



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:54 AM UTC

PDB ID : 6VZ8 / pdb_00006vz8
EMDB ID : EMD-21487
Title : Arabidopsis thaliana acetohydroxyacid synthase complex with valine bound
Authors : Guddat, L.W.; Low, Y.S.
Deposited on : 2020-02-27
Resolution : 3.45 Å(reported)
Based on initial models : 2PC6, 5K6Q

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

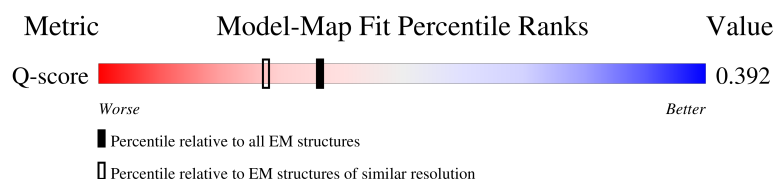
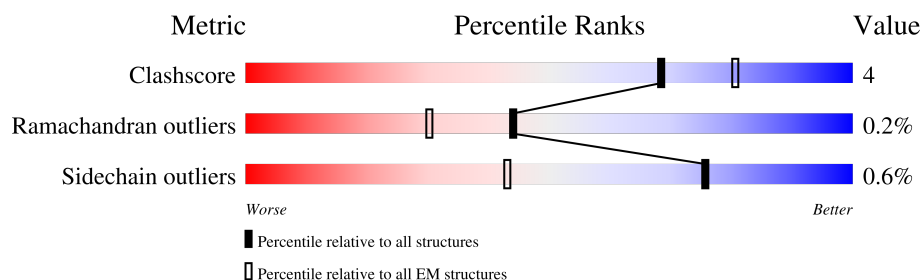
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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.



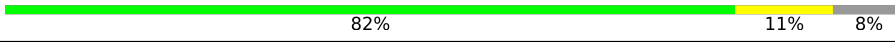
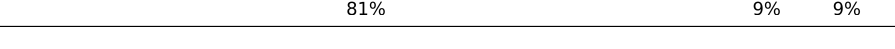
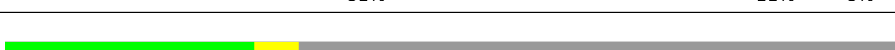
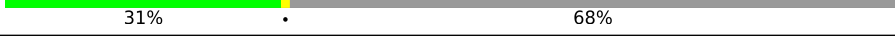
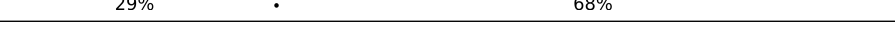
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13836 (2.95 - 3.95)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	586	
1	E	586	
1	H	586	
1	I	586	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	L	586	
1	M	586	
1	P	586	
1	Q	586	
2	F	491	
2	G	491	
2	J	491	
2	K	491	
2	N	491	
2	O	491	
2	R	491	
2	S	491	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 42132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Acetolactate synthase, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	531	Total	C	N	O	S	0	0
			3910	2490	675	725	20		
1	E	541	Total	C	N	O	S	0	0
			3953	2514	684	736	19		
1	H	531	Total	C	N	O	S	0	0
			3910	2490	675	725	20		
1	I	541	Total	C	N	O	S	0	0
			3953	2514	684	736	19		
1	L	531	Total	C	N	O	S	0	0
			3910	2490	675	725	20		
1	M	541	Total	C	N	O	S	0	0
			3953	2514	684	736	19		
1	P	531	Total	C	N	O	S	0	0
			3910	2490	675	725	20		
1	Q	541	Total	C	N	O	S	0	0
			3953	2514	684	736	19		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	85	MET	-	initiating methionine	UNP P17597
E	85	MET	-	initiating methionine	UNP P17597
H	85	MET	-	initiating methionine	UNP P17597
I	85	MET	-	initiating methionine	UNP P17597
L	85	MET	-	initiating methionine	UNP P17597
M	85	MET	-	initiating methionine	UNP P17597
P	85	MET	-	initiating methionine	UNP P17597
Q	85	MET	-	initiating methionine	UNP P17597

- Molecule 2 is a protein called Acetolactate synthase small subunit 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	159	Total	C	N	O	S	0	0
			1266	799	234	227	6		

Continued on next page...

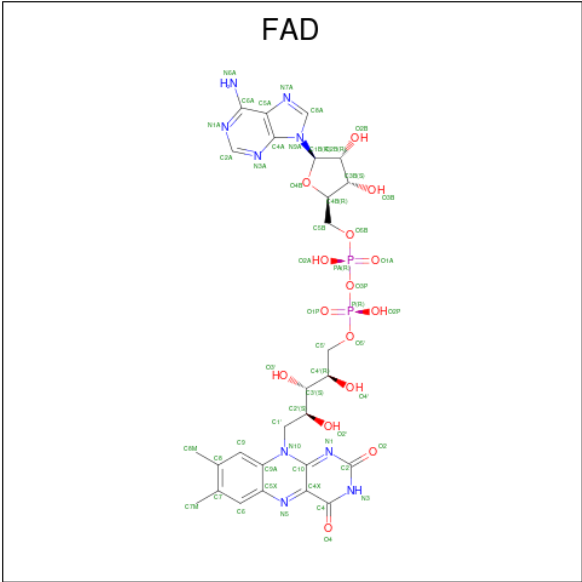
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	159	Total	C	N	O	S	0	0
			1228	775	222	228	3		
2	J	159	Total	C	N	O	S	0	0
			1266	799	234	227	6		
2	K	159	Total	C	N	O	S	0	0
			1228	775	222	228	3		
2	N	159	Total	C	N	O	S	0	0
			1266	799	234	227	6		
2	O	159	Total	C	N	O	S	0	0
			1228	775	222	228	3		
2	R	159	Total	C	N	O	S	0	0
			1266	799	234	227	6		
2	S	159	Total	C	N	O	S	0	0
			1228	775	222	228	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	H	1	Total	Mg	0
			1	1	
3	I	1	Total	Mg	0
			1	1	
3	L	1	Total	Mg	0
			1	1	
3	M	1	Total	Mg	0
			1	1	
3	P	1	Total	Mg	0
			1	1	
3	Q	1	Total	Mg	0
			1	1	

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).

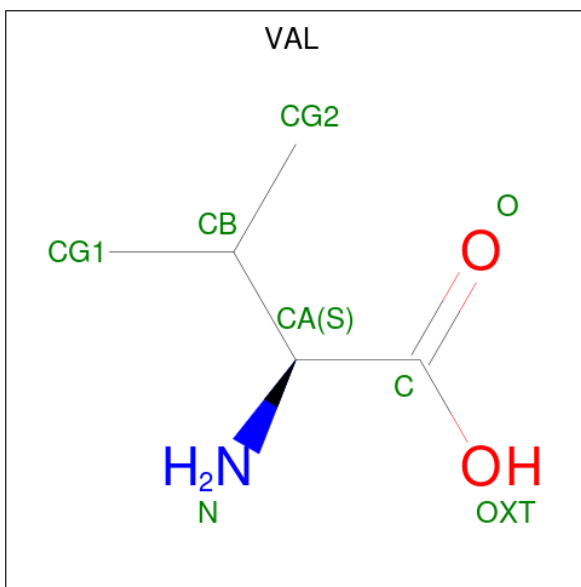


Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	E	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	H	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	I	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	L	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	M	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	P	1	Total	C	N	O	P	0
			53	27	9	15	2	
4	Q	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 5 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



- Molecule 6 is VALINE (CCD ID: VAL) (formula: $\text{C}_5\text{H}_{11}\text{NO}_2$) (labeled as "Ligand of Interest" by depositor).

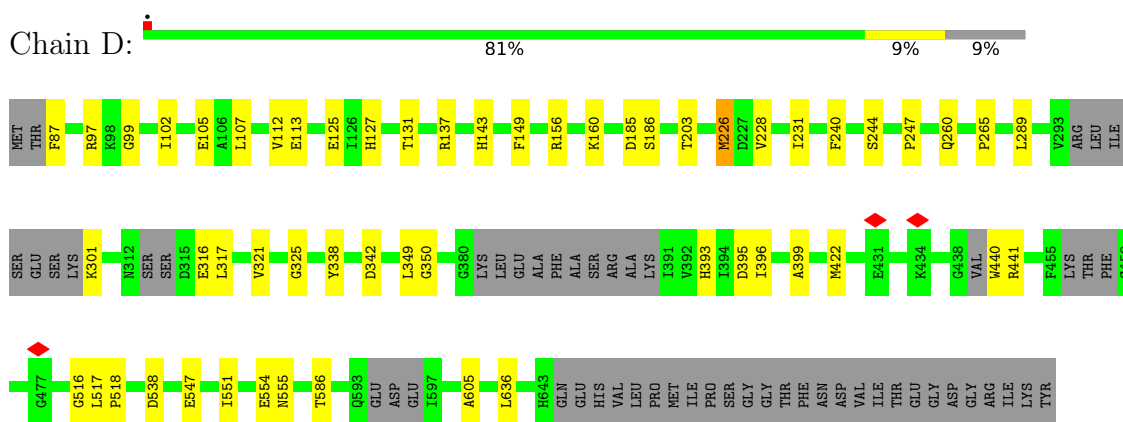


Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			8	5	1	2	
6	G	1	Total	C	N	O	0
			8	5	1	2	
6	J	1	Total	C	N	O	0
			8	5	1	2	
6	K	1	Total	C	N	O	0
			8	5	1	2	
6	N	1	Total	C	N	O	0
			8	5	1	2	
6	O	1	Total	C	N	O	0
			8	5	1	2	
6	R	1	Total	C	N	O	0
			8	5	1	2	
6	S	1	Total	C	N	O	0
			8	5	1	2	

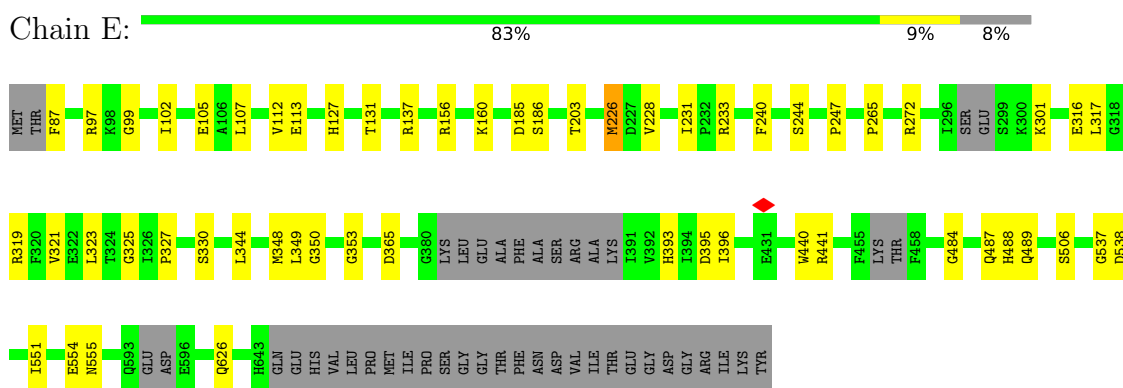
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

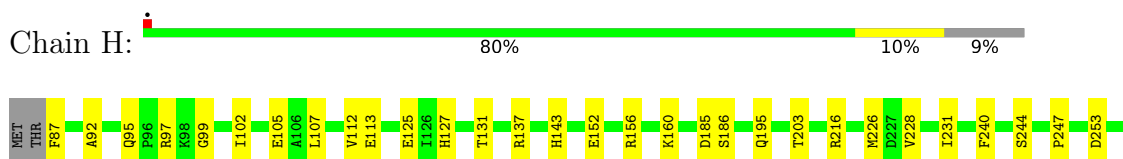
- Molecule 1: Acetolactate synthase, chloroplastic

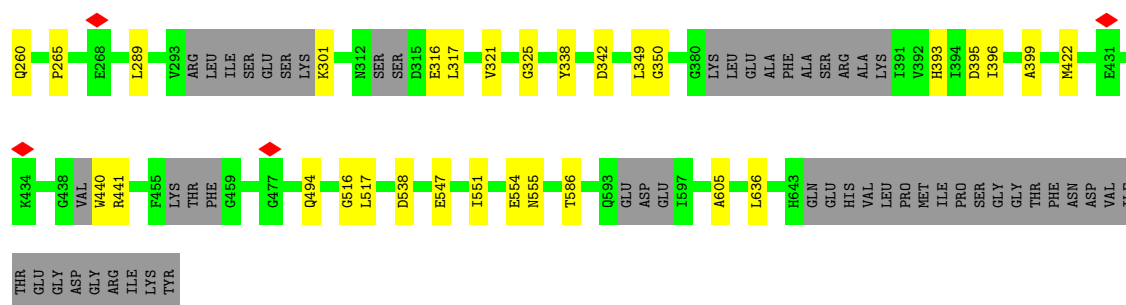


- Molecule 1: Acetolactate synthase, chloroplastic



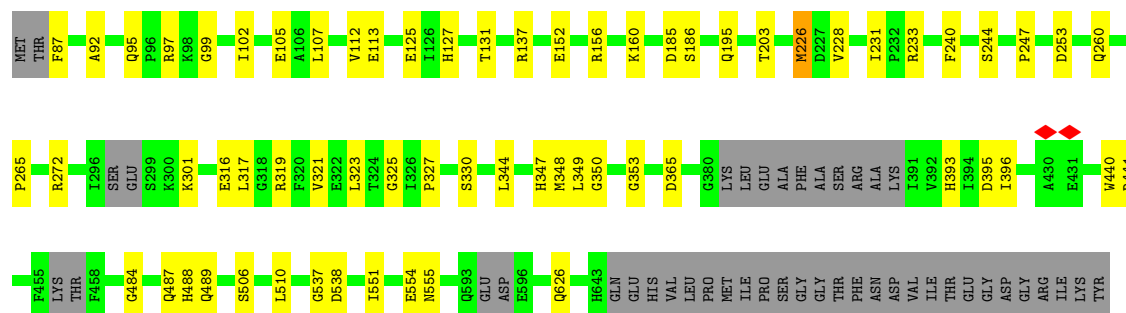
- Molecule 1: Acetolactate synthase, chloroplastic





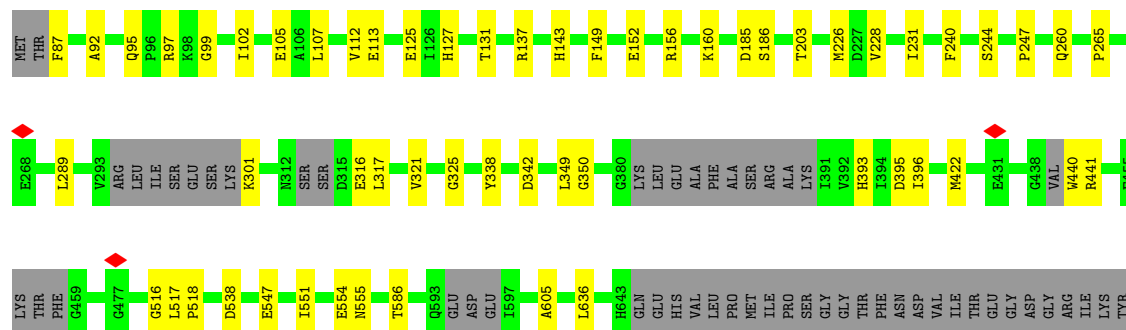
- Molecule 1: Acetolactate synthase, chloroplactic

Chain I: 81% 11% 8%



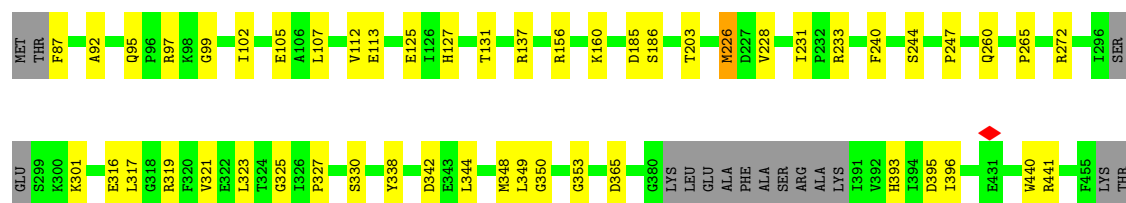
- Molecule 1: Acetolactate synthase, chloroplactic

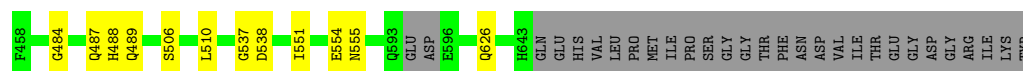
Chain L: 81% 10% 9%



- Molecule 1: Acetolactate synthase, chloroplactic

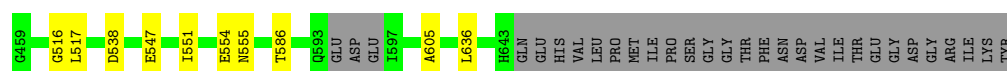
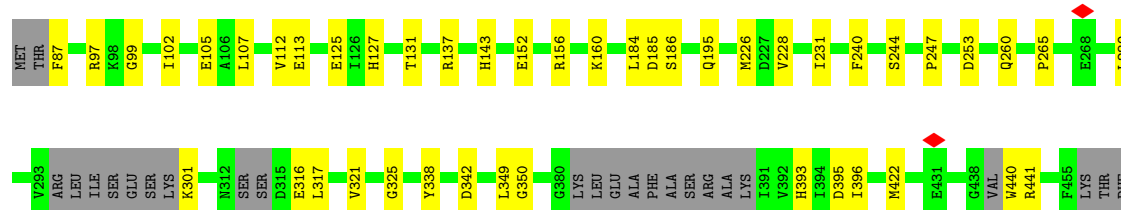
Chain M: 82% 11% 8%





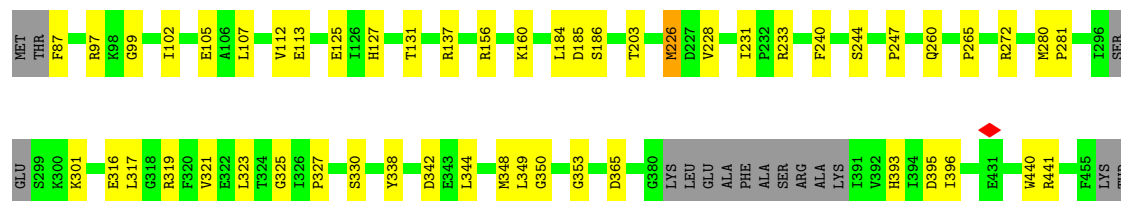
- Molecule 1: Acetolactate synthase, chloroplastic

Chain P: 81% 9% 9%



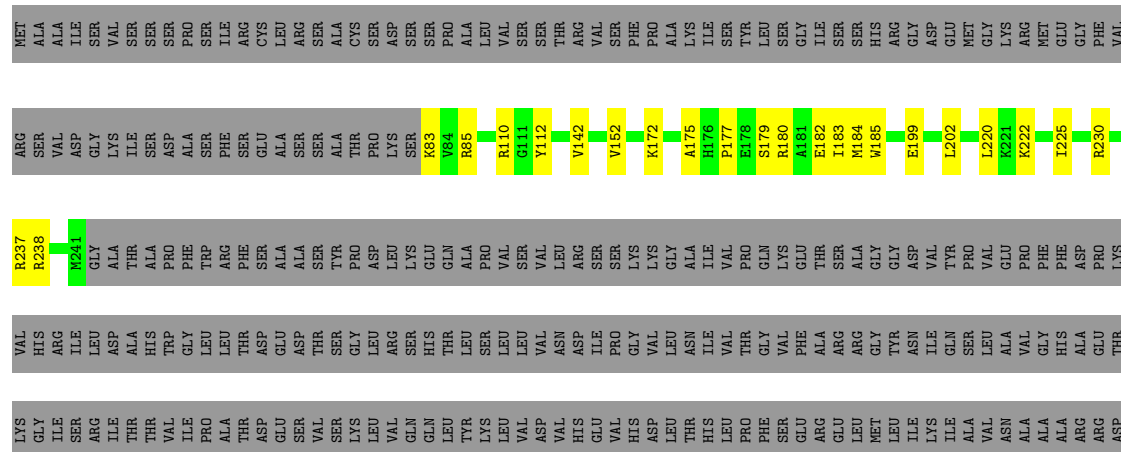
- Molecule 1: Acetolactate synthase, chloroplastic

Chain Q: 81% 11% 8%



- Molecule 2: Acetolactate synthase small subunit 2, chloroplastic

Chain F: 28% 5% 68%



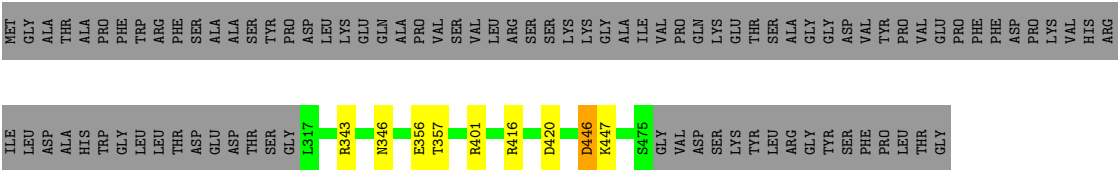
[illegible]

- Molecule 2: Acetolactate synthase small subunit 2, chloroplastic

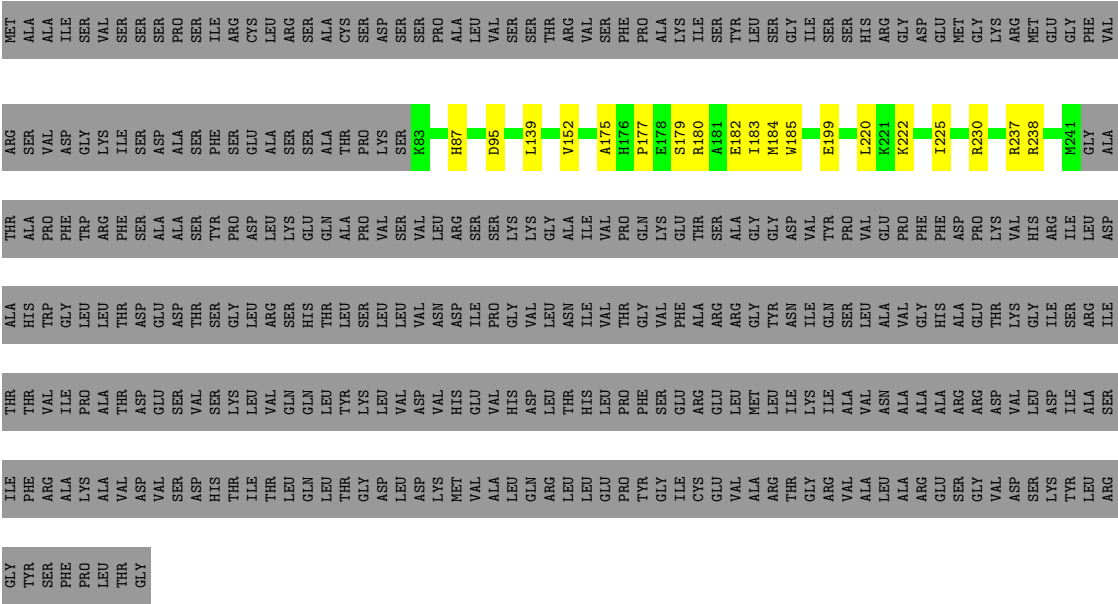
[illegible]

- Molecule 2: Acetolactate synthase small subunit 2, chloroplastic

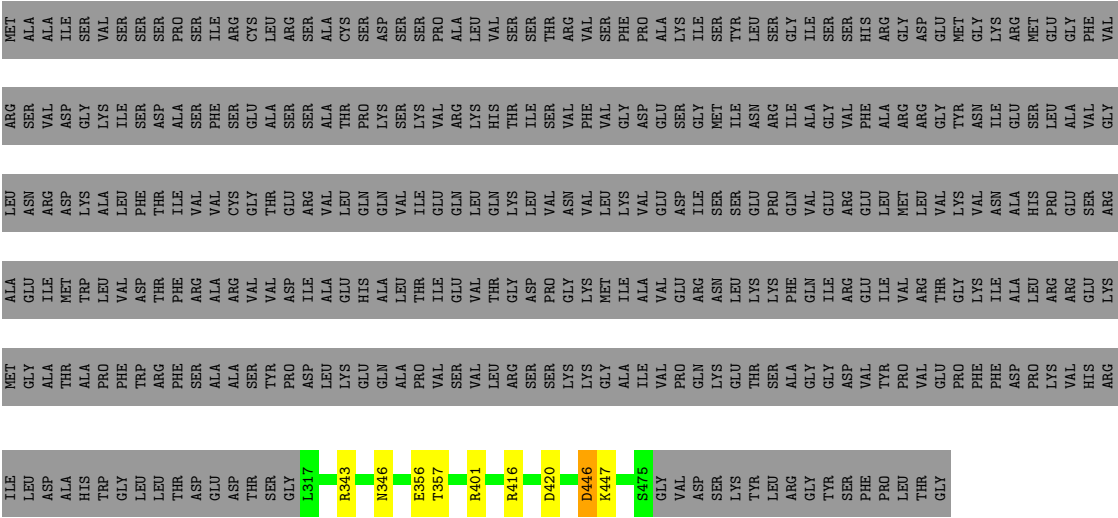
[illegible]



