



# Full wwPDB X-ray Structure Validation Report ⓘ

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

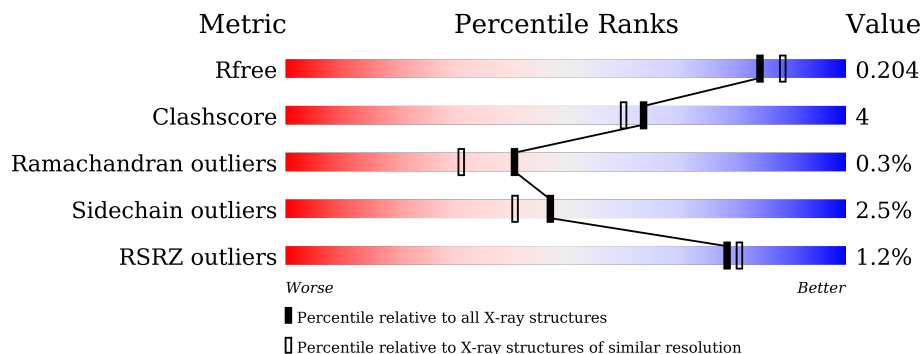
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . 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	 89% 9% ..
1	H	392	 91% 8% ..
1	I	392	 90% 9% ..
1	J	392	 89% 9% ..
1	K	392	 88% 10% ..
1	L	392	 90% 9% ..

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

There are 24 discrepancies between the modelled and reference sequences:

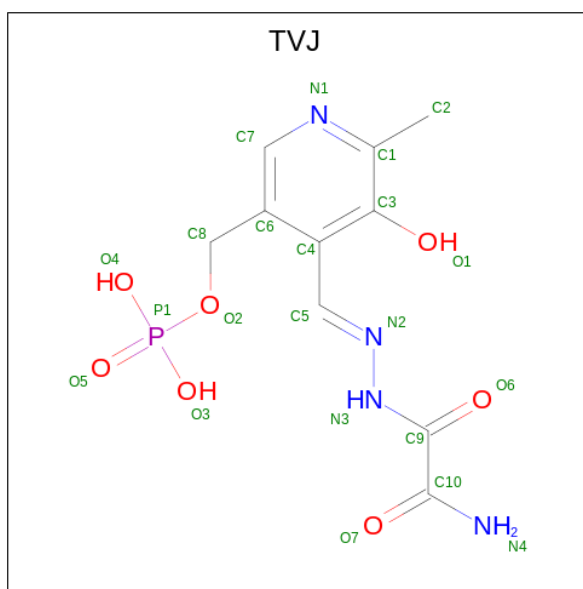
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	expression tag	UNP Q9EQS4
A	9	PRO	-	expression tag	UNP Q9EQS4
B	8	GLY	-	expression tag	UNP Q9EQS4
B	9	PRO	-	expression tag	UNP Q9EQS4
C	8	GLY	-	expression tag	UNP Q9EQS4

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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<sub>10</sub>H<sub>13</sub>N<sub>4</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



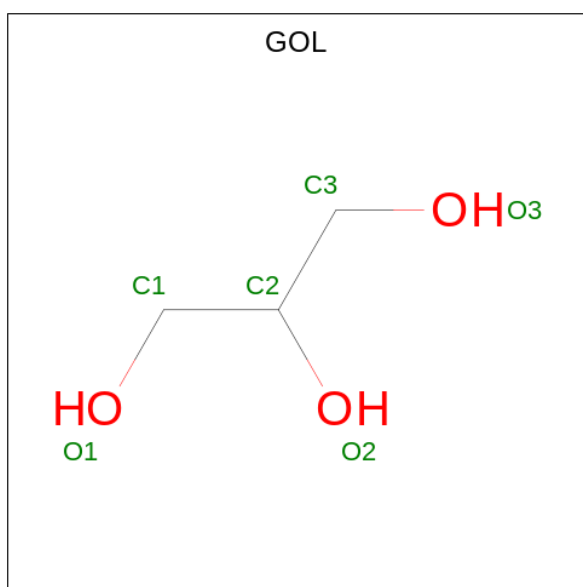
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	22	10	4	7	1	0	0

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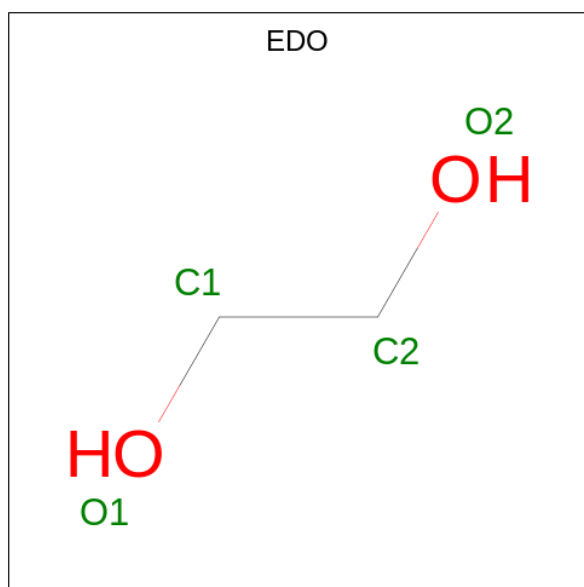
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	C	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	D	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	E	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	H	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	J	1	Total	C	N	O	P	0	0
			22	10	4	7	1		
2	K	1	Total	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<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 5 is water.

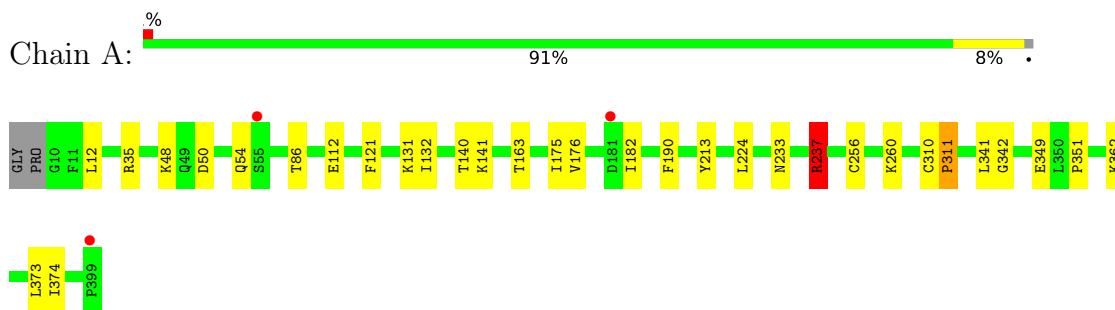
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	288	Total	O	0	0
			288	288		
5	B	285	Total	O	0	0
			285	285		
5	C	280	Total	O	0	0
			280	280		
5	D	299	Total	O	0	0
			299	299		
5	E	243	Total	O	0	0
			243	243		
5	H	237	Total	O	0	0
			237	237		
5	J	252	Total	O	0	0
			252	252		
5	K	228	Total	O	0	0
			228	228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



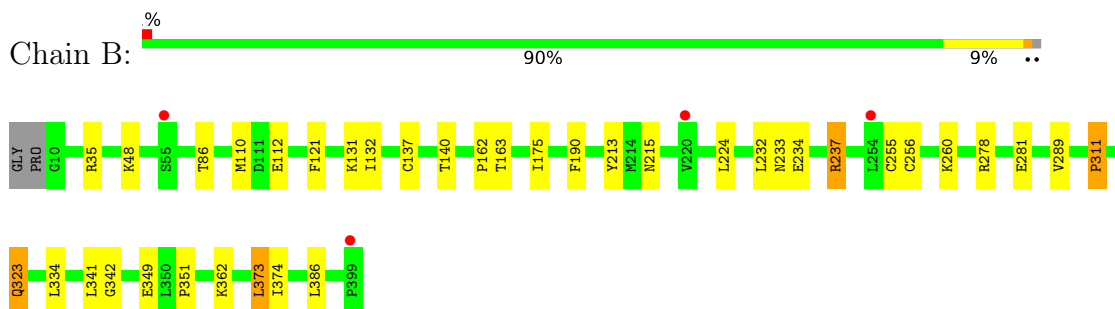
### 3 Residue-property plots [i](#)

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.

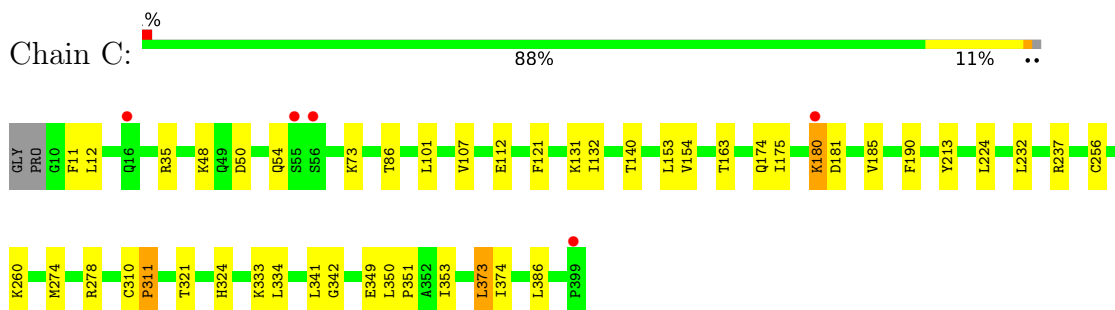
- Molecule 1: Cystathionine gamma-lyase



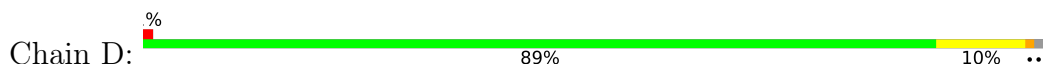
- Molecule 1: Cystathionine gamma-lyase



- Molecule 1: Cystathionine gamma-lyase

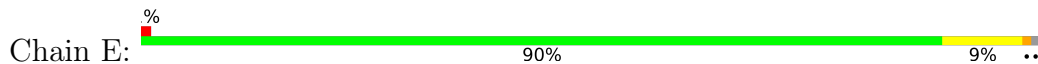


- Molecule 1: Cystathionine gamma-lyase

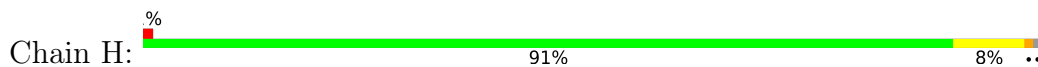




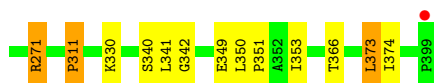
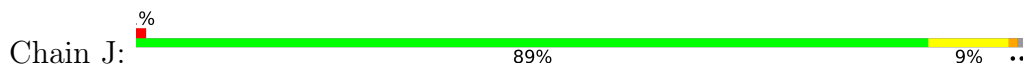
• Molecule 1: Cystathionine gamma-lyase



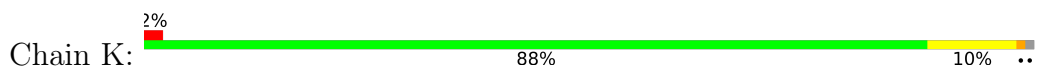
• Molecule 1: Cystathionine gamma-lyase



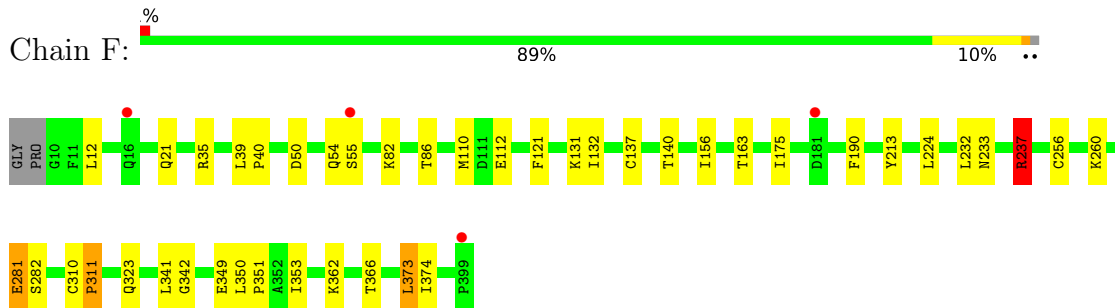
• Molecule 1: Cystathionine gamma-lyase



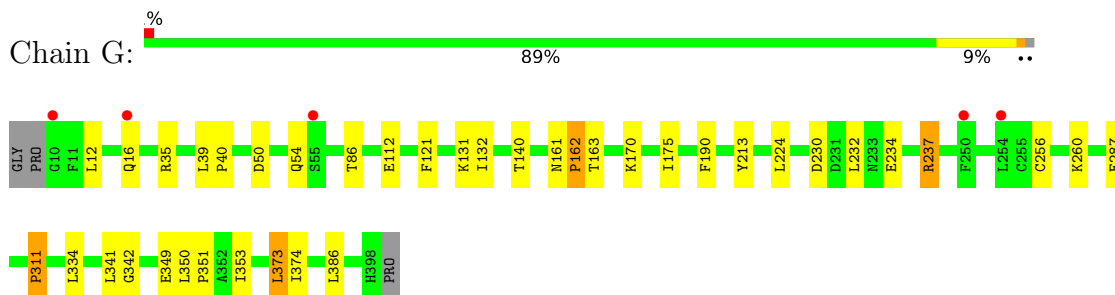
• Molecule 1: Cystathionine gamma-lyase



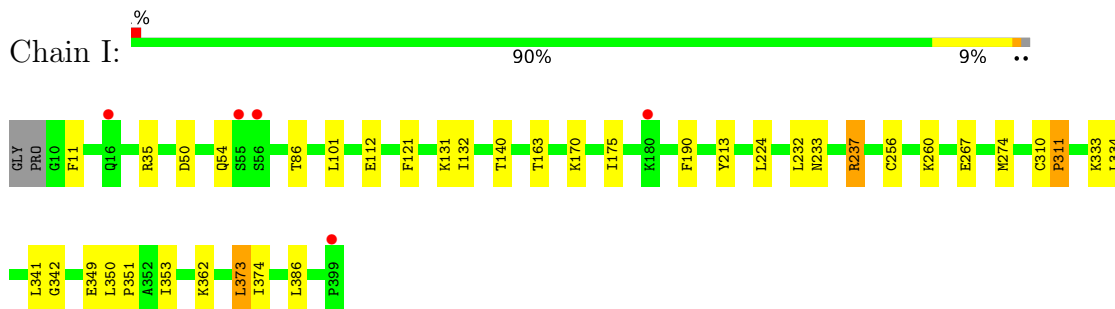
- Molecule 1: Cystathionine gamma-lyase



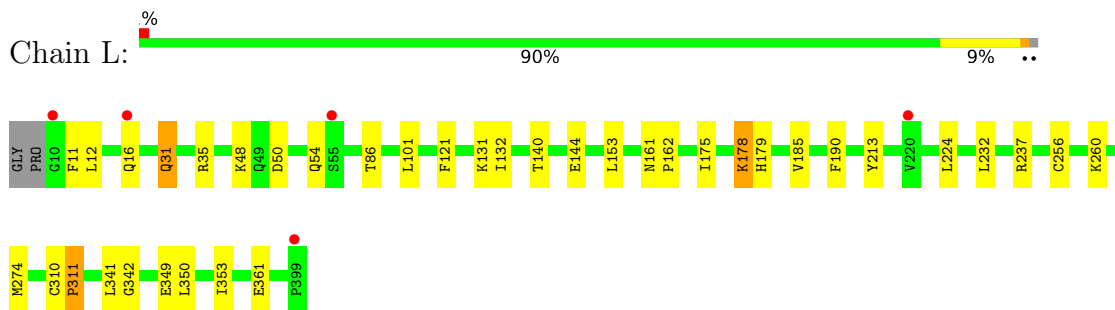
- Molecule 1: Cystathionine gamma-lyase



- Molecule 1: Cystathionine gamma-lyase



- Molecule 1: Cystathionine gamma-lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 1.90Å)	Xtrriage
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 <sup>2</sup> )	19.1	Xtrriage
Anisotropy	0.035	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	39772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: 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

