



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 10, 2025 – 04:13 pm BST

PDB ID : 9HY7 / pdb\_00009hy7  
Title : AlfB fucosidase in complex with Fucose  
Authors : Marina, A.; Gallego del Sol, F.  
Deposited on : 2025-01-09  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

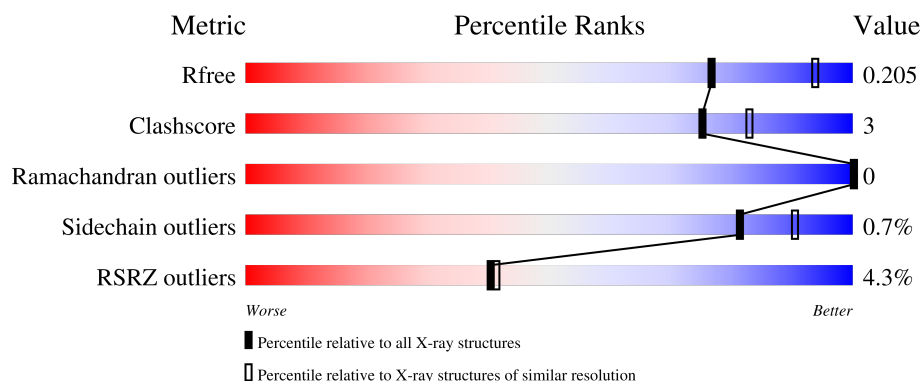
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	414	<div> <div>4%</div> <div>92%</div> <div>7%</div> </div>
1	B	414	<div> <div>5%</div> <div>92%</div> <div>7%</div> </div>
1	C	414	<div> <div>3%</div> <div>88%</div> <div>10%</div> </div>
1	D	414	<div> <div>4%</div> <div>91%</div> <div>7%</div> </div>
1	E	414	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	414	<div><div></div><div>6%</div><div>90%</div><div>9%</div><div></div></div>

## 2 Entry composition [i](#)

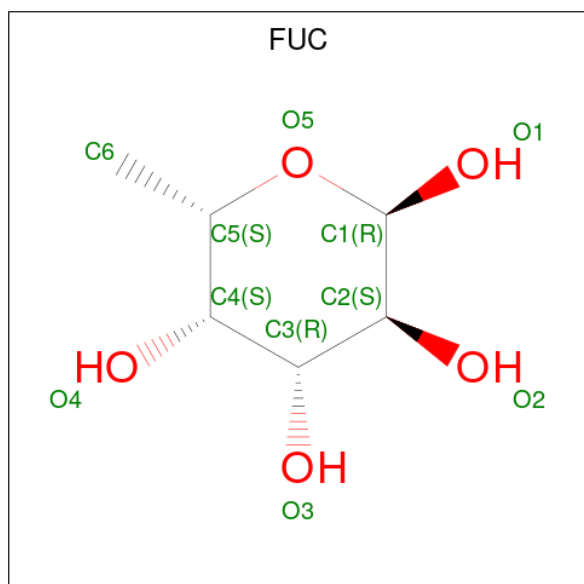
There are 3 unique types of molecules in this entry. The entry contains 21251 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-L-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	1	0
			3320	2133	568	609	10			
1	B	414	Total	C	N	O	S	0	1	0
			3322	2135	569	608	10			
1	C	407	Total	C	N	O	S	0	0	0
			3259	2097	554	599	9			
1	D	409	Total	C	N	O	S	0	0	0
			3275	2106	557	602	10			
1	E	413	Total	C	N	O	S	0	0	0
			3307	2125	566	607	9			
1	F	413	Total	C	N	O	S	0	0	0
			3307	2125	566	607	9			

- Molecule 2 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 6 5	0	0
2	B	1	Total C O 11 6 5	0	0
2	C	1	Total C O 11 6 5	0	0
2	D	1	Total C O 11 6 5	0	0
2	E	1	Total C O 11 6 5	0	0
2	F	1	Total C O 11 6 5	0	0

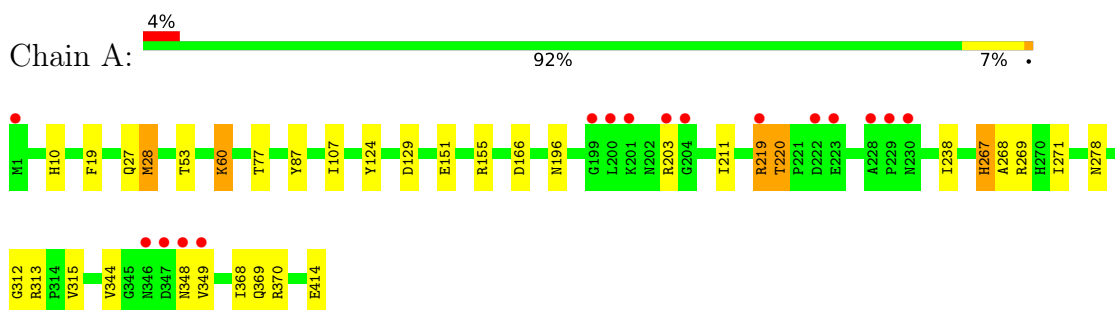
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	255	Total O 255 255	0	0
3	B	241	Total O 241 241	0	0
3	C	283	Total O 283 283	0	0
3	D	218	Total O 218 218	0	0
3	E	233	Total O 233 233	0	0
3	F	165	Total O 165 165	0	0

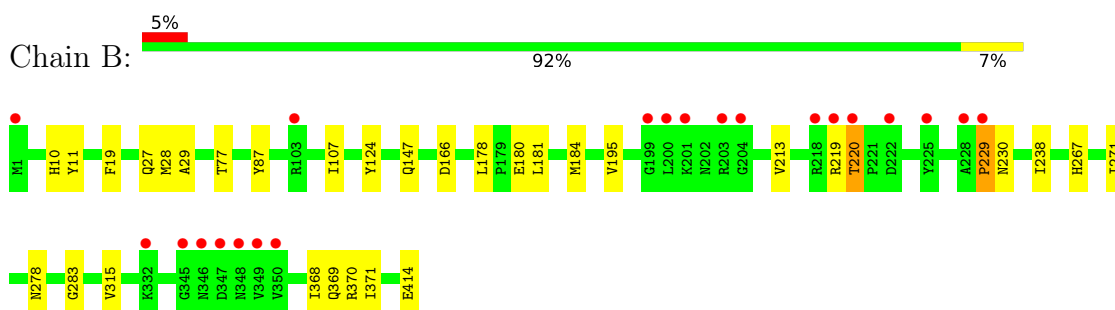
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

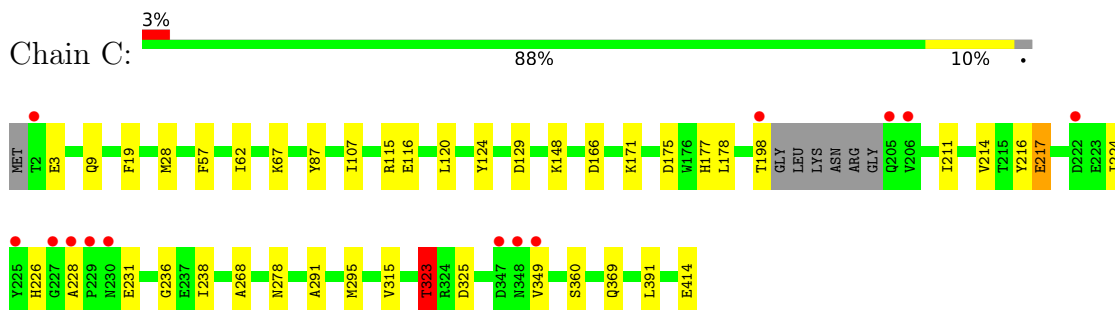
- Molecule 1: Alpha-L-fucosidase



- Molecule 1: Alpha-L-fucosidase

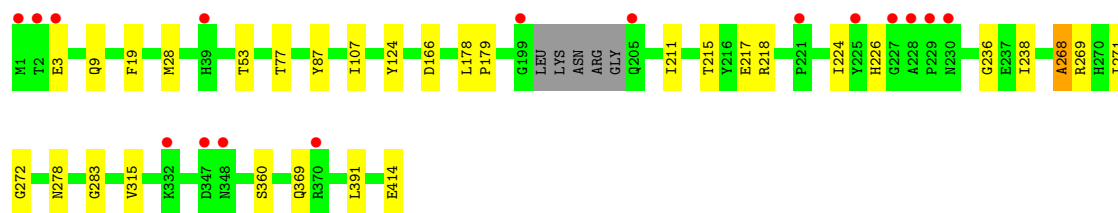


- Molecule 1: Alpha-L-fucosidase

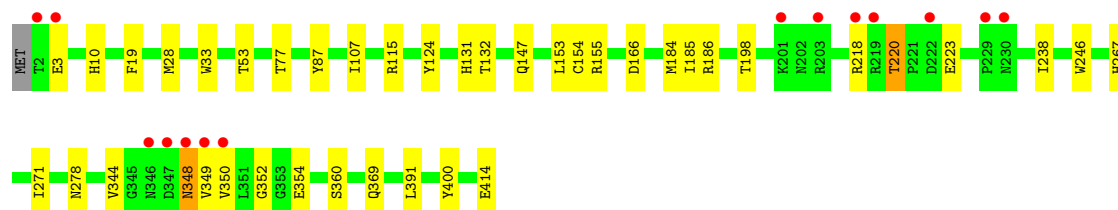
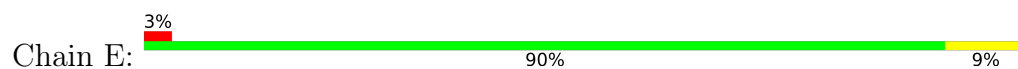