• Molecule 2: Acetolactate synthase small subunit 2, chloroplastic



• Molecule 2: Acetolactate synthase small subunit 2, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	290516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.134	Depositor
Minimum map value	-1.128	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, MG, TPP

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	D	0.57	0/3988	0.91	5/5427 (0.1%)
1	E	0.57	0/4033	0.94	6/5495 (0.1%)
1	H	0.57	0/3988	0.91	6/5427 (0.1%)
1	I	0.57	0/4033	0.94	6/5495 (0.1%)
1	L	0.57	0/3988	0.91	5/5427 (0.1%)
1	M	0.57	0/4033	0.95	6/5495 (0.1%)
1	P	0.57	0/3988	0.91	5/5427 (0.1%)
1	Q	0.57	0/4033	0.94	6/5495 (0.1%)
2	F	0.63	0/1279	1.08	2/1719 (0.1%)
2	G	0.66	0/1243	1.11	1/1687 (0.1%)
2	J	0.65	0/1279	1.14	4/1719 (0.2%)
2	K	0.66	0/1243	1.11	2/1687 (0.1%)
2	N	0.64	0/1279	1.11	2/1719 (0.1%)
2	O	0.67	0/1243	1.17	1/1687 (0.1%)
2	R	0.65	0/1279	1.10	3/1719 (0.2%)
2	S	0.67	0/1243	1.13	3/1687 (0.2%)
All	All	0.59	0/42172	0.98	63/57312 (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	H	0	1
2	F	0	3
2	G	0	1
2	J	0	2
2	N	0	1
2	O	0	1
2	R	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S	0	1
All	All	0	11

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	138	VAL	CA-CB-CG1	10.73	128.64	110.40
1	Q	538	ASP	CA-C-N	6.49	127.01	119.94
1	Q	538	ASP	C-N-CA	6.49	127.01	119.94
1	I	538	ASP	CA-C-N	6.44	126.96	119.94
1	I	538	ASP	C-N-CA	6.44	126.96	119.94
1	E	538	ASP	CA-C-N	6.44	126.96	119.94
1	E	538	ASP	C-N-CA	6.44	126.96	119.94
1	M	538	ASP	CA-C-N	6.42	126.94	119.94
1	M	538	ASP	C-N-CA	6.42	126.94	119.94
2	S	446	ASP	O-C-N	-6.04	115.72	122.12
2	G	446	ASP	O-C-N	-6.00	115.76	122.12
2	K	446	ASP	O-C-N	-6.00	115.76	122.12
2	O	446	ASP	O-C-N	-5.84	115.49	122.15
1	L	350	GLY	CA-C-N	5.76	128.00	120.28
1	L	350	GLY	C-N-CA	5.76	128.00	120.28
1	D	350	GLY	CA-C-N	5.75	127.98	120.28
1	D	350	GLY	C-N-CA	5.75	127.98	120.28
1	H	350	GLY	CA-C-N	5.74	127.98	120.28
1	H	350	GLY	C-N-CA	5.74	127.98	120.28
1	P	538	ASP	CA-C-N	5.74	126.20	119.94
1	P	538	ASP	C-N-CA	5.74	126.20	119.94
2	R	237	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	P	350	GLY	CA-C-N	5.73	127.95	120.28
1	P	350	GLY	C-N-CA	5.73	127.95	120.28
1	L	538	ASP	CA-C-N	5.67	126.12	119.94
1	L	538	ASP	C-N-CA	5.67	126.12	119.94
1	D	538	ASP	CA-C-N	5.66	126.11	119.94
1	D	538	ASP	C-N-CA	5.66	126.11	119.94
1	H	538	ASP	CA-C-N	5.65	126.10	119.94
1	H	538	ASP	C-N-CA	5.65	126.10	119.94
2	F	238	ARG	NE-CZ-NH2	5.56	124.20	119.20
2	J	237	ARG	NE-CZ-NH2	5.56	124.20	119.20
2	N	237	ARG	NE-CZ-NH2	5.51	124.16	119.20
2	K	415	ARG	NE-CZ-NH2	5.50	124.16	119.20
2	J	238	ARG	NE-CZ-NH2	5.47	124.12	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	487	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	Q	487	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	I	487	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	M	487	GLN	OE1-CD-NE2	-5.17	117.42	122.60
2	R	238	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	P	143	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	M	350	GLY	CA-C-N	5.10	127.37	120.38
1	M	350	GLY	C-N-CA	5.10	127.37	120.38
1	Q	626	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	I	626	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	Q	350	GLY	CA-C-N	5.08	127.33	120.38
1	Q	350	GLY	C-N-CA	5.08	127.33	120.38
1	I	350	GLY	CA-C-N	5.07	127.33	120.38
1	I	350	GLY	C-N-CA	5.07	127.33	120.38
2	F	237	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	D	143	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	L	143	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	M	626	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	H	143	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	H	494	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	E	626	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	E	350	GLY	CA-C-N	5.03	127.27	120.38
1	E	350	GLY	C-N-CA	5.03	127.27	120.38
2	N	238	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	S	446	ASP	CA-C-N	5.02	127.94	120.31
2	S	446	ASP	C-N-CA	5.02	127.94	120.31
2	J	87	HIS	CB-CG-CD2	-5.01	124.68	131.20
2	R	87	HIS	CB-CG-CD2	-5.00	124.69	131.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	110	ARG	Sidechain
2	F	112	TYR	Sidechain
2	F	230	ARG	Sidechain
2	G	343	ARG	Sidechain
1	H	216	ARG	Sidechain
2	J	112	TYR	Sidechain
2	J	230	ARG	Sidechain
2	N	230	ARG	Sidechain
2	O	343	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	R	230	ARG	Sidechain
2	S	343	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3910	0	3810	27	0
1	E	3953	0	3817	28	0
1	H	3910	0	3810	29	0
1	I	3953	0	3817	34	0
1	L	3910	0	3810	27	0
1	M	3953	0	3817	32	0
1	P	3910	0	3810	27	0
1	Q	3953	0	3817	32	0
2	F	1266	0	1338	17	0
2	G	1228	0	1283	8	0
2	J	1266	0	1338	17	0
2	K	1228	0	1283	7	0
2	N	1266	0	1338	12	0
2	O	1228	0	1283	7	0
2	R	1266	0	1338	13	0
2	S	1228	0	1283	7	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
4	D	53	0	31	0	0
4	E	53	0	31	0	0
4	H	53	0	31	0	0
4	I	53	0	31	0	0
4	L	53	0	31	0	0
4	M	53	0	31	0	0
4	P	53	0	31	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	53	0	31	0	0
5	D	26	0	16	0	0
5	E	26	0	16	0	0
5	H	26	0	16	0	0
5	I	26	0	16	0	0
5	L	26	0	16	0	0
5	M	26	0	16	0	0
5	P	26	0	16	0	0
5	Q	26	0	16	0	0
6	F	8	0	8	1	0
6	G	8	0	8	0	0
6	J	8	0	8	1	0
6	K	8	0	8	0	0
6	N	8	0	8	1	0
6	O	8	0	8	0	0
6	R	8	0	8	2	0
6	S	8	0	8	0	0
All	All	42132	0	41432	311	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 (311) 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:E:113:GLU:OE1	1:E:160:LYS:NZ	2.20	0.75
1:L:113:GLU:OE1	1:L:160:LYS:NZ	2.20	0.75
6:N:501:VAL:N	2:O:346:ASN:OD1	2.20	0.74
1:P:113:GLU:OE1	1:P:160:LYS:NZ	2.20	0.74
1:Q:113:GLU:OE1	1:Q:160:LYS:NZ	2.20	0.74
1:H:113:GLU:OE1	1:H:160:LYS:NZ	2.20	0.74
1:D:113:GLU:OE1	1:D:160:LYS:NZ	2.20	0.74
1:I:113:GLU:OE1	1:I:160:LYS:NZ	2.20	0.74
1:M:113:GLU:OE1	1:M:160:LYS:NZ	2.20	0.73
2:G:356:GLU:HG3	2:G:357:THR:HG23	1.70	0.73
2:K:356:GLU:HG3	2:K:357:THR:HG23	1.70	0.73
2:O:416:ARG:NH1	2:O:420:ASP:OD1	2.23	0.72
2:S:356:GLU:HG3	2:S:357:THR:HG23	1.70	0.72
2:N:177:PRO:HA	2:N:180:ARG:HD2	1.72	0.71
2:O:356:GLU:HG3	2:O:357:THR:HG23	1.70	0.71
1:Q:156:ARG:NH2	1:Q:185:ASP:OD2	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:416:ARG:NH1	2:K:420:ASP:OD1	2.23	0.71
2:J:177:PRO:HA	2:J:180:ARG:HD2	1.72	0.70
2:R:177:PRO:HA	2:R:180:ARG:HD2	1.72	0.70
2:J:185:TRP:CD1	2:N:184:MET:HE3	2.26	0.70
2:F:177:PRO:HA	2:F:180:ARG:HD2	1.72	0.69
1:M:156:ARG:NH2	1:M:185:ASP:OD2	2.24	0.69
1:D:156:ARG:NH2	1:D:185:ASP:OD2	2.24	0.69
2:S:416:ARG:NH1	2:S:420:ASP:OD1	2.23	0.69
1:I:156:ARG:NH2	1:I:185:ASP:OD2	2.24	0.68
2:G:416:ARG:NH1	2:G:420:ASP:OD1	2.23	0.68
1:H:156:ARG:NH2	1:H:185:ASP:OD2	2.24	0.68
1:E:156:ARG:NH2	1:E:185:ASP:OD2	2.24	0.68
2:N:180:ARG:NH2	2:N:199:GLU:O	2.27	0.67
2:R:180:ARG:NH2	2:R:199:GLU:O	2.27	0.67
2:F:180:ARG:NH2	2:F:199:GLU:O	2.27	0.66
2:J:180:ARG:NH2	2:J:199:GLU:O	2.27	0.66
1:P:156:ARG:NH2	1:P:185:ASP:OD2	2.24	0.65
2:F:175:ALA:O	2:F:180:ARG:NE	2.28	0.65
1:L:156:ARG:NH2	1:L:185:ASP:OD2	2.24	0.65
2:J:175:ALA:O	2:J:180:ARG:NE	2.28	0.64
6:R:501:VAL:N	2:S:346:ASN:OD1	2.31	0.63
2:N:175:ALA:O	2:N:180:ARG:NE	2.27	0.63
1:H:399:ALA:HA	2:K:379:GLN:NE2	2.14	0.63
6:F:501:VAL:N	2:G:346:ASN:OD1	2.32	0.62
2:F:185:TRP:CD1	2:J:184:MET:HE3	2.34	0.62
2:R:175:ALA:O	2:R:180:ARG:NE	2.27	0.62
2:R:179:SER:HA	2:R:182:GLU:OE2	2.04	0.58
2:N:179:SER:HA	2:N:182:GLU:OE2	2.04	0.58
2:F:179:SER:HA	2:F:182:GLU:OE2	2.04	0.58
2:F:199:GLU:HG3	2:R:222:LYS:HE3	1.86	0.58
2:J:179:SER:HA	2:J:182:GLU:OE2	2.04	0.58
2:F:222:LYS:HE3	2:J:199:GLU:HG3	1.86	0.57
2:F:185:TRP:HD1	2:J:184:MET:HE3	1.70	0.56
1:Q:327:PRO:HA	1:Q:344:LEU:HB3	1.88	0.56
1:E:327:PRO:HA	1:E:344:LEU:HB3	1.88	0.55
2:F:83:LYS:HE2	2:F:85:ARG:HD2	1.89	0.55
1:M:327:PRO:HA	1:M:344:LEU:HB3	1.88	0.55
1:M:87:PHE:CZ	1:M:105:GLU:HG3	2.42	0.55
1:Q:87:PHE:CZ	1:Q:105:GLU:HG3	2.42	0.55
1:L:87:PHE:CZ	1:L:105:GLU:HG3	2.42	0.54
1:E:87:PHE:CZ	1:E:105:GLU:HG3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:327:PRO:HA	1:I:344:LEU:HB3	1.88	0.54
2:R:179:SER:HA	2:R:182:GLU:CD	2.32	0.54
2:N:179:SER:HA	2:N:182:GLU:CD	2.32	0.54
2:F:179:SER:HA	2:F:182:GLU:CD	2.32	0.54
1:P:87:PHE:CZ	1:P:105:GLU:HG3	2.42	0.54
1:H:87:PHE:CZ	1:H:105:GLU:HG3	2.42	0.54
2:J:179:SER:HA	2:J:182:GLU:CD	2.32	0.54
2:R:220:LEU:HB3	2:R:225:ILE:HD11	1.90	0.54
2:F:220:LEU:HB3	2:F:225:ILE:HD11	1.90	0.54
1:I:87:PHE:CZ	1:I:105:GLU:HG3	2.42	0.53
2:N:185:TRP:CD1	2:R:184:MET:HE3	2.43	0.53
1:D:87:PHE:CZ	1:D:105:GLU:HG3	2.42	0.53
2:F:184:MET:HE3	2:R:185:TRP:CD1	2.43	0.53
2:J:220:LEU:HB3	2:J:225:ILE:HD11	1.90	0.53
2:N:220:LEU:HB3	2:N:225:ILE:HD11	1.90	0.53
1:D:395:ASP:OD1	1:D:396:ILE:N	2.43	0.52
1:L:517:LEU:HD23	1:L:547:GLU:HB2	1.91	0.52
1:E:395:ASP:OD1	1:E:396:ILE:N	2.43	0.52
1:D:517:LEU:HD23	1:D:547:GLU:HB2	1.91	0.52
1:H:517:LEU:HD23	1:H:547:GLU:HB2	1.91	0.52
1:P:517:LEU:HD23	1:P:547:GLU:HB2	1.91	0.52
1:Q:395:ASP:OD1	1:Q:396:ILE:N	2.43	0.52
1:E:99:GLY:HA2	1:E:102:ILE:HD12	1.92	0.52
1:H:99:GLY:HA2	1:H:102:ILE:HD12	1.92	0.52
1:L:395:ASP:OD1	1:L:396:ILE:N	2.43	0.52
1:H:137:ARG:NH2	1:H:554:GLU:OE1	2.44	0.52
1:I:99:GLY:HA2	1:I:102:ILE:HD12	1.92	0.52
1:P:395:ASP:OD1	1:P:396:ILE:N	2.43	0.52
1:M:488:HIS:CE1	1:M:537:GLY:H	2.28	0.51
1:Q:137:ARG:NH2	1:Q:554:GLU:OE1	2.43	0.51
1:D:99:GLY:HA2	1:D:102:ILE:HD12	1.92	0.51
1:I:137:ARG:NH2	1:I:554:GLU:OE1	2.44	0.51
1:I:395:ASP:OD1	1:I:396:ILE:N	2.43	0.51
1:D:137:ARG:NH2	1:D:554:GLU:OE1	2.43	0.51
1:I:488:HIS:CE1	1:I:537:GLY:H	2.28	0.51
1:P:137:ARG:NH2	1:P:554:GLU:OE1	2.44	0.51
1:Q:99:GLY:HA2	1:Q:102:ILE:HD12	1.92	0.51
1:E:137:ARG:NH2	1:E:554:GLU:OE1	2.43	0.51
1:H:395:ASP:OD1	1:H:396:ILE:N	2.43	0.51
1:M:137:ARG:NH2	1:M:554:GLU:OE1	2.44	0.51
1:M:395:ASP:OD1	1:M:396:ILE:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:99:GLY:HA2	1:M:102:ILE:HD12	1.92	0.51
1:L:99:GLY:HA2	1:L:102:ILE:HD12	1.92	0.51
1:Q:488:HIS:CE1	1:Q:537:GLY:H	2.28	0.51
2:F:185:TRP:CH2	2:J:180:ARG:HD3	2.46	0.50
1:P:99:GLY:HA2	1:P:102:ILE:HD12	1.92	0.50
1:E:488:HIS:CE1	1:E:537:GLY:H	2.28	0.50
1:L:137:ARG:NH2	1:L:554:GLU:OE1	2.44	0.50
1:E:316:GLU:OE1	1:E:316:GLU:N	2.45	0.49
1:E:330:SER:O	1:E:348:MET:HA	2.12	0.49
2:J:185:TRP:HD1	2:N:184:MET:HE3	1.75	0.49
1:H:338:TYR:OH	1:H:342:ASP:OD2	2.30	0.49
1:Q:330:SER:O	1:Q:348:MET:HA	2.12	0.49
2:N:177:PRO:O	2:N:180:ARG:HB2	2.13	0.49
2:R:177:PRO:O	2:R:180:ARG:HB2	2.13	0.49
1:M:349:LEU:C	1:M:353:GLY:HA3	2.38	0.49
1:E:349:LEU:C	1:E:353:GLY:HA3	2.38	0.49
1:Q:349:LEU:C	1:Q:353:GLY:HA3	2.38	0.49
1:I:330:SER:O	1:I:348:MET:HA	2.12	0.49
2:J:177:PRO:O	2:J:180:ARG:HB2	2.13	0.49
1:M:330:SER:O	1:M:348:MET:HA	2.12	0.49
2:S:446:ASP:OD2	2:S:447:LYS:N	2.46	0.48
2:F:177:PRO:O	2:F:180:ARG:HB2	2.13	0.48
1:I:349:LEU:C	1:I:353:GLY:HA3	2.38	0.48
2:G:446:ASP:OD2	2:G:447:LYS:N	2.46	0.48
1:Q:125:GLU:OE2	1:Q:260:GLN:NE2	2.30	0.48
1:Q:316:GLU:OE1	1:Q:316:GLU:N	2.45	0.48
1:D:125:GLU:OE2	1:D:260:GLN:NE2	2.30	0.48
1:D:316:GLU:OE1	1:D:316:GLU:N	2.45	0.48
1:I:125:GLU:OE2	1:I:260:GLN:NE2	2.31	0.48
1:L:338:TYR:OH	1:L:342:ASP:OD2	2.30	0.47
2:K:446:ASP:OD2	2:K:447:LYS:N	2.46	0.47
1:I:316:GLU:OE1	1:I:316:GLU:N	2.45	0.47
1:P:316:GLU:N	1:P:316:GLU:OE1	2.45	0.47
2:J:95:ASP:OD1	6:J:501:VAL:N	2.46	0.47
1:L:316:GLU:OE1	1:L:316:GLU:N	2.45	0.47
1:M:316:GLU:OE1	1:M:316:GLU:N	2.45	0.47
1:D:338:TYR:OH	1:D:342:ASP:OD2	2.30	0.47
1:M:125:GLU:OE2	1:M:260:GLN:NE2	2.30	0.47
2:G:416:ARG:HH21	2:G:416:ARG:HA	1.81	0.46
2:N:222:LYS:HE3	2:R:199:GLU:HG3	1.98	0.46
1:P:289:LEU:HD22	1:P:422:MET:HG3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:338:TYR:OH	1:P:342:ASP:OD2	2.30	0.46
1:H:289:LEU:HD22	1:H:422:MET:HG3	1.97	0.46
2:S:416:ARG:HH21	2:S:416:ARG:HA	1.81	0.46
2:J:220:LEU:HD23	2:J:220:LEU:HA	1.75	0.46
1:P:228:VAL:HG23	1:P:231:ILE:HD12	1.98	0.46
1:E:228:VAL:HG23	1:E:231:ILE:HD12	1.98	0.45
2:O:416:ARG:HA	2:O:416:ARG:HH21	1.81	0.45
1:Q:228:VAL:HG23	1:Q:231:ILE:HD12	1.99	0.45
1:I:228:VAL:HG23	1:I:231:ILE:HD12	1.99	0.45
2:O:446:ASP:OD2	2:O:447:LYS:N	2.47	0.45
1:Q:489:GLN:NE2	1:Q:506:SER:OG	2.43	0.45
1:D:127:HIS:O	1:D:131:THR:HG23	2.17	0.45
1:D:228:VAL:HG23	1:D:231:ILE:HD12	1.99	0.45
1:E:127:HIS:O	1:E:131:THR:HG23	2.17	0.45
1:I:127:HIS:O	1:I:131:THR:HG23	2.17	0.45
1:I:301:LYS:H	1:I:365:ASP:CG	2.24	0.45
1:P:127:HIS:O	1:P:131:THR:HG23	2.17	0.45
1:D:289:LEU:HD22	1:D:422:MET:HG3	1.97	0.45
1:I:489:GLN:NE2	1:I:506:SER:OG	2.43	0.45
1:L:289:LEU:HD22	1:L:422:MET:HG3	1.97	0.45
1:M:301:LYS:H	1:M:365:ASP:CG	2.24	0.45
1:E:301:LYS:H	1:E:365:ASP:CG	2.24	0.45
1:L:127:HIS:O	1:L:131:THR:HG23	2.17	0.45
1:M:228:VAL:HG23	1:M:231:ILE:HD12	1.98	0.45
1:Q:301:LYS:H	1:Q:365:ASP:CG	2.24	0.45
1:H:228:VAL:HG23	1:H:231:ILE:HD12	1.99	0.45
1:H:107:LEU:HB3	1:H:112:VAL:HG21	1.99	0.45
1:H:127:HIS:O	1:H:131:THR:HG23	2.17	0.45
1:Q:127:HIS:O	1:Q:131:THR:HG23	2.17	0.45
2:K:416:ARG:HA	2:K:416:ARG:HH21	1.81	0.44
1:L:107:LEU:HB3	1:L:112:VAL:HG21	1.99	0.44
1:E:107:LEU:HB3	1:E:112:VAL:HG21	1.99	0.44
1:H:125:GLU:OE2	1:H:260:GLN:NE2	2.30	0.44
1:M:107:LEU:HB3	1:M:112:VAL:HG21	1.99	0.44
1:M:489:GLN:NE2	1:M:506:SER:OG	2.43	0.44
1:L:228:VAL:HG23	1:L:231:ILE:HD12	1.98	0.44
1:M:127:HIS:O	1:M:131:THR:HG23	2.17	0.44
2:F:220:LEU:HD23	2:F:220:LEU:HA	1.75	0.44
1:H:316:GLU:OE1	1:H:316:GLU:N	2.45	0.44
1:M:338:TYR:OH	1:M:342:ASP:OD2	2.30	0.43
1:I:107:LEU:HB3	1:I:112:VAL:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:107:LEU:HB3	1:Q:112:VAL:HG21	1.99	0.43
1:H:186:SER:O	1:H:247:PRO:HG2	2.19	0.43
1:P:107:LEU:HB3	1:P:112:VAL:HG21	1.99	0.43
1:D:107:LEU:HB3	1:D:112:VAL:HG21	1.99	0.43
2:F:179:SER:O	2:F:183:ILE:HG12	2.19	0.43
1:H:152:GLU:OE1	1:H:156:ARG:NE	2.44	0.43
1:I:226:MET:HA	1:I:226:MET:HE2	2.00	0.43
1:P:317:LEU:O	1:P:321:VAL:HG23	2.19	0.43
1:Q:338:TYR:OH	1:Q:342:ASP:OD2	2.30	0.43
2:R:179:SER:O	2:R:183:ILE:HG12	2.19	0.43
1:Q:280:MET:HA	1:Q:281:PRO:HD3	1.94	0.43
1:E:393:HIS:CE1	1:E:395:ASP:HB2	2.54	0.43
1:H:399:ALA:HA	2:K:379:GLN:HE21	1.84	0.43
1:L:152:GLU:OE1	1:L:156:ARG:NE	2.44	0.43
1:M:186:SER:O	1:M:247:PRO:HG2	2.19	0.43
1:M:317:LEU:O	1:M:321:VAL:HG23	2.19	0.43
1:P:393:HIS:CE1	1:P:395:ASP:HB2	2.54	0.43
1:Q:186:SER:O	1:Q:247:PRO:HG2	2.19	0.43
1:H:393:HIS:CE1	1:H:395:ASP:HB2	2.54	0.43
1:L:605:ALA:HB2	1:L:636:LEU:HD23	2.01	0.43
1:Q:226:MET:HE2	1:Q:226:MET:HA	2.00	0.43
1:Q:317:LEU:O	1:Q:321:VAL:HG23	2.19	0.43
1:E:186:SER:O	1:E:247:PRO:HG2	2.19	0.43
1:H:317:LEU:O	1:H:321:VAL:HG23	2.19	0.43
1:H:605:ALA:HB2	1:H:636:LEU:HD23	2.01	0.43
1:L:317:LEU:O	1:L:321:VAL:HG23	2.19	0.43
1:M:226:MET:HE2	1:M:226:MET:HA	2.00	0.43
1:M:393:HIS:CE1	1:M:395:ASP:HB2	2.54	0.43
1:Q:393:HIS:CE1	1:Q:395:ASP:HB2	2.54	0.43
1:D:226:MET:HA	1:D:226:MET:HE2	2.00	0.43
1:I:240:PHE:CE1	1:I:244:SER:HB3	2.54	0.43
1:P:186:SER:O	1:P:247:PRO:HG2	2.19	0.43
1:L:393:HIS:CE1	1:L:395:ASP:HB2	2.54	0.42
1:L:97:ARG:NH1	1:L:265:PRO:HG3	2.35	0.42
1:L:301:LYS:HA	1:L:440:TRP:CD1	2.55	0.42
2:N:179:SER:O	2:N:183:ILE:HG12	2.19	0.42
1:P:97:ARG:NH1	1:P:265:PRO:HG3	2.34	0.42
1:D:399:ALA:HA	2:G:379:GLN:NE2	2.34	0.42
2:J:179:SER:O	2:J:183:ILE:HG12	2.19	0.42
1:L:186:SER:O	1:L:247:PRO:HG2	2.19	0.42
1:M:240:PHE:CE1	1:M:244:SER:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:301:LYS:HA	1:P:440:TRP:CD1	2.55	0.42
1:E:240:PHE:CE1	1:E:244:SER:HB3	2.54	0.42
1:E:317:LEU:O	1:E:321:VAL:HG23	2.19	0.42
1:H:97:ARG:NH1	1:H:265:PRO:HG3	2.34	0.42
1:I:301:LYS:HA	1:I:440:TRP:CD1	2.54	0.42
1:I:317:LEU:O	1:I:321:VAL:HG23	2.19	0.42
1:L:240:PHE:CE1	1:L:244:SER:HB3	2.54	0.42
1:D:186:SER:O	1:D:247:PRO:HG2	2.19	0.42
1:E:325:GLY:O	1:E:441:ARG:HD3	2.20	0.42
1:I:186:SER:O	1:I:247:PRO:HG2	2.19	0.42
1:Q:240:PHE:CE1	1:Q:244:SER:HB3	2.54	0.42
1:I:97:ARG:NH1	1:I:265:PRO:HG3	2.35	0.42
1:Q:97:ARG:NH1	1:Q:265:PRO:HG3	2.35	0.42
1:Q:325:GLY:O	1:Q:441:ARG:HD3	2.20	0.42
1:H:325:GLY:O	1:H:441:ARG:HD3	2.20	0.42
1:I:152:GLU:OE1	1:I:156:ARG:NE	2.44	0.42
1:L:325:GLY:O	1:L:441:ARG:HD3	2.20	0.42
1:P:240:PHE:CE1	1:P:244:SER:HB3	2.54	0.42
1:Q:301:LYS:HA	1:Q:440:TRP:CD1	2.54	0.42
1:D:301:LYS:HA	1:D:440:TRP:CD1	2.55	0.42
1:D:317:LEU:O	1:D:321:VAL:HG23	2.19	0.42
1:E:551:ILE:O	1:E:555:ASN:N	2.53	0.42
1:H:301:LYS:HA	1:H:440:TRP:CD1	2.54	0.42
1:M:301:LYS:HA	1:M:440:TRP:CD1	2.54	0.42
1:P:605:ALA:HB2	1:P:636:LEU:HD23	2.01	0.42
1:D:97:ARG:NH1	1:D:265:PRO:HG3	2.34	0.42
1:D:393:HIS:CE1	1:D:395:ASP:HB2	2.54	0.42
1:I:325:GLY:O	1:I:441:ARG:HD3	2.20	0.42
1:I:393:HIS:CE1	1:I:395:ASP:HB2	2.54	0.42
1:D:605:ALA:HB2	1:D:636:LEU:HD23	2.01	0.42
1:E:226:MET:HE2	1:E:226:MET:HA	2.00	0.42
1:H:349:LEU:HD23	1:H:349:LEU:H	1.85	0.42
1:P:325:GLY:O	1:P:441:ARG:HD3	2.20	0.42
1:I:551:ILE:O	1:I:555:ASN:N	2.53	0.41
1:D:240:PHE:CE1	1:D:244:SER:HB3	2.54	0.41
1:E:301:LYS:HA	1:E:440:TRP:CD1	2.54	0.41
1:D:325:GLY:O	1:D:441:ARG:HD3	2.20	0.41
2:S:416:ARG:HA	2:S:416:ARG:NH2	2.36	0.41
1:L:551:ILE:O	1:L:555:ASN:N	2.53	0.41
1:M:97:ARG:NH1	1:M:265:PRO:HG3	2.34	0.41
1:M:325:GLY:O	1:M:441:ARG:HD3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:416:ARG:HA	2:O:416:ARG:NH2	2.36	0.41
1:Q:319:ARG:NH2	1:Q:323:LEU:HG	2.35	0.41
1:H:240:PHE:CE1	1:H:244:SER:HB3	2.54	0.41
1:H:551:ILE:O	1:H:555:ASN:N	2.53	0.41
1:L:349:LEU:HD23	1:L:349:LEU:H	1.85	0.41
1:M:510:LEU:HD12	1:M:510:LEU:HA	1.86	0.41
1:M:551:ILE:O	1:M:555:ASN:N	2.53	0.41
1:Q:184:LEU:HD23	1:Q:184:LEU:HA	1.87	0.41
1:D:349:LEU:H	1:D:349:LEU:HD23	1.86	0.41
1:D:551:ILE:O	1:D:555:ASN:N	2.53	0.41
1:Q:551:ILE:O	1:Q:555:ASN:N	2.53	0.41
2:R:95:ASP:OD1	6:R:501:VAL:N	2.53	0.41
1:E:319:ARG:NH2	1:E:323:LEU:HG	2.35	0.41
1:Q:510:LEU:HD12	1:Q:510:LEU:HA	1.86	0.41
1:M:233:ARG:NH2	1:M:272:ARG:HD2	2.35	0.41
1:M:319:ARG:NH2	1:M:323:LEU:HG	2.35	0.41
1:P:551:ILE:O	1:P:555:ASN:N	2.53	0.41
1:E:97:ARG:NH1	1:E:265:PRO:HG3	2.35	0.41
1:E:233:ARG:NH2	1:E:272:ARG:HD2	2.36	0.41
1:I:319:ARG:NH2	1:I:323:LEU:HG	2.35	0.41
2:K:416:ARG:HA	2:K:416:ARG:NH2	2.36	0.41
1:L:125:GLU:OE2	1:L:260:GLN:NE2	2.30	0.41
1:M:321:VAL:O	1:M:325:GLY:N	2.38	0.41
2:O:401:ARG:NE	2:O:401:ARG:HA	2.36	0.41
1:P:195:GLN:NE2	1:P:253:ASP:OD1	2.52	0.41
2:S:401:ARG:NE	2:S:401:ARG:HA	2.36	0.41
1:E:349:LEU:HD23	1:E:349:LEU:H	1.86	0.41
2:G:401:ARG:NE	2:G:401:ARG:HA	2.36	0.41
1:I:195:GLN:NE2	1:I:253:ASP:OD1	2.52	0.41
1:I:233:ARG:NH2	1:I:272:ARG:HD2	2.36	0.41
1:P:152:GLU:OE1	1:P:156:ARG:NE	2.44	0.41
1:E:489:GLN:NE2	1:E:506:SER:OG	2.43	0.40
1:I:92:ALA:HB3	1:I:95:GLN:HB2	2.04	0.40
1:I:347:HIS:HB3	1:I:348:MET:H	1.80	0.40
1:I:510:LEU:HA	1:I:510:LEU:HD12	1.86	0.40
2:J:172:LYS:HA	2:J:202:LEU:O	2.22	0.40
1:P:125:GLU:OE2	1:P:260:GLN:NE2	2.30	0.40
1:P:349:LEU:H	1:P:349:LEU:HD23	1.85	0.40
1:H:92:ALA:HB3	1:H:95:GLN:HB2	2.04	0.40
1:I:349:LEU:HD23	1:I:349:LEU:H	1.86	0.40
1:L:149:PHE:CB	1:L:518:PRO:HB2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:172:LYS:HA	2:F:202:LEU:O	2.21	0.40
2:G:416:ARG:HA	2:G:416:ARG:NH2	2.36	0.40
1:L:92:ALA:HB3	1:L:95:GLN:HB2	2.04	0.40
1:M:92:ALA:HB3	1:M:95:GLN:HB2	2.04	0.40
1:P:184:LEU:HD23	1:P:184:LEU:HA	1.87	0.40
1:D:149:PHE:CB	1:D:518:PRO:HB2	2.51	0.40
1:H:195:GLN:NE2	1:H:253:ASP:OD1	2.52	0.40
1:Q:233:ARG:NH2	1:Q:272:ARG:HD2	2.36	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 PDB entries followed by that with respect to all EM entries.

