



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:32 AM UTC

PDB ID : 8IVP / pdb_00008ivp
Title : Crystal structure of MV in complex with LLP and FRU from Mycobacterium vanbaalenii
Authors : Li, Q.; Zhu, Y.M.; Gao, J.; Wei, H.L.; Han, X.; Liu, W.D.; Sun, Y.X.
Deposited on : 2023-03-28
Resolution : 1.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

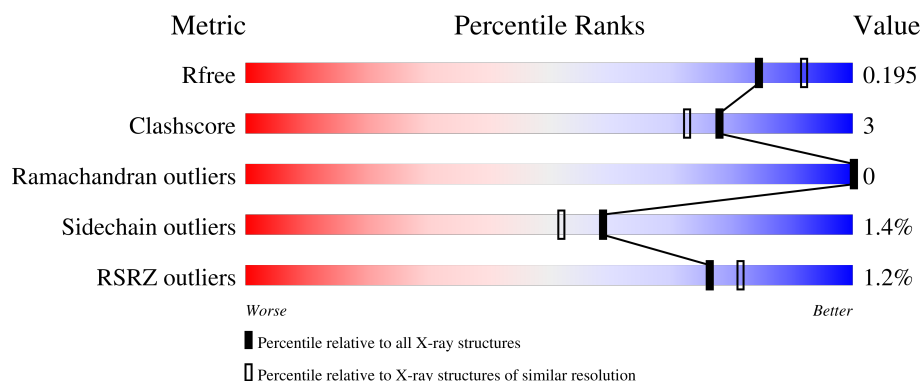
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	337	% 90% 5% 5%
1	B	337	% 89% 5% ••
1	C	337	% 89% 6% 5%
1	D	337	% 89% 6% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUD	A	401	-	X	-	-
2	FUD	B	401	-	X	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11496 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 Branched chain amino acid: 2-keto-4-methylthiobutyrate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	P	S	0	0	0
			2483	1574	419	481	1	8			
1	B	322	Total	C	N	O	P	S	0	0	0
			2493	1579	423	482	1	8			
1	C	319	Total	C	N	O	P	S	0	0	0
			2470	1565	417	479	1	8			
1	D	320	Total	C	N	O	P	S	0	0	0
			2468	1565	414	480	1	8			

There are 36 discrepancies between the modelled and reference sequences:

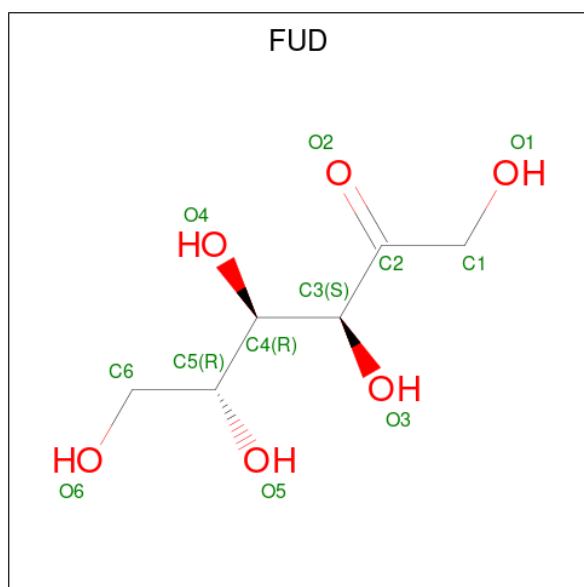
Chain	Residue	Modelled	Actual	Comment	Reference
A	69	LYS	HIS	engineered mutation	UNP A1TDP1
A	105	PRO	SER	engineered mutation	UNP A1TDP1
A	121	MET	SER	engineered mutation	UNP A1TDP1
A	142	PRO	LYS	engineered mutation	UNP A1TDP1
A	145	ARG	LYS	engineered mutation	UNP A1TDP1
A	152	ASN	HIS	engineered mutation	UNP A1TDP1
A	162	ILE	LEU	engineered mutation	UNP A1TDP1
A	168	GLU	ALA	engineered mutation	UNP A1TDP1
A	215	GLY	ARG	engineered mutation	UNP A1TDP1
B	69	LYS	HIS	engineered mutation	UNP A1TDP1
B	105	PRO	SER	engineered mutation	UNP A1TDP1
B	121	MET	SER	engineered mutation	UNP A1TDP1
B	142	PRO	LYS	engineered mutation	UNP A1TDP1
B	145	ARG	LYS	engineered mutation	UNP A1TDP1
B	152	ASN	HIS	engineered mutation	UNP A1TDP1
B	162	ILE	LEU	engineered mutation	UNP A1TDP1
B	168	GLU	ALA	engineered mutation	UNP A1TDP1
B	215	GLY	ARG	engineered mutation	UNP A1TDP1
C	69	LYS	HIS	engineered mutation	UNP A1TDP1
C	105	PRO	SER	engineered mutation	UNP A1TDP1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	121	MET	SER	engineered mutation	UNP A1TDP1
C	142	PRO	LYS	engineered mutation	UNP A1TDP1
C	145	ARG	LYS	engineered mutation	UNP A1TDP1
C	152	ASN	HIS	engineered mutation	UNP A1TDP1
C	162	ILE	LEU	engineered mutation	UNP A1TDP1
C	168	GLU	ALA	engineered mutation	UNP A1TDP1
C	215	GLY	ARG	engineered mutation	UNP A1TDP1
D	69	LYS	HIS	engineered mutation	UNP A1TDP1
D	105	PRO	SER	engineered mutation	UNP A1TDP1
D	121	MET	SER	engineered mutation	UNP A1TDP1
D	142	PRO	LYS	engineered mutation	UNP A1TDP1
D	145	ARG	LYS	engineered mutation	UNP A1TDP1
D	152	ASN	HIS	engineered mutation	UNP A1TDP1
D	162	ILE	LEU	engineered mutation	UNP A1TDP1
D	168	GLU	ALA	engineered mutation	UNP A1TDP1
D	215	GLY	ARG	engineered mutation	UNP A1TDP1

- Molecule 2 is D-fructose (CCD ID: FUD) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	385	Total	O	0	0
			385	385		
3	B	369	Total	O	0	0
			369	369		
3	C	404	Total	O	0	0
			404	404		
3	D	376	Total	O	0	0
			376	376		

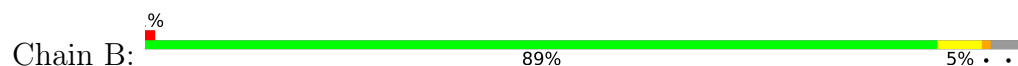
3 Residue-property plots [i](#)

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.

