wwPDB X-ray Structure Validation Summary Report (i)

Feb 8, 2024 – 04:20 PM JST

PDB ID	:	8J6N
Title	:	Crystal structure of Cystathionine gamma-lyase in complex with compound 1
Authors	:	Hibi, R.; Toma-Fukai, S.; Shimizu, T.; Hanaoka, K.
Deposited on	:	2023-04-26
Resolution	:	1.90 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:

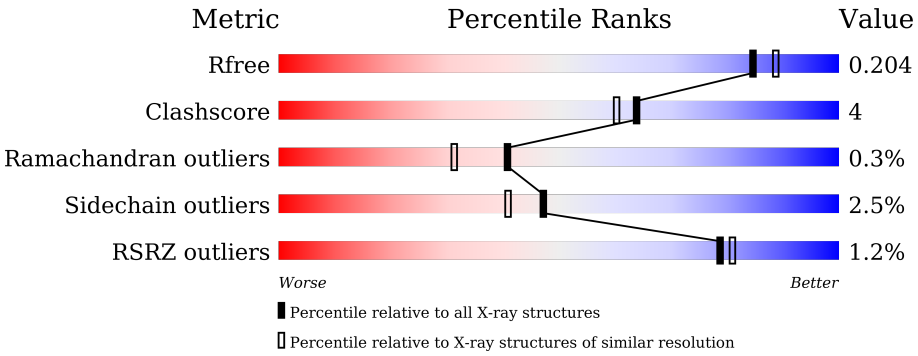
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	392	91% 8% •
1	B	392	90% 9% ••
1	C	392	88% 11% ••
1	D	392	89% 10% ••
1	E	392	90% 9% ••
1	F	392	89% 10% ••

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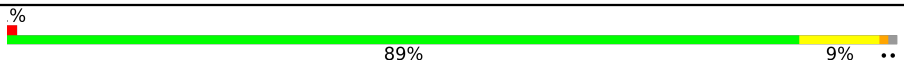
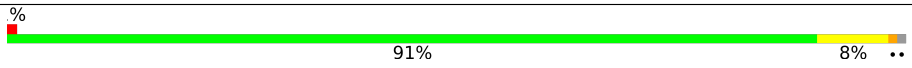
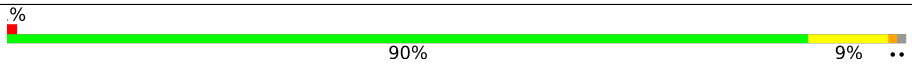
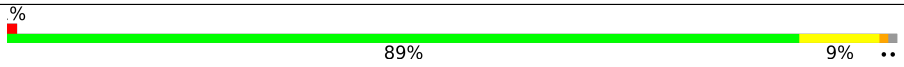
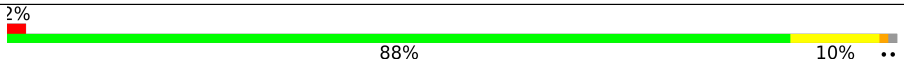
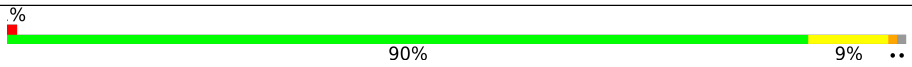
Mol	Chain	Length	Quality of chain
1	G	392	
1	H	392	
1	I	392	
1	J	392	
1	K	392	
1	L	392	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	J	403	-	-	X	-
4	EDO	J	405	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 39772 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 Cystathionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	6	0
			3024	1924	520	556	24			
1	B	390	Total	C	N	O	S	0	9	0
			3034	1932	520	557	25			
1	C	390	Total	C	N	O	S	0	10	0
			3049	1947	521	557	24			
1	D	390	Total	C	N	O	S	0	9	0
			3038	1937	520	557	24			
1	E	390	Total	C	N	O	S	0	7	0
			3027	1927	520	557	23			
1	H	390	Total	C	N	O	S	0	8	0
			3037	1935	523	556	23			
1	J	390	Total	C	N	O	S	0	10	0
			3043	1939	523	558	23			
1	K	390	Total	C	N	O	S	0	9	0
			3042	1940	523	556	23			
1	F	390	Total	C	N	O	S	0	8	0
			3031	1929	520	558	24			
1	G	389	Total	C	N	O	S	0	9	0
			3034	1932	522	557	23			
1	I	390	Total	C	N	O	S	0	9	0
			3040	1938	521	557	24			
1	L	390	Total	C	N	O	S	0	10	0
			3050	1947	521	559	23			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	expression tag	UNP Q9EQS4
A	9	PRO	-	expression tag	UNP Q9EQS4
B	8	GLY	-	expression tag	UNP Q9EQS4
B	9	PRO	-	expression tag	UNP Q9EQS4
C	8	GLY	-	expression tag	UNP Q9EQS4

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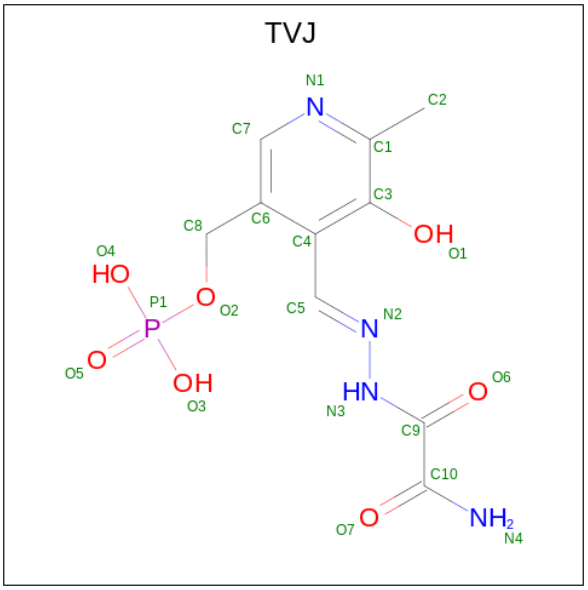
Chain	Residue	Modelled	Actual	Comment	Reference
C	9	PRO	-	expression tag	UNP Q9EQS4
D	8	GLY	-	expression tag	UNP Q9EQS4
D	9	PRO	-	expression tag	UNP Q9EQS4
E	8	GLY	-	expression tag	UNP Q9EQS4
E	9	PRO	-	expression tag	UNP Q9EQS4
H	8	GLY	-	expression tag	UNP Q9EQS4
H	9	PRO	-	expression tag	UNP Q9EQS4
J	8	GLY	-	expression tag	UNP Q9EQS4
J	9	PRO	-	expression tag	UNP Q9EQS4
K	8	GLY	-	expression tag	UNP Q9EQS4
K	9	PRO	-	expression tag	UNP Q9EQS4
F	8	GLY	-	expression tag	UNP Q9EQS4
F	9	PRO	-	expression tag	UNP Q9EQS4
G	8	GLY	-	expression tag	UNP Q9EQS4
G	9	PRO	-	expression tag	UNP Q9EQS4
I	8	GLY	-	expression tag	UNP Q9EQS4
I	9	PRO	-	expression tag	UNP Q9EQS4
L	8	GLY	-	expression tag	UNP Q9EQS4
L	9	PRO	-	expression tag	UNP Q9EQS4

- Molecule 2 is [6-methyl-4-[({E})-(oxamoylhydrazinylidene)methyl]-5-oxidanyl-pyridin-3-yl] methyl dihydrogen phosphate (three-letter code: TVJ) (formula: $C_{10}H_{13}N_4O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	4	7	1		

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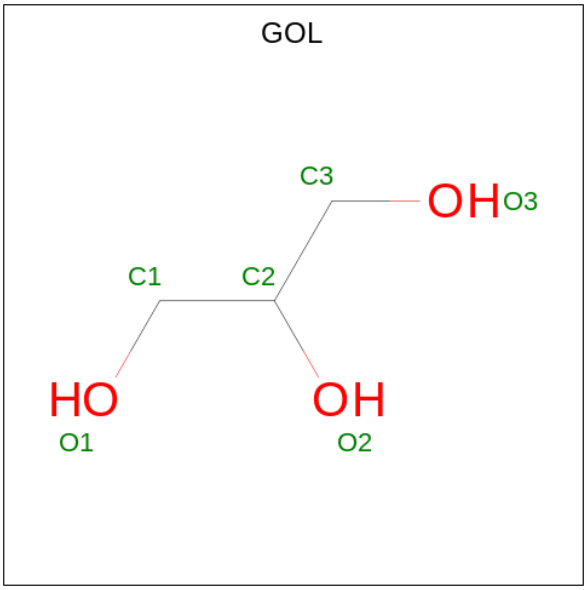
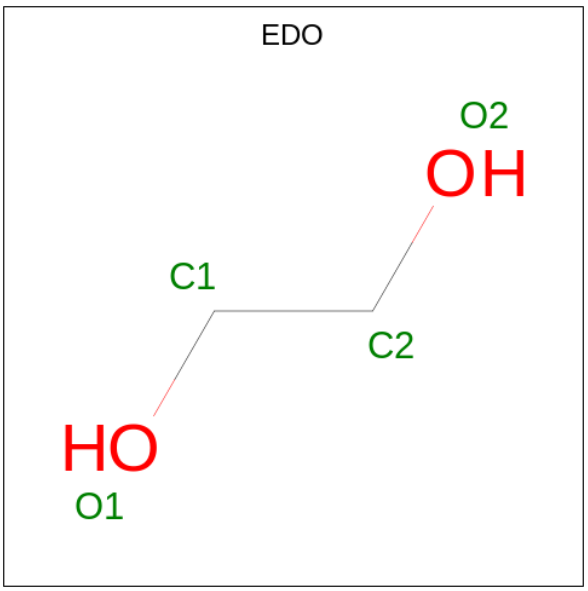
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	C	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	D	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	E	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	H	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	J	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	K	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	F	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	G	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	I	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	L	1	Total	C	N	O	P	0	0
			22	10	4	7	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	K	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

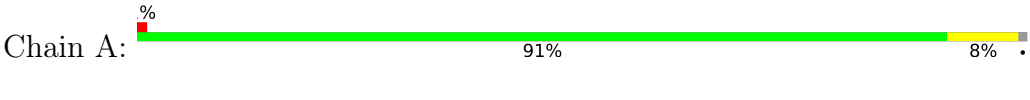
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	288	Total O 288 288	0	0
5	B	285	Total O 285 285	0	0
5	C	280	Total O 280 280	0	0
5	D	299	Total O 299 299	0	0
5	E	243	Total O 243 243	0	0
5	H	237	Total O 237 237	0	0
5	J	252	Total O 252 252	0	0
5	K	228	Total O 228 228	0	0
5	F	234	Total O 234 234	0	0
5	G	194	Total O 194 194	0	0
5	I	220	Total O 220 220	0	0
5	L	219	Total O 219 219	0	0

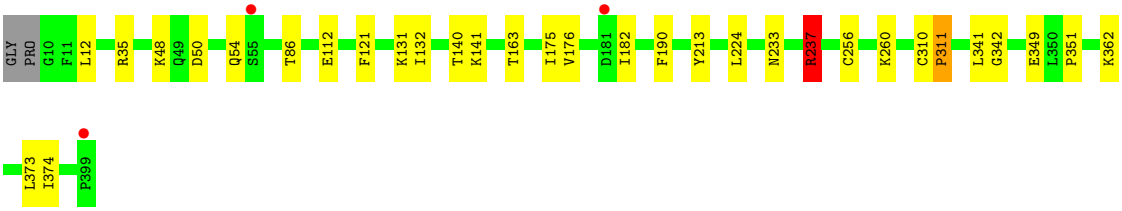
3 Residue-property plots (i)

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: Cystathionine gamma-lyase

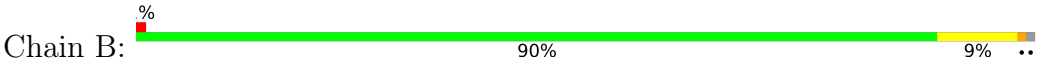
Chain A:

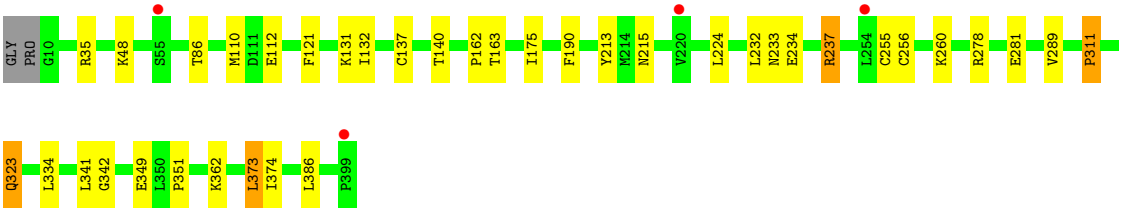




• Molecule 1: Cystathionine gamma-lyase

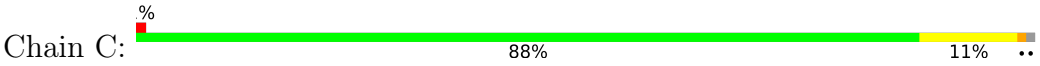
Chain B:

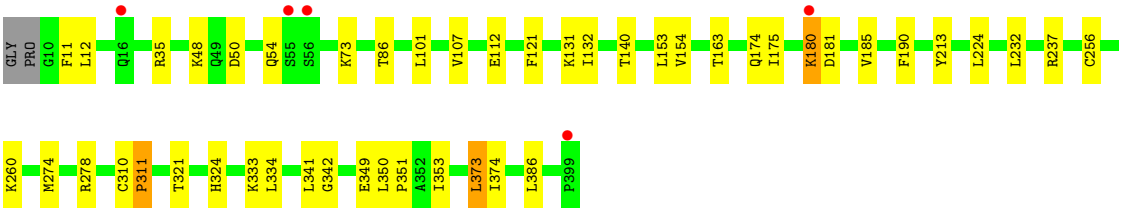




• Molecule 1: Cystathionine gamma-lyase

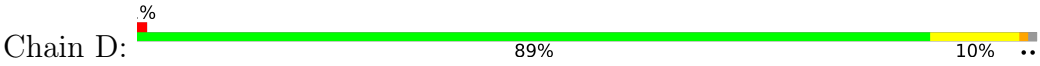
Chain C:

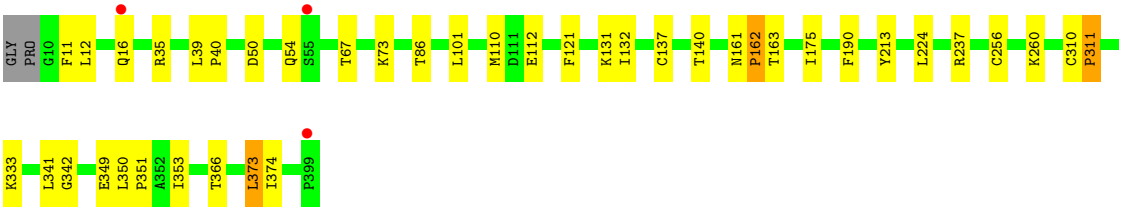




• Molecule 1: Cystathionine gamma-lyase

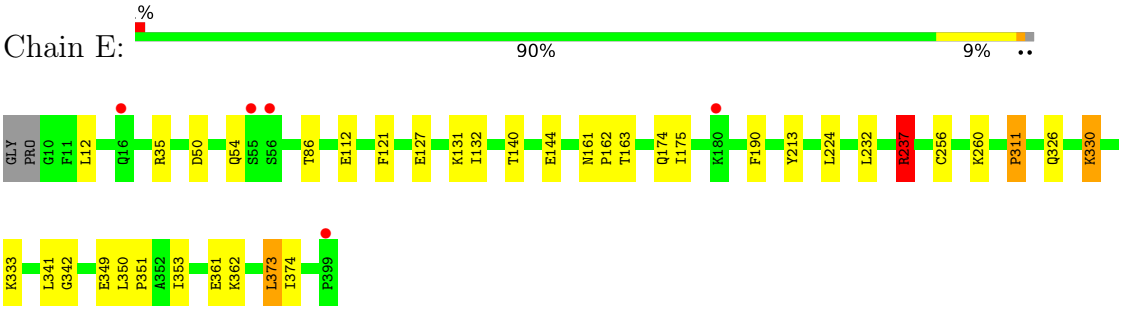
Chain D:





