wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2026 – 04:13 am BST

PDB ID	:	5EC5 / pdb_00005ec5
Title	:	Crystal structure of lysenin pore
Authors	:	Podobnik, M.; Savory, P.; Rojko, N.; Kisovec, M.; Bruce, M.; Jayasinghe, L.; Anderluh, G.
Deposited on	:	2015-10-20
Resolution	:	3.10 Å(reported)

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

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

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

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

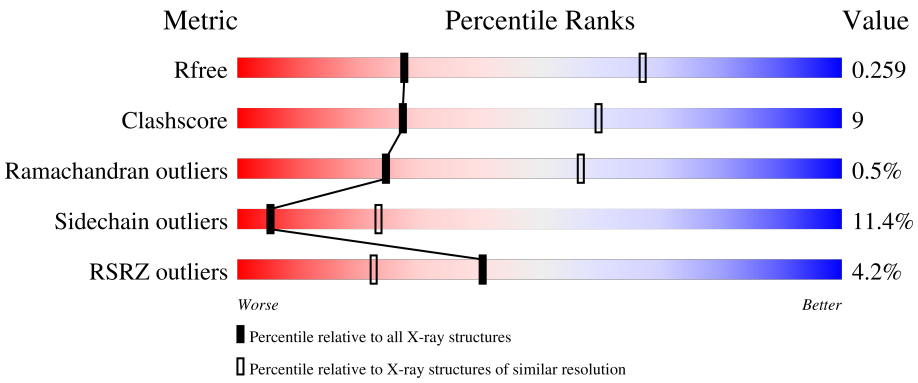
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	298	4%, 74%, 20%, • •
1	B	298	2%, 77%, 17%, • 5%
1	C	298	6%, 73%, 21%, • •
1	D	298	2%, 70%, 22%, • •
1	E	298	5%, 71%, 23%, • 5%

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Mol	Chain	Length	Quality of chain
1	F	298	5% 73% 20% 5%
1	G	298	4% 72% 20% 5%
1	H	298	2% 71% 20% 5%
1	I	298	% 71% 21% 5%
1	J	298	5% 74% 21%
1	K	298	5% 73% 20%
1	L	298	3% 74% 18% 5%
1	M	298	3% 72% 23%
1	N	298	4% 74% 20%
1	O	298	7% 73% 20%
1	P	298	5% 71% 24%
1	R	298	4% 74% 18% 5%
1	S	298	4% 73% 20% 5%

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	MBO	A	302	-	-	X	-
2	MBO	B	301	-	-	X	-
2	MBO	C	301	-	-	X	-
2	MBO	D	301	-	-	X	-
2	MBO	E	301	-	-	X	-
2	MBO	F	302	-	-	X	-
2	MBO	G	301	-	-	X	-
2	MBO	H	301	-	-	X	-
2	MBO	H	302	-	-	X	-
2	MBO	I	302	-	-	X	-
2	MBO	K	301	-	-	X	-
2	MBO	K	302	-	-	X	-
2	MBO	L	301	-	-	X	-
2	MBO	L	302	-	-	X	-
2	MBO	M	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MBO	O	301	-	-	X	-
2	MBO	P	302	-	-	X	-
2	MBO	R	301	-	-	X	-
2	MBO	S	301	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 41248 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 Lysenin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	2301	1459	390	444	8	0	0	0
1	B	284	2260	1432	384	436	8	0	0	0
1	C	286	2268	1436	386	438	8	0	0	0
1	D	285	2265	1435	385	437	8	0	0	0
1	E	283	2252	1428	383	433	8	0	0	0
1	F	283	2252	1428	383	433	8	0	0	0
1	G	290	2301	1459	390	444	8	0	0	0
1	H	283	2252	1428	383	433	8	0	0	0
1	I	282	2248	1426	382	432	8	0	0	0
1	J	290	2301	1459	390	444	8	0	0	0
1	K	290	2301	1459	390	444	8	0	0	0
1	L	284	2260	1434	384	434	8	0	0	0
1	M	289	2297	1457	389	443	8	0	0	0
1	N	289	2297	1457	389	443	8	0	0	0
1	O	289	2297	1457	389	443	8	0	0	0
1	P	289	2297	1457	389	443	8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	R	283	2252	1428	383	433	8	0	0	0
			Total	C	N	O	S			
1	S	283	2252	1428	383	433	8	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O18423
A	84	GLN	GLU	engineered mutation	UNP O18423
A	85	LYS	GLU	engineered mutation	UNP O18423
A	92	GLN	GLU	engineered mutation	UNP O18423
A	97	SER	GLU	engineered mutation	UNP O18423
A	126	GLY	ASP	engineered mutation	UNP O18423
B	0	GLY	-	expression tag	UNP O18423
B	84	GLN	GLU	engineered mutation	UNP O18423
B	85	LYS	GLU	engineered mutation	UNP O18423
B	92	GLN	GLU	engineered mutation	UNP O18423
B	97	SER	GLU	engineered mutation	UNP O18423
B	126	GLY	ASP	engineered mutation	UNP O18423
C	0	GLY	-	expression tag	UNP O18423
C	84	GLN	GLU	engineered mutation	UNP O18423
C	85	LYS	GLU	engineered mutation	UNP O18423
C	92	GLN	GLU	engineered mutation	UNP O18423
C	97	SER	GLU	engineered mutation	UNP O18423
C	126	GLY	ASP	engineered mutation	UNP O18423
D	0	GLY	-	expression tag	UNP O18423
D	84	GLN	GLU	engineered mutation	UNP O18423
D	85	LYS	GLU	engineered mutation	UNP O18423
D	92	GLN	GLU	engineered mutation	UNP O18423
D	97	SER	GLU	engineered mutation	UNP O18423
D	126	GLY	ASP	engineered mutation	UNP O18423
E	0	GLY	-	expression tag	UNP O18423
E	84	GLN	GLU	engineered mutation	UNP O18423
E	85	LYS	GLU	engineered mutation	UNP O18423
E	92	GLN	GLU	engineered mutation	UNP O18423
E	97	SER	GLU	engineered mutation	UNP O18423
E	126	GLY	ASP	engineered mutation	UNP O18423
F	0	GLY	-	expression tag	UNP O18423
F	84	GLN	GLU	engineered mutation	UNP O18423
F	85	LYS	GLU	engineered mutation	UNP O18423
F	92	GLN	GLU	engineered mutation	UNP O18423

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Chain	Residue	Modelled	Actual	Comment	Reference
F	97	SER	GLU	engineered mutation	UNP O18423
F	126	GLY	ASP	engineered mutation	UNP O18423
G	0	GLY	-	expression tag	UNP O18423
G	84	GLN	GLU	engineered mutation	UNP O18423
G	85	LYS	GLU	engineered mutation	UNP O18423
G	92	GLN	GLU	engineered mutation	UNP O18423
G	97	SER	GLU	engineered mutation	UNP O18423
G	126	GLY	ASP	engineered mutation	UNP O18423
H	0	GLY	-	expression tag	UNP O18423
H	84	GLN	GLU	engineered mutation	UNP O18423
H	85	LYS	GLU	engineered mutation	UNP O18423
H	92	GLN	GLU	engineered mutation	UNP O18423
H	97	SER	GLU	engineered mutation	UNP O18423
H	126	GLY	ASP	engineered mutation	UNP O18423
I	0	GLY	-	expression tag	UNP O18423
I	84	GLN	GLU	engineered mutation	UNP O18423
I	85	LYS	GLU	engineered mutation	UNP O18423
I	92	GLN	GLU	engineered mutation	UNP O18423
I	97	SER	GLU	engineered mutation	UNP O18423
I	126	GLY	ASP	engineered mutation	UNP O18423
J	0	GLY	-	expression tag	UNP O18423
J	84	GLN	GLU	engineered mutation	UNP O18423
J	85	LYS	GLU	engineered mutation	UNP O18423
J	92	GLN	GLU	engineered mutation	UNP O18423
J	97	SER	GLU	engineered mutation	UNP O18423
J	126	GLY	ASP	engineered mutation	UNP O18423
K	0	GLY	-	expression tag	UNP O18423
K	84	GLN	GLU	engineered mutation	UNP O18423
K	85	LYS	GLU	engineered mutation	UNP O18423
K	92	GLN	GLU	engineered mutation	UNP O18423
K	97	SER	GLU	engineered mutation	UNP O18423
K	126	GLY	ASP	engineered mutation	UNP O18423
L	0	GLY	-	expression tag	UNP O18423
L	84	GLN	GLU	engineered mutation	UNP O18423
L	85	LYS	GLU	engineered mutation	UNP O18423
L	92	GLN	GLU	engineered mutation	UNP O18423
L	97	SER	GLU	engineered mutation	UNP O18423
L	126	GLY	ASP	engineered mutation	UNP O18423
M	0	GLY	-	expression tag	UNP O18423
M	84	GLN	GLU	engineered mutation	UNP O18423
M	85	LYS	GLU	engineered mutation	UNP O18423
M	92	GLN	GLU	engineered mutation	UNP O18423

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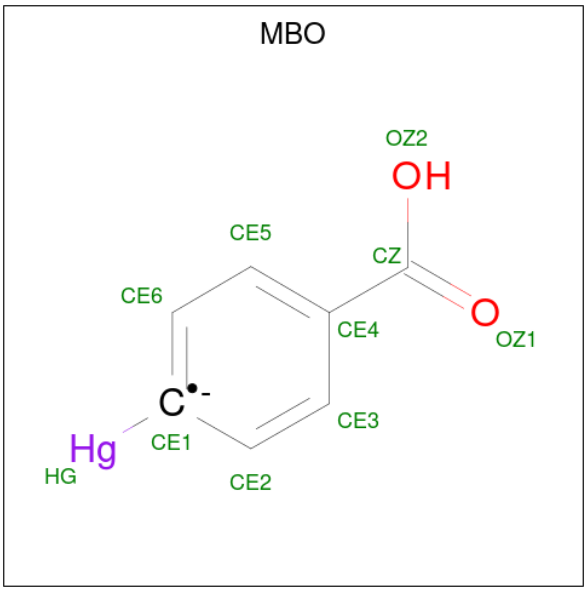
Chain	Residue	Modelled	Actual	Comment	Reference
M	97	SER	GLU	engineered mutation	UNP O18423
M	126	GLY	ASP	engineered mutation	UNP O18423
N	0	GLY	-	expression tag	UNP O18423
N	84	GLN	GLU	engineered mutation	UNP O18423
N	85	LYS	GLU	engineered mutation	UNP O18423
N	92	GLN	GLU	engineered mutation	UNP O18423
N	97	SER	GLU	engineered mutation	UNP O18423
N	126	GLY	ASP	engineered mutation	UNP O18423
O	0	GLY	-	expression tag	UNP O18423
O	84	GLN	GLU	engineered mutation	UNP O18423
O	85	LYS	GLU	engineered mutation	UNP O18423
O	92	GLN	GLU	engineered mutation	UNP O18423
O	97	SER	GLU	engineered mutation	UNP O18423
O	126	GLY	ASP	engineered mutation	UNP O18423
P	0	GLY	-	expression tag	UNP O18423
P	84	GLN	GLU	engineered mutation	UNP O18423
P	85	LYS	GLU	engineered mutation	UNP O18423
P	92	GLN	GLU	engineered mutation	UNP O18423
P	97	SER	GLU	engineered mutation	UNP O18423
P	126	GLY	ASP	engineered mutation	UNP O18423
R	0	GLY	-	expression tag	UNP O18423
R	84	GLN	GLU	engineered mutation	UNP O18423
R	85	LYS	GLU	engineered mutation	UNP O18423
R	92	GLN	GLU	engineered mutation	UNP O18423
R	97	SER	GLU	engineered mutation	UNP O18423
R	126	GLY	ASP	engineered mutation	UNP O18423
S	0	GLY	-	expression tag	UNP O18423
S	84	GLN	GLU	engineered mutation	UNP O18423
S	85	LYS	GLU	engineered mutation	UNP O18423
S	92	GLN	GLU	engineered mutation	UNP O18423
S	97	SER	GLU	engineered mutation	UNP O18423
S	126	GLY	ASP	engineered mutation	UNP O18423

- Molecule 2 is MERCURIBENZOIC ACID (CCD ID: MBO) (formula: $C_7H_5HgO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Hg	O		
2	A	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	A	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	B	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	B	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	C	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	D	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	E	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	F	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	G	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	H	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	H	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	I	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	K	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	K	1	10	7	1	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Hg	O		
2	L	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	L	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	M	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	M	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	O	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	P	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	R	1	10	7	1	2	0	0
			Total	C	Hg	O		
2	S	1	10	7	1	2	0	0

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
3	C	1	1	1	0	0
			Total	Hg		
3	D	1	1	1	0	0
			Total	Hg		
3	E	1	1	1	0	0
			Total	Hg		
3	F	1	1	1	0	0
			Total	Hg		
3	G	1	1	1	0	0
			Total	Hg		
3	I	1	1	1	0	0
			Total	Hg		
3	J	2	2	2	0	0
			Total	Hg		
3	N	2	2	2	0	0
			Total	Hg		
3	O	1	1	1	0	0
			Total	Hg		
3	P	1	1	1	0	0
			Total	Hg		
3	R	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
3	S	1	1	1	0	0

- Molecule 4 is water.

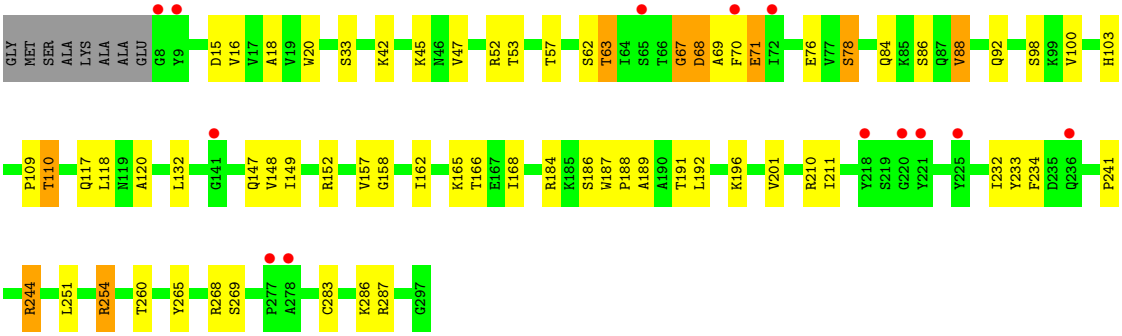
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	7	7	7	0	0
			Total	O		
4	B	2	2	2	0	0
			Total	O		
4	C	2	2	2	0	0
			Total	O		
4	D	7	7	7	0	0
			Total	O		
4	E	5	5	5	0	0
			Total	O		
4	F	5	5	5	0	0
			Total	O		
4	G	2	2	2	0	0
			Total	O		
4	H	2	2	2	0	0
			Total	O		
4	I	4	4	4	0	0
			Total	O		
4	J	4	4	4	0	0
			Total	O		
4	K	8	8	8	0	0
			Total	O		
4	L	2	2	2	0	0
			Total	O		
4	M	2	2	2	0	0
			Total	O		
4	N	2	2	2	0	0
			Total	O		
4	O	2	2	2	0	0
			Total	O		
4	P	1	1	1	0	0
			Total	O		
4	R	3	3	3	0	0
			Total	O		
4	S	1	1	1	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.