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	B	237	ARG	NE-CZ-NH2	13.93	127.26	120.30
1	G	237	ARG	NE-CZ-NH2	-13.83	113.39	120.30
1	F	237	ARG	NE-CZ-NH2	-13.55	113.53	120.30
1	A	237	ARG	NE-CZ-NH2	-13.53	113.53	120.30
1	K	237	ARG	NE-CZ-NH2	-13.19	113.70	120.30
1	J	237	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	B	35	ARG	NE-CZ-NH2	12.75	126.67	120.30
1	A	35	ARG	NE-CZ-NH2	11.75	126.17	120.30
1	E	237	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	A	237	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	H	237	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	J	237	ARG	NE-CZ-NH1	10.49	125.54	120.30
1	G	237	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	F	237	ARG	NE-CZ-NH1	10.25	125.42	120.30
1	H	35	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	G	35	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	K	35	ARG	NE-CZ-NH2	-9.73	115.44	120.30
1	D	237	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	L	35	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	K	237	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	I	35	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	F	35	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	C	237	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	D	35	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	J	35	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	L	31	GLN	CB-CA-C	-8.88	92.63	110.40
1	A	35	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	L	237	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	E	35	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	D	35	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	C	237	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	D	237	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	B	35	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	C	35	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	C	35	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	L	237	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	K	361	GLU	CB-CG-CD	6.73	132.37	114.20
1	E	35	ARG	NE-CZ-NH2	-5.91	117.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	237	ARG	CB-CG-CD	-5.68	96.83	111.60
1	H	237	ARG	CB-CG-CD	-5.64	96.93	111.60
1	A	237	ARG	CB-CG-CD	-5.58	97.09	111.60
1	E	237	ARG	CB-CG-CD	-5.54	97.19	111.60
1	K	237	ARG	CB-CG-CD	-5.53	97.21	111.60
1	G	35	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	F	237	ARG	CB-CG-CD	-5.41	97.53	111.60
1	J	237	ARG	CB-CG-CD	-5.34	97.72	111.60
1	L	178	LYS	CB-CG-CD	5.16	125.01	111.60
1	L	35	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	H	35	ARG	NE-CZ-NH1	5.03	122.81	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:F:54:GLN:O	1:F:55:SER:OG	1.99	0.80
1:C:274:MET:HE3	5:C:697:HOH:O	1.84	0.76
1:B:48:LYS:HE3	5:C:664:HOH:O	1.86	0.74
1:F:351:PRO:HG2	1:F:373[A]:LEU:HD13	1.71	0.72
1:G:351:PRO:HG2	1:G:373[A]:LEU:HD13	1.72	0.72
1:D:351:PRO:HG2	1:D:373[A]:LEU:HD13	1.72	0.72
1:B:351:PRO:HG2	1:B:373[A]:LEU:HD13	1.72	0.72
1:I:351:PRO:HG2	1:I:373[A]:LEU:HD13	1.71	0.71
1:J:330:LYS:HE2	5:J:709:HOH:O	1.91	0.71
1:D:39[B]:LEU:HD11	1:D:67:THR:HA	1.72	0.71
1:K:351:PRO:HG2	1:K:373[A]:LEU:HD13	1.72	0.70
1:L:274:MET:HE3	5:L:683:HOH:O	1.91	0.70
1:E:351:PRO:HG2	1:E:373[A]:LEU:HD13	1.73	0.70
1:C:351:PRO:HG2	1:C:373[A]:LEU:HD13	1.72	0.70
1:H:351:PRO:HG2	1:H:373[A]:LEU:HD13	1.72	0.70
1:A:351:PRO:HG2	1:A:373[B]:LEU:HD13	1.75	0.69
1:J:351:PRO:HG2	1:J:373[A]:LEU:HD13	1.72	0.69
1:F:237:ARG:HD3	5:F:4073:HOH:O	1.94	0.68
1:D:11:PHE:CZ	1:D:310[B]:CYS:SG	2.87	0.68
1:H:153[B]:LEU:HD13	1:H:154:VAL:N	2.10	0.67
1:C:153[B]:LEU:HD21	1:C:185:VAL:HG23	1.76	0.66
1:J:43:LEU:O	4:J:405:EDO:H12	1.95	0.66
1:G:230:ASP:O	1:G:234:GLU:HG2	1.98	0.64
1:C:11:PHE:CZ	1:C:310[B]:CYS:SG	2.91	0.64
1:G:334[B]:LEU:HD22	1:G:386:LEU:HD23	1.79	0.64
1:F:110[B]:MET:HG2	1:F:156[B]:ILE:HG12	1.80	0.64
1:K:153[B]:LEU:HD21	1:K:185:VAL:HG23	1.80	0.63
1:A:310[B]:CYS:SG	5:A:723:HOH:O	2.19	0.62
1:B:215:ASN:HB2	1:B:255[B]:CYS:SG	2.39	0.62
1:I:274[A]:MET:CE	5:I:630:HOH:O	2.44	0.61
1:J:271[A]:ARG:HH11	1:J:271[A]:ARG:HB3	1.65	0.61
1:H:50:ASP:H	1:H:54:GLN:HE22	1.48	0.61
1:C:50:ASP:H	1:C:54:GLN:NE2	1.99	0.61
1:I:50:ASP:H	1:I:54:GLN:NE2	1.99	0.60
1:B:190:PHE:O	1:B:311:PRO:HG3	2.02	0.60
1:H:50:ASP:H	1:H:54:GLN:NE2	2.00	0.60
1:A:50:ASP:H	1:A:54:GLN:NE2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:ASP:H	1:F:54:GLN:NE2	2.00	0.60
1:L:50:ASP:H	1:L:54:GLN:NE2	2.00	0.60
1:E:50:ASP:H	1:E:54:GLN:NE2	2.00	0.59
2:G:401:TVJ:O1	2:G:401:TVJ:N2	2.34	0.59
1:E:190:PHE:O	1:E:311:PRO:HG3	2.02	0.59
1:G:50:ASP:H	1:G:54:GLN:NE2	2.00	0.59
1:C:190[A]:PHE:O	1:C:311:PRO:HG3	2.02	0.59
1:J:110:MET:CE	1:J:156[A]:ILE:CD1	2.81	0.59
2:L:401:TVJ:N2	2:L:401:TVJ:O1	2.35	0.59
1:C:190[B]:PHE:O	1:C:311:PRO:HG3	2.02	0.59
1:H:190:PHE:O	1:H:311:PRO:HG3	2.02	0.59
1:A:190:PHE:O	1:A:311:PRO:HG3	2.02	0.59
1:I:190:PHE:O	1:I:311:PRO:HG3	2.03	0.59
1:L:153[B]:LEU:HD21	1:L:185:VAL:HG23	1.85	0.59
1:F:190:PHE:O	1:F:311:PRO:HG3	2.03	0.59
1:D:50:ASP:H	1:D:54:GLN:NE2	2.00	0.59
1:K:190:PHE:O	1:K:311:PRO:HG3	2.03	0.59
1:K:287:GLU:HG2	5:K:712:HOH:O	2.02	0.59
1:J:190:PHE:O	1:J:311:PRO:HG3	2.03	0.58
1:F:50:ASP:H	1:F:54:GLN:HE22	1.51	0.58
1:J:50:ASP:H	1:J:54:GLN:NE2	2.01	0.58
1:J:110:MET:HE2	1:J:156[A]:ILE:CD1	2.33	0.58
1:G:190:PHE:O	1:G:311:PRO:HG3	2.02	0.58
1:L:190[B]:PHE:O	1:L:311:PRO:HG3	2.04	0.58
1:C:256:CYS:SG	1:C:260:LYS:NZ	2.77	0.58
1:J:118:ASN:ND2	4:J:402:EDO:O1	2.36	0.57
1:G:256:CYS:SG	1:G:260:LYS:NZ	2.77	0.57
1:K:256:CYS:SG	1:K:260:LYS:NZ	2.78	0.57
1:J:340:SER:OG	4:J:403:EDO:O1	2.14	0.57
1:I:11:PHE:CZ	1:I:310[B]:CYS:SG	2.97	0.57
1:K:214:MET:HG2	4:K:403:EDO:H11	1.87	0.57
1:A:362:LYS:NZ	5:A:501:HOH:O	2.37	0.56
1:D:190:PHE:O	1:D:311:PRO:HG3	2.04	0.56
1:L:190[A]:PHE:O	1:L:311:PRO:HG3	2.04	0.56
1:H:256:CYS:SG	1:H:260:LYS:NZ	2.78	0.56
1:B:256:CYS:SG	1:B:260:LYS:NZ	2.79	0.56
1:B:323:GLN:NE2	5:B:506:HOH:O	2.38	0.56
1:J:16:GLN:HE21	1:J:16:GLN:HA	1.70	0.56
1:D:256:CYS:SG	1:D:260:LYS:NZ	2.79	0.56
2:C:401:TVJ:N2	2:C:401:TVJ:O1	2.38	0.56
1:J:111:ASP:O	4:J:402:EDO:H12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:256:CYS:SG	1:L:260:LYS:NZ	2.78	0.56
1:J:61:SER:OG	4:J:405:EDO:H11	2.06	0.55
1:K:107:VAL:HG13	1:K:153[B]:LEU:HD12	1.87	0.55
1:G:50:ASP:H	1:G:54:GLN:HE22	1.54	0.55
1:A:256:CYS:SG	1:A:260:LYS:NZ	2.79	0.55
1:C:321:THR:H	1:C:324:HIS:HD2	1.55	0.55
1:J:237:ARG:HD3	5:J:707:HOH:O	2.06	0.55
1:D:50:ASP:H	1:D:54:GLN:HE22	1.54	0.55
1:I:256:CYS:SG	1:I:260:LYS:NZ	2.79	0.55
1:E:174:GLN:HG3	5:E:647:HOH:O	2.06	0.55
1:F:281:GLU:HG3	5:F:3927:HOH:O	2.06	0.55
1:J:256:CYS:SG	1:J:260:LYS:NZ	2.80	0.55
1:F:256:CYS:SG	1:F:260:LYS:NZ	2.79	0.55
1:I:333:LYS:HE3	5:I:699:HOH:O	2.06	0.55
5:B:642:HOH:O	1:C:48:LYS:HE3	2.06	0.55
2:H:401:TVJ:O1	2:H:401:TVJ:N2	2.37	0.55
1:G:373[A]:LEU:HD22	1:G:374:ILE:N	2.21	0.55
1:J:373[A]:LEU:HD22	1:J:374:ILE:N	2.23	0.54
1:C:50:ASP:H	1:C:54:GLN:HE22	1.54	0.54
1:E:256:CYS:SG	1:E:260:LYS:NZ	2.81	0.54
1:H:373[A]:LEU:HD22	1:H:374:ILE:N	2.23	0.54
1:C:107:VAL:HG13	1:C:153[B]:LEU:HD12	1.90	0.54
1:J:218:SER:HA	4:J:403:EDO:H11	1.90	0.54
1:K:373[A]:LEU:HD22	1:K:374:ILE:N	2.23	0.54
1:A:50:ASP:H	1:A:54:GLN:HE22	1.57	0.53
1:I:373[A]:LEU:HD22	1:I:374:ILE:N	2.24	0.53
1:E:373[A]:LEU:HD22	1:E:374:ILE:N	2.23	0.53
2:D:401:TVJ:N2	2:D:401:TVJ:O1	2.41	0.53
1:F:373[A]:LEU:HD22	1:F:374:ILE:N	2.22	0.53
1:I:50:ASP:H	1:I:54:GLN:HE22	1.56	0.53
1:C:373[A]:LEU:HD22	1:C:374:ILE:N	2.23	0.53
1:D:373[A]:LEU:HD22	1:D:374:ILE:N	2.23	0.53
1:K:323:GLN:NE2	5:K:502:HOH:O	2.40	0.53
1:I:351:PRO:HG2	1:I:373[A]:LEU:CD1	2.39	0.53
1:B:373[A]:LEU:HD22	1:B:374:ILE:N	2.24	0.53
1:A:373[B]:LEU:HD22	1:A:374:ILE:N	2.23	0.53
1:D:11:PHE:HZ	1:D:310[B]:CYS:SG	2.32	0.53
1:E:50:ASP:H	1:E:54:GLN:HE22	1.56	0.53
1:H:351:PRO:HG2	1:H:373[A]:LEU:CD1	2.39	0.52
2:I:401:TVJ:O1	2:I:401:TVJ:N2	2.41	0.52
1:L:179:HIS:HE1	5:L:698:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:VAL:HG13	1:A:182:ILE:HB	1.91	0.52
1:G:351:PRO:HG2	1:G:373[A]:LEU:CD1	2.38	0.52
1:L:50:ASP:H	1:L:54:GLN:HE22	1.58	0.52
1:C:351:PRO:HG2	1:C:373[A]:LEU:CD1	2.39	0.52
1:J:61:SER:CB	4:J:405:EDO:H11	2.40	0.52
1:D:351:PRO:HG2	1:D:373[A]:LEU:CD1	2.39	0.52
1:H:237:ARG:HD3	5:H:696:HOH:O	2.10	0.52
1:F:310[B]:CYS:SG	5:F:4082:HOH:O	2.36	0.52
1:C:274:MET:CE	5:C:697:HOH:O	2.52	0.51
1:L:310[B]:CYS:SG	5:L:681:HOH:O	2.59	0.51
1:H:121:PHE:HB3	1:H:132:ILE:HG21	1.92	0.51
1:J:351:PRO:HG2	1:J:373[A]:LEU:CD1	2.39	0.51
2:F:401:TVJ:O1	2:F:401:TVJ:N2	2.42	0.51
1:E:326:GLN:O	1:E:330:LYS:HE3	2.11	0.51
1:J:50:ASP:H	1:J:54:GLN:HE22	1.57	0.51
1:F:86[A]:THR:HG22	1:F:224:LEU:CD2	2.41	0.51
1:B:334:LEU:HD22	1:B:386:LEU:HD23	1.93	0.51
1:B:351:PRO:HG2	1:B:373[A]:LEU:CD1	2.39	0.51
1:C:86:THR:HG22	1:C:224:LEU:CD2	2.41	0.51
1:D:101:LEU:O	3:D:402:GOL:H2	2.11	0.51
1:B:86:THR:HG22	1:B:224:LEU:CD2	2.41	0.51
1:J:121:PHE:HB3	1:J:132:ILE:HG21	1.93	0.51
1:K:86:THR:HG22	1:K:224:LEU:CD2	2.41	0.51
1:L:86:THR:HG22	1:L:224:LEU:CD2	2.41	0.51
1:A:121:PHE:HB3	1:A:132:ILE:HG21	1.93	0.50
1:K:121:PHE:HB3	1:K:132:ILE:HG21	1.93	0.50
1:B:234:GLU:HG3	5:B:751:HOH:O	2.12	0.50
1:E:86:THR:HG22	1:E:224:LEU:CD2	2.42	0.50
1:G:86:THR:HG22	1:G:224:LEU:CD2	2.41	0.50
1:D:86:THR:HG22	1:D:224:LEU:CD2	2.41	0.50
1:F:351:PRO:HG2	1:F:373[A]:LEU:CD1	2.39	0.50
1:D:121:PHE:HB3	1:D:132:ILE:HG21	1.94	0.50
1:I:334[B]:LEU:HD22	1:I:386:LEU:HD23	1.93	0.50
1:D:16:GLN:HE21	1:D:16:GLN:HA	1.76	0.50
1:J:86:THR:HG22	1:J:224:LEU:CD2	2.41	0.50
1:H:86:THR:HG22	1:H:224:LEU:CD2	2.42	0.50
1:F:21:GLN:NE2	5:F:3904:HOH:O	2.45	0.50
1:C:333:LYS:NZ	5:C:509:HOH:O	2.44	0.50
1:K:351:PRO:HG2	1:K:373[A]:LEU:CD1	2.40	0.50
1:A:86:THR:HG22	1:A:224:LEU:CD2	2.42	0.49
1:F:282:SER:HB3	5:F:4105:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86[A]:THR:HG22	1:F:224:LEU:HD23	1.95	0.49
1:C:121:PHE:HB3	1:C:132:ILE:HG21	1.94	0.49
1:E:351:PRO:HG2	1:E:373[A]:LEU:CD1	2.40	0.49
1:G:121:PHE:HB3	1:G:132:ILE:HG21	1.95	0.49
1:A:176:VAL:HG13	1:A:182:ILE:CG2	2.43	0.49
1:B:112:GLU:OE1	1:B:163:THR:OG1	2.27	0.49
2:J:401:TVJ:O1	2:J:401:TVJ:N2	2.45	0.49
1:A:351:PRO:HG2	1:A:373[B]:LEU:CD1	2.40	0.48
1:E:112:GLU:OE1	1:E:163:THR:OG1	2.27	0.48
1:L:121:PHE:HB3	1:L:132:ILE:HG21	1.95	0.48
1:B:234:GLU:CG	5:B:751:HOH:O	2.61	0.48
1:I:86:THR:HG22	1:I:224:LEU:CD2	2.42	0.48
1:B:86:THR:HG22	1:B:224:LEU:HD23	1.95	0.48
1:F:82:LYS:HA	1:F:82:LYS:HE2	1.94	0.48
1:B:121:PHE:HB3	1:B:132:ILE:HG21	1.95	0.48
1:C:86:THR:HG22	1:C:224:LEU:HD23	1.95	0.48
1:J:218:SER:CB	4:J:403:EDO:H22	2.40	0.48
1:E:333:LYS:HD2	5:E:701:HOH:O	2.14	0.48
1:K:86:THR:HG22	1:K:224:LEU:HD23	1.95	0.48
1:E:140:THR:HB	1:E:175:ILE:CD1	2.44	0.48
1:L:361:GLU:HG3	5:L:606:HOH:O	2.14	0.48
1:A:48:LYS:HE3	5:D:658:HOH:O	2.14	0.47
1:C:101:LEU:O	3:C:402:GOL:H2	2.15	0.47
2:E:401:TVJ:N2	2:E:401:TVJ:O1	2.46	0.47
1:J:112:GLU:OE1	1:J:163:THR:OG1	2.29	0.47
1:A:86:THR:HG22	1:A:224:LEU:HD23	1.96	0.47
1:H:86:THR:HG22	1:H:224:LEU:HD23	1.96	0.47
1:B:362:LYS:HG3	5:B:737:HOH:O	2.13	0.47
1:E:86:THR:HG22	1:E:224:LEU:HD23	1.97	0.47
1:I:101:LEU:O	3:I:402:GOL:H2	2.15	0.47
1:G:86:THR:HG22	1:G:224:LEU:HD23	1.96	0.47
1:C:153[B]:LEU:HD22	1:C:154:VAL:N	2.30	0.47
1:D:86:THR:HG22	1:D:224:LEU:HD23	1.95	0.47
1:H:153[B]:LEU:CD1	1:H:154:VAL:N	2.78	0.47
1:C:140:THR:HB	1:C:175:ILE:CD1	2.46	0.46
1:J:86:THR:HG22	1:J:224:LEU:HD23	1.96	0.46
2:B:401:TVJ:O1	2:B:401:TVJ:N2	2.46	0.46
1:F:121:PHE:HB3	1:F:132:ILE:HG21	1.97	0.46
1:B:278:ARG:NH1	5:B:503:HOH:O	2.36	0.46
1:E:127:GLU:HG3	3:H:402:GOL:H32	1.98	0.46
1:L:86:THR:HG22	1:L:224:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:LEU:HD22	1:C:386:LEU:HD23	1.97	0.46
1:I:121:PHE:HB3	1:I:132:ILE:HG21	1.96	0.46
1:E:121:PHE:HB3	1:E:132:ILE:HG21	1.96	0.46
1:B:140:THR:HB	1:B:175:ILE:CD1	2.45	0.46
1:E:174:GLN:HB3	5:E:712:HOH:O	2.15	0.46
1:G:334[B]:LEU:HD22	1:G:386:LEU:CD2	2.45	0.46
1:B:110[B]:MET:SD	1:B:137:CYS:HB2	2.55	0.46
1:C:278:ARG:NH1	5:C:502:HOH:O	2.32	0.46
1:E:237:ARG:HD3	5:E:707:HOH:O	2.15	0.46
1:K:30:GLU:OE1	1:L:48:LYS:HE2	2.16	0.46
1:I:333:LYS:CE	5:I:699:HOH:O	2.64	0.46
1:B:213:TYR:CE1	1:B:342:GLY:HA2	2.51	0.45
2:K:401:TVJ:O1	2:K:401:TVJ:N2	2.48	0.45
1:A:140:THR:HB	1:A:175:ILE:CD1	2.47	0.45
1:D:16:GLN:HA	1:D:16:GLN:NE2	2.31	0.45
5:I:651:HOH:O	1:L:48:LYS:HE3	2.17	0.45
1:H:140:THR:HB	1:H:175:ILE:CD1	2.47	0.45
1:C:174:GLN:HB3	5:C:738:HOH:O	2.15	0.45
1:K:192:SER:HA	4:K:403:EDO:C1	2.47	0.45
1:K:237:ARG:HD3	5:K:695:HOH:O	2.17	0.45
1:A:213:TYR:CE1	1:A:342:GLY:HA2	2.52	0.45
2:A:401:TVJ:O1	2:A:401:TVJ:N2	2.48	0.45
1:K:334[B]:LEU:HD21	1:K:381:GLU:HG2	1.99	0.45
1:I:140:THR:HB	1:I:175:ILE:CD1	2.46	0.45
1:J:110:MET:HE2	1:J:156[A]:ILE:HD11	1.99	0.44
1:D:110[B]:MET:SD	1:D:137:CYS:HB2	2.57	0.44
1:J:140:THR:HB	1:J:175:ILE:CD1	2.46	0.44
1:G:140:THR:HB	1:G:175:ILE:CD1	2.47	0.44
1:L:144:GLU:HG3	5:L:698:HOH:O	2.16	0.44
1:D:213:TYR:CE1	1:D:342:GLY:HA2	2.52	0.44
1:C:213:TYR:CE1	1:C:342:GLY:HA2	2.52	0.44
1:K:140:THR:HB	1:K:175:ILE:CD1	2.47	0.44
1:L:140:THR:HB	1:L:175:ILE:CD1	2.47	0.44
1:D:140:THR:HB	1:D:175:ILE:CD1	2.47	0.44
5:J:696:HOH:O	1:K:48:LYS:HE3	2.17	0.44
1:K:213:TYR:CE1	1:K:342:GLY:HA2	2.53	0.44
1:C:112:GLU:OE1	1:C:163:THR:OG1	2.28	0.44
1:J:110:MET:CE	1:J:156[A]:ILE:HD11	2.48	0.44
1:G:213:TYR:CE1	1:G:342:GLY:HA2	2.53	0.44
1:I:362:LYS:HG3	5:I:601:HOH:O	2.18	0.44
1:C:321:THR:H	1:C:324:HIS:CD2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39[B]:LEU:HA	1:D:40:PRO:HD3	1.88	0.44
1:D:112:GLU:OE1	1:D:163:THR:OG1	2.28	0.44
1:I:86:THR:HG22	1:I:224:LEU:HD23	1.99	0.44
1:I:112:GLU:OE1	1:I:163:THR:OG1	2.29	0.44
1:F:112:GLU:OE1	1:F:163:THR:OG1	2.28	0.44
1:I:350:LEU:HD23	1:I:353:ILE:HD12	2.00	0.44
4:J:403:EDO:C1	5:J:654:HOH:O	2.66	0.44
1:L:101:LEU:O	3:L:402:GOL:H2	2.18	0.44
1:E:213:TYR:CE1	1:E:342:GLY:HA2	2.53	0.43
1:J:43:LEU:O	4:J:405:EDO:C1	2.65	0.43
1:C:73:LYS:HE3	5:C:731:HOH:O	2.18	0.43
1:H:112:GLU:OE1	1:H:163:THR:OG1	2.28	0.43
1:H:278:ARG:NH1	5:H:504:HOH:O	2.40	0.43
1:G:161:ASN:HA	1:G:162:PRO:HA	1.88	0.43
1:J:61:SER:OG	4:J:405:EDO:C1	2.66	0.43
1:A:112:GLU:OE1	1:A:163:THR:OG1	2.28	0.43
1:L:350:LEU:HD23	1:L:353:ILE:HD12	2.01	0.43
1:I:213:TYR:CE1	1:I:342:GLY:HA2	2.53	0.43
1:L:11:PHE:CZ	1:L:310[B]:CYS:SG	3.11	0.43
1:H:213:TYR:CE1	1:H:342:GLY:HA2	2.53	0.43
1:J:213:TYR:CE1	1:J:342:GLY:HA2	2.54	0.43
1:F:140:THR:HB	1:F:175:ILE:CD1	2.49	0.43
1:F:350:LEU:HD23	1:F:353:ILE:HD12	2.00	0.43
1:B:281:GLU:HB2	1:B:289[B]:VAL:HG11	2.01	0.43
1:G:112:GLU:OE1	1:G:163:THR:OG1	2.29	0.43
1:L:213:TYR:CE1	1:L:342:GLY:HA2	2.54	0.43
1:D:333:LYS:CD	5:D:737:HOH:O	2.67	0.43
1:K:161:ASN:HA	1:K:162:PRO:HA	1.88	0.43
1:F:213:TYR:CE1	1:F:342:GLY:HA2	2.54	0.42
1:D:350:LEU:HD23	1:D:353:ILE:HD12	2.01	0.42
1:E:161:ASN:HA	1:E:162:PRO:HA	1.88	0.42
1:J:350:LEU:HD23	1:J:353:ILE:HD12	2.01	0.42
1:G:350:LEU:HD23	1:G:353:ILE:HD12	2.01	0.42
1:C:180:LYS:CE	1:C:181:ASP:HB2	2.49	0.42
1:C:350:LEU:HD23	1:C:353:ILE:HD12	2.01	0.42
1:F:39:LEU:HA	1:F:40:PRO:HD3	1.91	0.42
1:L:179:HIS:HD2	5:L:704:HOH:O	2.01	0.42
1:J:110:MET:HE1	1:J:156[A]:ILE:CD1	2.48	0.42
1:E:333:LYS:CD	5:E:701:HOH:O	2.68	0.42
1:E:350:LEU:HD23	1:E:353:ILE:HD12	2.02	0.42
1:E:330:LYS:HE2	1:H:52:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:TRP:HA	4:J:404:EDO:H11	2.01	0.42
1:J:271[A]:ARG:HB3	1:J:271[A]:ARG:NH1	2.34	0.42
1:K:214:MET:HG2	4:K:403:EDO:C1	2.50	0.42
1:G:39:LEU:HA	1:G:40:PRO:HD3	1.93	0.42
1:H:350:LEU:HD23	1:H:353:ILE:HD12	2.01	0.42
1:K:298:PRO:HG2	5:K:617:HOH:O	2.20	0.42
1:L:161:ASN:HA	1:L:162:PRO:HA	1.88	0.42
1:A:233:ASN:HD21	1:A:237:ARG:HH11	1.67	0.41
1:C:153[B]:LEU:HD21	1:C:185:VAL:CG2	2.47	0.41
1:K:153[B]:LEU:HD21	1:K:185:VAL:CG2	2.49	0.41
1:A:141:LYS:NZ	1:E:361:GLU:OE2	2.51	0.41
1:K:112:GLU:OE1	1:K:163:THR:OG1	2.28	0.41
1:I:233:ASN:HD21	1:I:237:ARG:HH11	1.69	0.41
1:D:73:LYS:HE3	5:D:590:HOH:O	2.21	0.41
1:H:233:ASN:HD21	1:H:237:ARG:HH11	1.68	0.41
1:F:233:ASN:HD21	1:F:237:ARG:HH11	1.67	0.41
1:L:361:GLU:CG	5:L:606:HOH:O	2.69	0.40
1:B:233:ASN:HD21	1:B:237:ARG:HH11	1.70	0.40
1:D:161:ASN:HA	1:D:162:PRO:HA	1.88	0.40
1:H:334:LEU:HD12	1:H:334:LEU:HA	1.94	0.40
1:C:180:LYS:HE2	1:C:181:ASP:HB2	2.04	0.40
1:J:233:ASN:HD21	1:J:237:ARG:HH11	1.70	0.40
4:J:405:EDO:C2	5:K:507:HOH:O	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	394/392 (100%)	383 (97%)	10 (2%)	1 (0%)	41 31
1	B	397/392 (101%)	387 (98%)	9 (2%)	1 (0%)	41 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	H	311	PRO
1	J	311	PRO
1	K	311	PRO
1	F	311	PRO
1	G	311	PRO
1	I	311	PRO
1	L	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

