



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2025 – 01:25 pm BST

PDB ID : 9HYX / pdb_00009hyx
Title : AlfB fucosidase in complex with Fucose
Authors : Marina, A.; Gallego del Sol, F.
Deposited on : 2025-01-11
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

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 Phenix2.0rc1
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

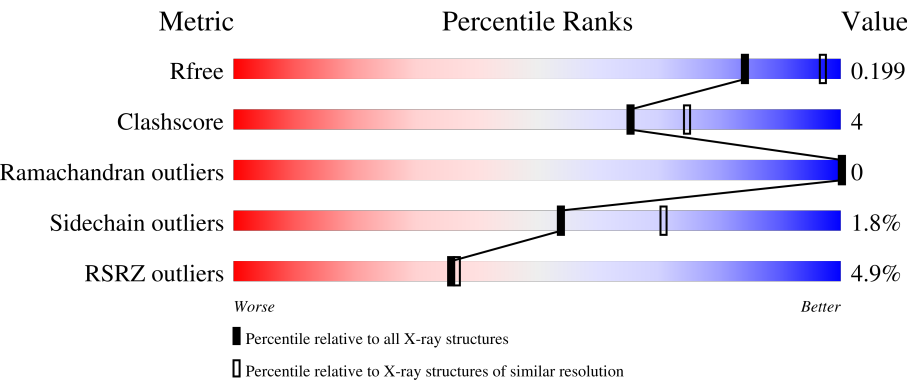
1 Overall quality at a glance i

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 ≥ 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>5%</div><div><div></div><div>89%</div><div>9%</div><div>..</div></div></div>
1	B	414	<div><div>3%</div><div><div></div><div>91%</div><div>7%</div><div>..</div></div></div>
1	C	414	<div><div>4%</div><div><div></div><div>89%</div><div>9%</div><div>.</div></div></div>
1	D	414	<div><div>5%</div><div><div></div><div>88%</div><div>10%</div><div>.</div></div></div>
1	E	414	<div><div>6%</div><div><div></div><div>90%</div><div>8%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	414	<div><div></div><div>6%</div><div>87%</div><div>11%</div><div>..</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20958 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	410	Total	C	N	O	S	0	2	0
			3296	2122	560	603	11			
1	B	409	Total	C	N	O	S	0	2	0
			3284	2115	558	601	10			
1	C	409	Total	C	N	O	S	0	0	0
			3275	2108	556	601	10			
1	D	413	Total	C	N	O	S	0	2	0
			3319	2135	567	606	11			
1	E	409	Total	C	N	O	S	0	0	0
			3271	2106	555	600	10			
1	F	410	Total	C	N	O	S	0	0	0
			3284	2114	558	602	10			

There are 18 discrepancies between the modelled and reference sequences:

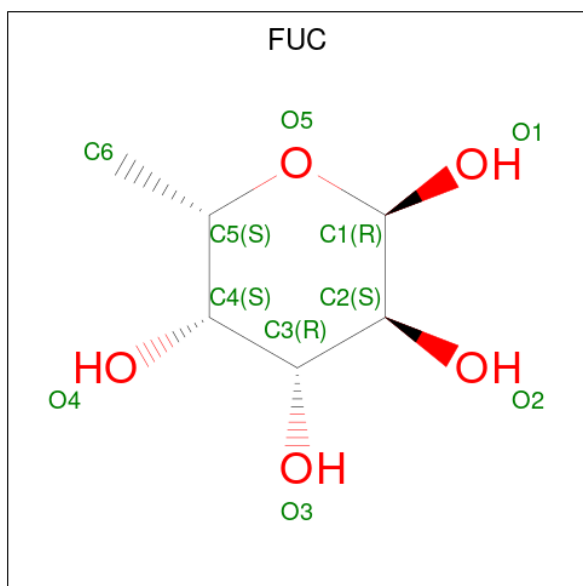
Chain	Residue	Modelled	Actual	Comment	Reference
A	196	SER	ASN	conflict	UNP A0AB36XDR5
A	261	MET	VAL	conflict	UNP A0AB36XDR5
A	346	LYS	ASN	conflict	UNP A0AB36XDR5
B	196	SER	ASN	conflict	UNP A0AB36XDR5
B	261	MET	VAL	conflict	UNP A0AB36XDR5
B	346	LYS	ASN	conflict	UNP A0AB36XDR5
C	196	SER	ASN	conflict	UNP A0AB36XDR5
C	261	MET	VAL	conflict	UNP A0AB36XDR5
C	346	LYS	ASN	conflict	UNP A0AB36XDR5
D	196	SER	ASN	conflict	UNP A0AB36XDR5
D	261	MET	VAL	conflict	UNP A0AB36XDR5
D	346	LYS	ASN	conflict	UNP A0AB36XDR5
E	196	SER	ASN	conflict	UNP A0AB36XDR5
E	261	MET	VAL	conflict	UNP A0AB36XDR5
E	346	LYS	ASN	conflict	UNP A0AB36XDR5
F	196	SER	ASN	conflict	UNP A0AB36XDR5
F	261	MET	VAL	conflict	UNP A0AB36XDR5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	346	LYS	ASN	conflict	UNP A0AB36XDR5

- Molecule 2 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C₆H₁₂O₅) (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	206	Total O 206 206	0	0
3	B	224	Total O 224 224	0	0

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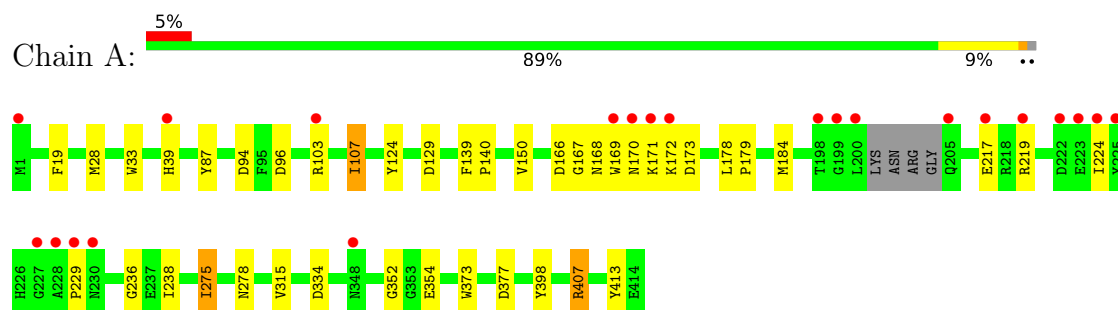
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	177	Total 177	O 177	0	0
3	D	244	Total 244	O 244	0	0
3	E	148	Total 148	O 148	0	0
3	F	164	Total 164	O 164	0	0

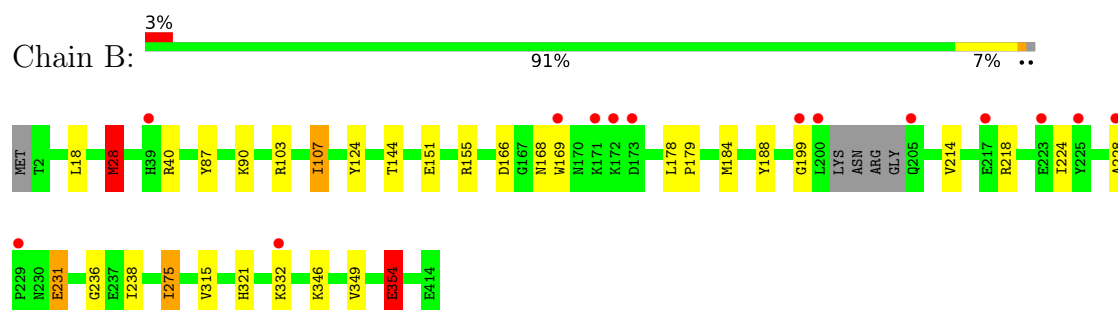
3 Residue-property plots [i](#)

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.