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	D	517/586 (88%)	499 (96%)	17 (3%)	1 (0%)	43	74
1	E	531/586 (91%)	512 (96%)	18 (3%)	1 (0%)	43	74
1	H	517/586 (88%)	499 (96%)	17 (3%)	1 (0%)	43	74
1	I	531/586 (91%)	511 (96%)	19 (4%)	1 (0%)	43	74
1	L	517/586 (88%)	498 (96%)	18 (4%)	1 (0%)	43	74
1	M	531/586 (91%)	512 (96%)	18 (3%)	1 (0%)	43	74
1	P	517/586 (88%)	497 (96%)	19 (4%)	1 (0%)	43	74
1	Q	531/586 (91%)	512 (96%)	18 (3%)	1 (0%)	43	74
2	F	157/491 (32%)	150 (96%)	7 (4%)	0	100	100
2	G	157/491 (32%)	153 (98%)	4 (2%)	0	100	100
2	J	157/491 (32%)	153 (98%)	3 (2%)	1 (1%)	21	53
2	K	157/491 (32%)	151 (96%)	6 (4%)	0	100	100
2	N	157/491 (32%)	151 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	157/491 (32%)	154 (98%)	3 (2%)	0	100	100
2	R	157/491 (32%)	154 (98%)	3 (2%)	0	100	100
2	S	157/491 (32%)	152 (97%)	5 (3%)	0	100	100
All	All	5448/8616 (63%)	5258 (96%)	181 (3%)	9 (0%)	44	74

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	123	ARG
1	D	516	GLY
1	H	516	GLY
1	L	516	GLY
1	P	516	GLY
1	E	484	GLY
1	I	484	GLY
1	M	484	GLY
1	Q	484	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	D	396/483 (82%)	393 (99%)	3 (1%)	73	77
1	E	395/483 (82%)	393 (100%)	2 (0%)	81	81
1	H	396/483 (82%)	393 (99%)	3 (1%)	73	77
1	I	395/483 (82%)	393 (100%)	2 (0%)	81	81
1	L	396/483 (82%)	393 (99%)	3 (1%)	73	77
1	M	395/483 (82%)	393 (100%)	2 (0%)	81	81
1	P	396/483 (82%)	394 (100%)	2 (0%)	81	81
1	Q	395/483 (82%)	393 (100%)	2 (0%)	81	81
2	F	139/418 (33%)	137 (99%)	2 (1%)	59	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	136/418 (32%)	136 (100%)	0	100	100
2	J	139/418 (33%)	138 (99%)	1 (1%)	76	78
2	K	136/418 (32%)	136 (100%)	0	100	100
2	N	139/418 (33%)	137 (99%)	2 (1%)	59	72
2	O	136/418 (32%)	136 (100%)	0	100	100
2	R	139/418 (33%)	137 (99%)	2 (1%)	59	72
2	S	136/418 (32%)	136 (100%)	0	100	100
All	All	4264/7208 (59%)	4238 (99%)	26 (1%)	76	80

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	203	THR
1	D	226	MET
1	D	586	THR
1	E	203	THR
1	E	226	MET
2	F	142	VAL
2	F	152	VAL
1	H	203	THR
1	H	226	MET
1	H	586	THR
1	I	203	THR
1	I	226	MET
2	J	138	VAL
1	L	203	THR
1	L	226	MET
1	L	586	THR
1	M	203	THR
1	M	226	MET
2	N	139	LEU
2	N	152	VAL
1	P	226	MET
1	P	586	THR
1	Q	203	THR
1	Q	226	MET
2	R	139	LEU
2	R	152	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49)

such sidechains are listed below:

Mol	Chain	Res	Type
1	D	269	GLN
1	D	393	HIS
1	D	487	GLN
1	D	582	ASN
1	E	128	GLN
1	E	269	GLN
1	E	393	HIS
2	F	122	ASN
2	F	163	GLN
2	G	346	ASN
2	G	452	GLN
1	H	259	GLN
1	H	269	GLN
1	H	393	HIS
1	H	487	GLN
1	H	497	ASN
1	H	582	ASN
1	I	128	GLN
1	I	259	GLN
1	I	269	GLN
1	I	393	HIS
2	J	113	ASN
2	J	163	GLN
2	K	327	ASN
1	L	259	GLN
1	L	269	GLN
1	L	393	HIS
1	L	487	GLN
1	L	582	ASN
1	M	128	GLN
1	M	269	GLN
1	M	393	HIS
1	M	487	GLN
2	N	163	GLN
2	O	327	ASN
2	O	348	GLN
2	O	380	GLN
1	P	259	GLN
1	P	269	GLN
1	P	393	HIS
1	P	487	GLN
1	P	582	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	128	GLN
1	Q	269	GLN
1	Q	393	HIS
1	Q	487	GLN
2	R	163	GLN
2	S	327	ASN
2	S	380	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	Q	702	-	58,58,58	1.06	3 (5%)	85,89,89	1.59	14 (16%)
5	TPP	M	703	3	26,27,27	1.23	3 (11%)	38,40,40	1.38	7 (18%)
5	TPP	P	703	3	26,27,27	1.24	4 (15%)	38,40,40	1.57	8 (21%)
4	FAD	L	702	-	58,58,58	0.99	1 (1%)	85,89,89	1.68	17 (20%)
5	TPP	H	703	3	26,27,27	1.24	4 (15%)	38,40,40	1.57	9 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	E	702	-	58,58,58	1.06	3 (5%)	85,89,89	1.59	14 (16%)
6	VAL	F	501	-	6,7,7	1.67	3 (50%)	8,9,9	0.97	0
4	FAD	D	702	-	58,58,58	0.99	1 (1%)	85,89,89	1.68	16 (18%)
6	VAL	R	501	-	6,7,7	1.71	3 (50%)	8,9,9	1.03	0
5	TPP	E	703	3	26,27,27	1.23	3 (11%)	38,40,40	1.39	7 (18%)
6	VAL	O	501	-	6,7,7	1.70	2 (33%)	8,9,9	0.96	1 (12%)
5	TPP	D	703	3	26,27,27	1.25	4 (15%)	38,40,40	1.58	9 (23%)
4	FAD	M	702	-	58,58,58	1.06	3 (5%)	85,89,89	1.59	14 (16%)
6	VAL	G	501	-	6,7,7	1.76	2 (33%)	8,9,9	1.07	1 (12%)
5	TPP	L	703	3	26,27,27	1.24	4 (15%)	38,40,40	1.56	8 (21%)
4	FAD	I	702	-	58,58,58	1.05	3 (5%)	85,89,89	1.59	14 (16%)
6	VAL	K	501	-	6,7,7	1.68	2 (33%)	8,9,9	1.04	1 (12%)
6	VAL	S	501	-	6,7,7	1.70	2 (33%)	8,9,9	1.01	1 (12%)
5	TPP	I	703	3	26,27,27	1.24	3 (11%)	38,40,40	1.38	8 (21%)
4	FAD	P	702	-	58,58,58	0.99	1 (1%)	85,89,89	1.68	16 (18%)
6	VAL	N	501	-	6,7,7	1.74	3 (50%)	8,9,9	1.05	1 (12%)
4	FAD	H	702	-	58,58,58	0.99	1 (1%)	85,89,89	1.68	16 (18%)
6	VAL	J	501	-	6,7,7	1.71	3 (50%)	8,9,9	1.02	1 (12%)
5	TPP	Q	703	3	26,27,27	1.23	3 (11%)	38,40,40	1.38	7 (18%)

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
4	FAD	Q	702	-	-	4/34/50/50	0/6/6/6
5	TPP	M	703	3	-	1/17/17/17	0/2/2/2
5	TPP	P	703	3	-	2/17/17/17	0/2/2/2
4	FAD	L	702	-	-	5/34/50/50	0/6/6/6
5	TPP	H	703	3	-	2/17/17/17	0/2/2/2
4	FAD	E	702	-	-	4/34/50/50	0/6/6/6
6	VAL	F	501	-	-	3/8/8/8	-
4	FAD	D	702	-	-	5/34/50/50	0/6/6/6
6	VAL	R	501	-	-	0/8/8/8	-
5	TPP	E	703	3	-	1/17/17/17	0/2/2/2
6	VAL	O	501	-	-	0/8/8/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TPP	D	703	3	-	2/17/17/17	0/2/2/2
4	FAD	M	702	-	-	4/34/50/50	0/6/6/6
6	VAL	G	501	-	-	0/8/8/8	-
5	TPP	L	703	3	-	2/17/17/17	0/2/2/2
4	FAD	I	702	-	-	4/34/50/50	0/6/6/6
6	VAL	K	501	-	-	0/8/8/8	-
6	VAL	S	501	-	-	0/8/8/8	-
5	TPP	I	703	3	-	1/17/17/17	0/2/2/2
4	FAD	P	702	-	-	5/34/50/50	0/6/6/6
6	VAL	N	501	-	-	3/8/8/8	-
4	FAD	H	702	-	-	5/34/50/50	0/6/6/6
6	VAL	J	501	-	-	1/8/8/8	-
5	TPP	Q	703	3	-	1/17/17/17	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	702	FAD	C5'-C4'	3.19	1.56	1.51
4	Q	702	FAD	C5'-C4'	3.19	1.56	1.51
4	I	702	FAD	C5'-C4'	3.13	1.56	1.51
4	M	702	FAD	C5'-C4'	3.10	1.56	1.51
5	L	703	TPP	C5'-C4'	-2.90	1.38	1.42
5	P	703	TPP	C5'-C4'	-2.89	1.38	1.42
5	D	703	TPP	C5'-C4'	-2.86	1.38	1.42
5	H	703	TPP	C5'-C4'	-2.82	1.38	1.42
6	G	501	VAL	CA-N	2.74	1.55	1.47
6	O	501	VAL	CA-N	2.68	1.54	1.47
6	S	501	VAL	CA-N	2.64	1.54	1.47
5	E	703	TPP	C5'-C4'	-2.62	1.38	1.42
5	D	703	TPP	PA-O3A	-2.61	1.56	1.59
6	G	501	VAL	OXT-C	-2.61	1.22	1.30
6	K	501	VAL	CA-N	2.60	1.54	1.47
5	I	703	TPP	C5'-C4'	-2.59	1.38	1.42
5	I	703	TPP	C4'-N3'	-2.59	1.31	1.35
6	O	501	VAL	OXT-C	-2.59	1.22	1.30
5	M	703	TPP	C5'-C4'	-2.58	1.38	1.42
5	Q	703	TPP	C4'-N3'	-2.58	1.31	1.35
6	S	501	VAL	OXT-C	-2.57	1.22	1.30
6	K	501	VAL	OXT-C	-2.57	1.22	1.30
6	R	501	VAL	OXT-C	-2.57	1.22	1.30
5	Q	703	TPP	C5'-C4'	-2.54	1.38	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	702	FAD	C5'-C4'	2.53	1.55	1.51
4	P	702	FAD	C5'-C4'	2.53	1.55	1.51
5	E	703	TPP	C4'-N3'	-2.53	1.31	1.35
4	I	702	FAD	C1'-C2'	2.52	1.56	1.52
5	P	703	TPP	C4'-N3'	-2.52	1.31	1.35
5	H	703	TPP	PA-O3A	-2.52	1.56	1.59
5	H	703	TPP	C4'-N3'	-2.52	1.31	1.35
5	L	703	TPP	PA-O3A	-2.51	1.56	1.59
6	J	501	VAL	OXT-C	-2.51	1.22	1.30
5	M	703	TPP	C4'-N3'	-2.51	1.31	1.35
5	P	703	TPP	PA-O3A	-2.51	1.56	1.59
6	N	501	VAL	OXT-C	-2.50	1.22	1.30
4	E	702	FAD	C1'-C2'	2.50	1.56	1.52
4	M	702	FAD	C1'-C2'	2.49	1.56	1.52
4	H	702	FAD	C5'-C4'	2.48	1.55	1.51
6	F	501	VAL	OXT-C	-2.47	1.22	1.30
5	L	703	TPP	C4'-N3'	-2.47	1.31	1.35
5	D	703	TPP	C4'-N3'	-2.47	1.31	1.35
4	D	702	FAD	C5'-C4'	2.46	1.55	1.51
4	Q	702	FAD	C1'-C2'	2.44	1.56	1.52
6	N	501	VAL	CA-C	2.44	1.57	1.52
6	J	501	VAL	CA-C	2.30	1.57	1.52
6	R	501	VAL	CA-N	2.28	1.53	1.47
6	J	501	VAL	CA-N	2.28	1.53	1.47
6	F	501	VAL	CA-C	2.28	1.57	1.52
6	N	501	VAL	CA-N	2.27	1.53	1.47
6	R	501	VAL	CA-C	2.22	1.57	1.52
5	H	703	TPP	C2-N3	2.18	1.37	1.32
5	D	703	TPP	C2-N3	2.16	1.37	1.32
6	F	501	VAL	CA-N	2.15	1.53	1.47
5	I	703	TPP	C2-N3	2.15	1.37	1.32
5	M	703	TPP	C2-N3	2.13	1.37	1.32
5	L	703	TPP	C2-N3	2.13	1.37	1.32
5	Q	703	TPP	C2-N3	2.12	1.37	1.32
5	P	703	TPP	C2-N3	2.12	1.37	1.32
4	M	702	FAD	C8A-N7A	2.07	1.35	1.31
5	E	703	TPP	C2-N3	2.06	1.37	1.32
4	Q	702	FAD	C8A-N7A	2.04	1.35	1.31
4	I	702	FAD	C8A-N7A	2.03	1.35	1.31
4	E	702	FAD	C8A-N7A	2.02	1.35	1.31