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	131	LYS
1	A	237	ARG
1	A	341	LEU
1	A	349	GLU
1	B	131	LYS
1	B	162	PRO
1	B	232	LEU
1	B	323	GLN
1	B	341	LEU
1	B	349	GLU
1	B	373[A]	LEU
1	B	373[B]	LEU
1	C	12	LEU
1	C	131	LYS
1	C	180	LYS
1	C	232[A]	LEU
1	C	232[B]	LEU
1	C	341	LEU
1	C	349	GLU
1	C	373[A]	LEU
1	C	373[B]	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	12	LEU
1	D	131	LYS
1	D	162	PRO
1	D	341	LEU
1	D	349	GLU
1	D	366[A]	THR
1	D	366[B]	THR
1	D	373[A]	LEU
1	D	373[B]	LEU
1	E	12	LEU
1	E	131	LYS
1	E	232[A]	LEU
1	E	232[B]	LEU
1	E	237	ARG
1	E	330	LYS
1	E	341	LEU
1	E	349	GLU
1	E	362	LYS
1	E	373[A]	LEU
1	E	373[B]	LEU
1	H	12	LEU
1	H	131	LYS
1	H	162	PRO
1	H	232[A]	LEU
1	H	232[B]	LEU
1	H	237	ARG
1	H	341	LEU
1	H	349	GLU
1	H	373[A]	LEU
1	H	373[B]	LEU
1	J	12	LEU
1	J	16	GLN
1	J	131	LYS
1	J	232[A]	LEU
1	J	232[B]	LEU
1	J	237	ARG
1	J	271[A]	ARG
1	J	271[B]	ARG
1	J	341	LEU
1	J	349	GLU
1	J	366	THR
1	J	373[A]	LEU

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Mol	Chain	Res	Type
1	J	373[B]	LEU
1	K	12	LEU
1	K	16	GLN
1	K	56	SER
1	K	131	LYS
1	K	180	LYS
1	K	232[A]	LEU
1	K	232[B]	LEU
1	K	237	ARG
1	K	341	LEU
1	K	349	GLU
1	K	361	GLU
1	K	362	LYS
1	K	366	THR
1	K	373[A]	LEU
1	K	373[B]	LEU
1	F	12	LEU
1	F	131	LYS
1	F	232	LEU
1	F	237	ARG
1	F	323	GLN
1	F	341	LEU
1	F	349	GLU
1	F	362	LYS
1	F	366	THR
1	F	373[A]	LEU
1	F	373[B]	LEU
1	G	12	LEU
1	G	16	GLN
1	G	131	LYS
1	G	162	PRO
1	G	170	LYS
1	G	232	LEU
1	G	237	ARG
1	G	341	LEU
1	G	349	GLU
1	G	373[A]	LEU
1	G	373[B]	LEU
1	I	131	LYS
1	I	170	LYS
1	I	232[A]	LEU
1	I	232[B]	LEU

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Mol	Chain	Res	Type
1	I	341	LEU
1	I	349	GLU
1	I	373[A]	LEU
1	I	373[B]	LEU
1	L	12	LEU
1	L	16	GLN
1	L	131	LYS
1	L	178	LYS
1	L	232[A]	LEU
1	L	232[B]	LEU
1	L	341	LEU
1	L	349	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	233	ASN
1	A	241	ASN
1	A	323	GLN
1	B	233	ASN
1	B	241	ASN
1	B	323	GLN
1	C	54	GLN
1	C	179	HIS
1	C	241	ASN
1	C	324	HIS
1	D	16	GLN
1	D	54	GLN
1	D	174	GLN
1	D	241	ASN
1	E	54	GLN
1	E	233	ASN
1	E	241	ASN
1	H	54	GLN
1	H	233	ASN
1	H	241	ASN
1	J	16	GLN
1	J	54	GLN
1	J	233	ASN
1	J	241	ASN
1	K	233	ASN

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Mol	Chain	Res	Type
1	K	241	ASN
1	F	54	GLN
1	F	179	HIS
1	F	233	ASN
1	F	241	ASN
1	F	323	GLN
1	G	54	GLN
1	G	233	ASN
1	G	241	ASN
1	G	323	GLN
1	G	398	HIS
1	I	54	GLN
1	I	233	ASN
1	I	241	ASN
1	L	54	GLN
1	L	179	HIS
1	L	241	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

All (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
2	L	401	TVJ	C10-N4	5.29	1.47	1.33
2	H	401	TVJ	C10-N4	5.29	1.47	1.33
2	E	401	TVJ	C10-N4	5.18	1.47	1.33
2	B	401	TVJ	C10-N4	4.96	1.46	1.33
2	F	401	TVJ	C10-N4	4.89	1.46	1.33
2	A	401	TVJ	C10-N4	4.78	1.46	1.33
2	J	401	TVJ	C10-N4	4.68	1.45	1.33
2	F	401	TVJ	P1-O2	3.16	1.70	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	401	TVJ	C3-C1	-2.93	1.38	1.40
2	L	401	TVJ	C3-C1	-2.76	1.38	1.40
2	C	401	TVJ	C3-C1	-2.62	1.38	1.40
2	E	401	TVJ	P1-O2	2.61	1.68	1.60
2	H	401	TVJ	C3-C1	-2.55	1.38	1.40
2	K	401	TVJ	P1-O5	2.30	1.58	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	F	401	TVJ	O2-P1-O5	-3.16	97.60	106.47
2	J	401	TVJ	O4-P1-O2	-2.86	99.12	106.73
2	C	401	TVJ	O2-P1-O5	-2.68	98.96	106.47
2	E	401	TVJ	O4-P1-O2	-2.62	99.77	106.73
2	F	401	TVJ	O6-C9-C10	2.47	124.36	121.30
2	L	401	TVJ	O7-C10-N4	-2.26	117.60	122.88
2	I	401	TVJ	O3-P1-O5	2.16	119.13	110.68
2	F	401	TVJ	O4-P1-O2	-2.13	101.08	106.73
2	J	401	TVJ	O4-P1-O3	2.12	115.76	107.64
2	C	401	TVJ	C3-C4-C5	-2.11	116.48	120.41
2	C	401	TVJ	C6-C4-C5	2.00	124.85	121.56

There are no chirality outliers.