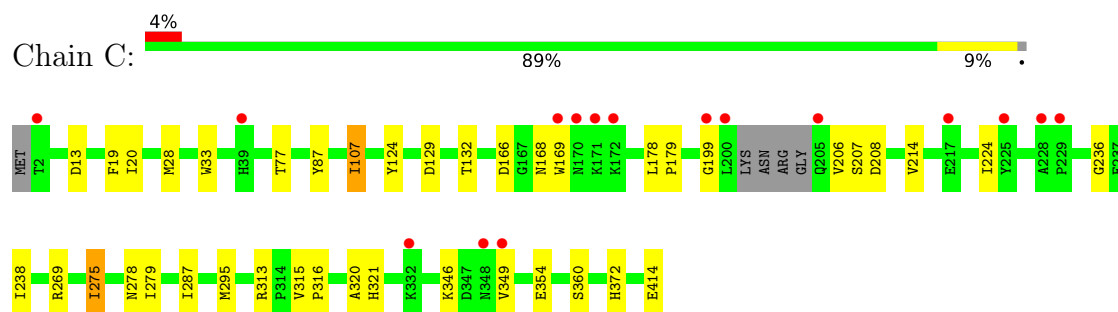
• Molecule 1: Alpha-L-fucosidase



• Molecule 1: Alpha-L-fucosidase

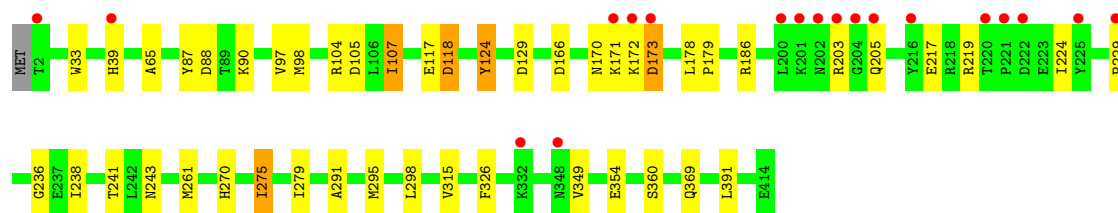


• Molecule 1: Alpha-L-fucosidase

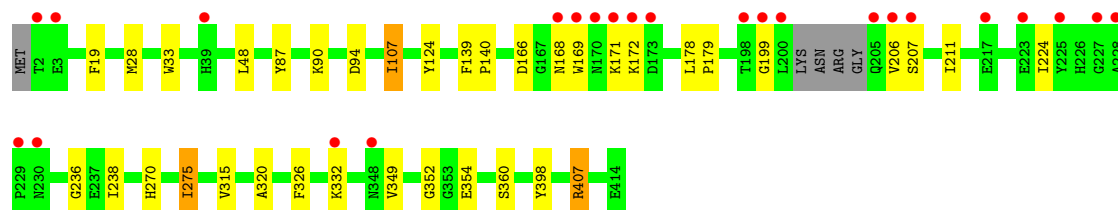
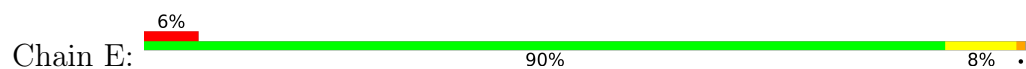


• Molecule 1: Alpha-L-fucosidase

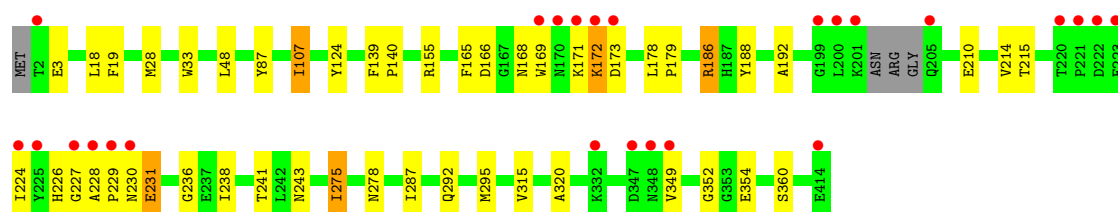
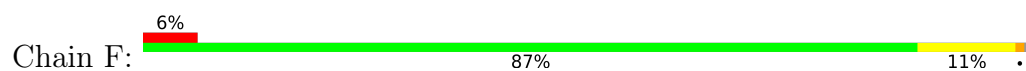




● Molecule 1: Alpha-L-fucosidase



● 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, α , β , γ	168.30Å 309.68Å 173.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.30 49.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.29-2.30) 100.0 (49.29-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.173 , 0.197 0.175 , 0.199	Depositor DCC
R_{free} test set	9862 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.1	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	0.96	EDS
Total number of atoms	20958	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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

5.1 Standard geometry

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	0.72	0/3400	1.07	7/4635 (0.2%)
1	B	0.73	0/3388	1.09	9/4620 (0.2%)
1	C	0.70	0/3372	1.07	3/4598 (0.1%)
1	D	0.75	0/3424	1.07	6/4667 (0.1%)
1	E	0.65	0/3368	1.06	6/4593 (0.1%)
1	F	0.72	0/3381	1.07	7/4609 (0.2%)
All	All	0.71	0/20333	1.07	38/27722 (0.1%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	GLU	N-CA-C	8.60	120.73	111.36
1	A	354	GLU	N-CA-C	7.86	119.84	111.28
1	F	227	GLY	N-CA-C	7.03	118.63	111.95
1	F	3	GLU	CB-CG-CD	-6.95	100.79	112.60
1	F	354	GLU	N-CA-C	6.85	118.75	111.28
1	D	315	VAL	N-CA-CB	-6.76	101.75	111.21
1	E	354	GLU	N-CA-C	6.70	118.59	111.28
1	C	354	GLU	N-CA-C	6.69	118.58	111.28
1	F	315	VAL	N-CA-CB	-6.18	102.56	111.21
1	E	352	GLY	N-CA-C	6.08	122.03	114.37
1	E	315	VAL	N-CA-CB	-6.07	102.71	111.21
1	A	315	VAL	N-CA-CB	-5.96	102.87	111.21
1	D	369	GLN	N-CA-C	5.91	117.52	111.14
1	D	354	GLU	N-CA-C	5.82	117.63	111.28
1	B	188	TYR	N-CA-C	5.80	117.68	111.36
1	A	352	GLY	N-CA-C	5.75	121.54	114.69
1	E	90	LYS	CB-CG-CD	5.72	124.45	111.30
1	B	231	GLU	CB-CG-CD	5.62	122.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	94	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	315	VAL	N-CA-CB	-5.57	103.41	111.21
1	C	132	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	94	ASP	CA-CB-CG	5.37	117.97	112.60
1	F	352	GLY	N-CA-C	5.37	121.13	114.37
1	A	229	PRO	CB-CA-C	5.23	118.16	111.21
1	B	332	LYS	CB-CG-CD	5.22	123.30	111.30
1	D	90	LYS	CG-CD-CE	5.21	123.29	111.30
1	B	144	THR	CA-CB-OG1	-5.18	101.83	109.60
1	D	129	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	229	PRO	CB-CA-C	5.14	118.09	111.46
1	A	129	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	129	ASP	CA-CB-CG	5.12	117.72	112.60
1	E	19	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	28	MET	N-CA-C	5.11	116.92	111.36
1	B	18	LEU	N-CA-CB	-5.08	102.16	110.43
1	B	218	ARG	CB-CA-C	-5.06	101.26	110.63
1	F	18	LEU	N-CA-CB	-5.06	102.19	110.43
1	F	165	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	96	ASP	CA-CB-CG	5.05	117.65	112.60

