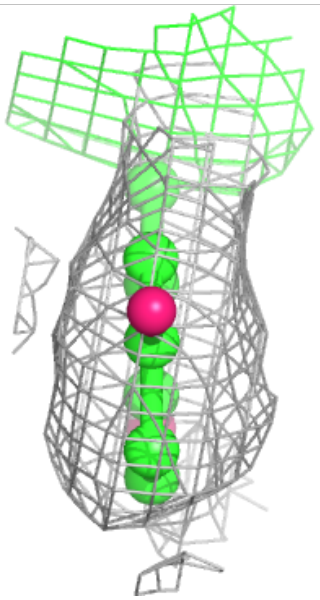


Electron density around 7DV E 302:

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

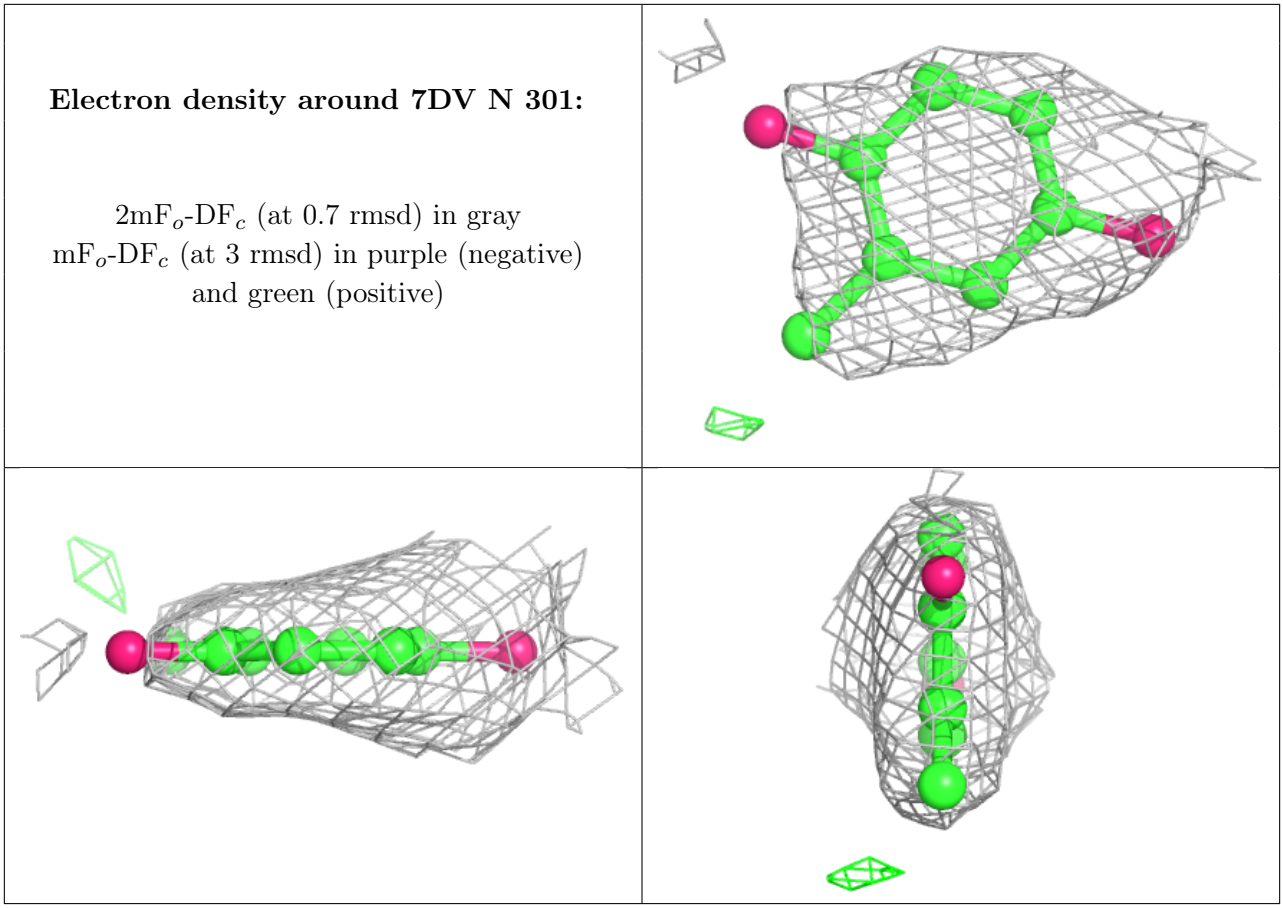






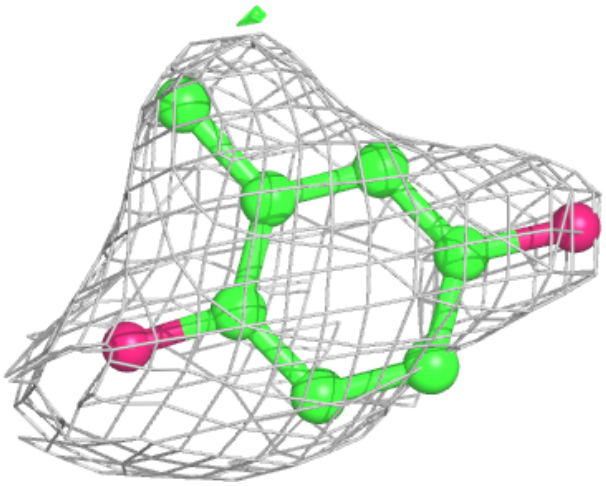
Electron density around 7DV N 301:

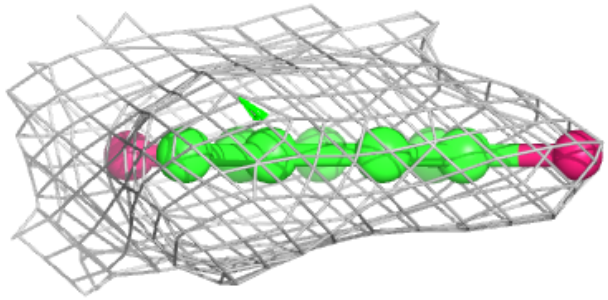
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

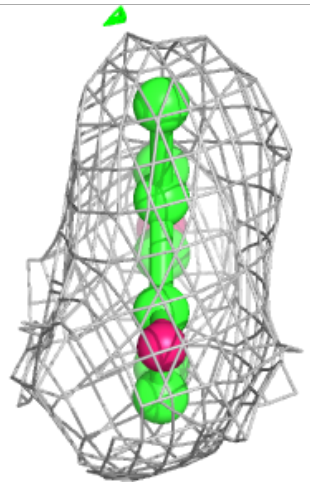


Electron density around 7DV A 301:

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

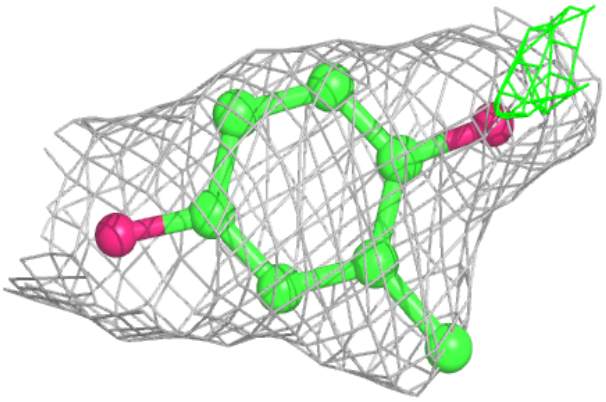


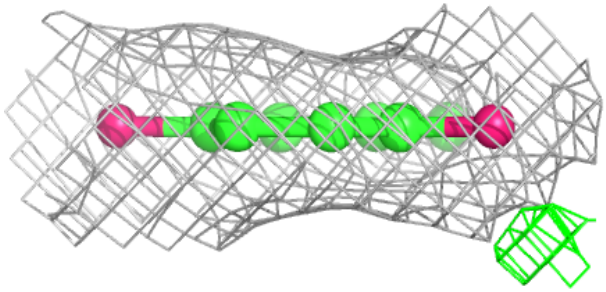


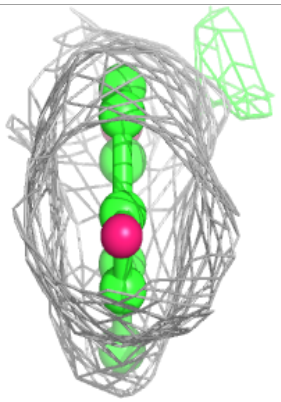


Electron density around 7DV F 301:

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

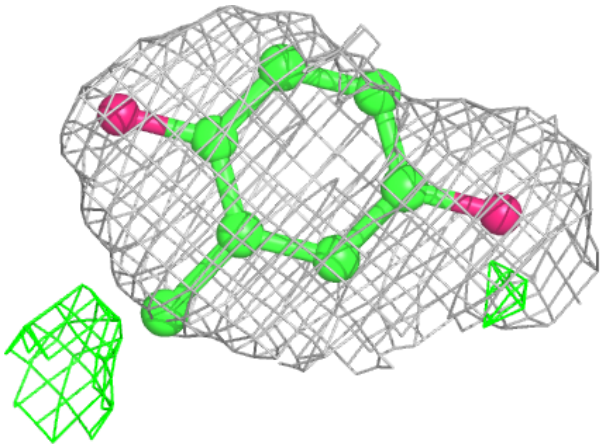


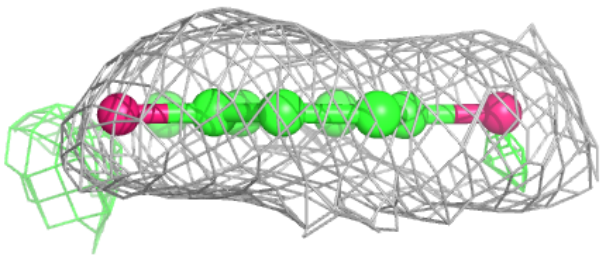


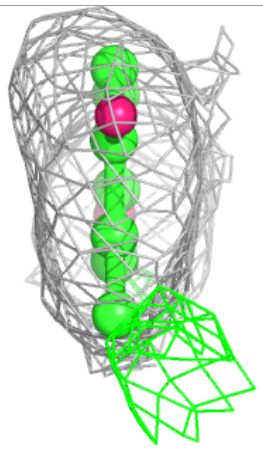


Electron density around 7DV I 302:

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

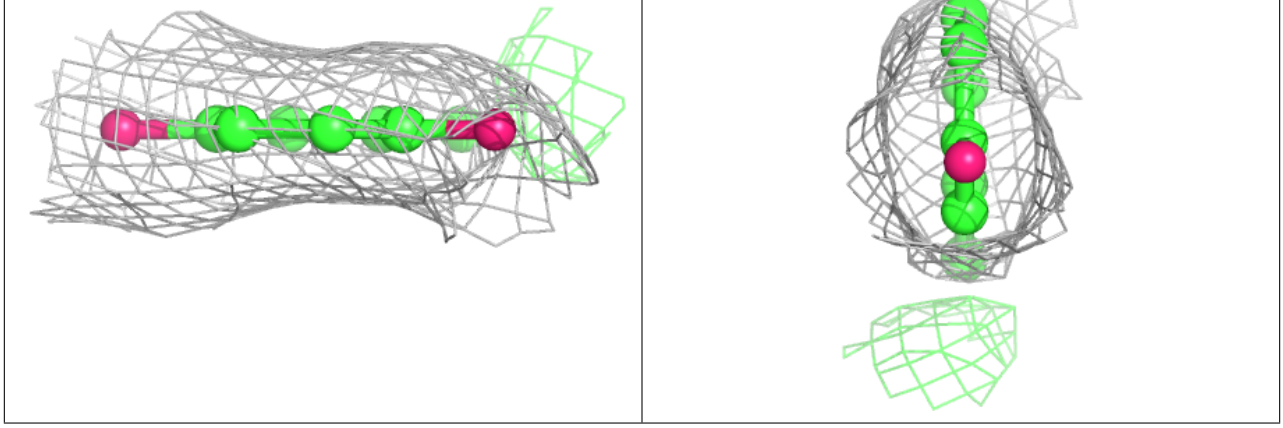






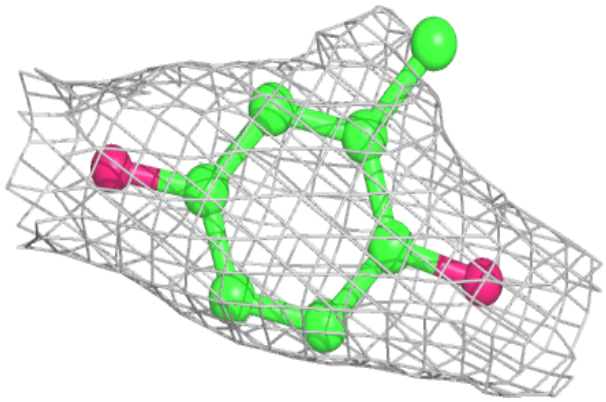
Electron density around 7DV J 301:

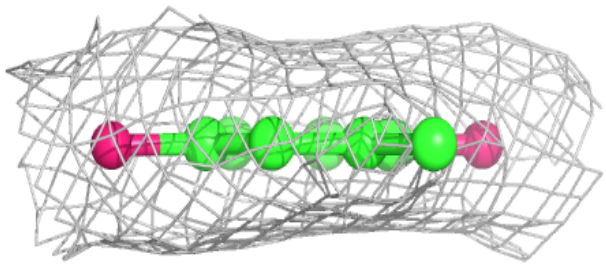
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

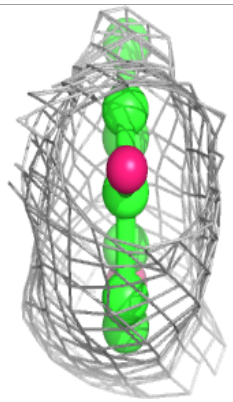


Electron density around 7DV D 301:

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

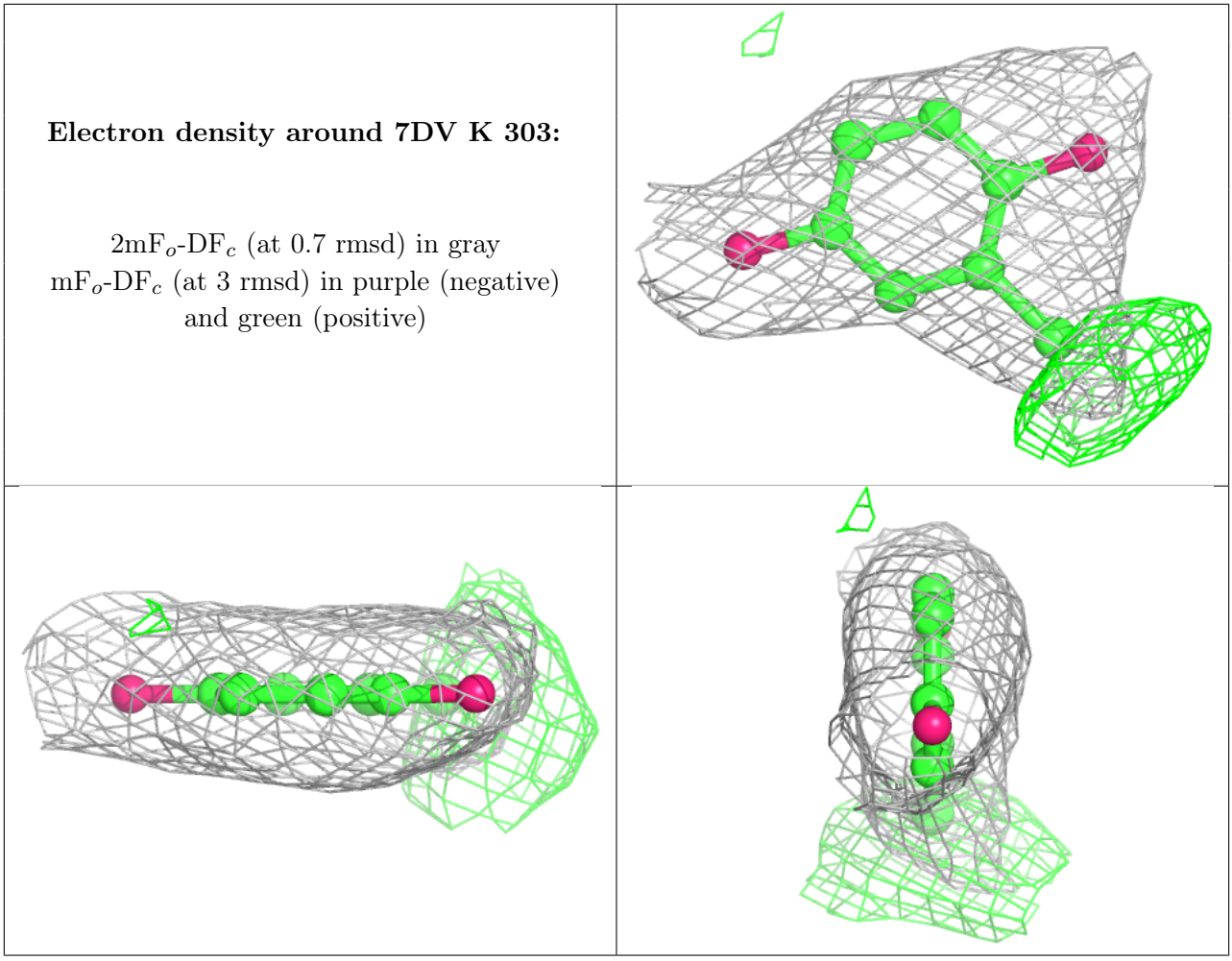






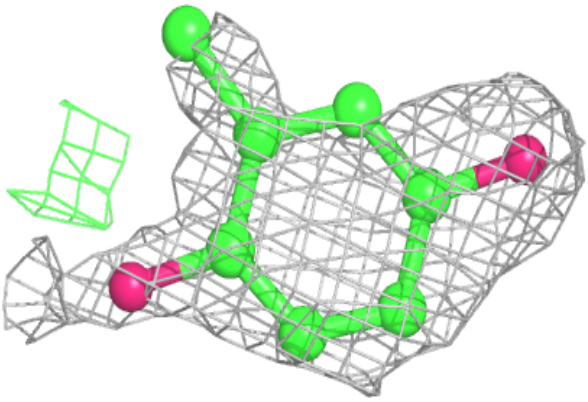
Electron density around 7DV K 303:

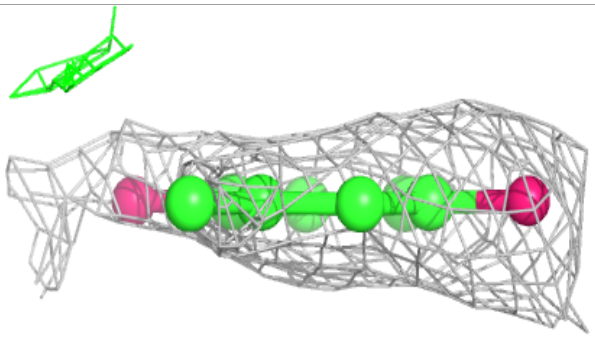
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

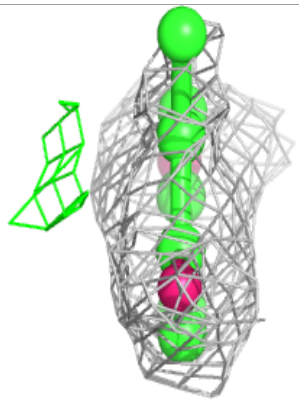


Electron density around 7DV M 301:

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

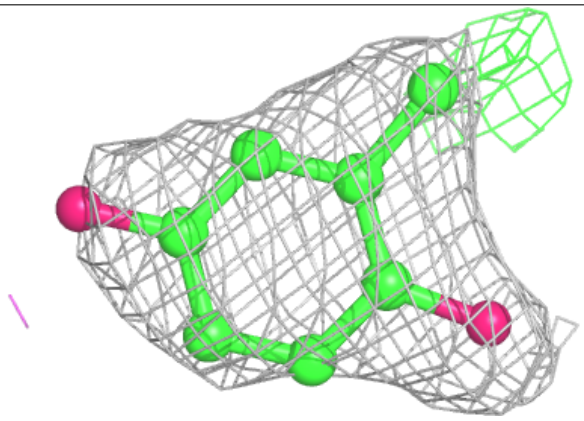


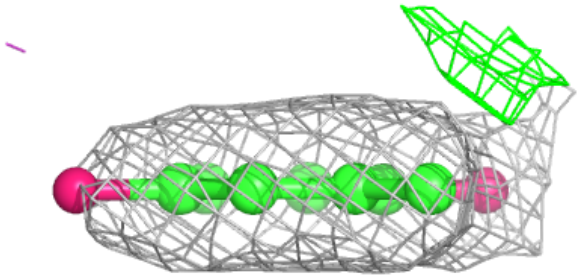


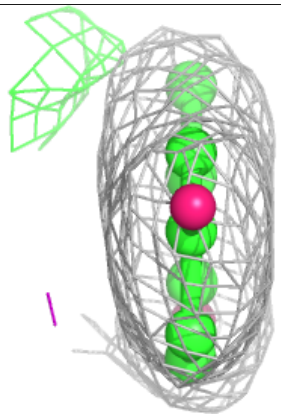


Electron density around 7DV G 301:

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

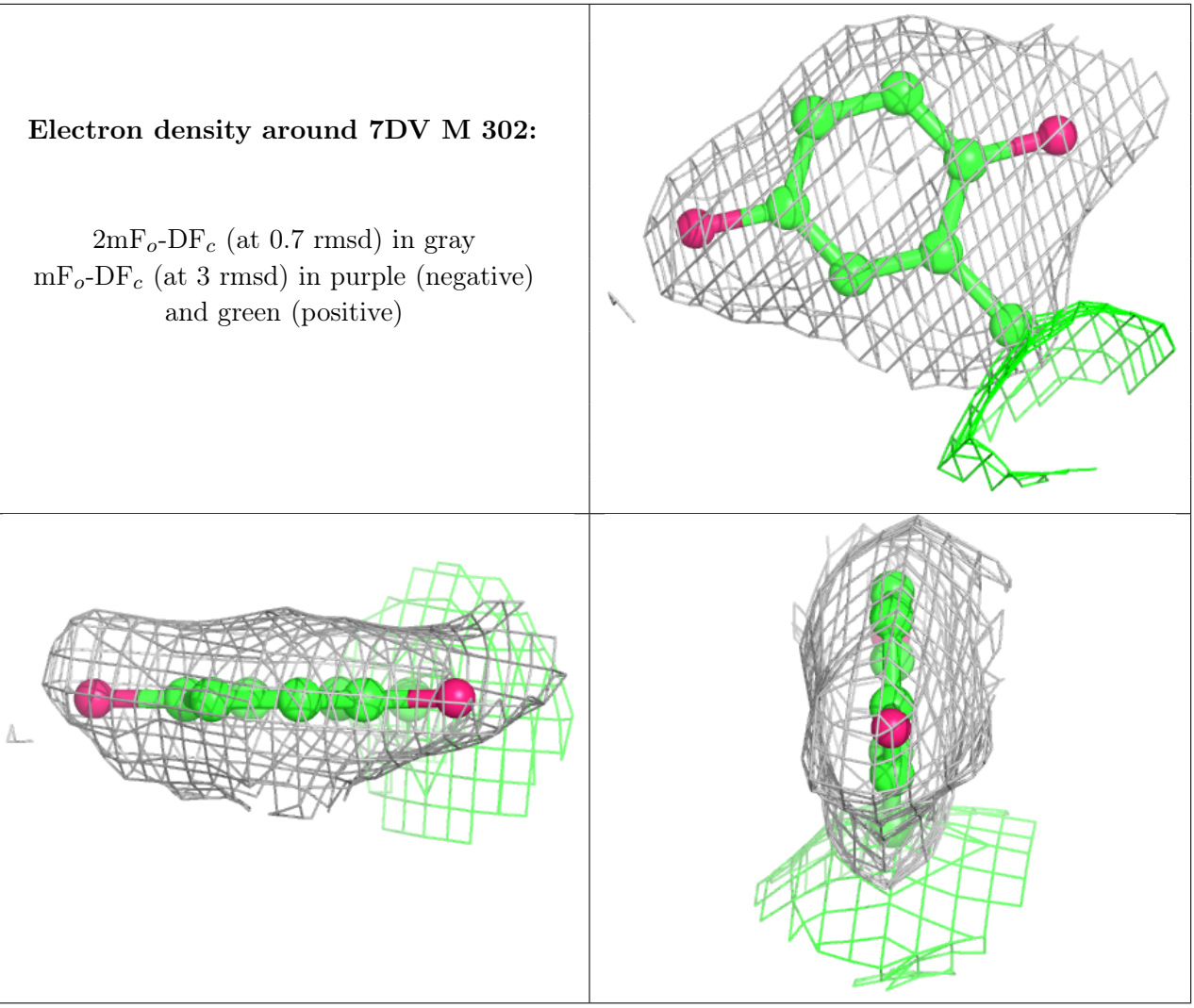






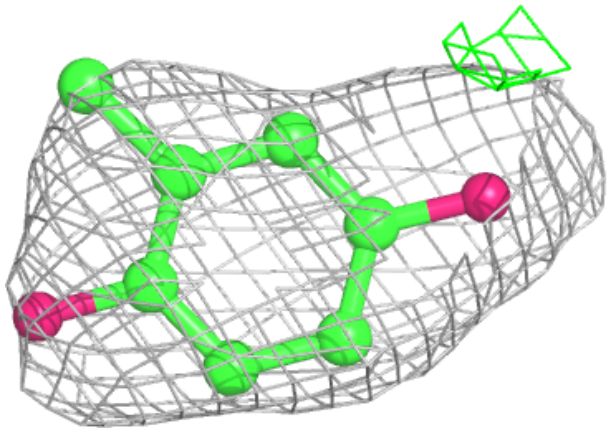
Electron density around 7DV M 302:

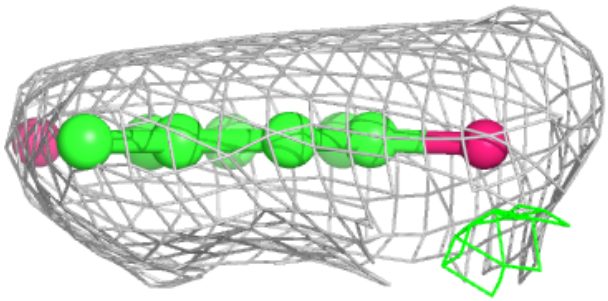
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