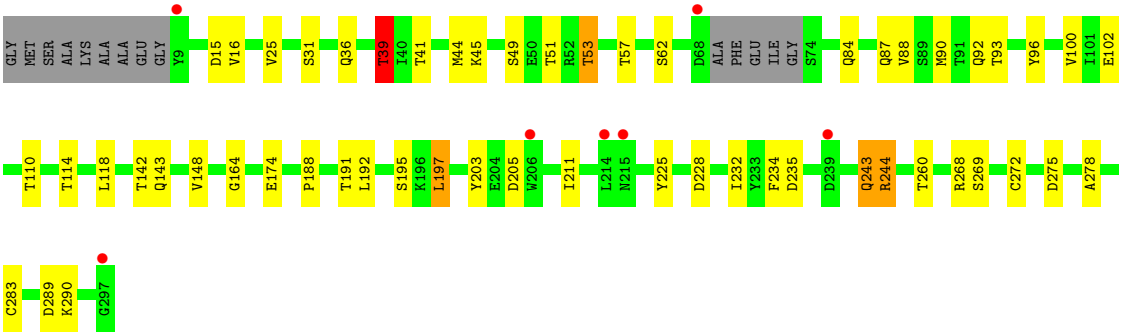
• Molecule 1: Lysenin

Chain A:



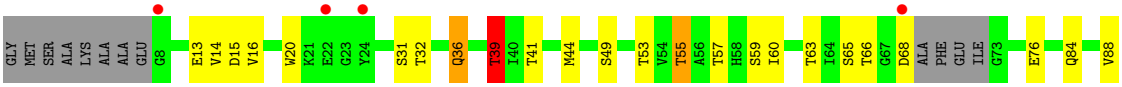
• Molecule 1: Lysenin

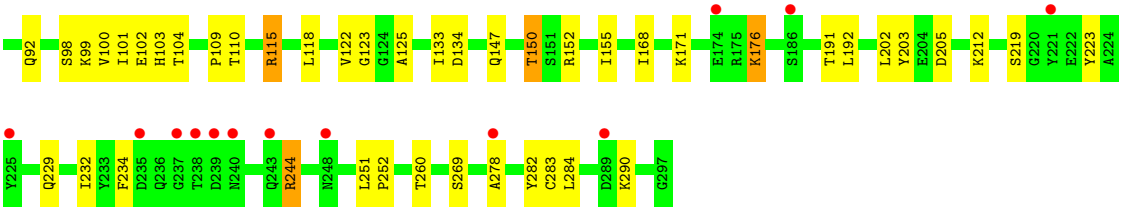
Chain B:



• Molecule 1: Lysenin

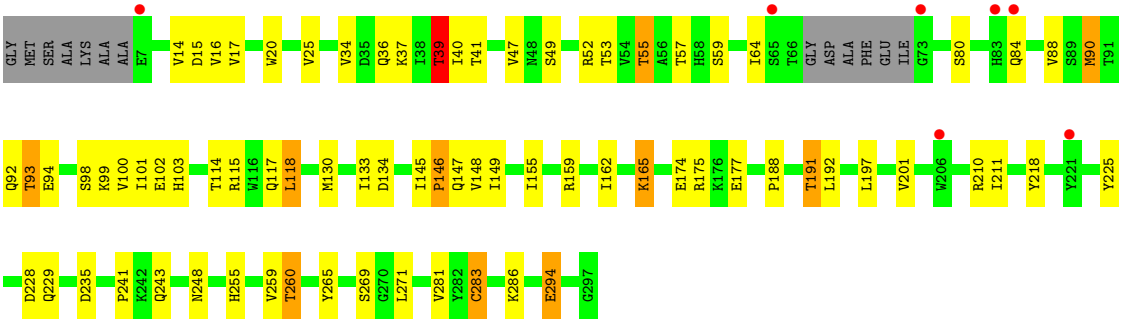
Chain C:





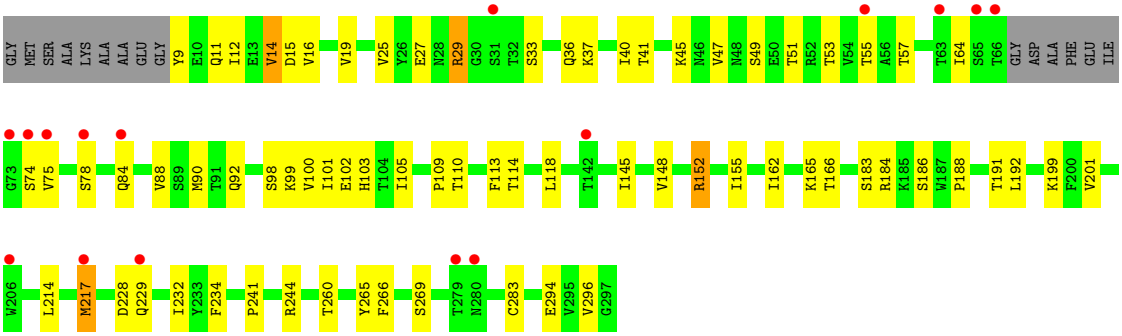
- Molecule 1: Lysenin

Chain D:



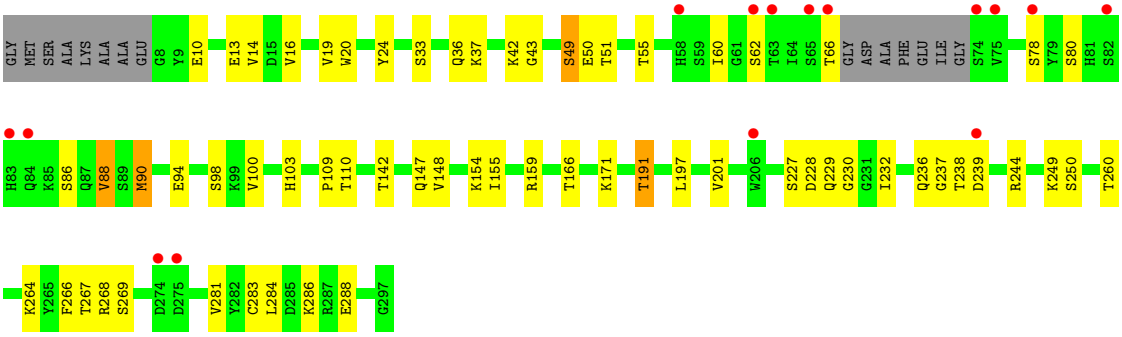
- Molecule 1: Lysenin

Chain E:



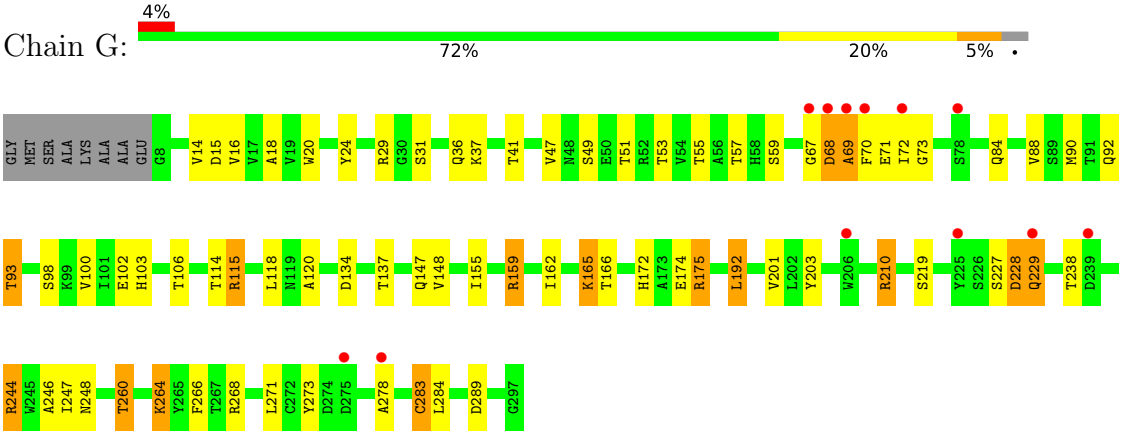
- Molecule 1: Lysenin

Chain F:



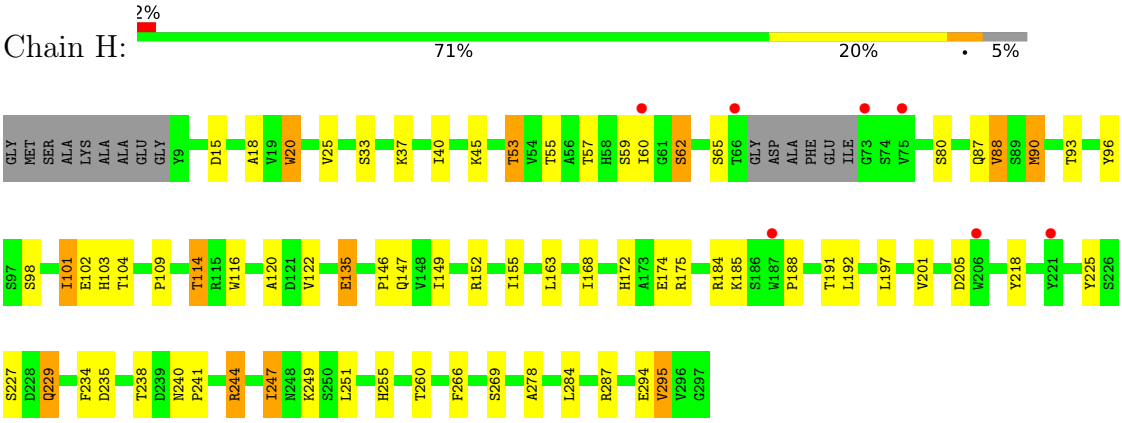
- Molecule 1: Lysenin

Chain G:



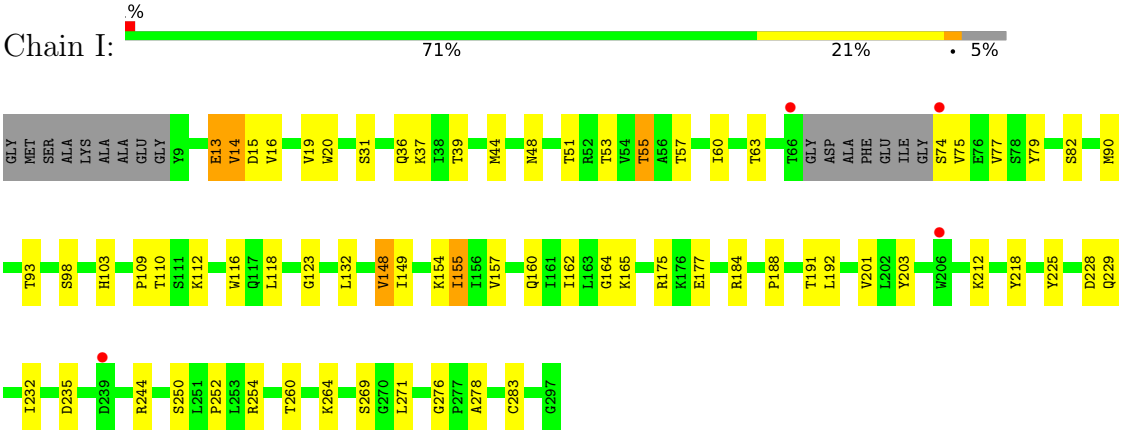
- Molecule 1: Lysenin

Chain H:



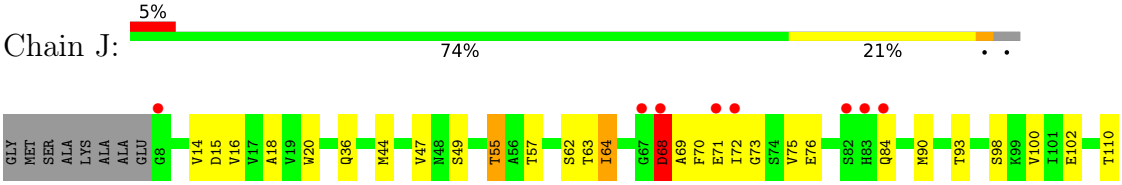
- Molecule 1: Lysenin

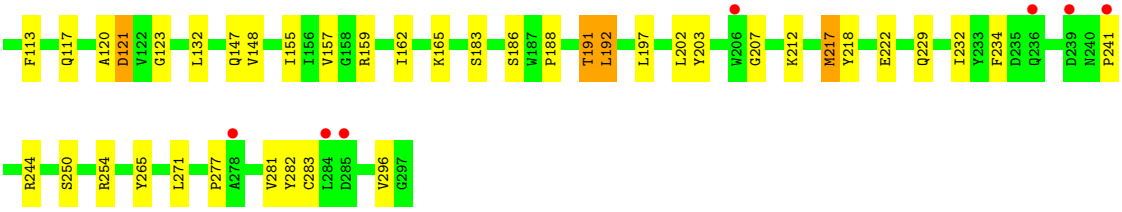
Chain I:



- Molecule 1: Lysenin

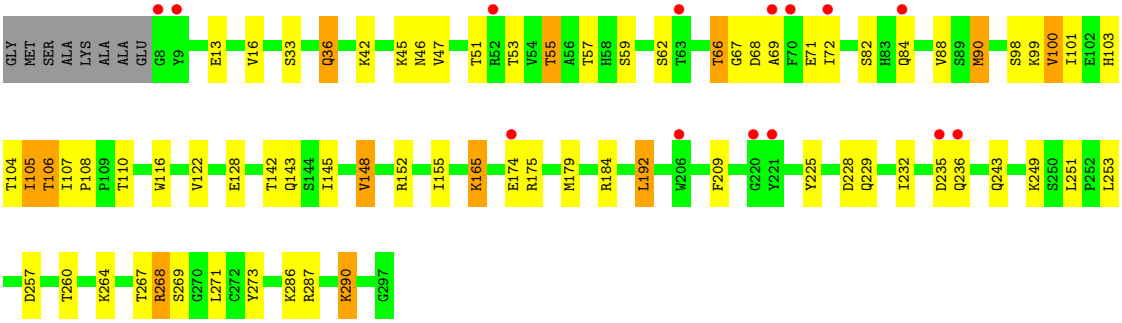
Chain J:





• Molecule 1: Lysenin

Chain K:

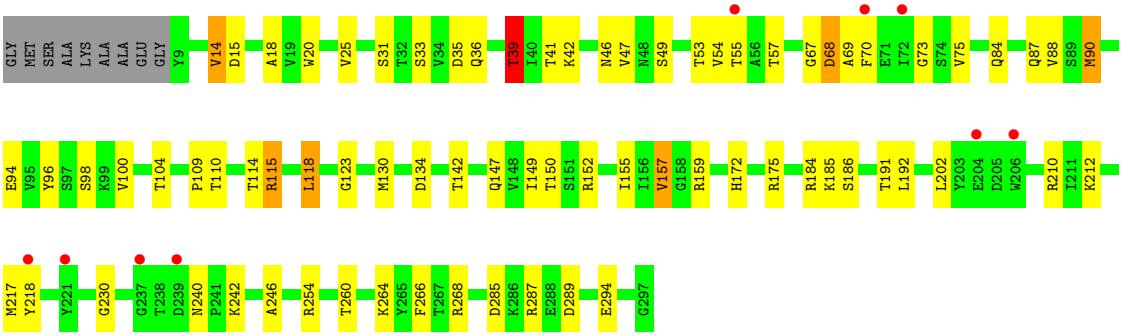


• Molecule 1: Lysenin

Chain L:

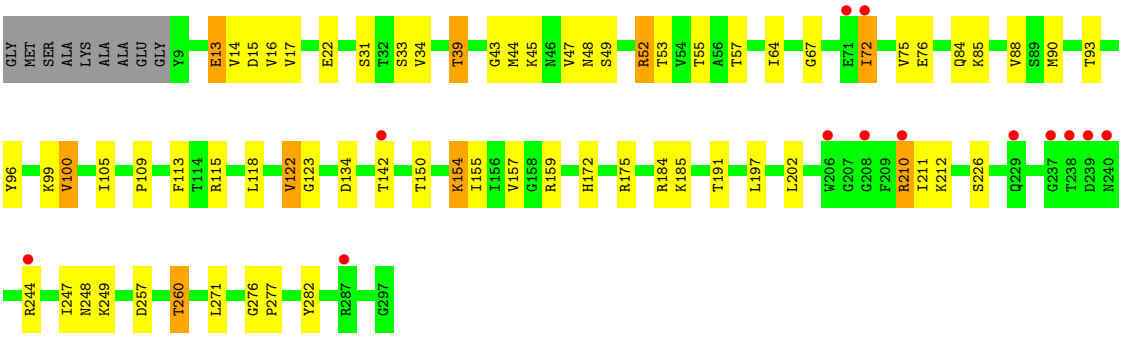
• Molecule 1: Lysenin

Chain M:



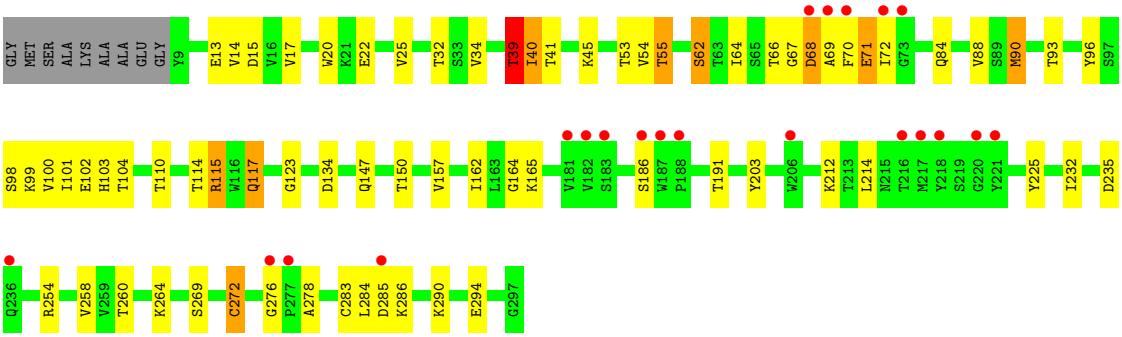
• Molecule 1: Lysenin

Chain N:



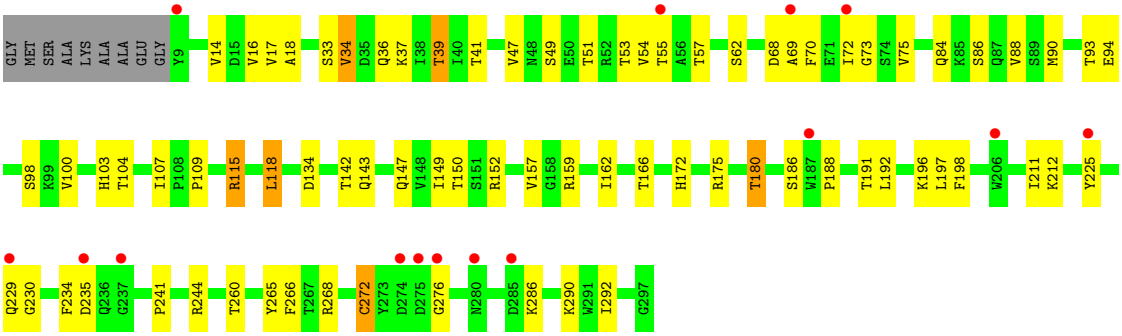
- Molecule 1: Lysenin

Chain O:



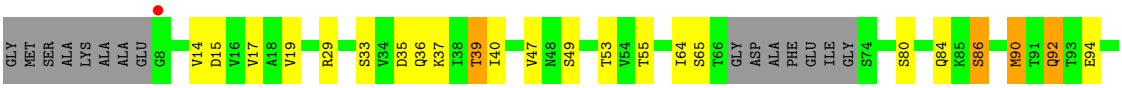
- Molecule 1: Lysenin

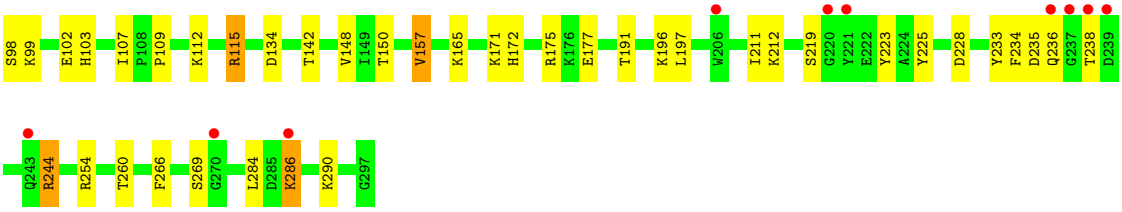
Chain P:



- Molecule 1: Lysenin

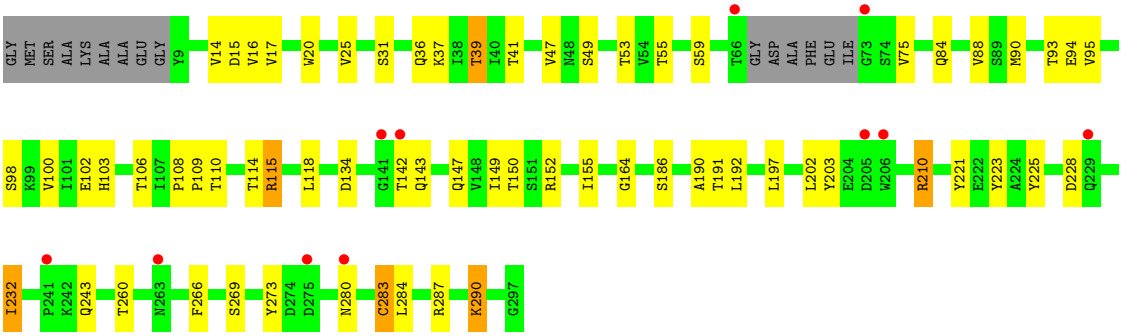
Chain R:





- Molecule 1: Lysenin

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	192.99Å 192.99Å 493.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 3.10 49.10 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.10-3.10) 99.9 (49.10-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.214 , 0.258 0.218 , 0.259	Depositor DCC
R_{free} test set	8448 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.6	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	41248	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MBO, HG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.66	0/2352	0.96	2/3186 (0.1%)
1	B	0.62	0/2309	0.89	1/3127 (0.0%)
1	C	0.65	0/2317	0.89	2/3137 (0.1%)
1	D	0.64	0/2314	0.92	2/3133 (0.1%)
1	E	0.66	0/2301	0.92	2/3116 (0.1%)
1	F	0.73	0/2301	0.99	2/3116 (0.1%)
1	G	0.71	0/2352	1.00	6/3186 (0.2%)
1	H	0.66	0/2301	0.96	2/3116 (0.1%)
1	I	0.67	0/2297	0.95	2/3111 (0.1%)
1	J	0.65	0/2352	0.92	1/3186 (0.0%)
1	K	0.67	0/2352	0.99	4/3186 (0.1%)
1	L	0.62	0/2309	0.91	2/3127 (0.1%)
1	M	0.66	0/2348	0.90	1/3181 (0.0%)
1	N	0.65	0/2348	0.92	3/3181 (0.1%)
1	O	0.66	0/2348	0.94	5/3181 (0.2%)
1	P	0.67	0/2348	0.95	2/3181 (0.1%)
1	R	0.65	0/2301	0.92	3/3116 (0.1%)
1	S	0.63	0/2301	0.91	1/3116 (0.0%)
All	All	0.66	0/41851	0.94	43/56683 (0.1%)

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	S	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	106	THR	CB-CA-C	7.80	123.50	110.79
1	G	73	GLY	N-CA-C	-6.62	102.02	111.42
1	H	101	ILE	CB-CA-C	6.32	118.71	110.12
1	O	68	ASP	N-CA-C	6.17	123.95	110.80
1	O	71	GLU	N-CA-C	-6.12	97.77	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	GLY	Peptide
1	S	221	TYR	Peptide

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	2301	0	2264	33	0
1	B	2260	0	2226	26	0
1	C	2268	0	2233	32	0
1	D	2265	0	2232	42	0
1	E	2252	0	2222	35	0
1	F	2252	0	2222	34	1
1	G	2301	0	2265	52	0
1	H	2252	0	2223	50	0
1	I	2248	0	2219	30	0
1	J	2301	0	2265	27	0
1	K	2301	0	2265	33	0
1	L	2260	0	2234	39	0
1	M	2297	0	2262	47	0
1	N	2297	0	2262	38	0
1	O	2297	0	2262	40	0
1	P	2297	0	2261	36	0
1	R	2252	0	2222	35	1
1	S	2252	0	2223	33	0
2	A	20	0	8	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	8	16	0
2	C	10	0	4	10	0
2	D	10	0	4	17	0
2	E	10	0	4	6	0
2	F	10	0	4	19	0
2	G	10	0	4	13	0
2	H	20	0	8	29	0
2	I	10	0	4	6	0
2	K	20	0	8	30	0
2	L	20	0	8	25	0
2	M	20	0	8	18	0
2	O	10	0	4	13	0
2	P	10	0	4	20	0
2	R	10	0	4	7	0
2	S	10	0	4	15	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	I	1	0	0	0	0
3	J	2	0	0	0	0
3	N	2	0	0	0	0
3	O	1	0	0	1	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
4	A	7	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	7	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	8	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	1	0	0	0	0
4	R	3	0	0	0	0
4	S	1	0	0	0	0
All	All	41248	0	40450	745	1

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 9.

The worst 5 of 745 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)
2:H:301:MBO:HE6	2:H:301:MBO:CE1	2.06	1.24
2:S:301:MBO:HE2	2:S:301:MBO:CE3	2.06	1.24
2:B:301:MBO:HE3	2:B:301:MBO:CE4	2.06	1.24
2:L:302:MBO:HE6	2:L:302:MBO:CE5	2.06	1.24
2:O:301:MBO:HE6	2:O:301:MBO:CE1	2.06	1.24

All (1) 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:F:239:ASP:OD2	1:R:236:GLN:OE1[7_556]	1.52	0.68

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	288/298 (97%)	273 (95%)	12 (4%)	3 (1%)	12 41
1	B	280/298 (94%)	269 (96%)	11 (4%)	0	100 100
1	C	282/298 (95%)	269 (95%)	13 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	281/298 (94%)	272 (97%)	8 (3%)	1 (0%)	30	61
1	E	279/298 (94%)	267 (96%)	12 (4%)	0	100	100
1	F	279/298 (94%)	259 (93%)	18 (6%)	2 (1%)	18	49
1	G	288/298 (97%)	273 (95%)	11 (4%)	4 (1%)	9	34
1	H	279/298 (94%)	272 (98%)	7 (2%)	0	100	100
1	I	278/298 (93%)	269 (97%)	9 (3%)	0	100	100
1	J	288/298 (97%)	274 (95%)	11 (4%)	3 (1%)	12	41
1	K	288/298 (97%)	272 (94%)	13 (4%)	3 (1%)	12	41
1	L	280/298 (94%)	268 (96%)	12 (4%)	0	100	100
1	M	287/298 (96%)	265 (92%)	20 (7%)	2 (1%)	18	49
1	N	287/298 (96%)	270 (94%)	16 (6%)	1 (0%)	36	67
1	O	287/298 (96%)	274 (96%)	10 (4%)	3 (1%)	12	41
1	P	287/298 (96%)	270 (94%)	15 (5%)	2 (1%)	18	49
1	R	279/298 (94%)	270 (97%)	9 (3%)	0	100	100
1	S	279/298 (94%)	263 (94%)	15 (5%)	1 (0%)	30	61
All	All	5096/5364 (95%)	4849 (95%)	222 (4%)	25 (0%)	24	57

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	70	PHE
1	A	71	GLU
1	G	68	ASP
1	G	72	ILE

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	253/257 (98%)	220 (87%)	33 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	250/257 (97%)	226 (90%)	24 (10%)	8	30
1	C	250/257 (97%)	223 (89%)	27 (11%)	6	25
1	D	250/257 (97%)	220 (88%)	30 (12%)	5	21
1	E	249/257 (97%)	218 (88%)	31 (12%)	4	19
1	F	249/257 (97%)	217 (87%)	32 (13%)	4	18
1	G	253/257 (98%)	223 (88%)	30 (12%)	5	21
1	H	249/257 (97%)	221 (89%)	28 (11%)	6	24
1	I	249/257 (97%)	218 (88%)	31 (12%)	4	19
1	J	253/257 (98%)	222 (88%)	31 (12%)	4	20
1	K	253/257 (98%)	219 (87%)	34 (13%)	4	17
1	L	250/257 (97%)	227 (91%)	23 (9%)	8	31
1	M	253/257 (98%)	229 (90%)	24 (10%)	8	30
1	N	253/257 (98%)	224 (88%)	29 (12%)	5	23
1	O	253/257 (98%)	228 (90%)	25 (10%)	7	29
1	P	253/257 (98%)	220 (87%)	33 (13%)	4	18
1	R	249/257 (97%)	224 (90%)	25 (10%)	7	29
1	S	249/257 (97%)	224 (90%)	25 (10%)	7	29
All	All	4518/4626 (98%)	4003 (89%)	515 (11%)	5	23

5 of 515 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	286	LYS
1	R	99	LYS
1	P	272	CYS
1	G	175	ARG
1	G	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	58	HIS
1	P	172	HIS
1	M	92	GLN
1	N	236	GLN

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Mol	Chain	Res	Type
1	R	92	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 14 are monoatomic - leaving 22 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	MBO	M	302	1	7,10,10	1.29	1 (14%)	10,13,13	1.81	4 (40%)
2	MBO	E	301	1	7,10,10	1.27	0	10,13,13	1.72	2 (20%)
2	MBO	C	301	1	7,10,10	1.29	1 (14%)	10,13,13	1.11	1 (10%)
2	MBO	S	301	1	7,10,10	1.17	0	10,13,13	1.59	2 (20%)
2	MBO	L	302	1	7,10,10	1.24	1 (14%)	10,13,13	1.17	0
2	MBO	O	301	1	7,10,10	1.29	1 (14%)	10,13,13	1.44	2 (20%)
2	MBO	A	301	1	7,10,10	1.28	1 (14%)	10,13,13	1.37	1 (10%)
2	MBO	M	301	1	7,10,10	1.23	0	10,13,13	1.15	1 (10%)
2	MBO	H	302	1	7,10,10	1.31	1 (14%)	10,13,13	1.33	0
2	MBO	L	301	1	7,10,10	1.25	0	10,13,13	1.32	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MBO	K	301	1	7,10,10	1.23	1 (14%)	10,13,13	1.85	2 (20%)
2	MBO	F	302	1	7,10,10	1.16	0	10,13,13	1.60	2 (20%)
2	MBO	I	302	1	7,10,10	1.29	1 (14%)	10,13,13	1.60	2 (20%)
2	MBO	R	301	1	7,10,10	1.27	0	10,13,13	1.14	1 (10%)
2	MBO	B	302	1	7,10,10	1.25	1 (14%)	10,13,13	1.30	1 (10%)
2	MBO	H	301	1	7,10,10	1.25	1 (14%)	10,13,13	1.27	0
2	MBO	P	302	1	7,10,10	1.26	1 (14%)	10,13,13	1.02	0
2	MBO	A	302	1	7,10,10	1.35	1 (14%)	10,13,13	1.43	1 (10%)
2	MBO	D	301	1	7,10,10	1.19	0	10,13,13	1.72	3 (30%)
2	MBO	B	301	1	7,10,10	1.25	0	10,13,13	1.54	1 (10%)
2	MBO	G	301	1	7,10,10	1.26	1 (14%)	10,13,13	1.36	2 (20%)
2	MBO	K	302	1	7,10,10	1.27	0	10,13,13	1.37	1 (10%)

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	MBO	M	302	1	-	4/4/14/14	0/1/1/1
2	MBO	E	301	1	-	0/4/14/14	0/1/1/1
2	MBO	C	301	1	-	4/4/14/14	0/1/1/1
2	MBO	S	301	1	-	4/4/14/14	0/1/1/1
2	MBO	L	302	1	-	4/4/14/14	0/1/1/1
2	MBO	O	301	1	-	4/4/14/14	0/1/1/1
2	MBO	A	301	1	-	2/4/14/14	0/1/1/1
2	MBO	M	301	1	-	4/4/14/14	0/1/1/1
2	MBO	H	302	1	-	4/4/14/14	0/1/1/1
2	MBO	L	301	1	-	1/4/14/14	0/1/1/1
2	MBO	K	301	1	-	4/4/14/14	0/1/1/1
2	MBO	F	302	1	-	4/4/14/14	0/1/1/1
2	MBO	I	302	1	-	3/4/14/14	0/1/1/1
2	MBO	R	301	1	-	4/4/14/14	0/1/1/1
2	MBO	B	302	1	-	4/4/14/14	0/1/1/1
2	MBO	H	301	1	-	3/4/14/14	0/1/1/1
2	MBO	P	302	1	-	0/4/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MBO	A	302	1	-	4/4/14/14	0/1/1/1
2	MBO	D	301	1	-	4/4/14/14	0/1/1/1
2	MBO	B	301	1	-	4/4/14/14	0/1/1/1
2	MBO	G	301	1	-	0/4/14/14	0/1/1/1
2	MBO	K	302	1	-	2/4/14/14	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	302	MBO	CE3-CE2	2.35	1.40	1.35
2	K	301	MBO	CE3-CE2	2.32	1.40	1.35
2	M	302	MBO	CE3-CE2	2.32	1.40	1.35
2	O	301	MBO	CE3-CE2	2.31	1.40	1.35
2	C	301	MBO	CE3-CE2	2.26	1.40	1.35

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	MBO	CE5-CE6-CE1	-3.99	118.33	121.79
2	K	301	MBO	CE5-CE6-CE1	-3.66	118.62	121.79
2	D	301	MBO	CE5-CE6-CE1	-3.65	118.62	121.79
2	I	302	MBO	CE5-CE6-CE1	-3.46	118.79	121.79
2	B	301	MBO	CE5-CE6-CE1	-3.41	118.84	121.79

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MBO	CE3-CE4-CZ-OZ1
2	A	302	MBO	CE3-CE4-CZ-OZ1
2	A	302	MBO	CE3-CE4-CZ-OZ2
2	A	302	MBO	CE5-CE4-CZ-OZ1
2	A	302	MBO	CE5-CE4-CZ-OZ2

There are no ring outliers.