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	3296	0	3177	20	0
1	B	3284	0	3159	22	0
1	C	3275	0	3150	30	0
1	D	3319	0	3202	31	0
1	E	3271	0	3144	21	0
1	F	3284	0	3163	26	0
2	A	11	0	12	1	0
2	B	11	0	12	1	0
2	C	11	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	11	0	12	1	0
2	E	11	0	12	2	0
2	F	11	0	12	2	0
3	A	206	0	0	2	0
3	B	224	0	0	0	0
3	C	177	0	0	1	0
3	D	244	0	0	1	0
3	E	148	0	0	0	0
3	F	164	0	0	0	0
All	All	20958	0	19067	142	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 (142) 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:228:ALA:HB3	1:B:231:GLU:HG3	1.50	0.91
1:F:186:ARG:HD3	1:F:210:GLU:OE1	1.79	0.82
1:B:166:ASP:OD2	2:B:501:FUC:H1	1.80	0.79
1:C:28:MET:HA	1:C:28:MET:HE2	1.66	0.77
1:F:287:ILE:HG21	1:F:295:MET:HE1	1.70	0.74
1:B:28:MET:HE3	1:B:40:ARG:CZ	2.19	0.73
1:D:87:TYR:HB3	1:D:107:ILE:HG12	1.70	0.73
1:D:224:ILE:HD13	1:D:236:GLY:HA3	1.70	0.72
1:B:224:ILE:HD13	1:B:236:GLY:HA3	1.72	0.72
1:C:224:ILE:HD13	1:C:236:GLY:HA3	1.71	0.71
1:E:224:ILE:HD13	1:E:236:GLY:HA3	1.73	0.71
1:F:224:ILE:HD13	1:F:236:GLY:HA3	1.72	0.71
1:B:87:TYR:HB3	1:B:107:ILE:HG12	1.73	0.70
1:D:171:LYS:HB3	1:D:173:ASP:OD1	1.91	0.70
1:F:228:ALA:O	1:F:231:GLU:HB2	1.92	0.70
1:B:28:MET:CE	1:B:40:ARG:CZ	2.71	0.68
1:E:87:TYR:HB3	1:E:107:ILE:HG12	1.75	0.68
1:F:166:ASP:OD2	2:F:501:FUC:H1	1.93	0.67
1:D:88:ASP:HB2	1:D:98:MET:HE3	1.75	0.67
1:D:291:ALA:O	1:D:295:MET:HG2	1.94	0.67
1:C:87:TYR:HB3	1:C:107:ILE:HG12	1.75	0.67
3:A:667:HOH:O	1:C:321:HIS:HE1	1.78	0.66
1:A:224:ILE:HD13	1:A:236:GLY:HA3	1.77	0.66
1:A:87:TYR:HB3	1:A:107:ILE:HG12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:MET:HE1	1:D:105:ASP:N	2.11	0.65
1:F:87:TYR:HB3	1:F:107:ILE:HG12	1.79	0.65
1:E:166:ASP:OD2	2:E:501:FUC:H1	1.98	0.64
1:E:398:TYR:HE1	1:E:407:ARG:HG3	1.63	0.64
1:C:166:ASP:OD2	2:C:501:FUC:H1	1.99	0.63
1:A:224:ILE:CD1	1:A:236:GLY:HA3	2.29	0.63
1:F:224:ILE:HD11	1:F:226:HIS:CE1	2.35	0.61
1:D:279:ILE:HD11	1:D:295:MET:HE2	1.84	0.60
1:C:346:LYS:HE3	1:D:39[B]:HIS:ND1	2.17	0.59
1:C:349:VAL:HG21	1:D:33:TRP:CZ3	2.37	0.59
1:F:229:PRO:O	1:F:230:ASN:HB2	2.02	0.58
1:F:186:ARG:NH2	1:F:192:ALA:O	2.37	0.58
1:D:166:ASP:OD2	2:D:501:FUC:H1	2.04	0.57
1:C:28:MET:HE2	1:C:28:MET:CA	2.35	0.56
1:E:33:TRP:CZ3	1:F:349:VAL:HG21	2.40	0.56
1:C:33:TRP:CZ3	1:D:349:VAL:HG21	2.40	0.56
1:E:207:SER:OG	1:E:211:ILE:CD1	2.53	0.55
1:C:315:VAL:CG2	1:C:316:PRO:HD2	2.37	0.55
1:A:167:GLY:O	1:A:170:ASN:ND2	2.40	0.55
1:D:97:VAL:HG13	1:D:98:MET:HE2	1.89	0.55
1:C:206:VAL:HG12	1:C:208:ASP:H	1.72	0.54
1:D:117:GLU:O	1:D:118:ASP:HB2	2.07	0.54
1:B:238:ILE:HG13	1:B:275:ILE:HD12	1.90	0.53
1:D:238:ILE:HG13	1:D:275:ILE:HD12	1.90	0.53
1:F:28:MET:HE3	1:F:48:LEU:HD21	1.91	0.53
1:E:28:MET:HE3	1:E:48:LEU:HD21	1.91	0.53
1:F:238:ILE:HG13	1:F:275:ILE:HD12	1.91	0.53
1:C:287:ILE:HG21	1:C:295:MET:HE1	1.91	0.53
1:A:166:ASP:OD2	2:A:501:FUC:H1	2.09	0.52
1:F:228:ALA:HB3	1:F:231:GLU:HG3	1.91	0.52
1:E:238:ILE:HG13	1:E:275:ILE:HD12	1.90	0.52
1:A:238:ILE:HG13	1:A:275:ILE:HD12	1.91	0.52
1:C:238:ILE:HG13	1:C:275:ILE:HD12	1.91	0.52
1:B:28:MET:CE	1:B:40:ARG:NE	2.74	0.51
1:B:28:MET:HE1	1:B:40:ARG:CZ	2.41	0.51
1:D:224:ILE:CD1	1:D:236:GLY:HA3	2.39	0.51
1:C:124:TYR:C	1:C:124:TYR:CD1	2.89	0.50
1:B:321:HIS:HE1	3:D:753:HOH:O	1.94	0.49
1:E:349:VAL:HG21	1:F:33:TRP:CZ3	2.46	0.49
1:D:279:ILE:HD11	1:D:295:MET:CE	2.42	0.49
1:D:261[A]:MET:HE3	1:D:298:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ASP:OD1	1:D:173:ASP:N	2.46	0.48
1:B:151:GLU:O	1:B:155:ARG:HG3	2.13	0.48
1:B:224:ILE:CD1	1:B:236:GLY:HA3	2.41	0.48
1:A:28:MET:HA	1:A:28:MET:HE2	1.94	0.48
1:C:199:GLY:HA3	1:C:214:VAL:HG22	1.95	0.48
1:C:77:THR:HA	1:C:124:TYR:HB3	1.96	0.48
1:B:28:MET:HE3	1:B:40:ARG:NH2	2.29	0.48
1:C:224:ILE:CD1	1:C:236:GLY:HA3	2.41	0.48
1:B:199:GLY:HA3	1:B:214:VAL:HG22	1.95	0.47
1:B:178:LEU:N	1:B:179:PRO:CD	2.77	0.47
1:D:124:TYR:C	1:D:124:TYR:CD1	2.93	0.47
1:B:124:TYR:C	1:B:124:TYR:CD1	2.92	0.47
1:F:124:TYR:C	1:F:124:TYR:CD1	2.93	0.47
1:E:124:TYR:C	1:E:124:TYR:CD1	2.92	0.47
1:E:224:ILE:CD1	1:E:236:GLY:HA3	2.41	0.47
1:D:65:ALA:HB1	1:D:295:MET:HE3	1.97	0.47
1:D:170:ASN:H	1:D:172:LYS:HZ3	1.62	0.47
1:A:373:TRP:CE3	1:A:407:ARG:HD3	2.50	0.46
1:D:270:HIS:HB2	1:D:326:PHE:CE2	2.50	0.46
1:A:124:TYR:C	1:A:124:TYR:CD1	2.93	0.46
1:A:33:TRP:CZ3	1:B:349:VAL:HG21	2.50	0.46
1:A:398:TYR:HE1	1:A:407:ARG:HG3	1.81	0.46
1:C:206:VAL:HG12	1:C:207:SER:N	2.30	0.46
1:D:98:MET:HE1	1:D:105:ASP:CA	2.46	0.46
1:D:261[B]:MET:HB3	1:D:261[B]:MET:HE3	1.76	0.46
1:B:168:ASN:HB3	1:B:169:TRP:CD1	2.52	0.45
1:B:28:MET:HE3	1:B:40:ARG:NE	2.31	0.45
1:F:166:ASP:OD2	2:F:501:FUC:C1	2.60	0.45
1:C:269:ARG:HA	1:C:269:ARG:HD2	1.83	0.45
1:C:168:ASN:HB3	1:C:169:TRP:CD1	2.52	0.45
1:C:178:LEU:N	1:C:179:PRO:CD	2.80	0.45
1:C:320:ALA:HB2	1:C:360:SER:HB2	1.99	0.45
1:C:20:ILE:HD13	1:C:279:ILE:HG12	1.98	0.44
1:E:398:TYR:CE1	1:E:407:ARG:HG3	2.48	0.44
1:F:172:LYS:O	1:F:173:ASP:HB2	2.17	0.44
1:C:346:LYS:CE	1:D:39[B]:HIS:ND1	2.80	0.44
1:E:168:ASN:O	1:E:169:TRP:CD1	2.70	0.44
1:D:178:LEU:N	1:D:179:PRO:CD	2.81	0.44
1:E:168:ASN:OD1	1:E:169:TRP:CD1	2.70	0.44
1:E:199:GLY:O	1:E:206:VAL:HA	2.18	0.44
1:D:261[A]:MET:CE	1:D:298:LEU:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:GLU:H	1:B:354:GLU:CD	2.26	0.44
1:F:168:ASN:HB3	1:F:169:TRP:CD1	2.53	0.43
1:F:178:LEU:N	1:F:179:PRO:CD	2.82	0.43
1:A:217:GLU:HB2	3:A:730:HOH:O	2.17	0.43
1:E:178:LEU:N	1:E:179:PRO:CD	2.82	0.43
1:B:184:MET:HE2	1:B:184:MET:HB3	1.96	0.43
1:A:168:ASN:HB3	1:A:169:TRP:CE3	2.53	0.43
1:F:214:VAL:HG12	1:F:215:THR:N	2.34	0.43
1:F:320:ALA:HB2	1:F:360:SER:HB2	2.01	0.42
1:E:166:ASP:OD2	2:E:501:FUC:C1	2.67	0.42
1:E:270:HIS:HB2	1:E:326:PHE:CE1	2.55	0.42
1:A:150:VAL:HG12	1:A:184:MET:HE1	2.02	0.42
1:C:315:VAL:HG22	1:C:316:PRO:HD2	2.01	0.42
1:A:178:LEU:N	1:A:179:PRO:CD	2.82	0.42
1:E:332:LYS:HE3	1:E:332:LYS:HB2	1.67	0.42
1:F:155:ARG:HD2	1:F:188:TYR:CZ	2.55	0.42
1:C:372:HIS:ND1	3:C:601:HOH:O	2.37	0.41
1:D:98:MET:HE1	1:D:104:ARG:C	2.45	0.41
1:E:320:ALA:HB2	1:E:360:SER:HB2	2.02	0.41
1:A:19:PHE:HB3	1:A:278:ASN:HA	2.03	0.41
1:A:139:PHE:N	1:A:140:PRO:CD	2.84	0.41
1:F:292:GLN:HA	1:F:295:MET:HE3	2.02	0.41
1:A:39[A]:HIS:HB2	1:B:346:LYS:NZ	2.36	0.41
1:D:186:ARG:HD3	1:D:186:ARG:HA	1.88	0.41
1:C:28:MET:HA	1:C:28:MET:CE	2.45	0.41
1:A:172:LYS:O	1:A:173:ASP:HB2	2.21	0.41
1:C:13:ASP:OD1	1:C:313:ARG:NH2	2.54	0.40
1:D:360:SER:HA	1:D:391:LEU:O	2.22	0.40
1:F:19:PHE:HB3	1:F:278:ASN:HA	2.03	0.40
1:F:139:PHE:N	1:F:140:PRO:CD	2.84	0.40
1:C:19:PHE:HB3	1:C:278:ASN:HA	2.02	0.40
1:C:206:VAL:CG1	1:C:207:SER:N	2.85	0.40
1:D:241:THR:HG23	1:D:243:ASN:O	2.22	0.40
1:E:139:PHE:N	1:E:140:PRO:CD	2.84	0.40
1:F:241:THR:HG23	1:F:243:ASN:O	2.22	0.40
1:A:334:ASP:OD2	1:A:413:TYR:OH	2.32	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	408/414 (99%)	402 (98%)	6 (2%)	0	100	100
1	B	407/414 (98%)	399 (98%)	8 (2%)	0	100	100
1	C	405/414 (98%)	395 (98%)	10 (2%)	0	100	100
1	D	413/414 (100%)	403 (98%)	10 (2%)	0	100	100
1	E	405/414 (98%)	394 (97%)	11 (3%)	0	100	100
1	F	406/414 (98%)	398 (98%)	8 (2%)	0	100	100
All	All	2444/2484 (98%)	2391 (98%)	53 (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	345/346 (100%)	338 (98%)	7 (2%)	50	68
1	B	343/346 (99%)	337 (98%)	6 (2%)	56	72
1	C	342/346 (99%)	339 (99%)	3 (1%)	75	87
1	D	347/346 (100%)	338 (97%)	9 (3%)	41	58
1	E	341/346 (99%)	336 (98%)	5 (2%)	60	76
1	F	343/346 (99%)	337 (98%)	6 (2%)	56	72
All	All	2061/2076 (99%)	2025 (98%)	36 (2%)	54	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	107	ILE
1	A	171	LYS
1	A	219	ARG
1	A	275	ILE
1	A	377	ASP
1	A	407	ARG
1	B	28	MET
1	B	90	LYS
1	B	103	ARG
1	B	107	ILE
1	B	275	ILE
1	B	354	GLU
1	C	107	ILE
1	C	275	ILE
1	C	414	GLU
1	D	107	ILE
1	D	118	ASP
1	D	124	TYR
1	D	173	ASP
1	D	203	ARG
1	D	205	GLN
1	D	217	GLU
1	D	219	ARG
1	D	275	ILE
1	E	107	ILE
1	E	171	LYS
1	E	172	LYS
1	E	275	ILE
1	E	407	ARG
1	F	107	ILE
1	F	171	LYS
1	F	172	LYS
1	F	186	ARG
1	F	231	GLU
1	F	275	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	HIS