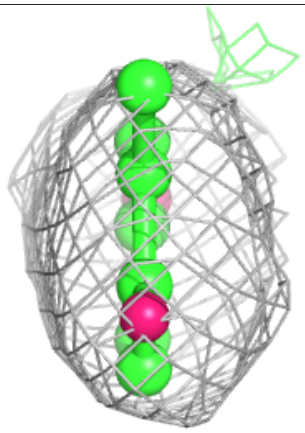


Electron density around 7DV J 303:

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

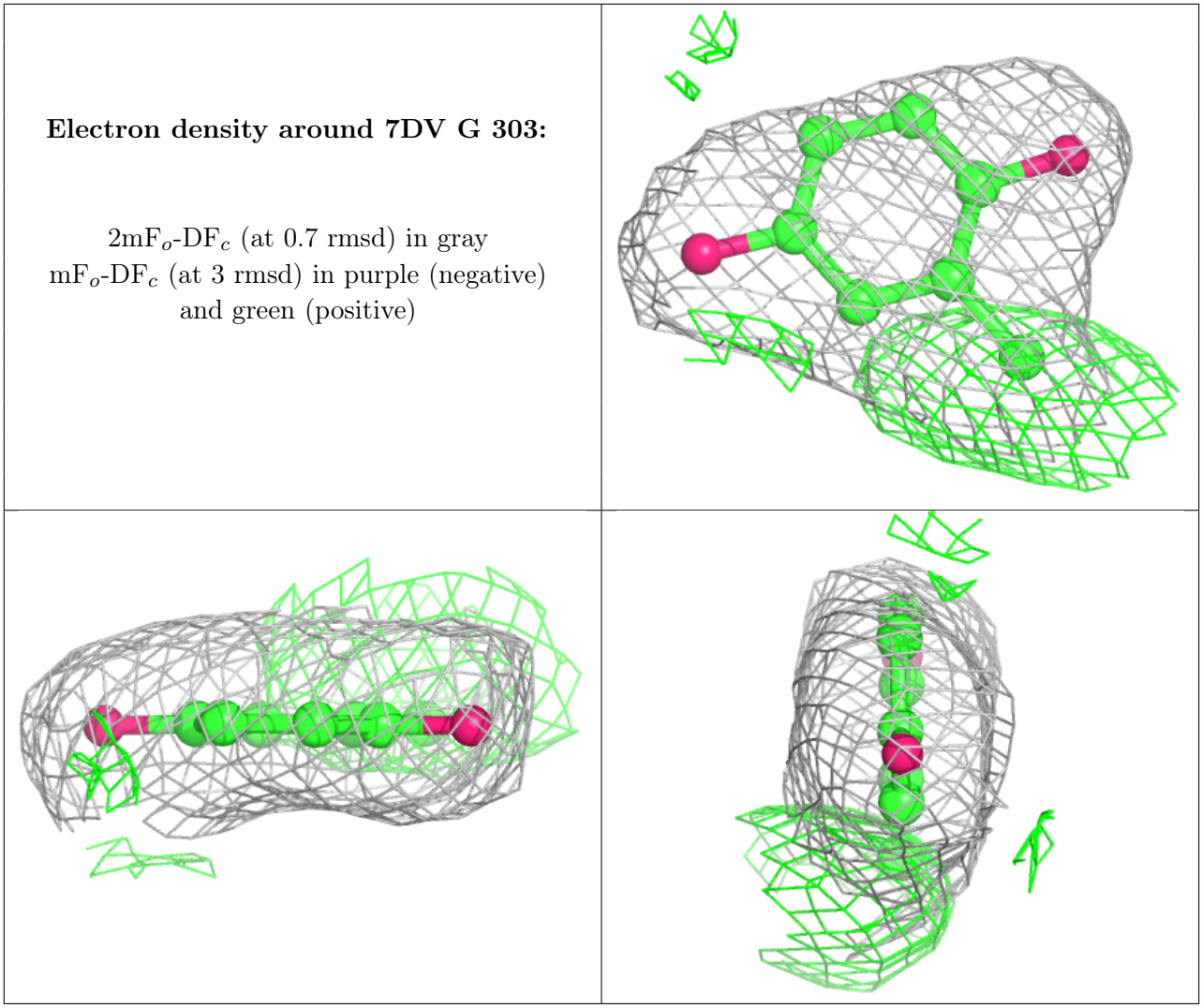






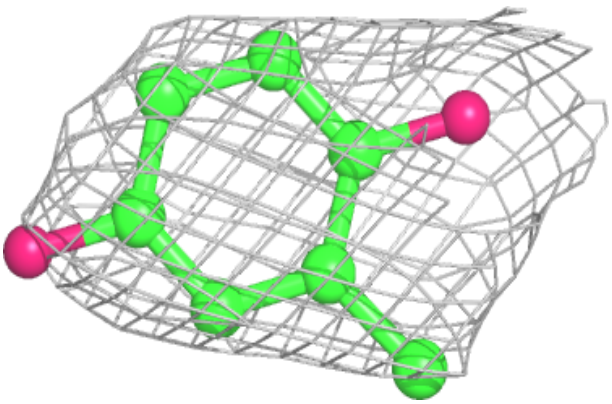
Electron density around 7DV G 303:

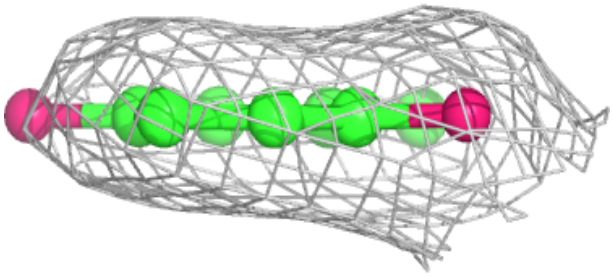
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

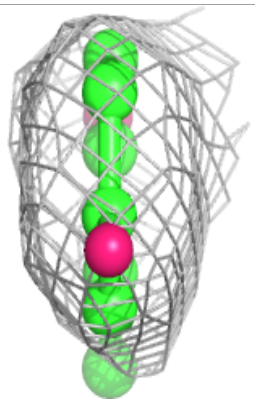


Electron density around 7DV C 301:

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

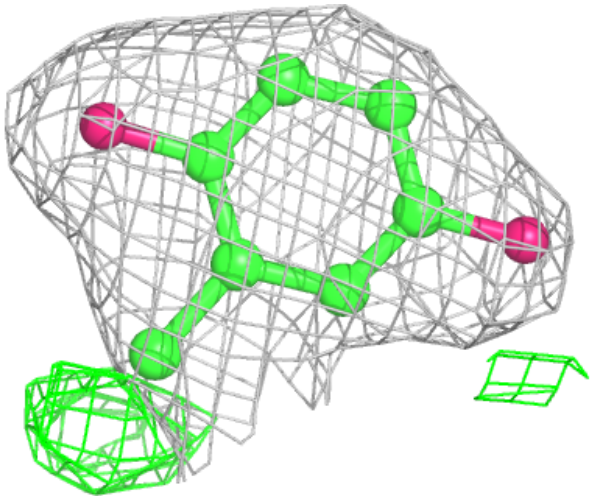


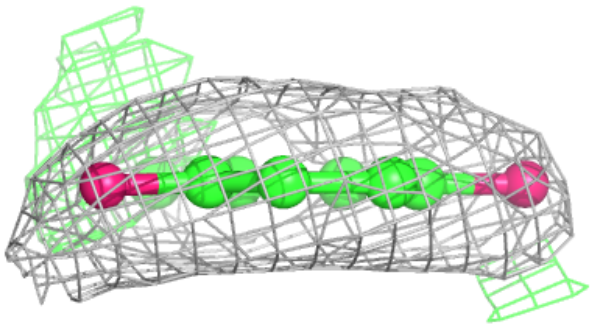


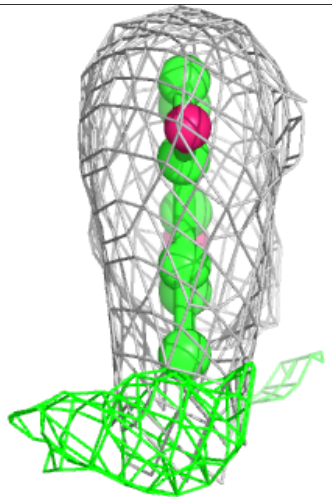


Electron density around 7DV G 302:

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

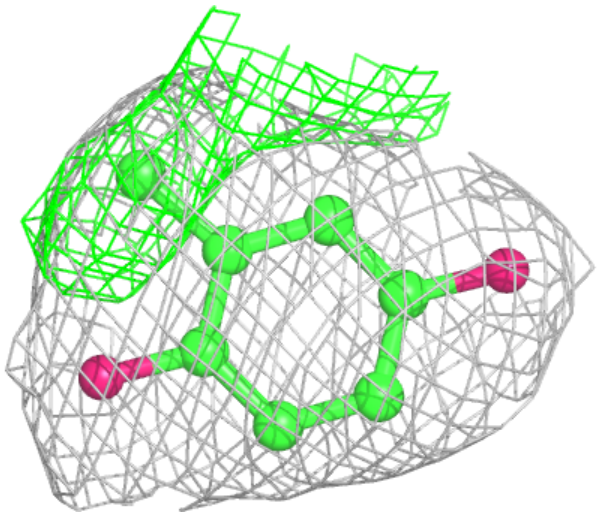


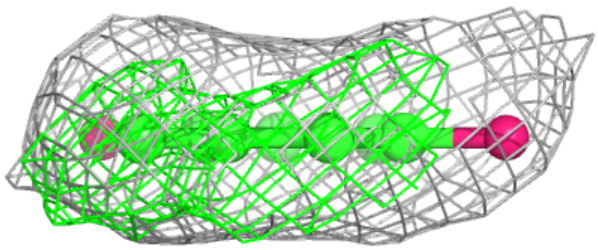


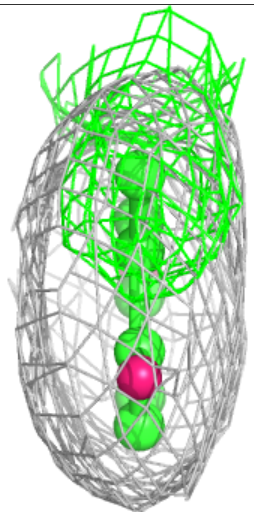


Electron density around 7DV O 303:

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

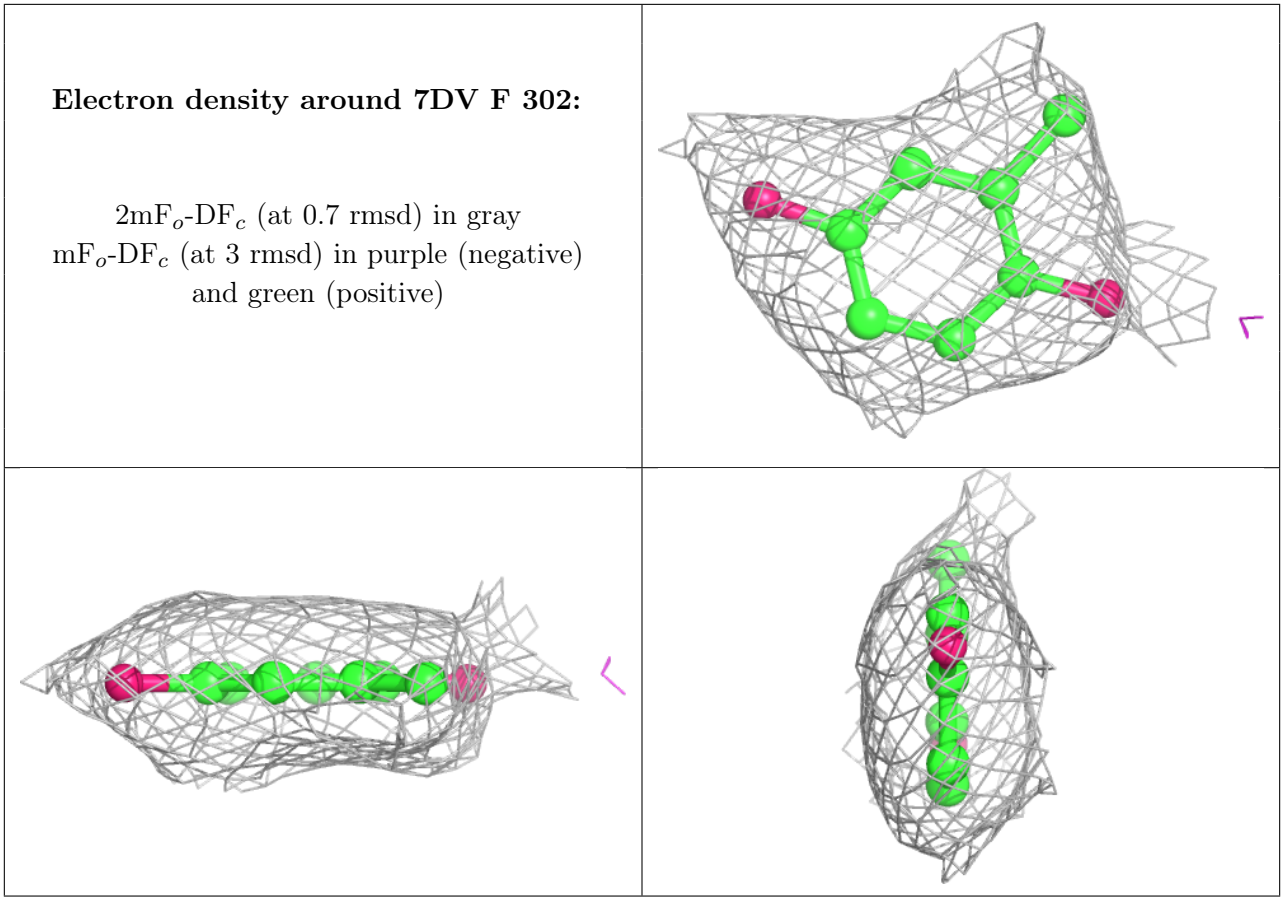






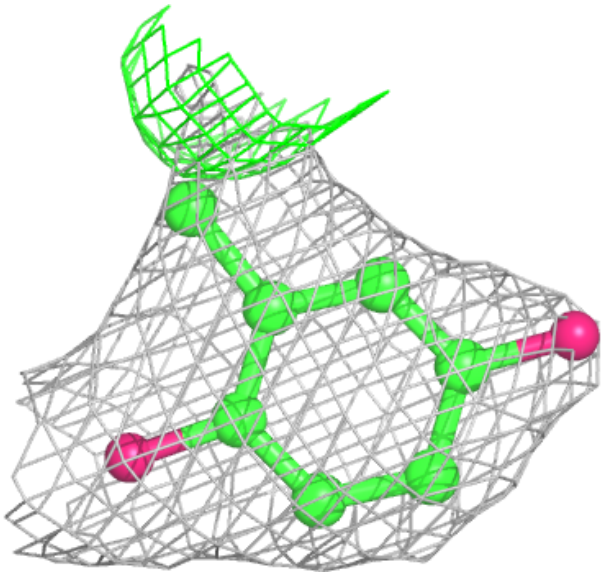
Electron density around 7DV F 302:

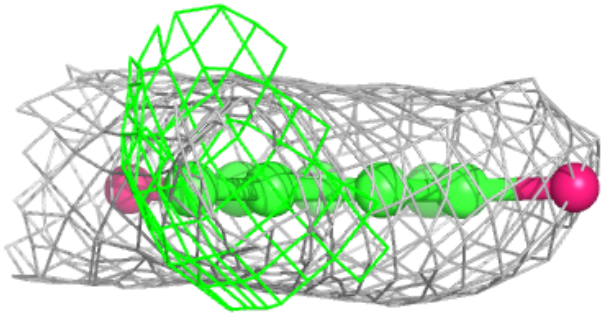
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

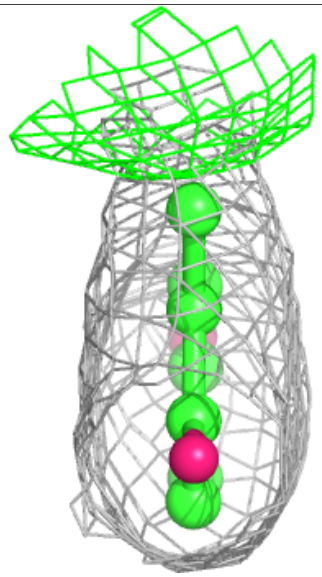


Electron density around 7DV C 303:

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

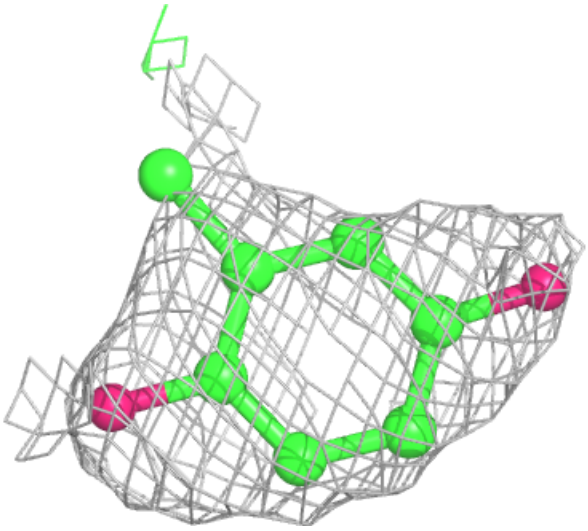


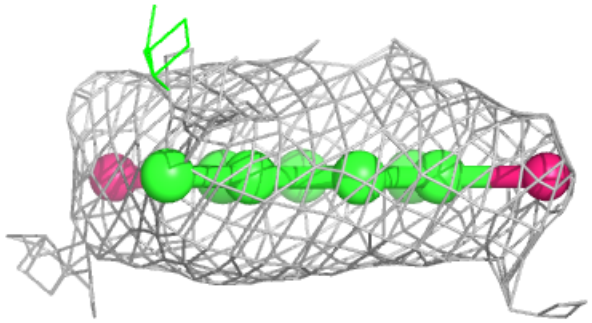


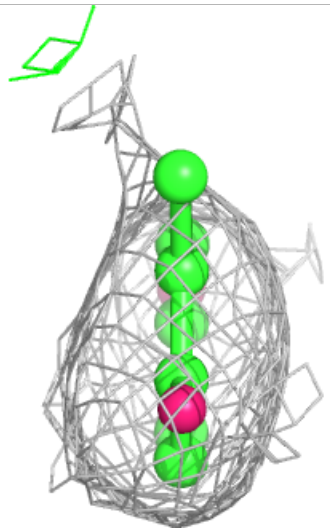


Electron density around 7DV N 302:

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

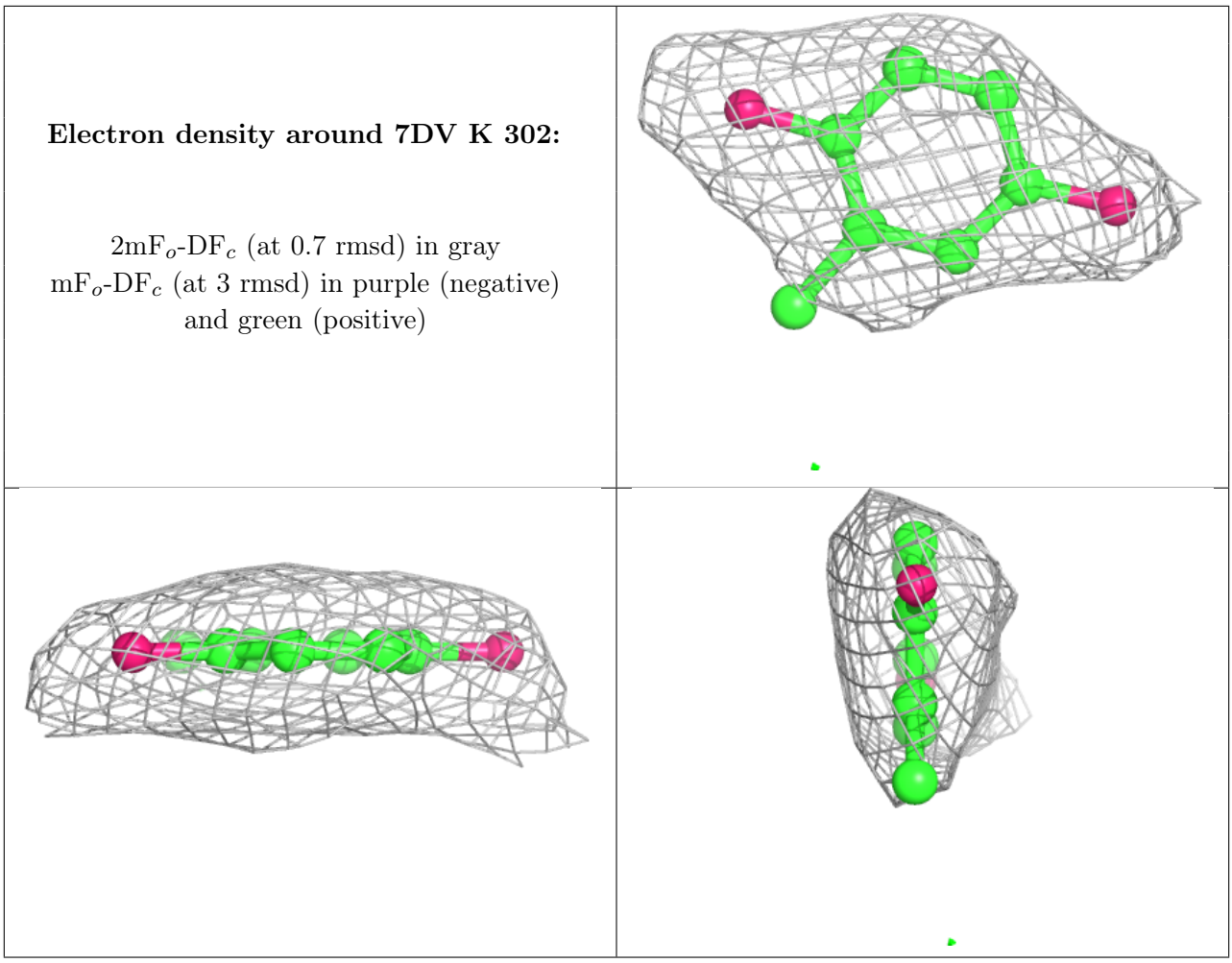






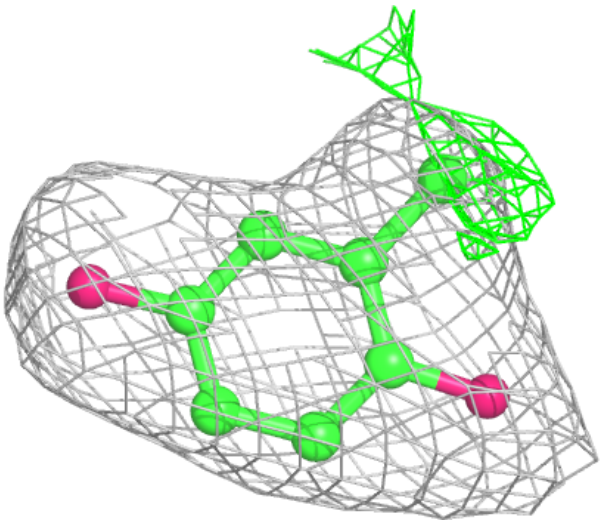
Electron density around 7DV K 302:

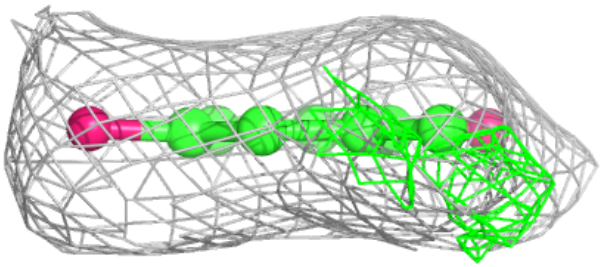
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

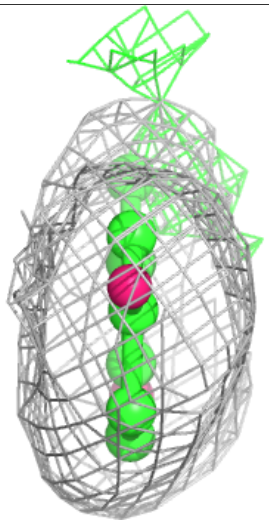


Electron density around 7DV I 303:

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

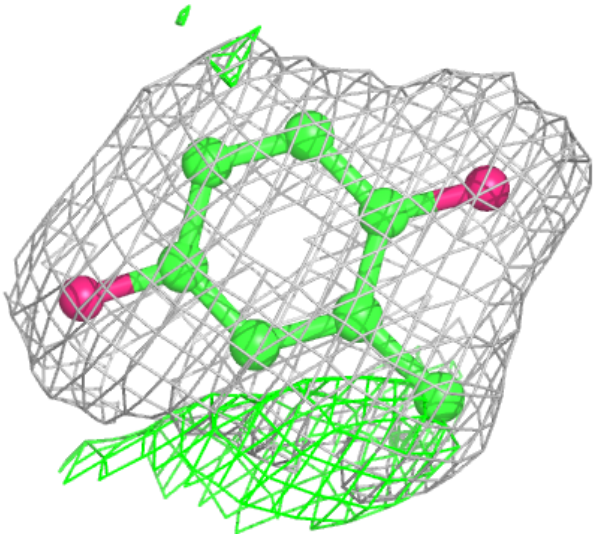


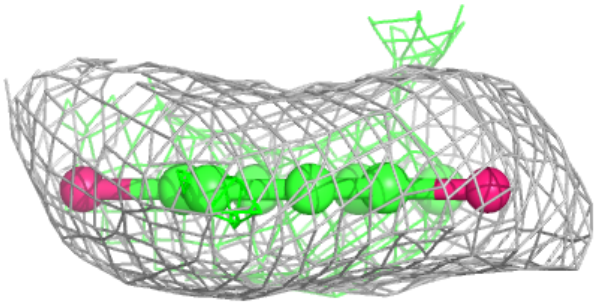


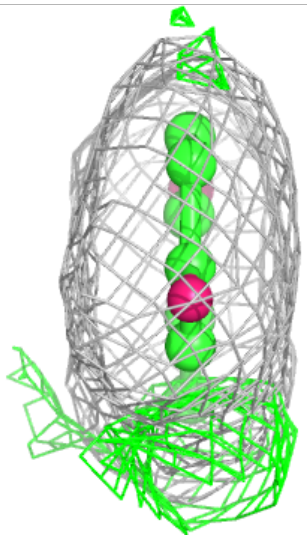


Electron density around 7DV M 303:

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

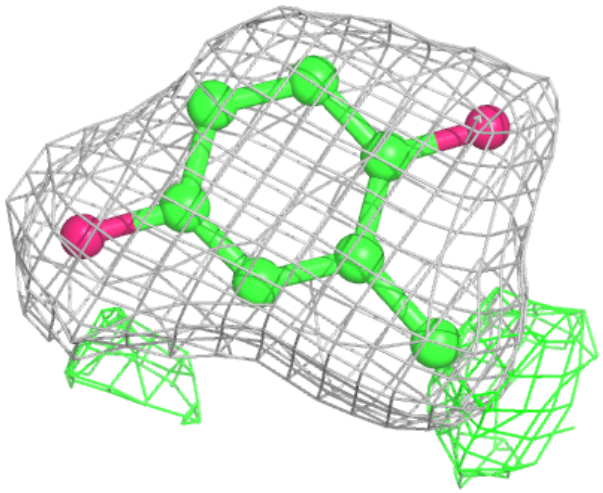


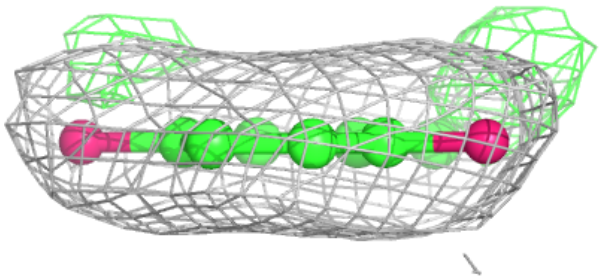


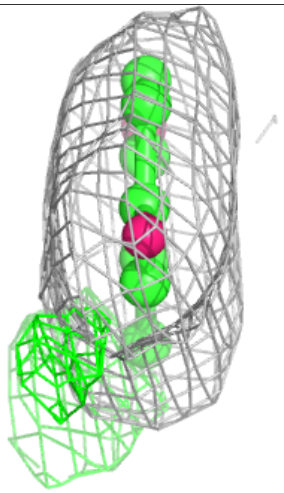


Electron density around 7DV A 302:

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

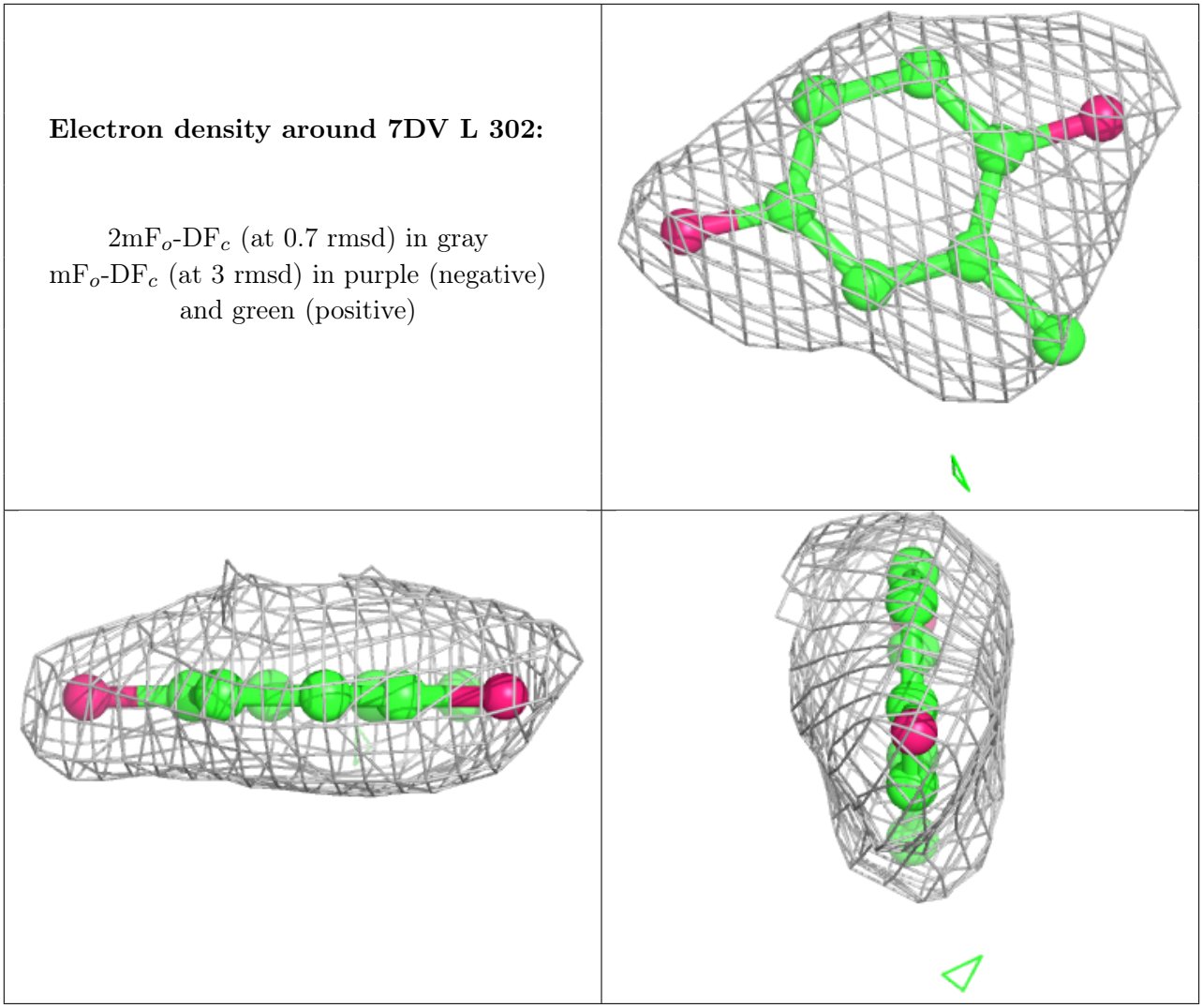






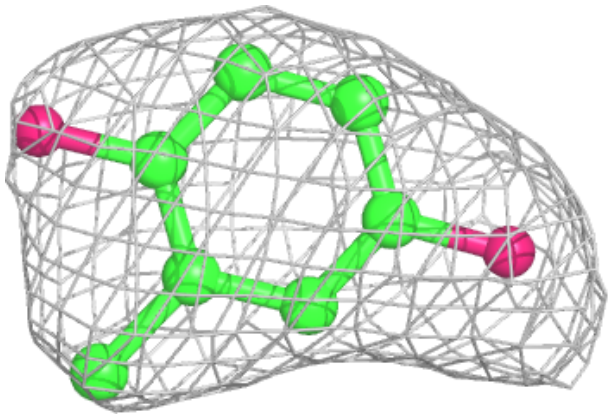
Electron density around 7DV L 302:

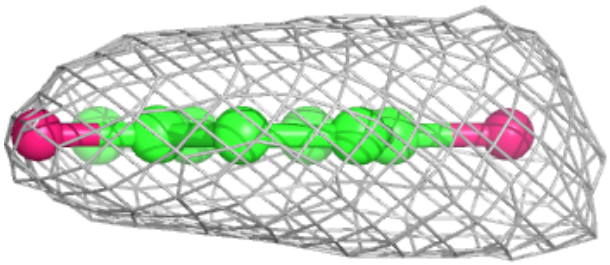
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

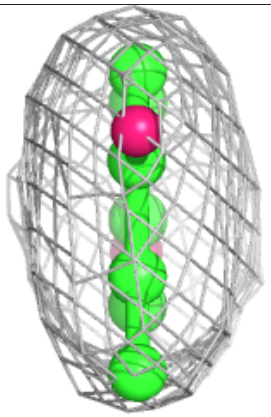


Electron density around 7DV L 303:

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

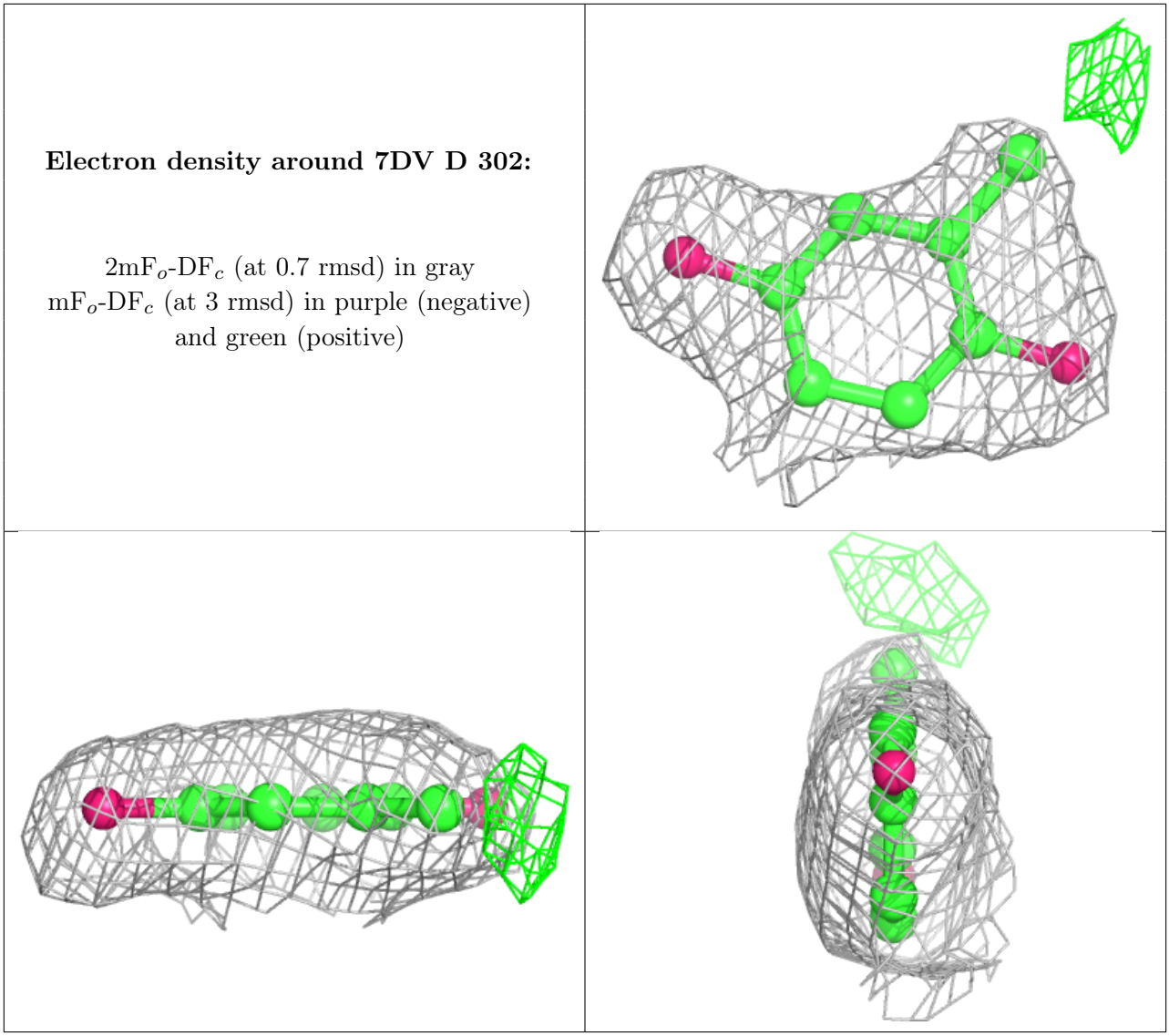






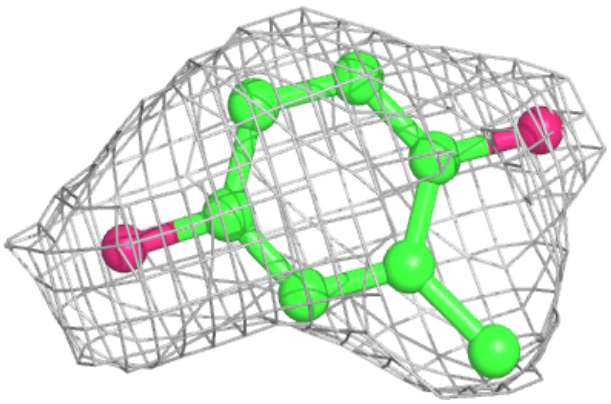
Electron density around 7DV D 302:

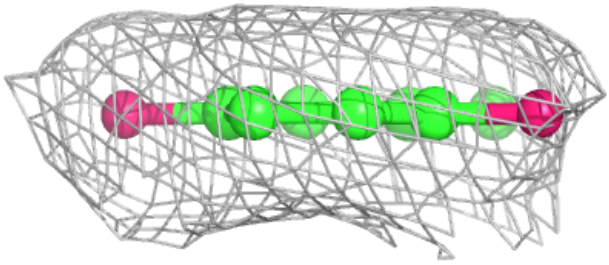
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