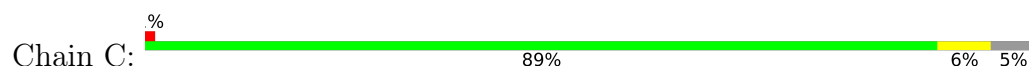
- Molecule 1: Branched chain amino acid: 2-keto-4-methylthiobutyrate aminotransferase



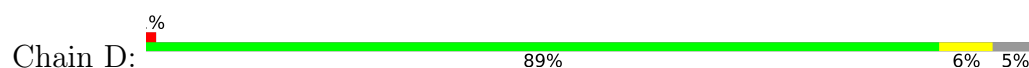
- Molecule 1: Branched chain amino acid: 2-keto-4-methylthiobutyrate aminotransferase



- Molecule 1: Branched chain amino acid: 2-keto-4-methylthiobutyrate aminotransferase



- Molecule 1: Branched chain amino acid: 2-keto-4-methylthiobutyrate aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.71Å 112.24Å 92.10Å 90.00° 112.31° 90.00°	Depositor
Resolution (Å)	45.14 – 1.93 45.14 – 1.93	Depositor EDS
% Data completeness (in resolution range)	92.7 (45.14-1.93) 93.1 (45.14-1.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.151 , 0.188 0.162 , 0.195	Depositor DCC
R_{free} test set	5344 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11496	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: LLP, FUD

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	1.11	1/2515 (0.0%)	1.26	0/3423
1	B	1.08	2/2525 (0.1%)	1.26	2/3435 (0.1%)
1	C	1.08	4/2502 (0.2%)	1.24	0/3405
1	D	1.08	0/2500	1.27	4/3405 (0.1%)
All	All	1.09	7/10042 (0.1%)	1.26	6/13668 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	GLY	C-O	6.05	1.31	1.23
1	C	134	ILE	C-O	5.81	1.30	1.24
1	C	90	HIS	CE1-NE2	5.68	1.38	1.32
1	C	288	VAL	C-O	5.57	1.29	1.24
1	A	232	PHE	C-O	5.32	1.30	1.23
1	C	177	VAL	C-O	5.18	1.29	1.24
1	B	181	HIS	CE1-NE2	5.09	1.37	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	141	ARG	CB-CA-C	6.16	118.58	109.22
1	D	165	PHE	CA-C-N	5.96	124.01	119.66
1	D	165	PHE	C-N-CA	5.96	124.01	119.66
1	B	245	PRO	N-CA-C	5.58	119.62	111.03
1	D	90	HIS	CA-CB-CG	-5.45	108.35	113.80

There are no chirality outliers.

There are no planarity outliers.

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	A	2483	0	2418	15	0
1	B	2493	0	2432	17	0
1	C	2470	0	2402	10	0
1	D	2468	0	2391	10	0
2	A	12	0	12	4	0
2	B	12	0	12	7	0
2	C	24	0	24	0	0
3	A	385	0	0	2	0
3	B	369	0	0	5	0
3	C	404	0	0	1	0
3	D	376	0	0	3	0
All	All	11496	0	9691	55	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 3.

All (55) 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:B:141:ARG:HB2	3:B:615:HOH:O	1.74	0.87
1:A:199:TRP:CE3	1:B:69:LYS:HE2	2.11	0.84
1:A:33:TYR:HE2	1:A:35:ILE:HD11	1.48	0.78
1:B:141:ARG:CB	3:B:615:HOH:O	2.36	0.69
2:A:401:FUD:O6	2:A:401:FUD:H12	1.97	0.64
1:A:17:ALA:N	3:A:501:HOH:O	2.32	0.62
1:A:33:TYR:CE2	1:A:35:ILE:HD11	2.33	0.60
1:B:72:LEU:C	1:B:72:LEU:HD12	2.27	0.59
1:A:207:PHE:CZ	1:B:147:LEU:HD23	2.39	0.58
2:A:401:FUD:O6	2:A:401:FUD:C1	2.50	0.58
2:A:401:FUD:H12	2:A:401:FUD:H5	1.86	0.58
1:A:35:ILE:HD12	1:A:124:GLN:CB	2.36	0.55
1:B:143:GLY:HA2	1:B:145:ARG:NH1	2.22	0.55
1:B:74:TYR:OH	2:B:401:FUD:H61	2.09	0.53
1:A:35:ILE:HD12	1:A:124:GLN:HB3	1.90	0.53
1:A:72:LEU:C	1:A:72:LEU:HD12	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:THR:HG22	3:D:556:HOH:O	2.09	0.53
1:B:141:ARG:CA	3:B:615:HOH:O	2.55	0.52
2:B:401:FUD:O6	2:B:401:FUD:H12	2.11	0.50
1:A:146:ASP:HB3	1:A:149:LYS:HG3	1.93	0.50
1:C:100:LYS:HE3	1:C:194:ILE:HD11	1.95	0.49
1:B:74:TYR:CE1	1:B:195:LLP:HG3	2.48	0.49
1:B:121:MET:HG3	1:B:336:GLN:O	2.13	0.48
2:A:401:FUD:H12	2:A:401:FUD:C5	2.45	0.47
1:C:52:TYR:CZ	1:C:118:LYS:HD3	2.50	0.47
1:B:291:ALA:HB3	2:B:401:FUD:H3	1.98	0.46
1:A:35:ILE:HD12	1:A:124:GLN:HB2	1.98	0.45
2:B:401:FUD:O6	2:B:401:FUD:O4	2.34	0.45
1:C:147:LEU:HD13	1:D:207:PHE:CZ	2.52	0.45
2:B:401:FUD:O4	2:B:401:FUD:C1	2.65	0.45
1:A:207:PHE:CZ	1:B:147:LEU:CD2	2.99	0.44
1:A:79:VAL:O	1:A:127:GLU:HA	2.17	0.44
2:B:401:FUD:O6	2:B:401:FUD:C1	2.66	0.44
1:C:100:LYS:NZ	3:C:517:HOH:O	2.50	0.44
1:A:147:LEU:HD23	1:B:207:PHE:CZ	2.53	0.43
1:D:35:ILE:HB	1:D:37:TYR:CE2	2.53	0.43
1:B:97:GLY:HA3	3:B:602:HOH:O	2.17	0.43
2:B:401:FUD:O4	2:B:401:FUD:O1	2.36	0.43
1:D:48:ILE:CD1	1:D:58:ALA:HB1	2.48	0.43
1:D:48:ILE:HD11	1:D:58:ALA:HB1	2.01	0.43
1:C:336:GLN:HE21	1:C:336:GLN:HB3	1.70	0.43
1:A:199:TRP:CE3	1:B:69:LYS:CE	2.92	0.42
1:C:251:PRO:HA	1:C:255:ARG:NH2	2.34	0.42
1:D:56:GLU:HB2	3:D:585:HOH:O	2.19	0.42
1:D:52:TYR:CZ	1:D:118:LYS:HD2	2.55	0.42
1:D:118:LYS:HB2	1:D:118:LYS:HE2	1.92	0.42
1:C:41:PHE:HB3	1:C:45:VAL:HG22	2.02	0.42
1:A:97:GLY:HA3	3:A:613:HOH:O	2.20	0.42
1:C:118:LYS:HG3	1:C:121:MET:CE	2.50	0.41
1:C:147:LEU:HD11	3:D:750:HOH:O	2.20	0.41
1:B:76:VAL:HA	1:B:130:VAL:O	2.20	0.41
1:B:320:ARG:NH2	3:B:510:HOH:O	2.49	0.41
1:C:65:THR:OG1	1:C:136:ARG:HB3	2.21	0.40
1:D:177:VAL:O	1:D:217:ALA:HA	2.21	0.40
1:D:66:GLY:O	1:D:70:SER:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	318/337 (94%)	310 (98%)	8 (2%)	0	100	100
1	B	319/337 (95%)	311 (98%)	8 (2%)	0	100	100
1	C	316/337 (94%)	308 (98%)	8 (2%)	0	100	100
1	D	317/337 (94%)	309 (98%)	8 (2%)	0	100	100
All	All	1270/1348 (94%)	1238 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 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	256/269 (95%)	253 (99%)	3 (1%)	63	57
1	B	257/269 (96%)	253 (98%)	4 (2%)	55	46
1	C	255/269 (95%)	253 (99%)	2 (1%)	73	71
1	D	254/269 (94%)	249 (98%)	5 (2%)	48	39
All	All	1022/1076 (95%)	1008 (99%)	14 (1%)	59	52