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	702	FAD	C4X-C10-N10	6.70	126.07	116.48
4	P	702	FAD	C4X-C10-N10	6.68	126.05	116.48
4	L	702	FAD	C4X-C10-N10	6.68	126.04	116.48
4	D	702	FAD	C4X-C10-N10	6.67	126.03	116.48
4	Q	702	FAD	C4X-C10-N10	6.58	125.91	116.48
4	M	702	FAD	C4X-C10-N10	6.57	125.89	116.48
4	E	702	FAD	C4X-C10-N10	6.56	125.88	116.48
4	I	702	FAD	C4X-C10-N10	6.53	125.83	116.48
4	M	702	FAD	C9A-N10-C10	-6.23	111.26	120.75
4	Q	702	FAD	C9A-N10-C10	-6.21	111.28	120.75
4	E	702	FAD	C9A-N10-C10	-6.21	111.29	120.75
4	I	702	FAD	C9A-N10-C10	-6.18	111.33	120.75
4	L	702	FAD	C9A-N10-C10	-5.94	111.70	120.75
4	P	702	FAD	C9A-N10-C10	-5.92	111.73	120.75
4	H	702	FAD	C9A-N10-C10	-5.91	111.74	120.75
4	D	702	FAD	C9A-N10-C10	-5.88	111.78	120.75
4	D	702	FAD	C10-N1-C2	3.79	125.06	116.85
4	H	702	FAD	C10-N1-C2	3.78	125.04	116.85
4	P	702	FAD	C10-N1-C2	3.77	125.02	116.85
4	L	702	FAD	C10-N1-C2	3.74	124.95	116.85
4	D	702	FAD	O2A-PA-O3P	3.60	117.00	107.27
4	P	702	FAD	O2A-PA-O3P	3.59	116.98	107.27
4	H	702	FAD	O2A-PA-O3P	3.58	116.95	107.27
4	L	702	FAD	O2A-PA-O3P	3.54	116.85	107.27
5	H	703	TPP	O2B-PB-O3A	3.51	116.40	104.64
5	L	703	TPP	O2B-PB-O3A	3.51	116.40	104.64
5	P	703	TPP	O2B-PB-O3A	3.50	116.39	104.64
5	D	703	TPP	O2B-PB-O3A	3.50	116.38	104.64
4	M	702	FAD	C10-N1-C2	3.47	124.36	116.85
4	I	702	FAD	C10-N1-C2	3.47	124.36	116.85
4	Q	702	FAD	C10-N1-C2	3.45	124.31	116.85
4	E	702	FAD	C10-N1-C2	3.43	124.28	116.85
4	P	702	FAD	O2P-P-O3P	3.43	116.53	107.27
4	H	702	FAD	O2P-P-O3P	3.42	116.52	107.27
4	L	702	FAD	O2P-P-O3P	3.40	116.45	107.27
4	D	702	FAD	O2P-P-O3P	3.39	116.45	107.27
4	H	702	FAD	C10-C4X-N5	-3.21	118.26	124.81
4	L	702	FAD	C10-C4X-N5	-3.20	118.28	124.81
5	P	703	TPP	CM4-C4-N3	3.19	127.92	120.57
4	D	702	FAD	C10-C4X-N5	-3.18	118.31	124.81
5	D	703	TPP	CM4-C4-N3	3.16	127.86	120.57
4	L	702	FAD	C4-C4X-N5	3.15	122.55	118.21
5	H	703	TPP	CM4-C4-N3	3.15	127.83	120.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	702	FAD	C10-C4X-N5	-3.14	118.39	124.81
5	L	703	TPP	CM4-C4-N3	3.14	127.82	120.57
4	M	702	FAD	C10-C4X-N5	-3.13	118.43	124.81
4	D	702	FAD	C4-C4X-N5	3.12	122.52	118.21
4	H	702	FAD	C4-C4X-N5	3.12	122.52	118.21
4	I	702	FAD	C10-C4X-N5	-3.10	118.47	124.81
4	E	702	FAD	C10-C4X-N5	-3.10	118.47	124.81
4	Q	702	FAD	C10-C4X-N5	-3.10	118.48	124.81
4	H	702	FAD	C4A-C5A-N7A	3.07	114.10	110.58
4	D	702	FAD	C4A-C5A-N7A	3.07	114.09	110.58
4	P	702	FAD	C4-C4X-N5	3.04	122.41	118.21
4	P	702	FAD	C4A-C5A-N7A	3.02	114.04	110.58
5	D	703	TPP	N4'-C4'-N3'	-2.99	113.00	117.03
5	E	703	TPP	N4'-C4'-N3'	-2.98	113.00	117.03
4	L	702	FAD	C4A-C5A-N7A	2.98	113.98	110.58
5	I	703	TPP	N4'-C4'-N3'	-2.97	113.03	117.03
5	P	703	TPP	N4'-C4'-N3'	-2.97	113.03	117.03
5	L	703	TPP	N4'-C4'-N3'	-2.95	113.05	117.03
5	Q	703	TPP	C2-S1-C5	-2.94	89.27	91.22
4	L	702	FAD	C5X-C9A-N10	2.94	120.63	117.97
5	M	703	TPP	N4'-C4'-N3'	-2.94	113.06	117.03
5	H	703	TPP	N4'-C4'-N3'	-2.93	113.08	117.03
5	Q	703	TPP	N4'-C4'-N3'	-2.92	113.09	117.03
5	E	703	TPP	C2-S1-C5	-2.91	89.29	91.22
4	M	702	FAD	C4-C4X-N5	2.91	122.22	118.21
4	P	702	FAD	C5X-C9A-N10	2.90	120.59	117.97
4	I	702	FAD	C4-C4X-N5	2.88	122.19	118.21
4	E	702	FAD	C4-C4X-N5	2.88	122.19	118.21
4	H	702	FAD	C5X-C9A-N10	2.88	120.57	117.97
4	Q	702	FAD	C4-C4X-N5	2.88	122.18	118.21
5	M	703	TPP	C2-S1-C5	-2.86	89.32	91.22
5	I	703	TPP	C2-S1-C5	-2.86	89.32	91.22
4	D	702	FAD	C5X-C9A-N10	2.84	120.53	117.97
5	Q	703	TPP	CM4-C4-N3	2.82	127.08	120.57
5	E	703	TPP	CM4-C4-N3	2.81	127.06	120.57
4	D	702	FAD	C4X-C10-N1	-2.79	117.74	124.59
4	M	702	FAD	C5X-C9A-N10	2.79	120.49	117.97
5	I	703	TPP	CM4-C4-N3	2.79	127.00	120.57
4	H	702	FAD	C4X-C10-N1	-2.79	117.76	124.59
4	Q	702	FAD	C5X-C9A-N10	2.78	120.48	117.97
5	M	703	TPP	CM4-C4-N3	2.78	126.99	120.57
4	P	702	FAD	C4X-C10-N1	-2.78	117.78	124.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	702	FAD	C4A-C5A-N7A	2.78	113.75	110.58
4	L	702	FAD	C4X-C10-N1	-2.76	117.82	124.59
4	P	702	FAD	C5A-C4A-N3A	-2.76	122.92	126.72
4	M	702	FAD	C4A-C5A-N7A	2.75	113.72	110.58
4	L	702	FAD	C5A-C4A-N3A	-2.75	122.93	126.72
4	E	702	FAD	C5X-C9A-N10	2.73	120.44	117.97
4	I	702	FAD	C5X-C9A-N10	2.73	120.43	117.97
4	E	702	FAD	C4A-C5A-N7A	2.72	113.69	110.58
4	I	702	FAD	C4A-C5A-N7A	2.70	113.67	110.58
4	D	702	FAD	C5A-C4A-N3A	-2.70	123.00	126.72
4	H	702	FAD	C5A-C4A-N3A	-2.70	123.00	126.72
5	D	703	TPP	C2-S1-C5	-2.68	89.44	91.22
5	H	703	TPP	C2-S1-C5	-2.67	89.45	91.22
4	I	702	FAD	C5A-C4A-N3A	-2.65	123.06	126.72
5	P	703	TPP	C2-S1-C5	-2.65	89.46	91.22
4	M	702	FAD	C4X-C10-N1	-2.64	118.11	124.59
4	I	702	FAD	C4X-C10-N1	-2.63	118.14	124.59
4	Q	702	FAD	C4X-C10-N1	-2.62	118.17	124.59
4	E	702	FAD	C4X-C10-N1	-2.61	118.19	124.59
4	E	702	FAD	C5A-C4A-N3A	-2.60	123.14	126.72
5	L	703	TPP	C2-S1-C5	-2.58	89.50	91.22
4	M	702	FAD	C5A-C4A-N3A	-2.55	123.20	126.72
4	Q	702	FAD	C5A-C4A-N3A	-2.54	123.22	126.72
6	G	501	VAL	C-CA-N	2.48	114.69	109.49
5	P	703	TPP	C5'-C4'-N3'	2.47	124.94	121.31
5	D	703	TPP	C5'-C4'-N3'	2.46	124.92	121.31
4	M	702	FAD	C1'-N10-C9A	2.46	125.42	120.63
4	I	702	FAD	C1'-N10-C9A	2.46	125.41	120.63
4	Q	702	FAD	C1'-N10-C9A	2.45	125.40	120.63
5	L	703	TPP	C5'-C4'-N3'	2.45	124.90	121.31
4	E	702	FAD	C1'-N10-C9A	2.44	125.37	120.63
4	M	702	FAD	O3P-PA-O1A	2.43	118.02	110.70
5	E	703	TPP	C2-N3-C4	2.43	117.34	114.06
5	H	703	TPP	C5'-C4'-N3'	2.43	124.87	121.31
4	I	702	FAD	O3P-PA-O1A	2.42	118.00	110.70
5	M	703	TPP	C2-N3-C4	2.42	117.33	114.06
4	E	702	FAD	O3P-PA-O1A	2.42	117.99	110.70
4	Q	702	FAD	O3P-PA-O1A	2.42	117.98	110.70
5	Q	703	TPP	C2-N3-C4	2.41	117.32	114.06
5	I	703	TPP	O3B-PB-O3A	2.40	112.69	104.64
5	Q	703	TPP	O3B-PB-O3A	2.38	112.62	104.64
5	E	703	TPP	O3B-PB-O3A	2.37	112.60	104.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	703	TPP	O3B-PB-O3A	2.37	112.59	104.64
5	I	703	TPP	C2-N3-C4	2.37	117.26	114.06
4	I	702	FAD	N6A-C6A-N1A	-2.33	113.18	118.38
4	Q	702	FAD	N6A-C6A-N1A	-2.32	113.21	118.38
5	P	703	TPP	C2-N3-C4	2.32	117.19	114.06
4	M	702	FAD	N6A-C6A-N1A	-2.31	113.22	118.38
5	D	703	TPP	C2-N3-C4	2.30	117.16	114.06
4	E	702	FAD	N6A-C6A-N1A	-2.29	113.27	118.38
5	L	703	TPP	C2-N3-C4	2.27	117.12	114.06
6	K	501	VAL	C-CA-N	2.26	114.25	109.49
5	H	703	TPP	C2-N3-C4	2.25	117.10	114.06
6	O	501	VAL	C-CA-N	2.24	114.20	109.49
5	Q	703	TPP	C4-C5-S1	2.24	114.05	110.56
5	E	703	TPP	C4-C5-S1	2.23	114.05	110.56
5	M	703	TPP	C4-C5-S1	2.21	114.02	110.56
5	I	703	TPP	C4-C5-S1	2.20	113.99	110.56
4	P	702	FAD	N3A-C4A-N9A	2.19	130.89	127.17
6	S	501	VAL	C-CA-N	2.18	114.08	109.49
4	L	702	FAD	C2A-N1A-C6A	-2.18	115.14	118.73
4	L	702	FAD	N3A-C4A-N9A	2.18	130.88	127.17
4	D	702	FAD	N3A-C4A-N9A	2.18	130.88	127.17
5	L	703	TPP	C6-C5-C4	-2.18	122.71	128.17
5	D	703	TPP	C6-C5-C4	-2.18	122.71	128.17
5	H	703	TPP	C6-C5-C4	-2.17	122.74	128.17
5	P	703	TPP	C6-C5-C4	-2.16	122.75	128.17
4	H	702	FAD	N3A-C4A-N9A	2.15	130.83	127.17
4	P	702	FAD	C2A-N1A-C6A	-2.15	115.19	118.73
4	D	702	FAD	C2A-N1A-C6A	-2.15	115.20	118.73
4	L	702	FAD	C5A-C6A-N1A	2.14	122.94	117.51
4	D	702	FAD	C5A-C6A-N1A	2.12	122.89	117.51
4	H	702	FAD	C5A-C6A-N1A	2.11	122.88	117.51
4	P	702	FAD	C5A-C6A-N1A	2.11	122.86	117.51
4	H	702	FAD	C2A-N1A-C6A	-2.11	115.27	118.73
4	Q	702	FAD	C2A-N1A-C6A	-2.10	115.28	118.73
6	N	501	VAL	C-CA-N	2.10	113.90	109.49
4	M	702	FAD	C2A-N1A-C6A	-2.09	115.29	118.73
4	I	702	FAD	C2A-N1A-C6A	-2.09	115.30	118.73
4	I	702	FAD	C5A-C6A-N1A	2.08	122.80	117.51
4	M	702	FAD	C5A-C6A-N1A	2.08	122.80	117.51
4	E	702	FAD	C5A-C6A-N1A	2.08	122.78	117.51
4	Q	702	FAD	C5A-C6A-N1A	2.07	122.77	117.51
4	E	702	FAD	C2A-N1A-C6A	-2.06	115.34	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	703	TPP	C7'-N3-C2	-2.06	119.18	123.48
5	D	703	TPP	C2'-N3'-C4'	-2.06	114.93	118.10
6	J	501	VAL	C-CA-N	2.06	113.82	109.49
5	H	703	TPP	C2'-N3'-C4'	-2.05	114.94	118.10
4	P	702	FAD	O5B-C5B-C4B	2.05	115.97	108.99
5	P	703	TPP	C2'-N3'-C4'	-2.05	114.95	118.10
4	L	702	FAD	O5B-C5B-C4B	2.04	115.95	108.99
4	D	702	FAD	N6A-C6A-N1A	-2.04	113.83	118.38
5	L	703	TPP	C2'-N3'-C4'	-2.04	114.96	118.10
4	P	702	FAD	N6A-C6A-N1A	-2.03	113.84	118.38
4	L	702	FAD	N6A-C6A-N1A	-2.03	113.85	118.38
4	H	702	FAD	N6A-C6A-N1A	-2.03	113.85	118.38
4	H	702	FAD	O5B-C5B-C4B	2.03	115.90	108.99
4	D	702	FAD	O5B-C5B-C4B	2.03	115.90	108.99
5	Q	703	TPP	C7'-N3-C2	-2.03	119.25	123.48
5	D	703	TPP	C4-C5-S1	2.02	113.71	110.56
4	L	702	FAD	C1'-N10-C9A	2.01	124.55	120.63
5	I	703	TPP	C7'-N3-C2	-2.01	119.28	123.48
5	E	703	TPP	C7'-N3-C2	-2.01	119.29	123.48
5	H	703	TPP	C4-C5-S1	2.01	113.69	110.56
5	I	703	TPP	C5'-C4'-N3'	2.00	124.25	121.31

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	702	FAD	C4B-C5B-O5B-PA
4	D	702	FAD	N10-C1'-C2'-O2'
4	D	702	FAD	N10-C1'-C2'-C3'
4	D	702	FAD	C5'-O5'-P-O1P
4	D	702	FAD	C5'-O5'-P-O3P
4	H	702	FAD	C4B-C5B-O5B-PA
4	H	702	FAD	N10-C1'-C2'-O2'
4	H	702	FAD	N10-C1'-C2'-C3'
4	H	702	FAD	C5'-O5'-P-O1P
4	H	702	FAD	C5'-O5'-P-O3P
4	L	702	FAD	C4B-C5B-O5B-PA
4	L	702	FAD	N10-C1'-C2'-O2'
4	L	702	FAD	N10-C1'-C2'-C3'
4	L	702	FAD	C5'-O5'-P-O1P
4	L	702	FAD	C5'-O5'-P-O3P
4	P	702	FAD	C4B-C5B-O5B-PA

Continued on next page...

Continued from previous page...

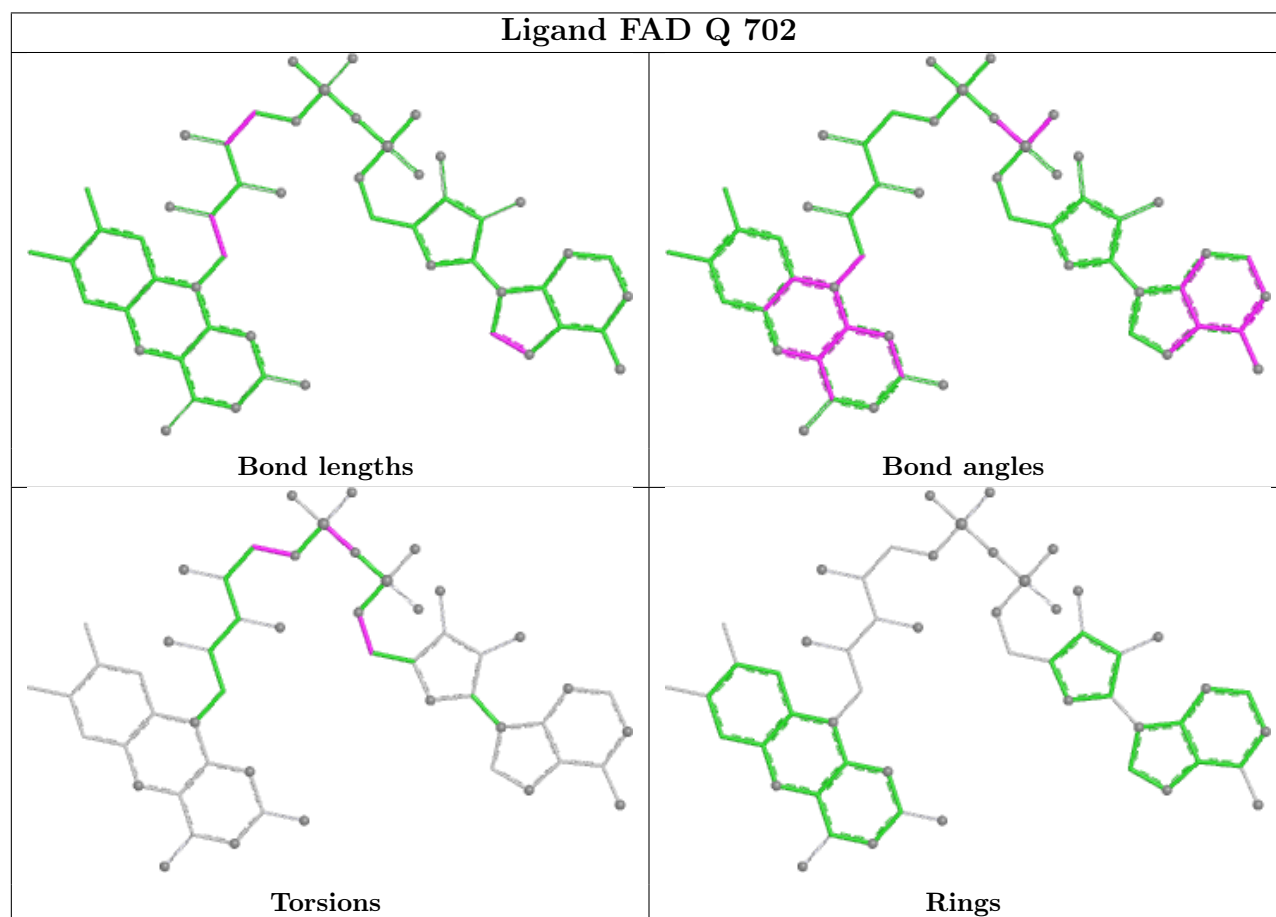
Mol	Chain	Res	Type	Atoms
4	P	702	FAD	N10-C1'-C2'-O2'
4	P	702	FAD	N10-C1'-C2'-C3'
4	P	702	FAD	C5'-O5'-P-O1P
4	P	702	FAD	C5'-O5'-P-O3P
4	E	702	FAD	PA-O3P-P-O5'
4	I	702	FAD	PA-O3P-P-O5'
4	M	702	FAD	PA-O3P-P-O5'
4	Q	702	FAD	PA-O3P-P-O5'
5	D	703	TPP	PB-O3A-PA-O7
5	E	703	TPP	PB-O3A-PA-O7
5	H	703	TPP	PB-O3A-PA-O7
5	I	703	TPP	PB-O3A-PA-O7
5	L	703	TPP	PB-O3A-PA-O7
5	M	703	TPP	PB-O3A-PA-O7
5	P	703	TPP	PB-O3A-PA-O7
5	Q	703	TPP	PB-O3A-PA-O7
6	F	501	VAL	OXT-C-CA-CB
6	N	501	VAL	OXT-C-CA-CB
4	E	702	FAD	C4'-C5'-O5'-P
4	I	702	FAD	C4'-C5'-O5'-P
4	M	702	FAD	C4'-C5'-O5'-P
4	Q	702	FAD	C4'-C5'-O5'-P
6	F	501	VAL	OXT-C-CA-N
4	E	702	FAD	C4B-C5B-O5B-PA
4	I	702	FAD	C4B-C5B-O5B-PA
4	M	702	FAD	C4B-C5B-O5B-PA
4	Q	702	FAD	C4B-C5B-O5B-PA
4	M	702	FAD	PA-O3P-P-O2P
6	N	501	VAL	OXT-C-CA-N
6	F	501	VAL	C-CA-CB-CG2
6	J	501	VAL	C-CA-CB-CG2
6	N	501	VAL	C-CA-CB-CG2
4	E	702	FAD	PA-O3P-P-O2P
4	I	702	FAD	PA-O3P-P-O2P
4	Q	702	FAD	PA-O3P-P-O2P
5	D	703	TPP	S1-C5-C6-C7
5	H	703	TPP	S1-C5-C6-C7
5	L	703	TPP	S1-C5-C6-C7
5	P	703	TPP	S1-C5-C6-C7

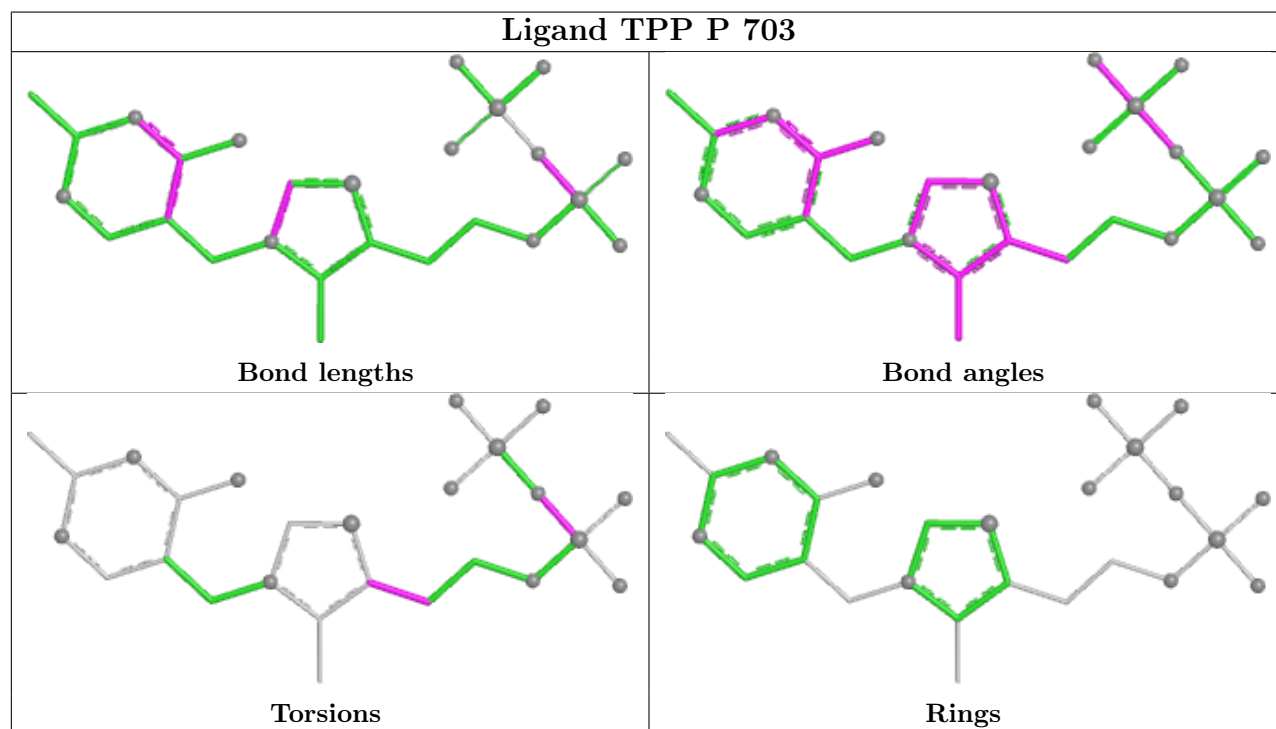
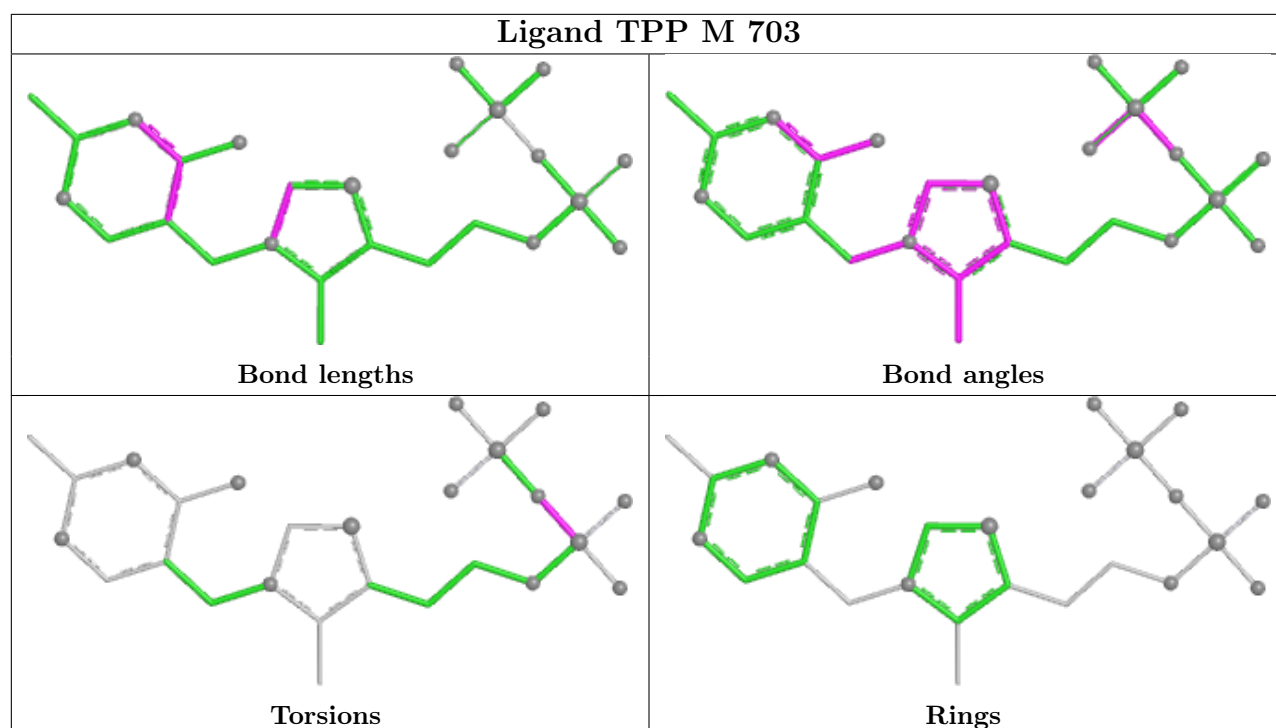
There are no ring outliers.