All (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
2	J	401	TVJ	N4-C10-C9-O6
2	F	401	TVJ	O7-C10-C9-N3
2	F	401	TVJ	N4-C10-C9-O6
2	I	401	TVJ	O7-C10-C9-N3
2	I	401	TVJ	N4-C10-C9-O6
3	C	402	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	D	402	GOL	O1-C1-C2-C3
3	D	402	GOL	C1-C2-C3-O3
3	H	402	GOL	O1-C1-C2-C3
3	K	402	GOL	C1-C2-C3-O3
3	I	402	GOL	C1-C2-C3-O3
3	L	402	GOL	O1-C1-C2-C3
2	A	401	TVJ	O7-C10-C9-O6
2	E	401	TVJ	O7-C10-C9-O6
2	I	401	TVJ	O7-C10-C9-O6
2	B	401	TVJ	O7-C10-C9-O6
2	C	401	TVJ	O7-C10-C9-O6
2	D	401	TVJ	O7-C10-C9-O6
2	H	401	TVJ	O7-C10-C9-O6
2	J	401	TVJ	O7-C10-C9-O6
2	K	401	TVJ	O7-C10-C9-O6
2	F	401	TVJ	O7-C10-C9-O6
2	G	401	TVJ	O7-C10-C9-O6
2	L	401	TVJ	O7-C10-C9-O6
3	E	402	GOL	O1-C1-C2-C3
3	E	402	GOL	C1-C2-C3-O3
3	D	402	GOL	O1-C1-C2-O2
3	L	402	GOL	O1-C1-C2-O2
4	J	404	EDO	O1-C1-C2-O2
4	K	403	EDO	O1-C1-C2-O2
3	C	402	GOL	O2-C2-C3-O3
3	E	402	GOL	O2-C2-C3-O3
3	H	402	GOL	O1-C1-C2-O2
3	K	402	GOL	O2-C2-C3-O3
3	I	402	GOL	O2-C2-C3-O3
2	B	401	TVJ	O7-C10-C9-N3
2	C	401	TVJ	O7-C10-C9-N3
2	D	401	TVJ	O7-C10-C9-N3
2	J	401	TVJ	O7-C10-C9-N3
2	K	401	TVJ	O7-C10-C9-N3
2	G	401	TVJ	O7-C10-C9-N3
2	L	401	TVJ	O7-C10-C9-N3
3	L	402	GOL	C1-C2-C3-O3
4	J	403	EDO	O1-C1-C2-O2
2	K	401	TVJ	C6-C4-C5-N2
4	J	402	EDO	O1-C1-C2-O2
3	F	402	GOL	O1-C1-C2-O2
3	F	402	GOL	C1-C2-C3-O3

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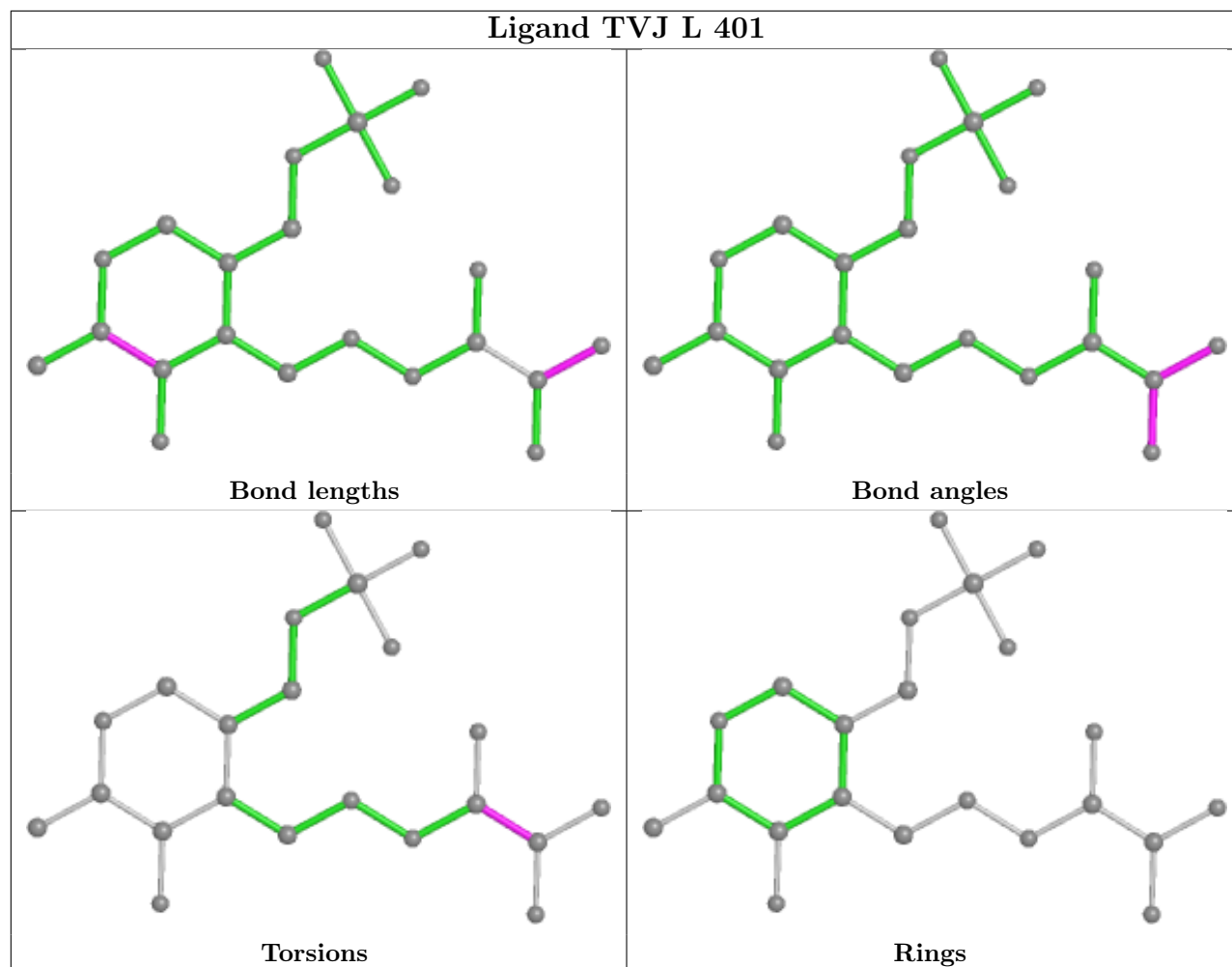
Mol	Chain	Res	Type	Atoms
2	E	401	TVJ	C5-N2-N3-C9
3	D	402	GOL	O2-C2-C3-O3

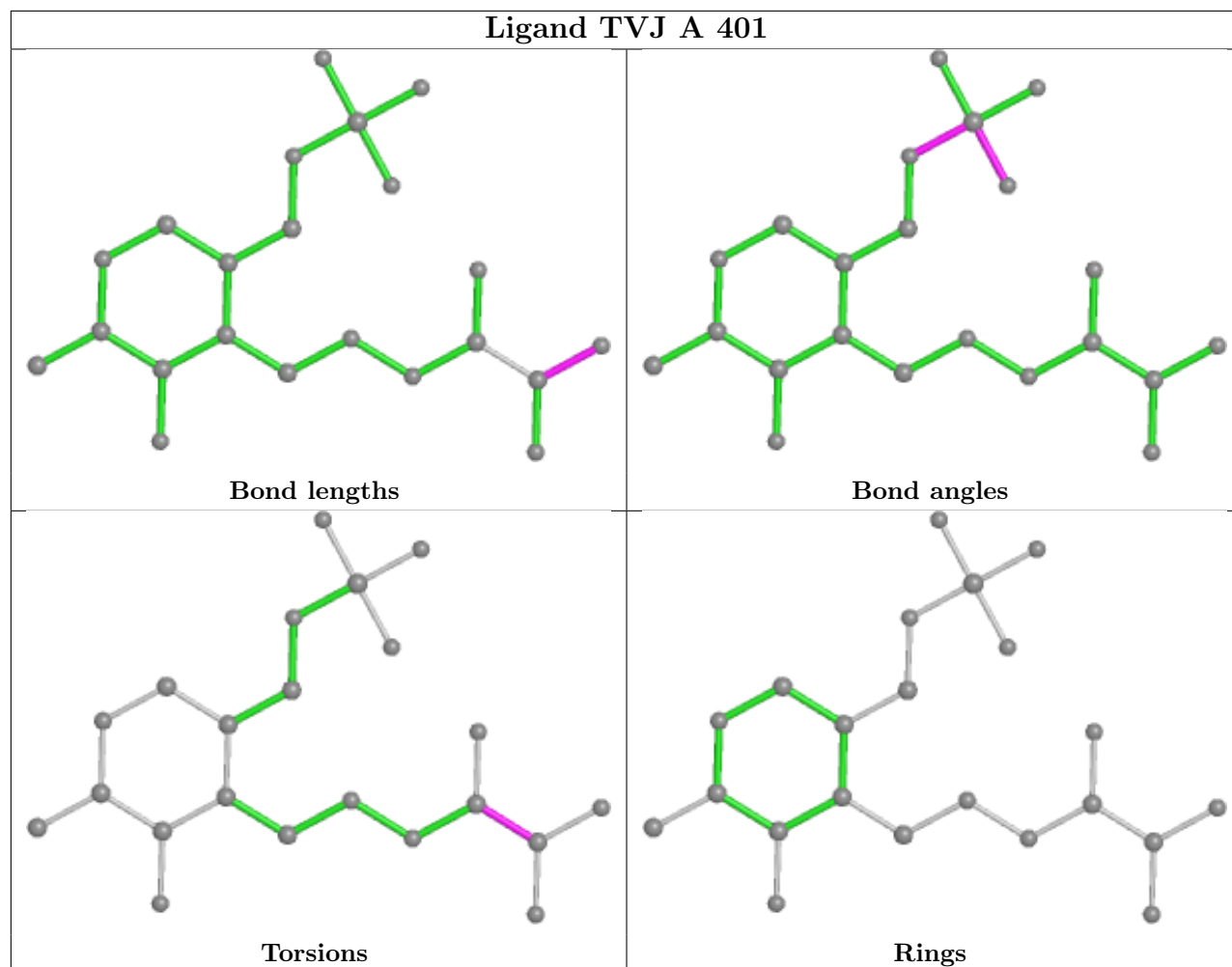
There are no ring outliers.

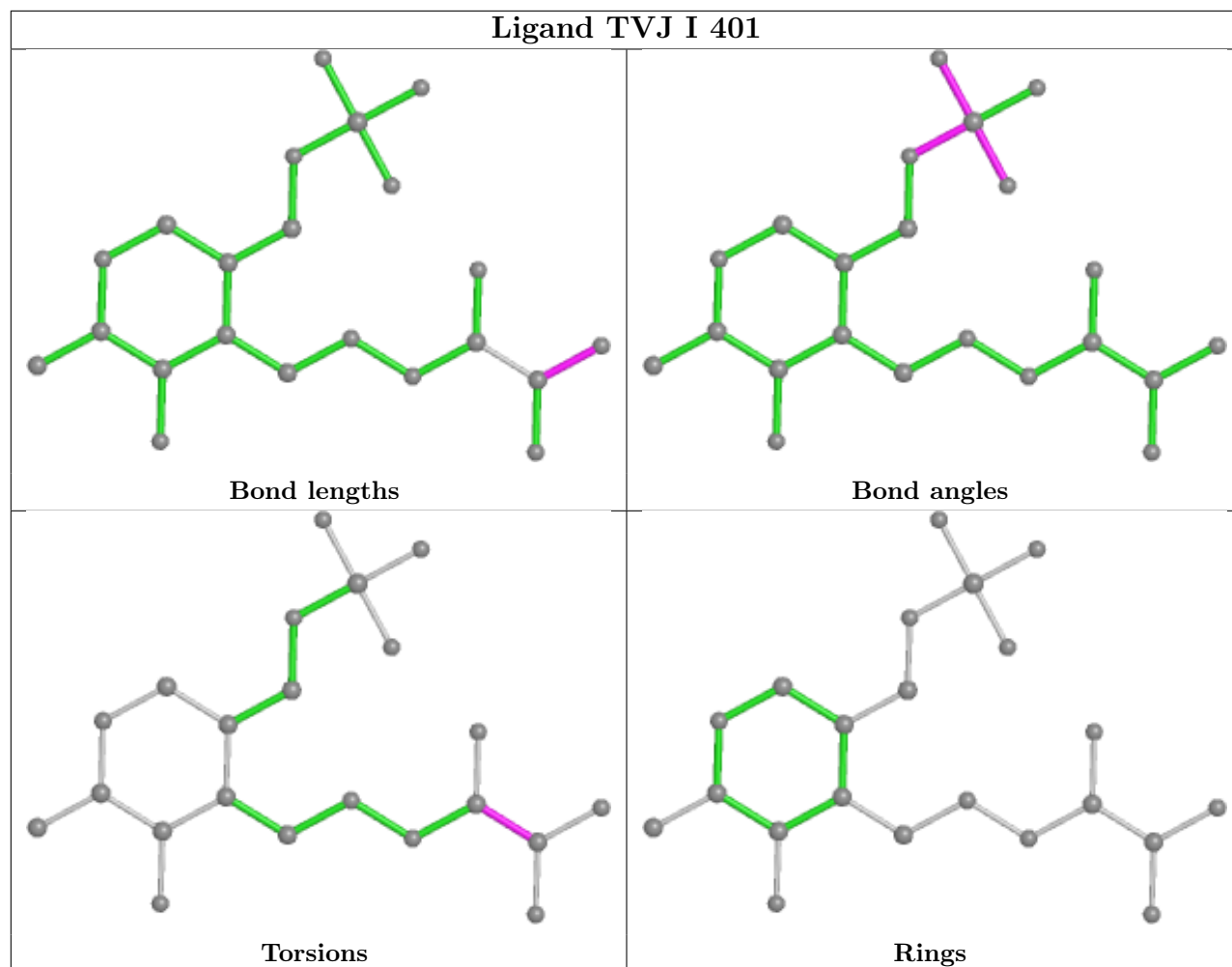
22 monomers are involved in 35 short contacts:

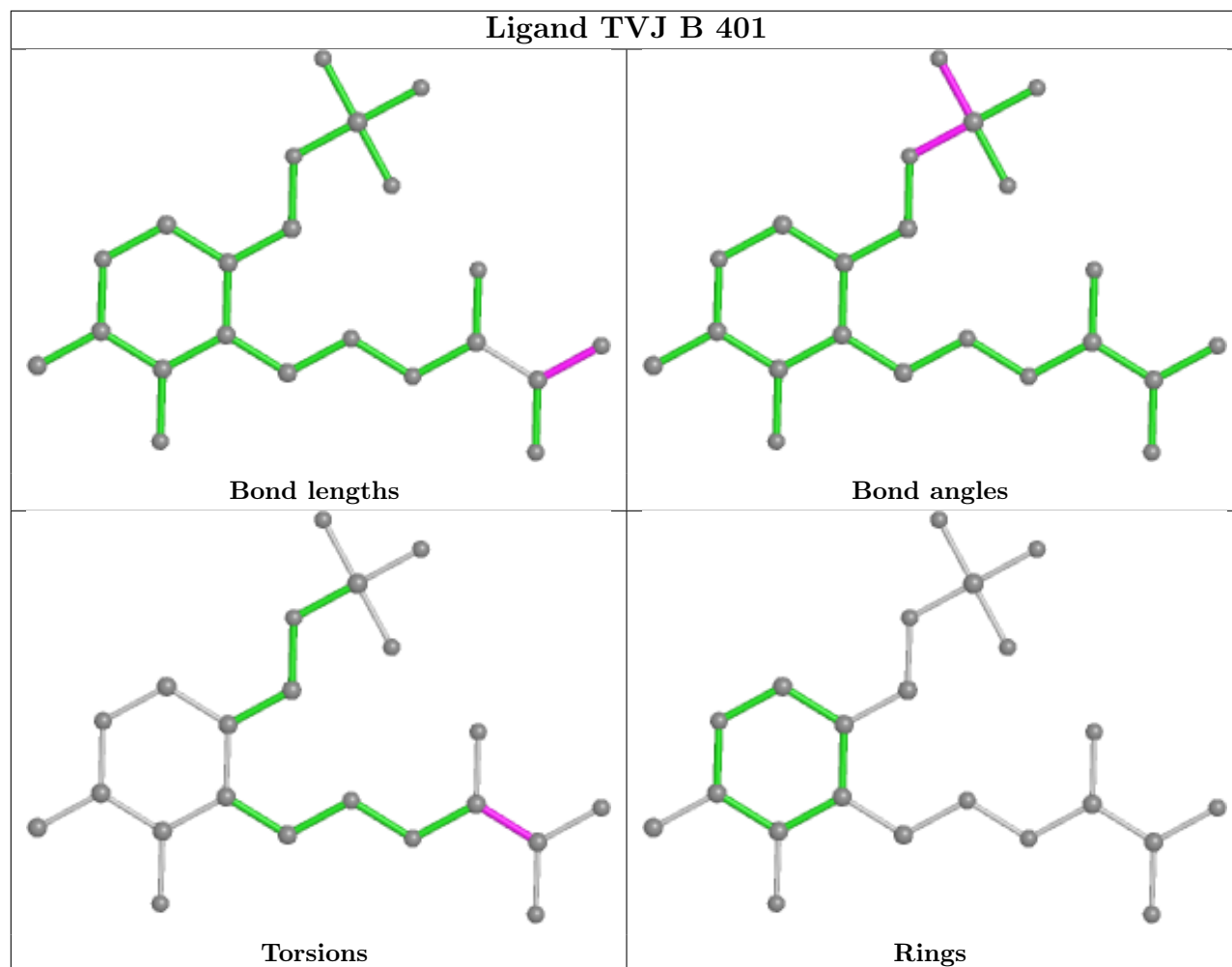
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	401	TVJ	1	0
2	A	401	TVJ	1	0
3	I	402	GOL	1	0
2	I	401	TVJ	1	0
2	B	401	TVJ	1	0
2	G	401	TVJ	1	0
4	J	402	EDO	2	0
3	H	402	GOL	1	0
2	C	401	TVJ	1	0
4	J	405	EDO	6	0
2	H	401	TVJ	1	0
3	C	402	GOL	1	0
4	J	404	EDO	1	0
2	E	401	TVJ	1	0
3	D	402	GOL	1	0
4	K	403	EDO	3	0
2	F	401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

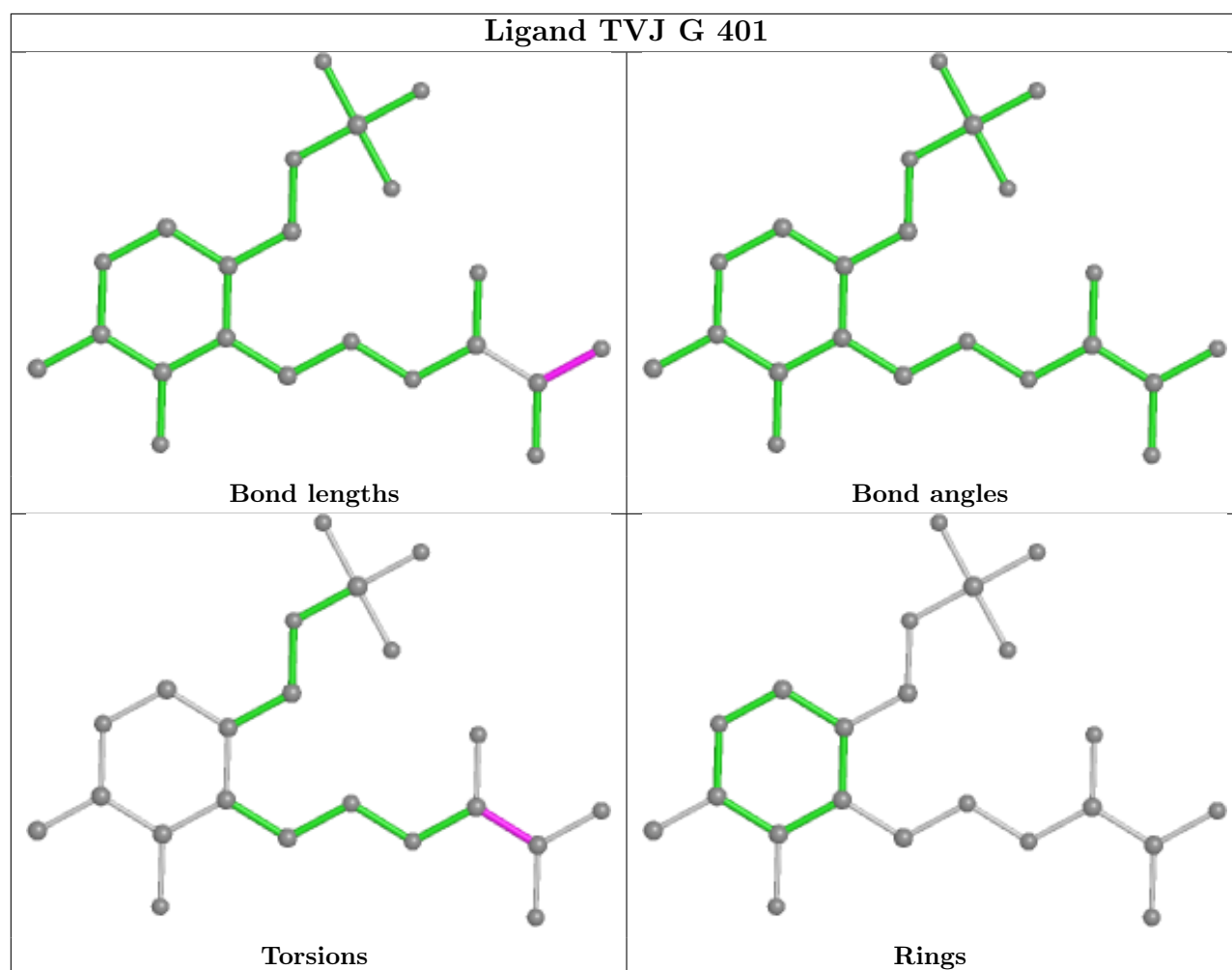
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