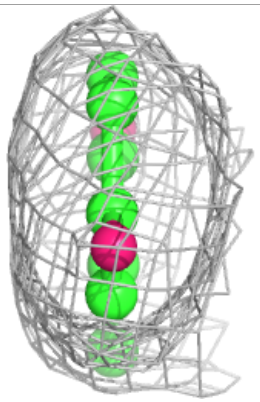


Electron density around 7DV H 303:

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

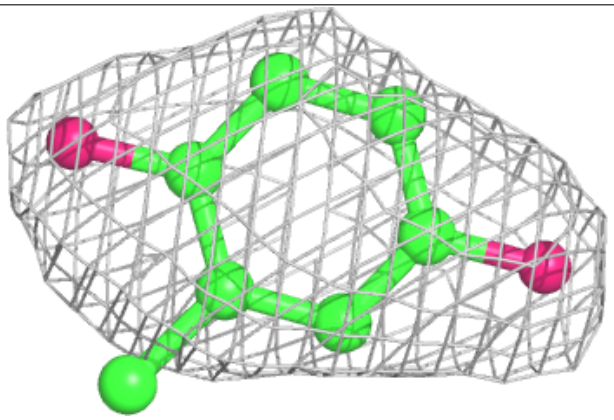


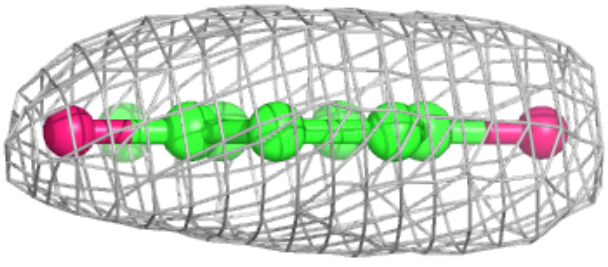


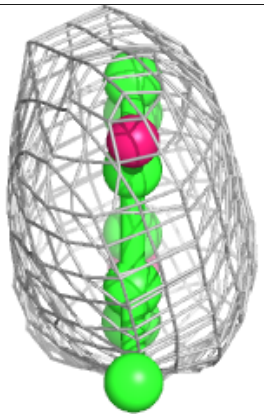


Electron density around 7DV B 303:

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

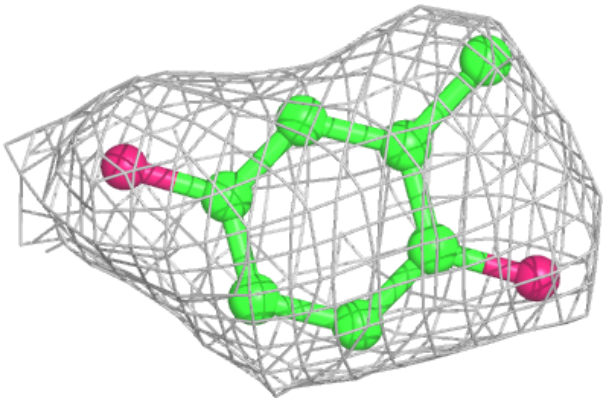


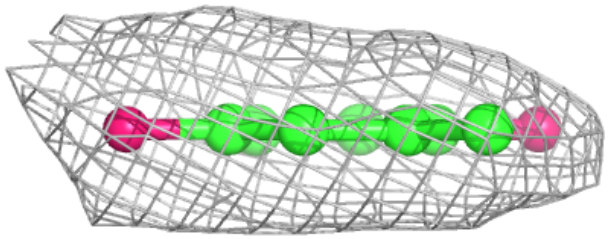


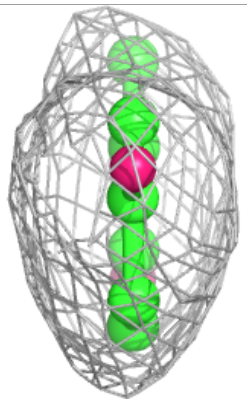


Electron density around 7DV F 303:

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

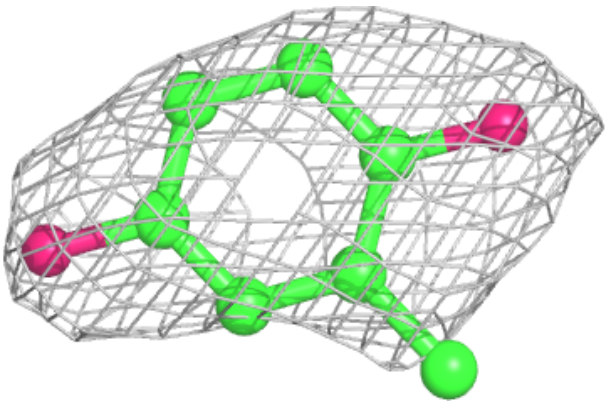


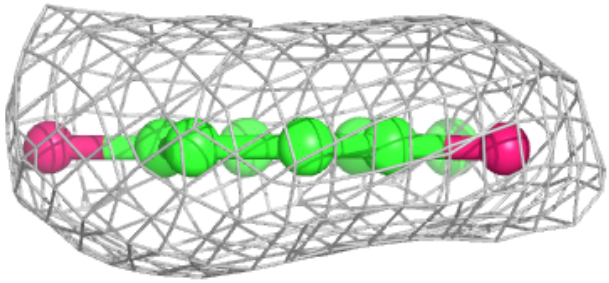


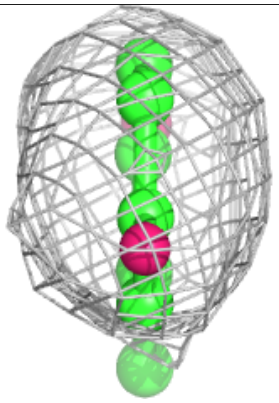


Electron density around 7DV D 303:

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

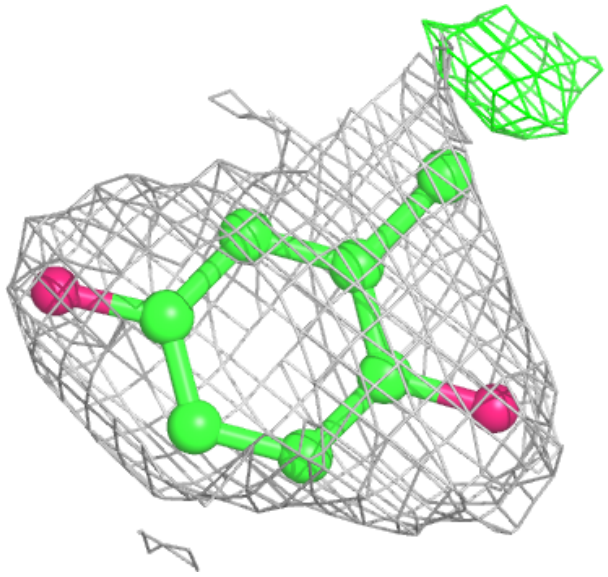


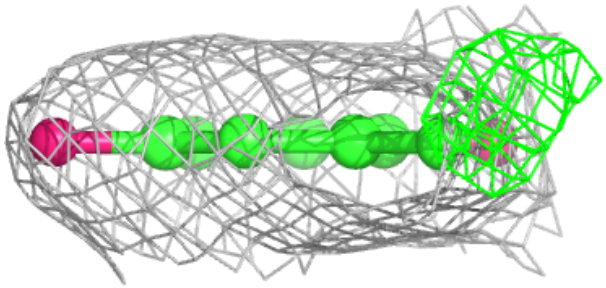


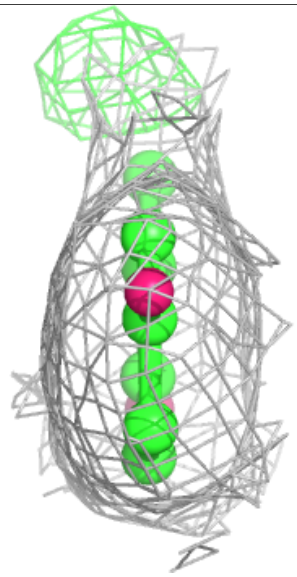


Electron density around 7DV J 302:

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

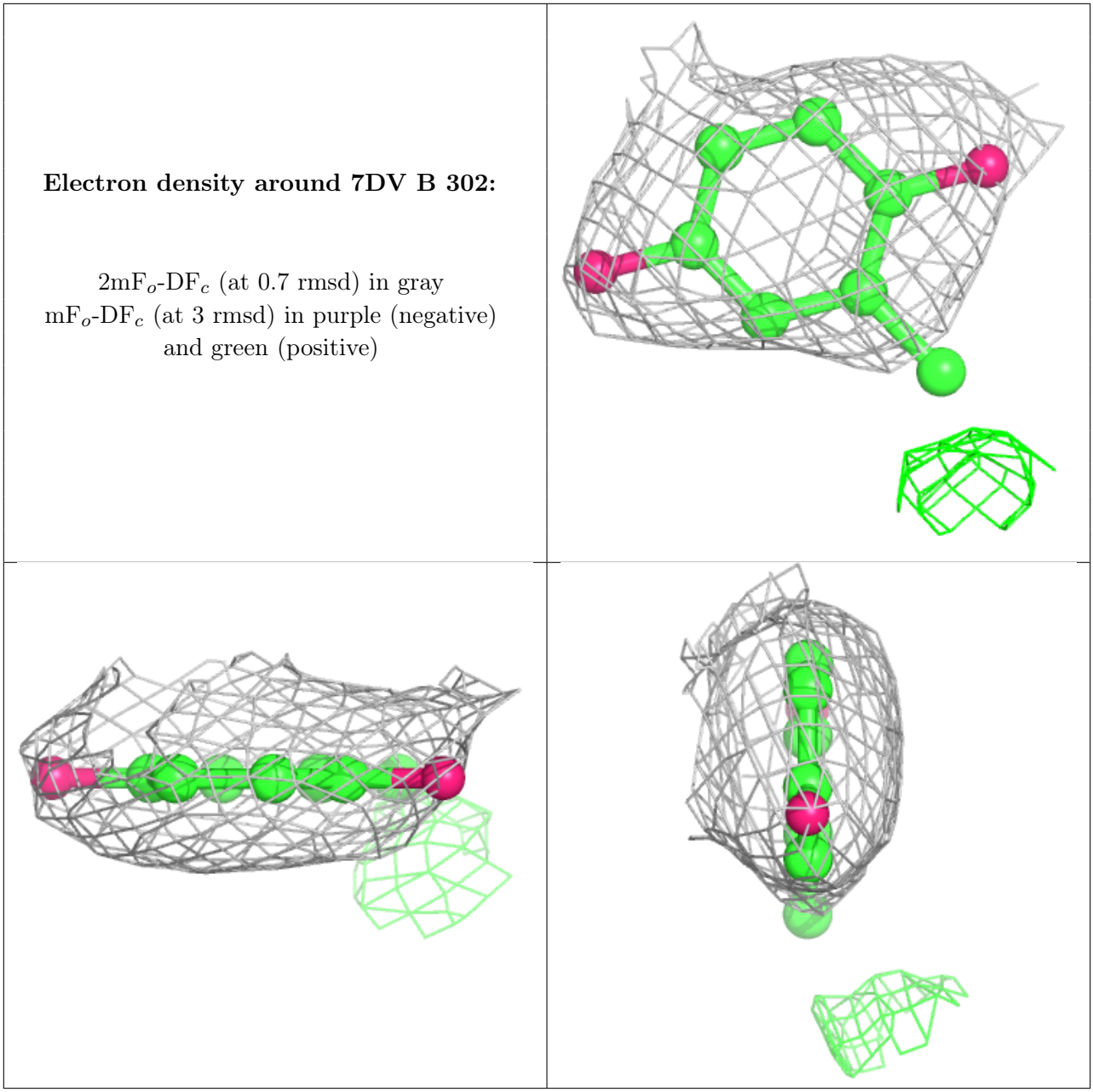






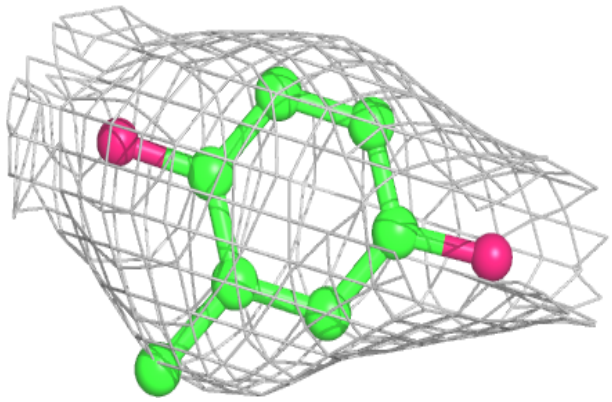
Electron density around 7DV B 302:

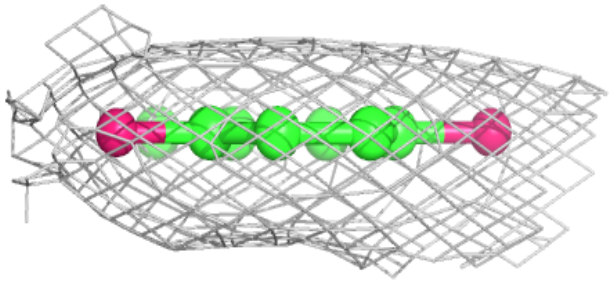
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