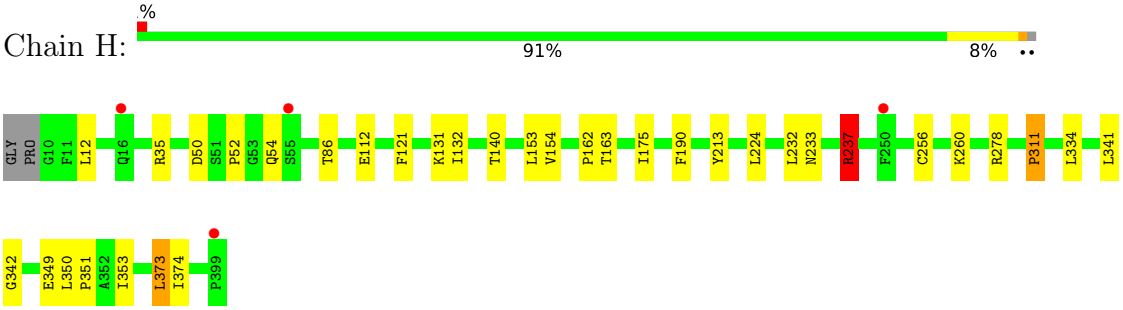
• Molecule 1: Cystathionine gamma-lyase

Chain E:



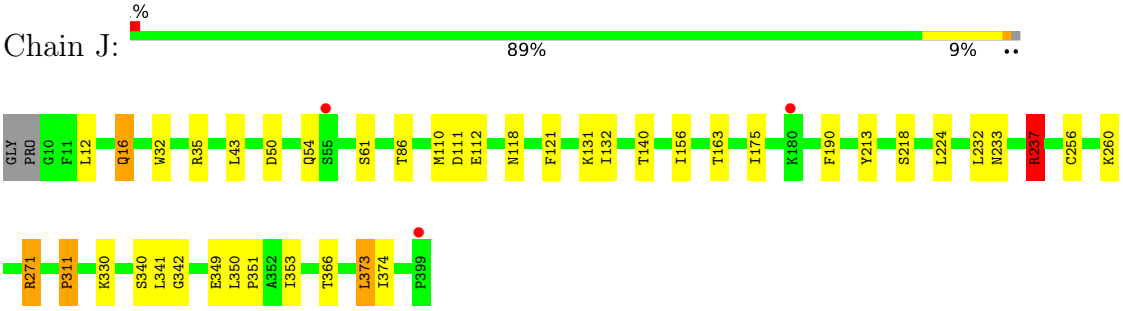
• Molecule 1: Cystathionine gamma-lyase

Chain H:



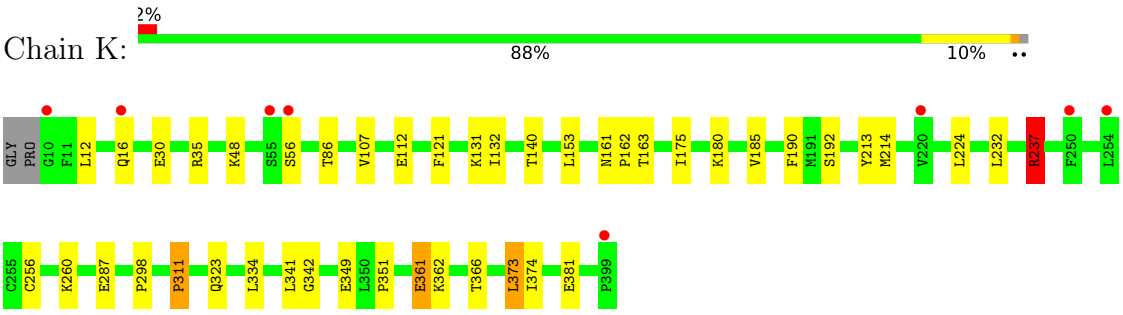
• Molecule 1: Cystathionine gamma-lyase

Chain J:



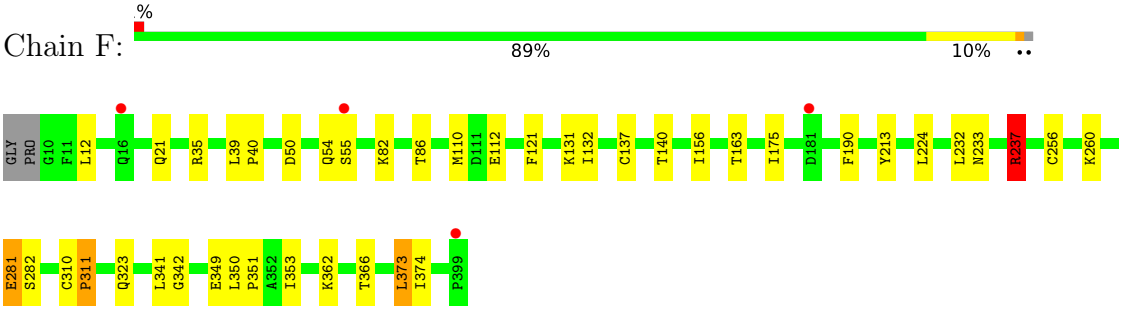
• Molecule 1: Cystathionine gamma-lyase

Chain K:



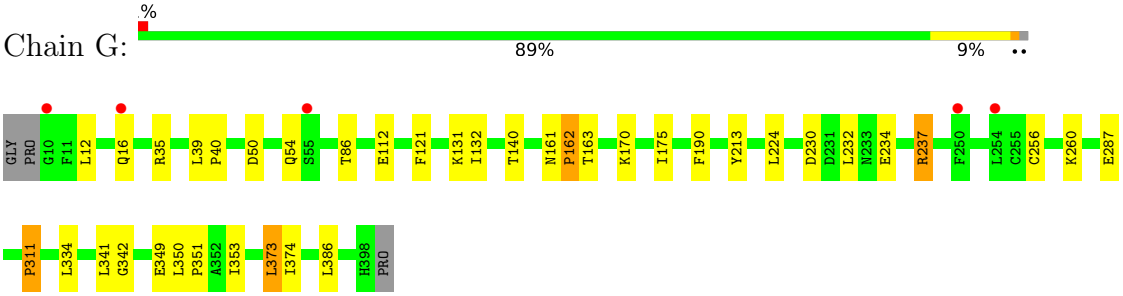
• Molecule 1: Cystathionine gamma-lyase

Chain F:



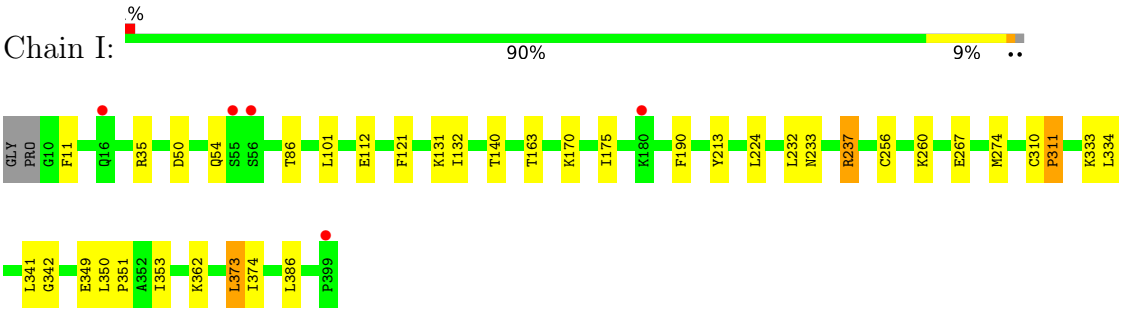
• Molecule 1: Cystathionine gamma-lyase

Chain G:



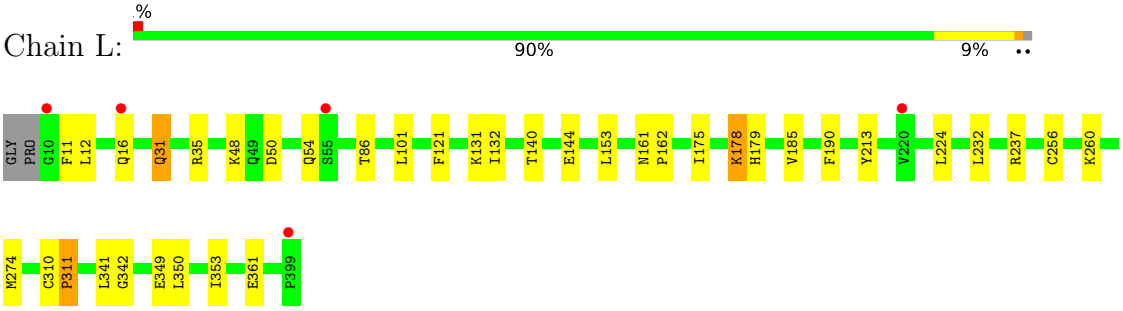
• Molecule 1: Cystathionine gamma-lyase

Chain I:



• Molecule 1: Cystathionine gamma-lyase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	176.21Å 184.12Å 175.94Å 90.00° 99.46° 90.00°	Depositor
Resolution (Å)	48.98 – 1.90 48.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.98-1.90) 99.4 (48.98-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.172 , 0.196 0.182 , 0.204	Depositor DCC
R_{free} test set	21313 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	39772	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5183e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO, TVJ

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	0.73	0/3104	0.86	5/4203 (0.1%)
1	B	0.72	0/3123	0.88	4/4229 (0.1%)
1	C	0.71	0/3139	0.83	4/4251 (0.1%)
1	D	0.72	0/3127	0.84	4/4236 (0.1%)
1	E	0.73	1/3110 (0.0%)	0.85	5/4212 (0.1%)
1	F	0.72	1/3117 (0.0%)	0.86	4/4221 (0.1%)
1	G	0.69	1/3122 (0.0%)	0.85	5/4228 (0.1%)
1	H	0.70	0/3123	0.86	5/4229 (0.1%)
1	I	0.71	1/3129 (0.0%)	0.87	3/4237 (0.1%)
1	J	0.71	0/3135	0.84	4/4245 (0.1%)
1	K	0.70	0/3131	0.86	5/4240 (0.1%)
1	L	0.70	0/3140	0.84	6/4253 (0.1%)
All	All	0.71	4/37500 (0.0%)	0.85	54/50784 (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	L	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	144	GLU	CD-OE1	6.52	1.32	1.25
1	G	287	GLU	CD-OE2	5.58	1.31	1.25
1	I	267	GLU	CD-OE1	5.36	1.31	1.25
1	F	281	GLU	CD-OE2	-5.01	1.20	1.25

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	237	ARG	NE-CZ-NH1	-16.28	112.16	120.30
1	B	237	ARG	NE-CZ-NH1	-15.76	112.42	120.30
1	I	237	ARG	NE-CZ-NH2	15.07	127.83	120.30
1	E	237	ARG	NE-CZ-NH2	-14.02	113.29	120.30
1	H	237	ARG	NE-CZ-NH2	-13.95	113.33	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	31	GLN	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	3024	0	3073	21	0
1	B	3034	0	3092	22	0
1	C	3049	0	3112	33	0
1	D	3038	0	3102	25	0
1	E	3027	0	3080	24	0
1	F	3031	0	3085	25	0
1	G	3034	0	3094	19	0
1	H	3037	0	3099	22	0
1	I	3040	0	3103	24	0
1	J	3043	0	3109	38	0
1	K	3042	0	3110	25	0
1	L	3050	0	3109	24	0
2	A	22	0	0	1	0
2	B	22	0	0	1	0
2	C	22	0	0	1	0
2	D	22	0	0	1	0
2	E	22	0	0	1	0
2	F	22	0	0	1	0
2	G	22	0	0	1	0
2	H	22	0	0	1	0
2	I	22	0	0	1	0
2	J	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	22	0	0	1	0
2	L	22	0	0	1	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	1	0
3	D	6	0	8	1	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	H	6	0	8	1	0
3	I	6	0	8	1	0
3	K	6	0	8	0	0
3	L	6	0	8	1	0
4	J	16	0	22	15	0
4	K	4	0	6	3	0
5	A	288	0	0	3	0
5	B	285	0	0	6	0
5	C	280	0	0	7	0
5	D	299	0	0	3	0
5	E	243	0	0	5	0
5	F	234	0	0	5	0
5	G	194	0	0	0	0
5	H	237	0	0	2	0
5	I	220	0	0	6	0
5	J	252	0	0	4	0
5	K	228	0	0	5	0
5	L	219	0	0	7	0
All	All	39772	0	37276	313	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 313 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:J:218:SER:OG	4:J:403:EDO:H22	1.40	1.18
1:J:218:SER:OG	4:J:403:EDO:C2	2.13	0.94
1:A:237:ARG:HD3	5:A:715:HOH:O	1.76	0.85
1:F:110[B]:MET:SD	1:F:137:CYS:HB2	2.18	0.83
1:I:274[A]:MET:HE3	5:I:630:HOH:O	1.81	0.80

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/392 (100%)	383 (97%)	10 (2%)	1 (0%)	41	31
1	B	397/392 (101%)	387 (98%)	9 (2%)	1 (0%)	41	31
1	C	398/392 (102%)	389 (98%)	8 (2%)	1 (0%)	41	31
1	D	397/392 (101%)	387 (98%)	9 (2%)	1 (0%)	41	31
1	E	395/392 (101%)	384 (97%)	10 (2%)	1 (0%)	41	31
1	F	396/392 (101%)	385 (97%)	10 (2%)	1 (0%)	41	31
1	G	396/392 (101%)	386 (98%)	9 (2%)	1 (0%)	41	31
1	H	396/392 (101%)	386 (98%)	9 (2%)	1 (0%)	41	31
1	I	397/392 (101%)	385 (97%)	11 (3%)	1 (0%)	41	31
1	J	398/392 (102%)	387 (97%)	10 (2%)	1 (0%)	41	31
1	K	397/392 (101%)	387 (98%)	9 (2%)	1 (0%)	41	31
1	L	398/392 (102%)	388 (98%)	9 (2%)	1 (0%)	41	31
All	All	4759/4704 (101%)	4634 (97%)	113 (2%)	12 (0%)	41	31

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	PRO
1	B	311	PRO
1	C	311	PRO
1	D	311	PRO
1	E	311	PRO