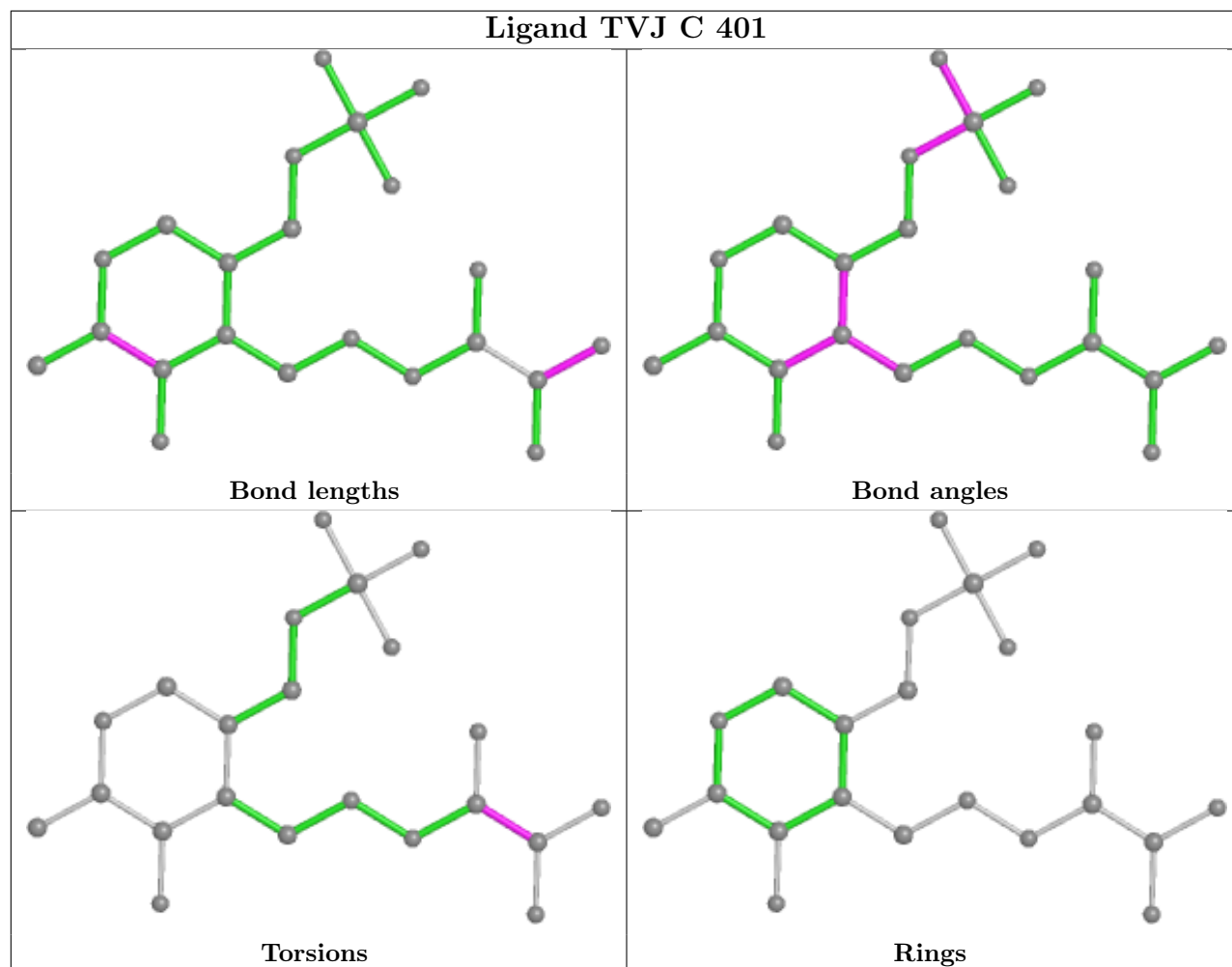


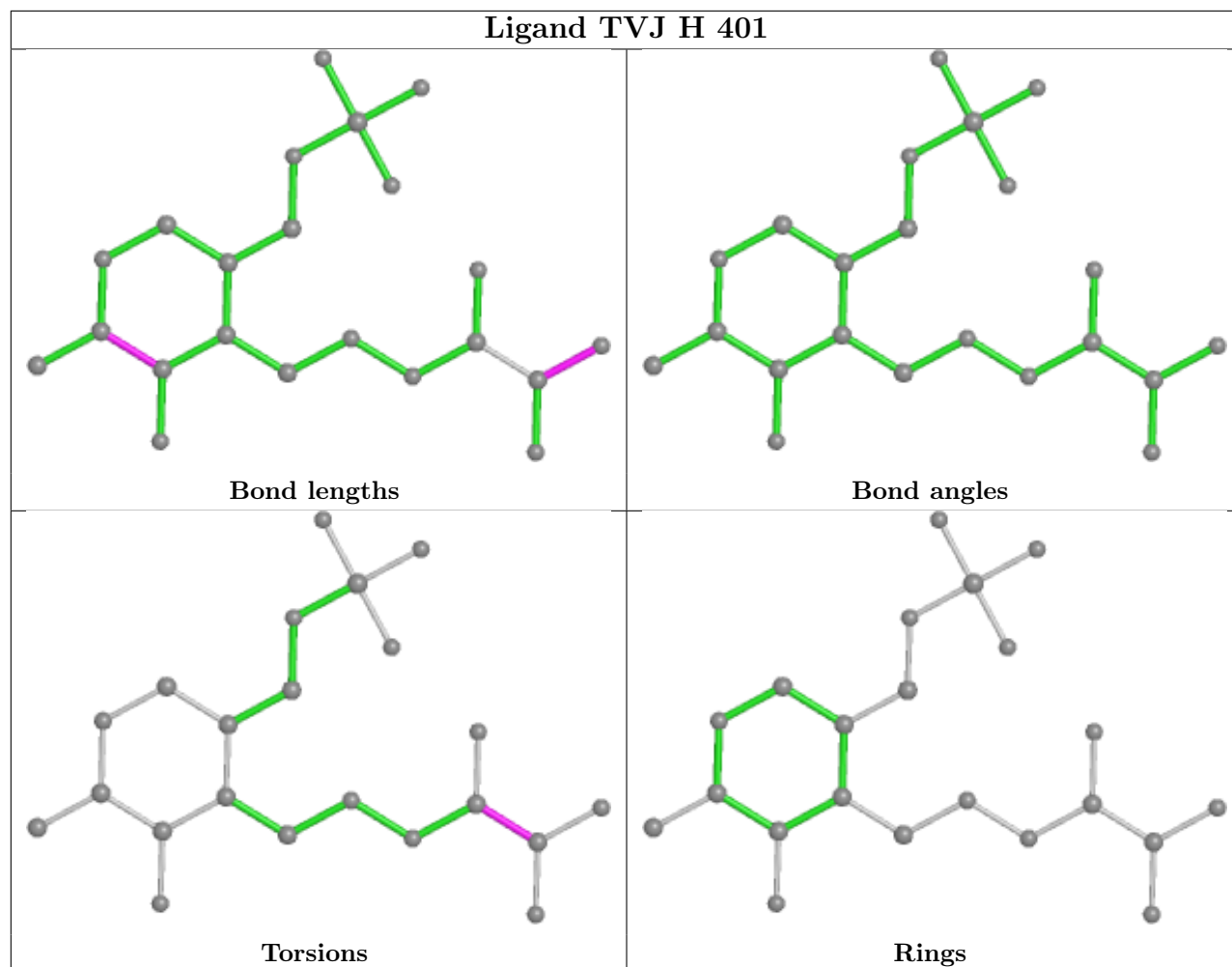


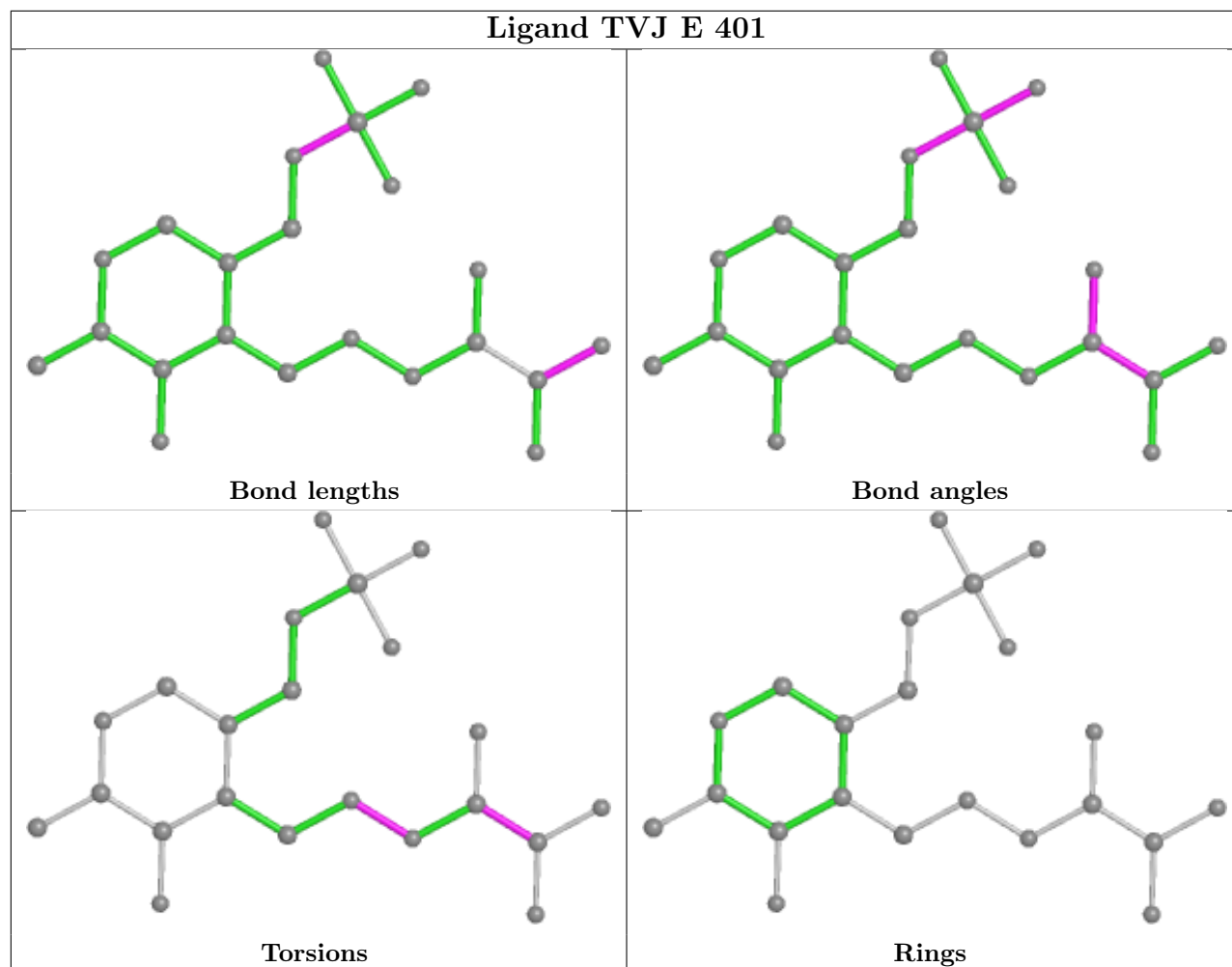


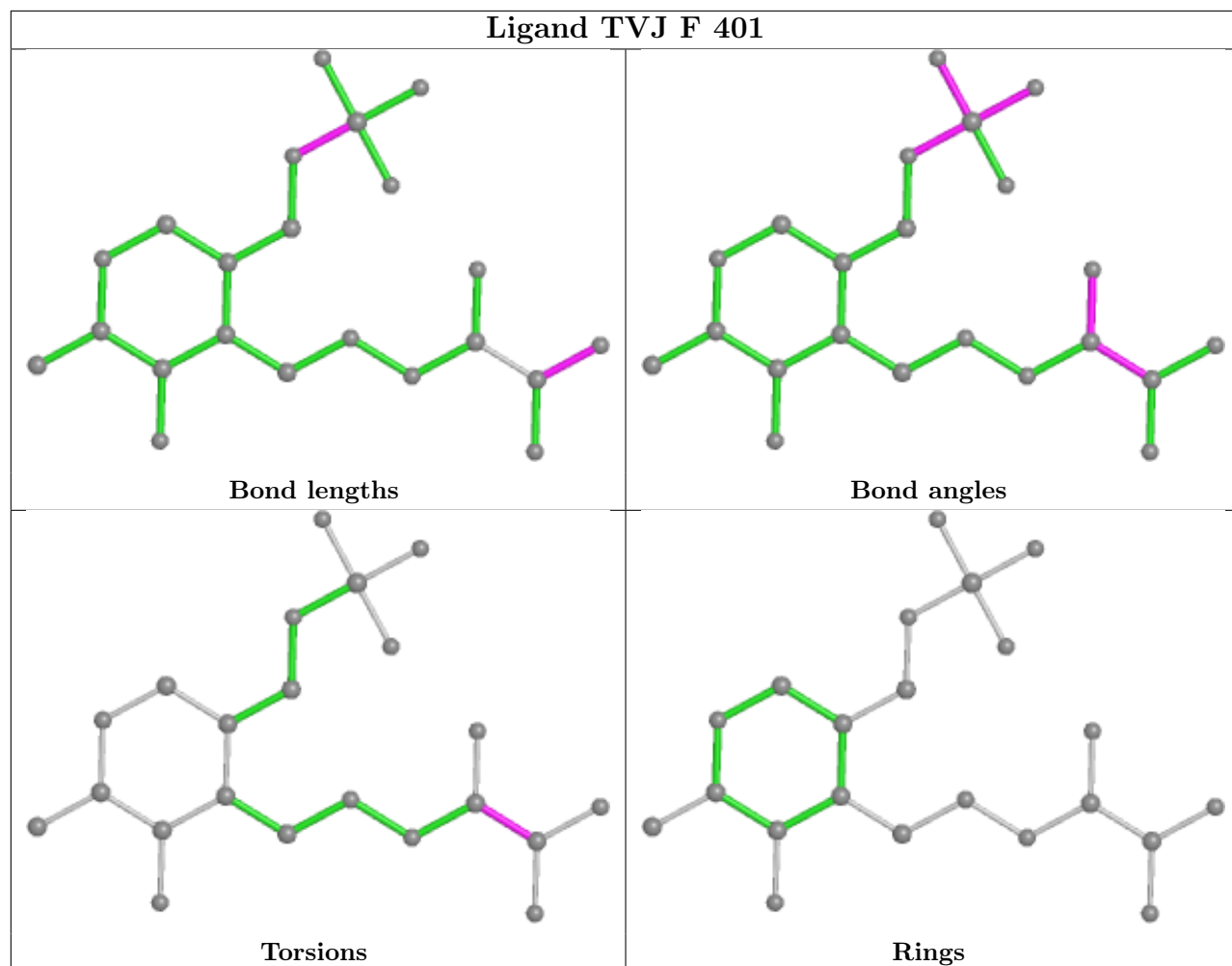


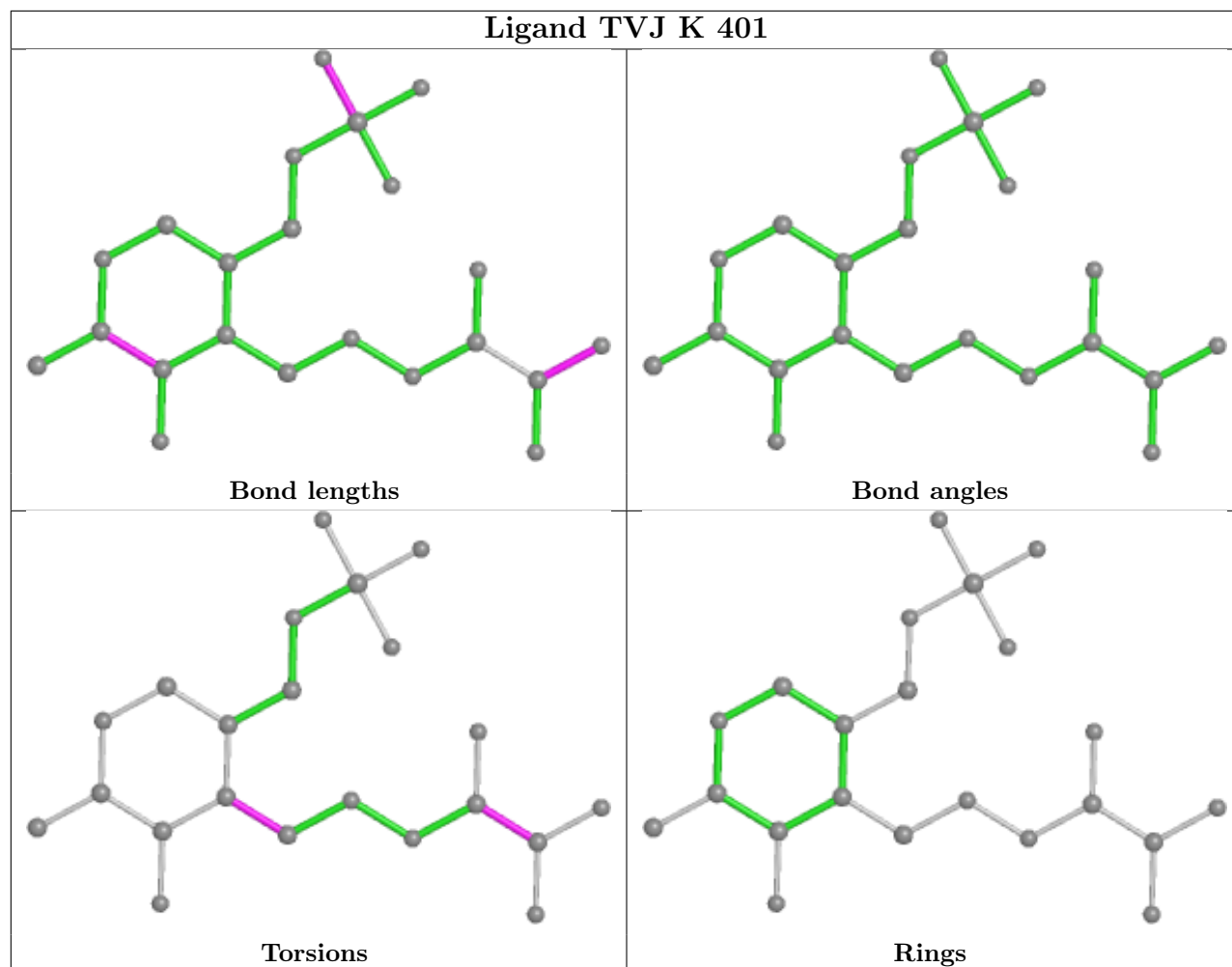


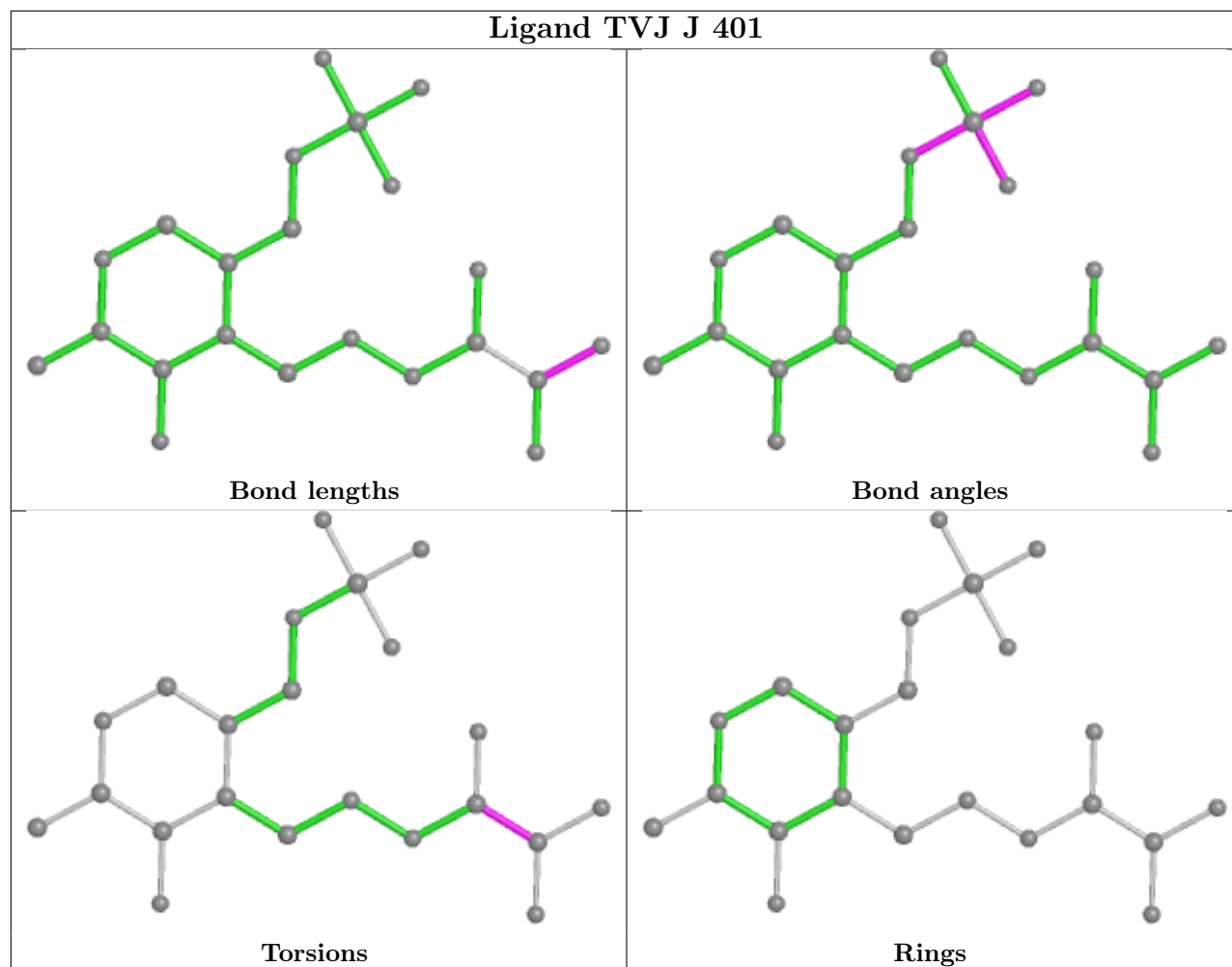


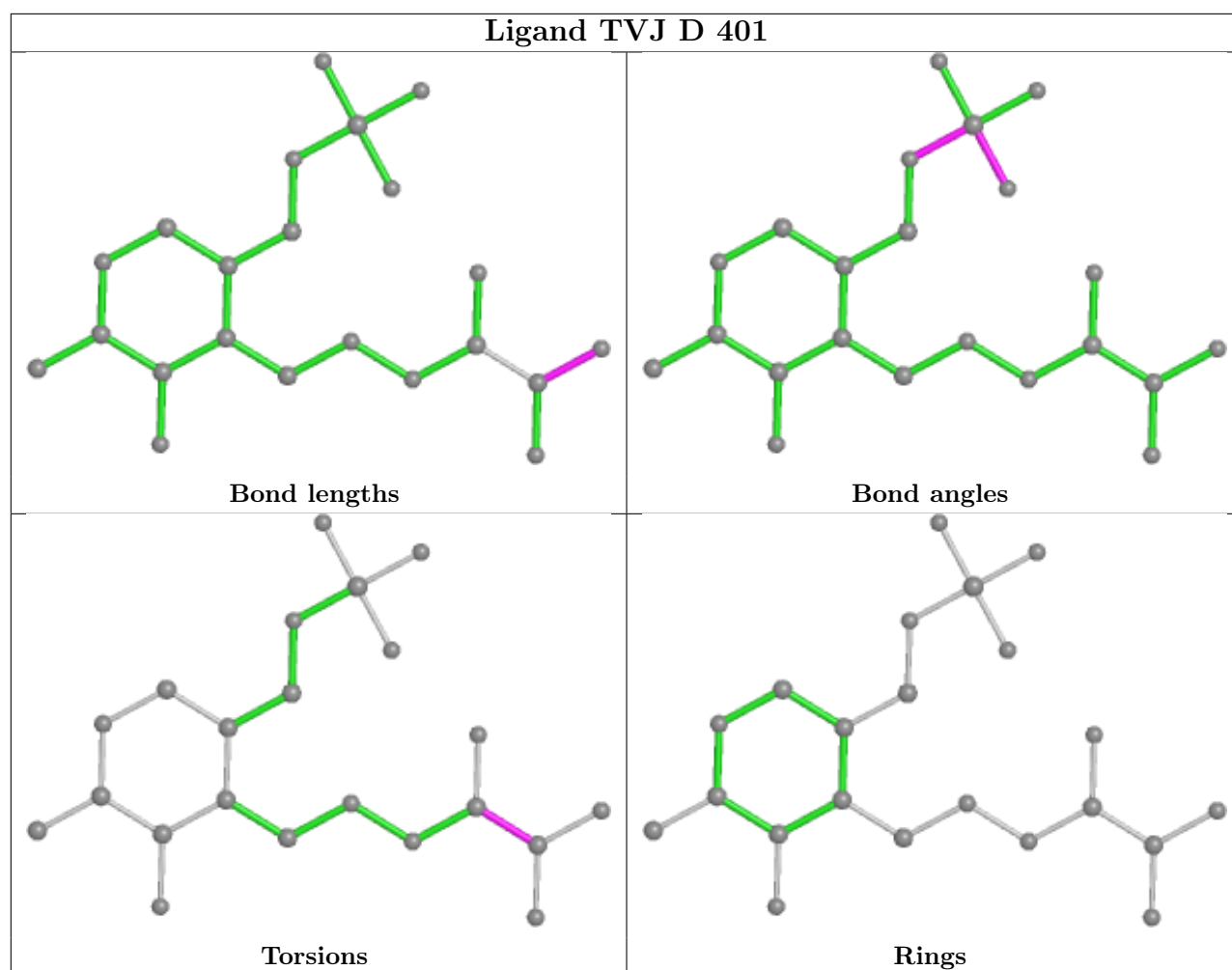












## 5.7 Other polymers [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	K	55	SER	4.8
1	L	55	SER	4.5
1	I	399	PRO	4.2
1	K	16	GLN	4.0
1	D	55	SER	4.0
1	I	56	SER	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	55	SER	3.9
1	C	399	PRO	3.9
1	G	16	GLN	3.7
1	B	55	SER	3.4
1	H	399	PRO	3.4
1	D	399	PRO	3.1
1	B	399	PRO	3.0
1	J	399	PRO	3.0
1	E	16	GLN	2.9
1	L	16	GLN	2.9
1	H	16	GLN	2.8
1	J	180	LYS	2.7
1	K	56	SER	2.7
1	K	399	PRO	2.7
1	A	181	ASP	2.6
1	E	180	LYS	2.6
1	I	16	GLN	2.6
1	L	399	PRO	2.5
1	K	254	LEU	2.5
1	H	250	PHE	2.5
1	G	254	LEU	2.5
1	K	250	PHE	2.4
1	G	250	PHE	2.4
1	F	16	GLN	2.4
1	K	220	VAL	2.4
1	H	55	SER	2.4
1	I	180	LYS	2.3
1	L	10	GLY	2.3
1	A	399	PRO	2.3
1	C	16	GLN	2.3
1	G	10	GLY	2.3
1	D	16	GLN	2.3
1	E	399	PRO	2.2
1	E	56	SER	2.2
1	F	181	ASP	2.2
1	F	399	PRO	2.2
1	B	254	LEU	2.1
1	B	220	VAL	2.1
1	C	56	SER	2.1
1	C	180	LYS	2.1
1	K	10	GLY	2.1
1	L	220	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	55	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

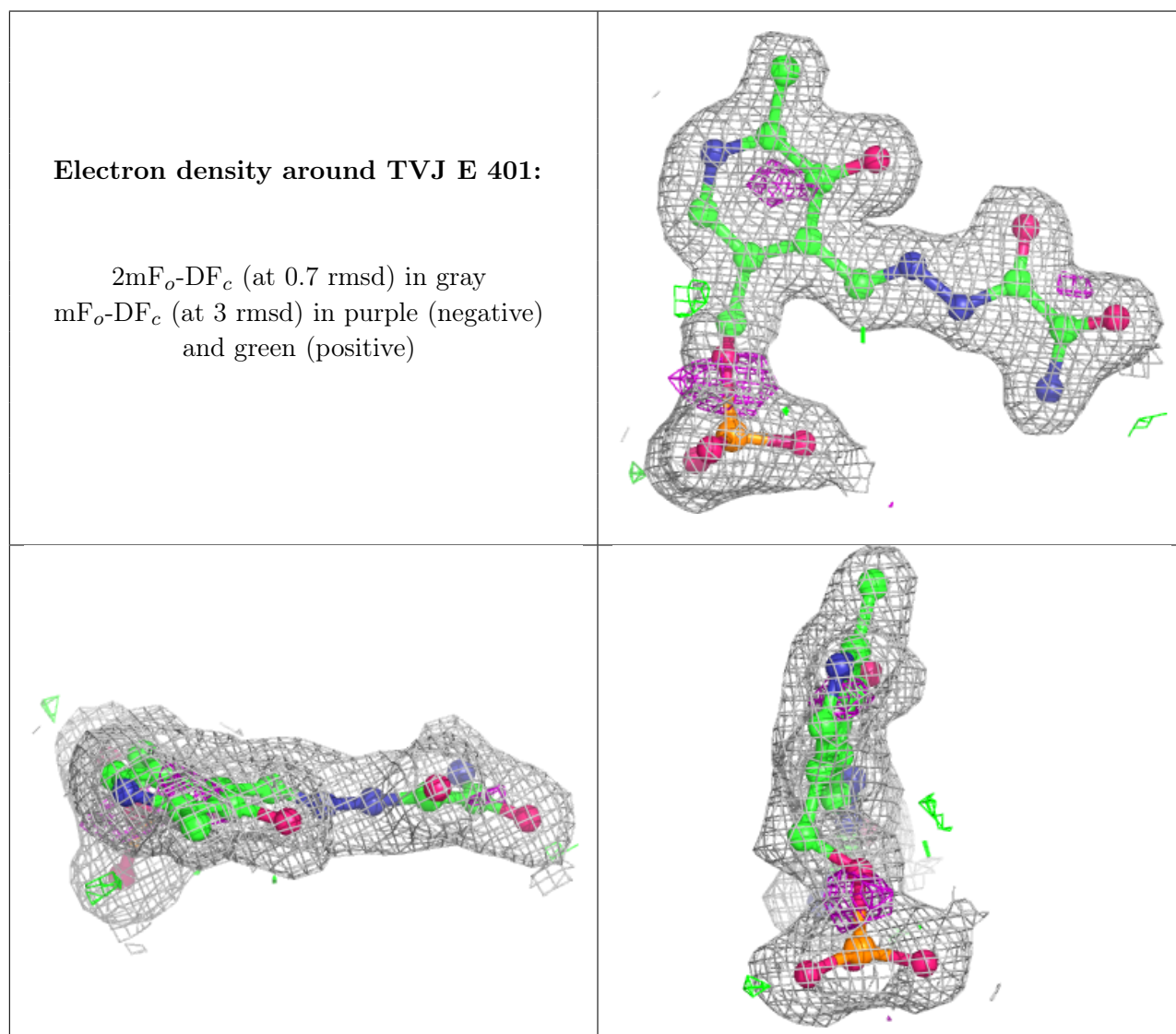
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	J	405	4/4	0.83	0.23	38,41,42,47	0