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Mol	Chain	Res	Type
1	A	410	GLN
1	B	43	HIS
1	B	147	GLN
1	B	187	HIS
1	B	270	HIS
1	B	321	HIS
1	B	366	GLN
1	C	9	GLN
1	C	27	GLN
1	C	43	HIS
1	C	296	HIS
1	C	321	HIS
1	D	9	GLN
1	D	27	GLN
1	D	270	HIS
1	D	296	HIS
1	D	410	GLN
1	E	9	GLN
1	E	56	GLN
1	F	9	GLN
1	F	27	GLN
1	F	43	HIS
1	F	226	HIS
1	F	292	GLN
1	F	296	HIS
1	F	342	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

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	E	501	-	11,11,11	0.45	0	15,16,16	1.06	1 (6%)
2	FUC	F	501	-	11,11,11	0.40	0	15,16,16	1.08	1 (6%)
2	FUC	A	501	-	11,11,11	0.44	0	15,16,16	1.09	1 (6%)
2	FUC	B	501	-	11,11,11	0.50	0	15,16,16	1.07	1 (6%)
2	FUC	C	501	-	11,11,11	0.46	0	15,16,16	1.00	1 (6%)
2	FUC	D	501	-	11,11,11	0.43	0	15,16,16	1.10	1 (6%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FUC	O5-C1-C2	2.87	115.40	110.28
2	D	501	FUC	O5-C5-C4	2.86	114.66	109.52
2	A	501	FUC	O5-C5-C4	2.74	114.43	109.52
2	F	501	FUC	O5-C5-C4	2.72	114.40	109.52
2	C	501	FUC	O5-C5-C4	2.70	114.36	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	FUC	O5-C5-C4	2.64	114.26	109.52

There are no chirality outliers.