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	334/329 (102%)	329 (98%)	5 (2%)	65	62
1	B	337/329 (102%)	329 (98%)	8 (2%)	49	43
1	C	338/329 (103%)	329 (97%)	9 (3%)	44	38
1	D	337/329 (102%)	328 (97%)	9 (3%)	44	38
1	E	335/329 (102%)	324 (97%)	11 (3%)	38	29
1	F	336/329 (102%)	325 (97%)	11 (3%)	38	29
1	G	336/329 (102%)	325 (97%)	11 (3%)	38	29
1	H	336/329 (102%)	326 (97%)	10 (3%)	41	33
1	I	337/329 (102%)	329 (98%)	8 (2%)	49	43
1	J	338/329 (103%)	325 (96%)	13 (4%)	33	24
1	K	337/329 (102%)	322 (96%)	15 (4%)	27	18
1	L	338/329 (103%)	330 (98%)	8 (2%)	49	43
All	All	4039/3948 (102%)	3921 (97%)	118 (3%)	47	35

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	237	ARG
1	L	12	LEU
1	K	232[B]	LEU
1	I	373[B]	LEU
1	G	349	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	179	HIS
1	G	323	GLN
1	F	233	ASN
1	G	54	GLN
1	I	54	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TVJ	L	401	-	21,22,22	1.45	2 (9%)	26,31,31	1.04	1 (3%)
2	TVJ	A	401	-	21,22,22	1.38	1 (4%)	26,31,31	1.20	1 (3%)
3	GOL	I	402	-	5,5,5	0.21	0	5,5,5	0.44	0
2	TVJ	I	401	-	21,22,22	1.47	1 (4%)	26,31,31	1.02	2 (7%)
2	TVJ	B	401	-	21,22,22	1.32	1 (4%)	26,31,31	1.06	1 (3%)
2	TVJ	G	401	-	21,22,22	1.43	1 (4%)	26,31,31	1.02	0
4	EDO	J	402	-	3,3,3	0.13	0	2,2,2	0.37	0
3	GOL	F	402	-	5,5,5	0.09	0	5,5,5	0.25	0
3	GOL	H	402	-	5,5,5	0.12	0	5,5,5	0.51	0
3	GOL	E	402	-	5,5,5	0.10	0	5,5,5	0.30	0
2	TVJ	C	401	-	21,22,22	1.49	2 (9%)	26,31,31	1.01	3 (11%)
4	EDO	J	405	-	3,3,3	0.75	0	2,2,2	1.37	0
2	TVJ	H	401	-	21,22,22	1.43	2 (9%)	26,31,31	1.02	0
3	GOL	C	402	-	5,5,5	0.18	0	5,5,5	0.59	0
4	EDO	J	404	-	3,3,3	0.91	0	2,2,2	0.58	0
2	TVJ	E	401	-	21,22,22	1.42	2 (9%)	26,31,31	1.23	2 (7%)
3	GOL	K	402	-	5,5,5	0.10	0	5,5,5	0.48	0
3	GOL	D	402	-	5,5,5	0.12	0	5,5,5	0.59	0
4	EDO	K	403	-	3,3,3	0.87	0	2,2,2	0.89	0
2	TVJ	F	401	-	21,22,22	1.43	2 (9%)	26,31,31	1.24	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	L	402	-	5,5,5	0.17	0	5,5,5	0.42	0
4	EDO	J	403	-	3,3,3	0.76	0	2,2,2	0.11	0
2	TVJ	K	401	-	21,22,22	1.61	3 (14%)	26,31,31	0.96	0
3	GOL	B	402	-	5,5,5	0.16	0	5,5,5	0.46	0
2	TVJ	J	401	-	21,22,22	1.33	1 (4%)	26,31,31	1.05	2 (7%)
3	GOL	A	402	-	5,5,5	0.19	0	5,5,5	0.52	0
2	TVJ	D	401	-	21,22,22	1.52	1 (4%)	26,31,31	1.06	1 (3%)

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	TVJ	L	401	-	-	2/15/16/16	0/1/1/1
2	TVJ	A	401	-	-	2/15/16/16	0/1/1/1
3	GOL	I	402	-	-	2/4/4/4	-
2	TVJ	I	401	-	-	3/15/16/16	0/1/1/1
2	TVJ	B	401	-	-	2/15/16/16	0/1/1/1
2	TVJ	G	401	-	-	2/15/16/16	0/1/1/1
4	EDO	J	402	-	-	1/1/1/1	-
3	GOL	F	402	-	-	2/4/4/4	-
3	GOL	H	402	-	-	2/4/4/4	-
3	GOL	E	402	-	-	3/4/4/4	-
2	TVJ	C	401	-	-	2/15/16/16	0/1/1/1
4	EDO	J	405	-	-	0/1/1/1	-
2	TVJ	H	401	-	-	2/15/16/16	0/1/1/1
3	GOL	C	402	-	-	2/4/4/4	-
4	EDO	J	404	-	-	1/1/1/1	-
2	TVJ	E	401	-	-	4/15/16/16	0/1/1/1
3	GOL	K	402	-	-	2/4/4/4	-
3	GOL	D	402	-	-	4/4/4/4	-
4	EDO	K	403	-	-	1/1/1/1	-
2	TVJ	F	401	-	-	3/15/16/16	0/1/1/1
3	GOL	L	402	-	-	3/4/4/4	-
4	EDO	J	403	-	-	1/1/1/1	-
2	TVJ	K	401	-	-	3/15/16/16	0/1/1/1
3	GOL	B	402	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TVJ	J	401	-	-	3/15/16/16	0/1/1/1
3	GOL	A	402	-	-	0/4/4/4	-
2	TVJ	D	401	-	-	3/15/16/16	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	TVJ	C10-N4	6.07	1.49	1.33
2	G	401	TVJ	C10-N4	6.02	1.49	1.33
2	I	401	TVJ	C10-N4	5.95	1.49	1.33
2	K	401	TVJ	C10-N4	5.79	1.48	1.33
2	C	401	TVJ	C10-N4	5.44	1.47	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	TVJ	O3-P1-O2	-3.65	97.03	106.73
2	D	401	TVJ	O3-P1-O2	-3.57	97.24	106.73
2	E	401	TVJ	O6-C9-C10	3.45	125.57	121.30
2	I	401	TVJ	O3-P1-O2	-3.32	97.90	106.73
2	B	401	TVJ	O2-P1-O5	-3.23	97.42	106.47

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	TVJ	O7-C10-C9-N3
2	D	401	TVJ	N4-C10-C9-O6
2	E	401	TVJ	O7-C10-C9-N3
2	E	401	TVJ	N4-C10-C9-O6
2	H	401	TVJ	O7-C10-C9-N3

There are no ring outliers.

22 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	401	TVJ	1	0
2	A	401	TVJ	1	0
3	I	402	GOL	1	0
2	I	401	TVJ	1	0

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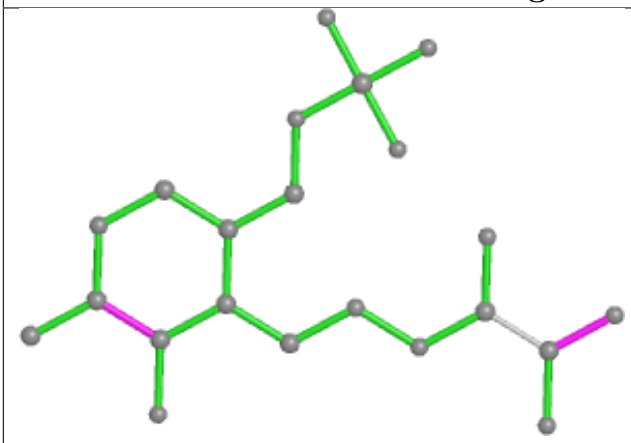
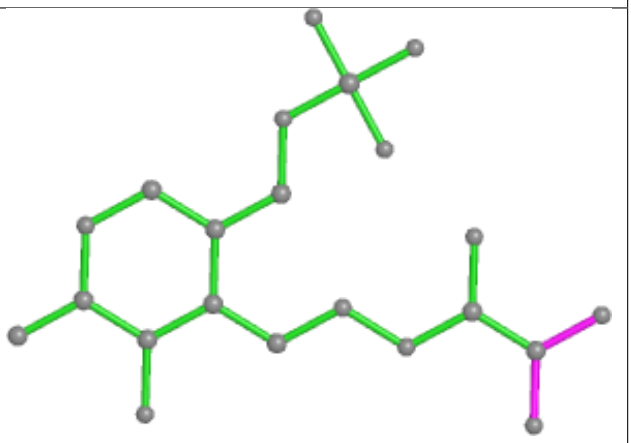
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	TVJ	1	0
2	G	401	TVJ	1	0
4	J	402	EDO	2	0
3	H	402	GOL	1	0
2	C	401	TVJ	1	0
4	J	405	EDO	6	0
2	H	401	TVJ	1	0
3	C	402	GOL	1	0
4	J	404	EDO	1	0
2	E	401	TVJ	1	0
3	D	402	GOL	1	0
4	K	403	EDO	3	0
2	F	401	TVJ	1	0
3	L	402	GOL	1	0
4	J	403	EDO	6	0
2	K	401	TVJ	1	0
2	J	401	TVJ	1	0
2	D	401	TVJ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

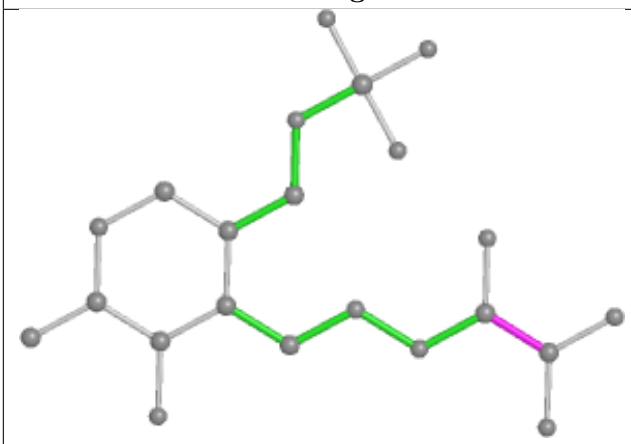
Ligand TVJ L 401



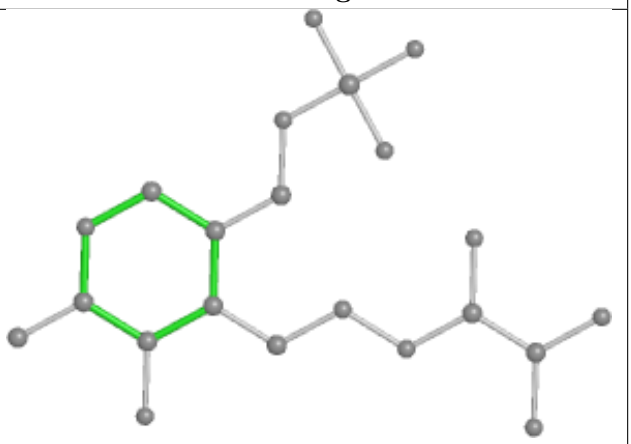
Bond lengths



Bond angles

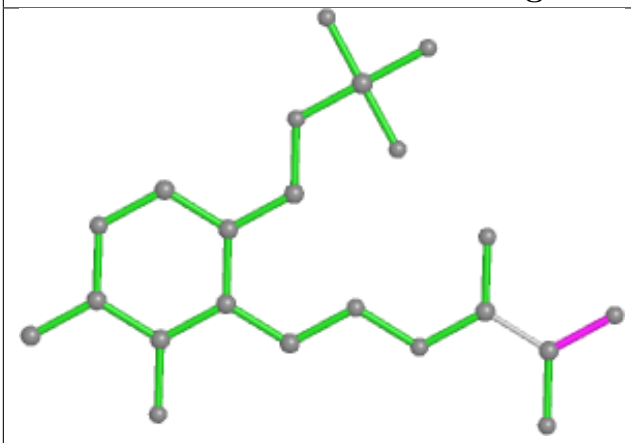


Torsions



Rings

Ligand TVJ A 401



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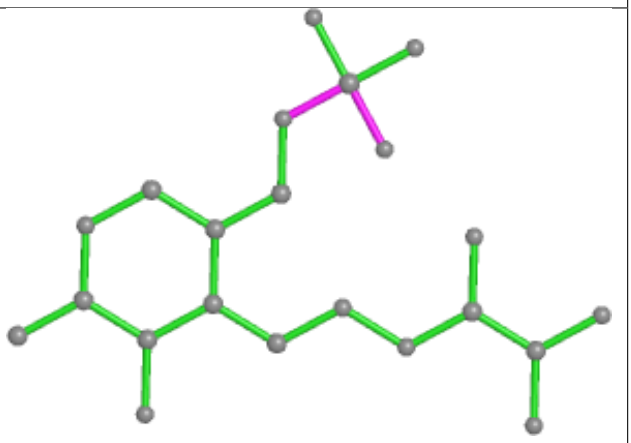

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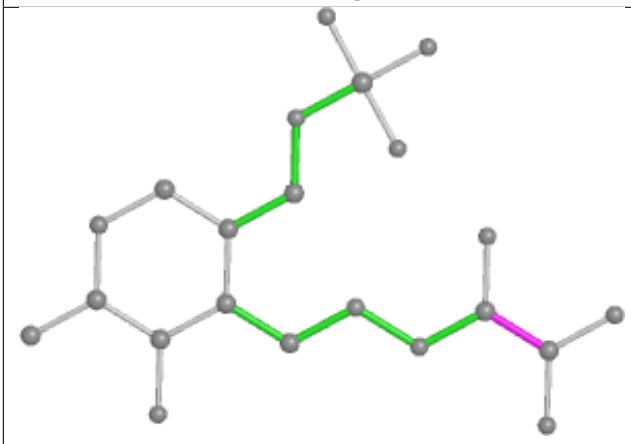

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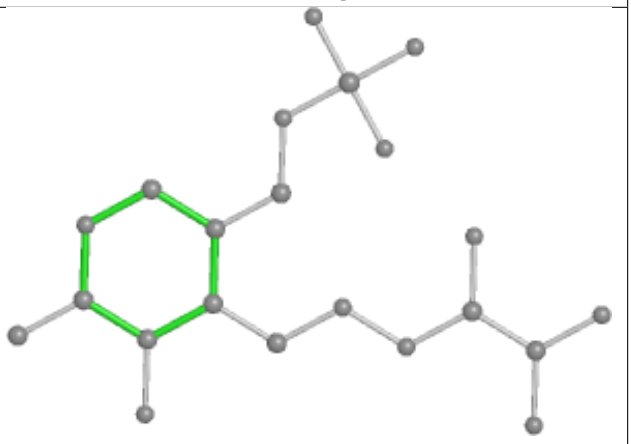
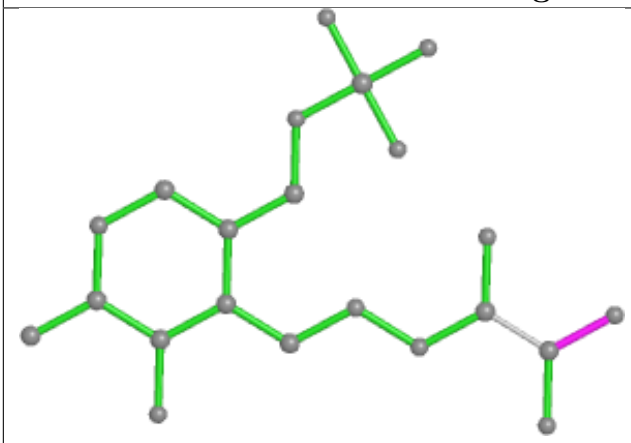