4	EDO	K	403	4/4	0.85	0.22	33,39,42,55	0
3	GOL	E	402	6/6	0.89	0.19	34,40,44,44	0
4	EDO	J	404	4/4	0.90	0.14	23,24,33,34	0
3	GOL	D	402	6/6	0.90	0.14	27,30,34,37	0
4	EDO	J	402	4/4	0.90	0.28	39,40,41,42	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

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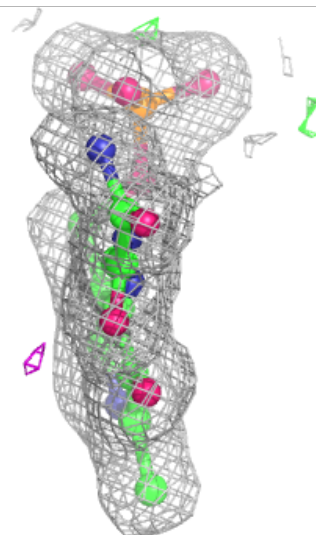
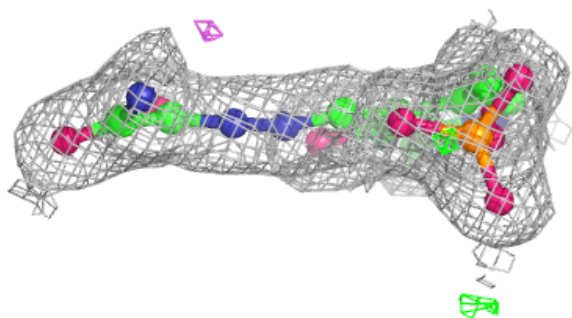
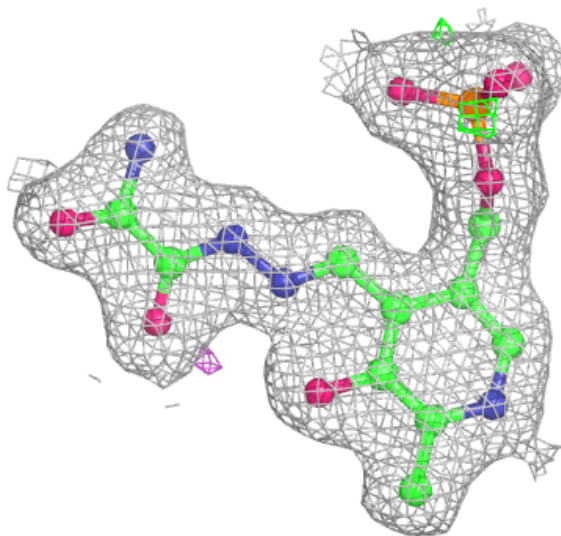
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TVJ	C	401	22/22	0.98	0.10	10,13,21,25	0
2	TVJ	F	401	22/22	0.98	0.06	15,19,25,27	0
2	TVJ	G	401	22/22	0.98	0.11	18,20,31,32	0
2	TVJ	I	401	22/22	0.98	0.07	12,16,22,25	0
2	TVJ	D	401	22/22	0.99	0.09	9,12,18,21	0

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.



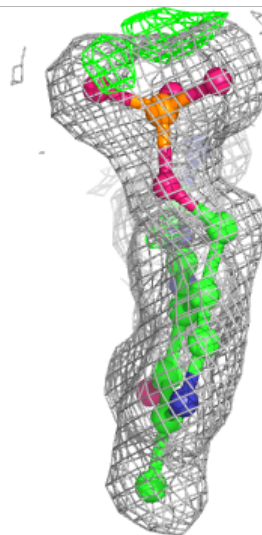
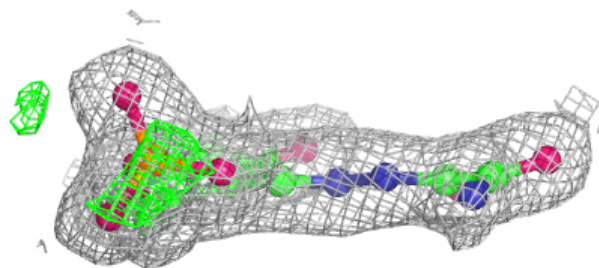
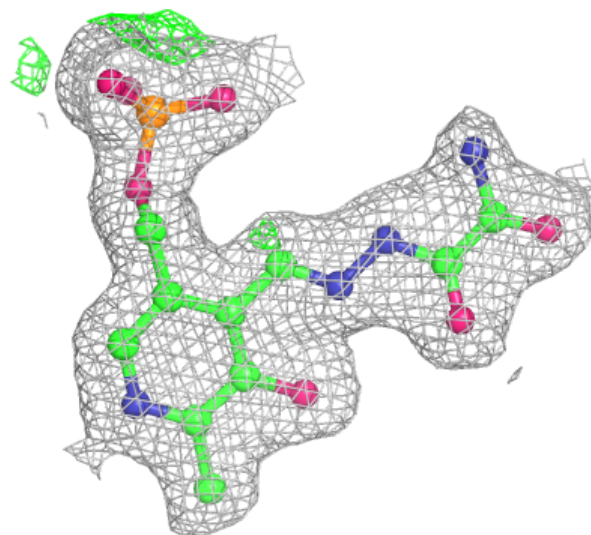
**Electron density around TVJ H 401:**

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



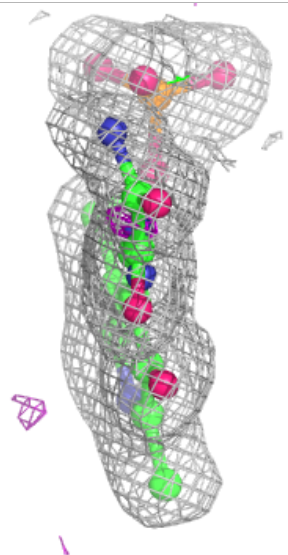
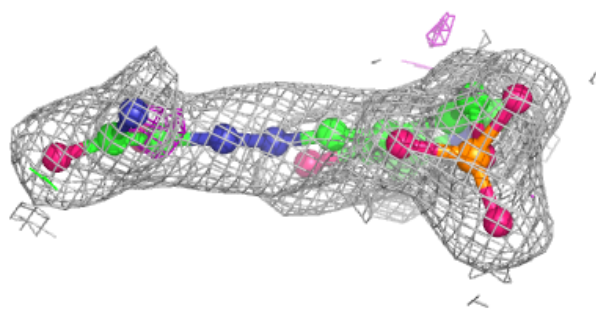
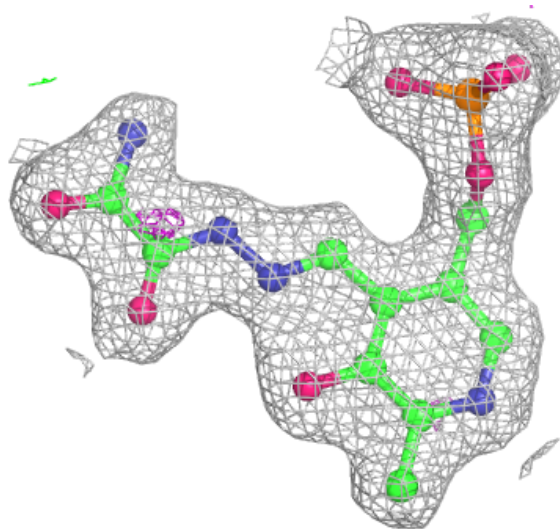
**Electron density around TVJ K 401:**

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



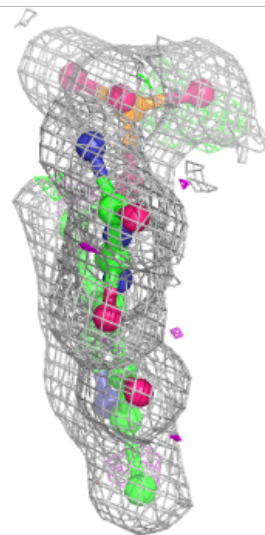
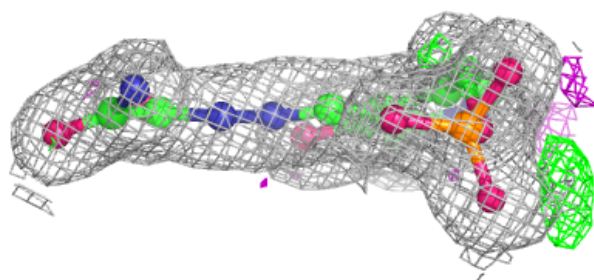
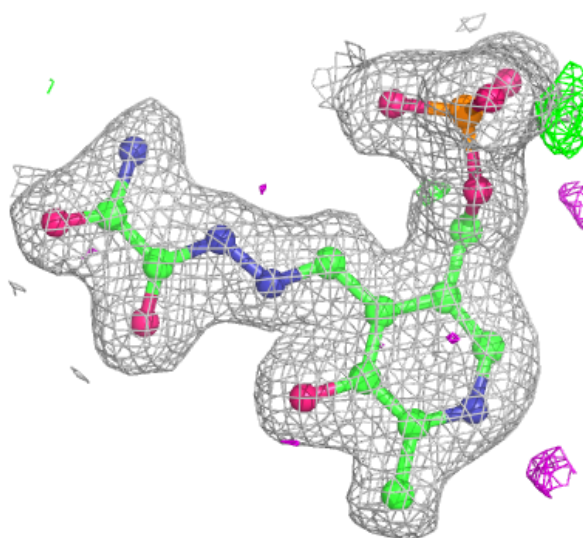
**Electron density around TVJ L 401:**