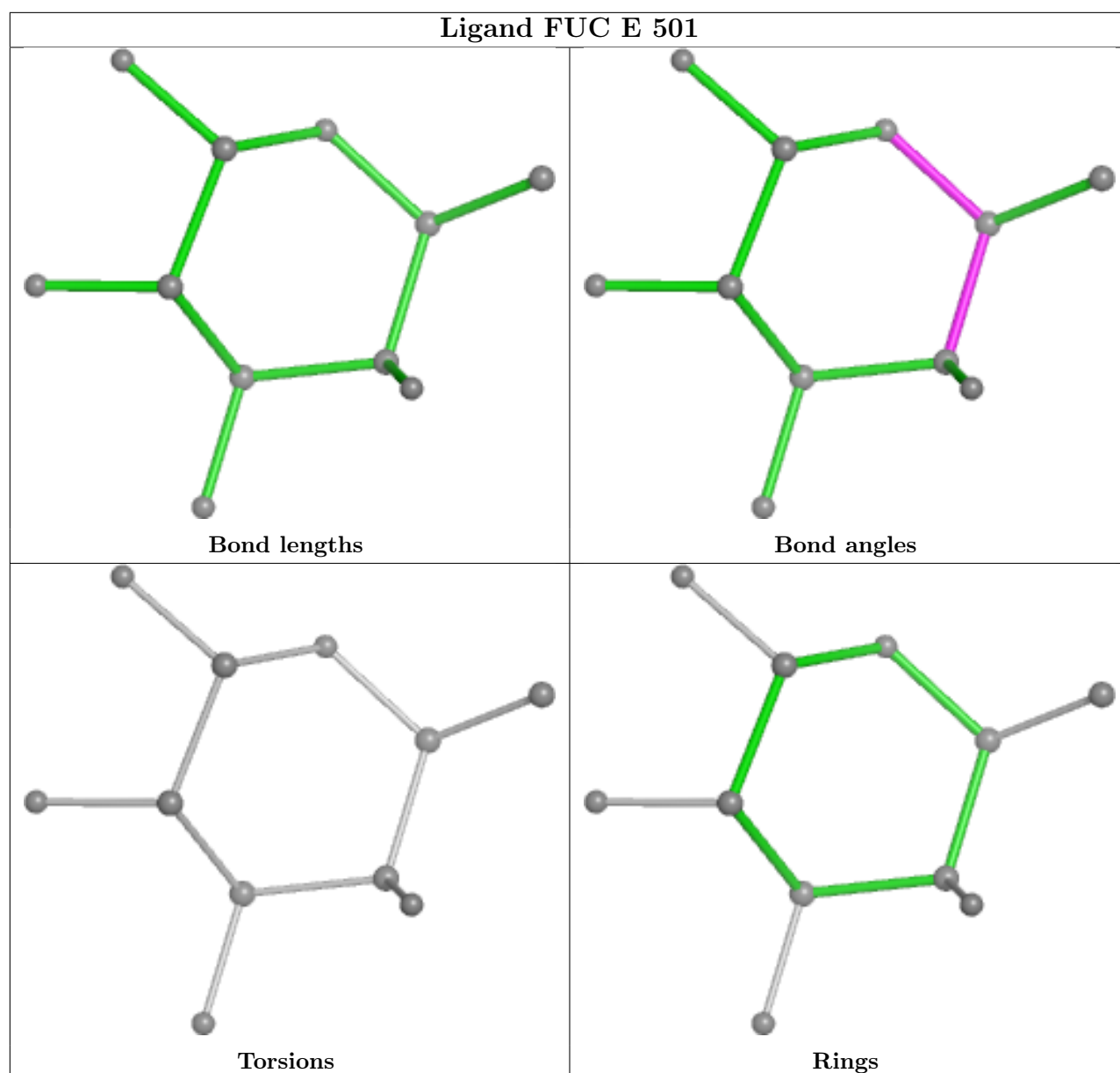
There are no torsion outliers.

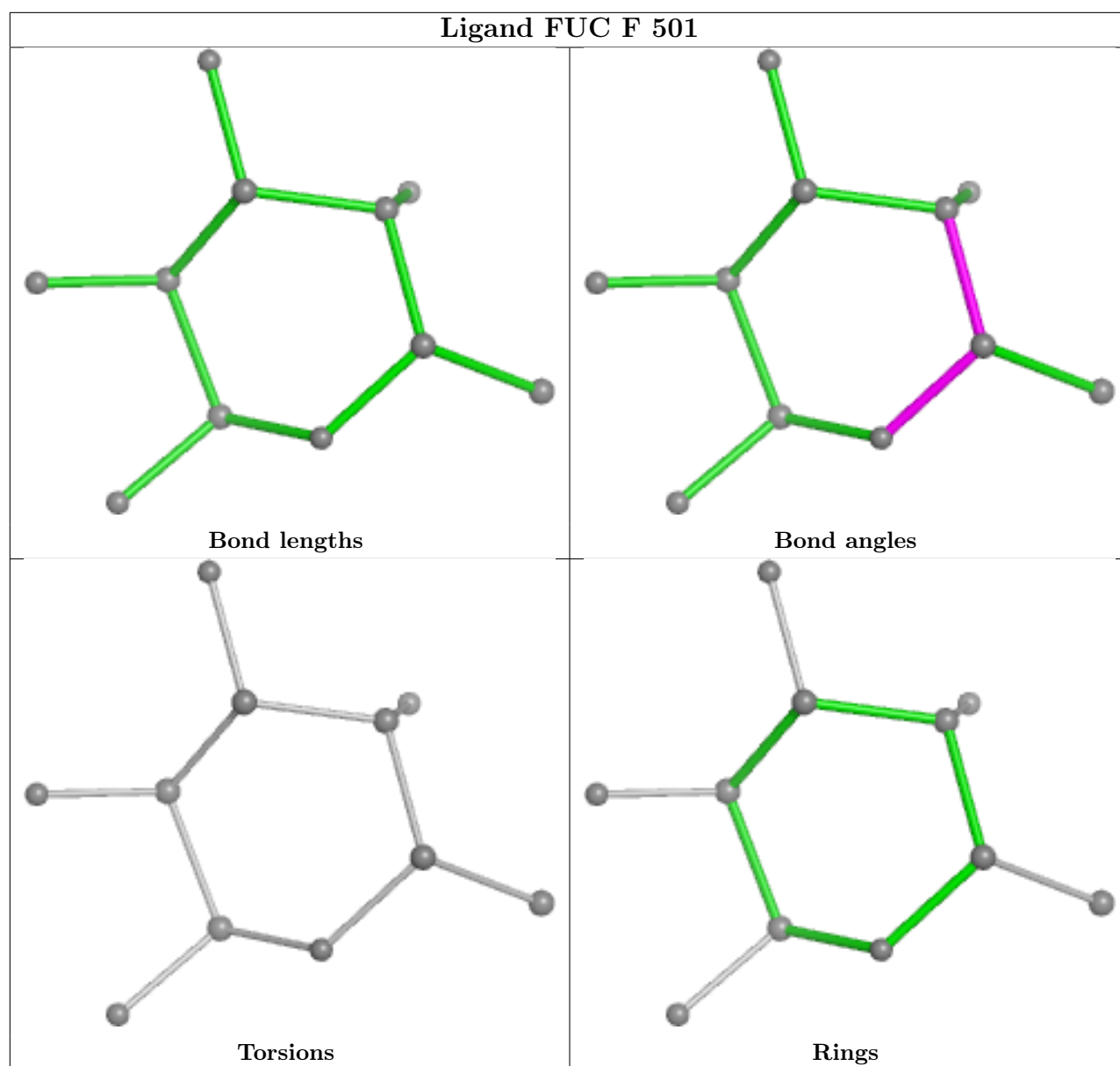
There are no ring outliers.