22 monomers are involved in 253 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	302	MBO	1	0
2	E	301	MBO	6	0

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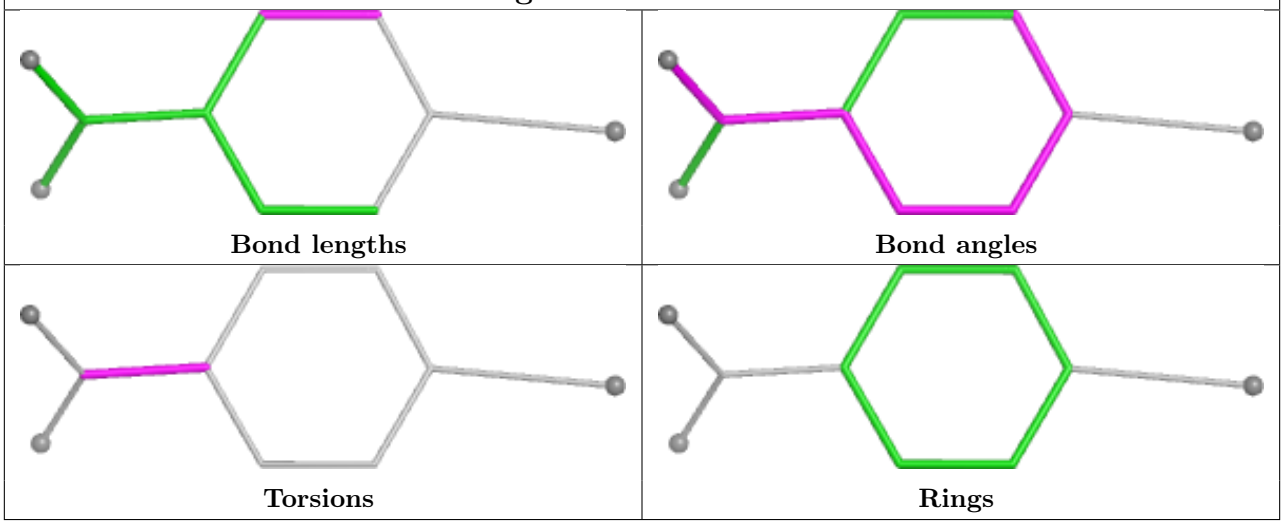
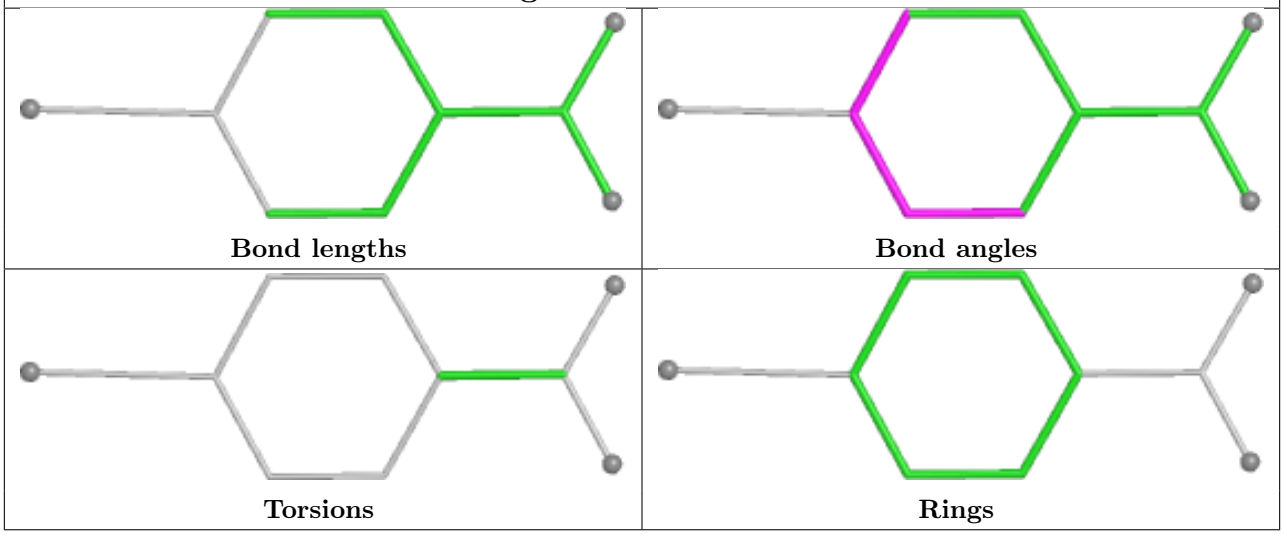
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	MBO	10	0
2	S	301	MBO	15	0
2	L	302	MBO	8	0
2	O	301	MBO	13	0
2	A	301	MBO	1	0
2	M	301	MBO	17	0
2	H	302	MBO	14	0
2	L	301	MBO	17	0
2	K	301	MBO	16	0
2	F	302	MBO	19	0
2	I	302	MBO	6	0
2	R	301	MBO	7	0
2	B	302	MBO	3	0
2	H	301	MBO	15	0
2	P	302	MBO	20	0
2	A	302	MBO	8	0
2	D	301	MBO	17	0
2	B	301	MBO	13	0
2	G	301	MBO	13	0
2	K	302	MBO	14	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.

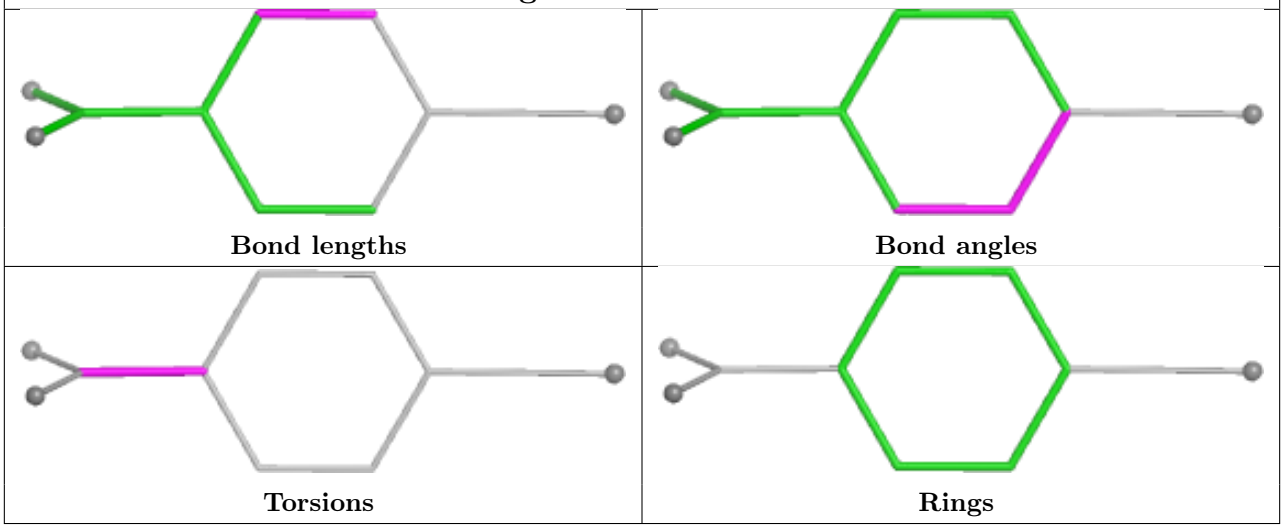
Ligand MBO M 302



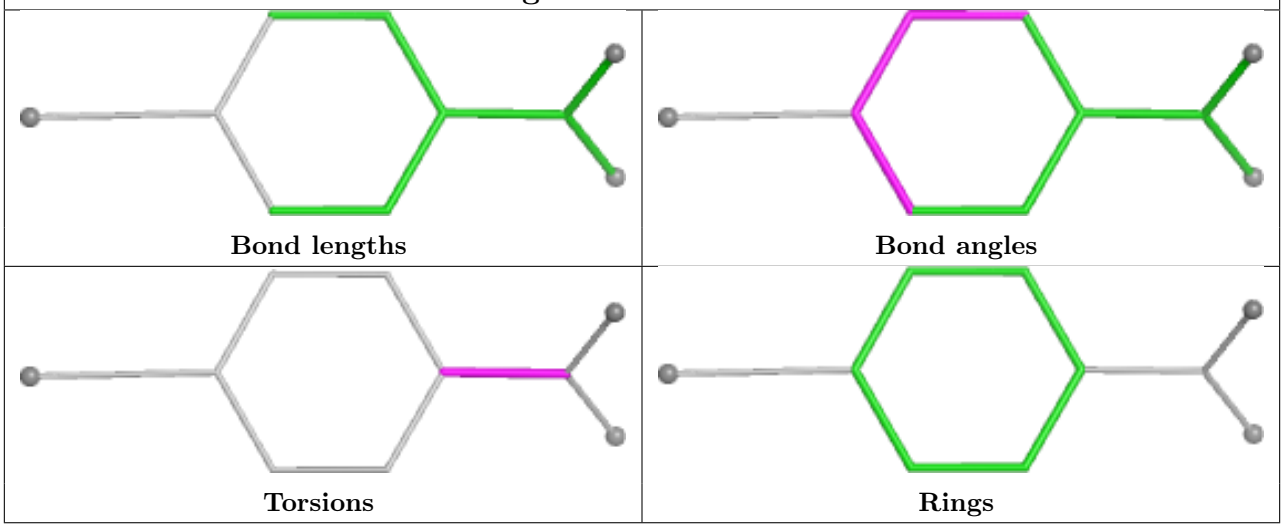
Ligand MBO E 301



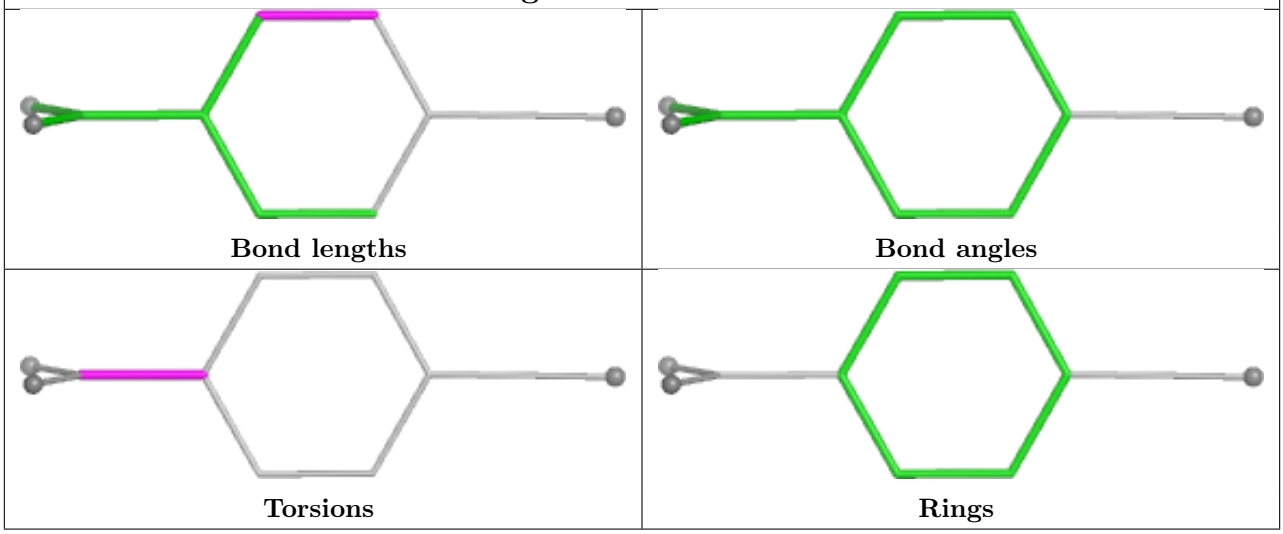
Ligand MBO C 301



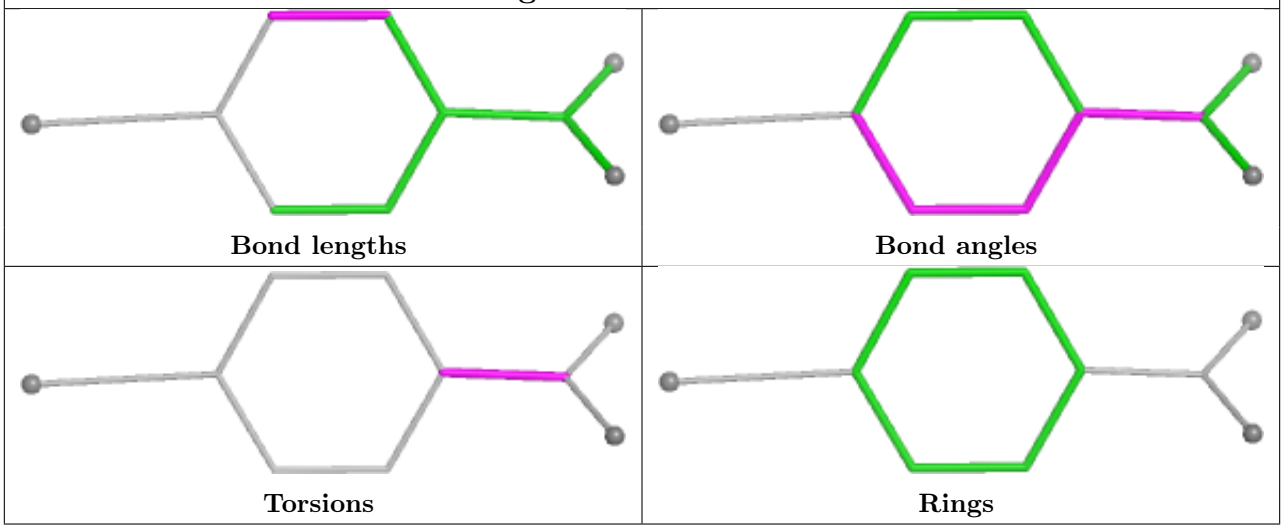
Ligand MBO S 301



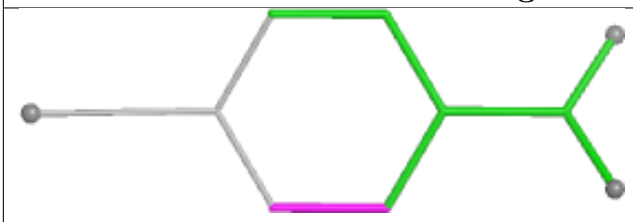
Ligand MBO L 302



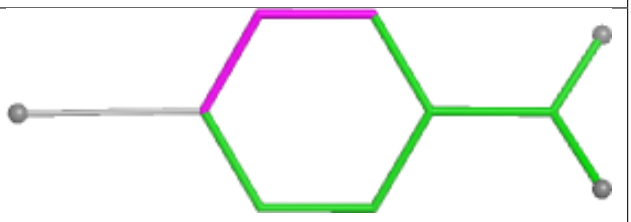
Ligand MBO O 301



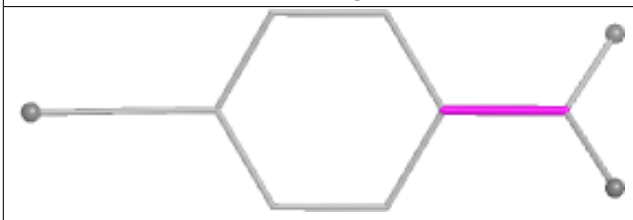
Ligand MBO A 301



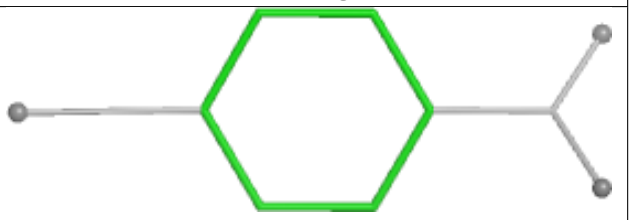
Bond lengths



Bond angles

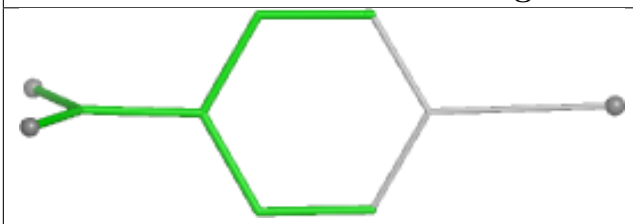


Torsions

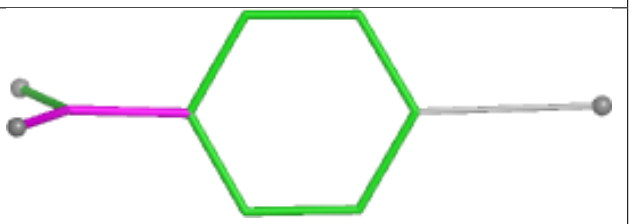


Rings

Ligand MBO M 301



Bond lengths



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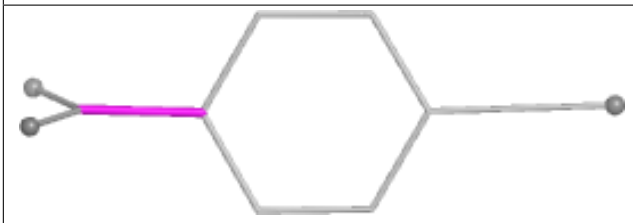