4 monomers are involved in 5 short contacts:

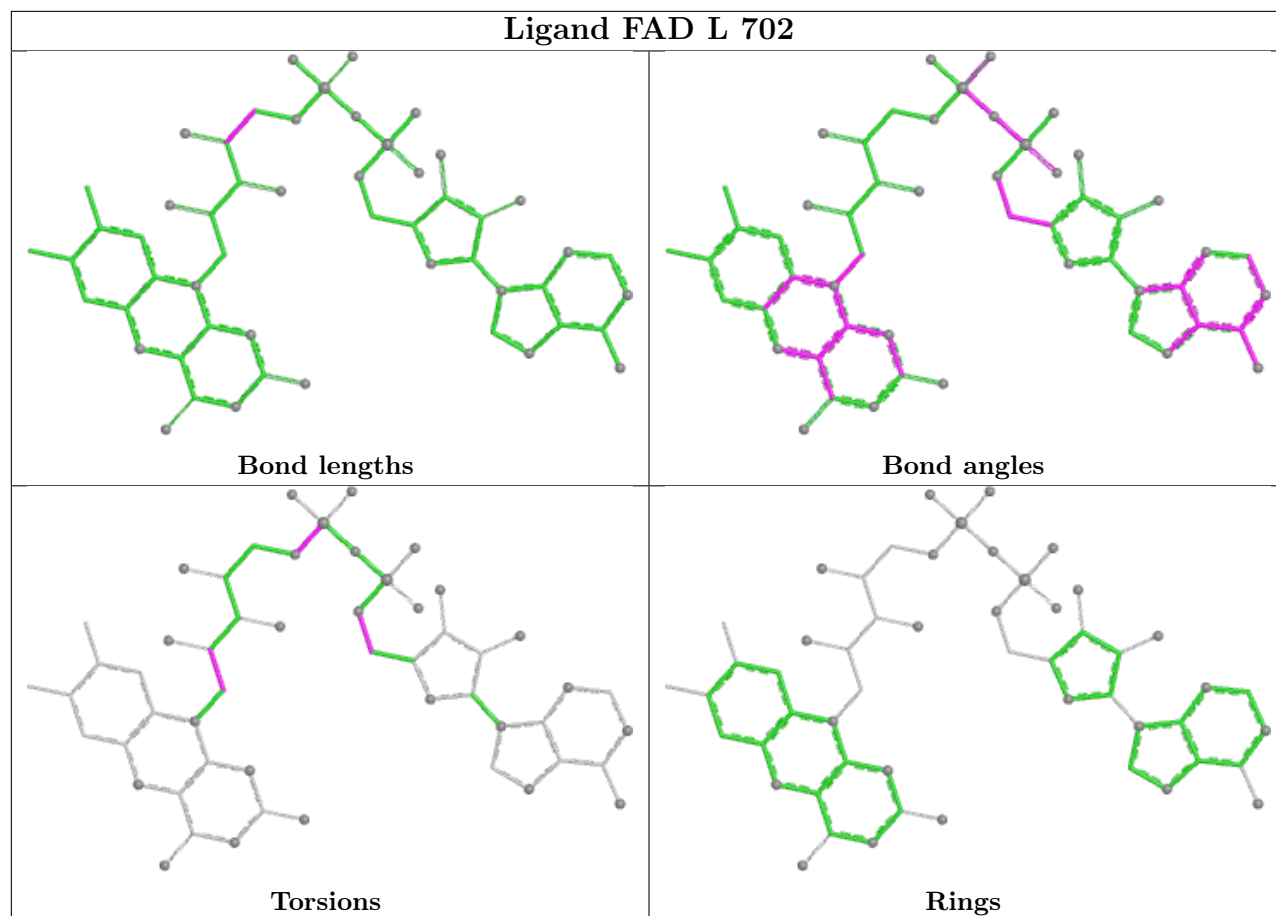
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	501	VAL	1	0
6	R	501	VAL	2	0
6	N	501	VAL	1	0
6	J	501	VAL	1	0

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.

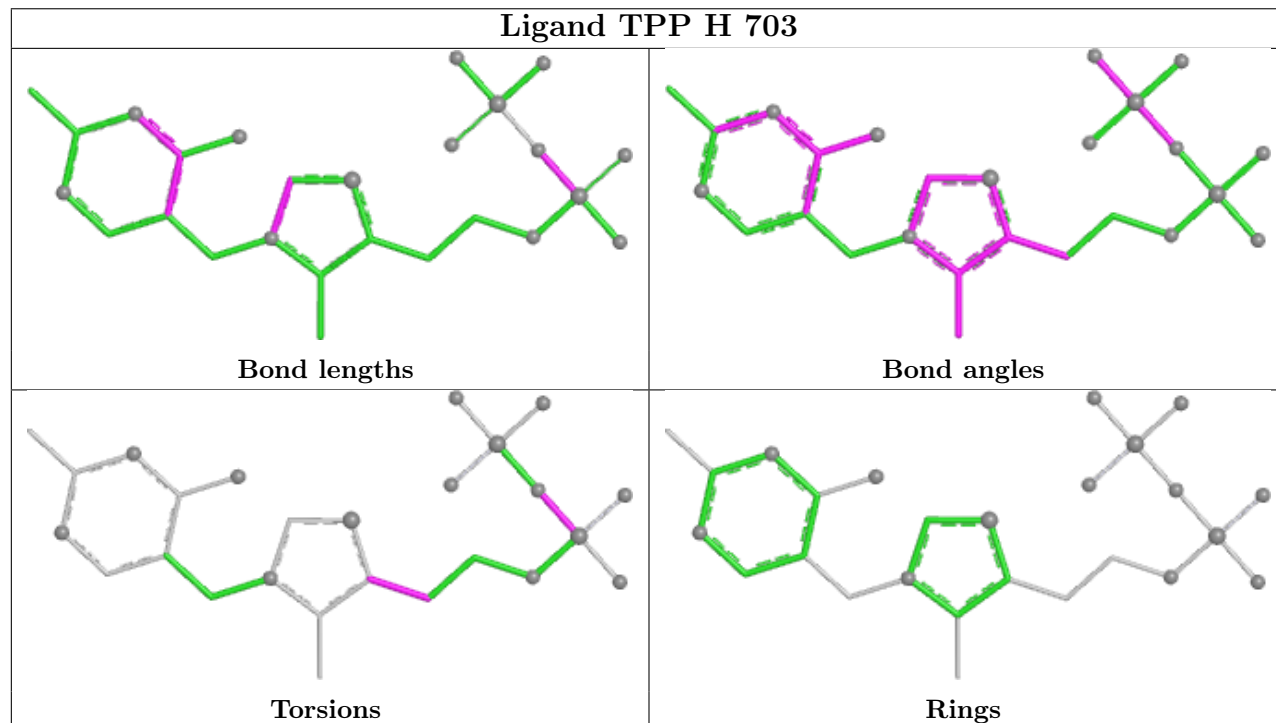


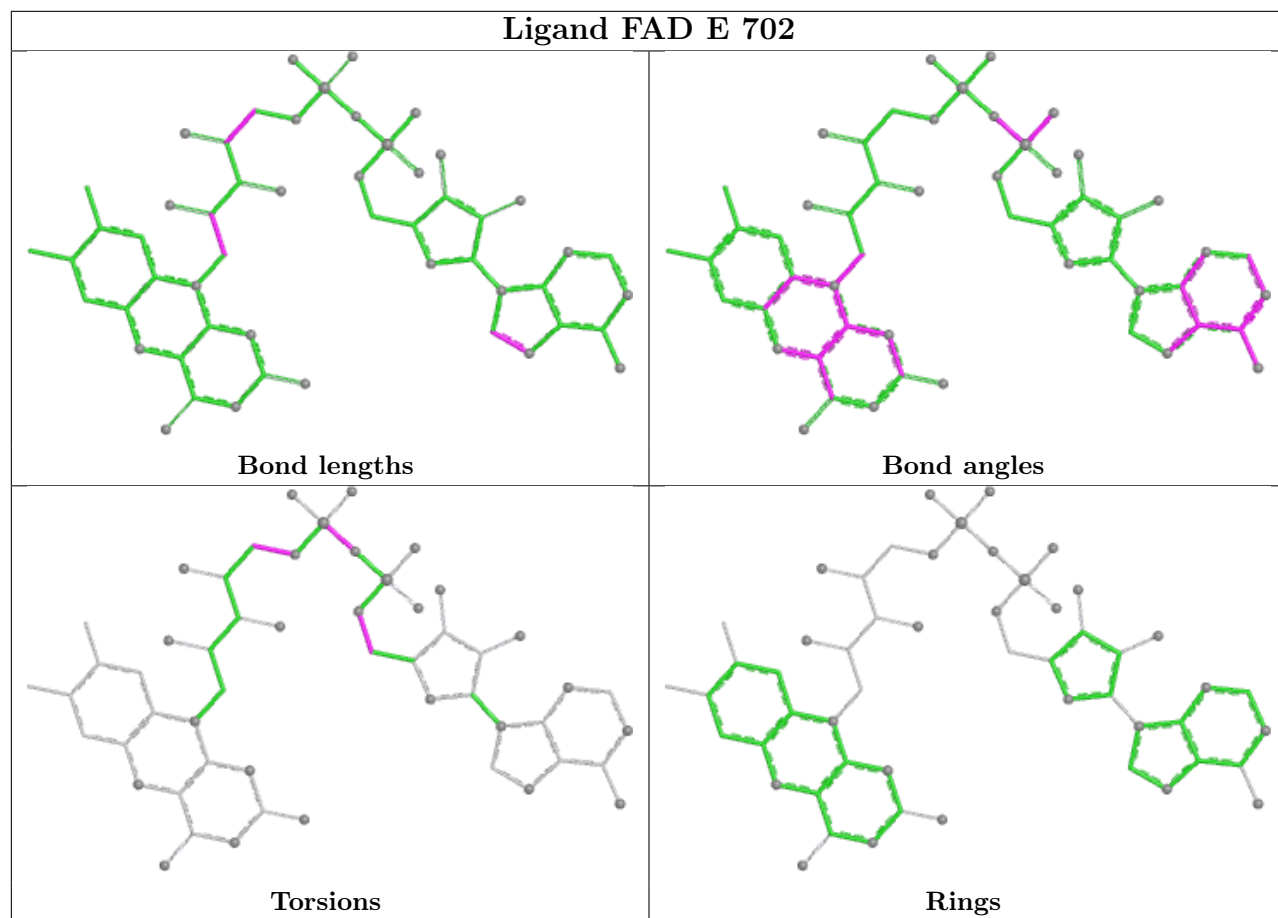


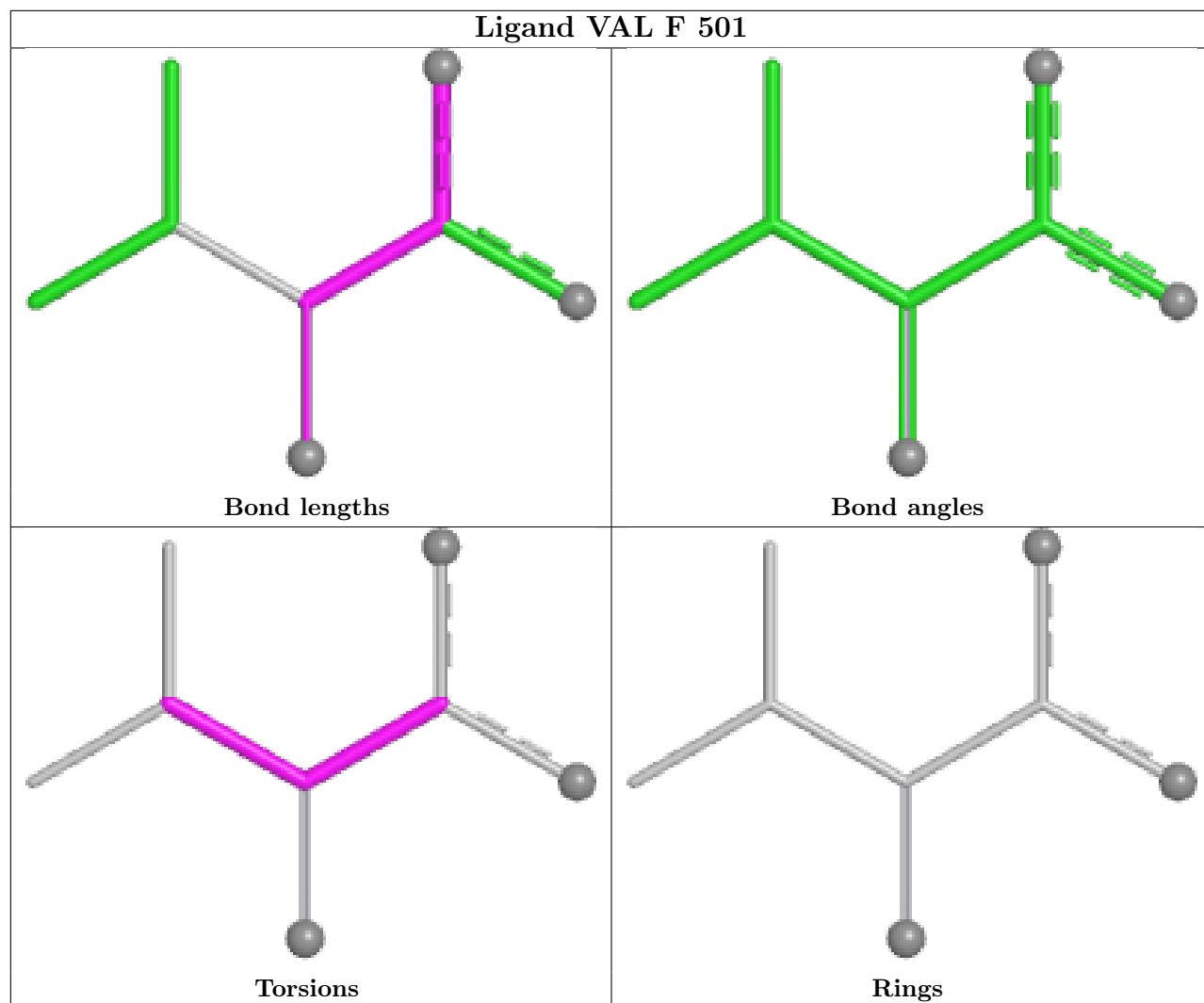
Ligand FAD L 702

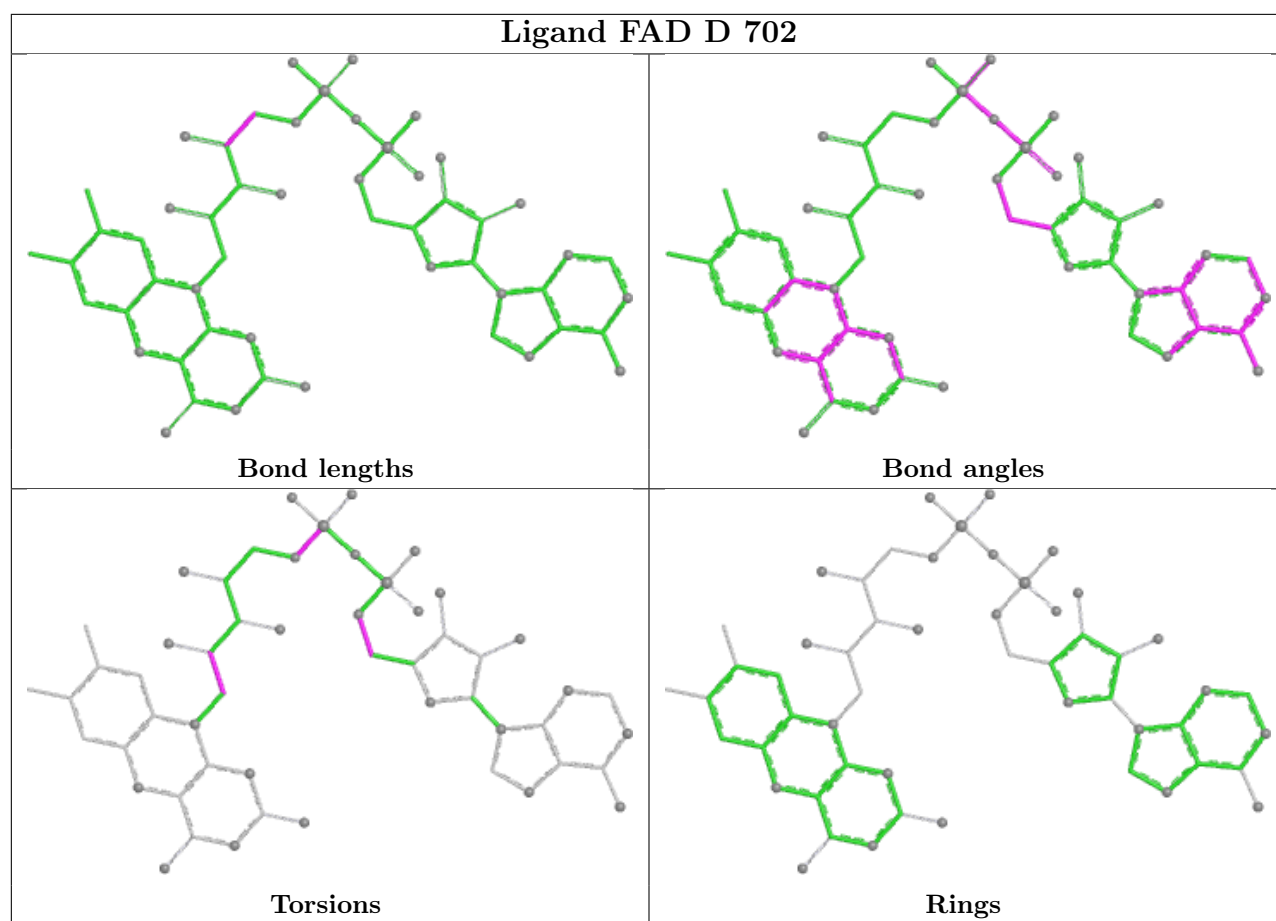


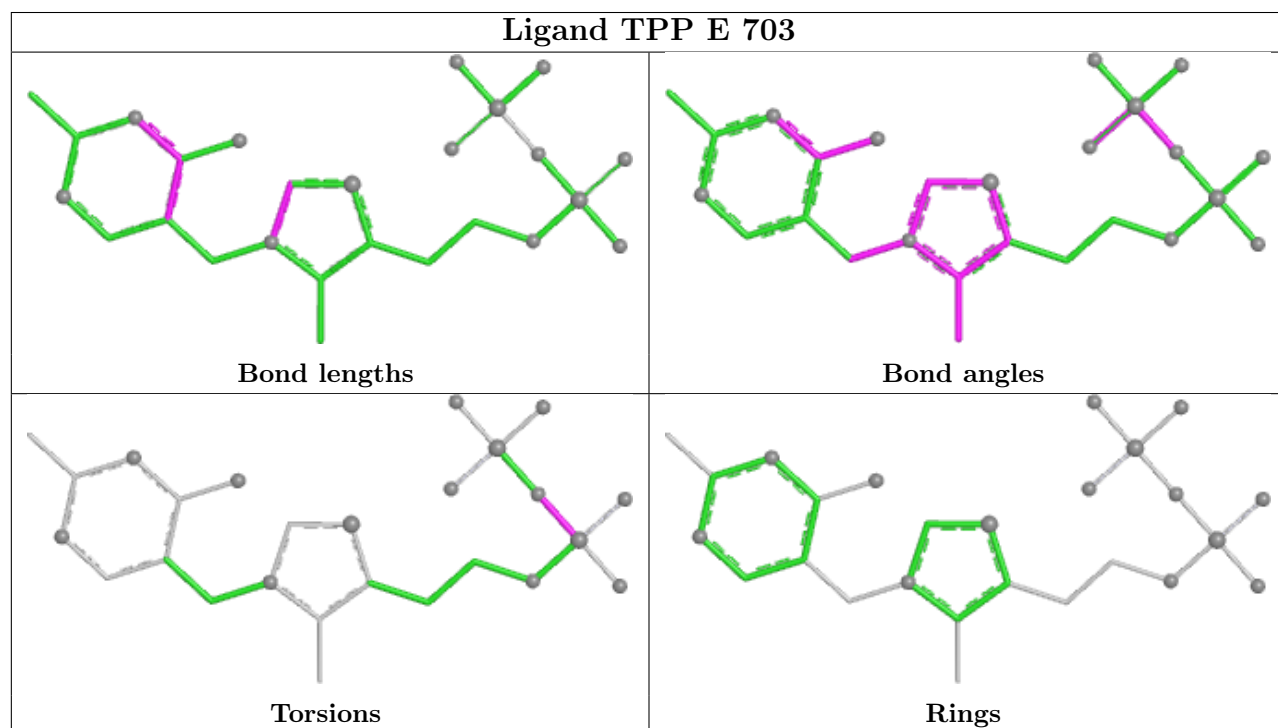
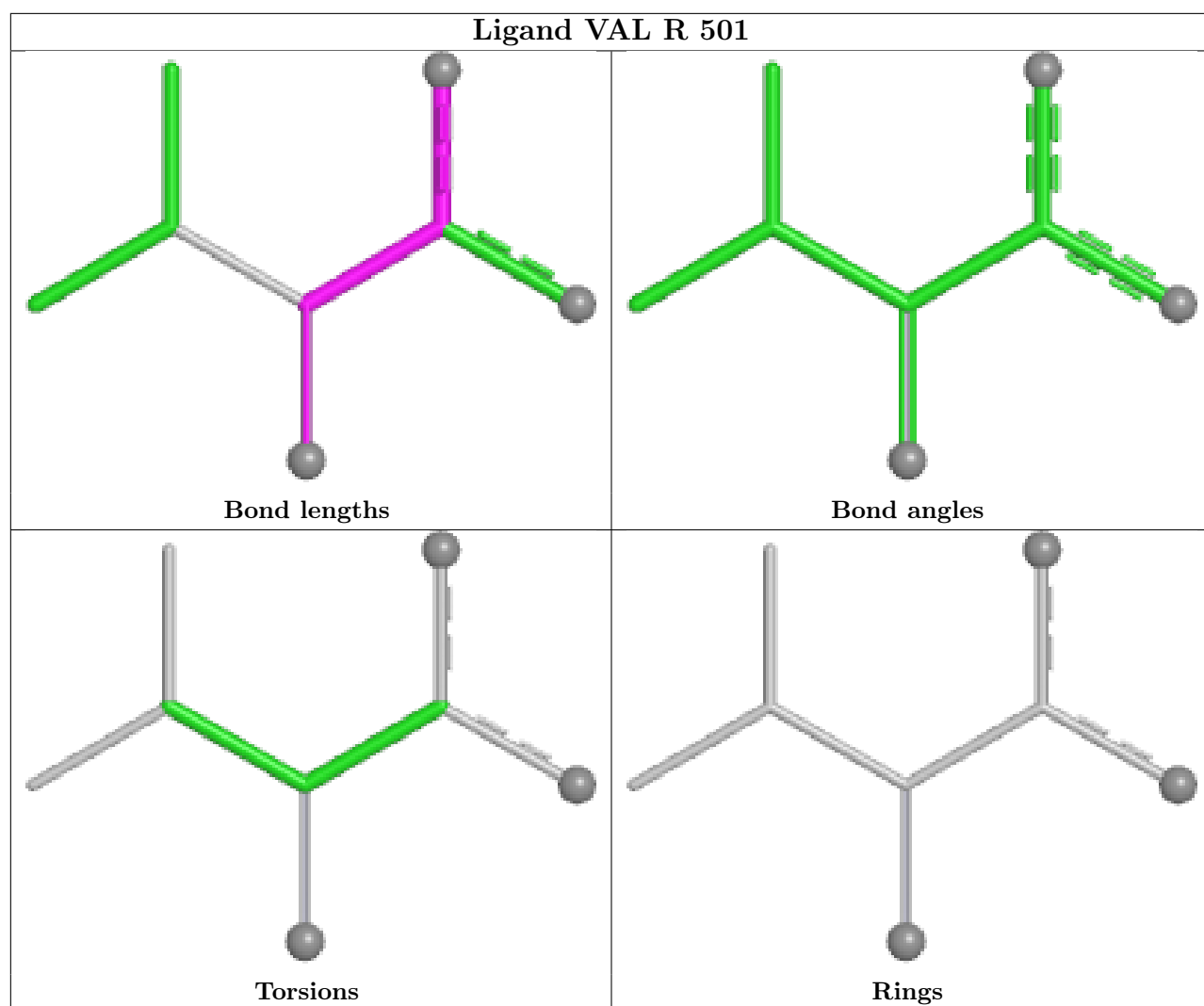
Ligand TPP H 703