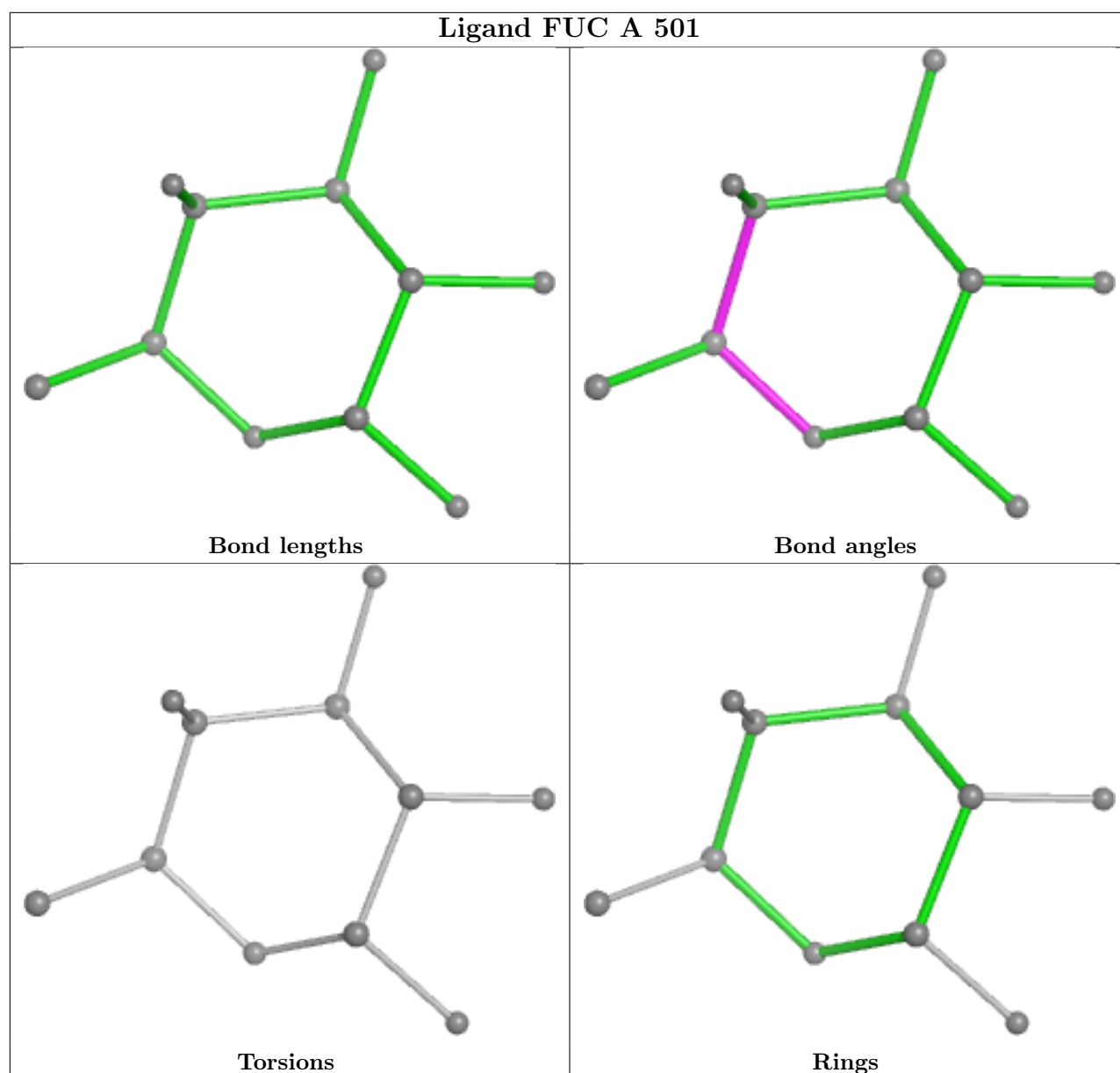
6 monomers are involved in 8 short contacts:

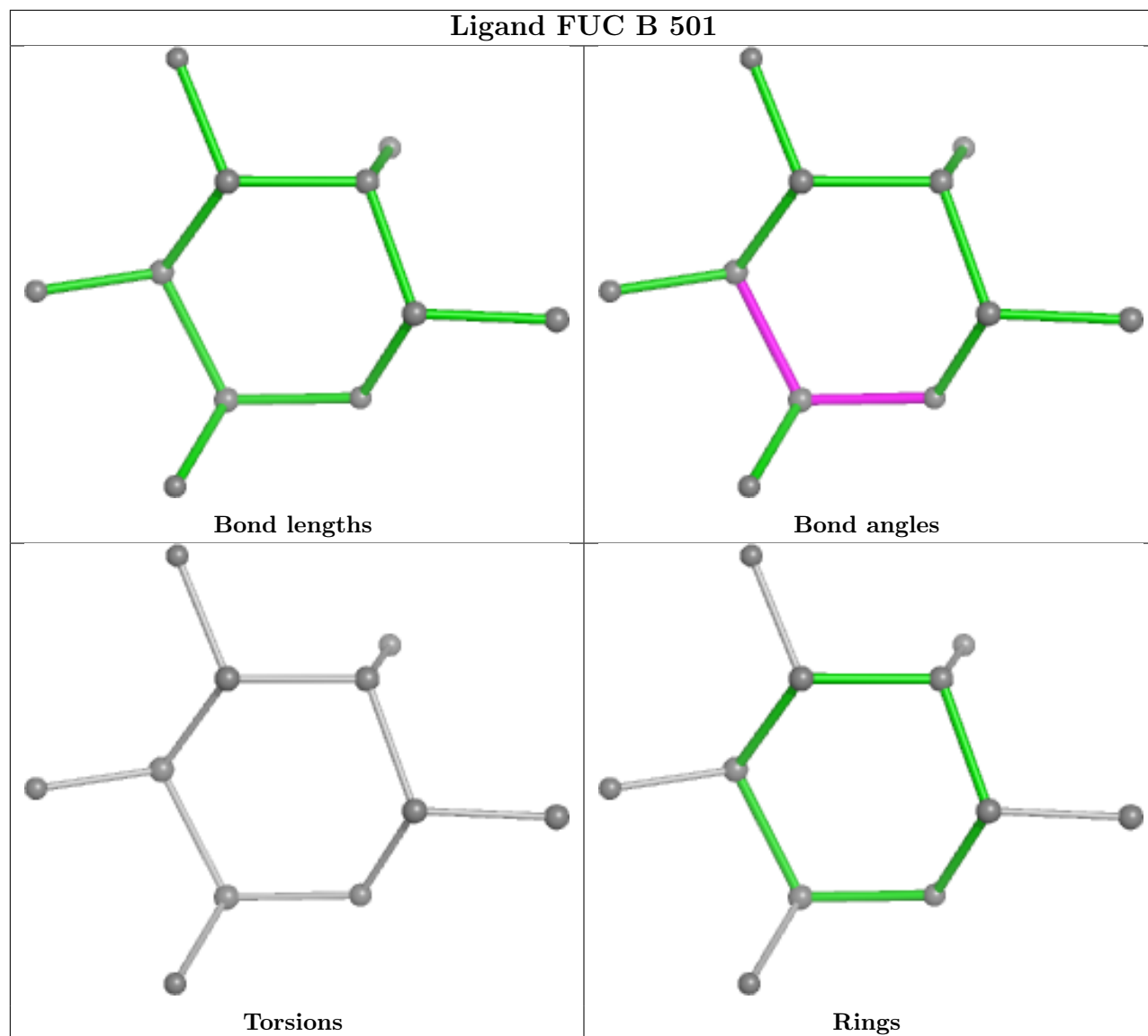
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	FUC	2	0
2	F	501	FUC	2	0
2	A	501	FUC	1	0
2	B	501	FUC	1	0
2	C	501	FUC	1	0
2	D	501	FUC	1	0