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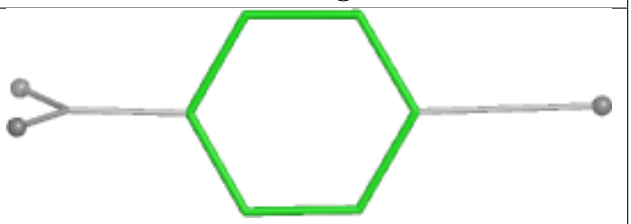
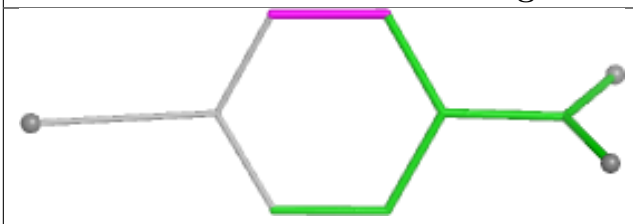


Rings

Ligand MBO H 302



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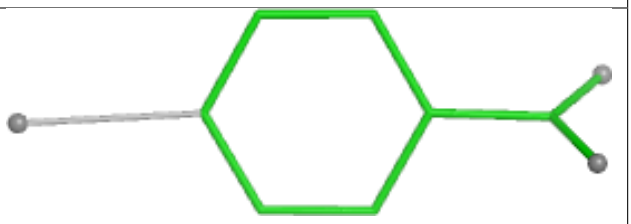
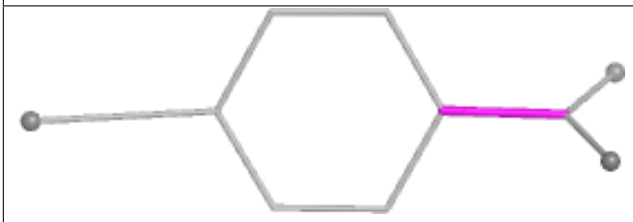


Bond angles



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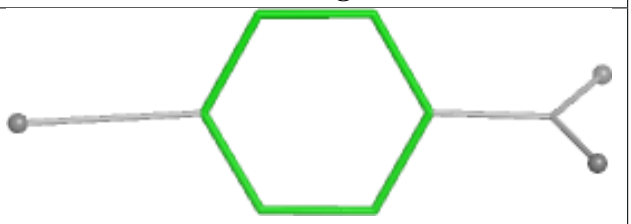
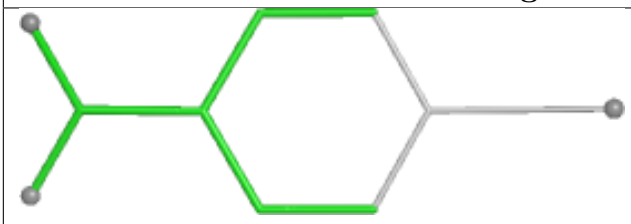


Rings

Ligand MBO L 301



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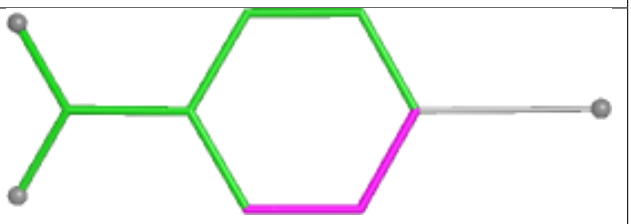

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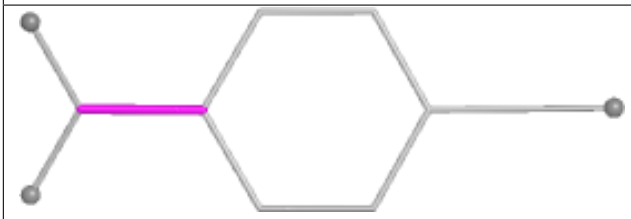

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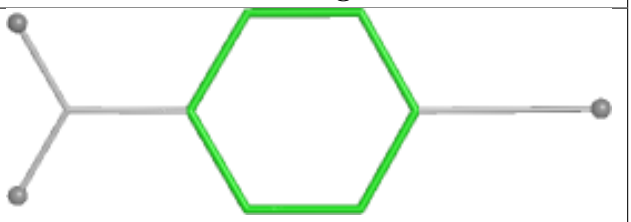

Rings

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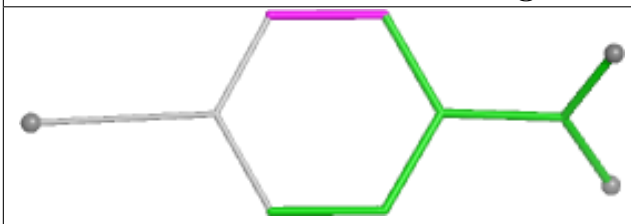

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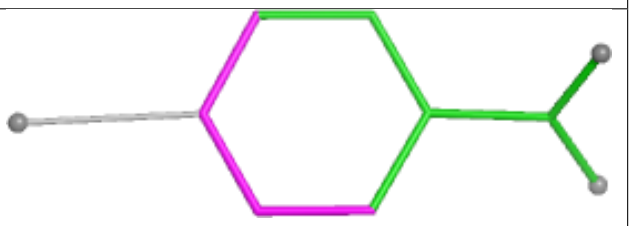

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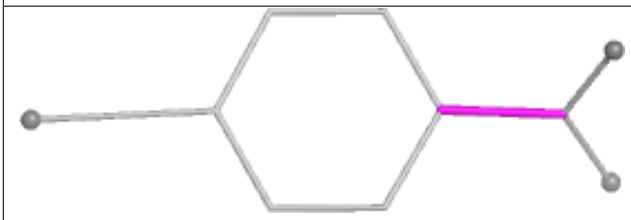

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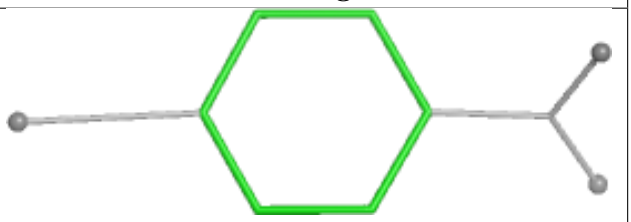
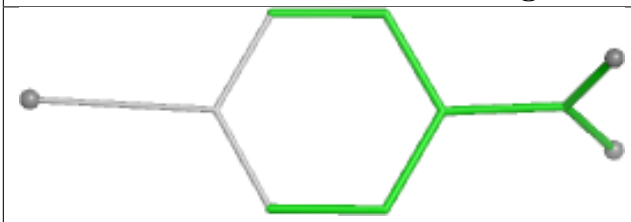


Rings

Ligand MBO F 302



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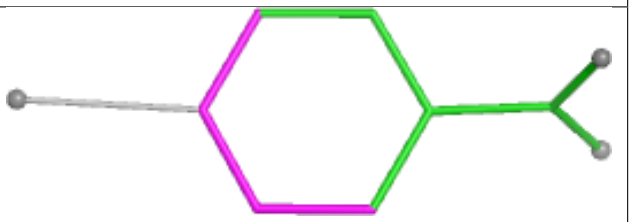
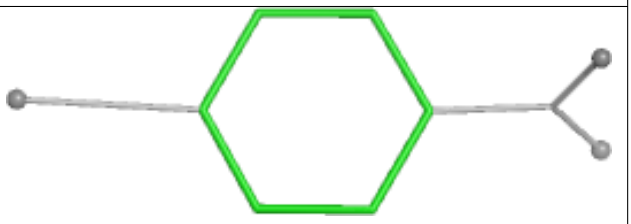


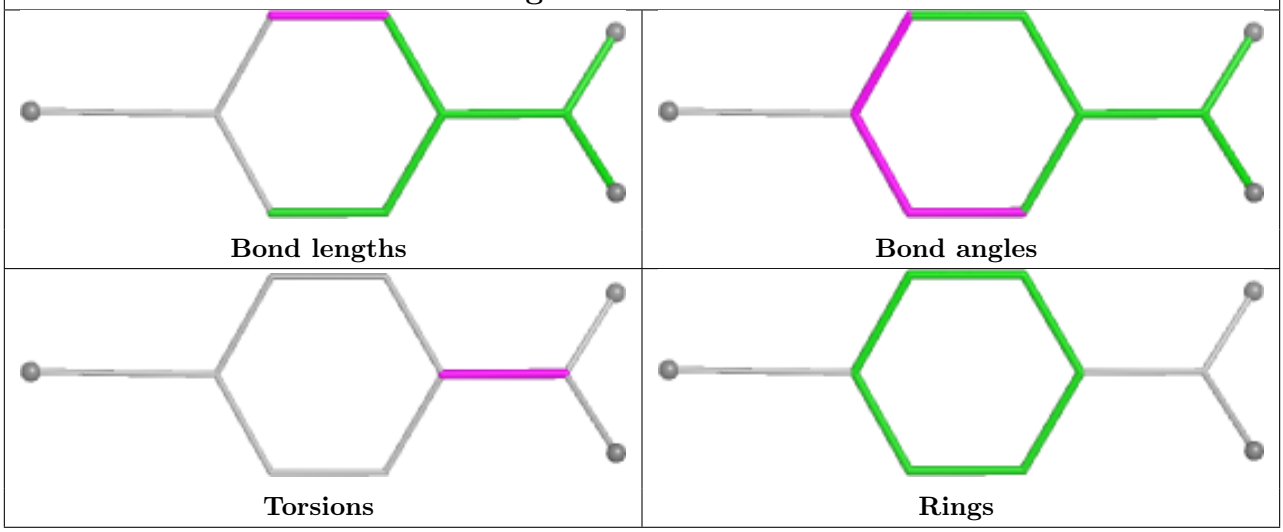
Bond angles

Torsions

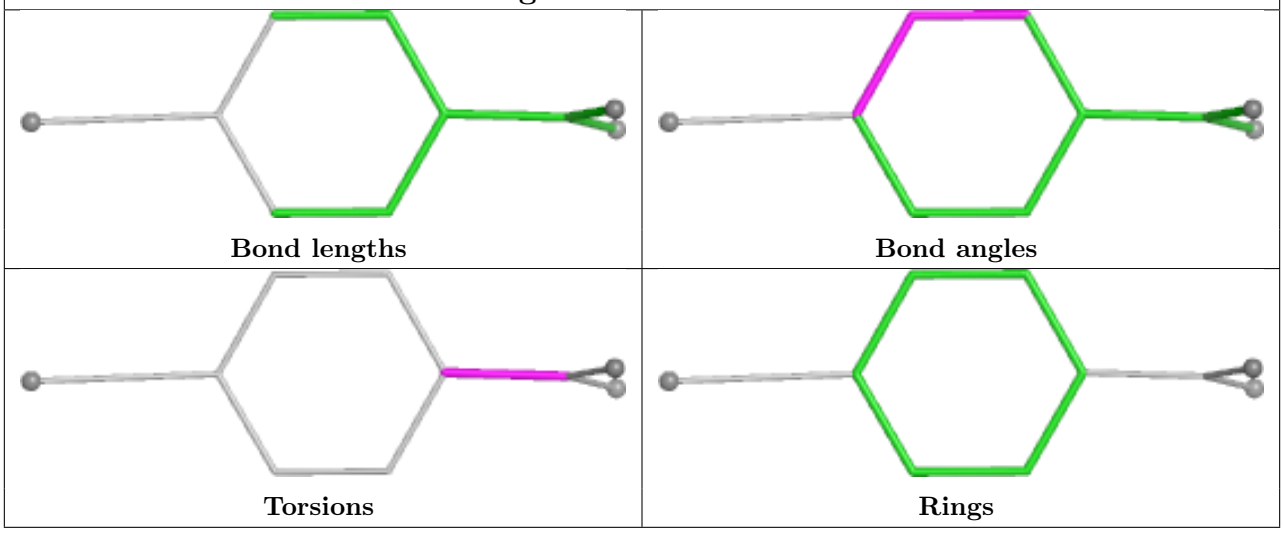


Rings

Ligand MBO I 302



Ligand MBO R 301



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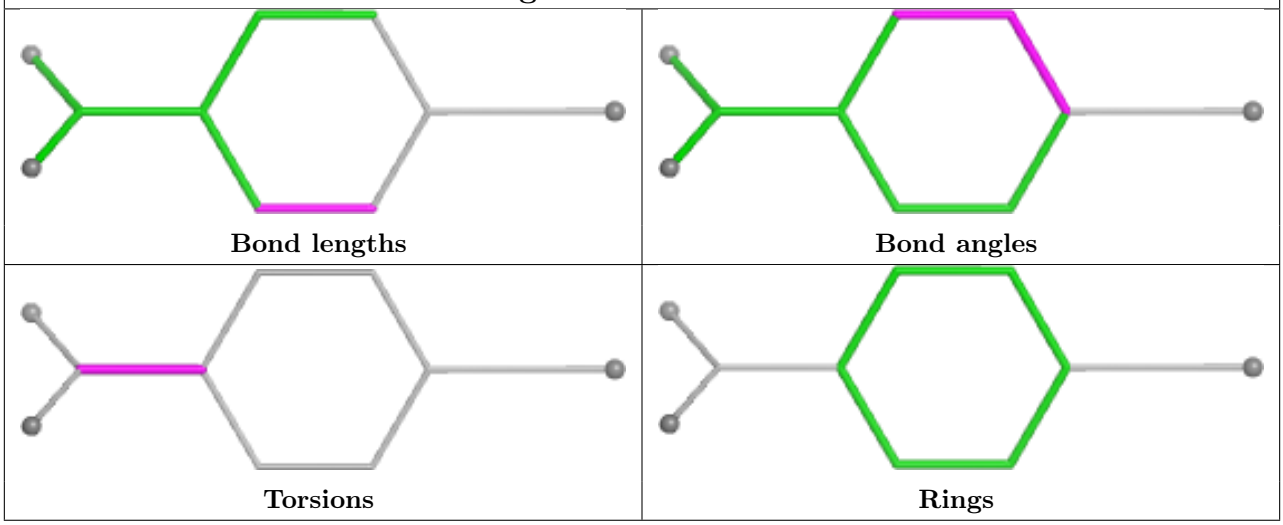