Rings

Ligand TVJ I 401



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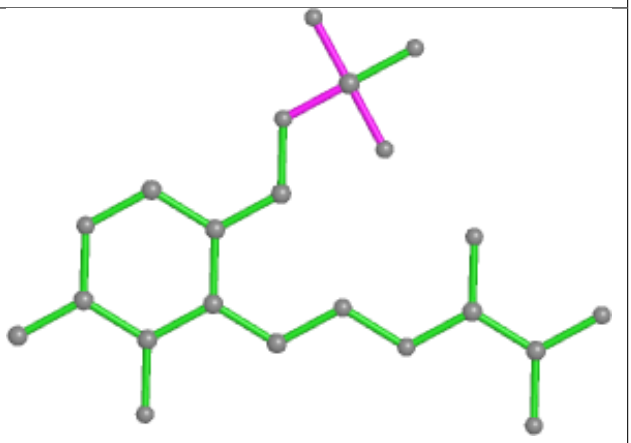
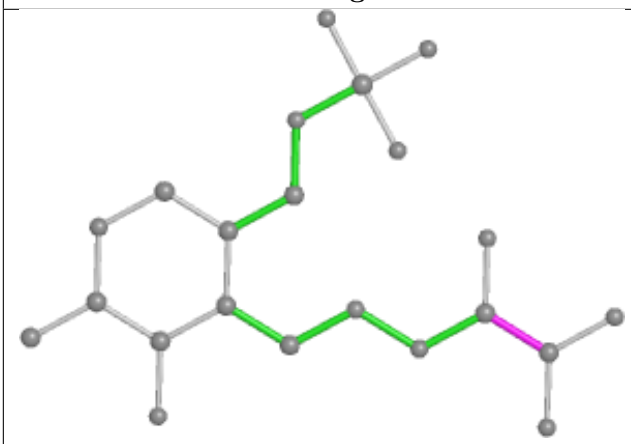
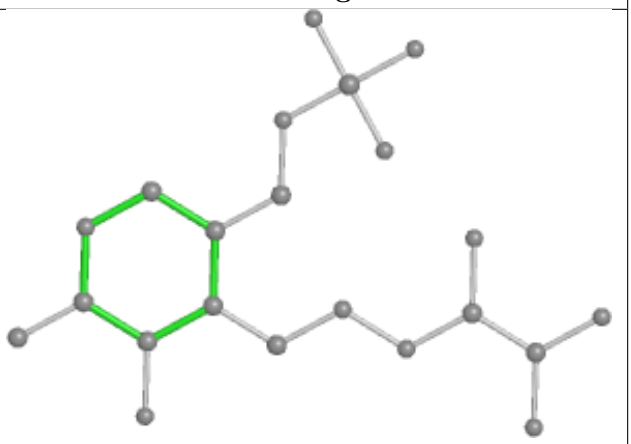