- Molecule 1: Alpha-L-fucosidase

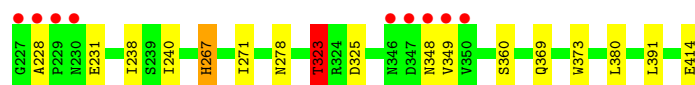
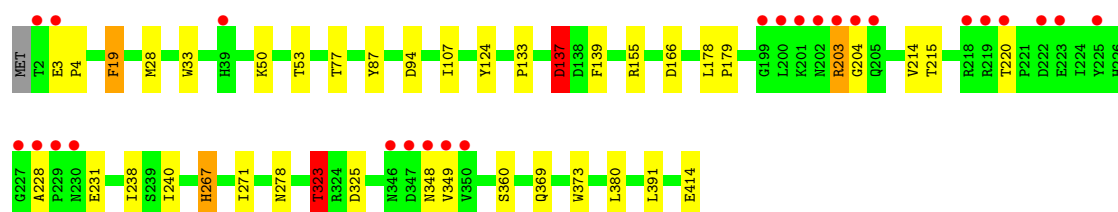
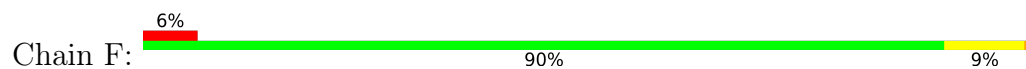




● Molecule 1: Alpha-L-fucosidase



● Molecule 1: Alpha-L-fucosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.18Å 309.56Å 175.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.72 – 2.30 87.72 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (87.72-2.30) 96.8 (87.72-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.177 , 0.205 0.178 , 0.205	Depositor DCC
$R_{free}$ test set	9650 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.85	7/3421 (0.2%)	1.10	9/4666 (0.2%)
1	B	0.87	10/3424 (0.3%)	1.12	7/4670 (0.1%)
1	C	0.85	8/3356 (0.2%)	1.09	5/4580 (0.1%)
1	D	0.77	4/3372 (0.1%)	1.07	7/4600 (0.2%)
1	E	0.78	7/3405 (0.2%)	1.11	13/4645 (0.3%)
1	F	0.69	2/3405 (0.1%)	1.11	10/4645 (0.2%)
All	All	0.81	38/20383 (0.2%)	1.10	51/27806 (0.2%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10[A]	HIS	CA-C	9.96	1.65	1.52
1	B	10[B]	HIS	CA-C	9.96	1.65	1.52
1	B	178	LEU	C-O	-7.10	1.17	1.24
1	C	178	LEU	C-O	-7.09	1.17	1.24
1	C	115	ARG	C-O	-7.00	1.16	1.24
1	A	268	ALA	C-O	-6.99	1.16	1.24
1	C	325	ASP	C-O	-6.78	1.15	1.23
1	C	120	LEU	C-O	-6.74	1.15	1.24
1	A	27	GLN	C-O	-6.69	1.16	1.24
1	A	312	GLY	C-O	-6.45	1.17	1.23
1	D	268	ALA	C-O	-6.43	1.16	1.24
1	C	177	HIS	C-O	-6.35	1.15	1.23
1	E	154	CYS	C-O	-6.31	1.15	1.24
1	A	344	VAL	C-O	-6.22	1.17	1.24
1	A	267	HIS	C-O	-6.14	1.17	1.24
1	D	269	ARG	C-O	-6.14	1.17	1.24
1	D	272	GLY	C-O	-6.13	1.16	1.24
1	C	323	THR	C-O	-6.13	1.16	1.23
1	A	368	ILE	C-O	-6.07	1.17	1.24
1	D	271	ILE	C-O	-6.06	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	185	ILE	C-O	-6.06	1.17	1.24
1	E	344	VAL	C-O	-6.05	1.17	1.24
1	B	11	TYR	C-O	-5.96	1.17	1.24
1	B	27	GLN	C-O	-5.94	1.17	1.24
1	C	116	GLU	C-O	-5.86	1.16	1.24
1	E	153	LEU	C-O	-5.72	1.17	1.24
1	E	186	ARG	C-O	-5.54	1.17	1.24
1	A	313	ARG	C-O	-5.45	1.19	1.24
1	F	139	PHE	C-O	-5.45	1.19	1.24
1	B	181	LEU	C-O	-5.43	1.17	1.24
1	E	132	THR	C-O	-5.40	1.17	1.24
1	F	155	ARG	C-O	-5.27	1.17	1.24
1	B	29	ALA	C-O	-5.21	1.17	1.23
1	B	180	GLU	C-O	-5.11	1.18	1.24
1	B	371	ILE	C-O	-5.04	1.19	1.24
1	B	368	ILE	C-O	-5.02	1.18	1.24
1	C	175	ASP	C-O	-5.02	1.18	1.24
1	E	155	ARG	C-O	-5.01	1.17	1.24

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	203	ARG	N-CA-C	11.55	123.43	111.07
1	E	354	GLU	N-CA-C	9.40	121.52	111.28
1	E	220	THR	CA-C-N	7.09	127.55	120.52
1	E	220	THR	C-N-CA	7.09	127.55	120.52
1	E	352	GLY	N-CA-C	6.62	122.70	114.37
1	F	348	ASN	N-CA-C	6.52	118.47	111.36
1	B	229	PRO	CB-CA-C	6.43	120.07	111.71
1	B	219	ARG	N-CA-C	6.41	119.63	109.50
1	D	3	GLU	N-CA-CB	-6.15	101.98	110.29
1	E	132	THR	CA-C-N	6.14	125.76	119.56
1	E	132	THR	C-N-CA	6.14	125.76	119.56
1	A	348	ASN	N-CA-C	6.14	118.05	111.36
1	E	3	GLU	CB-CA-C	5.91	117.21	108.87
1	E	350	VAL	N-CA-C	5.85	117.18	108.23
1	D	315	VAL	N-CA-CB	-5.83	103.04	111.21
1	E	3	GLU	N-CA-CB	-5.75	102.53	110.29
1	B	220	THR	CA-C-N	5.72	126.98	119.84
1	B	220	THR	C-N-CA	5.72	126.98	119.84
1	F	137	ASP	N-CA-C	5.66	117.53	111.36
1	B	315	VAL	N-CA-CB	-5.66	103.28	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	THR	CB-CA-C	-5.58	100.66	109.42
1	E	53	THR	CA-CB-OG1	-5.58	101.24	109.60
1	D	3	GLU	CB-CA-C	5.57	116.73	108.87
1	A	28	MET	N-CA-C	5.54	118.24	111.82
1	F	50	LYS	CB-CG-CD	5.53	124.03	111.30
1	C	217	GLU	N-CA-CB	-5.48	101.92	109.97
1	F	323	THR	N-CA-CB	-5.46	102.35	111.20
1	D	217	GLU	CA-C-N	5.41	127.52	120.28
1	D	217	GLU	C-N-CA	5.41	127.52	120.28
1	A	60	LYS	CG-CD-CE	5.39	123.70	111.30
1	A	370	ARG	N-CA-C	5.37	117.24	108.76
1	A	315	VAL	N-CA-CB	-5.34	103.73	111.21
1	F	267	HIS	CA-CB-CG	-5.32	108.48	113.80
1	C	148	LYS	CG-CD-CE	5.31	123.51	111.30
1	F	53	THR	CA-CB-OG1	-5.26	101.71	109.60
1	B	370	ARG	N-CA-C	5.26	116.84	108.79
1	F	94	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	129	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	129	ASP	CA-CB-CG	5.22	117.82	112.60
1	D	215	THR	CA-CB-OG1	-5.22	101.77	109.60
1	D	53	THR	CA-CB-OG1	-5.21	101.79	109.60
1	E	131	HIS	N-CA-C	5.20	117.74	111.40
1	C	3	GLU	CB-CA-C	5.19	115.69	109.31
1	E	115	ARG	CA-CB-CG	-5.19	103.73	114.10
1	F	3	GLU	CB-CA-C	5.15	115.84	108.68
1	A	220	THR	CA-C-N	5.09	125.56	120.52
1	A	220	THR	C-N-CA	5.09	125.56	120.52
1	C	315	VAL	N-CA-CB	-5.08	104.09	111.21
1	A	53	THR	CA-CB-OG1	-5.03	102.06	109.60
1	F	19	PHE	CA-CB-CG	5.01	118.81	113.80
1	E	198	THR	CA-CB-OG1	-5.01	102.09	109.60