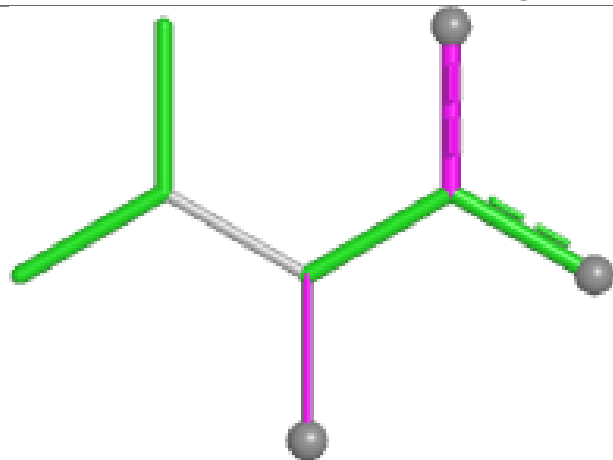




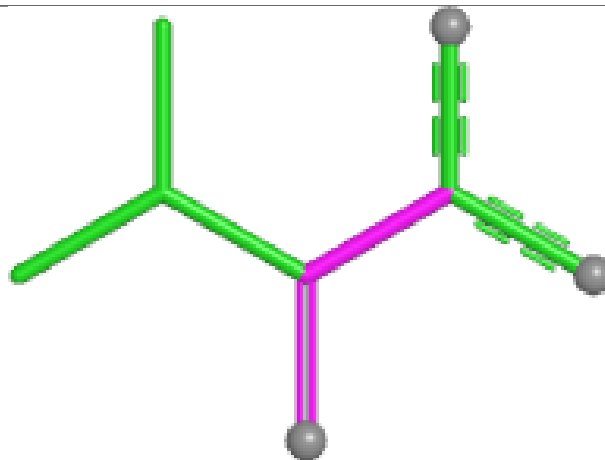




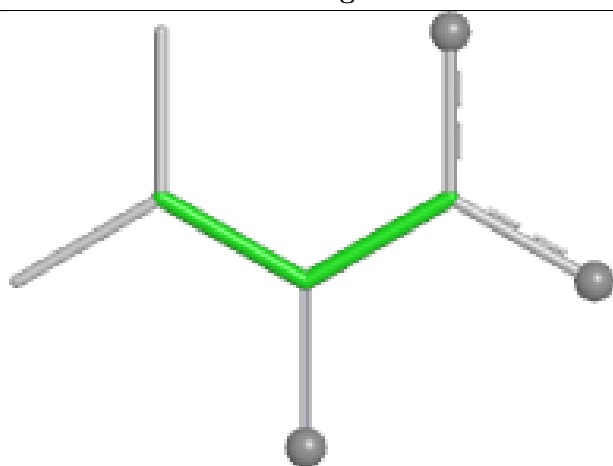
Ligand VAL O 501



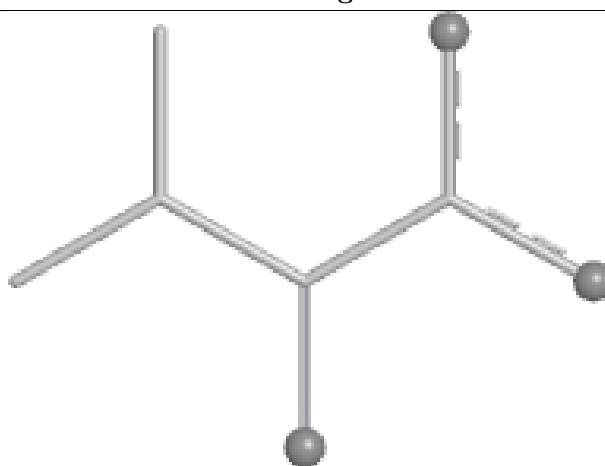
Bond lengths



Bond angles

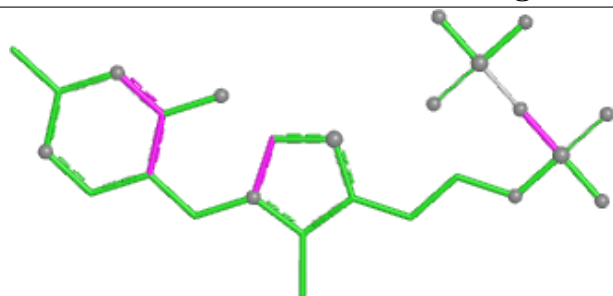


Torsions

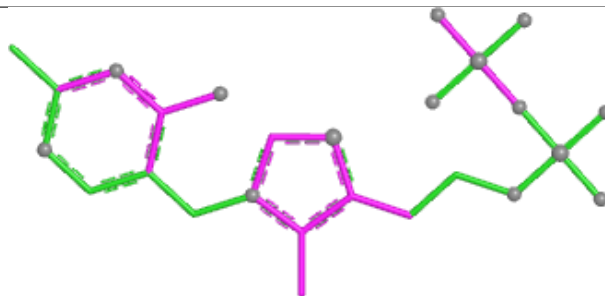


Rings

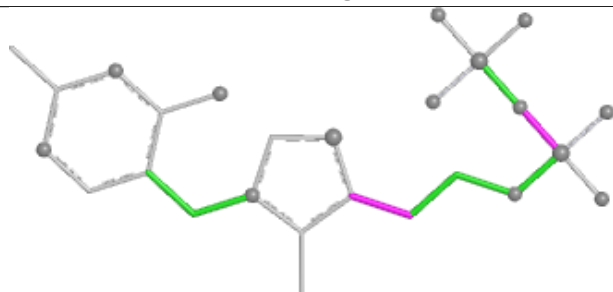
Ligand TPP D 703



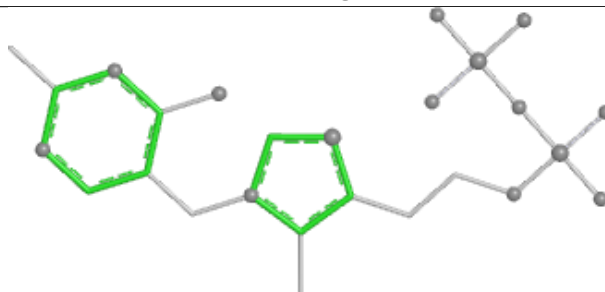
Bond lengths



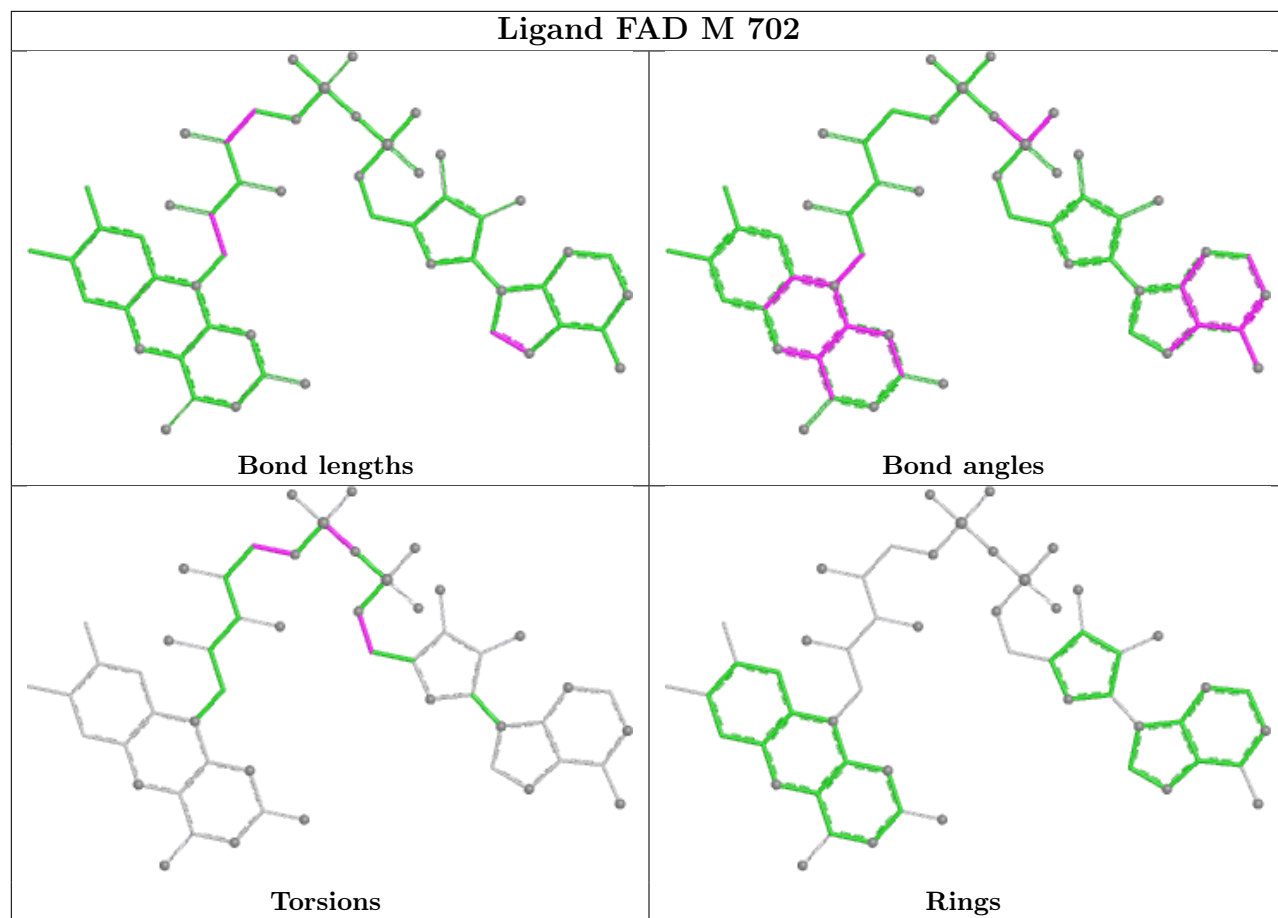
Bond angles

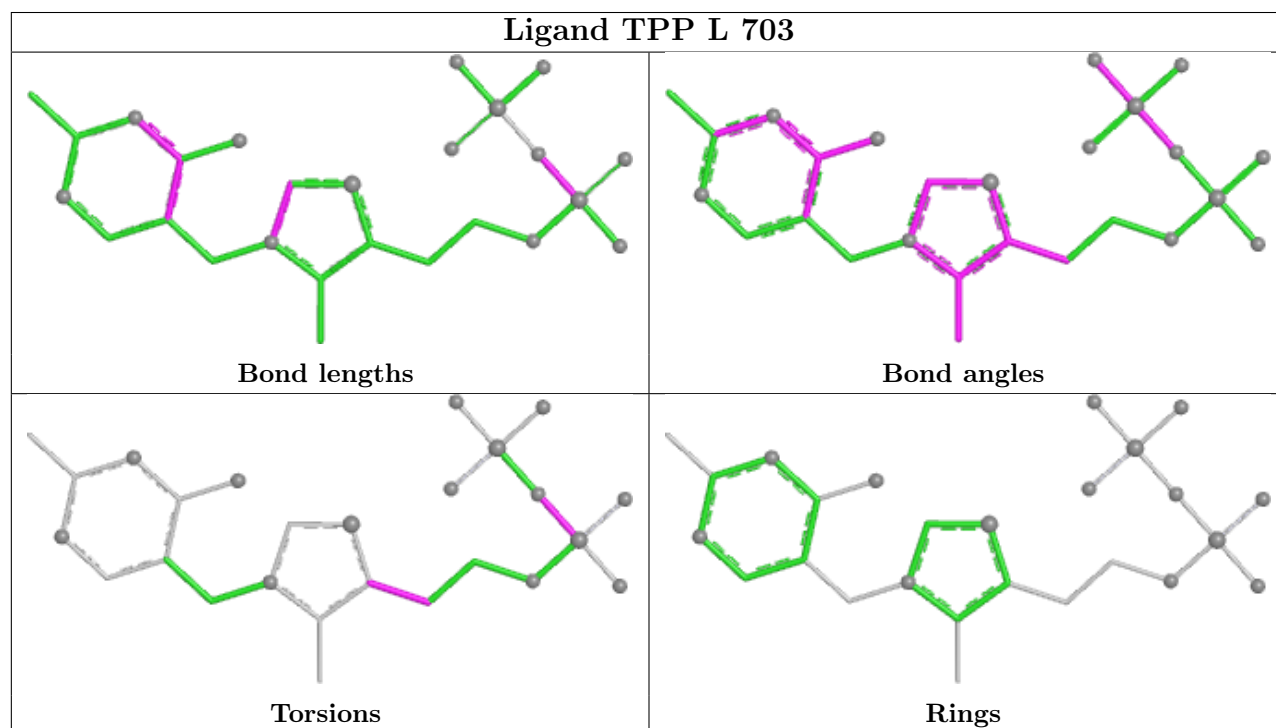
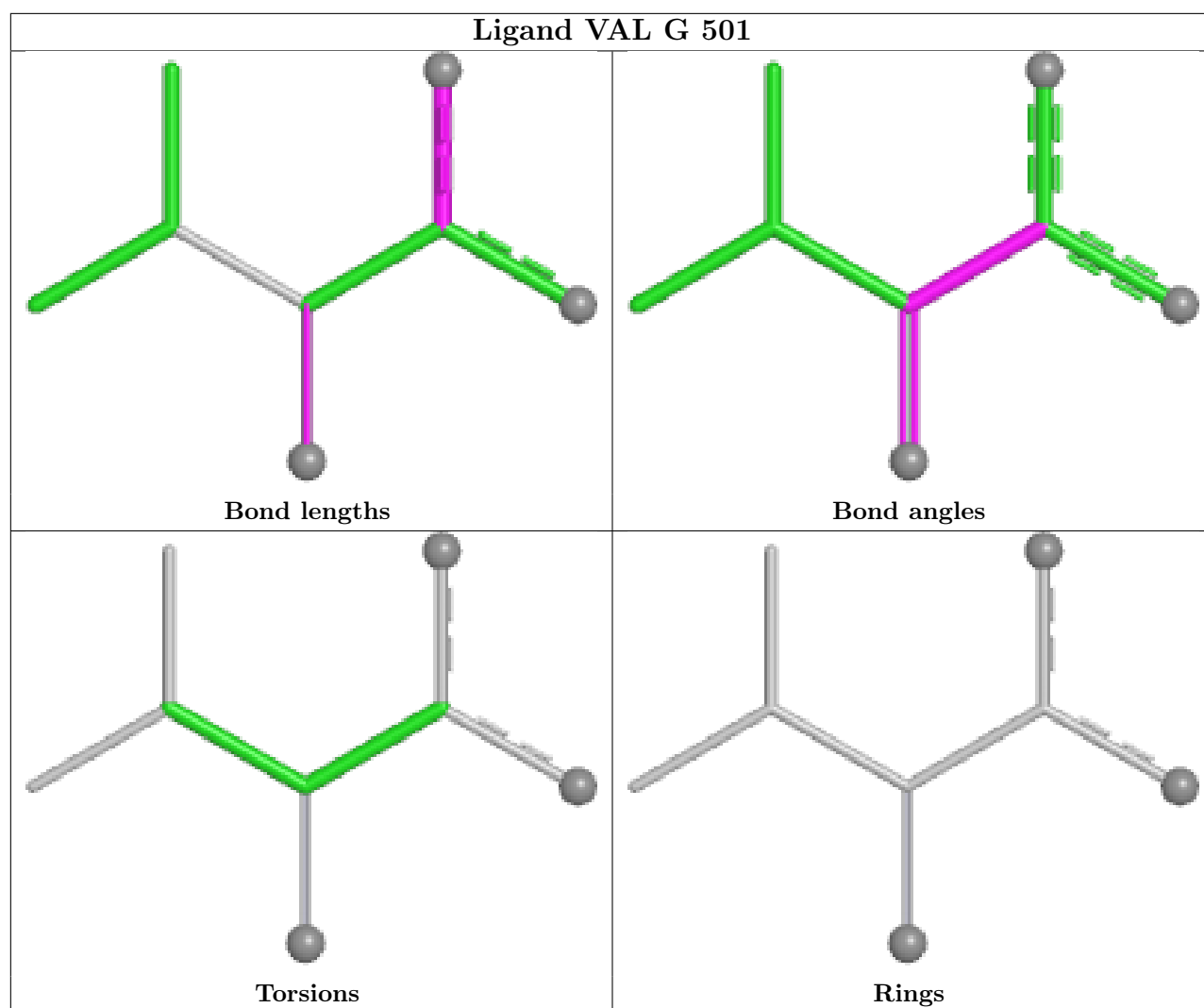