Bond angles

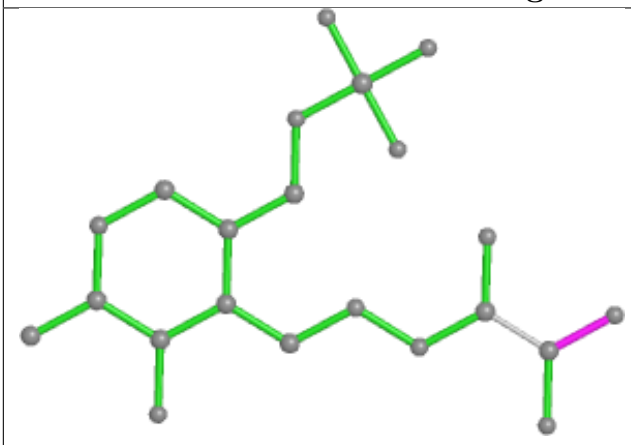


Torsions

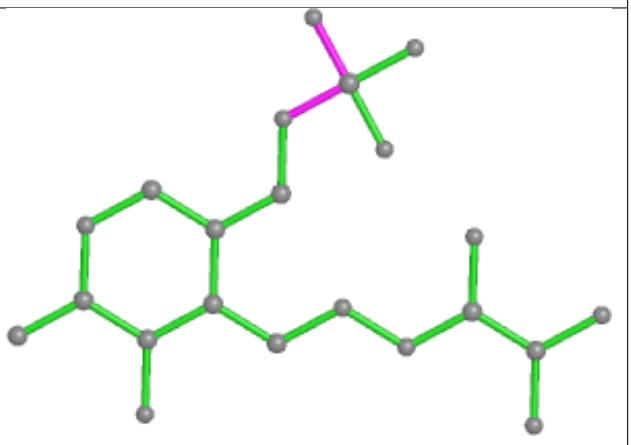


Rings

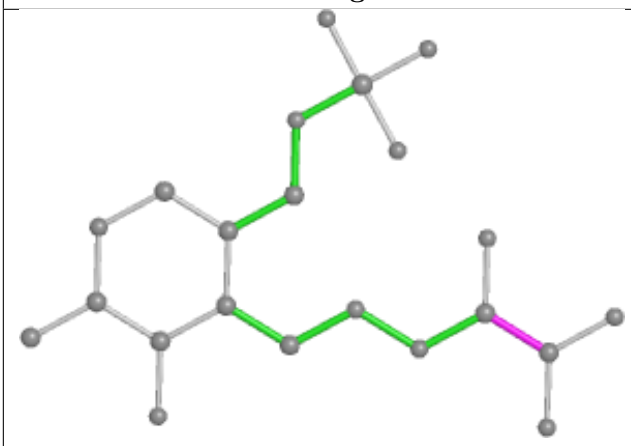
Ligand TVJ B 401



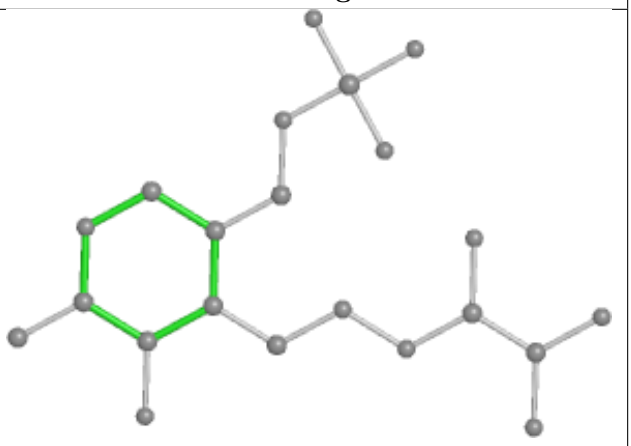
Bond lengths



Bond angles

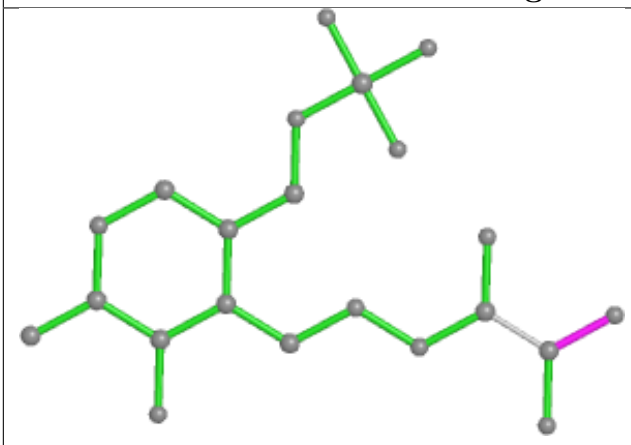


Torsions

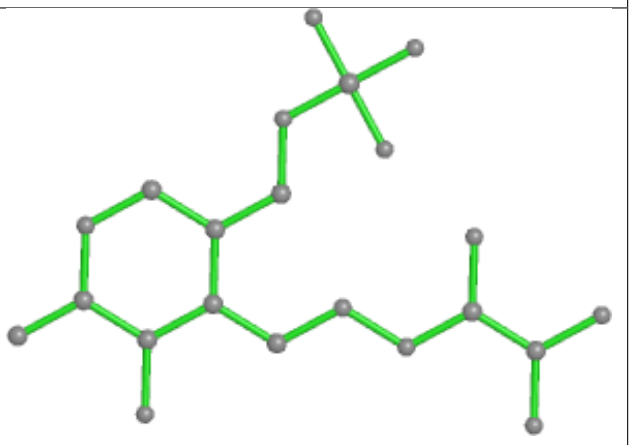


Rings

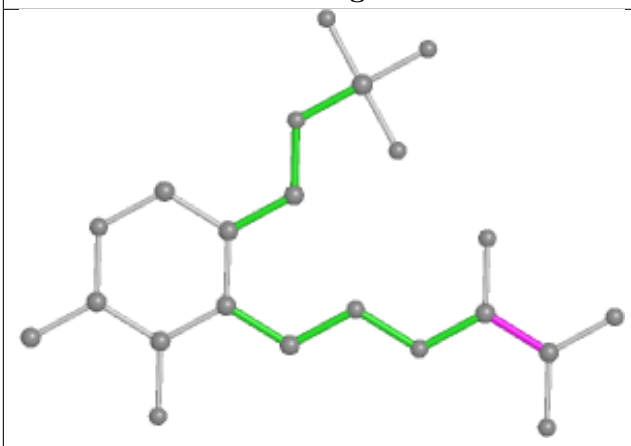
Ligand TVJ G 401



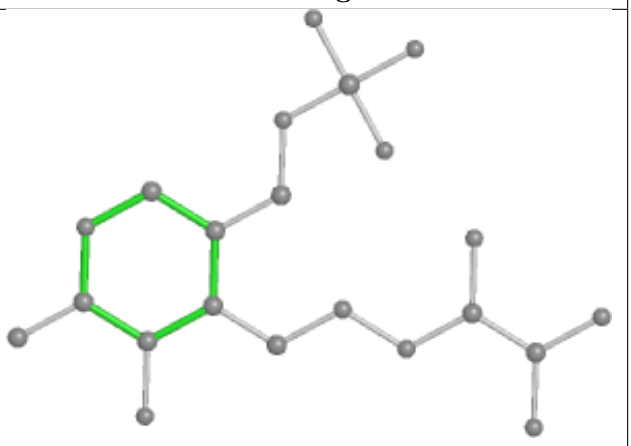
Bond lengths



Bond angles

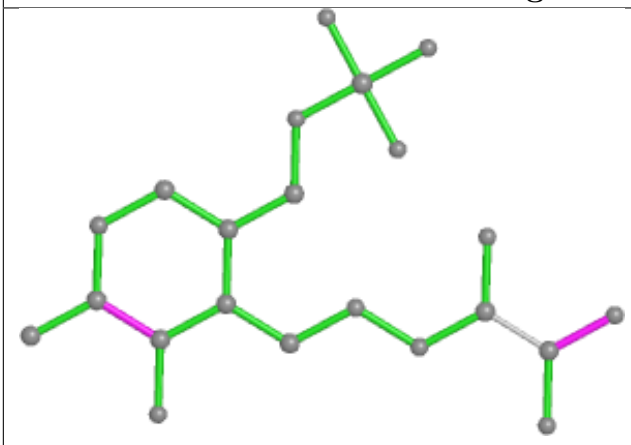


Torsions

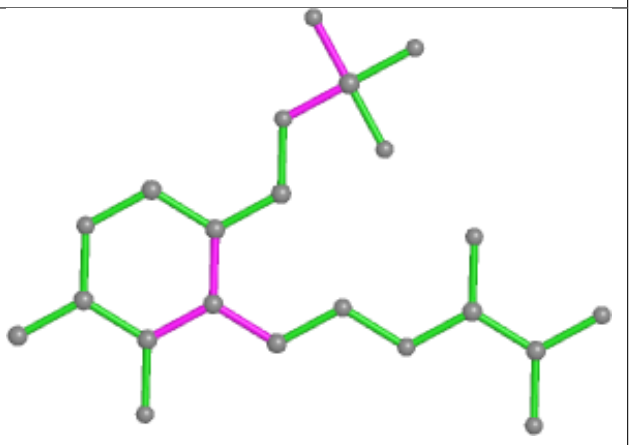


Rings

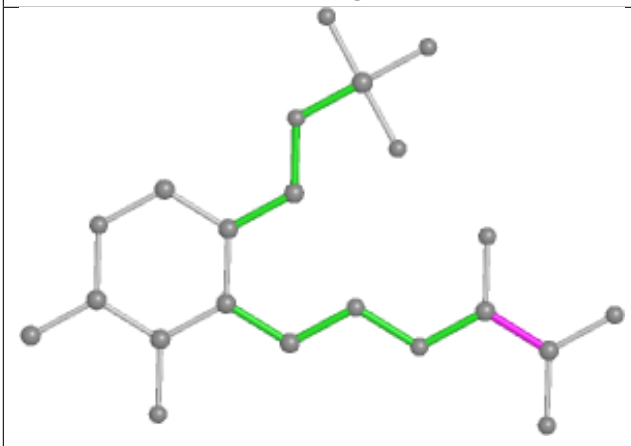
Ligand TVJ C 401



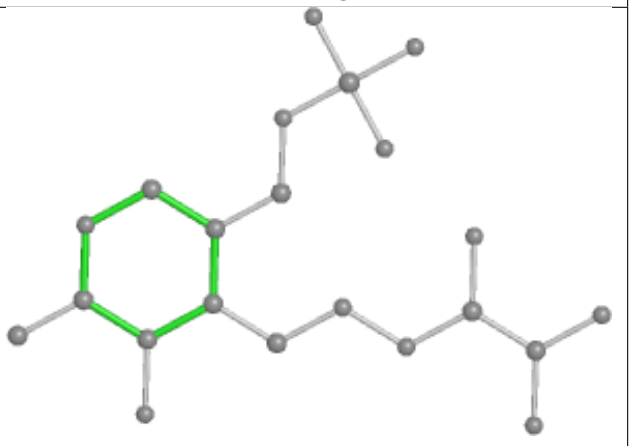
Bond lengths



Bond angles

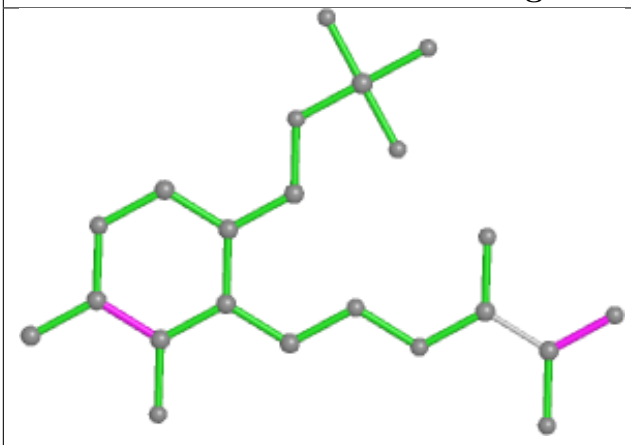


Torsions

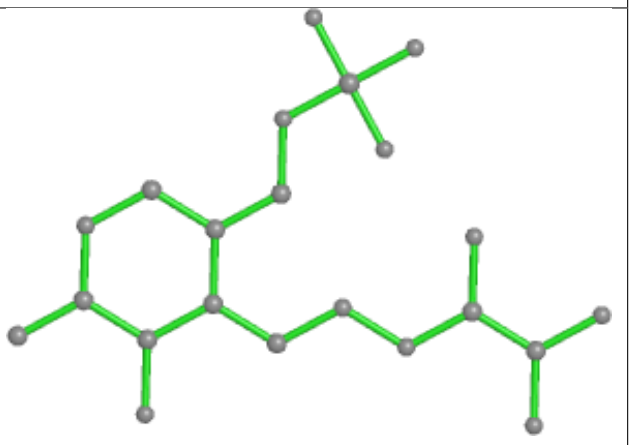


Rings

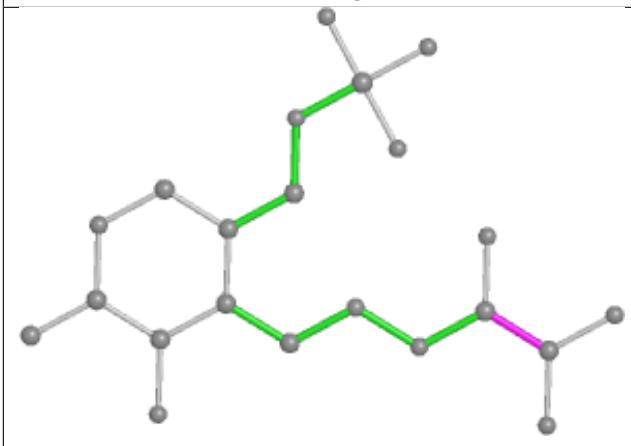
Ligand TVJ H 401



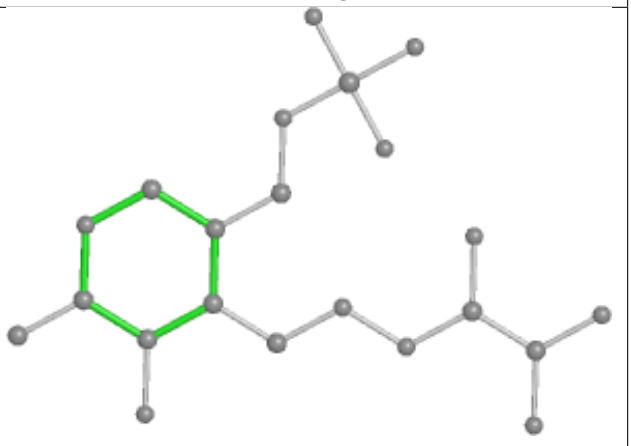
Bond lengths



Bond angles

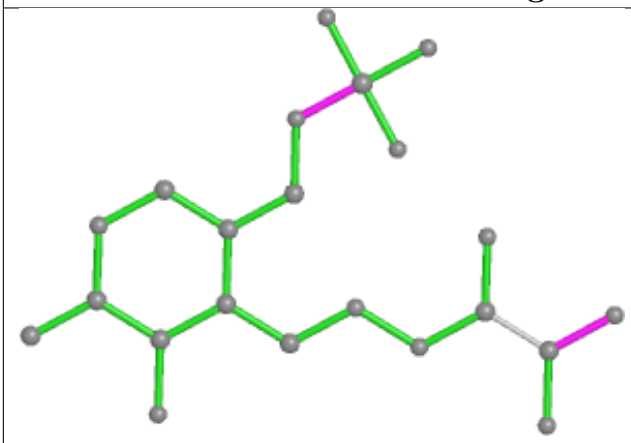


Torsions

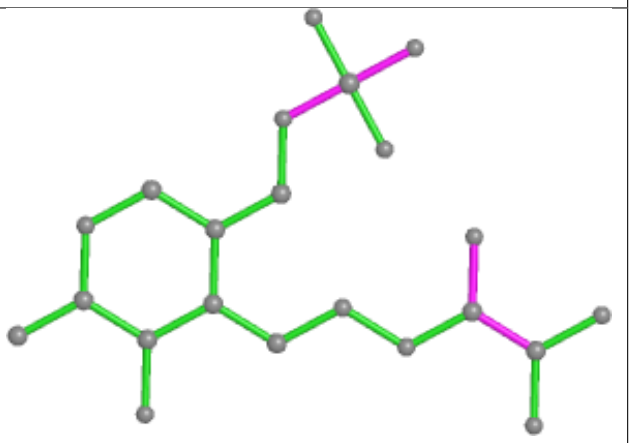


Rings

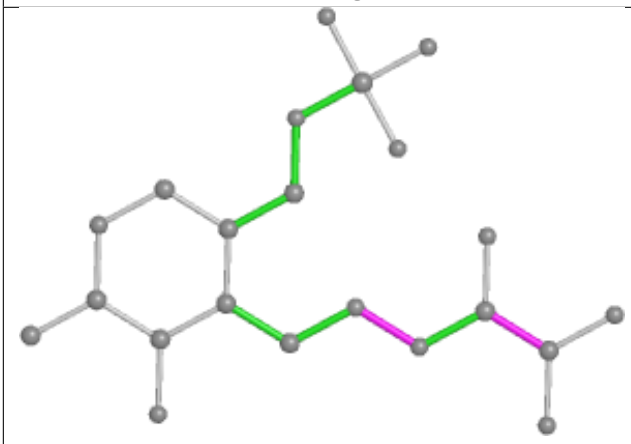
Ligand TVJ E 401



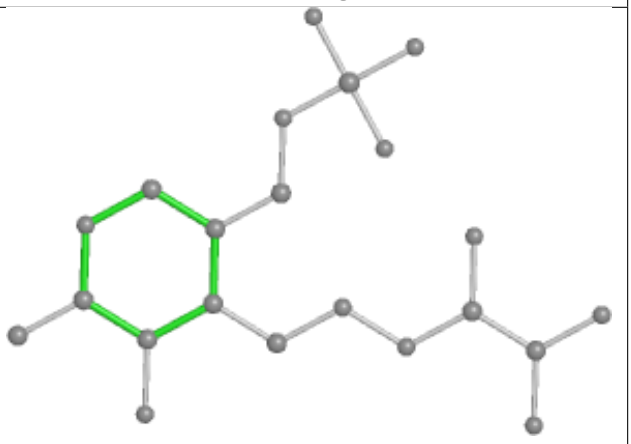
Bond lengths



Bond angles

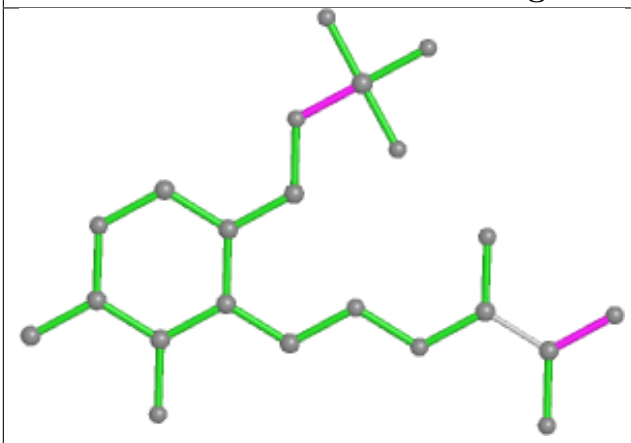


Torsions

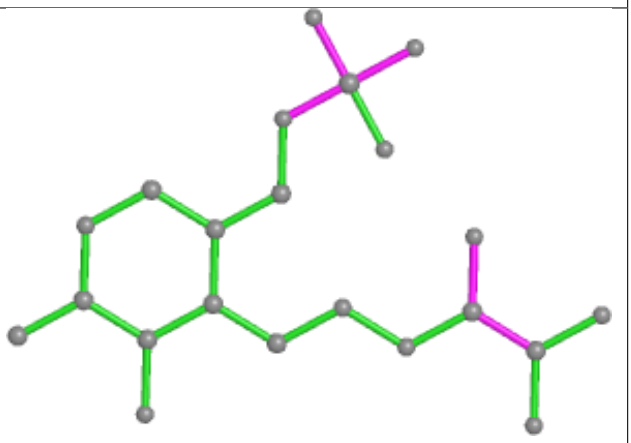


Rings

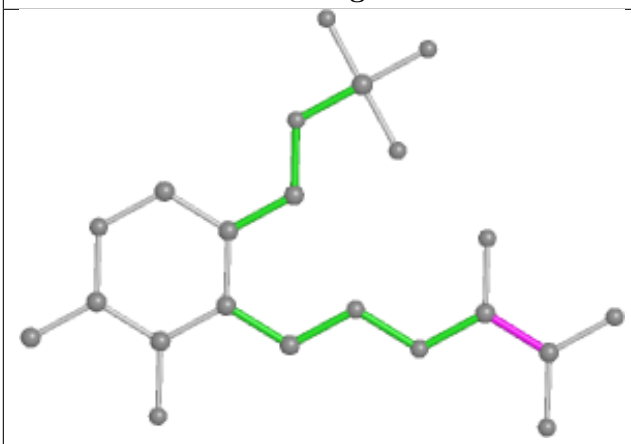
Ligand TVJ F 401



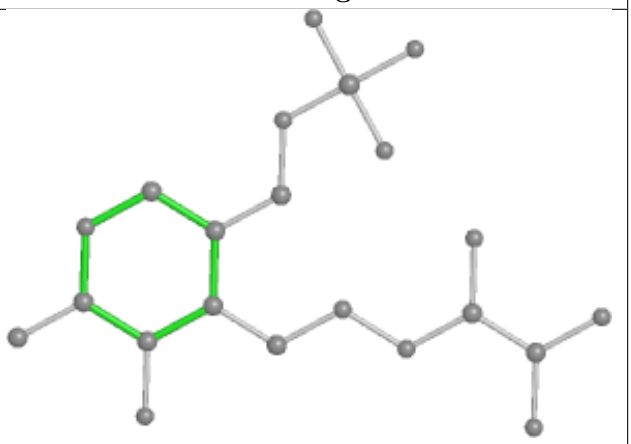
Bond lengths



Bond angles

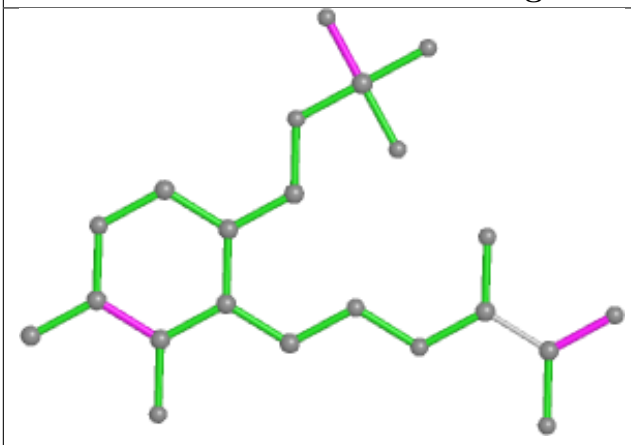


Torsions

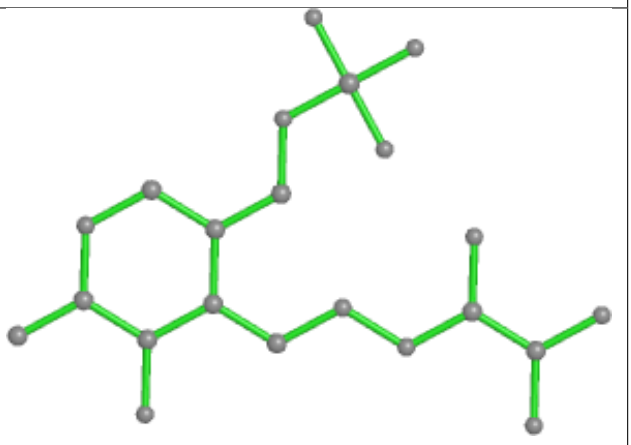


Rings

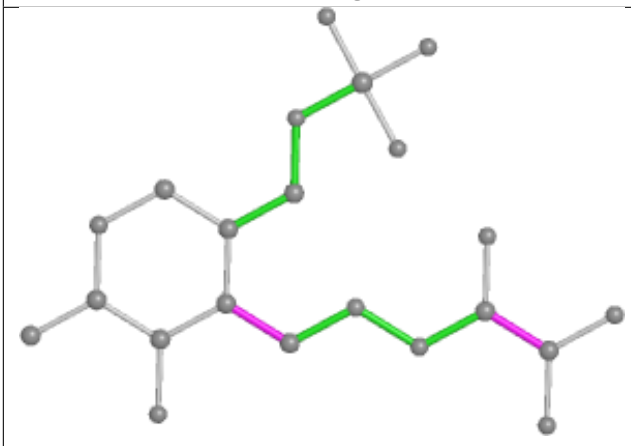
Ligand TVJ K 401



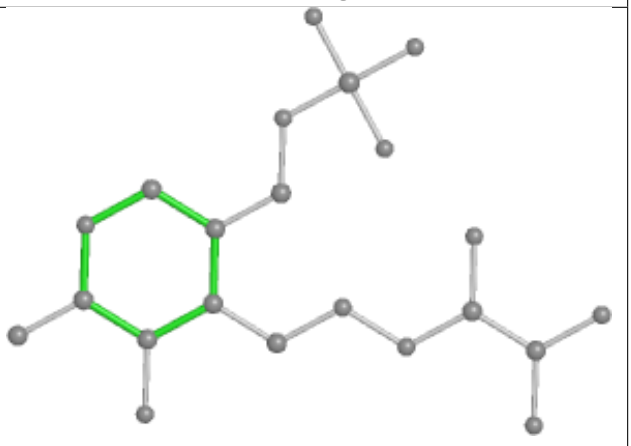
Bond lengths



Bond angles

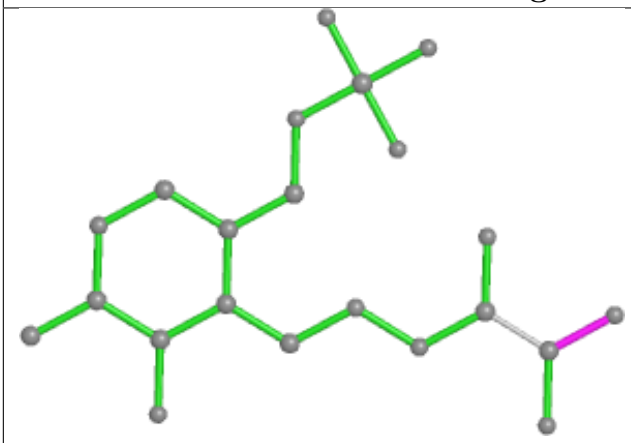


Torsions

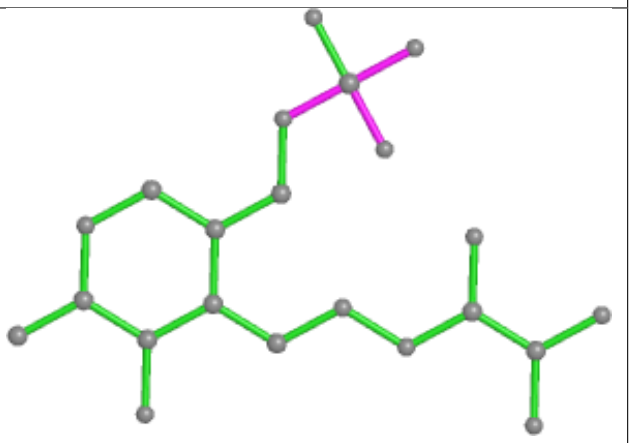


Rings

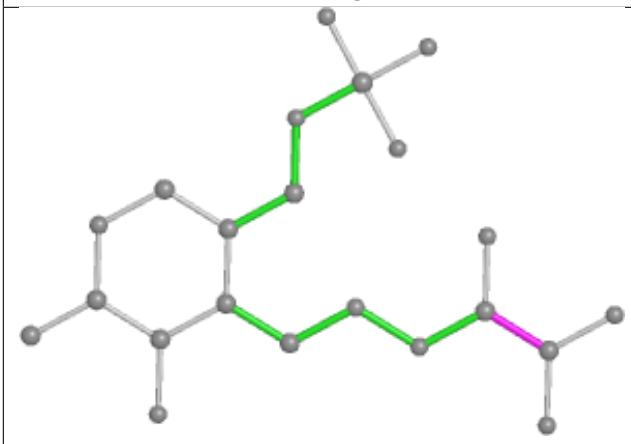
Ligand TVJ J 401



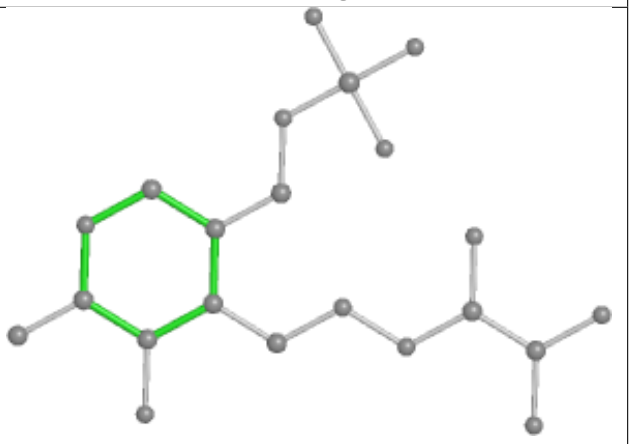
Bond lengths



Bond angles

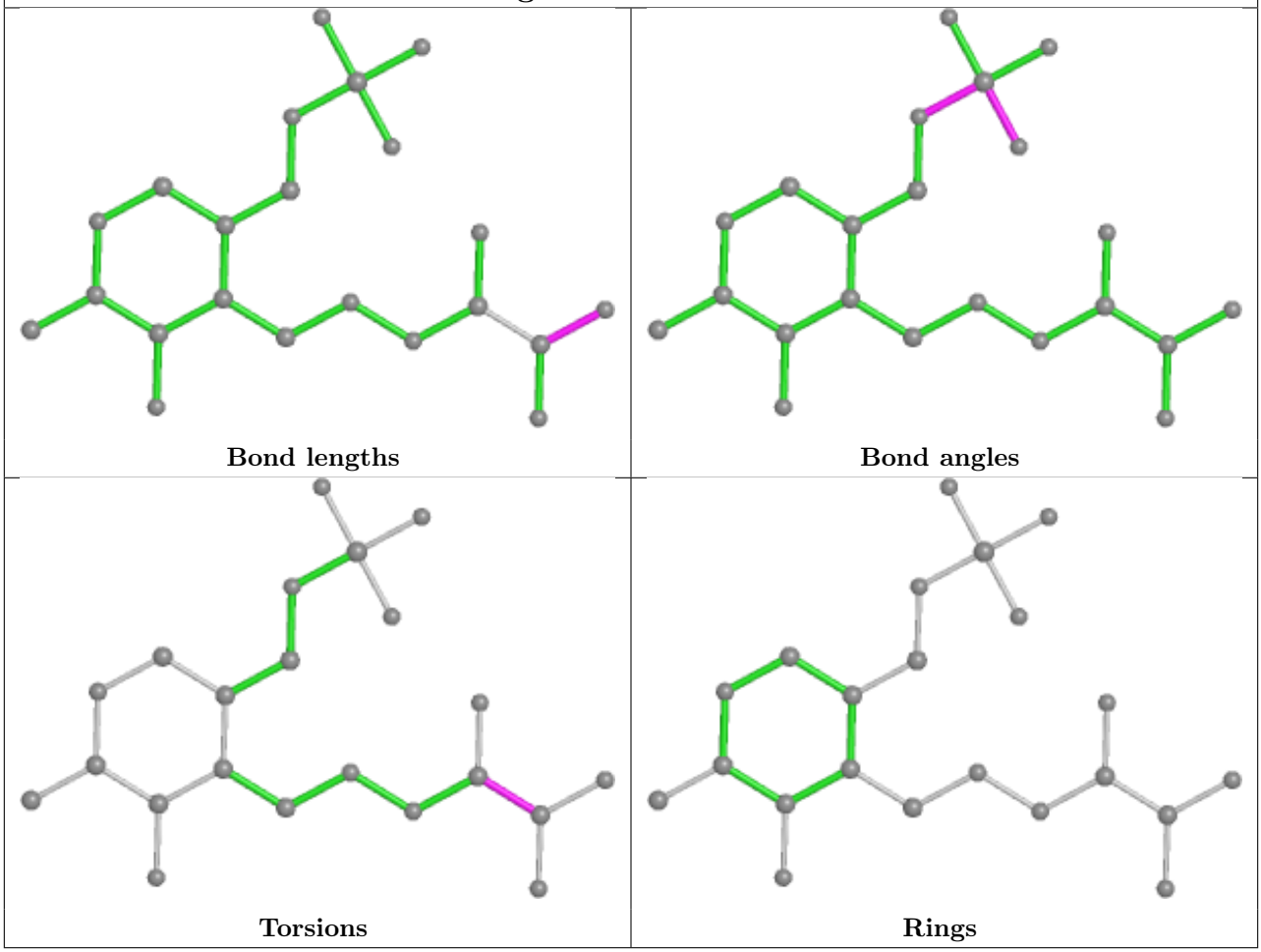


Torsions



Rings

Ligand TVJ D 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	390/392 (99%)	-0.34	3 (0%)	86	87	9, 17, 33, 58	0
1	B	390/392 (99%)	-0.32	4 (1%)	82	84	10, 17, 35, 59	0
1	C	390/392 (99%)	-0.29	5 (1%)	77	79	10, 17, 34, 62	0
1	D	390/392 (99%)	-0.31	3 (0%)	86	87	8, 17, 33, 62	0