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	140	LYS

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Mol	Chain	Res	Type
1	A	141	ARG
1	B	34	GLU
1	B	78	HIS
1	B	141	ARG
1	B	336	GLN
1	C	78	HIS
1	C	140	LYS
1	D	18	ILE
1	D	34	GLU
1	D	56	GLU
1	D	78	HIS
1	D	182	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	298	ASN
1	A	336	GLN
1	B	298	ASN
1	B	336	GLN
1	C	298	ASN
1	C	336	GLN
1	D	233	ASN
1	D	298	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	LLP	D	195	1	23,24,25	2.36	6 (26%)	25,32,34	2.14	7 (28%)
1	LLP	C	195	1	23,24,25	2.12	5 (21%)	25,32,34	1.81	5 (20%)
1	LLP	B	195	1	23,24,25	2.06	4 (17%)	25,32,34	1.79	6 (24%)
1	LLP	A	195	1	23,24,25	2.18	4 (17%)	25,32,34	1.82	6 (24%)

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
1	LLP	D	195	1	-	4/16/17/19	0/1/1/1
1	LLP	C	195	1	-	4/16/17/19	0/1/1/1
1	LLP	B	195	1	-	3/16/17/19	0/1/1/1
1	LLP	A	195	1	-	4/16/17/19	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	195	LLP	CD-CE	6.21	1.72	1.51
1	D	195	LLP	CD-CE	6.08	1.72	1.51
1	A	195	LLP	C4'-NZ	5.91	1.47	1.27
1	A	195	LLP	CD-CE	5.81	1.71	1.51
1	B	195	LLP	CD-CE	5.60	1.70	1.51
1	D	195	LLP	C4'-NZ	5.43	1.45	1.27
1	D	195	LLP	C4-C4'	5.18	1.57	1.46
1	C	195	LLP	C4'-NZ	5.13	1.44	1.27
1	B	195	LLP	C4'-NZ	4.78	1.43	1.27
1	A	195	LLP	C4-C4'	4.16	1.55	1.46
1	B	195	LLP	C4-C4'	4.13	1.55	1.46
1	C	195	LLP	C4-C4'	4.03	1.55	1.46
1	D	195	LLP	C3-C2	3.49	1.44	1.41
1	B	195	LLP	C3-C2	3.13	1.44	1.41
1	C	195	LLP	C3-C2	2.93	1.44	1.41
1	D	195	LLP	CE-NZ	2.29	1.51	1.46
1	A	195	LLP	C3-C2	2.18	1.43	1.41
1	C	195	LLP	CE-NZ	2.06	1.51	1.46
1	D	195	LLP	C4-C3	2.02	1.44	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	LLP	C3-C4-C5	-5.79	113.62	118.28
1	D	195	LLP	CD-CE-NZ	4.60	123.01	110.83
1	A	195	LLP	CD-CE-NZ	4.53	122.82	110.83
1	C	195	LLP	CD-CE-NZ	4.49	122.72	110.83
1	C	195	LLP	C3-C4-C5	-4.44	114.71	118.28
1	B	195	LLP	CD-CE-NZ	4.08	121.62	110.83
1	A	195	LLP	C3-C4-C5	-3.84	115.19	118.28
1	B	195	LLP	CD-CG-CB	3.65	127.39	113.62
1	D	195	LLP	CD-CG-CB	3.60	127.18	113.62
1	B	195	LLP	C3-C4-C5	-3.54	115.43	118.28
1	A	195	LLP	C4-C3-C2	3.40	122.06	120.14
1	B	195	LLP	OP3-P-OP4	-3.35	97.94	106.67
1	A	195	LLP	CD-CG-CB	3.22	125.77	113.62
1	C	195	LLP	CD-CG-CB	3.13	125.42	113.62
1	D	195	LLP	C5'-C5-C6	-2.94	114.58	119.36
1	C	195	LLP	C4-C3-C2	2.90	121.78	120.14
1	D	195	LLP	OP3-P-OP4	-2.78	99.43	106.67
1	C	195	LLP	OP3-P-OP4	-2.66	99.73	106.67
1	D	195	LLP	C5-C4-C4'	2.61	125.50	121.47
1	A	195	LLP	C5-C4-C4'	2.46	125.27	121.47
1	A	195	LLP	CE-NZ-C4'	2.24	125.91	118.72
1	D	195	LLP	OP3-P-OP2	2.15	115.88	107.80
1	B	195	LLP	C4-C3-C2	2.12	121.34	120.14
1	B	195	LLP	C5-C4-C4'	2.02	124.58	121.47