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



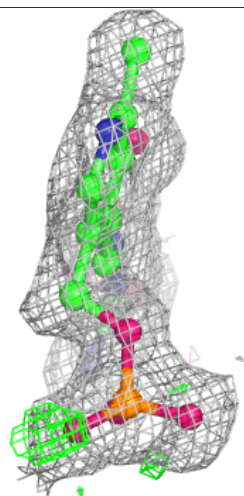
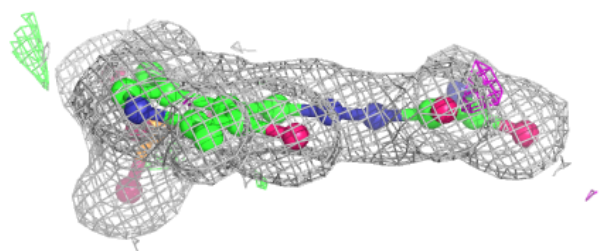
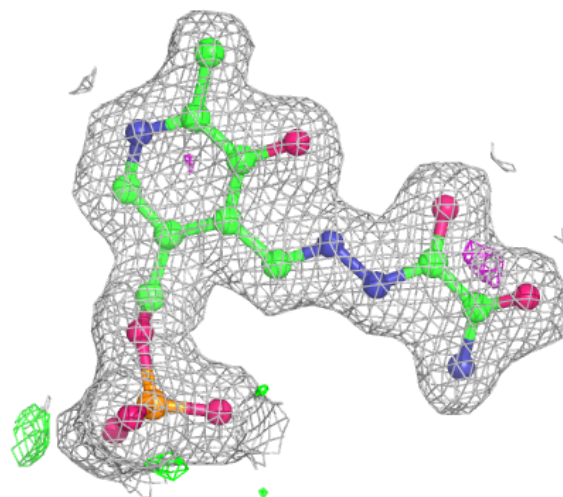
**Electron density around TVJ A 401:**

$2mF_o-DF_c$  (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:**

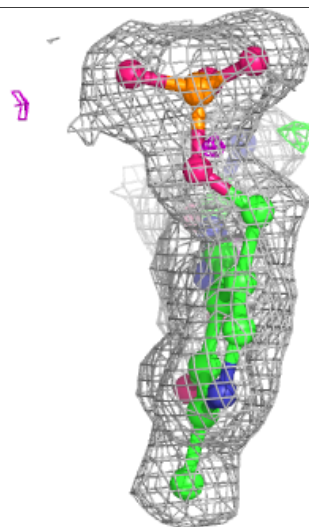
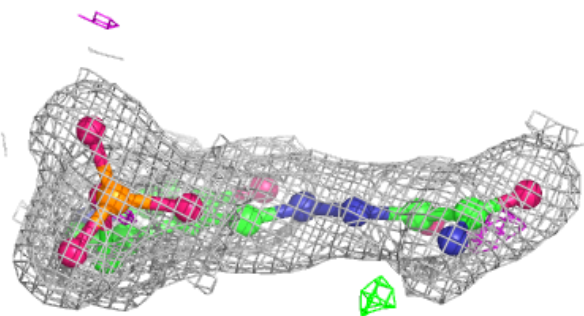
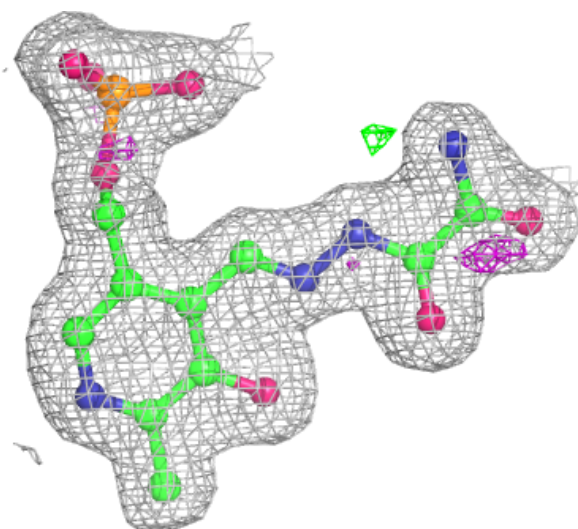
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





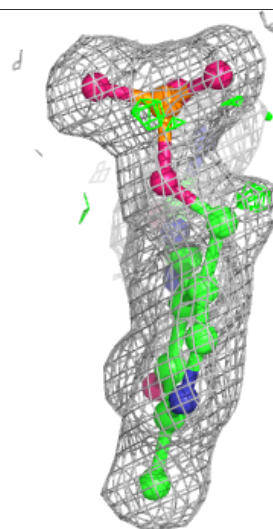
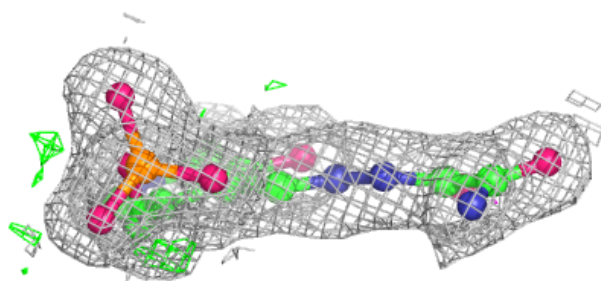
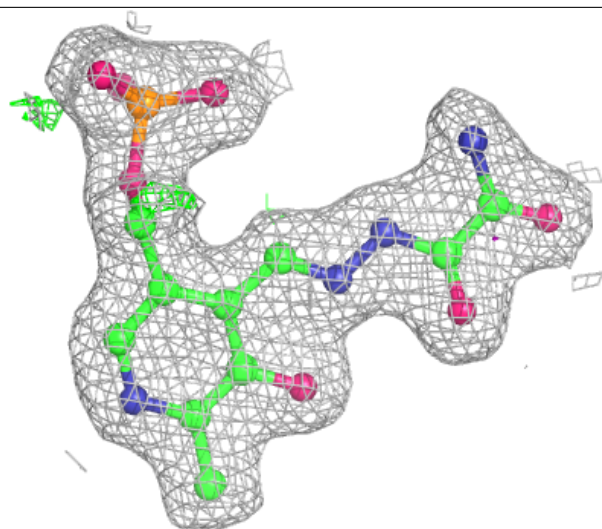
**Electron density around TVJ J 401:**

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



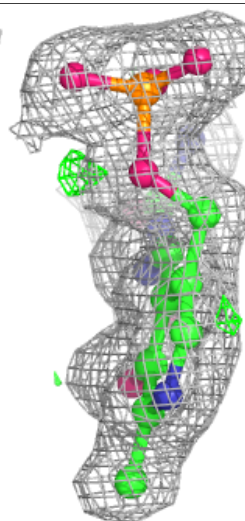
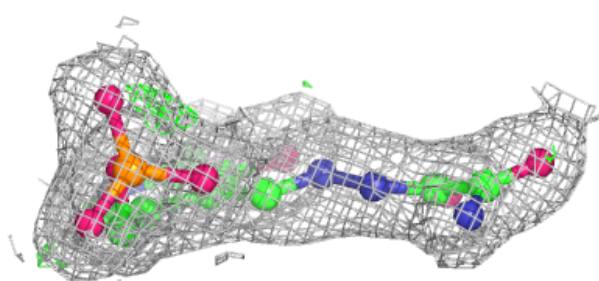
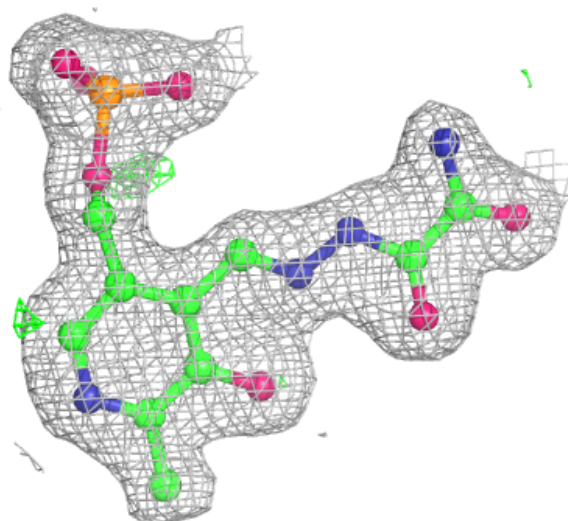
**Electron density around TVJ C 401:**

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



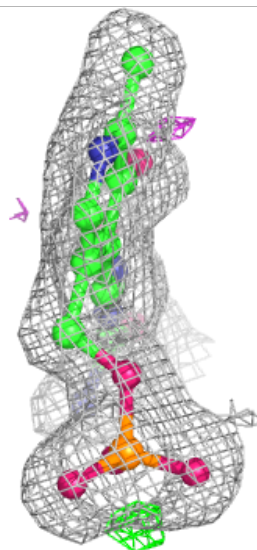
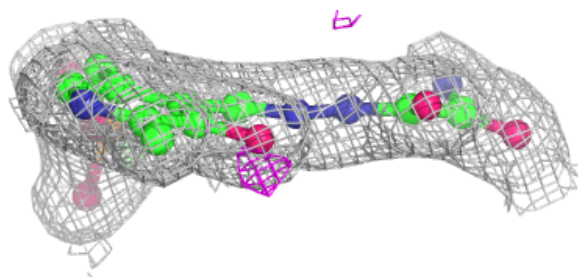
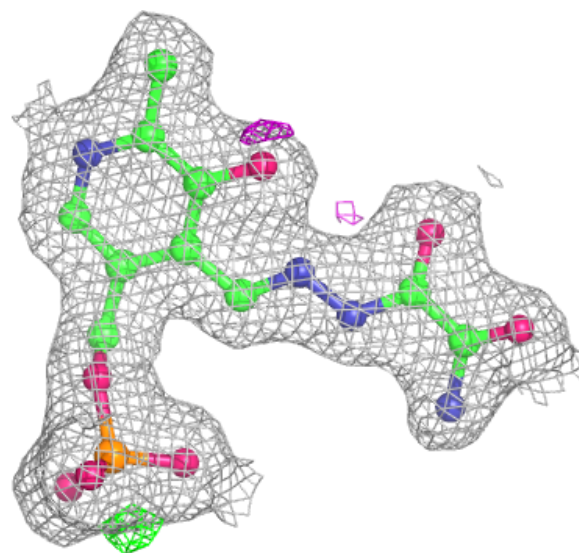
**Electron density around TVJ F 401:**

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



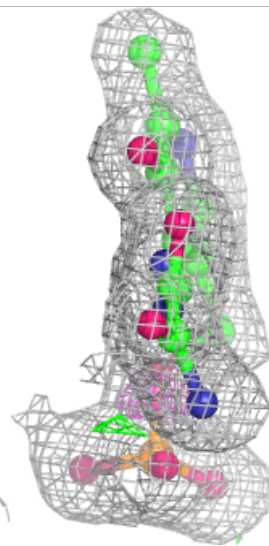
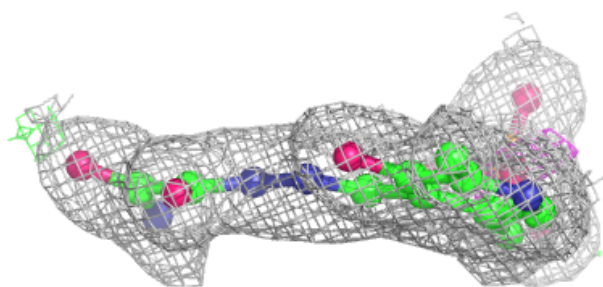
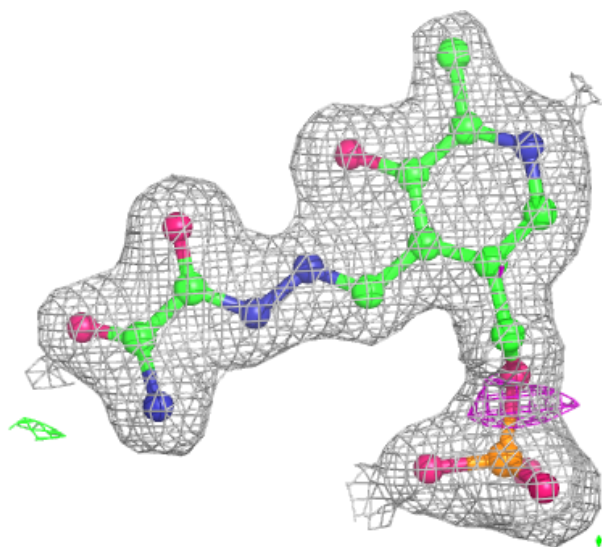
**Electron density around TVJ G 401:**

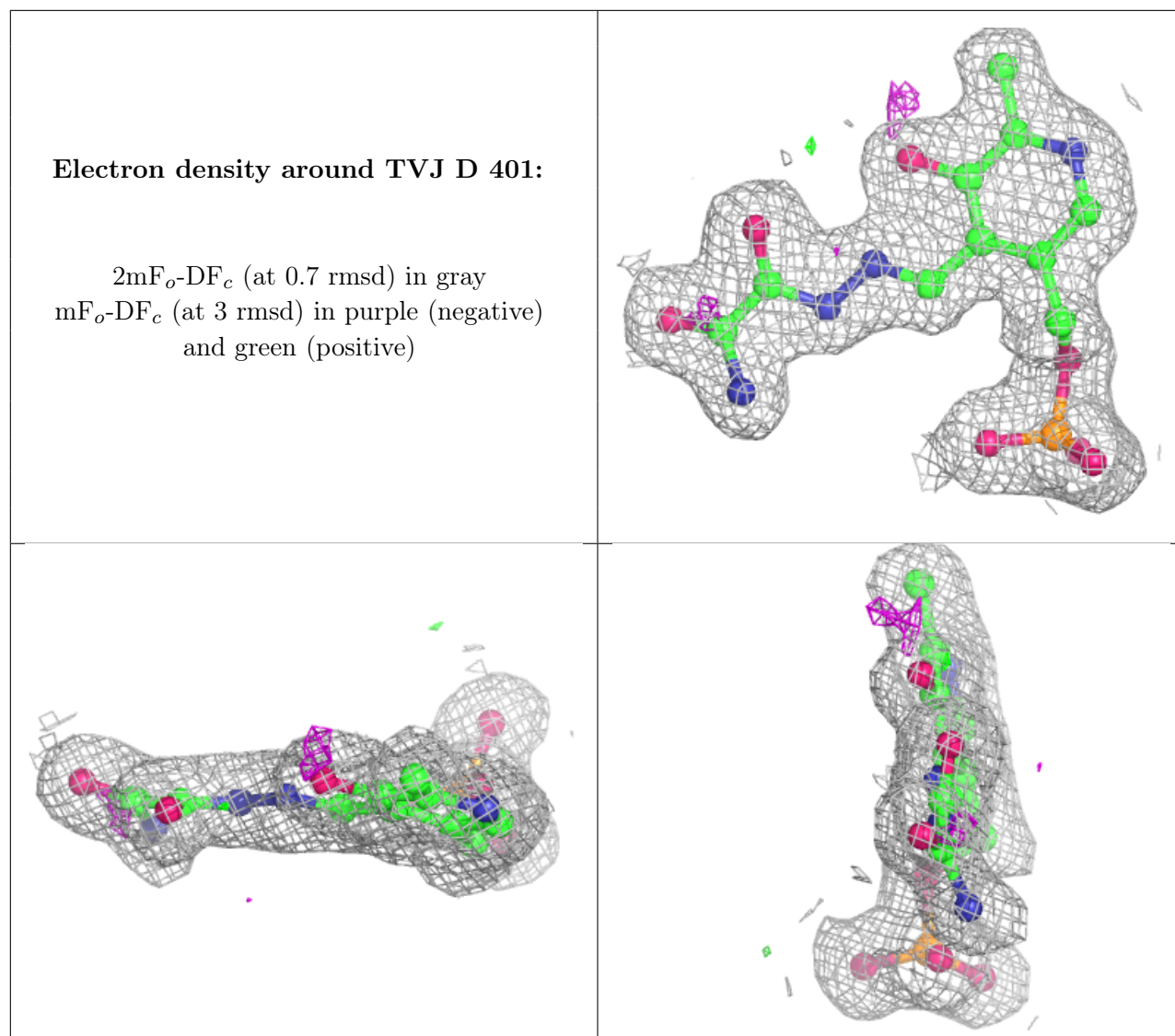
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.