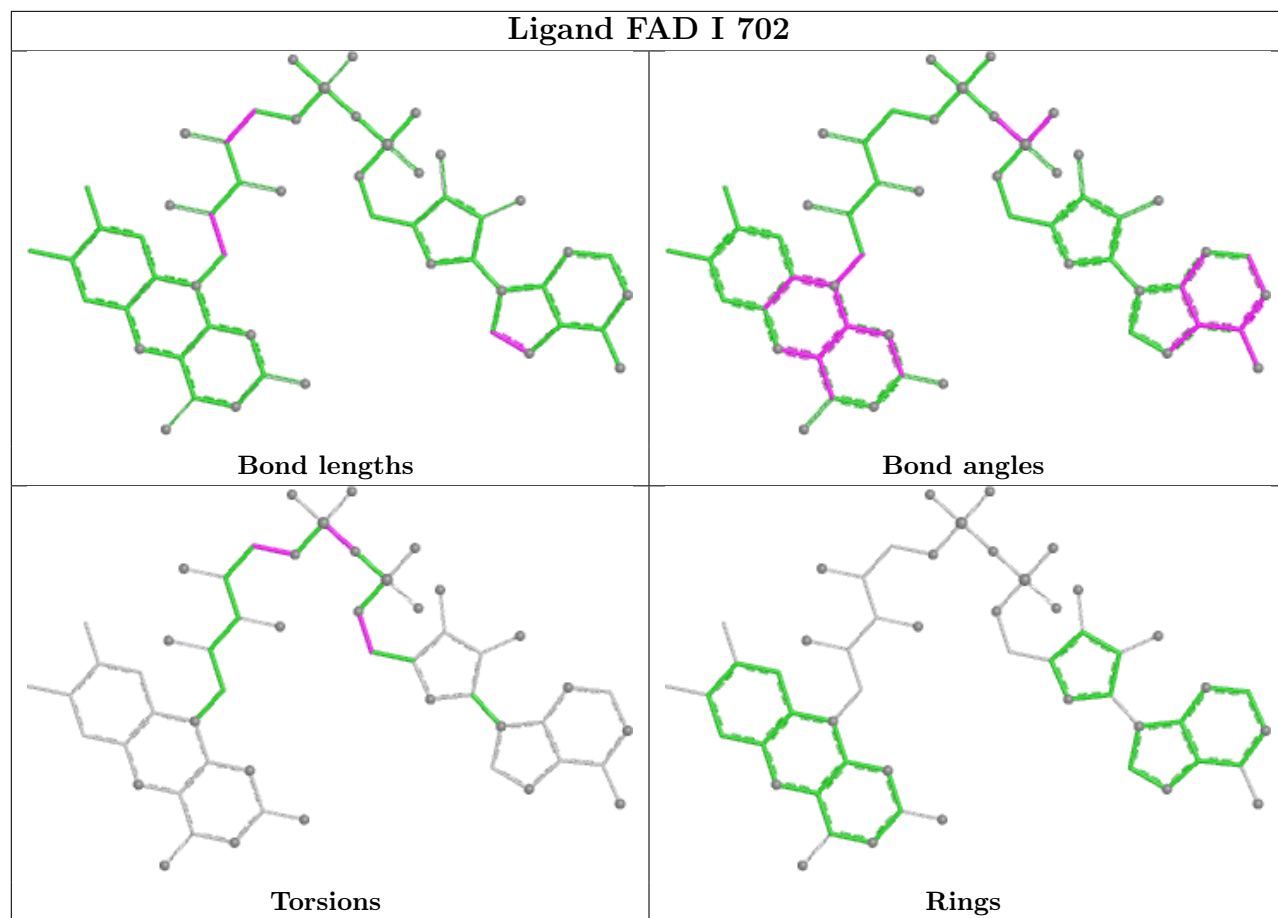
Torsions

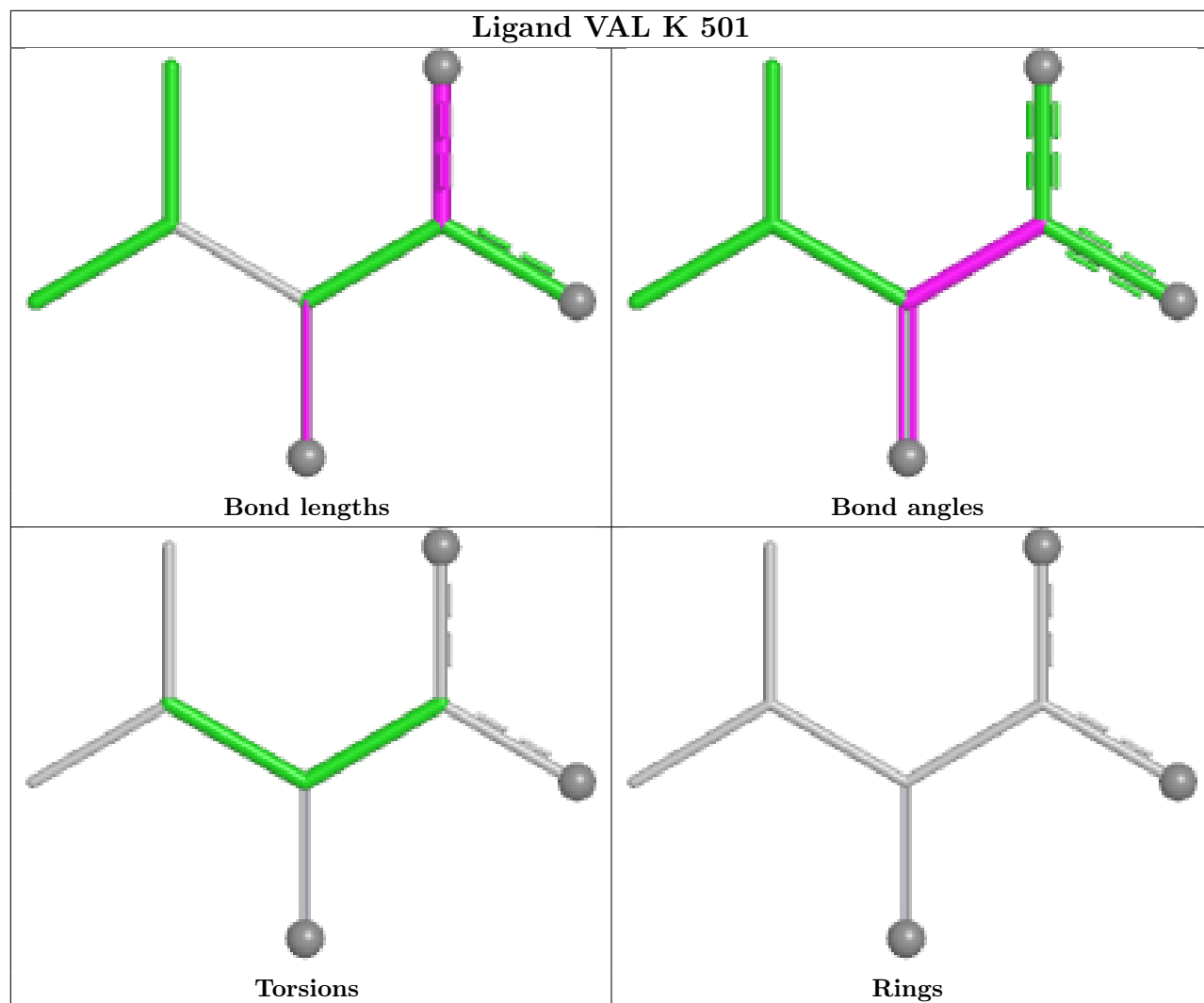


Rings

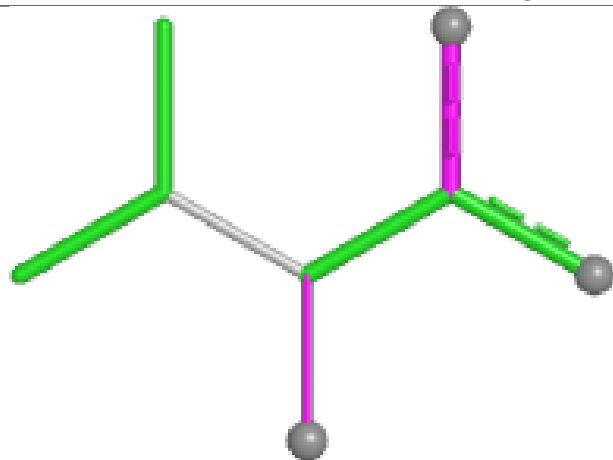




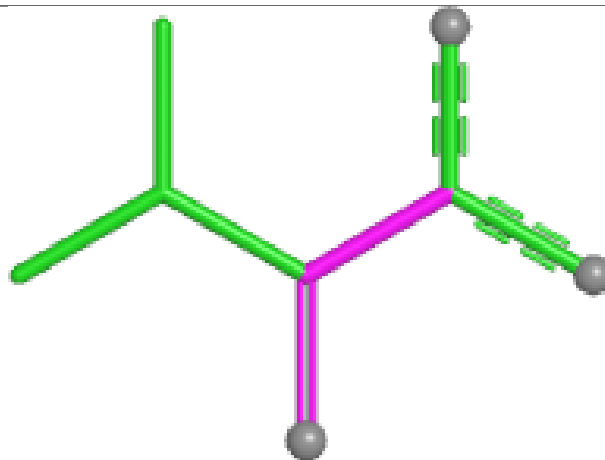




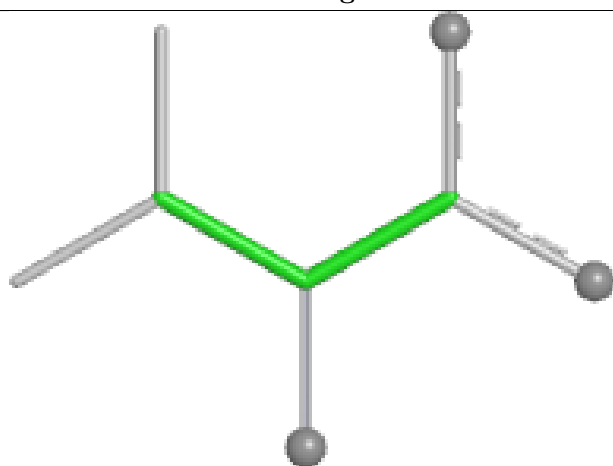
Ligand VAL S 501



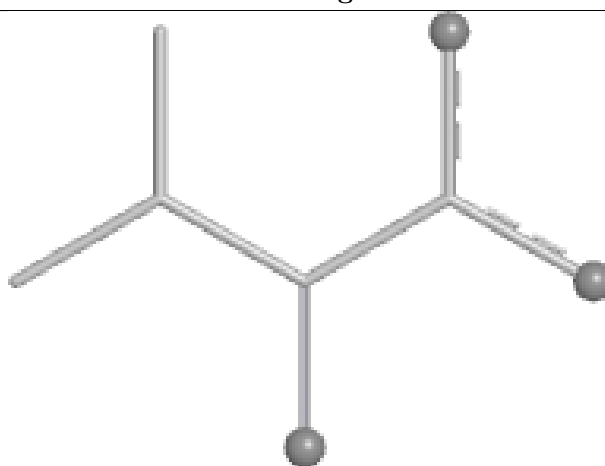
Bond lengths



Bond angles

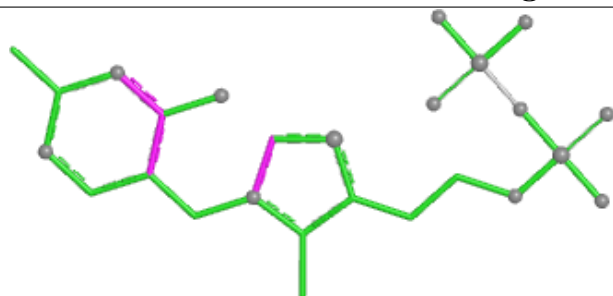


Torsions

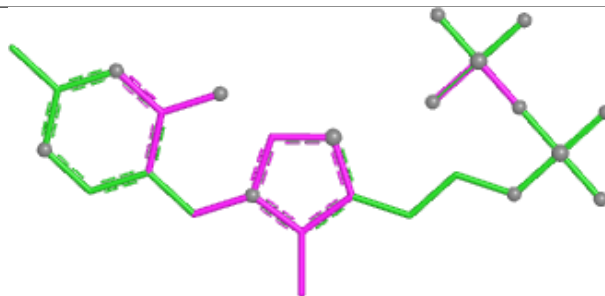


Rings

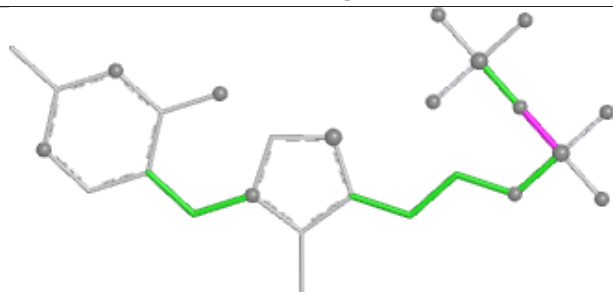
Ligand TPP I 703



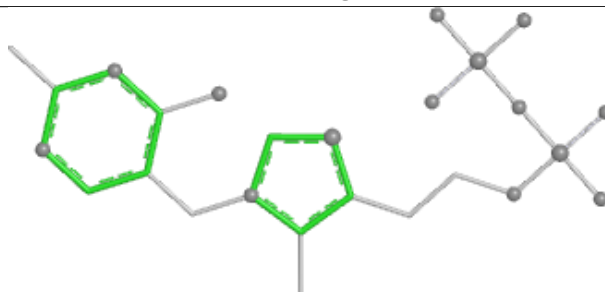
Bond lengths



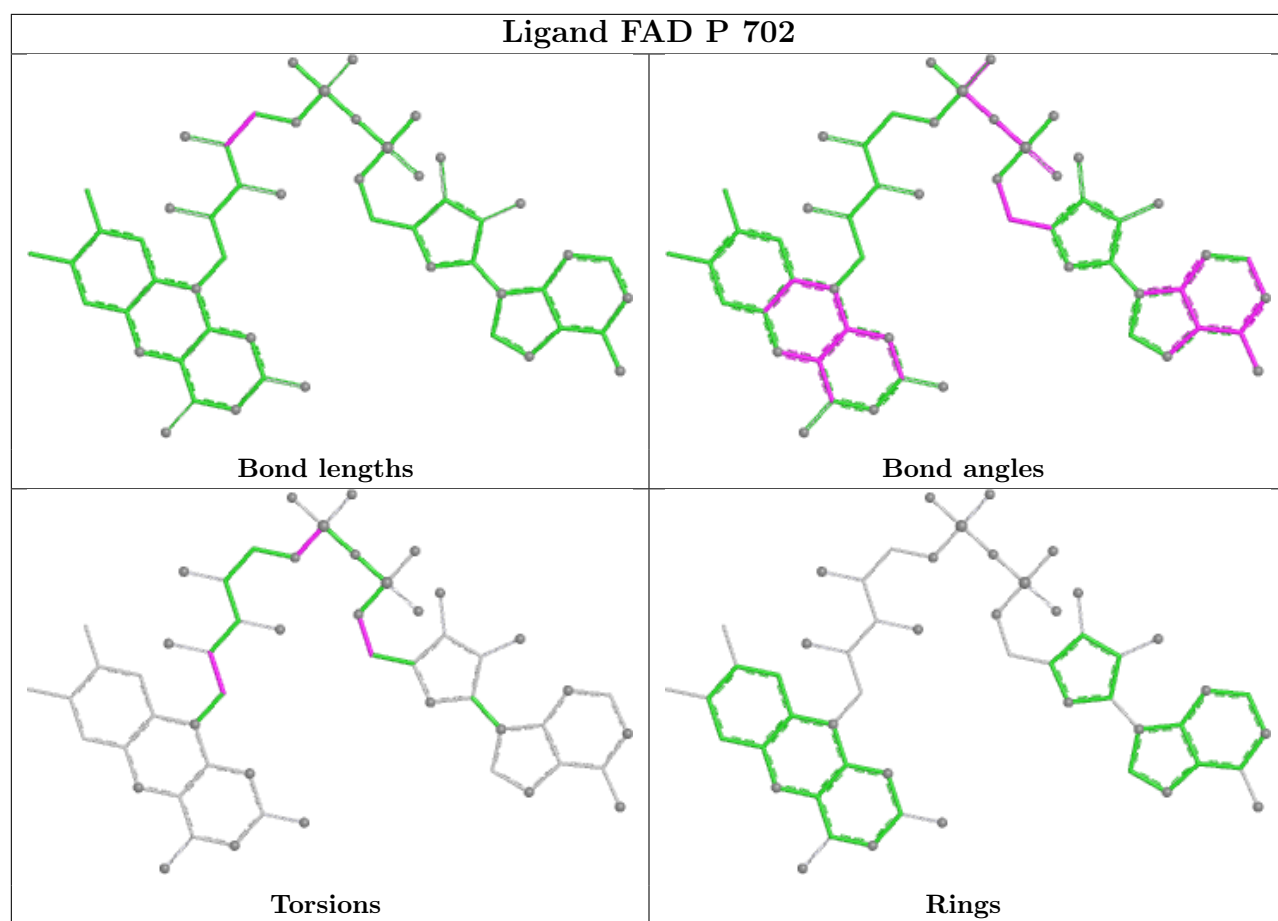
Bond angles

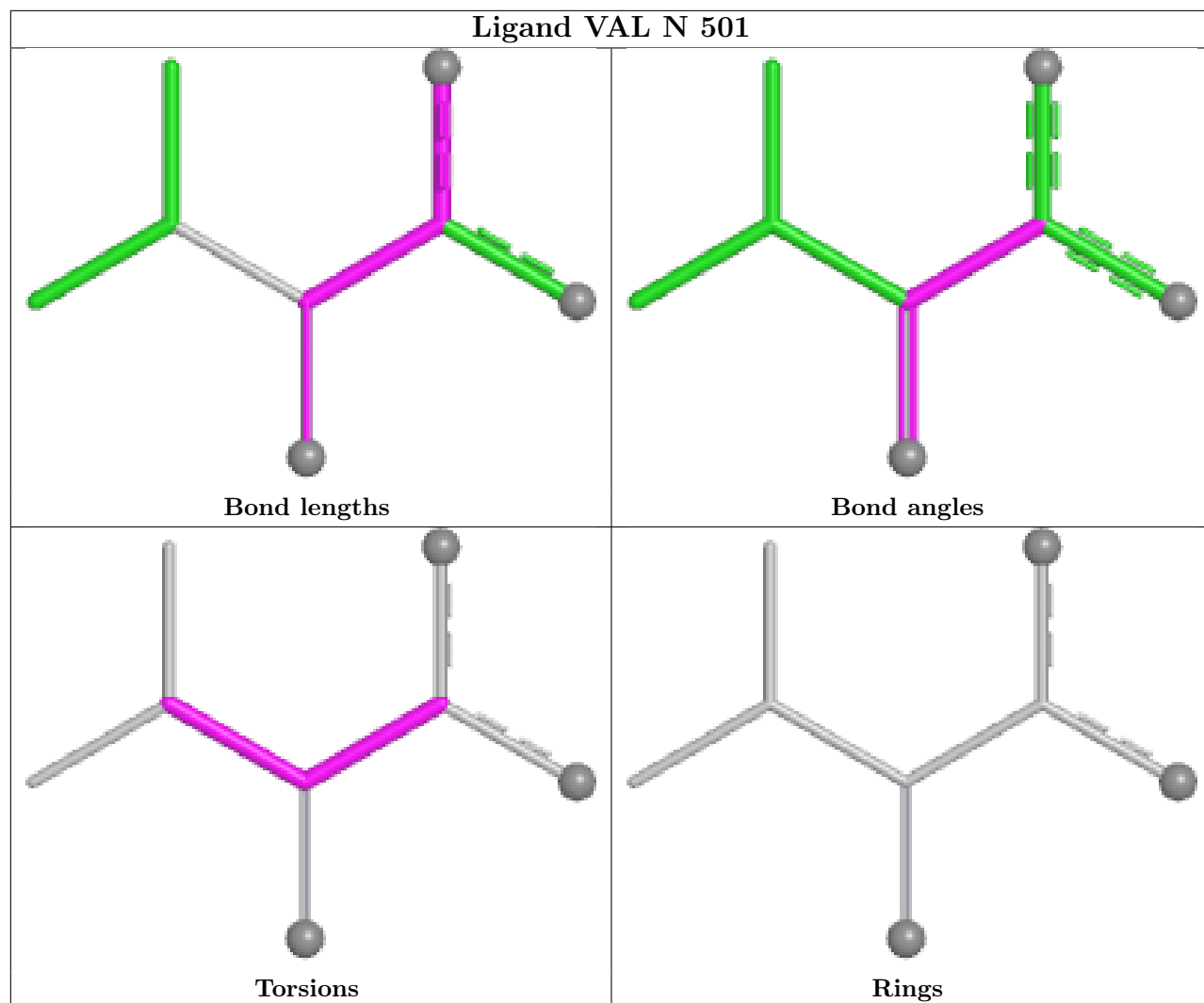


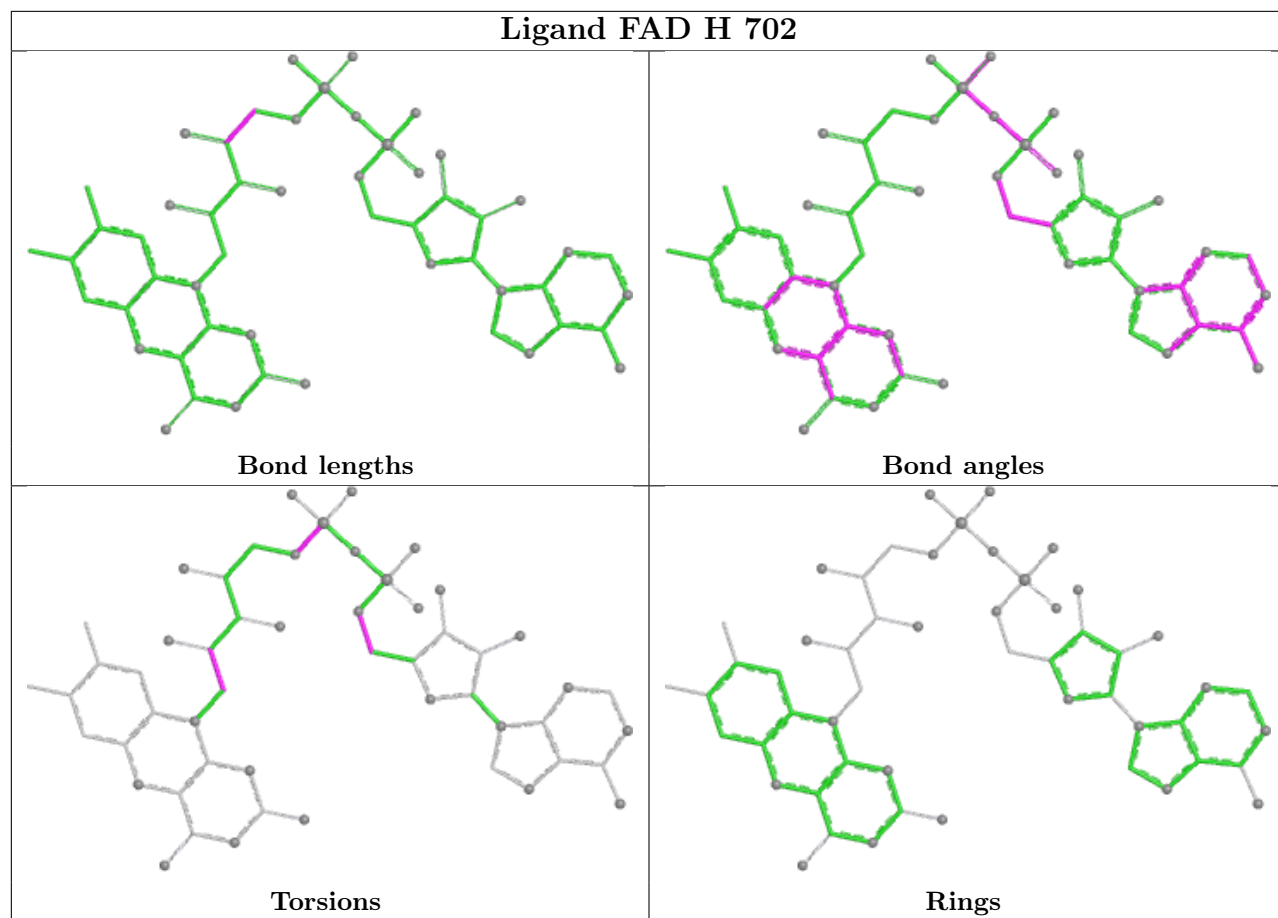
Torsions



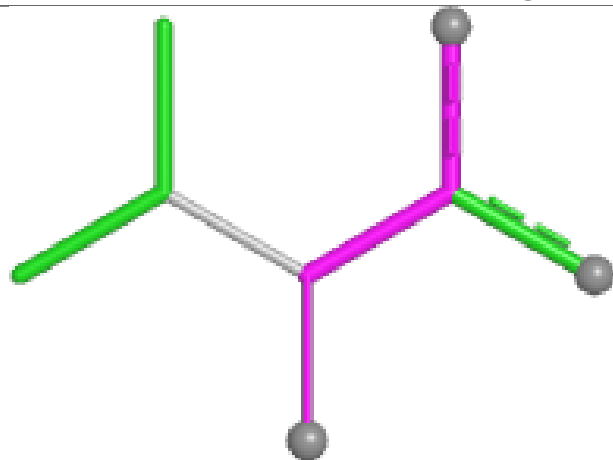
Rings



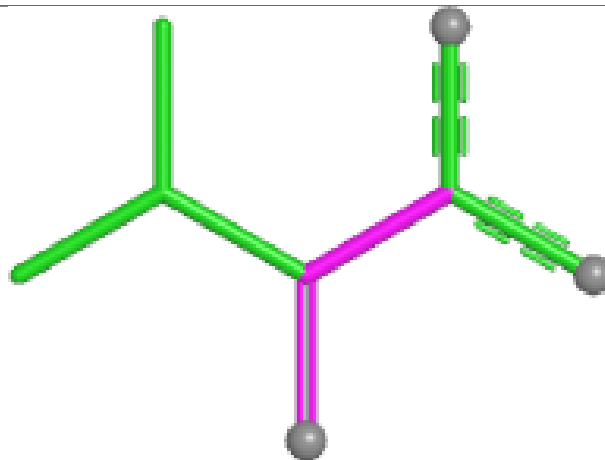




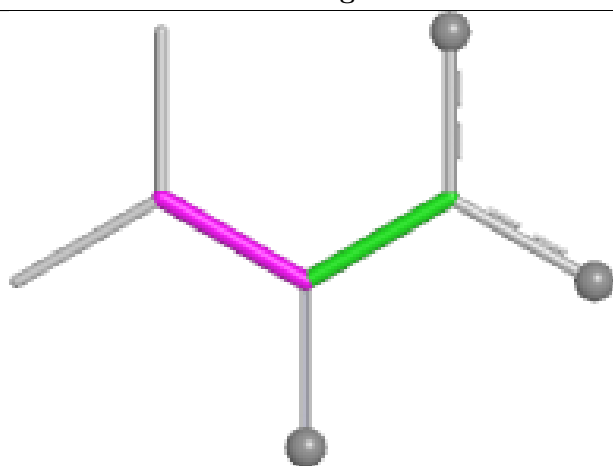
Ligand VAL J 501



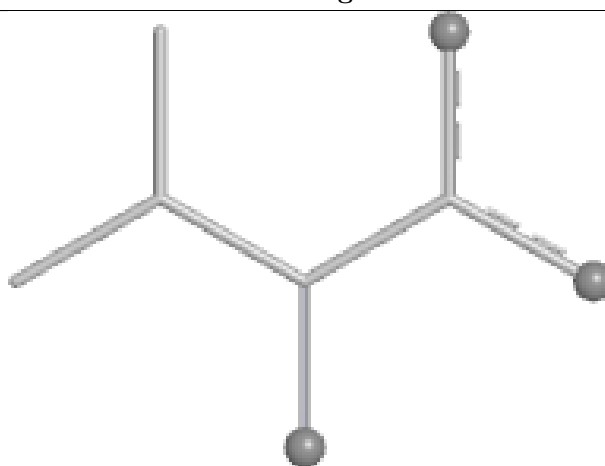
Bond lengths



Bond angles

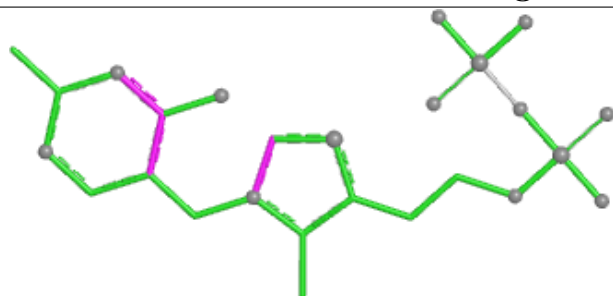


Torsions

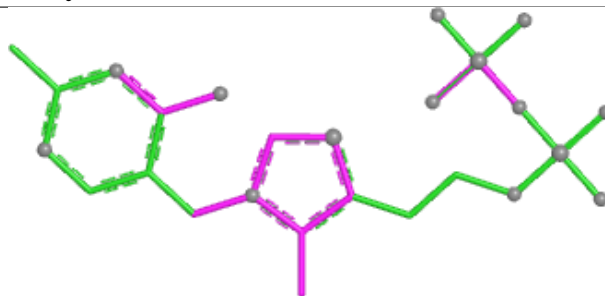


Rings

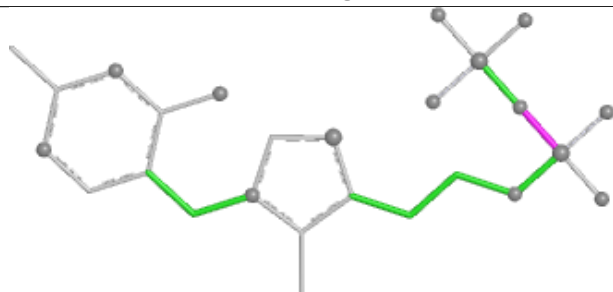
Ligand TPP Q 703



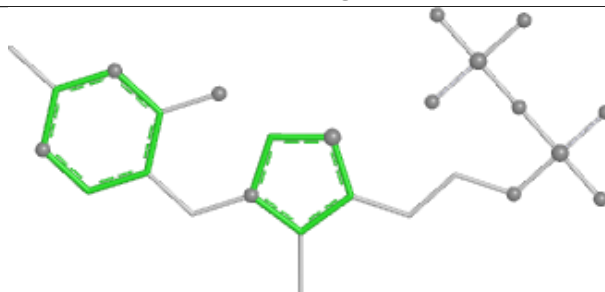
Bond lengths



Bond angles



Torsions



Rings

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.

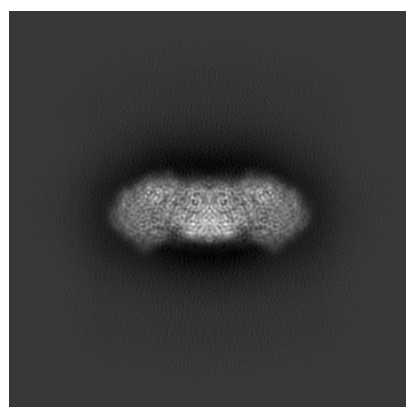
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21487. These allow visual inspection of the internal detail of the map and identification of artifacts.