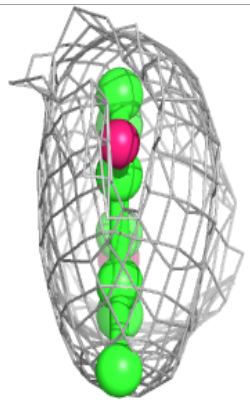


Electron density around 7DV H 301:

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

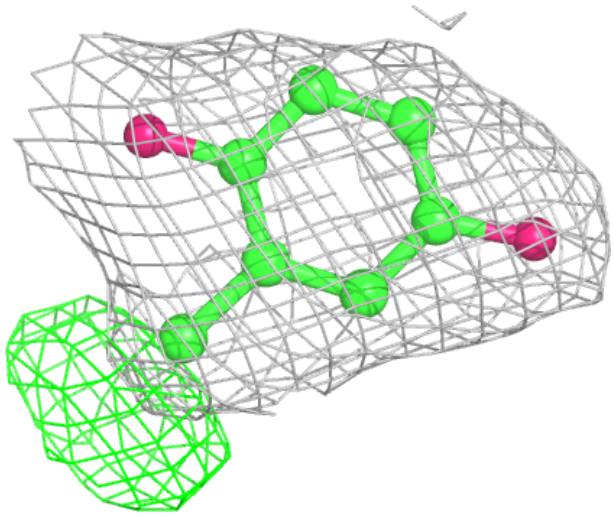


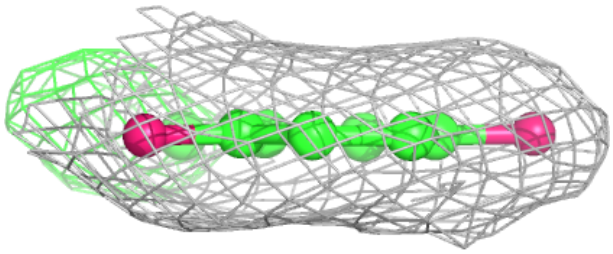


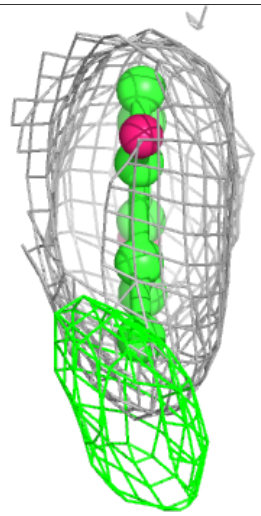


Electron density around 7DV P 302:

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

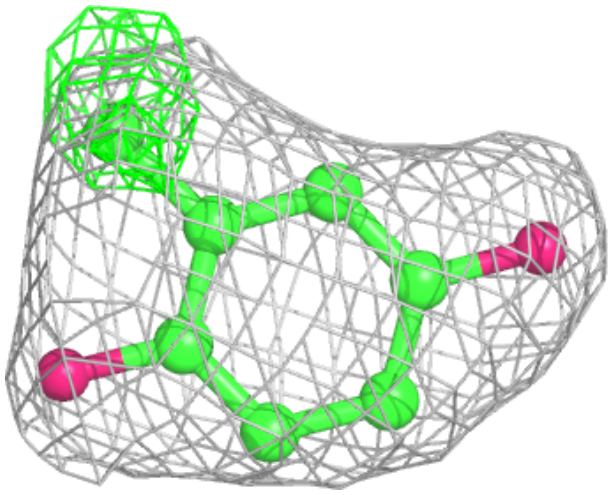


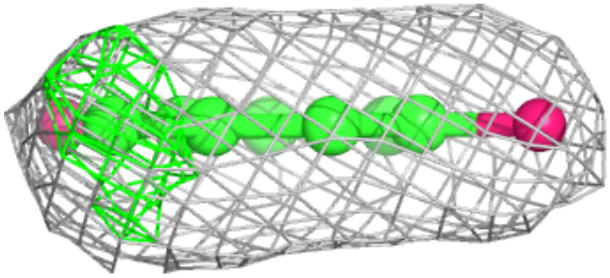


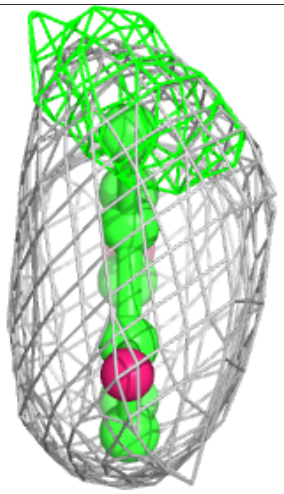


Electron density around 7DV L 301:

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

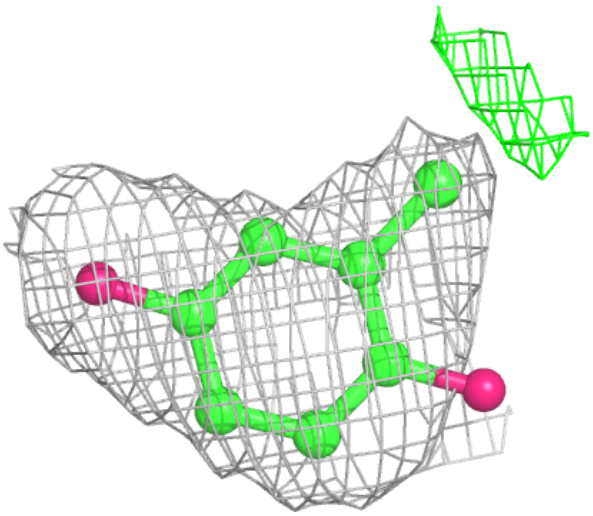


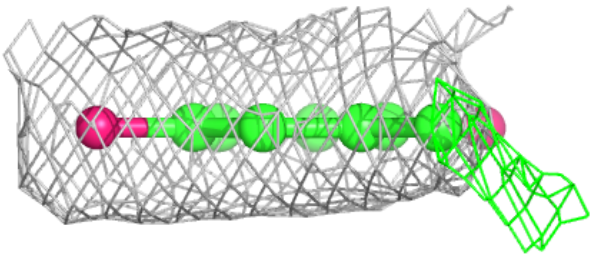


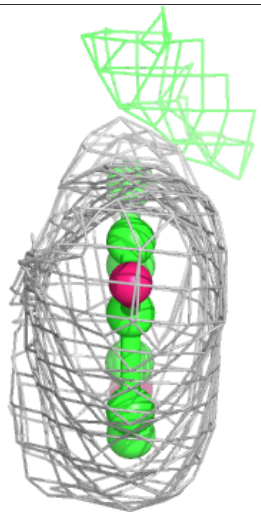


Electron density around 7DV C 302:

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

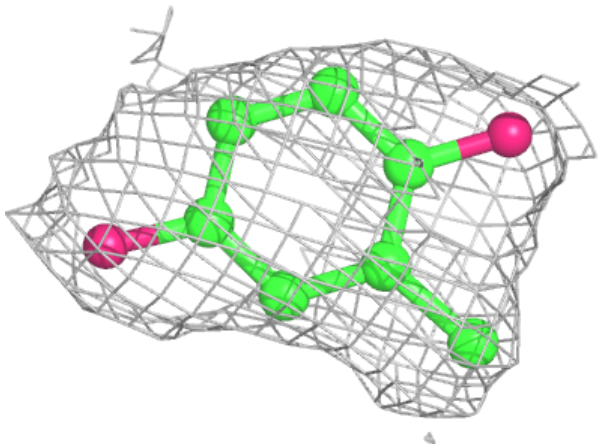


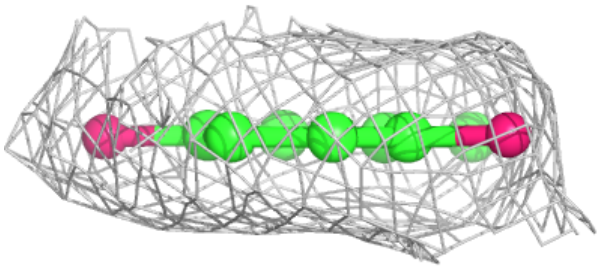


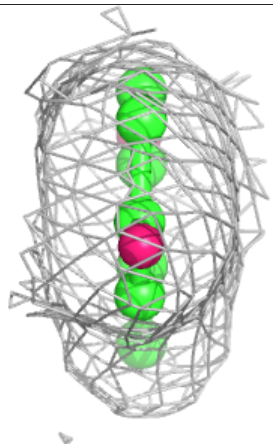


Electron density around 7DV H 302:

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

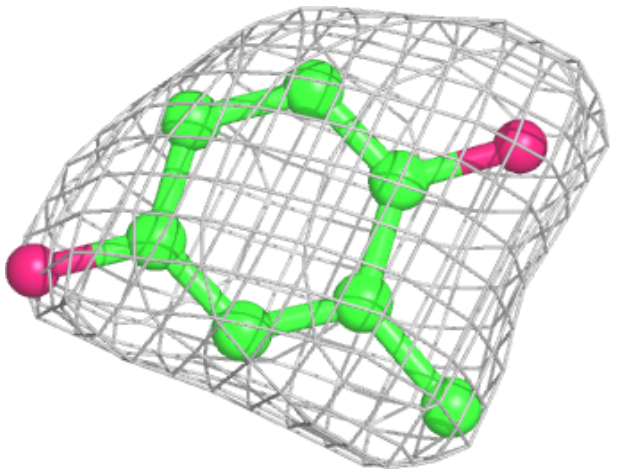


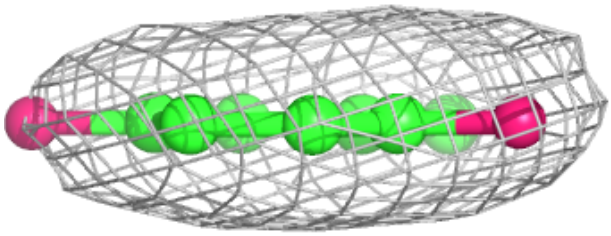


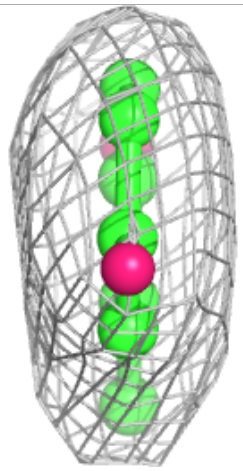


Electron density around 7DV L 304:

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

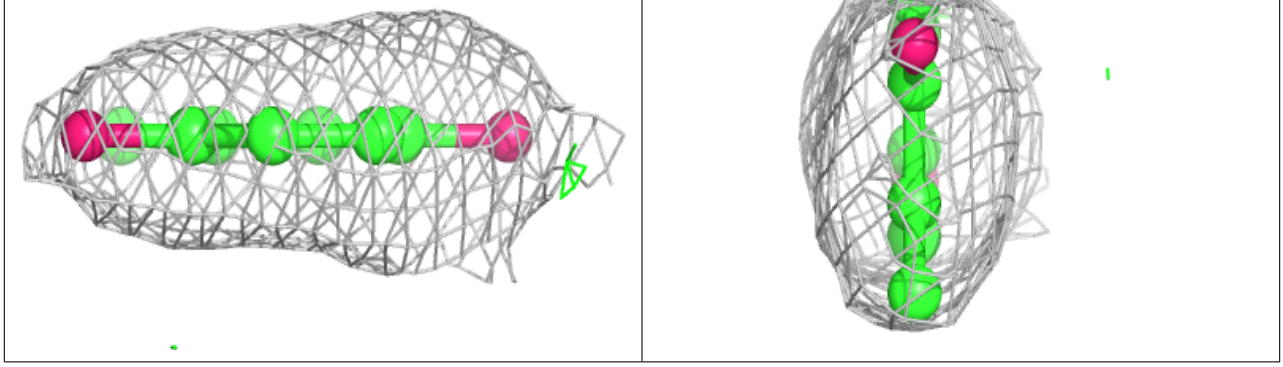






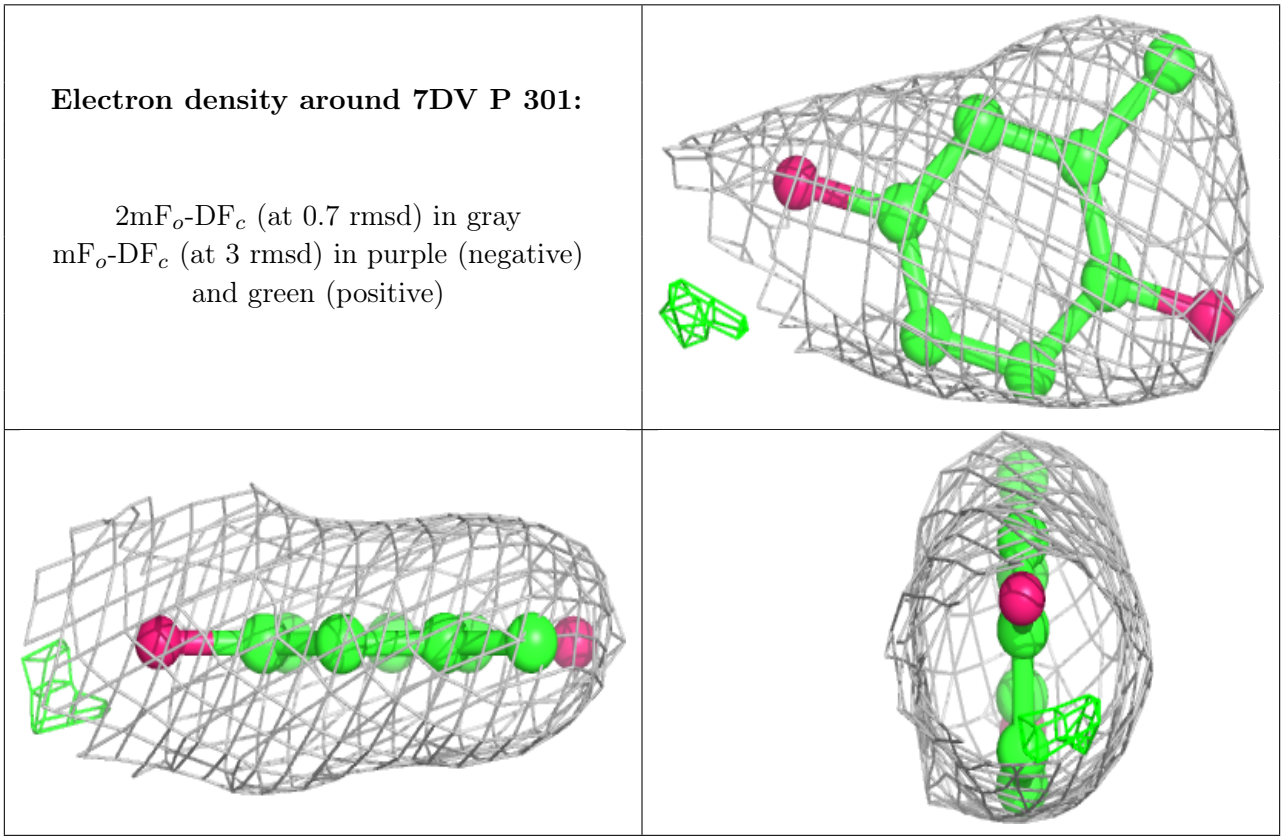
Electron density around 7DV B 301:

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



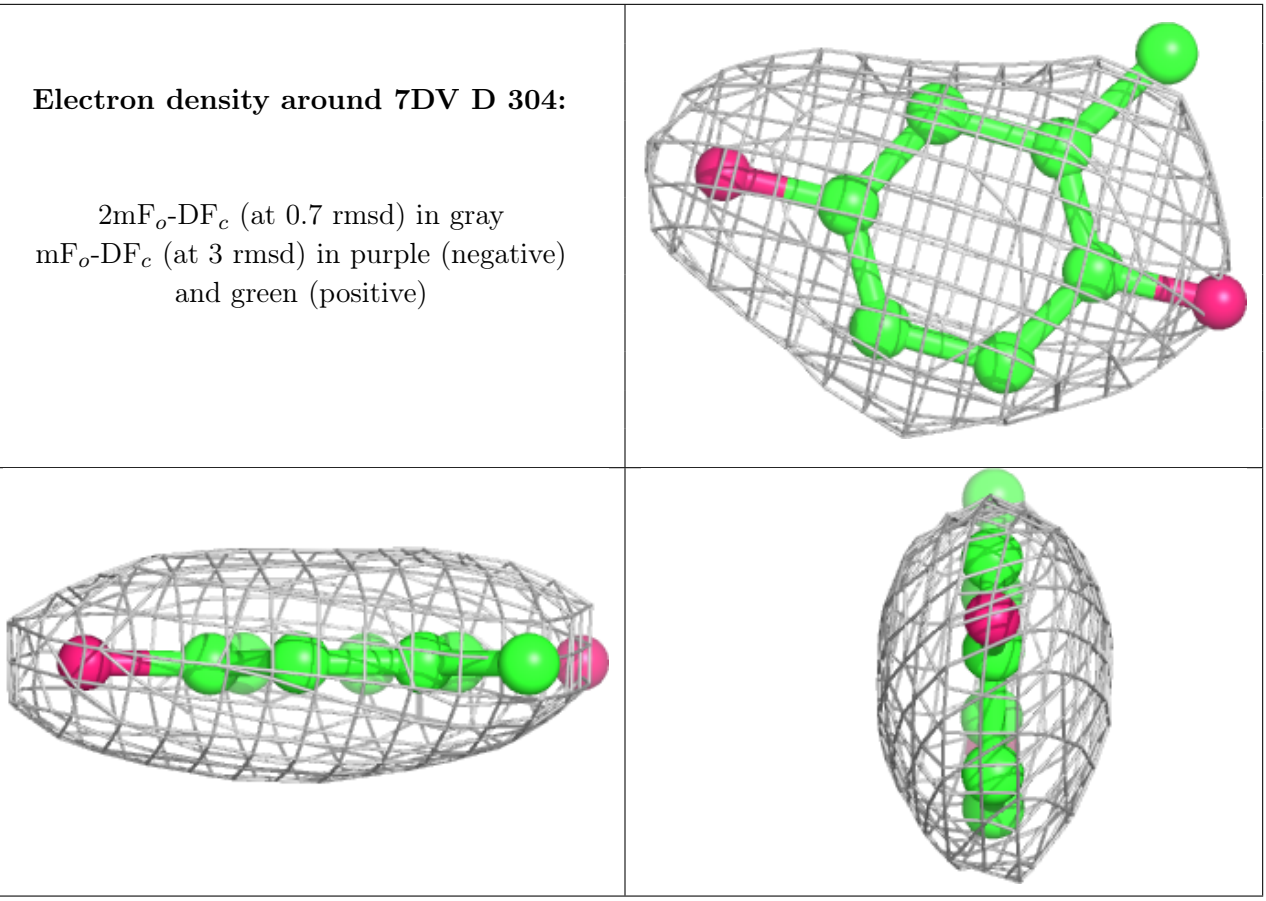
Electron density around 7DV P 301:

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



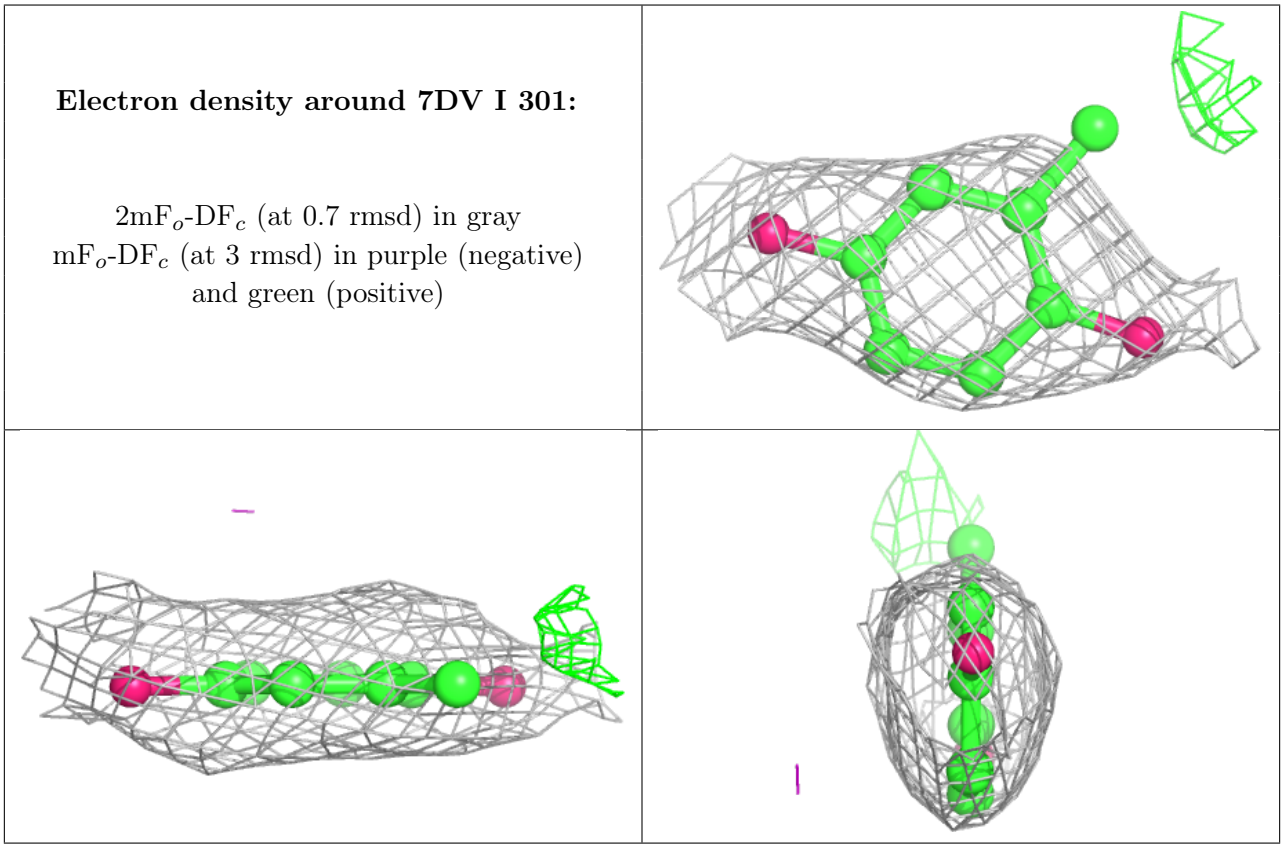
Electron density around 7DV D 304:

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



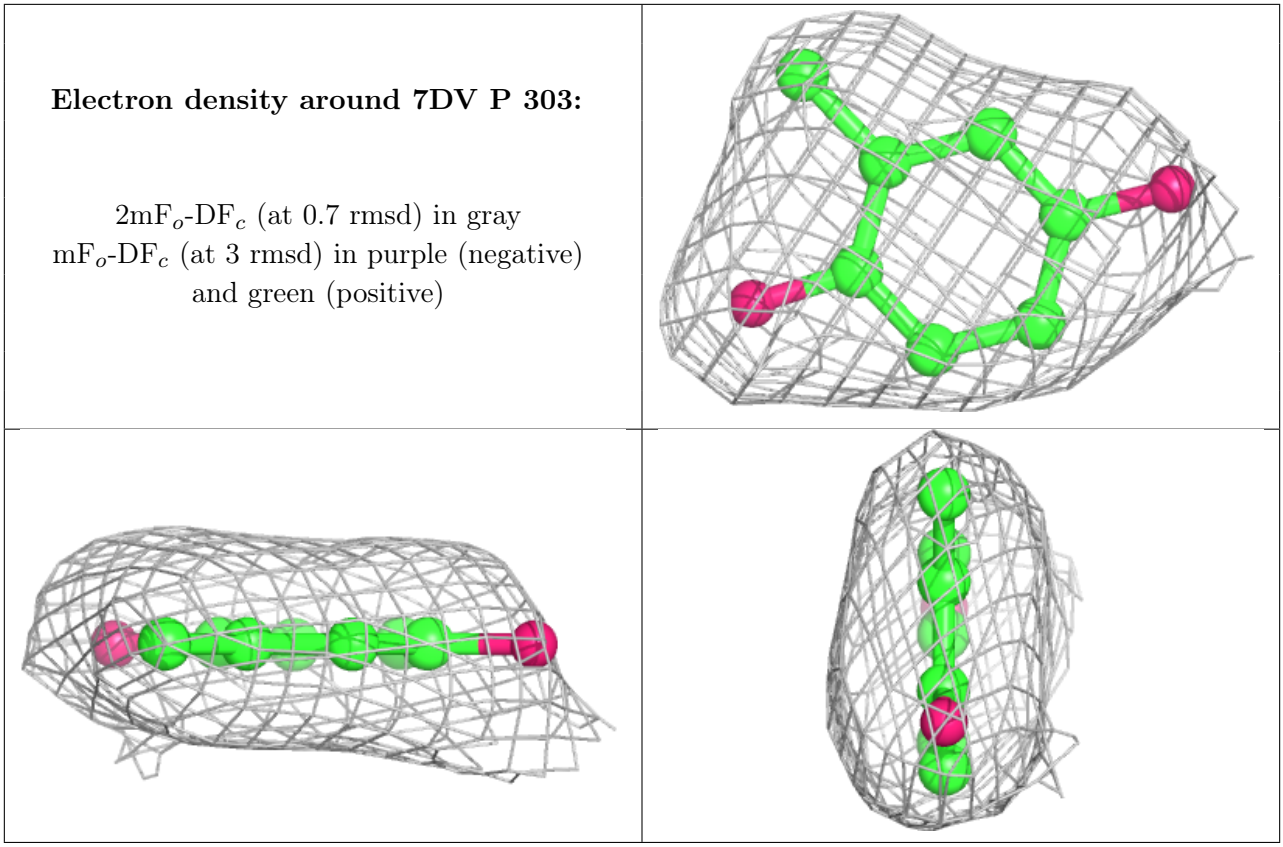
Electron density around 7DV I 301:

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



Electron density around 7DV P 303:

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



6.5 Other polymers

There are no such residues in this entry.