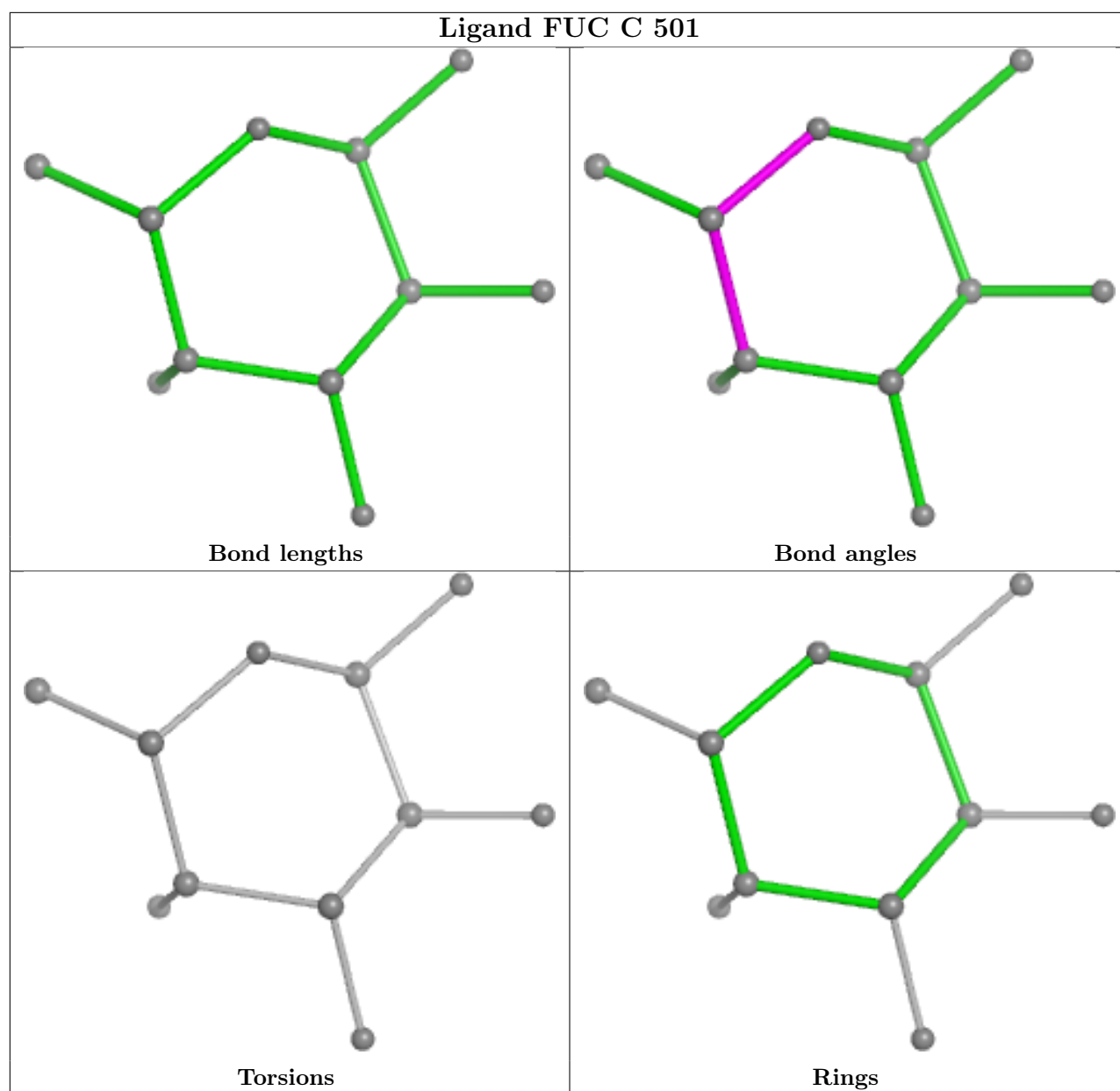
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