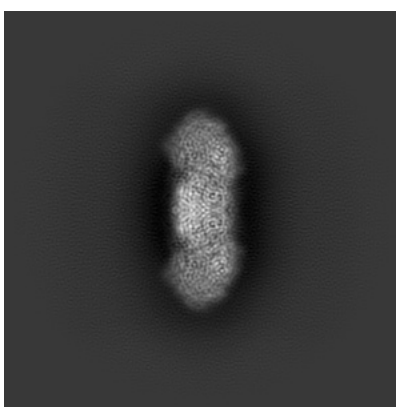
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

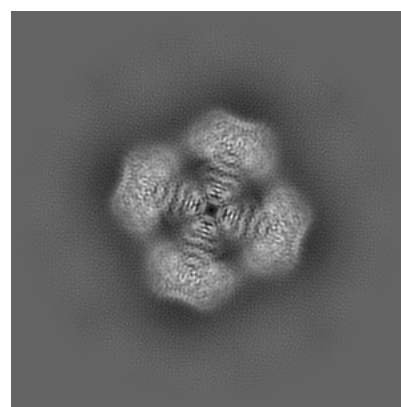
6.1.1 Primary map



X



Y

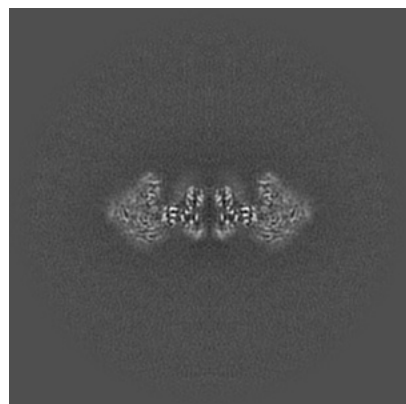


Z

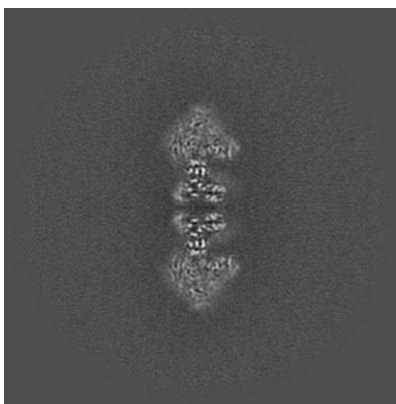
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

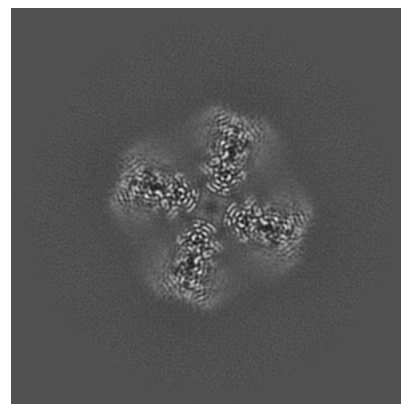
6.2.1 Primary map



X Index: 256



Y Index: 256

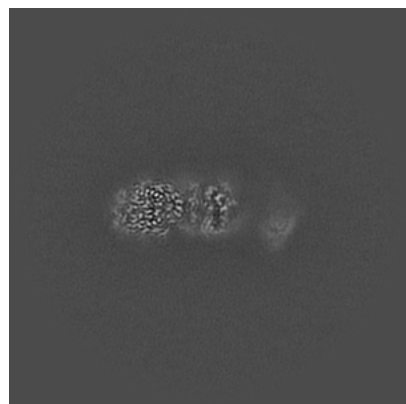


Z Index: 256

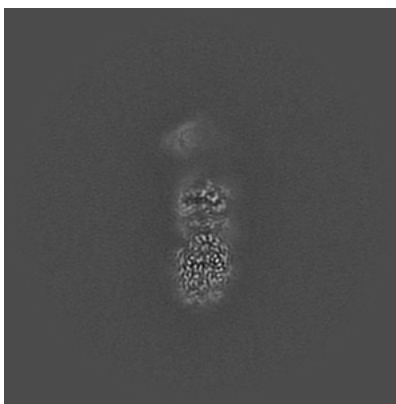
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

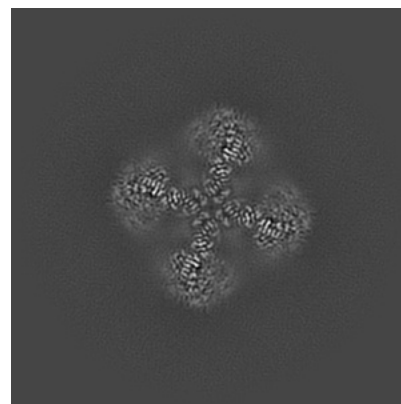
6.3.1 Primary map



X Index: 233



Y Index: 279

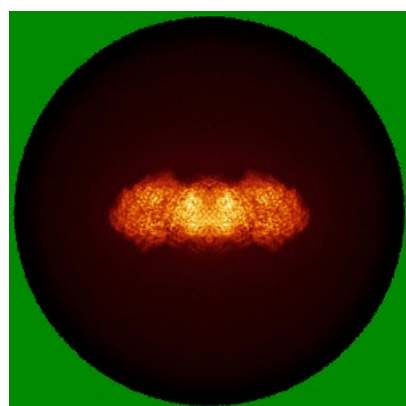


Z Index: 238

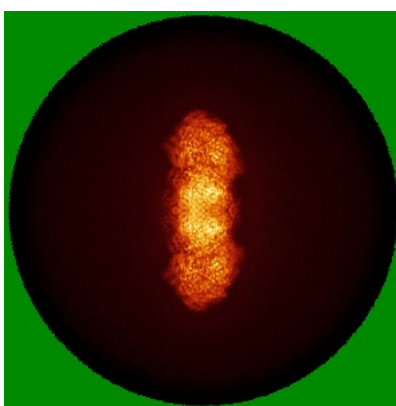
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

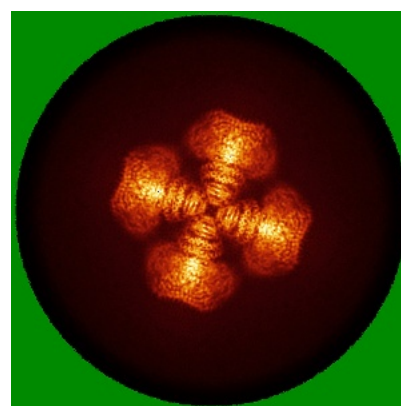
6.4.1 Primary map



X



Y

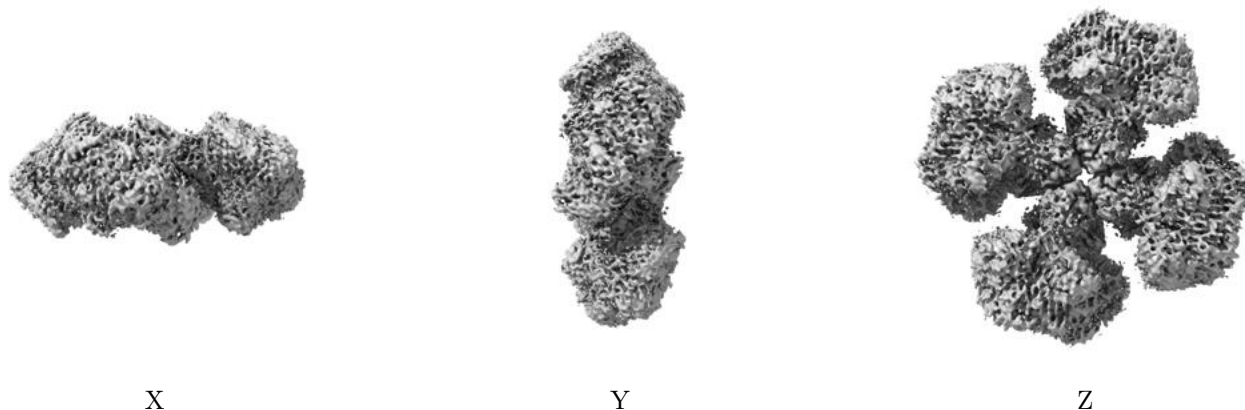


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

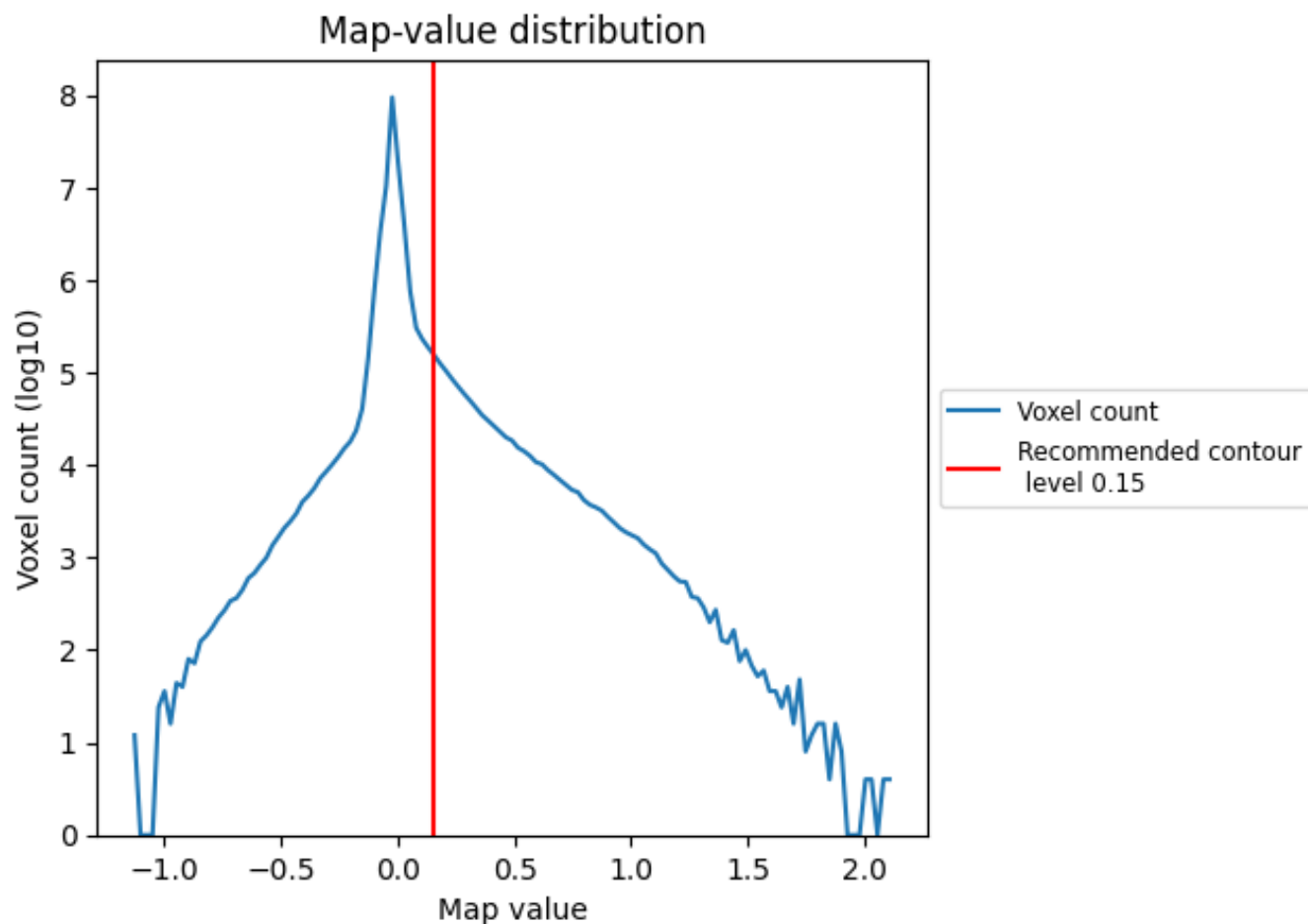
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

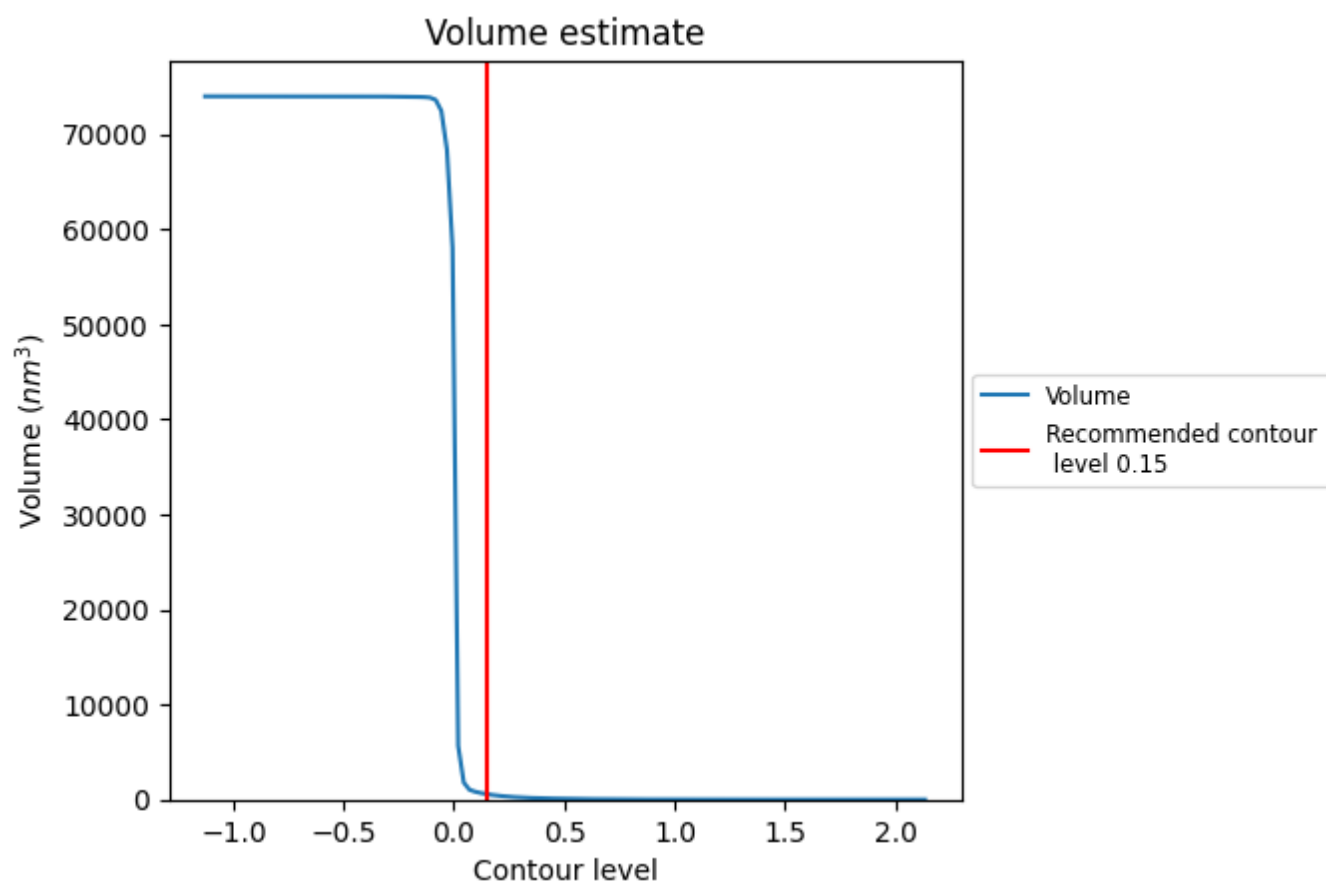
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

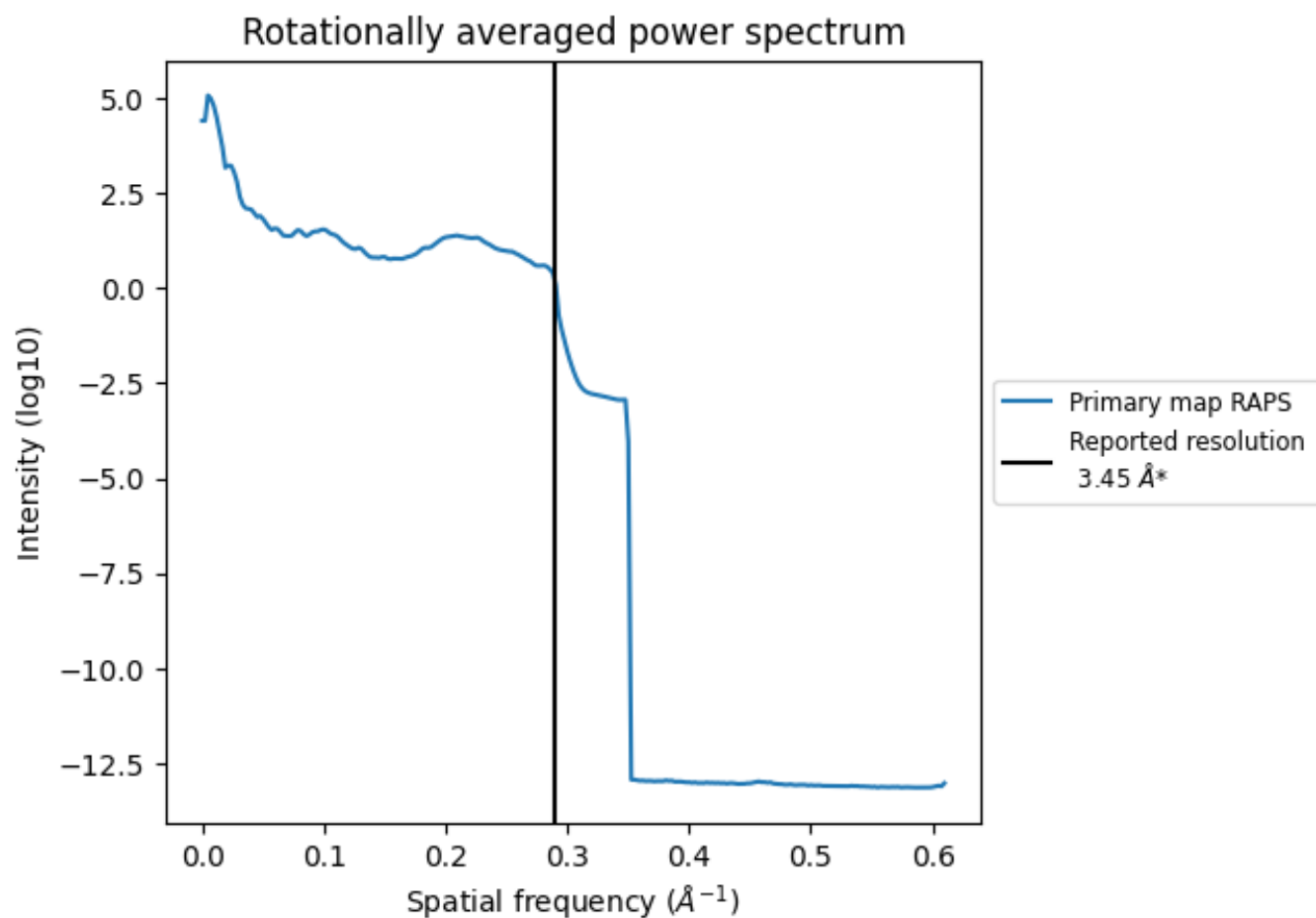
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 568 nm^3 ; this corresponds to an approximate mass of 513 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

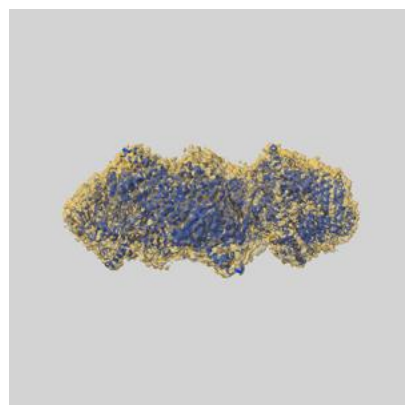
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

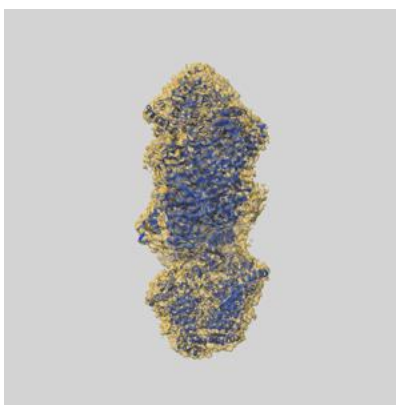
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21487 and PDB model 6VZ8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

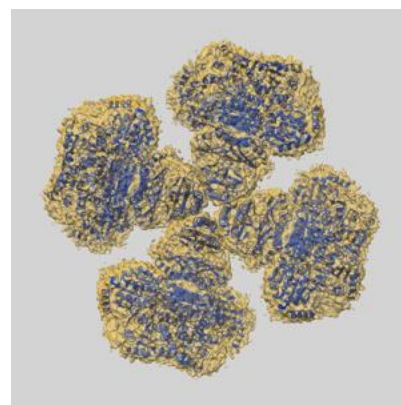
9.1 Map-model overlay [i](#)



X



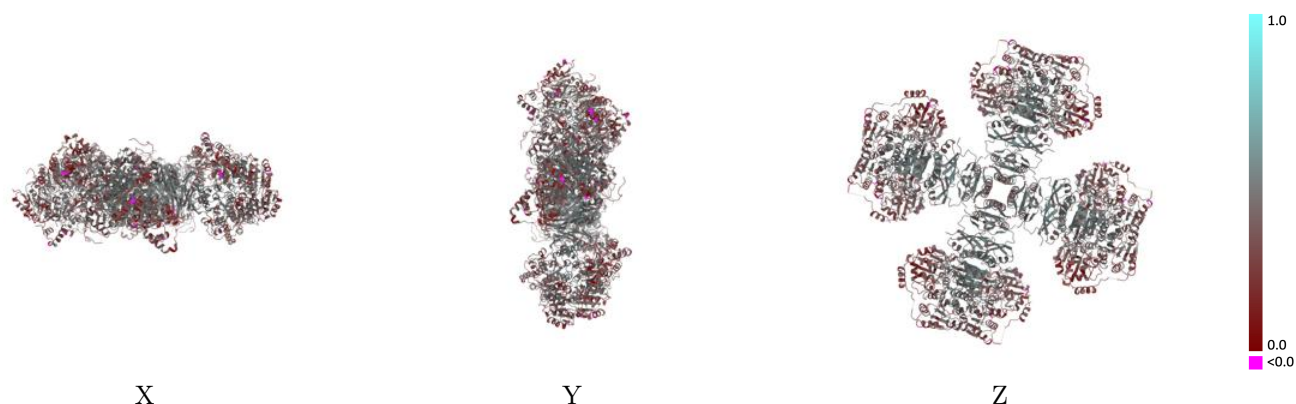
Y



Z

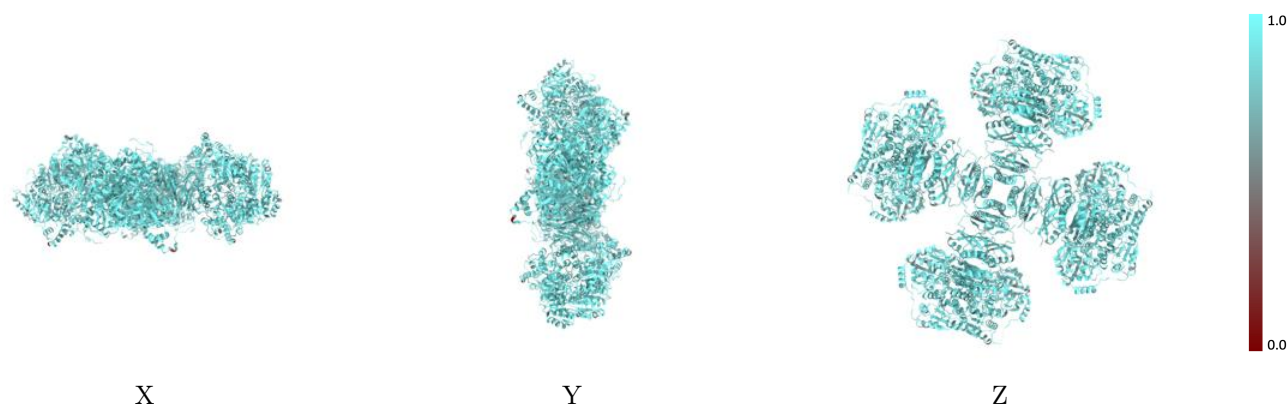
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



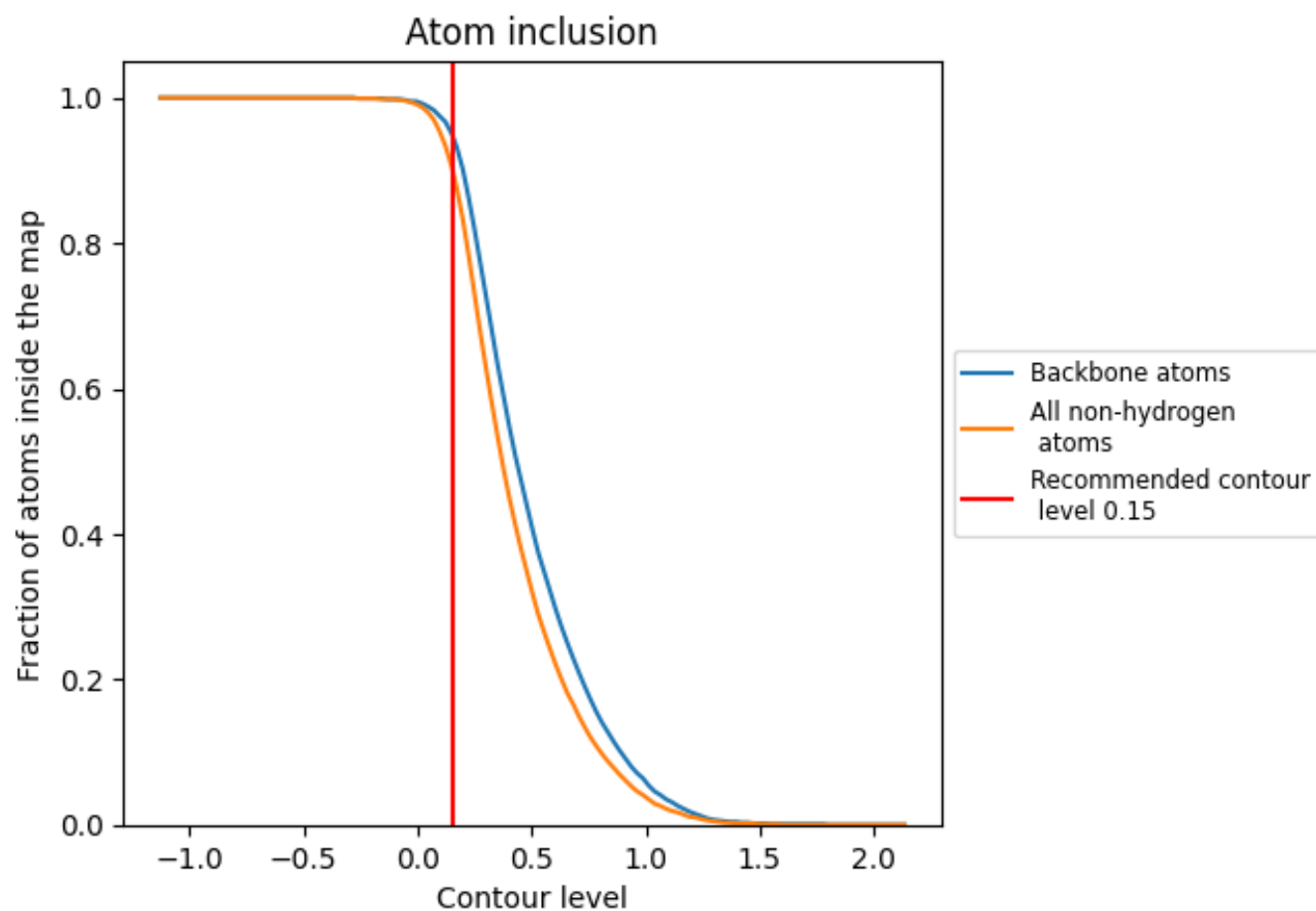
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9040	0.3920
D	0.8950	0.3670
E	0.9020	0.3720
F	0.9030	0.4450
G	0.9280	0.4770
H	0.8940	0.3670
I	0.9050	0.3710
J	0.9000	0.4450
K	0.9260	0.4790
L	0.8970	0.3700
M	0.9090	0.3740
N	0.9060	0.4460
O	0.9220	0.4780
P	0.8940	0.3670
Q	0.9090	0.3770
R	0.9040	0.4480
S	0.9250	0.4790

1.0

0.0

<0.0