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	3320	0	3198	18	0
1	B	3322	0	3199	18	0
1	C	3259	0	3124	20	0
1	D	3275	0	3145	14	0
1	E	3307	0	3180	19	0
1	F	3307	0	3180	28	0
2	A	11	0	12	2	0
2	B	11	0	12	1	0
2	C	11	0	12	1	0
2	D	11	0	12	1	0
2	E	11	0	12	1	0
2	F	11	0	12	2	0
3	A	255	0	0	2	0
3	B	241	0	0	1	0
3	C	283	0	0	5	0
3	D	218	0	0	2	0
3	E	233	0	0	2	0
3	F	165	0	0	2	0
All	All	21251	0	19098	114	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 (114) 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:A:166:ASP:OD2	2:A:501:FUC:H1	1.54	1.07
1:C:171:LYS:HE3	3:C:789:HOH:O	1.63	0.96
1:F:220:THR:HG21	1:F:267:HIS:ND1	1.80	0.96
1:E:166:ASP:OD2	2:E:501:FUC:H1	1.64	0.95
1:B:220:THR:HG21	1:B:267:HIS:CD2	2.04	0.92
1:F:166:ASP:OD2	2:F:501:FUC:H1	1.72	0.89
1:D:166:ASP:OD2	2:D:501:FUC:H1	1.73	0.88
1:B:166:ASP:OD2	2:B:501:FUC:H1	1.74	0.88
1:C:228:ALA:HB3	1:C:231:GLU:HG3	1.60	0.82
1:C:166:ASP:OD2	2:C:501:FUC:H1	1.81	0.79
1:A:203:ARG:NH1	1:A:219:ARG:O	2.17	0.75
1:C:217:GLU:HG2	3:C:841:HOH:O	1.87	0.75
1:F:323:THR:HG23	1:F:325:ASP:H	1.52	0.74
1:B:220:THR:HG21	1:B:267:HIS:HD2	1.53	0.72
1:E:220:THR:HG21	1:E:267:HIS:ND1	2.08	0.68
1:F:220:THR:HG21	1:F:267:HIS:CE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:THR:HG21	3:F:690:HOH:O	1.93	0.67
1:C:87:TYR:HB3	1:C:107:ILE:HG12	1.77	0.65
1:A:220:THR:HG21	1:A:267:HIS:CE1	2.31	0.65
1:C:171:LYS:CE	3:C:789:HOH:O	2.34	0.64
1:C:224:ILE:HD11	1:C:226:HIS:CE1	2.34	0.63
1:E:223:GLU:HA	3:E:613:HOH:O	1.99	0.61
1:C:214:VAL:HG23	1:C:216:TYR:CE1	2.35	0.61
1:A:220:THR:HG21	1:A:267:HIS:ND1	2.17	0.60
1:D:28:MET:HA	1:D:28:MET:HE2	1.84	0.59
1:D:224:ILE:HD13	1:D:236:GLY:HA3	1.85	0.59
1:A:238:ILE:HD11	1:A:271:ILE:HD11	1.85	0.59
1:D:87:TYR:HB3	1:D:107:ILE:HG12	1.85	0.58
1:F:238:ILE:HD11	1:F:271:ILE:HD11	1.86	0.58
1:F:228:ALA:HB3	1:F:231:GLU:HG3	1.87	0.57
1:A:87:TYR:HB3	1:A:107:ILE:HG12	1.87	0.56
1:C:28:MET:HA	1:C:28:MET:HE2	1.86	0.56
1:B:87:TYR:HB3	1:B:107:ILE:HG12	1.86	0.56
1:C:224:ILE:HD13	1:C:236:GLY:HA3	1.88	0.56
1:F:28:MET:HA	1:F:28:MET:HE2	1.87	0.56
1:F:323:THR:CG2	1:F:325:ASP:H	2.17	0.56
1:E:28:MET:HA	1:E:28:MET:HE2	1.88	0.55
1:C:323:THR:HG21	3:C:713:HOH:O	2.06	0.55
1:E:87:TYR:HB3	1:E:107:ILE:HG12	1.89	0.55
1:F:87:TYR:HB3	1:F:107:ILE:HG12	1.88	0.54
1:F:203:ARG:O	1:F:215:THR:O	2.26	0.54
1:E:238:ILE:HD11	1:E:271:ILE:HD11	1.89	0.53
1:B:238:ILE:HD11	1:B:271:ILE:HD11	1.90	0.53
1:F:204:GLY:HA2	1:F:214:VAL:CG1	2.38	0.53
1:A:10:HIS:CE1	3:A:719:HOH:O	2.62	0.53
1:D:218:ARG:NH1	3:D:601:HOH:O	2.27	0.53
1:E:147:GLN:HG3	1:E:184:MET:CE	2.41	0.51
1:E:220:THR:HG21	1:E:267:HIS:CE1	2.45	0.51
1:D:238:ILE:HD11	1:D:268:ALA:HB2	1.92	0.50
1:A:10:HIS:HB2	3:A:820:HOH:O	2.11	0.50
1:A:166:ASP:CG	2:A:501:FUC:H1	2.32	0.50
1:E:33:TRP:CZ3	1:F:349:VAL:HG11	2.47	0.50
1:F:204:GLY:HA2	1:F:214:VAL:HG13	1.92	0.49
1:D:369:GLN:HB2	1:D:414:GLU:HG2	1.95	0.48
1:C:238:ILE:HD11	1:C:268:ALA:HB2	1.94	0.48
1:E:19:PHE:HB3	1:E:278:ASN:HA	1.95	0.48
1:E:369:GLN:HB2	1:E:414:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:ARG:HD3	1:E:246:TRP:CZ2	2.49	0.47
1:B:220:THR:HG23	1:B:238:ILE:HD13	1.97	0.47
1:C:369:GLN:HB2	1:C:414:GLU:HG2	1.97	0.47
1:C:19:PHE:HB3	1:C:278:ASN:HA	1.97	0.47
1:A:369:GLN:HB2	1:A:414:GLU:HG2	1.95	0.47
1:F:369:GLN:HB2	1:F:414:GLU:HG2	1.97	0.47
1:F:133:PRO:O	1:F:137:ASP:HB2	2.15	0.46
1:A:19:PHE:HB3	1:A:278:ASN:HA	1.97	0.46
1:A:28:MET:HA	1:A:28:MET:HE2	1.97	0.46
1:B:28:MET:HA	1:B:28:MET:HE2	1.96	0.46
1:B:369:GLN:HB2	1:B:414:GLU:HG2	1.95	0.46
1:D:283:GLY:HA3	3:D:801:HOH:O	2.15	0.46
1:D:19:PHE:HB3	1:D:278:ASN:HA	1.96	0.46
1:C:57:PHE:CE1	1:C:62:ILE:HD12	2.51	0.46
1:A:196:ASN:HB2	1:A:211:ILE:HD11	1.98	0.46
1:B:229:PRO:O	1:B:230:ASN:HB2	2.15	0.46
1:E:10:HIS:CE1	3:E:628:HOH:O	2.69	0.46
1:F:19:PHE:HB3	1:F:278:ASN:HA	1.97	0.46
1:B:147:GLN:HG3	1:B:184:MET:HE2	1.98	0.45
1:E:33:TRP:CH2	1:F:349:VAL:HG11	2.51	0.45
1:B:283:GLY:HA3	3:B:816:HOH:O	2.16	0.45
1:F:220:THR:CG2	1:F:267:HIS:CE1	2.99	0.45
1:B:19:PHE:HB3	1:B:278:ASN:HA	1.97	0.45
1:F:4:PRO:HA	3:F:621:HOH:O	2.17	0.45
1:B:220:THR:HG23	1:B:238:ILE:CD1	2.47	0.45
1:A:151:GLU:OE2	1:A:155:ARG:NH1	2.48	0.44
1:D:224:ILE:HD11	1:D:226:HIS:CE1	2.52	0.43
1:C:291:ALA:O	1:C:295:MET:HG2	2.19	0.43
1:C:214:VAL:HG22	3:C:606:HOH:O	2.19	0.43
1:E:77:THR:HA	1:E:124:TYR:HB3	2.00	0.43
1:F:203:ARG:HD3	1:F:203:ARG:HA	1.60	0.43
1:F:77:THR:HA	1:F:124:TYR:HB3	2.01	0.43
1:B:184:MET:HE3	1:B:184:MET:HB3	1.97	0.42
1:A:124:TYR:C	1:A:124:TYR:CD1	2.97	0.42
1:E:348:ASN:OD1	1:E:348:ASN:N	2.52	0.42
1:A:349:VAL:O	1:A:349:VAL:HG13	2.18	0.42
1:E:124:TYR:CD1	1:E:124:TYR:C	2.98	0.42
1:E:400:TYR:CZ	1:F:33:TRP:HB2	2.55	0.42
1:B:124:TYR:C	1:B:124:TYR:CD1	2.98	0.42
1:D:77:THR:HA	1:D:124:TYR:HB3	2.02	0.42
1:B:220:THR:HG21	1:B:267:HIS:NE2	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:TYR:C	1:F:124:TYR:CD1	2.98	0.42
1:B:77:THR:HA	1:B:124:TYR:HB3	2.01	0.41
1:C:360:SER:HA	1:C:391:LEU:O	2.20	0.41
1:D:178:LEU:N	1:D:179:PRO:CD	2.83	0.41
1:F:178:LEU:N	1:F:179:PRO:CD	2.83	0.41
1:C:124:TYR:CD1	1:C:124:TYR:C	2.99	0.41
1:F:166:ASP:CG	2:F:501:FUC:H1	2.41	0.41
1:F:373:TRP:NE1	1:F:380:LEU:HD21	2.36	0.41
1:B:195:VAL:HG22	1:B:213:VAL:HB	2.03	0.41
1:C:67:LYS:HA	1:C:67:LYS:HD2	1.81	0.40
1:A:77:THR:HA	1:A:124:TYR:HB3	2.03	0.40
1:A:269:ARG:HA	1:A:269:ARG:HD2	1.93	0.40
1:D:124:TYR:CD1	1:D:124:TYR:C	2.98	0.40
1:F:360:SER:HA	1:F:391:LEU:O	2.22	0.40
1:D:360:SER:HA	1:D:391:LEU:O	2.22	0.40
1:E:360:SER:HA	1:E:391:LEU:O	2.22	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	413/414 (100%)	403 (98%)	10 (2%)	0	100	100
1	B	413/414 (100%)	403 (98%)	10 (2%)	0	100	100
1	C	403/414 (97%)	393 (98%)	10 (2%)	0	100	100
1	D	405/414 (98%)	395 (98%)	10 (2%)	0	100	100
1	E	411/414 (99%)	401 (98%)	10 (2%)	0	100	100
1	F	411/414 (99%)	398 (97%)	13 (3%)	0	100	100
All	All	2456/2484 (99%)	2393 (97%)	63 (3%)	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	347/346 (100%)	345 (99%)	2 (1%)	84	92
1	B	347/346 (100%)	347 (100%)	0	100	100
1	C	340/346 (98%)	335 (98%)	5 (2%)	60	76
1	D	342/346 (99%)	340 (99%)	2 (1%)	84	92
1	E	345/346 (100%)	343 (99%)	2 (1%)	84	92
1	F	345/346 (100%)	342 (99%)	3 (1%)	75	87
All	All	2066/2076 (100%)	2052 (99%)	14 (1%)	81	90

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

Mol	Chain	Res	Type
1	A	60	LYS
1	A	219	ARG
1	C	9	GLN
1	C	198	THR
1	C	211	ILE
1	C	323	THR
1	C	349	VAL
1	D	9	GLN
1	D	211	ILE
1	E	348	ASN
1	E	349	VAL
1	F	137	ASP
1	F	240	ILE
1	F	323	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	27	GLN
1	A	196	ASN
1	A	410	GLN
1	B	177	HIS
1	B	187	HIS
1	B	230	ASN
1	B	270	HIS
1	B	348	ASN
1	B	410	GLN
1	C	64	HIS
1	C	147	GLN
1	C	170	ASN
1	D	170	ASN
1	D	270	HIS
1	D	410	GLN
1	E	27	GLN
1	E	196	ASN
1	E	270	HIS
1	E	410	GLN
1	F	270	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	FUC	B	501	-	11,11,11	1.06	0	15,16,16	1.95	4 (26%)
2	FUC	C	501	-	11,11,11	0.93	0	15,16,16	2.09	5 (33%)
2	FUC	F	501	-	11,11,11	1.03	0	15,16,16	1.68	2 (13%)
2	FUC	A	501	-	11,11,11	1.16	1 (9%)	15,16,16	1.57	4 (26%)
2	FUC	E	501	-	11,11,11	1.17	1 (9%)	15,16,16	2.00	5 (33%)
2	FUC	D	501	-	11,11,11	1.07	1 (9%)	15,16,16	1.86	4 (26%)