1	E	390/392 (99%)	-0.24	5 (1%)	77	79	13, 22, 41, 70	0
1	F	390/392 (99%)	-0.25	4 (1%)	82	84	14, 23, 42, 87	0
1	G	389/392 (99%)	-0.05	5 (1%)	77	79	15, 27, 46, 69	0
1	H	390/392 (99%)	-0.16	4 (1%)	82	84	14, 23, 41, 65	0
1	I	390/392 (99%)	-0.29	5 (1%)	77	79	13, 22, 40, 72	0
1	J	390/392 (99%)	-0.27	3 (0%)	86	87	13, 22, 40, 77	0
1	K	390/392 (99%)	-0.05	8 (2%)	63	66	13, 25, 44, 72	0
1	L	390/392 (99%)	-0.16	5 (1%)	77	79	13, 23, 41, 65	0
All	All	4679/4704 (99%)	-0.23	54 (1%)	79	81	8, 21, 41, 87	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	55	SER	7.8
1	J	55	SER	7.2
1	E	55	SER	6.4
1	I	55	SER	5.8
1	G	55	SER	5.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

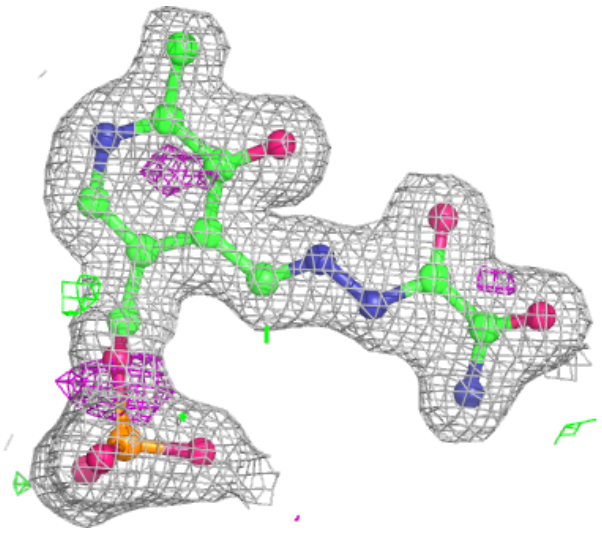
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

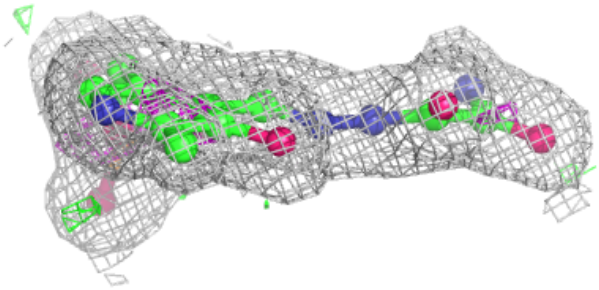
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	J	405	4/4	0.83	0.23	38,41,42,47	0
4	EDO	K	403	4/4	0.85	0.22	33,39,42,55	0
3	GOL	E	402	6/6	0.89	0.19	34,40,44,44	0
4	EDO	J	404	4/4	0.90	0.14	23,24,33,34	0
3	GOL	D	402	6/6	0.90	0.14	27,30,34,37	0
4	EDO	J	402	4/4	0.90	0.28	39,40,41,42	0
3	GOL	I	402	6/6	0.92	0.18	33,38,39,40	0
3	GOL	C	402	6/6	0.93	0.16	26,32,35,36	0
3	GOL	L	402	6/6	0.93	0.15	36,37,38,39	0
3	GOL	B	402	6/6	0.94	0.13	29,30,33,35	0
3	GOL	A	402	6/6	0.94	0.12	27,30,31,32	0
3	GOL	F	402	6/6	0.94	0.11	35,38,40,41	0
4	EDO	J	403	4/4	0.95	0.20	25,31,33,46	0
3	GOL	H	402	6/6	0.95	0.10	31,35,39,42	0
3	GOL	K	402	6/6	0.96	0.11	30,33,37,37	0
2	TVJ	E	401	22/22	0.97	0.07	14,17,23,24	0
2	TVJ	H	401	22/22	0.97	0.11	15,18,26,29	0
2	TVJ	K	401	22/22	0.97	0.11	15,20,28,34	0
2	TVJ	L	401	22/22	0.98	0.10	14,17,26,30	0
2	TVJ	A	401	22/22	0.98	0.10	8,12,18,22	0
2	TVJ	B	401	22/22	0.98	0.10	10,13,20,24	0
2	TVJ	J	401	22/22	0.98	0.07	14,18,23,26	0
2	TVJ	C	401	22/22	0.98	0.10	10,13,21,25	0
2	TVJ	F	401	22/22	0.98	0.06	15,19,25,27	0
2	TVJ	G	401	22/22	0.98	0.11	18,20,31,32	0
2	TVJ	I	401	22/22	0.98	0.07	12,16,22,25	0
2	TVJ	D	401	22/22	0.99	0.09	9,12,18,21	0

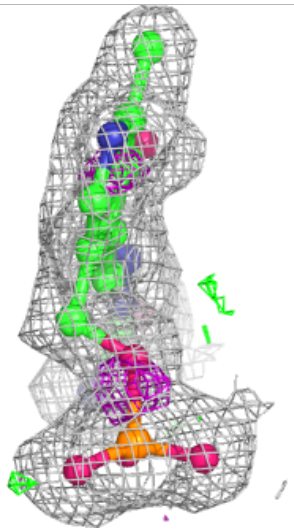
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TVJ E 401:

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

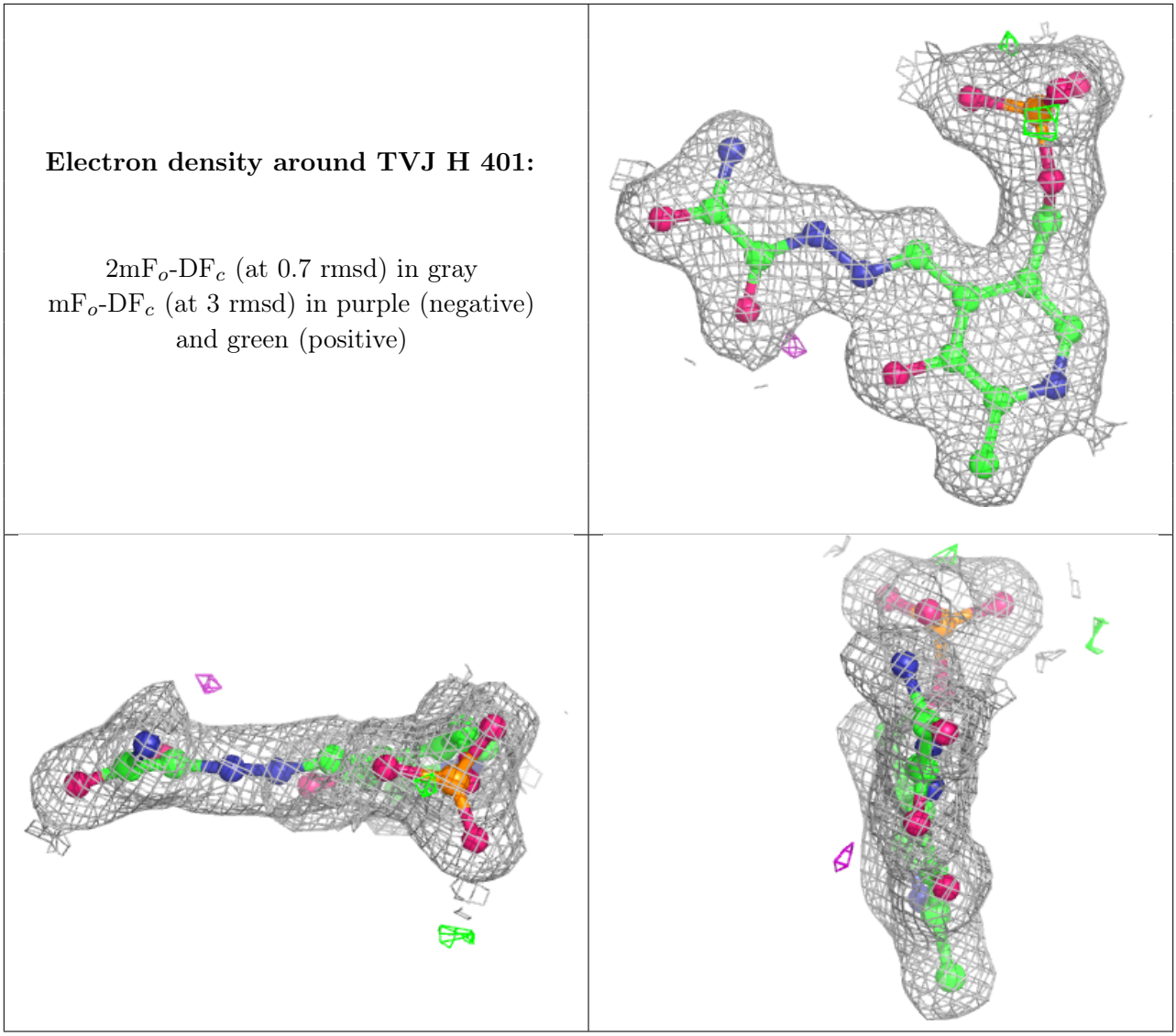






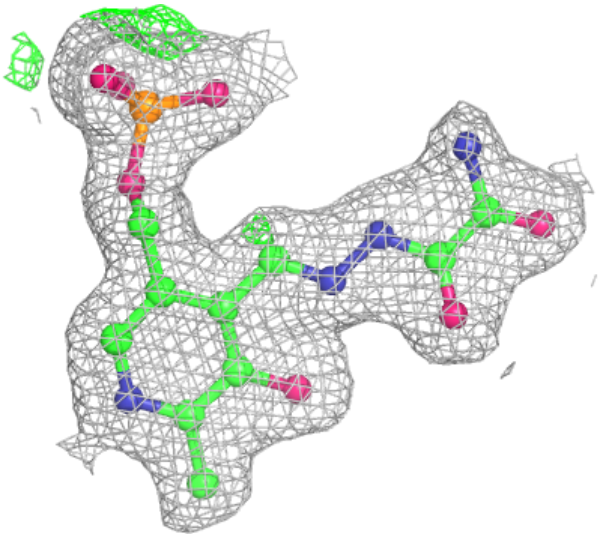
Electron density around TVJ H 401:

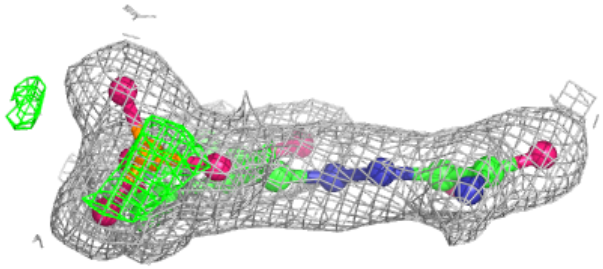
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

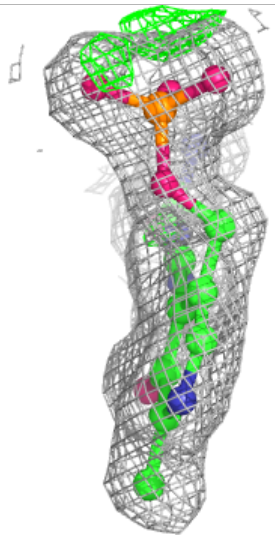


Electron density around TVJ K 401:

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

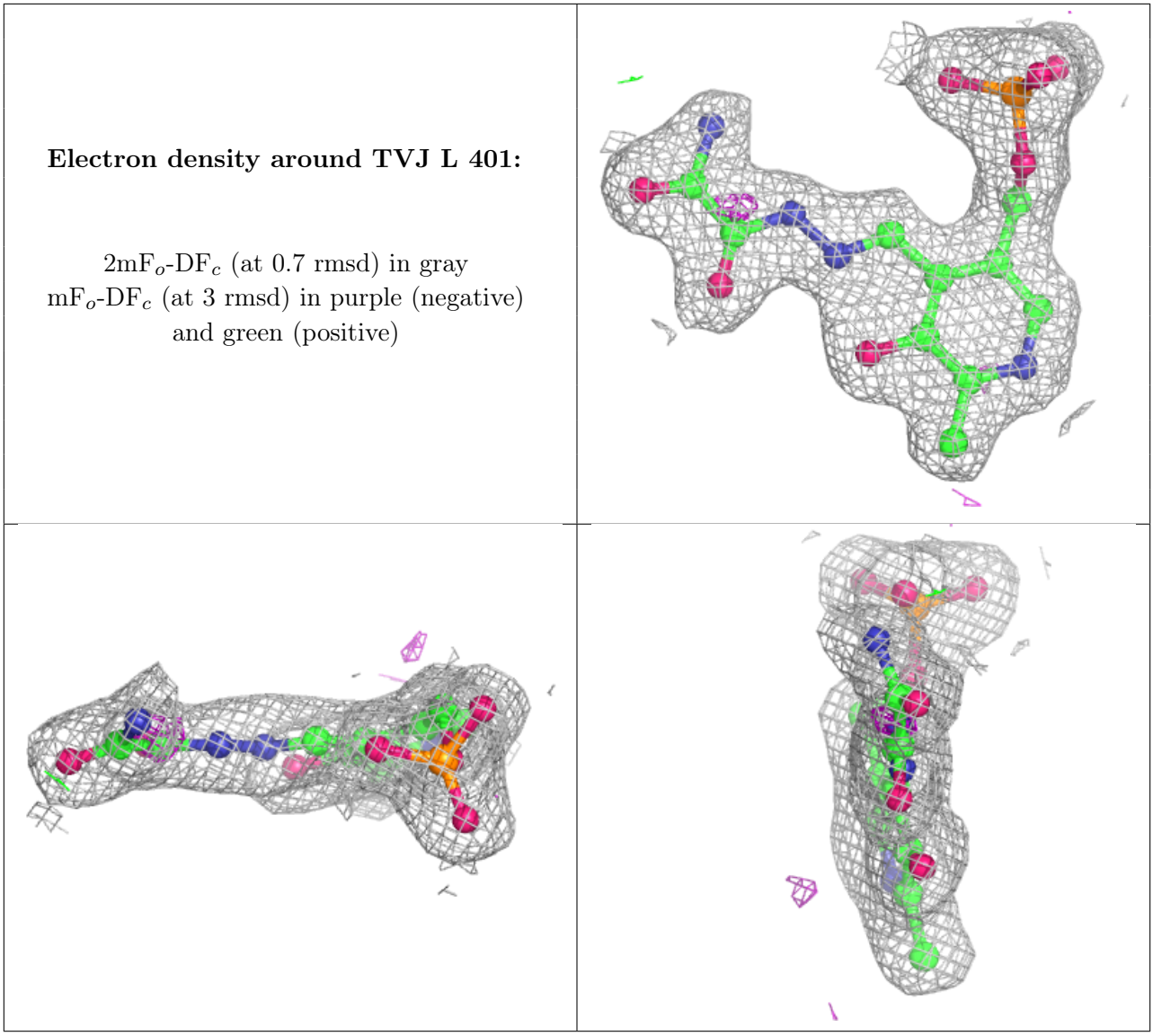






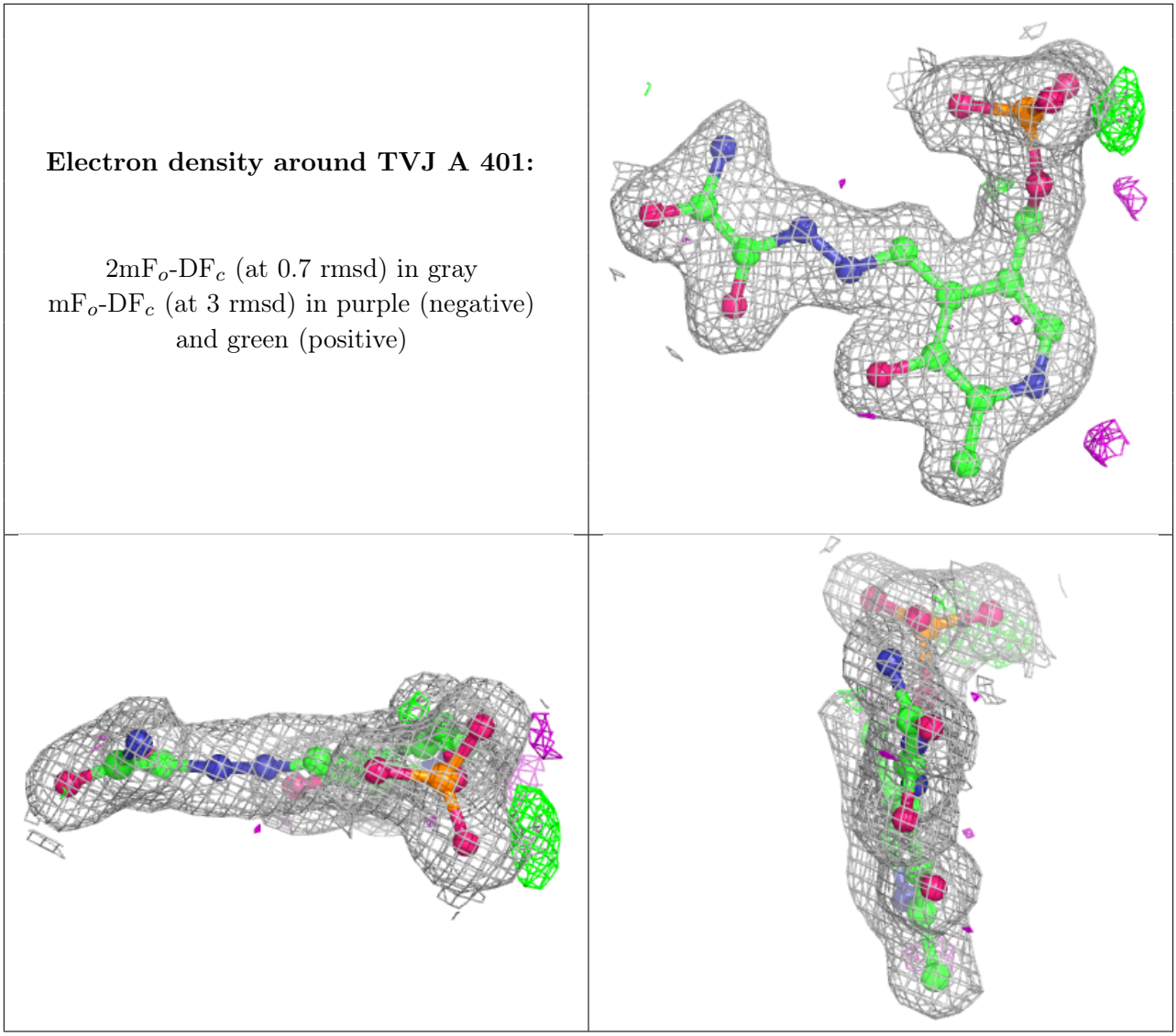
Electron density around TVJ L 401:

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



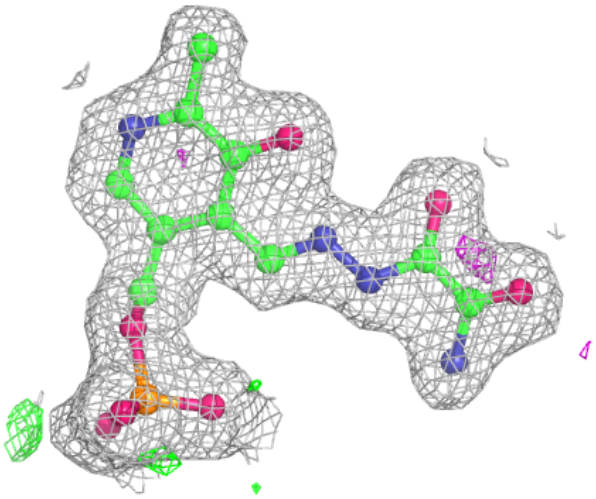
Electron density around TVJ A 401:

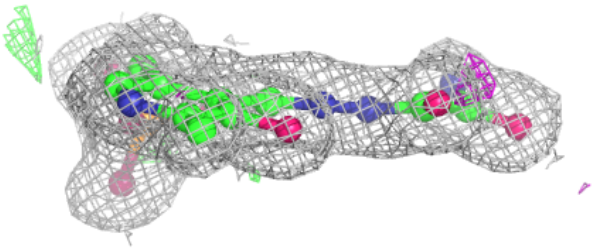
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

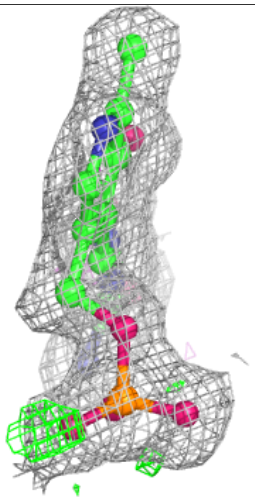


Electron density around TVJ B 401:

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

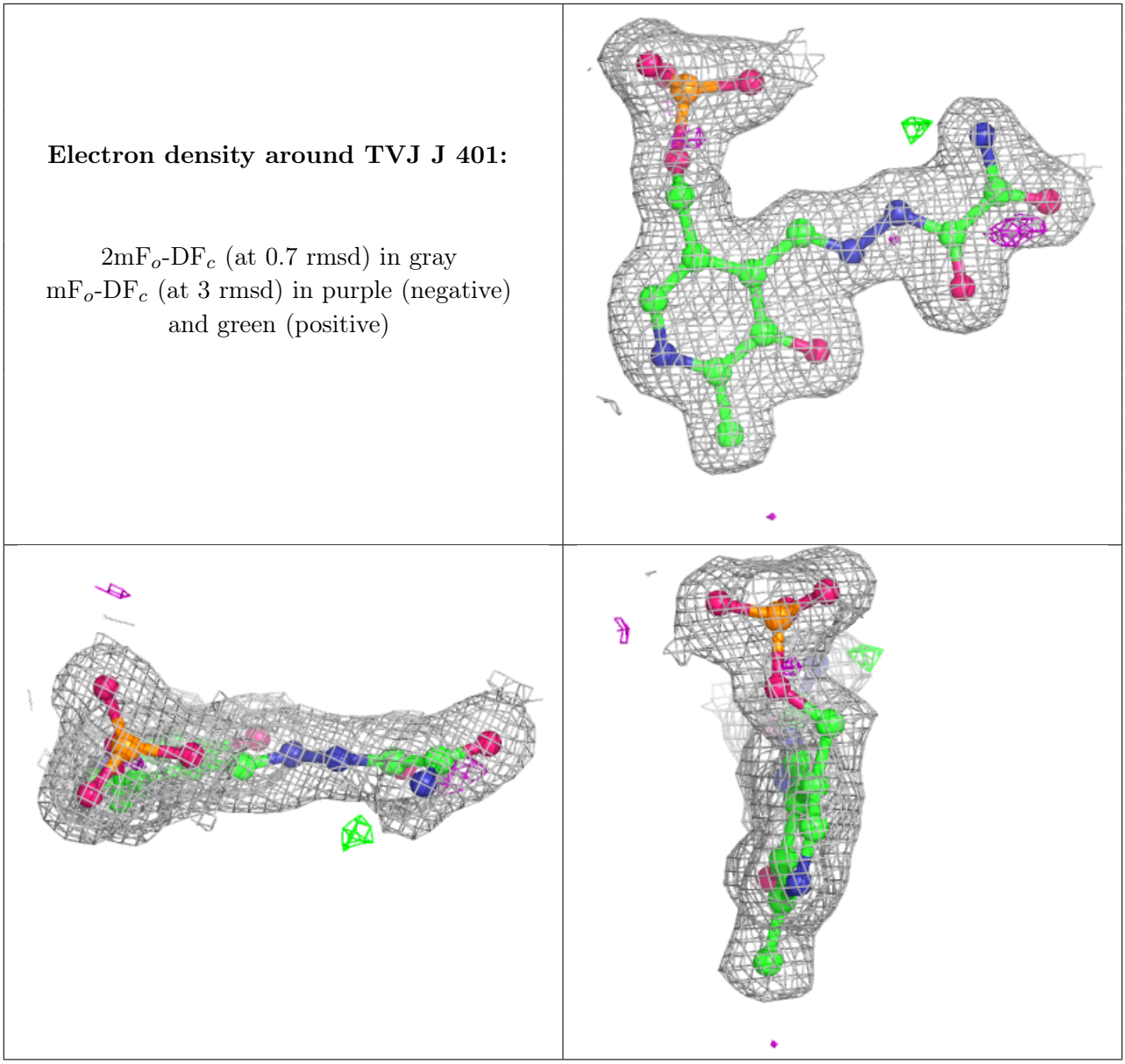






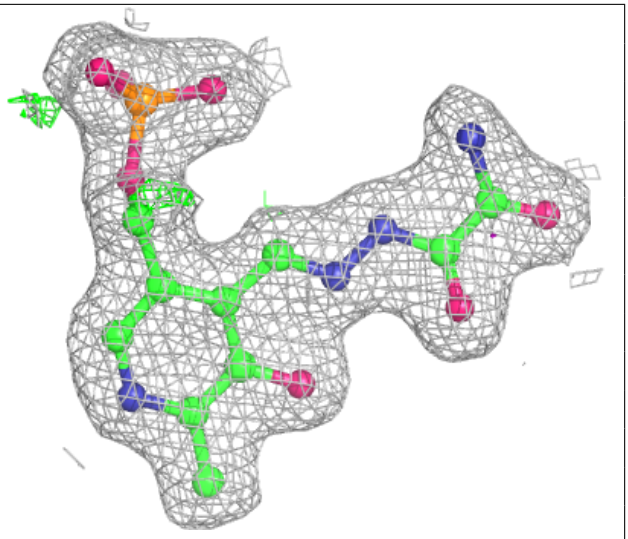
Electron density around TVJ J 401:

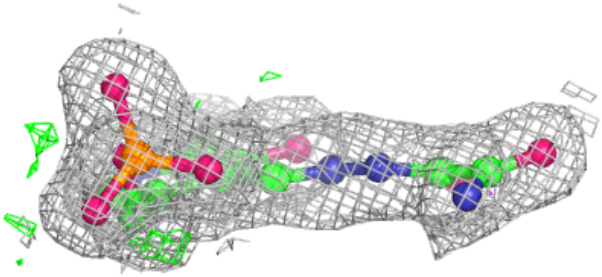
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

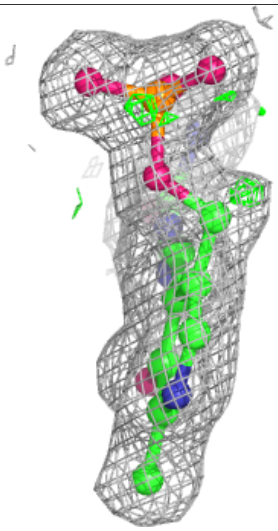


Electron density around TVJ C 401:

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

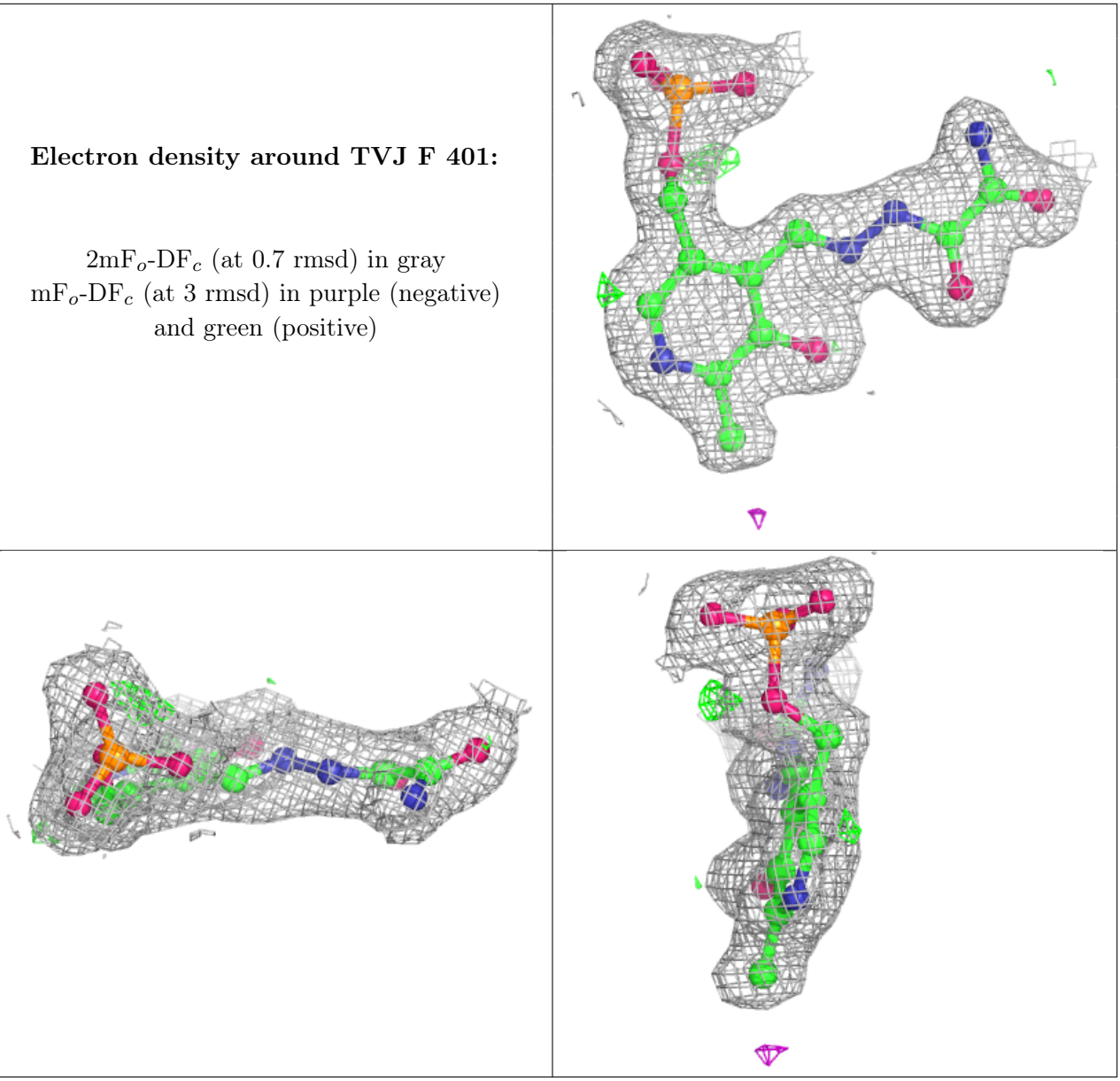






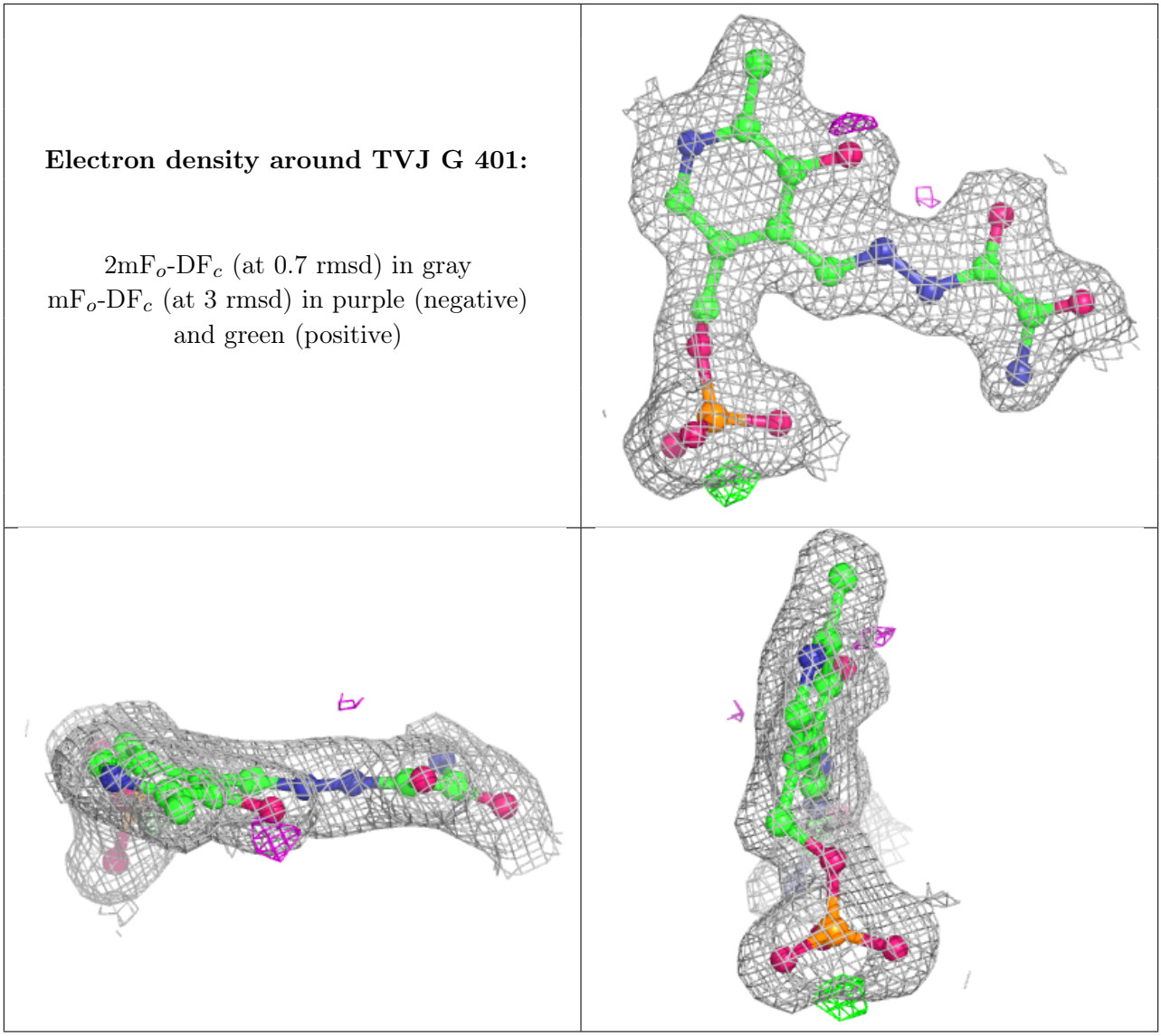
Electron density around TVJ F 401:

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



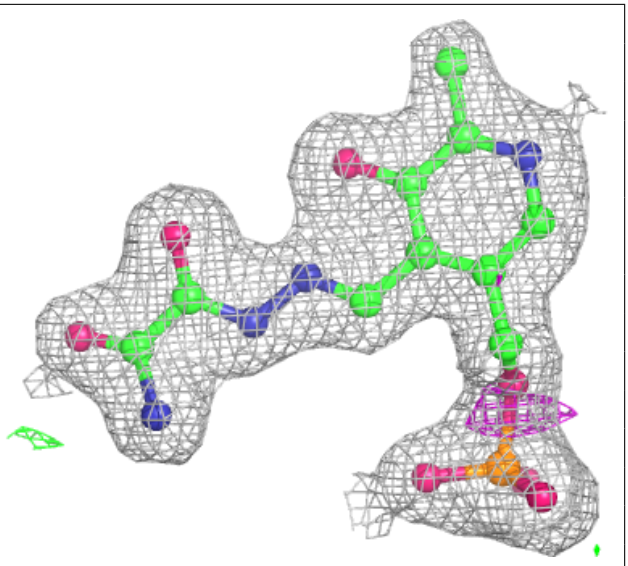
Electron density around TVJ G 401:

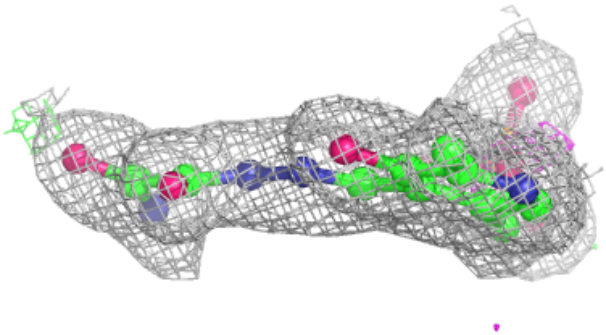
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

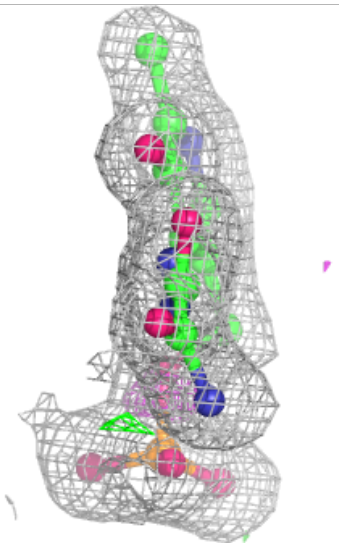


Electron density around TVJ I 401:

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

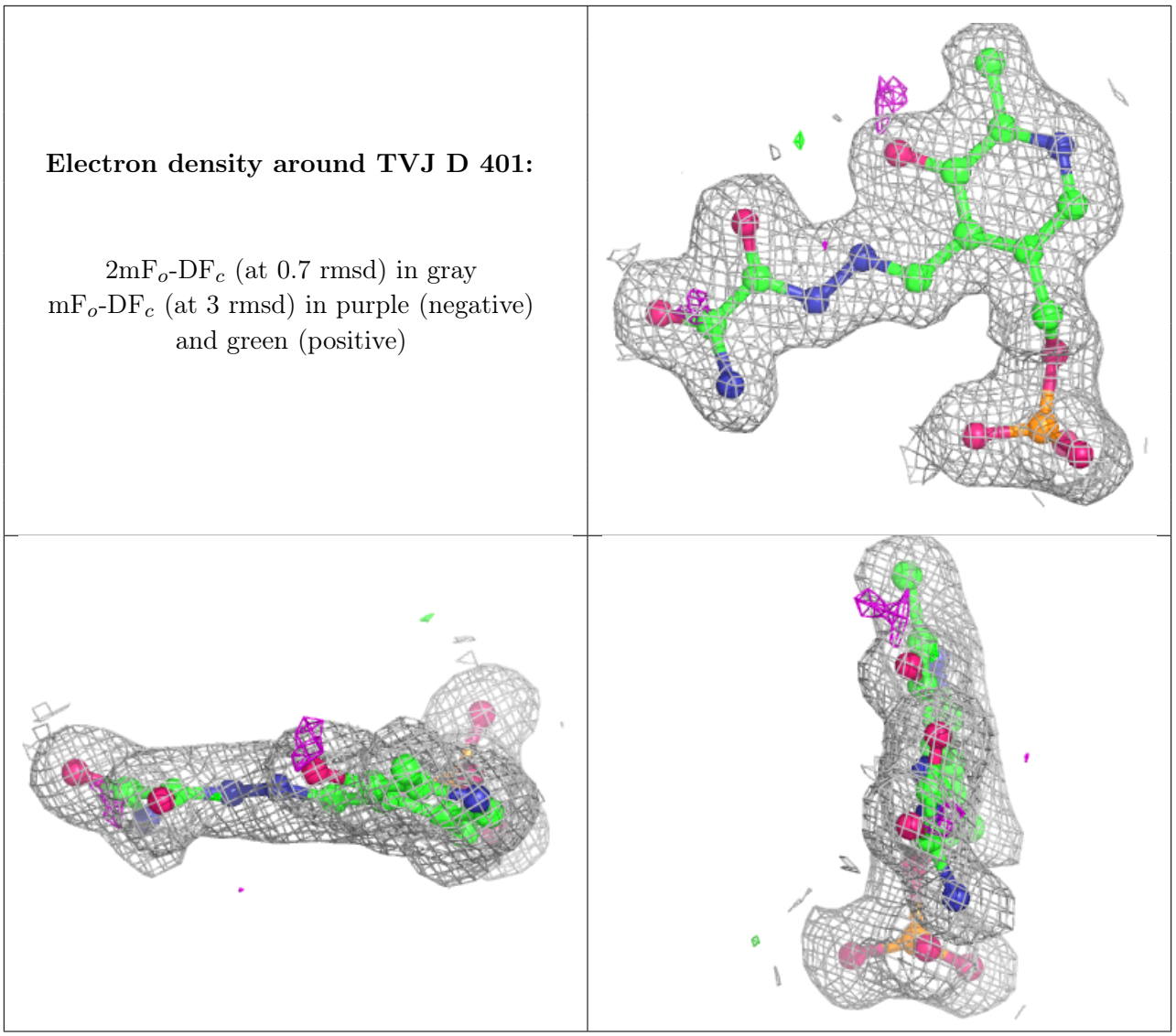






Electron density around TVJ D 401:

$2mF_o$-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.