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	195	LLP	C4-C4'-NZ-CE
1	B	195	LLP	C4-C4'-NZ-CE
1	B	195	LLP	CG-CD-CE-NZ
1	C	195	LLP	C4-C4'-NZ-CE
1	C	195	LLP	CG-CD-CE-NZ
1	D	195	LLP	C4-C4'-NZ-CE
1	A	195	LLP	CG-CD-CE-NZ
1	D	195	LLP	CG-CD-CE-NZ
1	C	195	LLP	C3-C4-C4'-NZ
1	A	195	LLP	C3-C4-C4'-NZ
1	B	195	LLP	C3-C4-C4'-NZ
1	D	195	LLP	C3-C4-C4'-NZ
1	A	195	LLP	N-CA-CB-CG
1	C	195	LLP	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	D	195	LLP	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	195	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	FUD	A	401	-	11,11,11	1.03	1 (9%)	10,14,14	2.74	7 (70%)
2	FUD	B	401	-	11,11,11	0.88	1 (9%)	10,14,14	2.05	5 (50%)
2	FUD	C	402	-	11,11,11	1.04	0	10,14,14	3.66	3 (30%)
2	FUD	C	401	-	11,11,11	0.73	0	10,14,14	1.95	3 (30%)

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	FUD	A	401	-	-	10/16/16/16	-
2	FUD	B	401	-	-	13/16/16/16	-
2	FUD	C	402	-	-	12/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUD	C	401	-	-	11/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FUD	C5-C4	-2.20	1.49	1.53
2	B	401	FUD	C5-C4	-2.07	1.49	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	FUD	C5-C4-C3	8.48	125.97	112.05
2	C	402	FUD	O6-C6-C5	5.59	122.89	111.16
2	A	401	FUD	C5-C4-C3	4.85	120.01	112.05
2	C	402	FUD	O4-C4-C3	-4.77	100.72	109.29
2	C	401	FUD	O1-C1-C2	-3.35	103.85	112.73
2	B	401	FUD	O5-C5-C4	-3.25	101.65	109.25
2	A	401	FUD	O3-C3-C4	-3.11	103.63	110.38
2	B	401	FUD	O1-C1-C2	-2.93	104.95	112.73
2	A	401	FUD	C6-C5-C4	2.91	118.10	112.17
2	C	401	FUD	C6-C5-C4	-2.89	106.29	112.17
2	A	401	FUD	O4-C4-C3	-2.80	104.27	109.29
2	B	401	FUD	C5-C4-C3	2.67	116.44	112.05
2	A	401	FUD	O1-C1-C2	-2.50	106.10	112.73
2	C	401	FUD	O3-C3-C4	-2.48	105.00	110.38
2	A	401	FUD	O4-C4-C5	-2.39	103.50	108.93
2	A	401	FUD	O5-C5-C4	-2.26	103.96	109.25
2	B	401	FUD	O2-C2-C1	-2.12	116.57	120.16
2	B	401	FUD	O4-C4-C3	-2.10	105.53	109.29

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FUD	O1-C1-C2-O2
2	A	401	FUD	O2-C2-C3-C4
2	A	401	FUD	C3-C4-C5-C6
2	B	401	FUD	O1-C1-C2-O2
2	B	401	FUD	O2-C2-C3-O3
2	B	401	FUD	C2-C3-C4-C5
2	B	401	FUD	C2-C3-C4-O4

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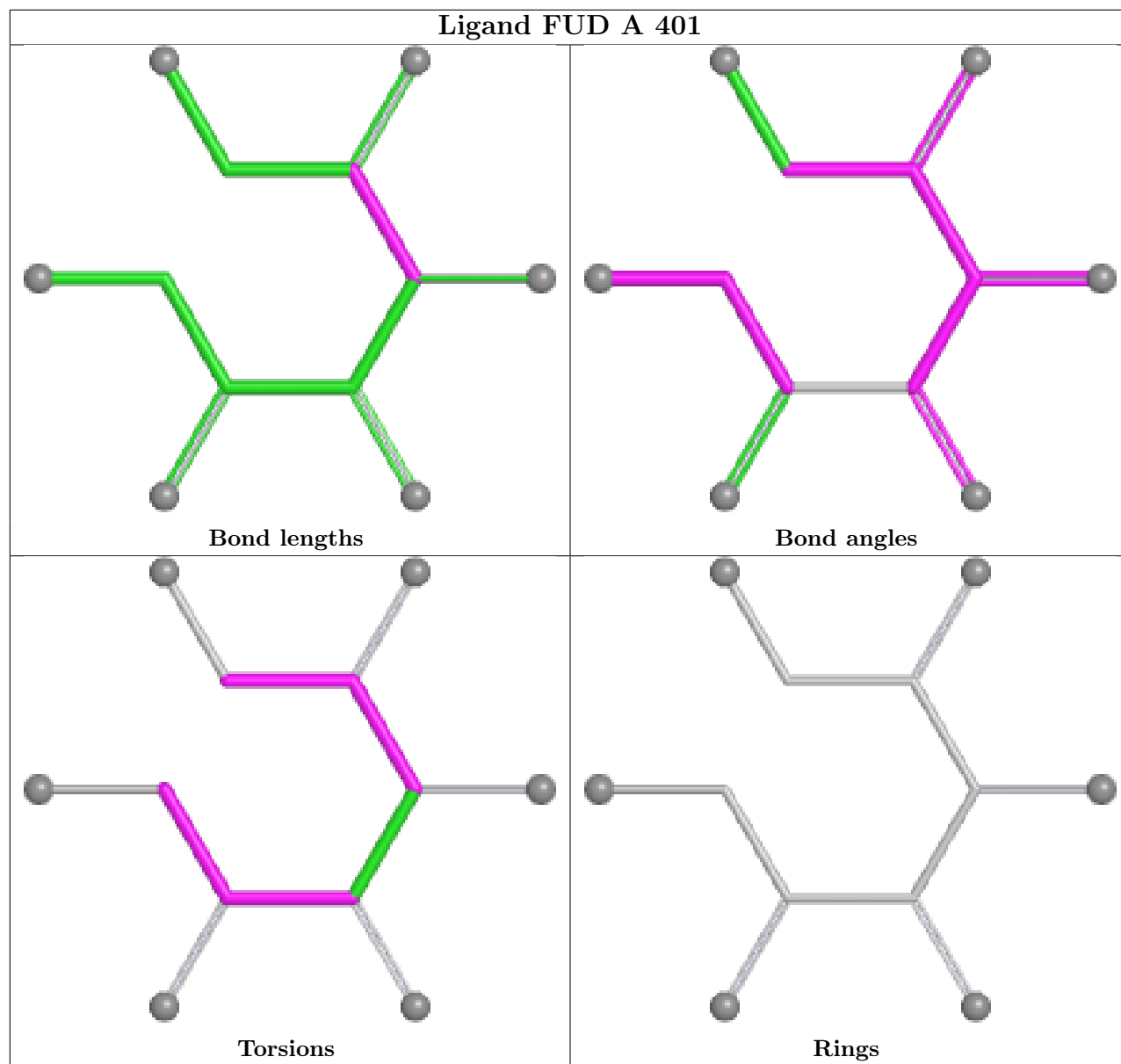
Mol	Chain	Res	Type	Atoms
2	B	401	FUD	O3-C3-C4-C5
2	B	401	FUD	O3-C3-C4-O4
2	B	401	FUD	C3-C4-C5-O5
2	B	401	FUD	O4-C4-C5-C6
2	B	401	FUD	O4-C4-C5-O5
2	C	401	FUD	O1-C1-C2-C3
2	C	401	FUD	O1-C1-C2-O2
2	C	401	FUD	C2-C3-C4-C5
2	C	401	FUD	C2-C3-C4-O4
2	C	401	FUD	O3-C3-C4-C5
2	C	401	FUD	O3-C3-C4-O4
2	C	402	FUD	O1-C1-C2-C3
2	C	402	FUD	O1-C1-C2-O2
2	C	402	FUD	C1-C2-C3-C4
2	C	402	FUD	O2-C2-C3-C4
2	C	402	FUD	O2-C2-C3-O3
2	C	402	FUD	C3-C4-C5-O5
2	C	402	FUD	O4-C4-C5-O5
2	C	402	FUD	O4-C4-C5-C6
2	B	401	FUD	C3-C4-C5-C6
2	C	402	FUD	C3-C4-C5-C6
2	A	401	FUD	O4-C4-C5-C6
2	A	401	FUD	O5-C5-C6-O6
2	A	401	FUD	C3-C4-C5-O5
2	A	401	FUD	C4-C5-C6-O6
2	C	402	FUD	O5-C5-C6-O6
2	C	401	FUD	O5-C5-C6-O6
2	A	401	FUD	O4-C4-C5-O5
2	C	402	FUD	C4-C5-C6-O6
2	A	401	FUD	C1-C2-C3-C4
2	B	401	FUD	C1-C2-C3-C4
2	B	401	FUD	O2-C2-C3-C4
2	C	401	FUD	C3-C4-C5-O5
2	A	401	FUD	O1-C1-C2-C3
2	B	401	FUD	O1-C1-C2-C3
2	C	401	FUD	C3-C4-C5-C6
2	C	402	FUD	C1-C2-C3-O3
2	C	401	FUD	C4-C5-C6-O6
2	C	401	FUD	O4-C4-C5-C6