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	FUC	B	501	-	-	-	0/1/1/1
2	FUC	C	501	-	-	-	0/1/1/1
2	FUC	F	501	-	-	-	0/1/1/1
2	FUC	A	501	-	-	-	0/1/1/1
2	FUC	E	501	-	-	-	0/1/1/1
2	FUC	D	501	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	FUC	O5-C5	-2.14	1.39	1.44
2	A	501	FUC	O2-C2	-2.06	1.38	1.43
2	D	501	FUC	O5-C5	-2.01	1.40	1.44

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	FUC	O5-C1-C2	5.16	119.48	110.28
2	B	501	FUC	O5-C1-C2	4.68	118.63	110.28
2	F	501	FUC	O5-C1-C2	4.56	118.42	110.28
2	C	501	FUC	C4-C3-C2	-3.88	104.05	110.82
2	D	501	FUC	O5-C1-C2	3.82	117.11	110.28
2	C	501	FUC	O5-C1-C2	3.60	116.72	110.28
2	C	501	FUC	O5-C5-C4	3.54	115.87	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FUC	O5-C5-C4	3.43	115.68	109.52
2	A	501	FUC	O5-C1-C2	3.33	116.22	110.28
2	D	501	FUC	O3-C3-C4	-2.94	103.55	110.35
2	E	501	FUC	O5-C5-C4	2.54	114.08	109.52
2	F	501	FUC	O5-C5-C4	2.53	114.06	109.52
2	C	501	FUC	C3-C4-C5	-2.50	105.88	109.77
2	D	501	FUC	C3-C4-C5	-2.46	105.94	109.77
2	B	501	FUC	C3-C4-C5	-2.42	106.00	109.77
2	A	501	FUC	O5-C5-C4	2.41	113.84	109.52
2	A	501	FUC	O1-C1-C2	2.40	115.79	109.03
2	C	501	FUC	C1-C2-C3	2.39	115.27	110.31
2	E	501	FUC	O2-C2-C3	2.36	115.80	110.35
2	E	501	FUC	O1-C1-C2	2.34	115.61	109.03
2	D	501	FUC	C4-C3-C2	-2.26	106.89	110.82
2	A	501	FUC	C3-C4-C5	-2.16	106.40	109.77
2	B	501	FUC	C1-C2-C3	2.15	114.78	110.31
2	E	501	FUC	O4-C4-C3	2.02	115.01	110.35

There are no chirality outliers.

There are no torsion outliers.

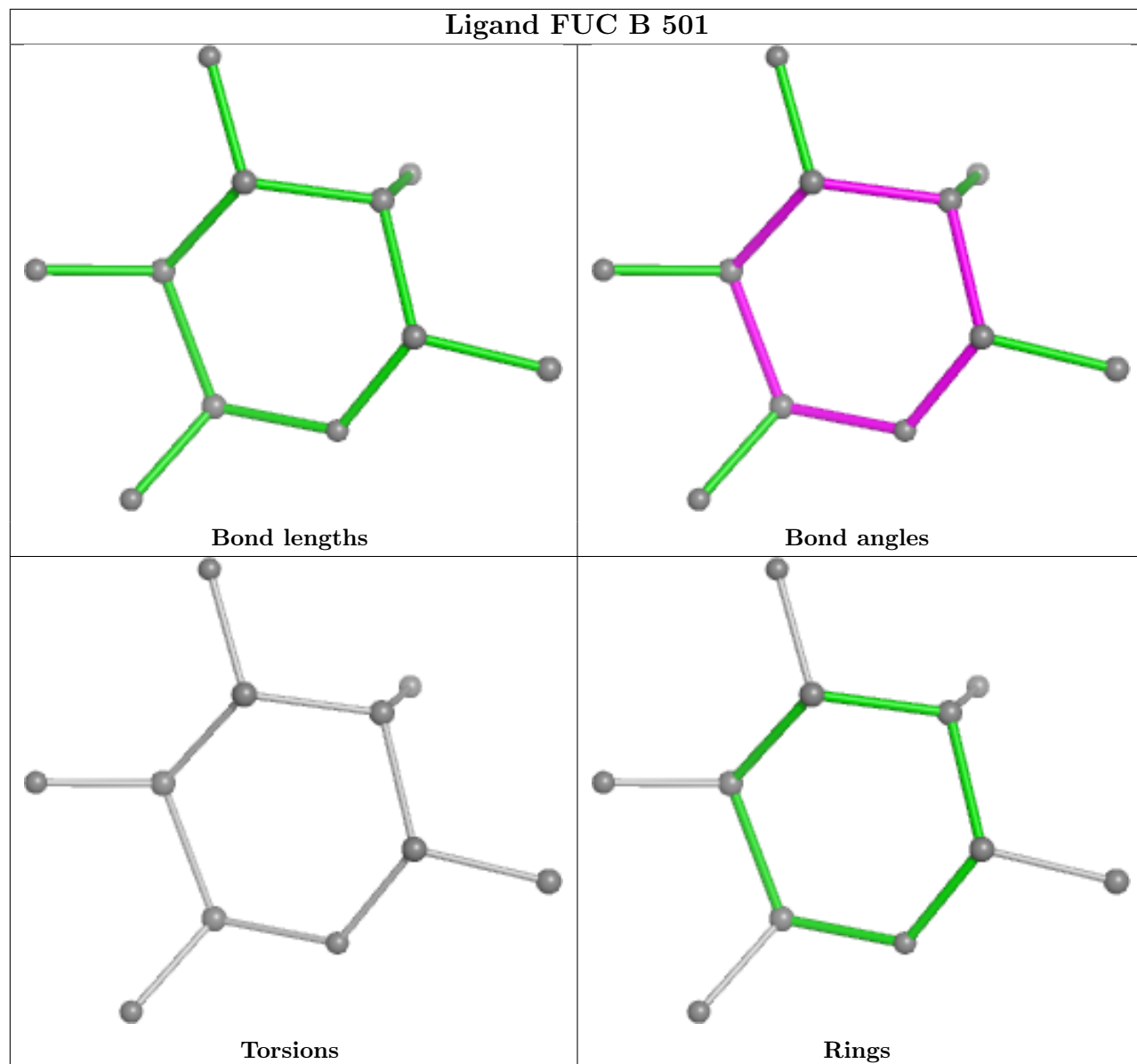
There are no ring outliers.

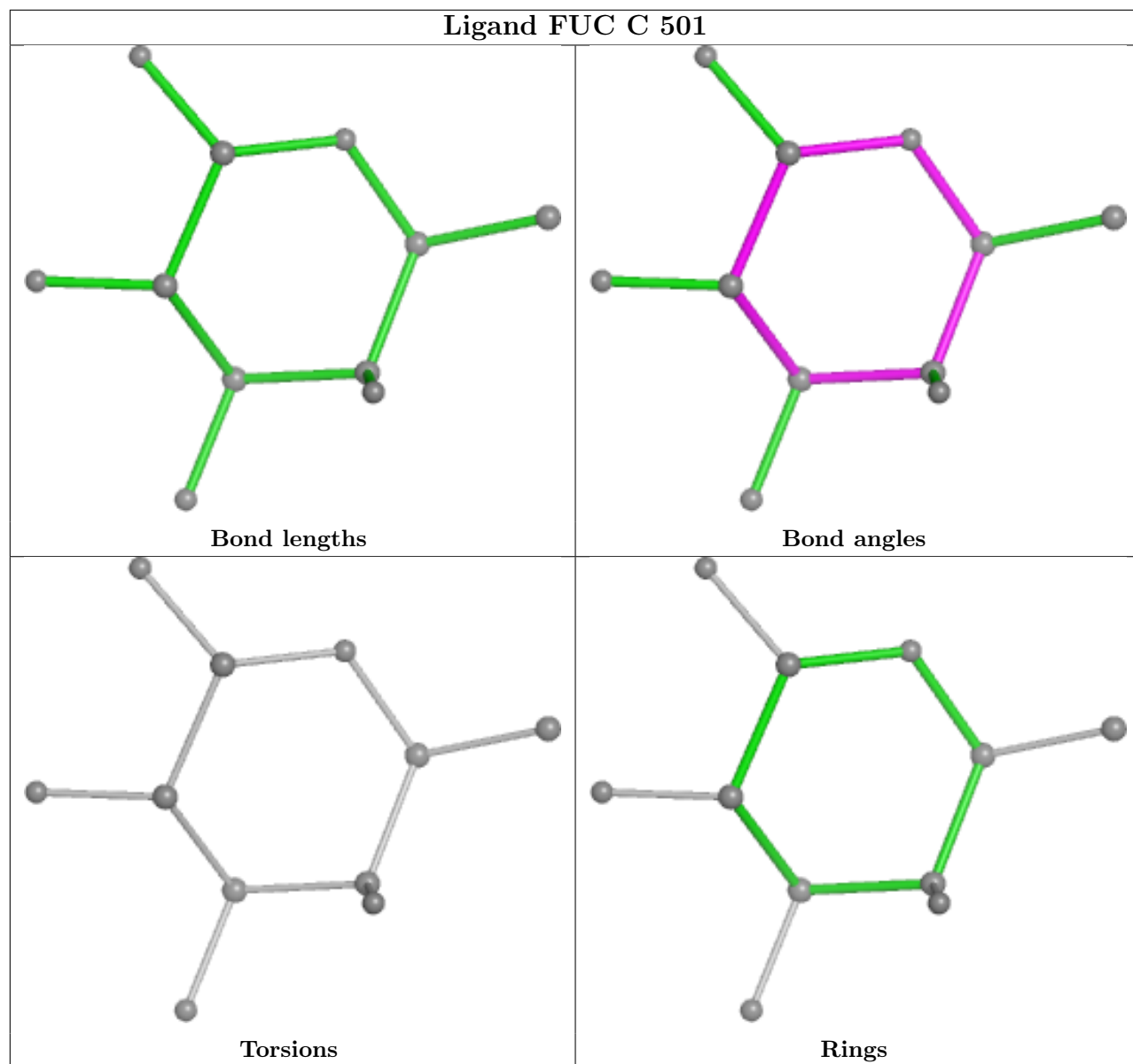
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FUC	1	0
2	C	501	FUC	1	0
2	F	501	FUC	2	0
2	A	501	FUC	2	0
2	E	501	FUC	1	0
2	D	501	FUC	1	0