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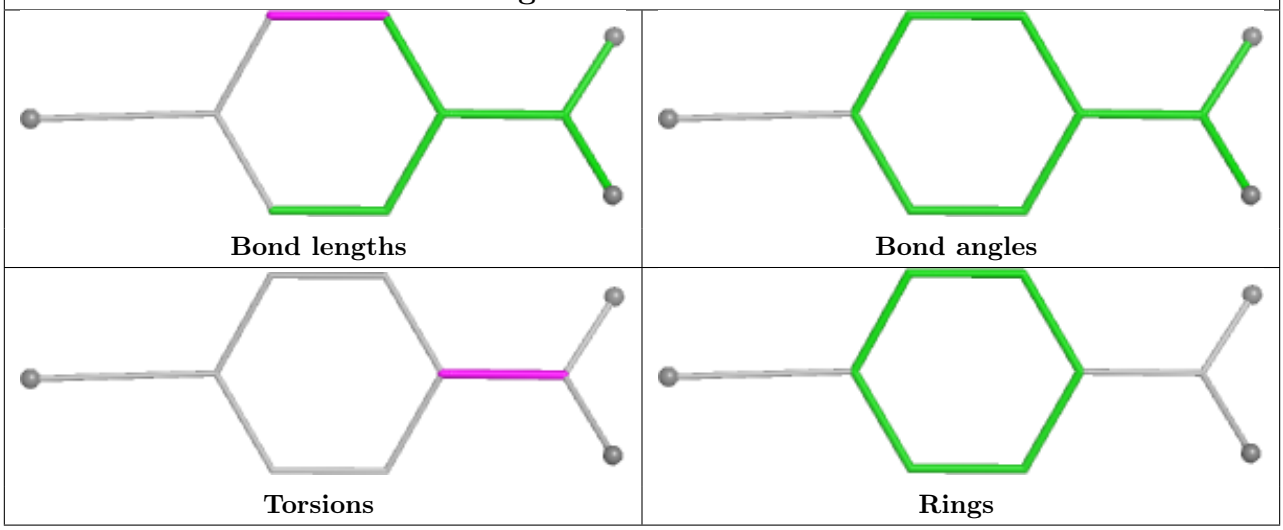

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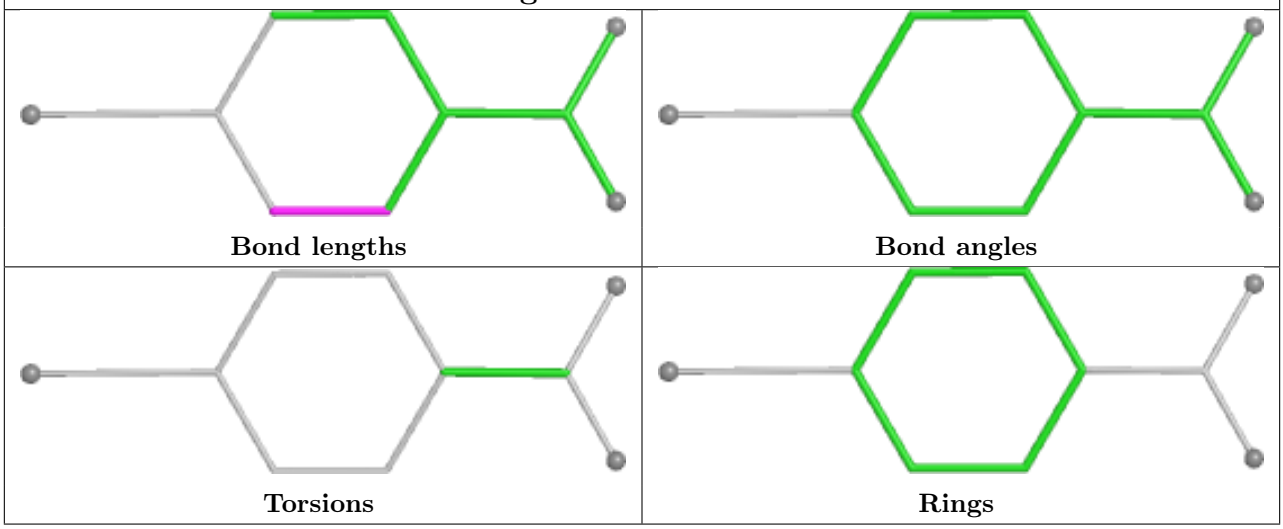

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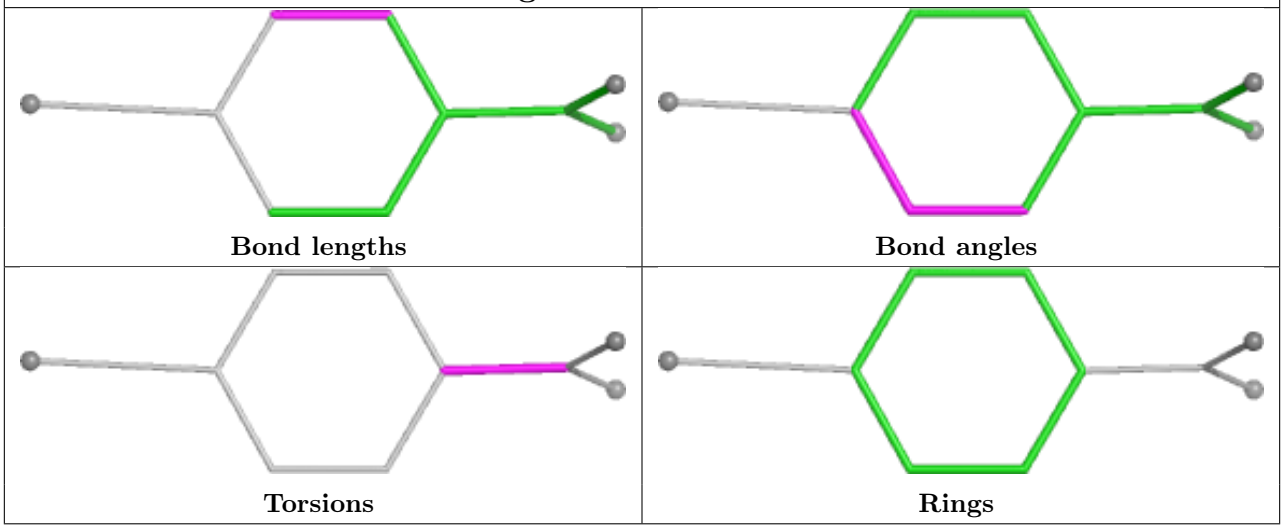

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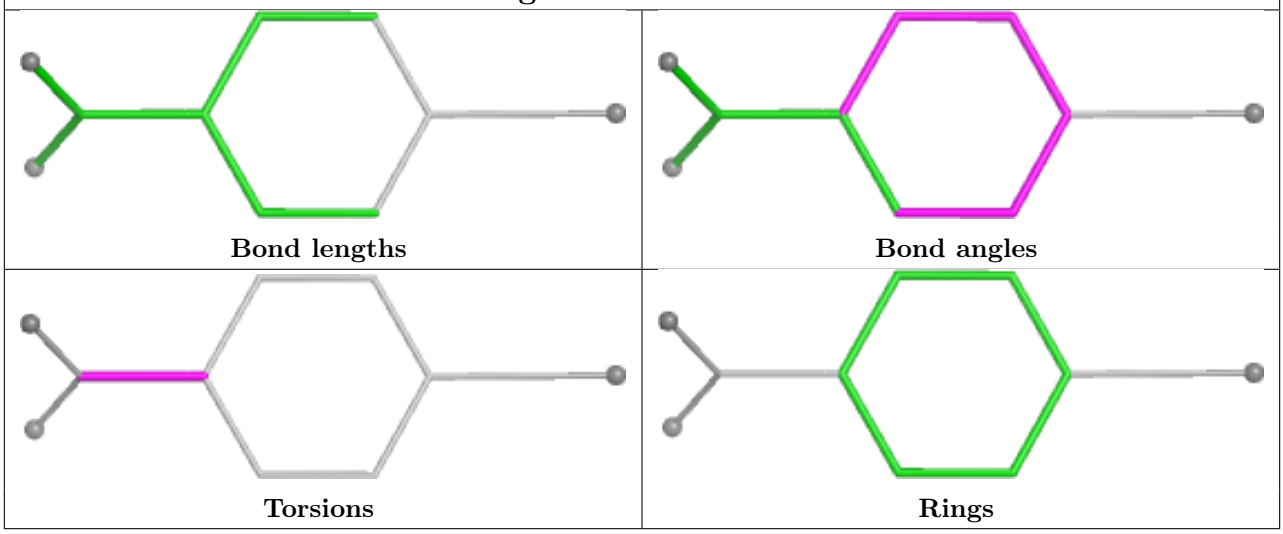

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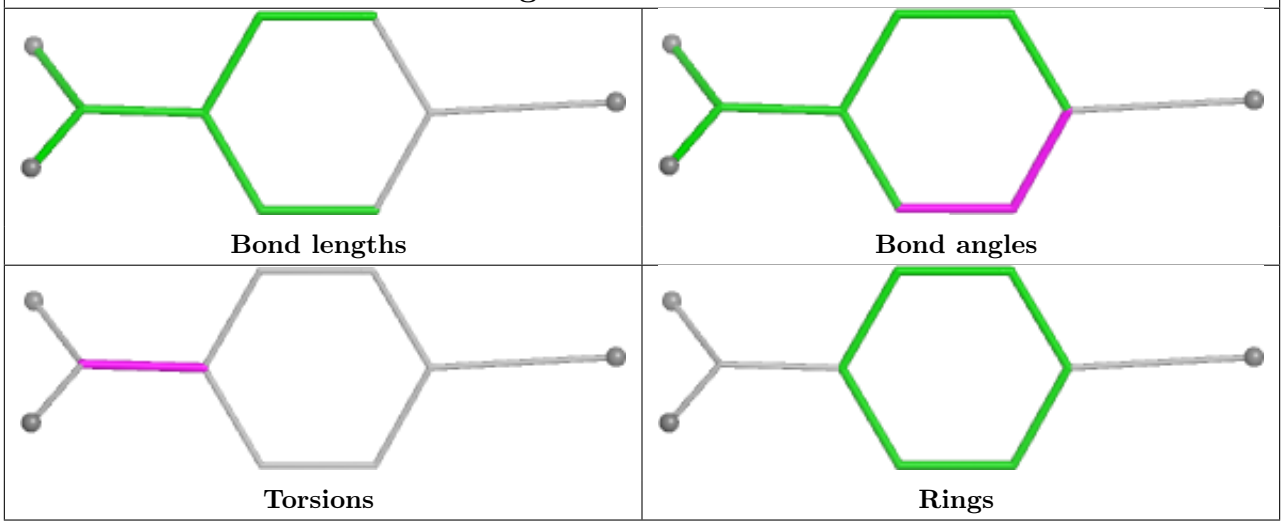
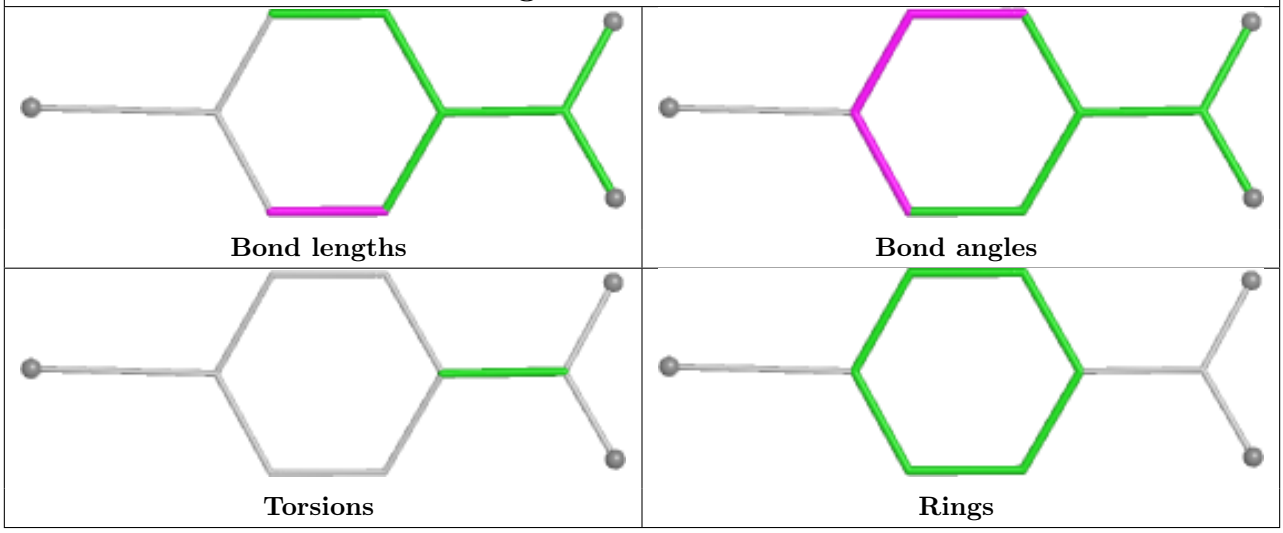
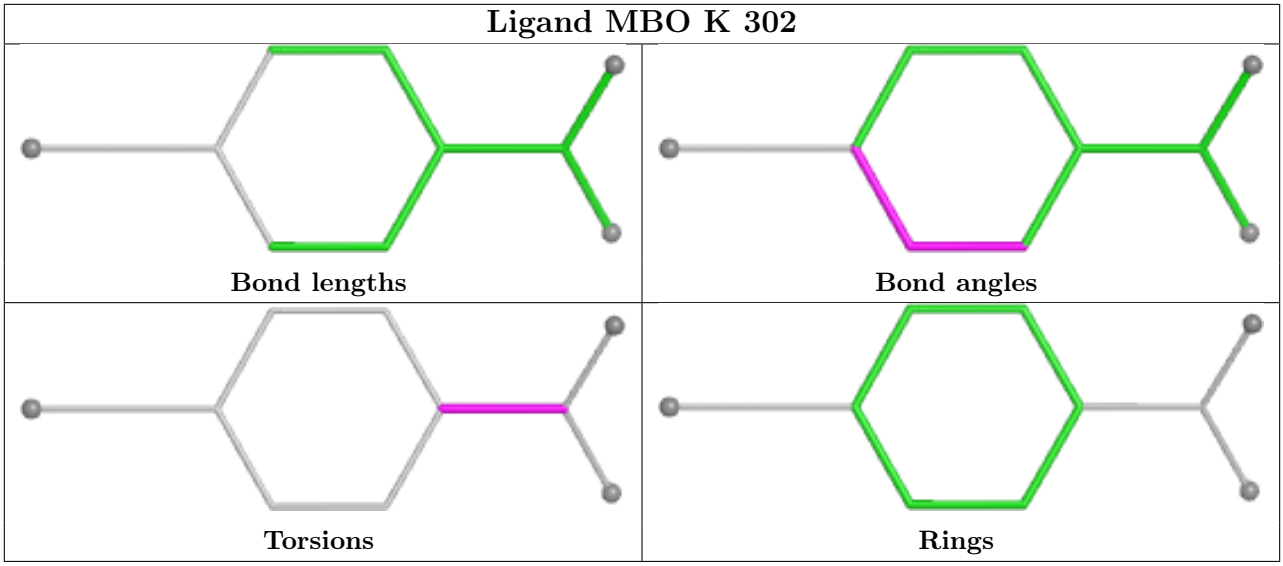


Ligand MBO G 301





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	290/298 (97%)	0.08	13 (4%)	38	20	28, 53, 90, 141	0
1	B	284/298 (95%)	0.10	7 (2%)	58	37	26, 59, 86, 126	0
1	C	286/298 (95%)	0.33	17 (5%)	28	15	31, 62, 94, 134	0
1	D	285/298 (95%)	0.16	7 (2%)	58	37	32, 55, 86, 132	0
1	E	283/298 (94%)	0.06	16 (5%)	29	16	28, 49, 81, 111	0
1	F	283/298 (94%)	0.12	15 (5%)	32	17	28, 47, 90, 124	0
1	G	290/298 (97%)	0.10	12 (4%)	41	23	26, 45, 97, 145	0
1	H	283/298 (94%)	0.04	7 (2%)	58	37	28, 46, 87, 112	0
1	I	282/298 (94%)	-0.05	4 (1%)	73	53	27, 48, 82, 111	0
1	J	290/298 (97%)	0.24	15 (5%)	33	17	29, 56, 96, 141	0
1	K	290/298 (97%)	0.20	14 (4%)	35	19	29, 51, 100, 155	0
1	L	284/298 (95%)	0.02	10 (3%)	47	27	28, 48, 87, 114	0
1	M	289/298 (96%)	0.13	9 (3%)	51	30	28, 53, 91, 145	0
1	N	289/298 (96%)	0.28	13 (4%)	38	20	26, 61, 96, 161	0
1	O	289/298 (96%)	0.40	21 (7%)	21	11	32, 62, 103, 155	0
1	P	289/298 (96%)	0.39	15 (5%)	33	17	30, 63, 100, 151	0
1	R	283/298 (94%)	0.32	11 (3%)	43	24	30, 61, 86, 115	0
1	S	283/298 (94%)	0.20	11 (3%)	43	24	28, 59, 89, 121	0
All	All	5152/5364 (96%)	0.17	217 (4%)	40	22	26, 54, 92, 161	0