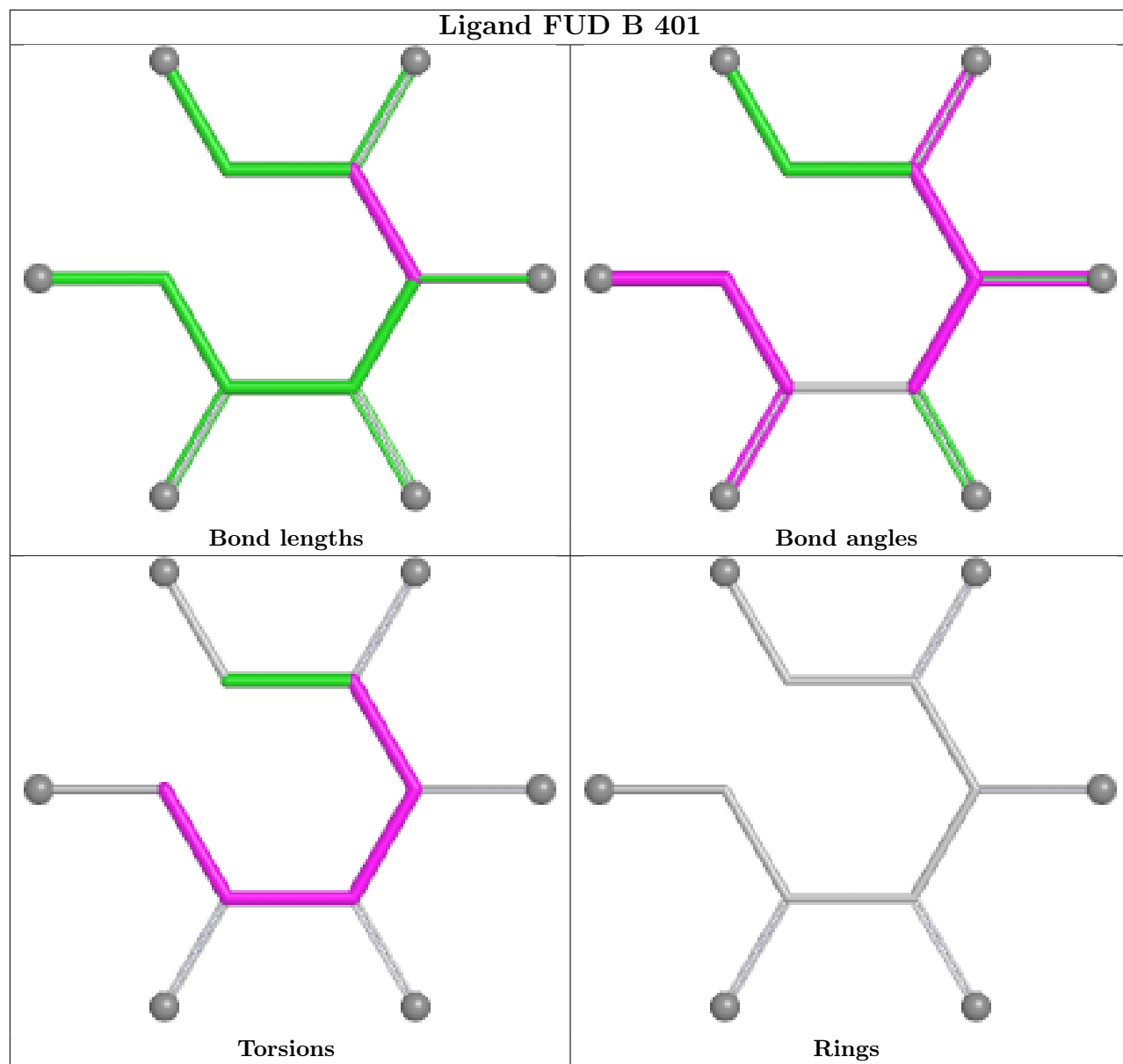
There are no ring outliers.