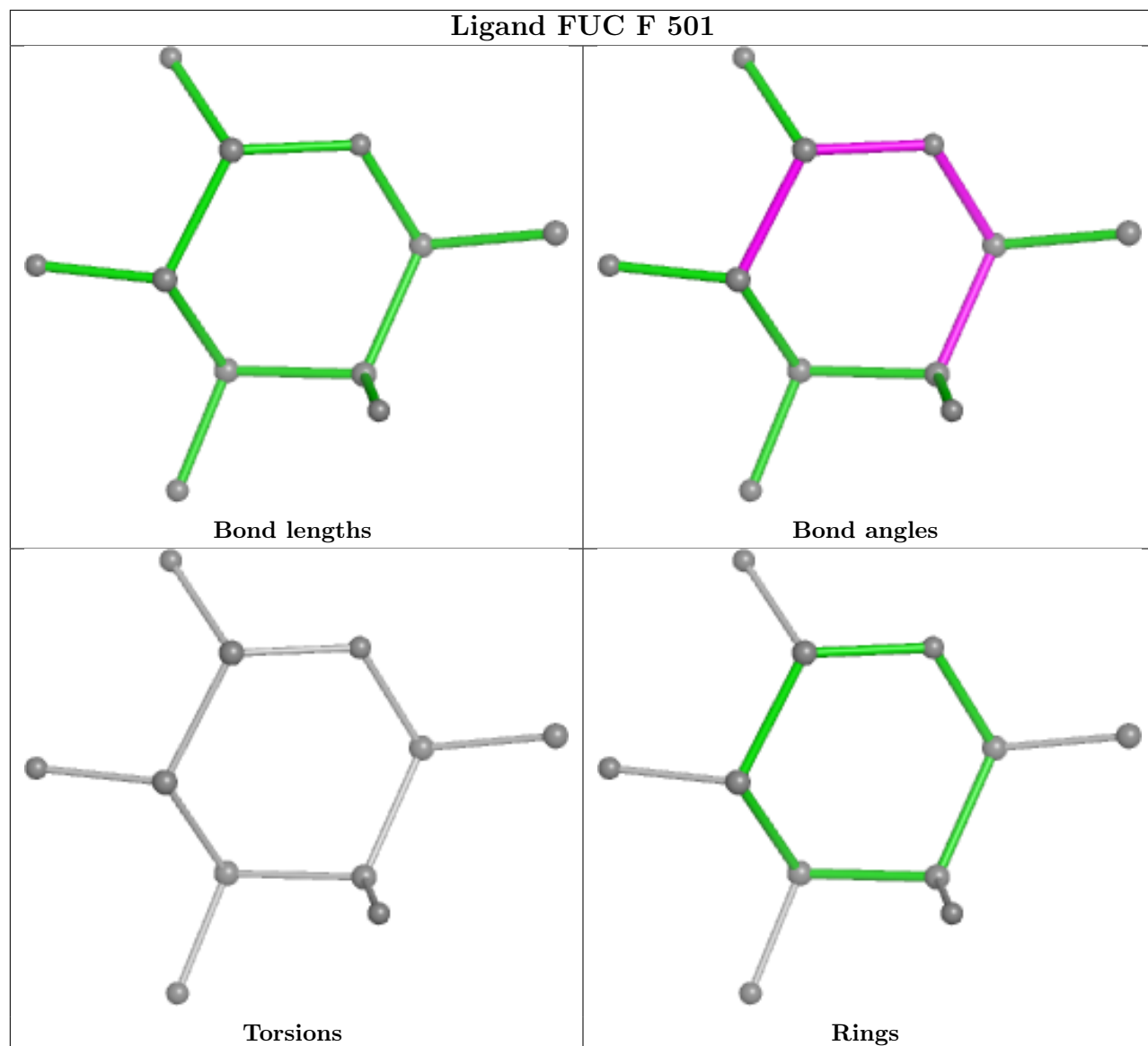
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

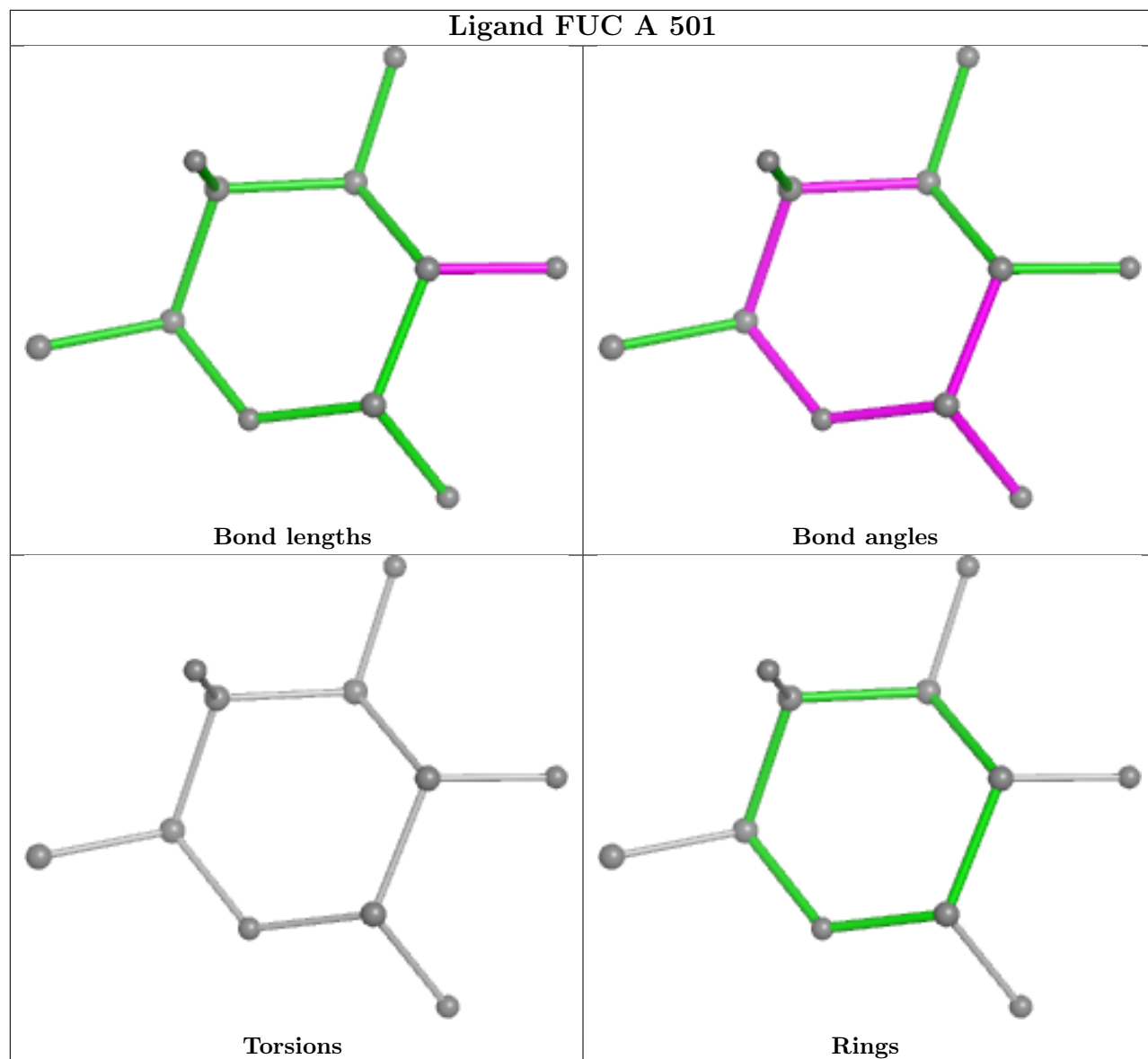
equivalents in the CSD to analyse the geometry.