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	74	SER	5.7
1	O	72	ILE	5.5
1	F	75	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	66	THR	5.2
1	N	72	ILE	5.0

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 oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HG	O	302	1/1	0.98	0.04	88,88,88,88	0
2	MBO	H	302	10/10	0.99	0.09	55,71,77,78	0
2	MBO	K	301	10/10	0.99	0.08	63,80,84,86	0
2	MBO	M	302	10/10	0.99	0.10	68,75,82,83	0
2	MBO	O	301	10/10	0.99	0.08	78,86,97,98	0
2	MBO	P	302	10/10	0.99	0.07	83,95,99,99	0
2	MBO	R	301	10/10	0.99	0.07	79,104,113,119	0
3	HG	C	302	1/1	0.99	0.04	80,80,80,80	0
3	HG	E	302	1/1	0.99	0.03	66,66,66,66	0
3	HG	G	302	1/1	0.99	0.02	58,58,58,58	0
3	HG	I	301	1/1	0.99	0.05	67,67,67,67	0
3	HG	J	301	1/1	0.99	0.03	66,66,66,66	0
3	HG	J	302	1/1	0.99	0.03	79,79,79,79	0
3	HG	N	301	1/1	0.99	0.03	70,70,70,70	0
3	HG	N	302	1/1	0.99	0.04	78,78,78,78	0
2	MBO	C	301	10/10	0.99	0.06	80,96,100,101	0
3	HG	P	301	1/1	0.99	0.03	81,81,81,81	0
3	HG	R	302	1/1	0.99	0.03	83,83,83,83	0
3	HG	S	302	1/1	0.99	0.02	77,77,77,77	0
2	MBO	D	301	10/10	1.00	0.06	61,75,86,93	0
2	MBO	E	301	10/10	1.00	0.05	50,58,66,68	0

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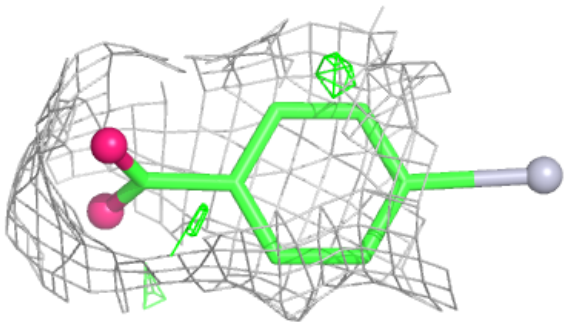
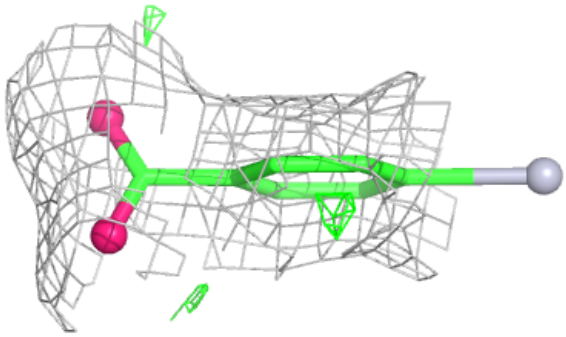
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MBO	S	301	10/10	1.00	0.05	74,84,89,93	0
2	MBO	F	302	10/10	1.00	0.07	45,70,86,92	0
3	HG	D	302	1/1	1.00	0.03	73,73,73,73	0
2	MBO	G	301	10/10	1.00	0.06	52,75,79,82	0
3	HG	F	301	1/1	1.00	0.03	60,60,60,60	0
2	MBO	H	301	10/10	1.00	0.06	62,76,90,90	0
2	MBO	A	302	10/10	1.00	0.07	68,80,85,87	0
2	MBO	I	302	10/10	1.00	0.06	56,67,80,81	0
2	MBO	B	301	10/10	1.00	0.07	79,97,103,105	0
2	MBO	K	302	10/10	1.00	0.07	72,82,90,93	0
2	MBO	L	301	10/10	1.00	0.05	54,71,77,79	0
2	MBO	L	302	10/10	1.00	0.06	65,86,96,100	0
2	MBO	M	301	10/10	1.00	0.07	63,81,100,100	0
2	MBO	B	302	10/10	1.00	0.07	76,103,112,112	0
2	MBO	A	301	10/10	1.00	0.06	61,73,77,79	0

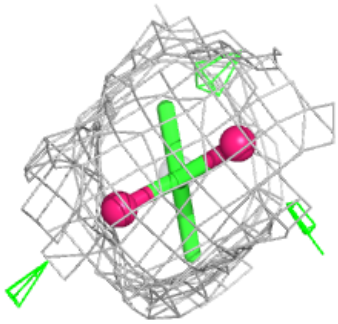
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MBO 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)

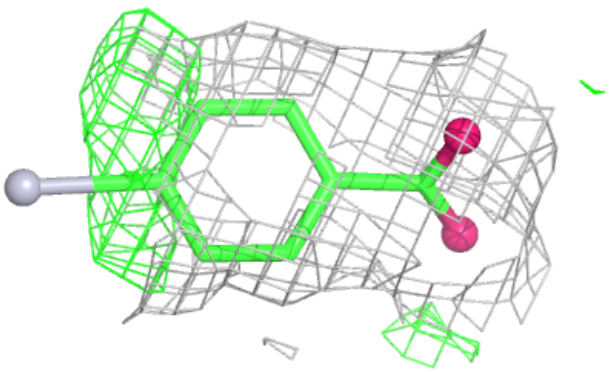


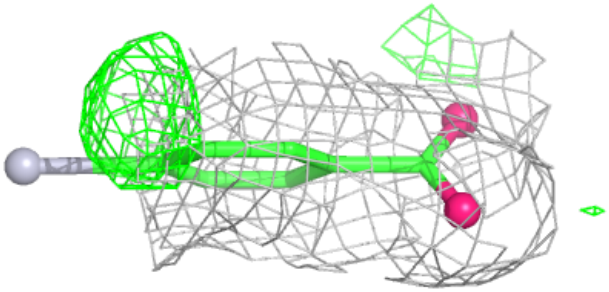


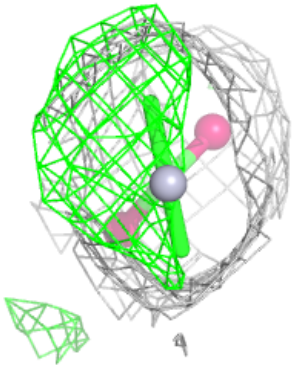


Electron density around MBO K 301:

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







Electron density around MBO M 302:

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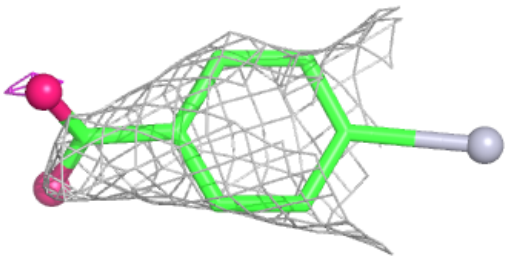
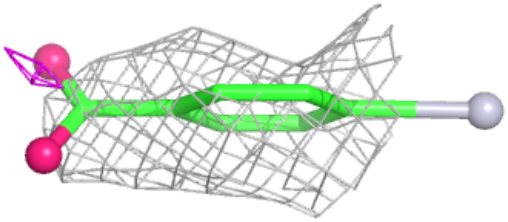
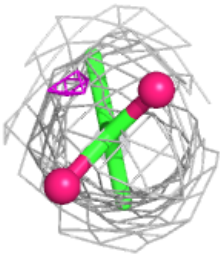
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

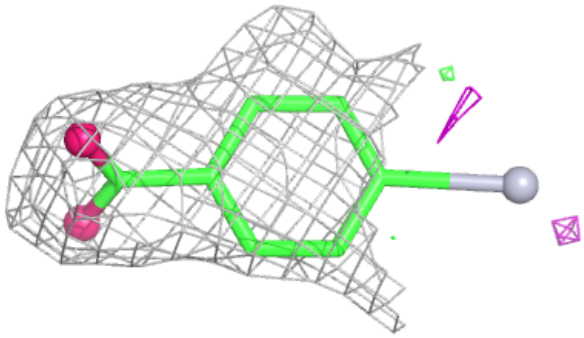


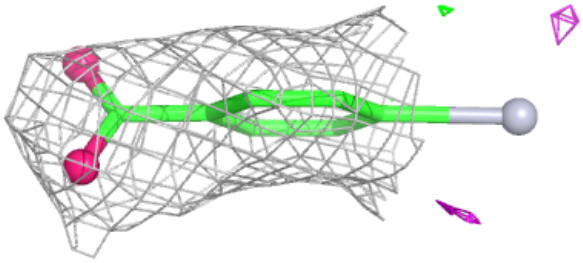


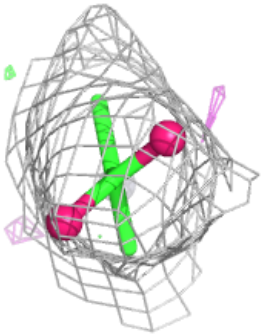


Electron density around MBO O 301:

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







Electron density around MBO P 302:

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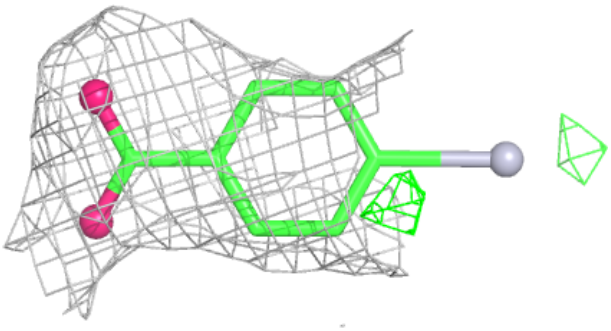
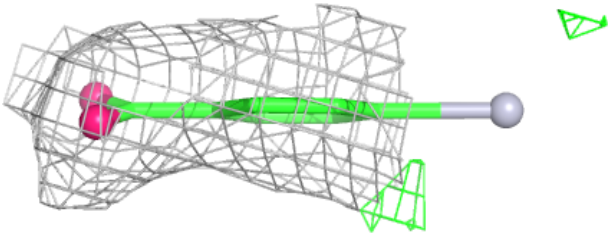
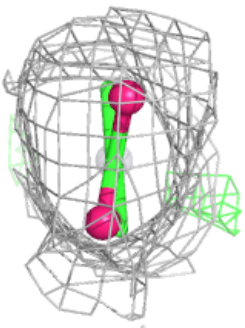
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

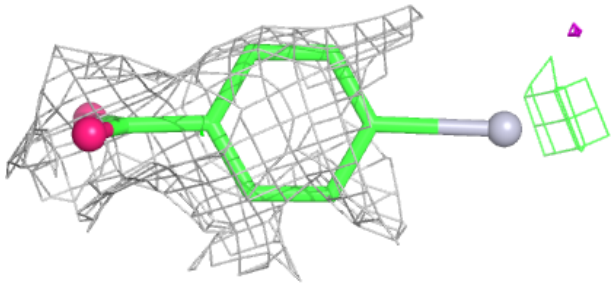


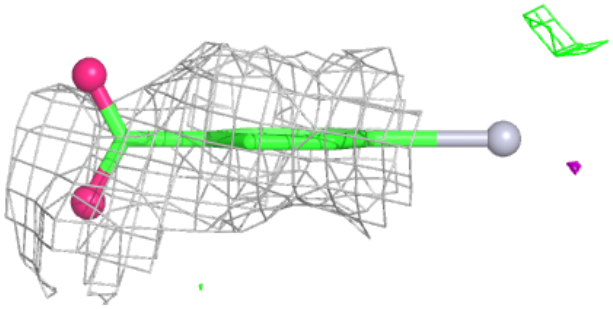


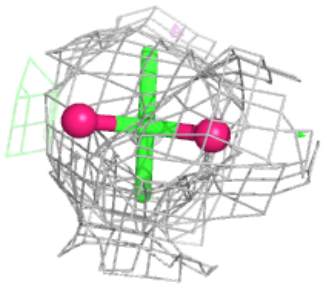


Electron density around MBO R 301:

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

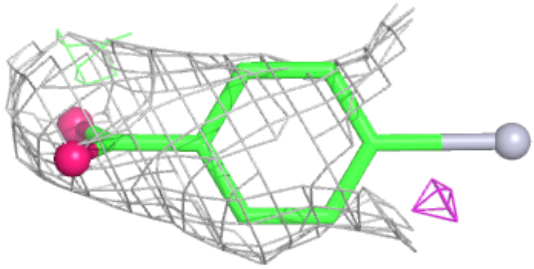


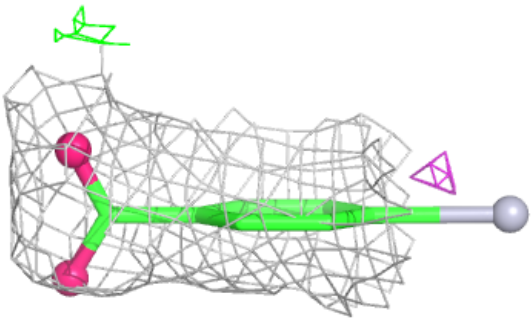


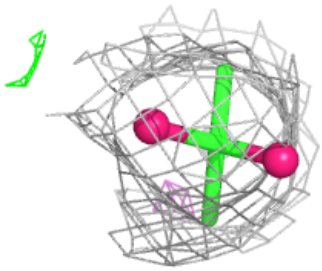


Electron density around MBO C 301:

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







Electron density around MBO D 301:

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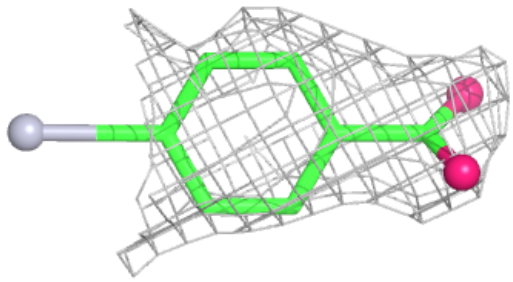
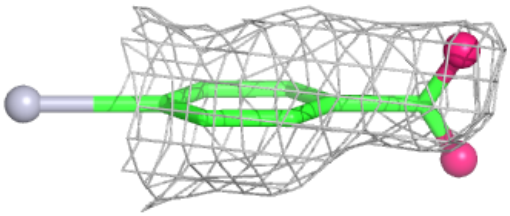
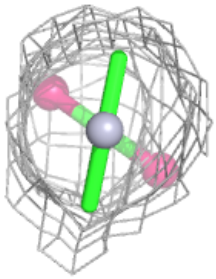
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around MBO E 301:

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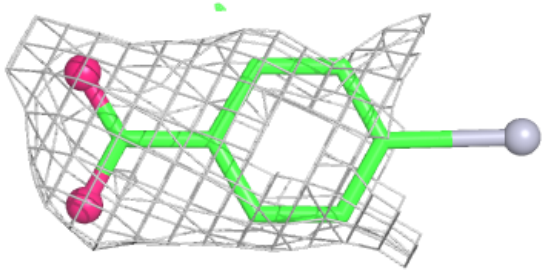
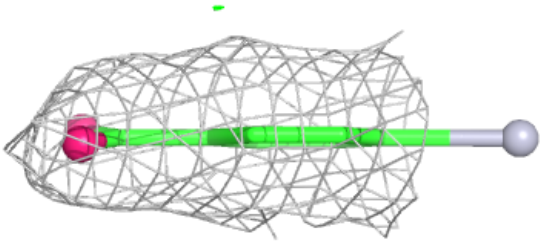
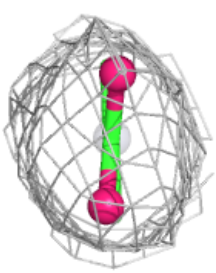
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