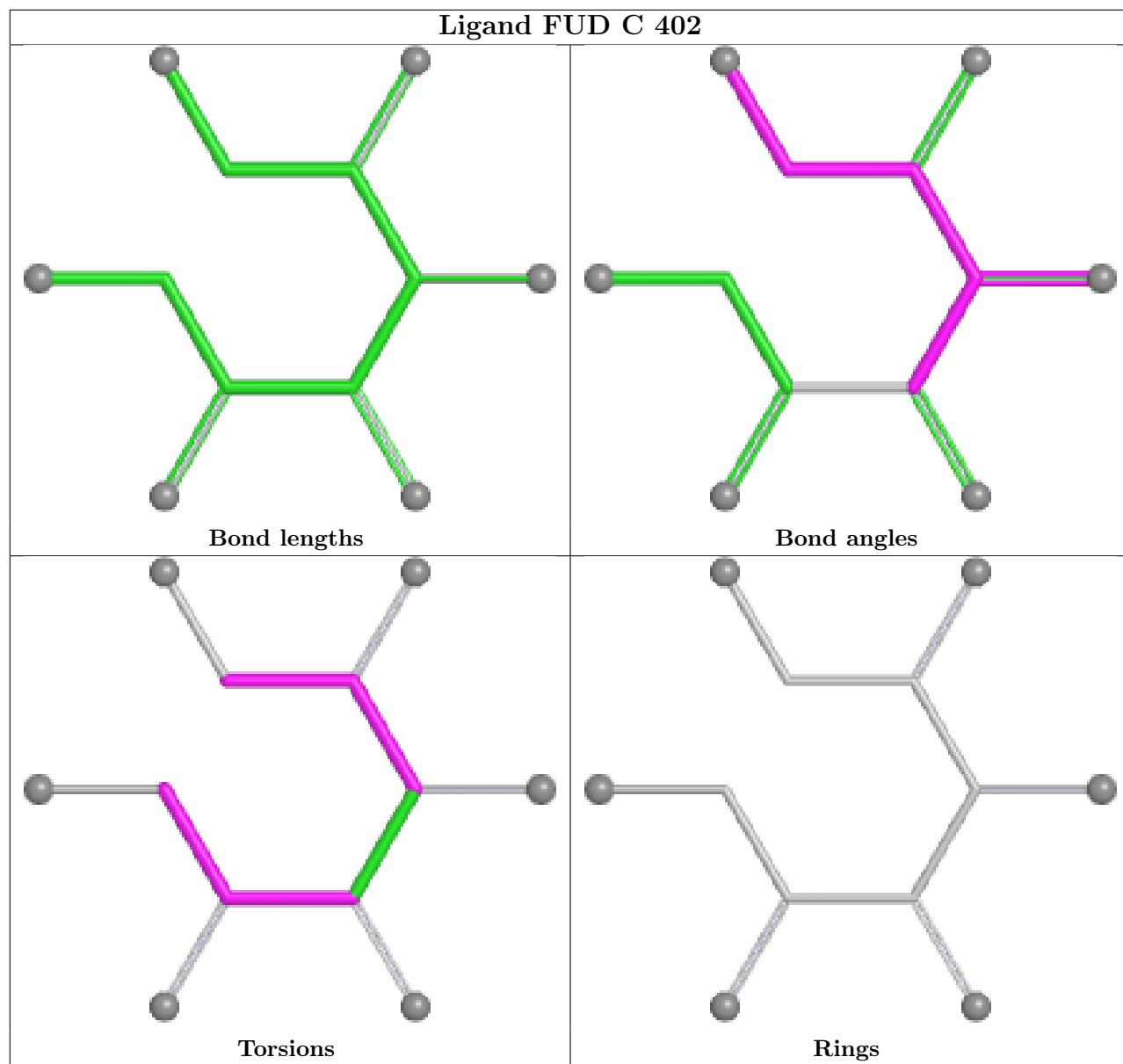
2 monomers are involved in 11 short contacts:

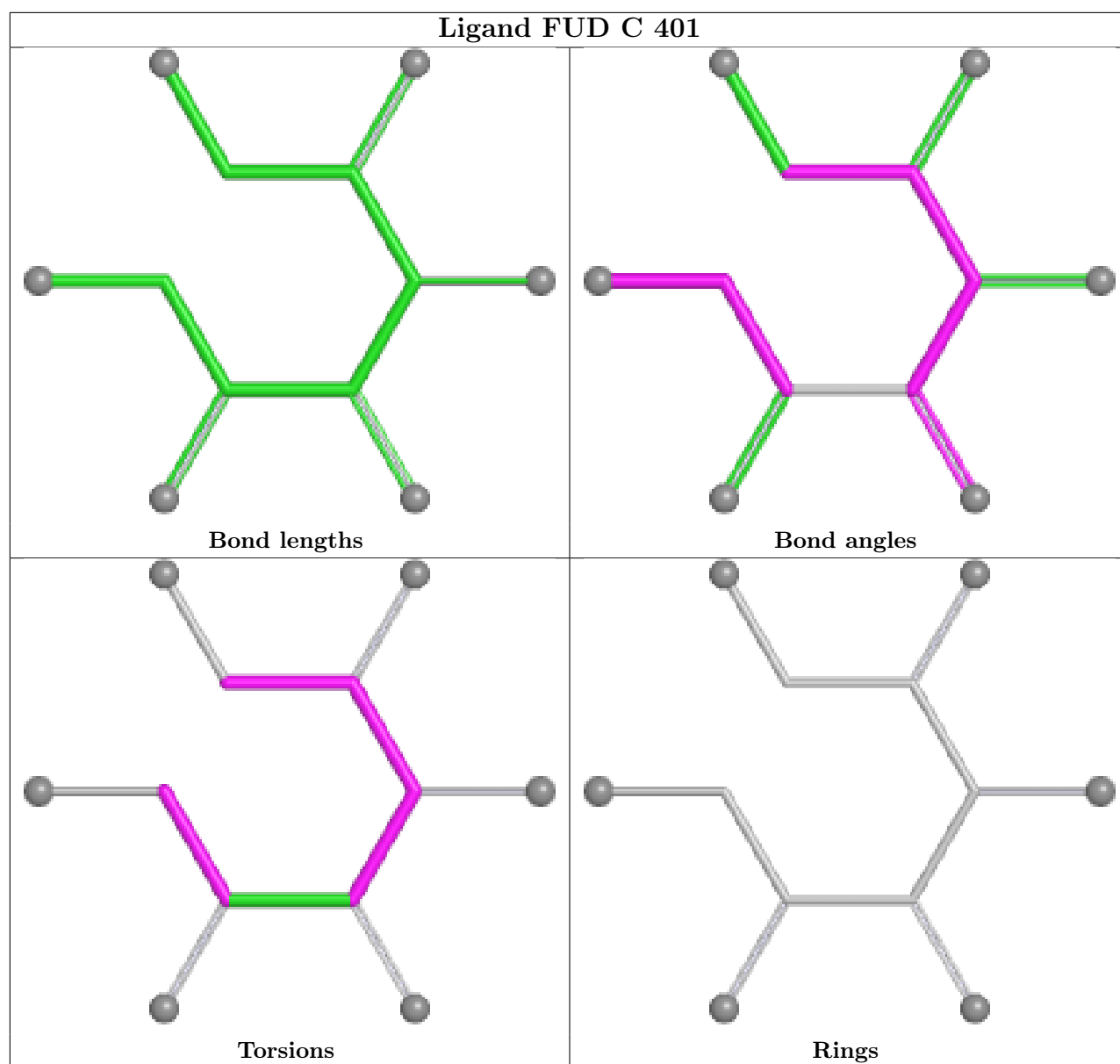
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FUD	4	0
2	B	401	FUD	7	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/337 (94%)	-0.40	5 (1%) 70 77	8, 12, 31, 52	0
1	B	321/337 (95%)	-0.31	2 (0%) 85 89	9, 14, 31, 54	0
1	C	318/337 (94%)	-0.39	4 (1%) 75 80	8, 13, 30, 49	0
1	D	319/337 (94%)	-0.25	4 (1%) 75 80	8, 16, 31, 54	0
All	All	1278/1348 (94%)	-0.34	15 (1%) 76 81	8, 14, 31, 54	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	ILE	4.8
1	C	336	GLN	3.9
1	D	145	ARG	3.6
1	A	183	ARG	3.4
1	C	147	LEU	3.3
1	B	143	GLY	3.2
1	D	143	GLY	3.1
1	C	145	ARG	3.0
1	A	141	ARG	2.7
1	A	140	LYS	2.7
1	A	147	LEU	2.7
1	B	141	ARG	2.6
1	D	147	LEU	2.3
1	C	143	GLY	2.3
1	A	145	ARG	2.1