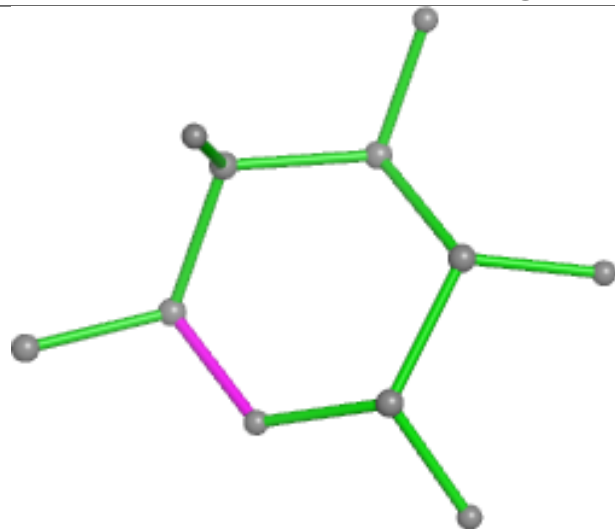


## Ligand FUC F 501

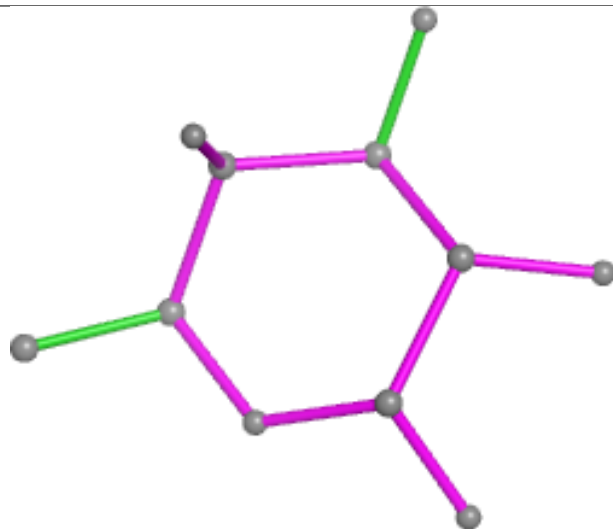




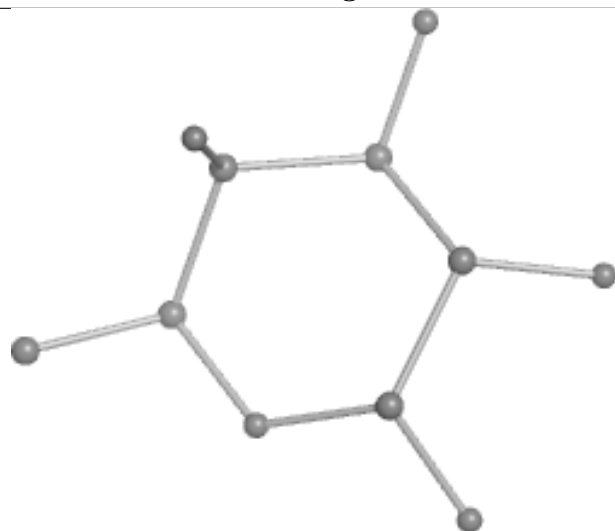
## Ligand FUC E 501



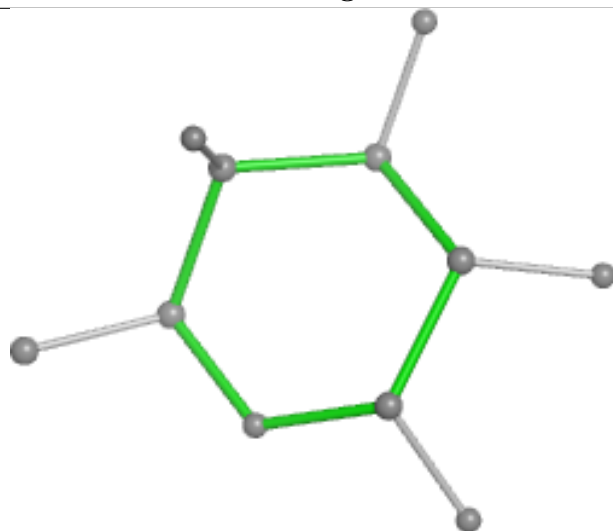
Bond lengths



Bond angles

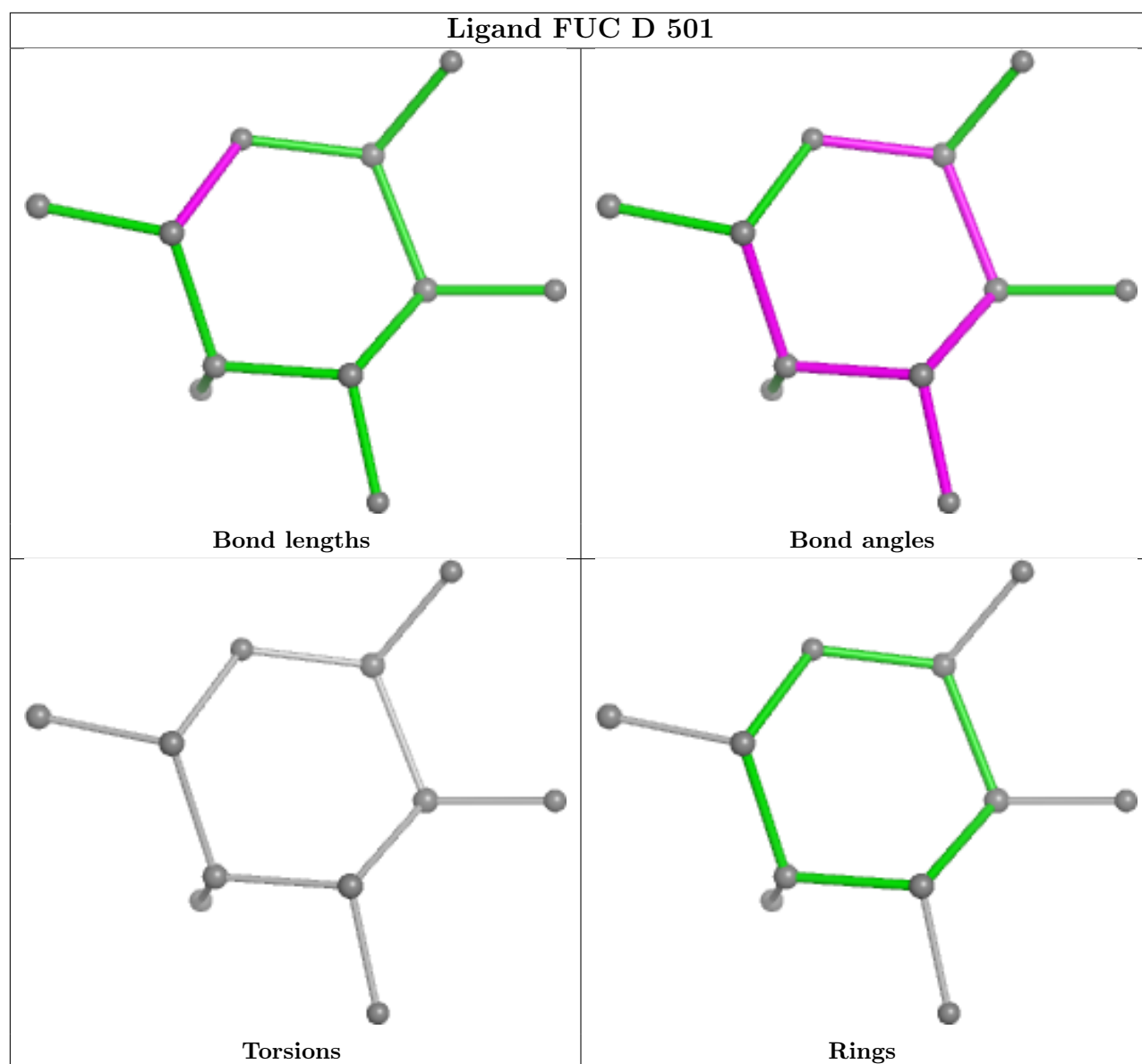


Torsions



Rings





## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	414/414 (100%)	-0.50	16 (3%)	44	45	8, 18, 52, 117	1 (0%)
1	B	414/414 (100%)	-0.43	21 (5%)	34	35	8, 16, 54, 105	1 (0%)
1	C	407/414 (98%)	-0.56	13 (3%)	50	52	9, 16, 50, 114	0
1	D	409/414 (98%)	-0.29	16 (3%)	44	45	10, 21, 56, 118	0
1	E	413/414 (99%)	-0.41	14 (3%)	48	50	12, 20, 54, 121	0
1	F	413/414 (99%)	-0.23	25 (6%)	28	30	11, 23, 66, 102	0
All	All	2470/2484 (99%)	-0.40	105 (4%)	40	41	8, 19, 56, 121	2 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	229	PRO	7.0
1	B	347	ASP	7.0
1	D	1	MET	6.8
1	C	229	PRO	6.5
1	E	2	THR	6.5
1	F	347	ASP	6.3
1	F	222	ASP	6.2
1	C	228	ALA	6.0
1	D	225	TYR	5.9
1	C	225	TYR	5.9
1	A	1	MET	5.9
1	B	1	MET	5.5
1	A	347	ASP	5.2
1	E	347	ASP	5.1
1	C	348	ASN	5.1
1	F	203	ARG	5.1
1	E	219	ARG	4.9
1	B	349	VAL	4.7
1	B	346	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	4.7
1	C	205	GLN	4.7
1	D	205	GLN	4.7
1	F	2	THR	4.6
1	C	227	GLY	4.5
1	F	204	GLY	4.5
1	B	218	ARG	4.4
1	A	348	ASN	4.4
1	A	200	LEU	4.3
1	F	219	ARG	4.3
1	F	200	LEU	4.2
1	F	348	ASN	4.2
1	D	199	GLY	4.2
1	E	350	VAL	4.1
1	D	227	GLY	4.0
1	D	230	ASN	4.0
1	F	346	ASN	4.0
1	D	228	ALA	3.9
1	F	230	ASN	3.9
1	D	347	ASP	3.9
1	A	346	ASN	3.8
1	B	222	ASP	3.8
1	F	218	ARG	3.8
1	B	204	GLY	3.8
1	B	229	PRO	3.7
1	B	201	LYS	3.7
1	C	347	ASP	3.7
1	F	223	GLU	3.6
1	A	229	PRO	3.6
1	C	2	THR	3.5
1	D	2	THR	3.5
1	F	349	VAL	3.5
1	B	219	ARG	3.5
1	F	202	ASN	3.4
1	C	198	THR	3.4
1	E	346	ASN	3.4
1	E	203	ARG	3.3
1	F	228	ALA	3.3
1	E	348	ASN	3.3
1	F	201	LYS	3.3
1	F	350	VAL	3.3
1	A	230	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	349	VAL	3.2
1	C	230	ASN	3.2
1	B	220	THR	3.2
1	E	218	ARG	3.2
1	F	229	PRO	3.1
1	C	206	VAL	3.1
1	A	199	GLY	3.0
1	E	3	GLU	3.0
1	F	225	TYR	3.0
1	F	199	GLY	3.0
1	B	348	ASN	3.0
1	A	203	ARG	3.0
1	E	230	ASN	3.0
1	B	203	ARG	3.0
1	B	199	GLY	2.9
1	E	201	LYS	2.9
1	C	222	ASP	2.7
1	E	222	ASP	2.7
1	B	350	VAL	2.7
1	F	3	GLU	2.7
1	E	229	PRO	2.6
1	A	219	ARG	2.6
1	A	222	ASP	2.6
1	F	205	GLN	2.6
1	D	348	ASN	2.6
1	A	201	LYS	2.6
1	F	39	HIS	2.4
1	D	370	ARG	2.3
1	A	349	VAL	2.2
1	C	349	VAL	2.2
1	A	204	GLY	2.2
1	F	227	GLY	2.2
1	D	39	HIS	2.1
1	A	228	ALA	2.1
1	B	228	ALA	2.1
1	A	223	GLU	2.1
1	F	220	THR	2.1
1	B	225	TYR	2.1
1	B	345	GLY	2.1
1	D	3	GLU	2.0
1	D	332	LYS	2.0
1	B	103	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	332	LYS	2.0
1	D	221	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