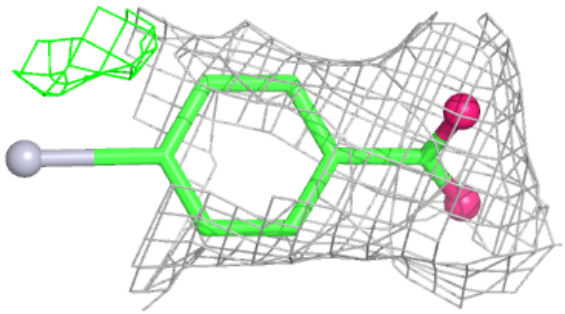


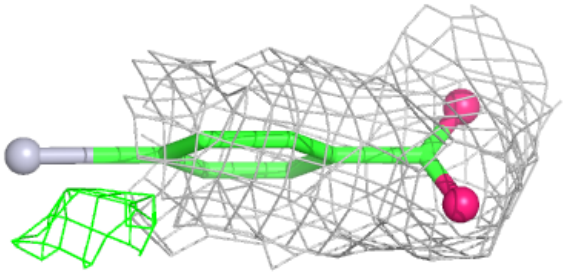


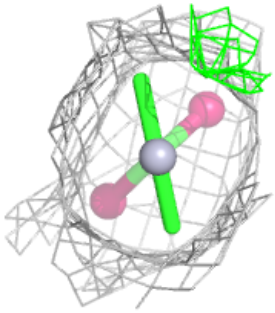


Electron density around MBO S 301:

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

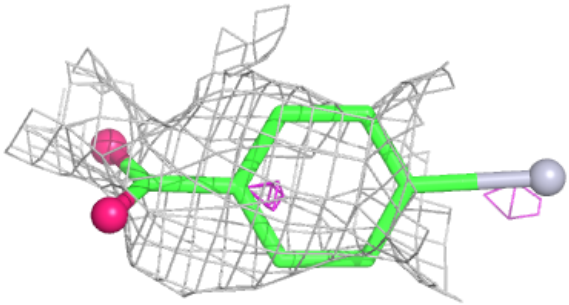


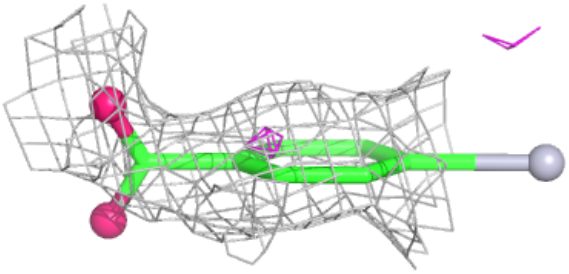


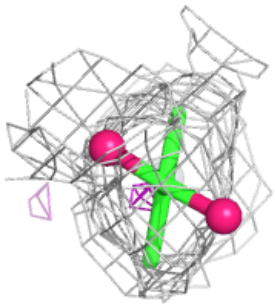


Electron density around MBO F 302:

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







Electron density around MBO G 301:

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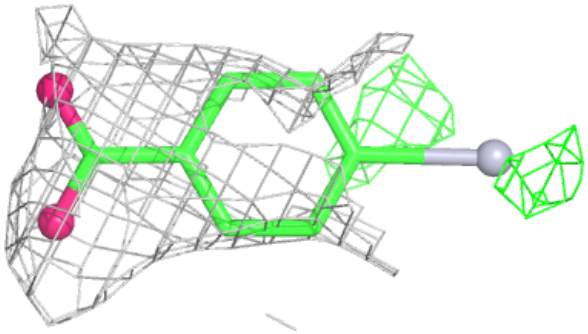
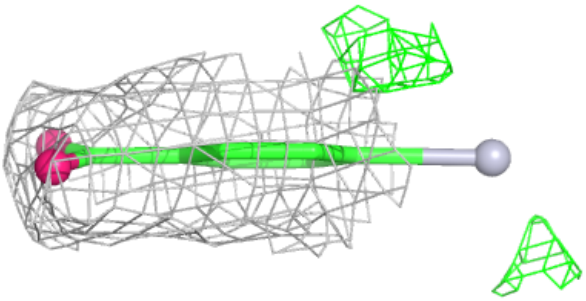
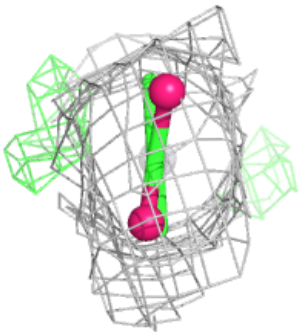
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around MBO H 301:

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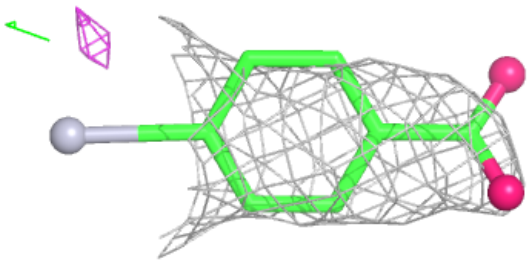
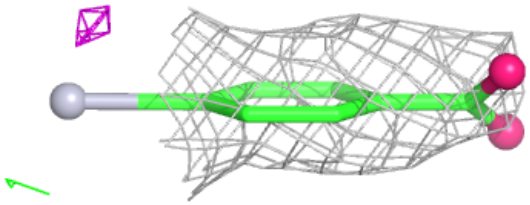
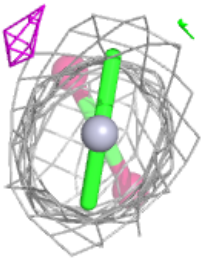
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around MBO A 302:

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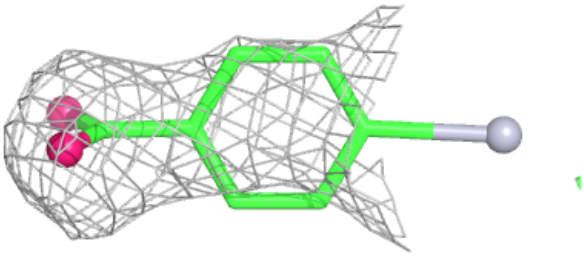
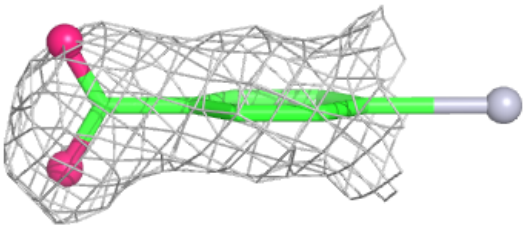
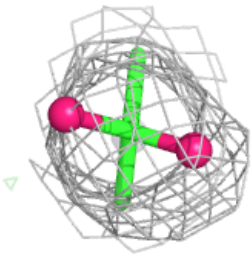
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

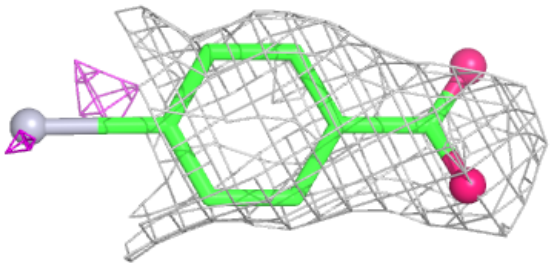


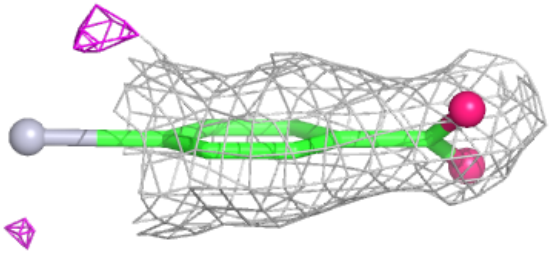


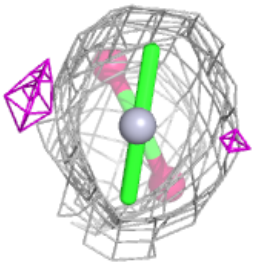


Electron density around MBO I 302:

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

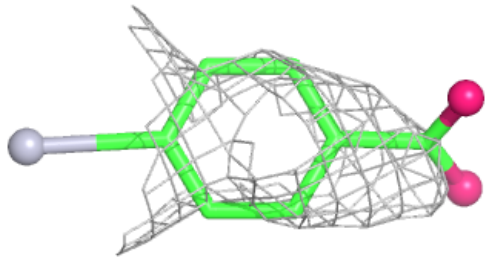


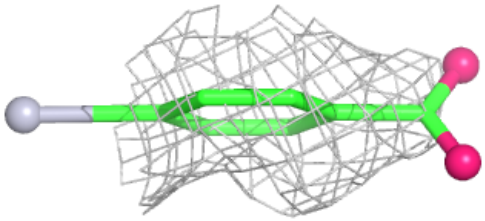


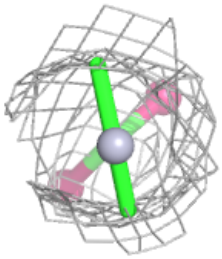


Electron density around MBO B 301:

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

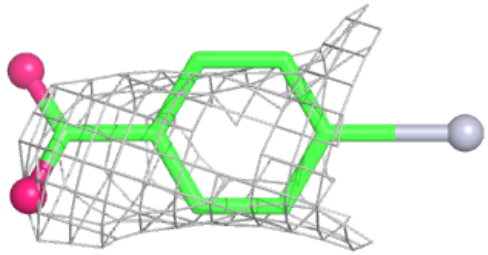


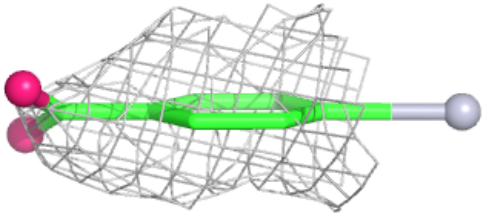


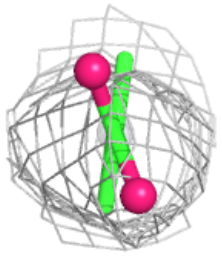


Electron density around MBO K 302:

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

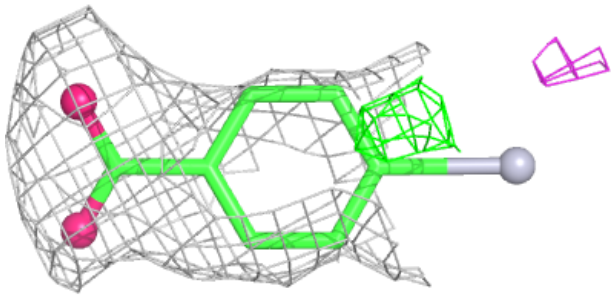


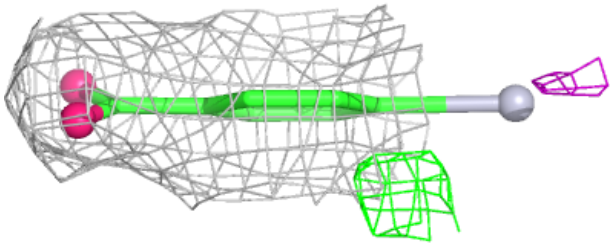


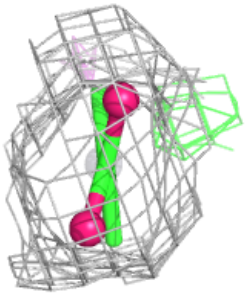


Electron density around MBO L 301:

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

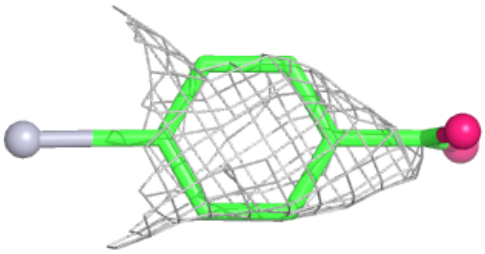


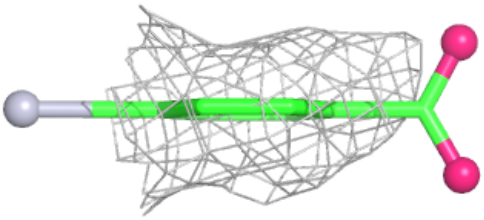


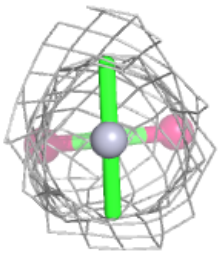


Electron density around MBO L 302:

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

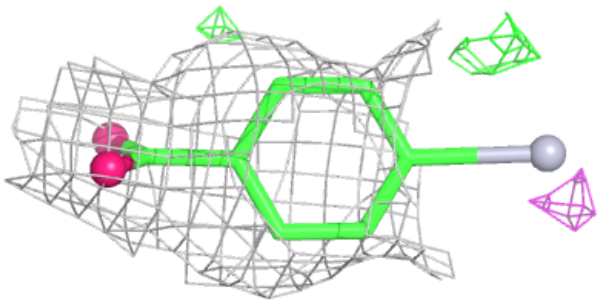


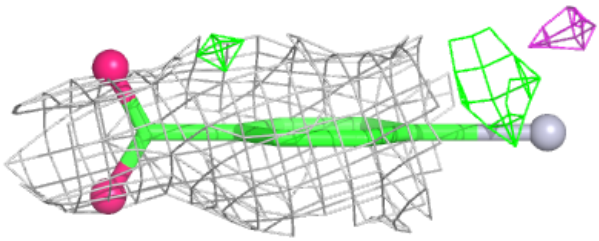


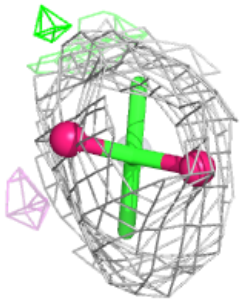


Electron density around MBO M 301:

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

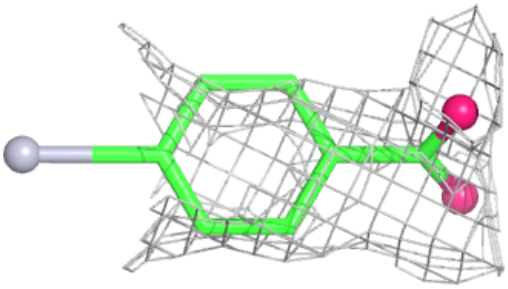


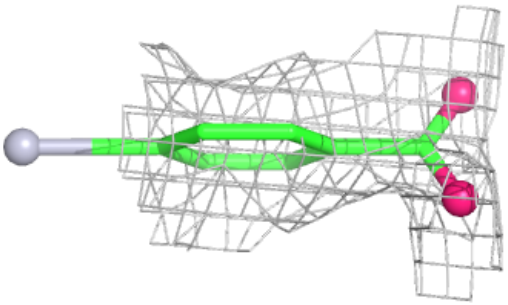


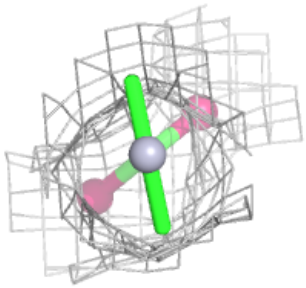


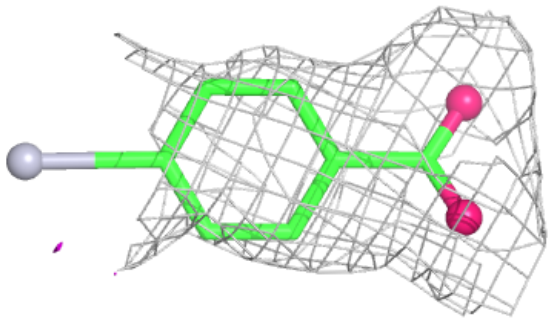
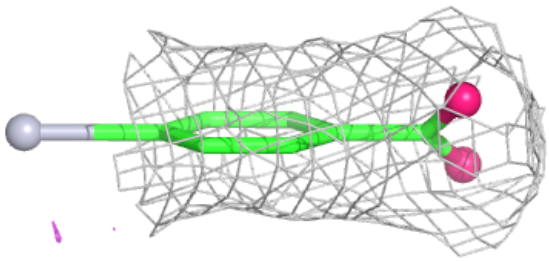
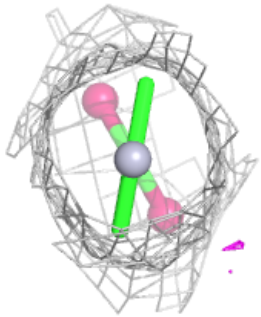
Electron density around MBO B 302:

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







Electron density around MBO 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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.