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

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

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	C	195	24/25	0.95	0.07	9,10,17,19	0
1	LLP	B	195	24/25	0.96	0.07	10,11,15,16	0
1	LLP	A	195	24/25	0.96	0.07	9,10,13,14	0
1	LLP	D	195	24/25	0.96	0.06	9,10,12,13	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

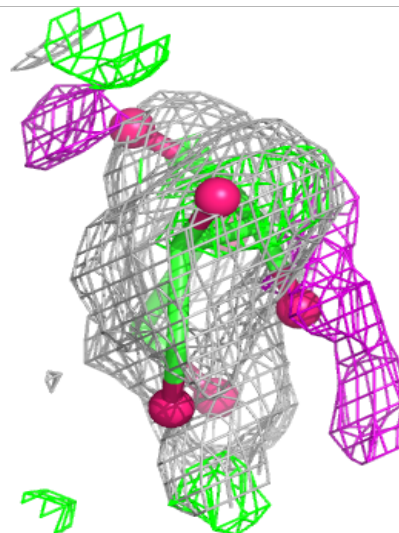
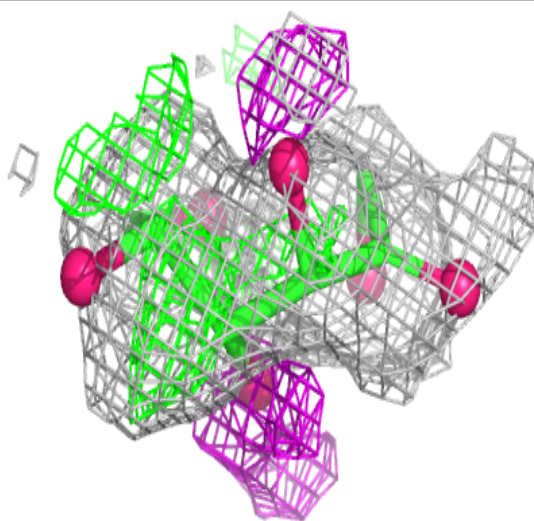
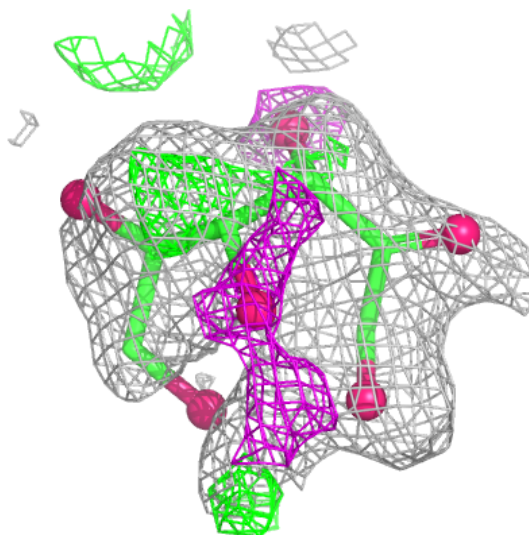
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUD	B	401	12/12	0.81	0.21	43,50,66,66	0
2	FUD	A	401	12/12	0.86	0.18	29,36,47,49	0
2	FUD	C	401	12/12	0.86	0.16	34,44,48,58	0
2	FUD	C	402	12/12	0.88	0.13	32,37,41,46	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.

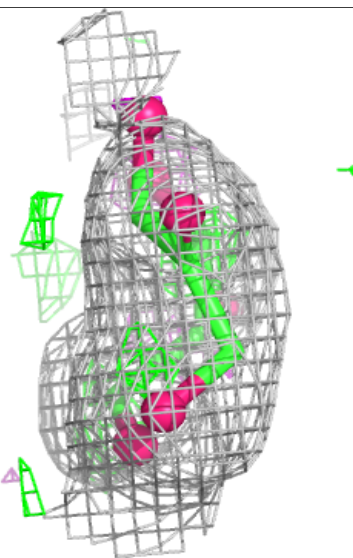
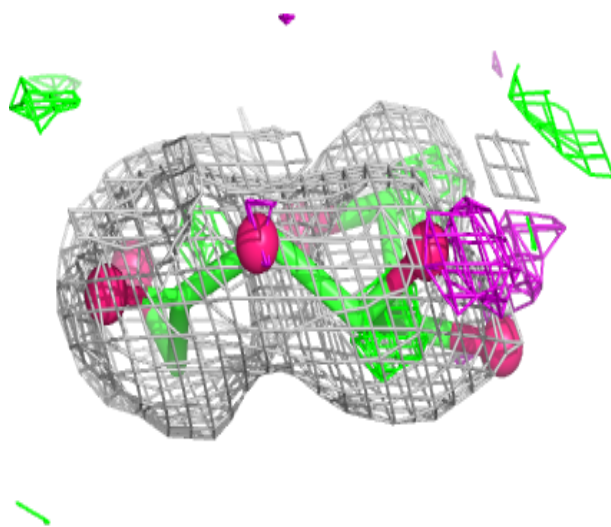
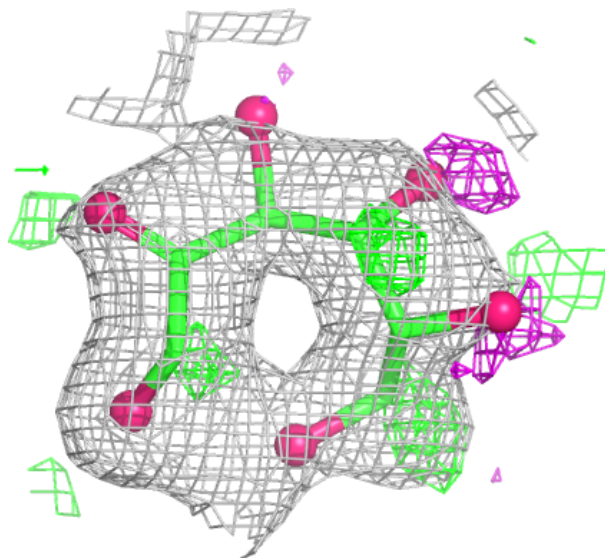
Electron density around FUD B 401:

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



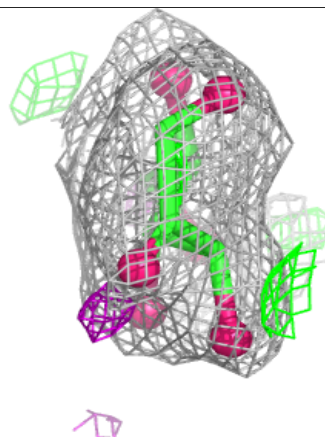
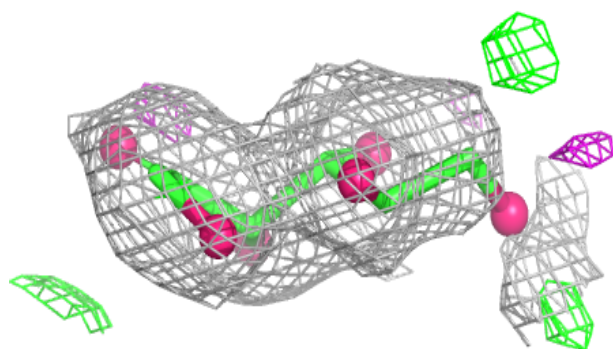
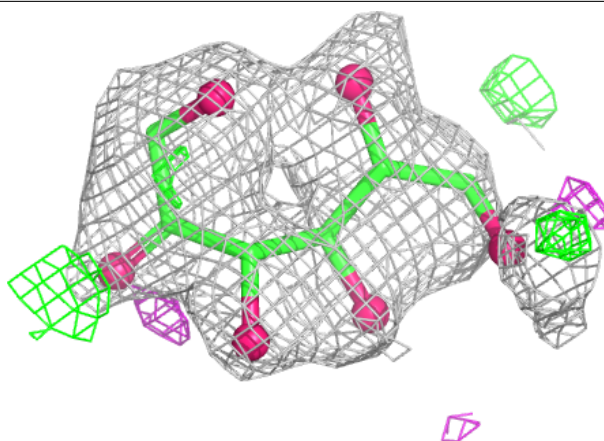
Electron density around FUD A 401:

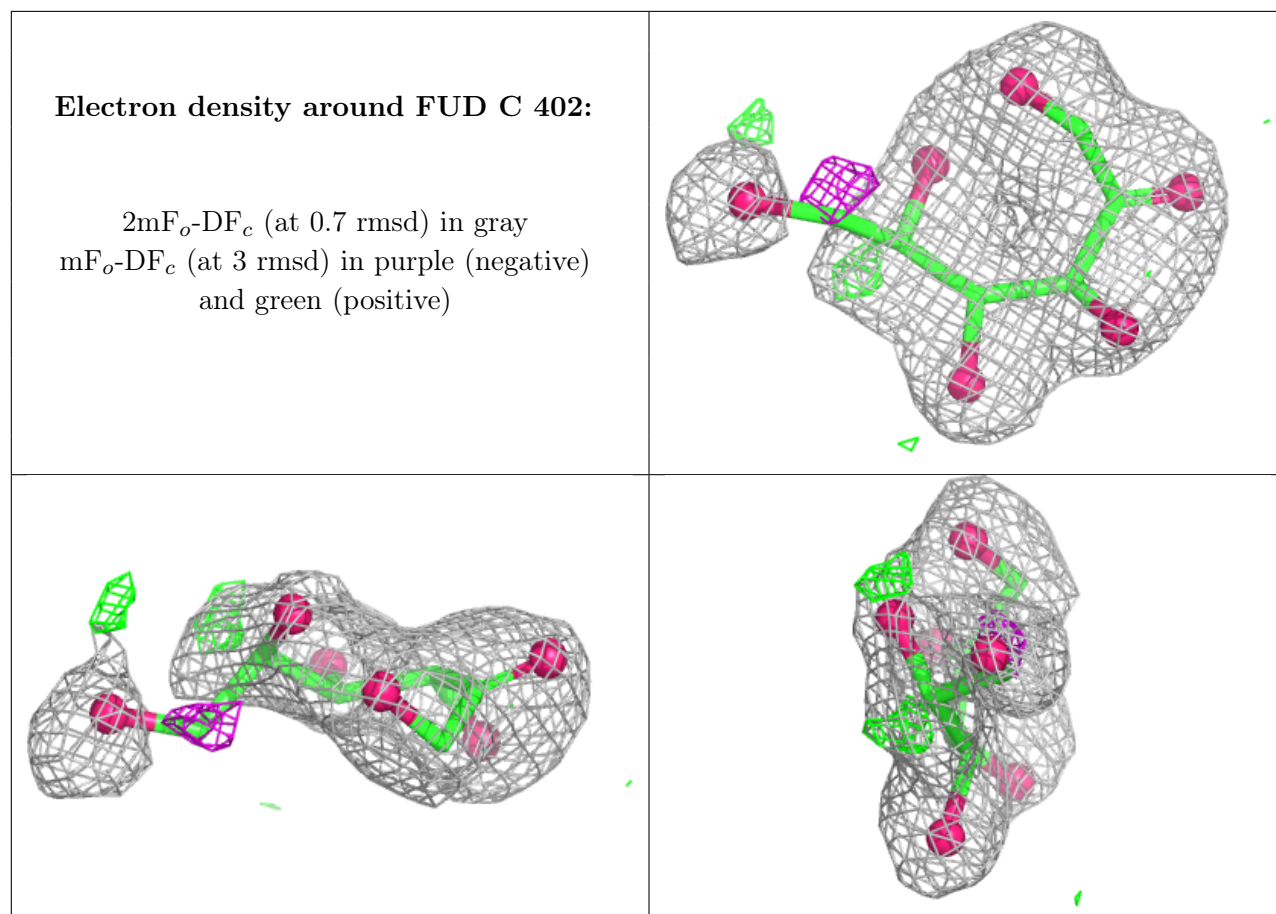
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FUD 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.