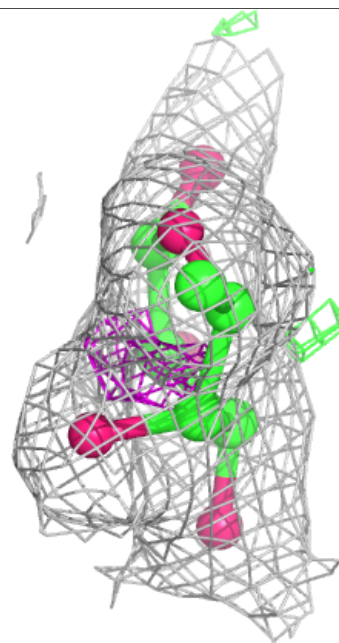
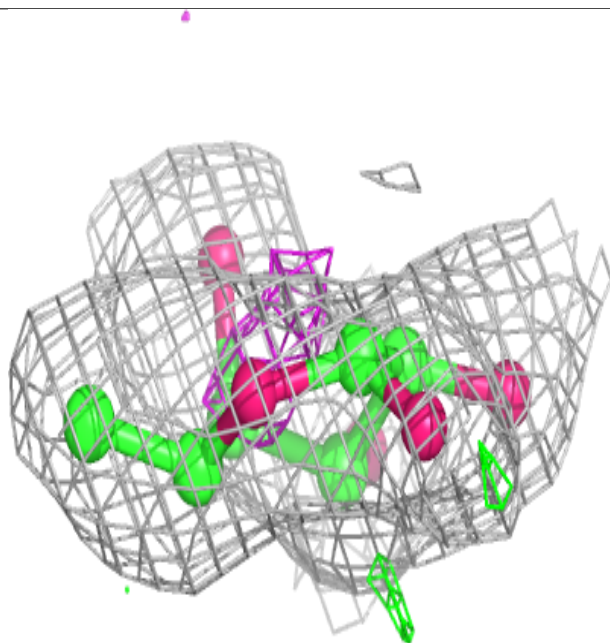
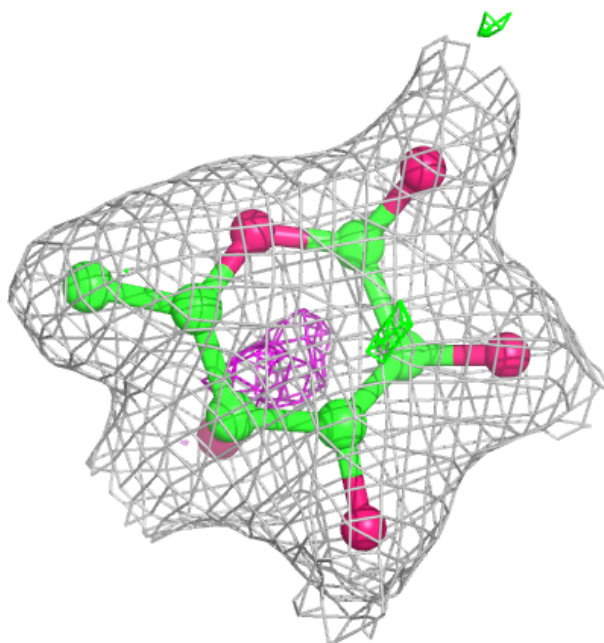
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FUC	D	501	11/11	0.93	0.10	19,22,27,27	0
2	FUC	F	501	11/11	0.93	0.09	22,27,32,39	0
2	FUC	A	501	11/11	0.94	0.07	17,21,26,27	0
2	FUC	C	501	11/11	0.94	0.08	17,22,28,30	0
2	FUC	E	501	11/11	0.96	0.07	16,18,23,23	0
2	FUC	B	501	11/11	0.97	0.06	12,15,20,20	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.

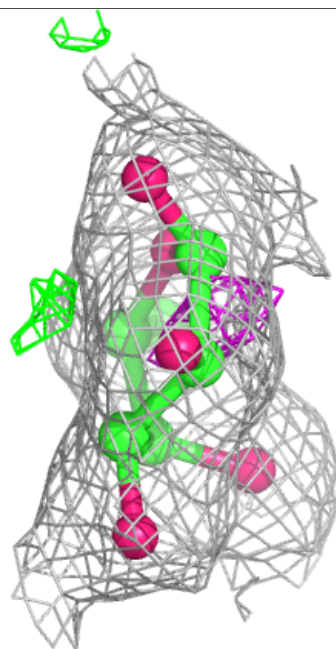
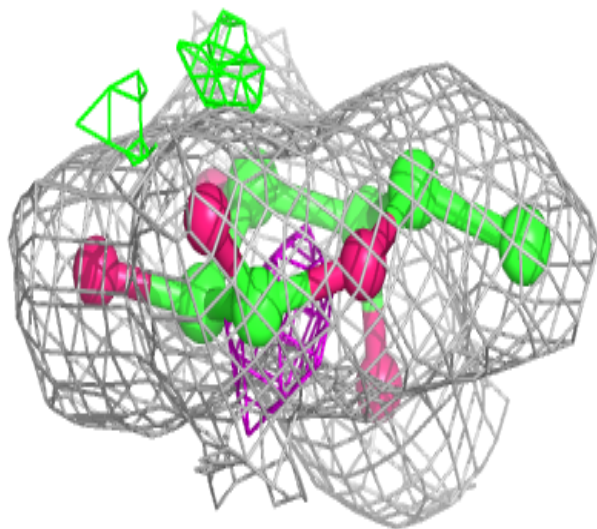
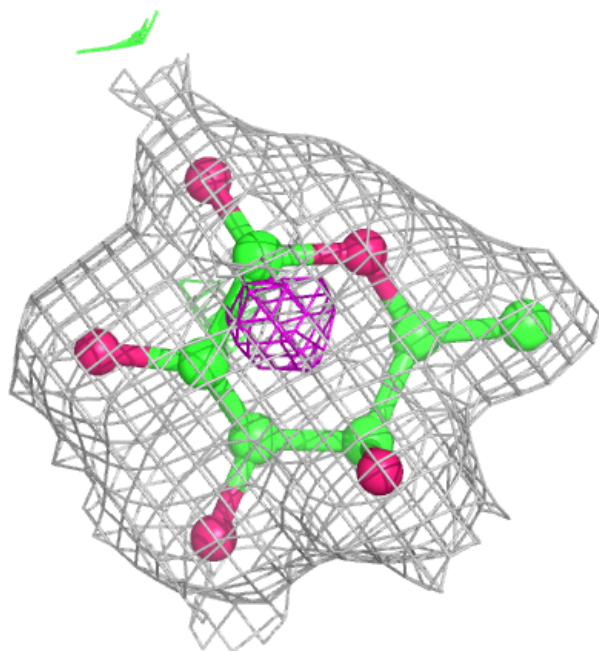
**Electron density around FUC D 501:**

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



**Electron density around FUC F 501:**

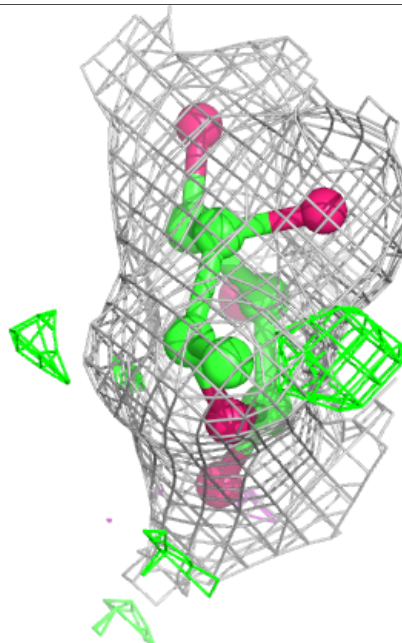
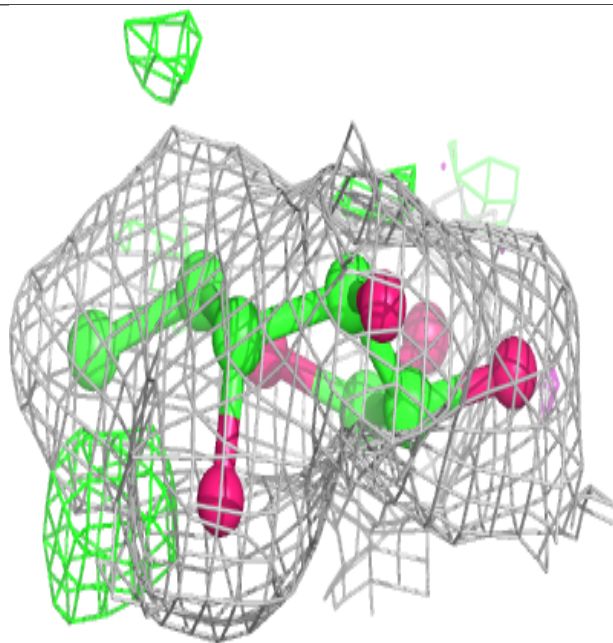
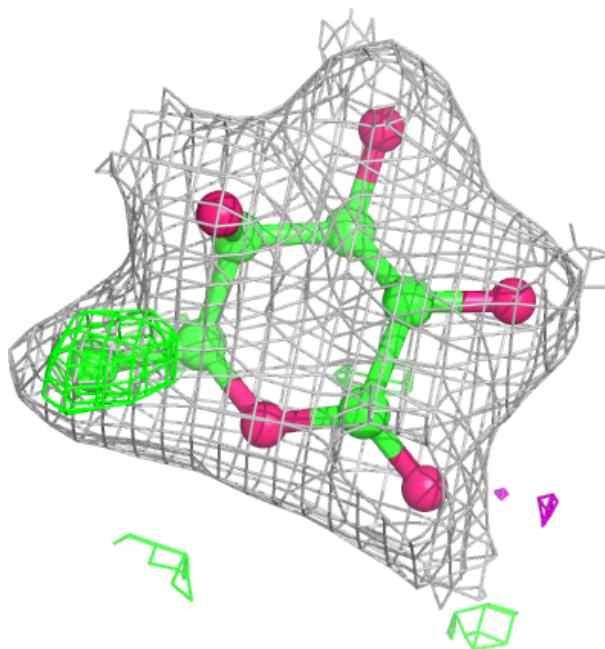
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FUC A 501:**

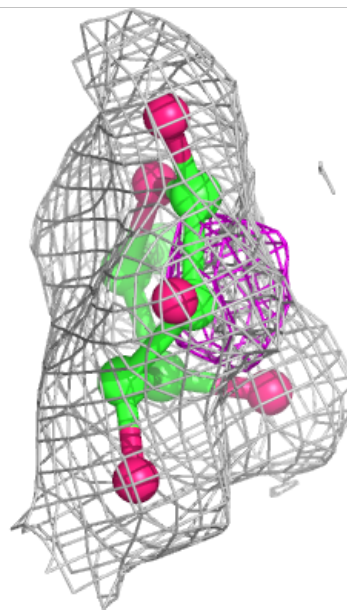
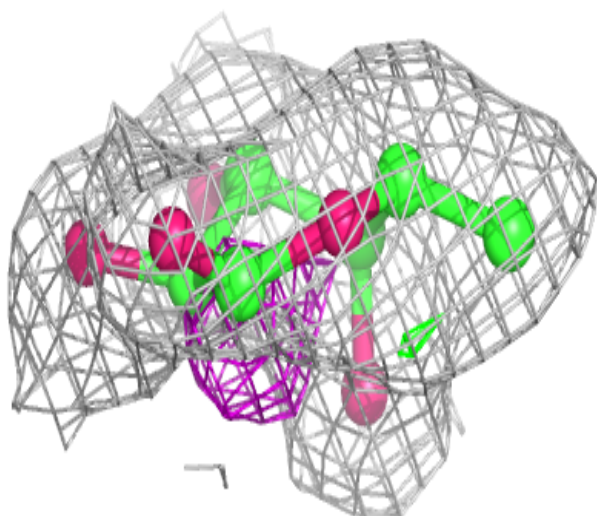
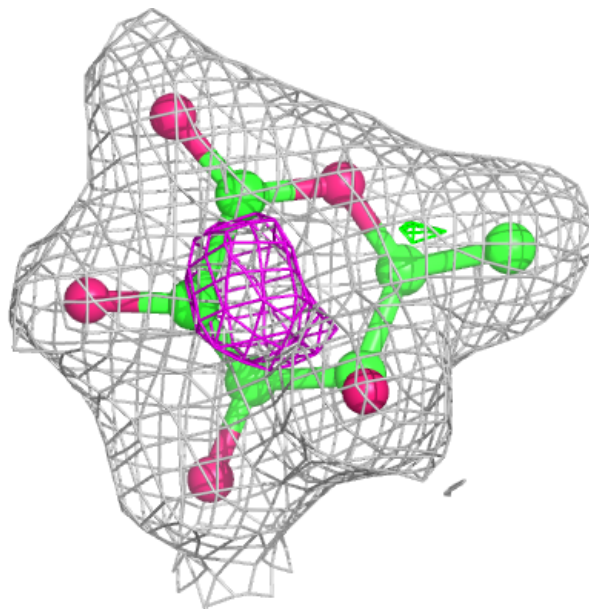
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





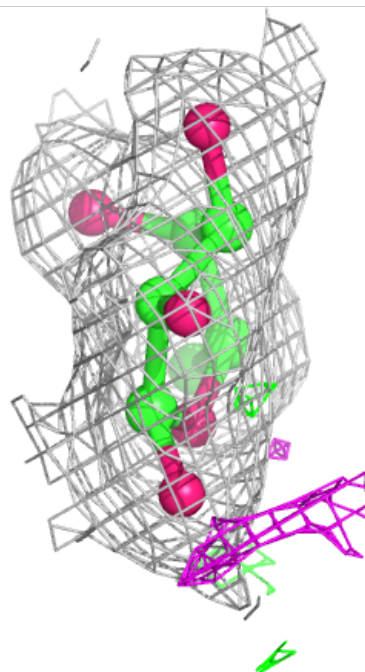
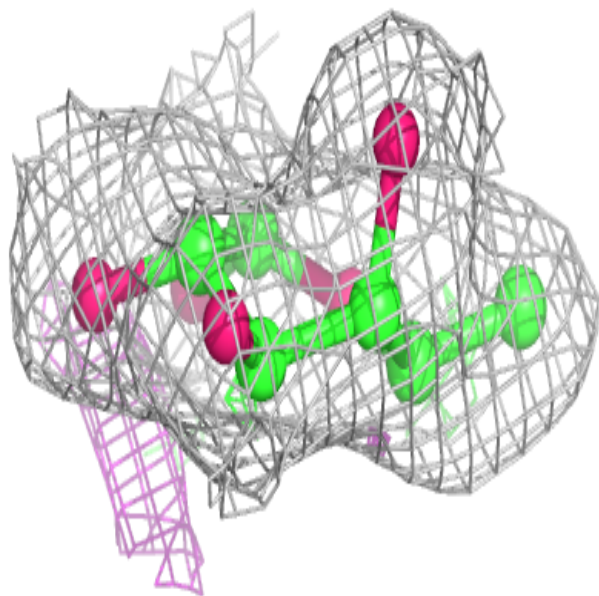
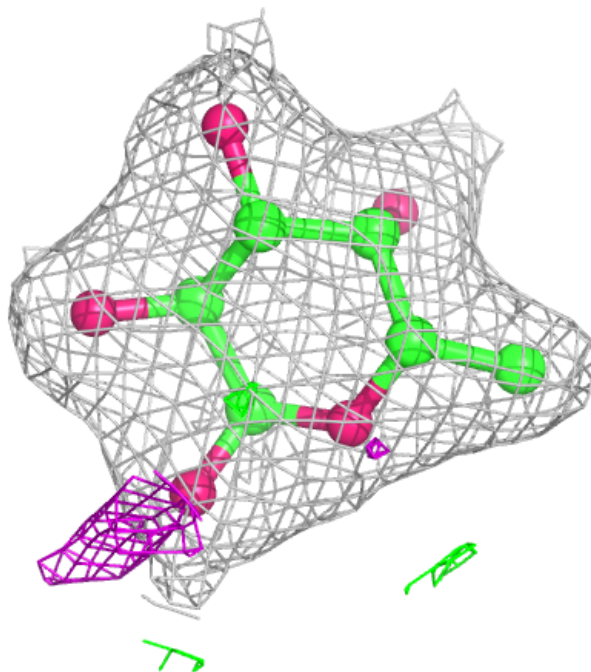
**Electron density around FUC C 501:**

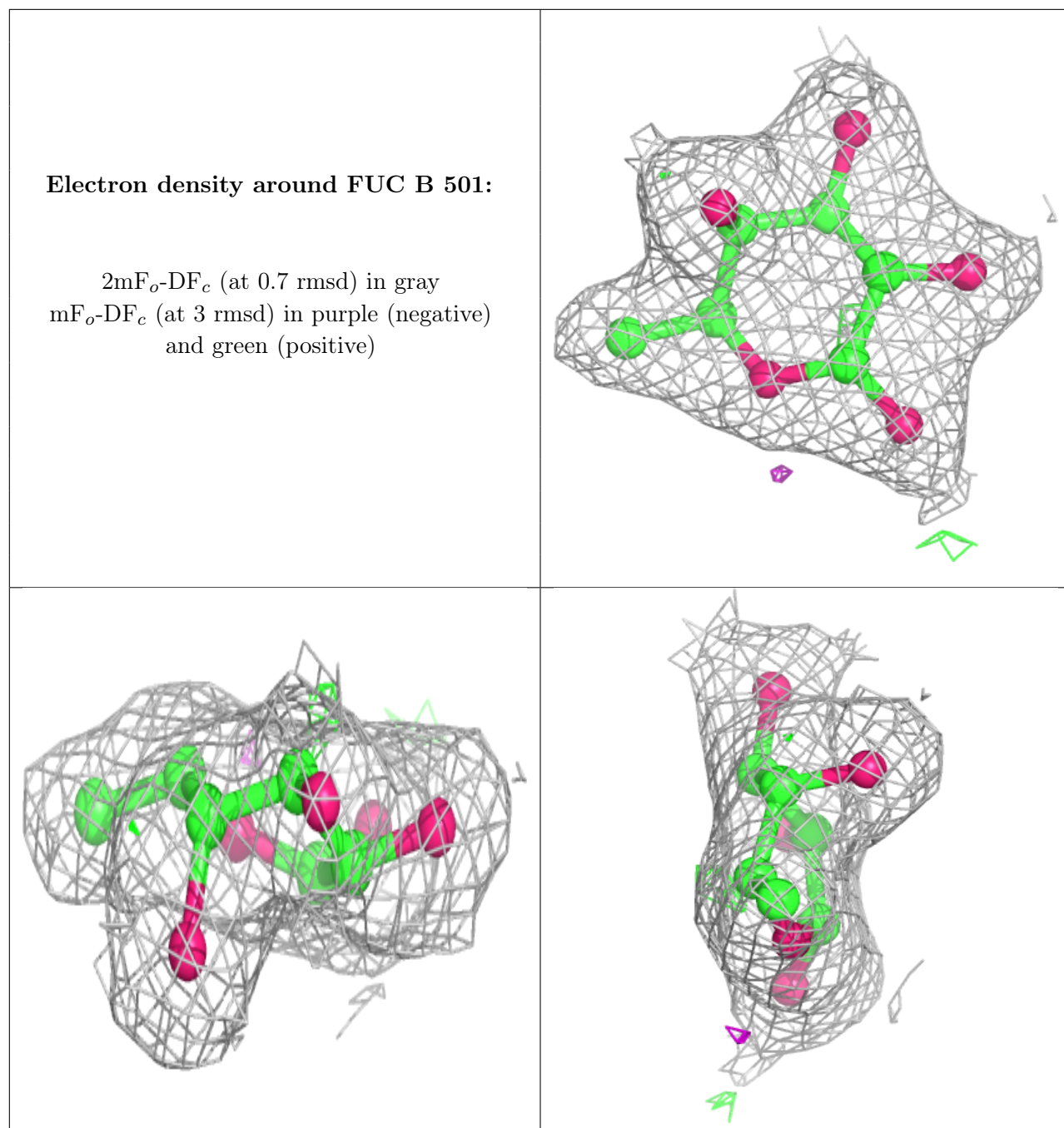
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FUC E 501:**

$2mF_o-DF_c$  (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.