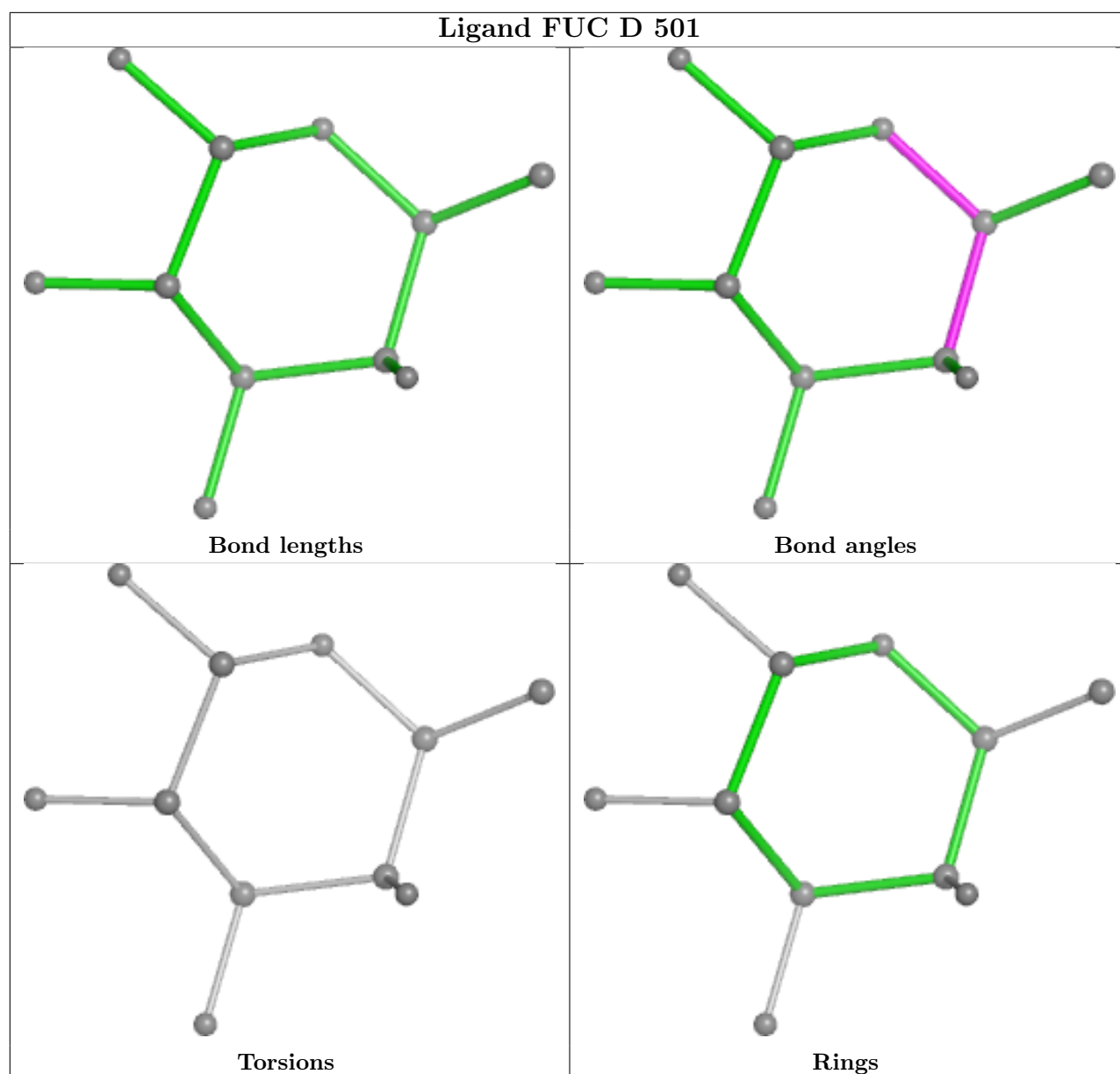












5.7 Other polymers [i](#)

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, 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	410/414 (99%)	-0.41	22 (5%)	32	34	20, 30, 72, 117	2 (0%)
1	B	409/414 (98%)	-0.53	14 (3%)	48	50	17, 27, 62, 112	2 (0%)
1	C	409/414 (98%)	-0.30	16 (3%)	44	45	20, 32, 72, 113	0
1	D	413/414 (99%)	-0.47	19 (4%)	38	39	16, 28, 72, 107	2 (0%)
1	E	409/414 (98%)	-0.14	24 (5%)	29	31	21, 36, 81, 113	0
1	F	410/414 (99%)	-0.25	25 (6%)	28	30	20, 33, 78, 137	0
All	All	2460/2484 (99%)	-0.35	120 (4%)	36	37	16, 31, 73, 137	6 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.5
1	F	2	THR	7.1
1	F	225	TYR	6.4
1	E	172	LYS	6.2
1	A	200	LEU	6.2
1	D	172	LYS	6.1
1	F	201	LYS	5.5
1	E	225	TYR	5.4
1	B	172	LYS	5.3
1	E	200	LEU	5.2
1	D	203	ARG	5.2
1	B	171	LYS	5.0
1	D	205	GLN	4.9
1	E	171	LYS	4.8
1	D	204	GLY	4.7
1	A	172	LYS	4.7
1	A	225	TYR	4.6
1	E	169	TRP	4.5
1	E	228	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	225	TYR	4.4
1	E	205	GLN	4.3
1	F	229	PRO	4.3
1	A	169	TRP	4.2
1	A	228	ALA	4.2
1	F	172	LYS	4.2
1	A	229	PRO	4.2
1	C	171	LYS	4.1
1	E	229	PRO	4.1
1	B	229	PRO	4.1
1	D	225	TYR	4.1
1	A	205	GLN	4.0
1	F	171	LYS	3.9
1	E	227	GLY	3.9
1	C	200	LEU	3.8
1	C	229	PRO	3.8
1	F	223	GLU	3.8
1	C	205	GLN	3.7
1	C	169	TRP	3.7
1	D	202	ASN	3.7
1	F	349	VAL	3.6
1	D	39[A]	HIS	3.6
1	C	172	LYS	3.5
1	F	228	ALA	3.5
1	A	39[A]	HIS	3.5
1	A	348	ASN	3.4
1	D	171	LYS	3.4
1	A	171	LYS	3.2
1	A	199	GLY	3.2
1	F	230	ASN	3.1
1	D	229	PRO	3.1
1	F	205	GLN	3.1
1	B	199	GLY	3.1
1	B	332	LYS	3.0
1	C	39	HIS	3.0
1	D	201	LYS	3.0
1	E	168	ASN	2.9
1	E	206	VAL	2.9
1	E	199	GLY	2.9
1	A	222	ASP	2.8
1	C	199	GLY	2.8
1	B	205	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	173	ASP	2.8
1	E	217	GLU	2.8
1	A	219	ARG	2.8
1	C	348	ASN	2.8
1	F	224	ILE	2.7
1	D	173	ASP	2.7
1	F	221	PRO	2.7
1	F	347	ASP	2.7
1	F	332	LYS	2.7
1	A	230	ASN	2.7
1	B	200	LEU	2.6
1	D	348	ASN	2.6
1	F	222	ASP	2.6
1	B	225	TYR	2.5
1	F	227	GLY	2.5
1	E	173	ASP	2.5
1	B	169	TRP	2.5
1	B	173	ASP	2.4
1	A	227	GLY	2.4
1	D	2	THR	2.4
1	E	170	ASN	2.4
1	D	221	PRO	2.4
1	F	200	LEU	2.4
1	F	348	ASN	2.4
1	B	223	GLU	2.3
1	C	228	ALA	2.3
1	E	348	ASN	2.3
1	C	2	THR	2.3
1	E	198	THR	2.3
1	D	222	ASP	2.3
1	D	332	LYS	2.3
1	F	220	THR	2.3
1	F	169	TRP	2.3
1	A	224	ILE	2.3
1	B	217	GLU	2.3
1	A	217	GLU	2.2
1	D	220	THR	2.2
1	E	207	SER	2.2
1	D	200	LEU	2.2
1	D	216	TYR	2.2
1	C	217	GLU	2.2
1	A	198	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	170	ASN	2.2
1	C	332	LYS	2.2
1	A	170	ASN	2.1
1	E	230	ASN	2.1
1	E	223	GLU	2.1
1	B	39	HIS	2.1
1	E	2	THR	2.1
1	A	103	ARG	2.1
1	F	199	GLY	2.1
1	E	39	HIS	2.1
1	E	332	LYS	2.1
1	F	414	GLU	2.1
1	E	3	GLU	2.0
1	C	349	VAL	2.0
1	F	170	ASN	2.0
1	A	223	GLU	2.0
1	B	228	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

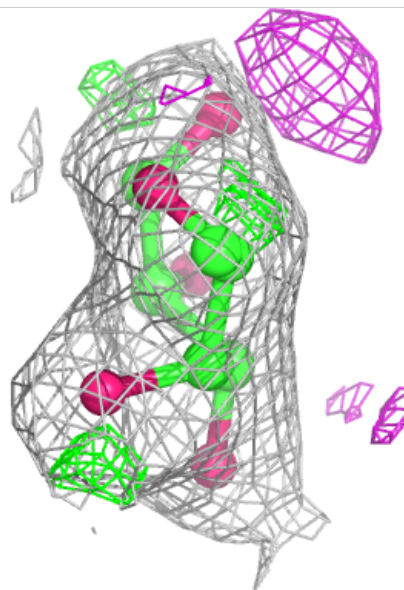
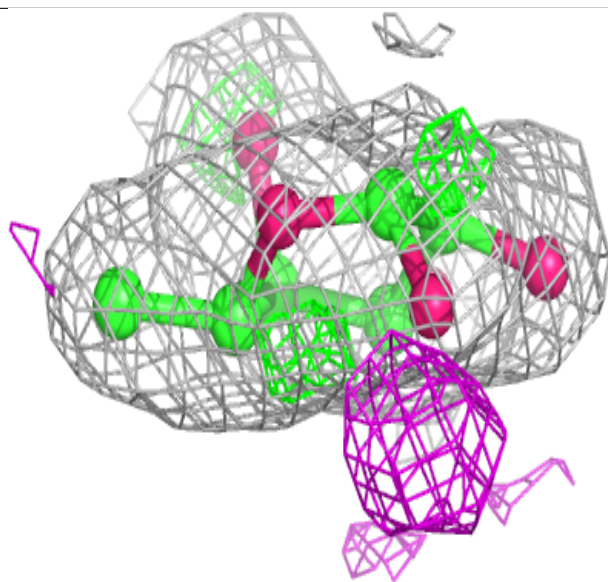
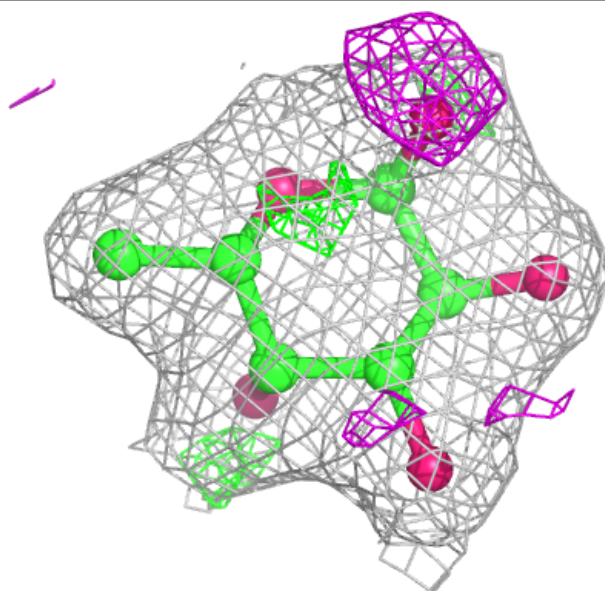
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUC	B	501	11/11	0.92	0.10	20,28,38,42	0
2	FUC	C	501	11/11	0.92	0.10	30,34,39,40	0
2	FUC	E	501	11/11	0.92	0.10	33,38,46,49	0
2	FUC	D	501	11/11	0.94	0.08	22,26,35,35	0
2	FUC	A	501	11/11	0.94	0.09	23,32,40,44	0
2	FUC	F	501	11/11	0.94	0.09	27,32,39,39	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.

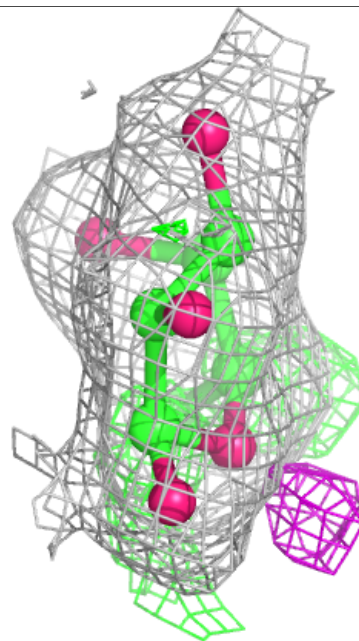
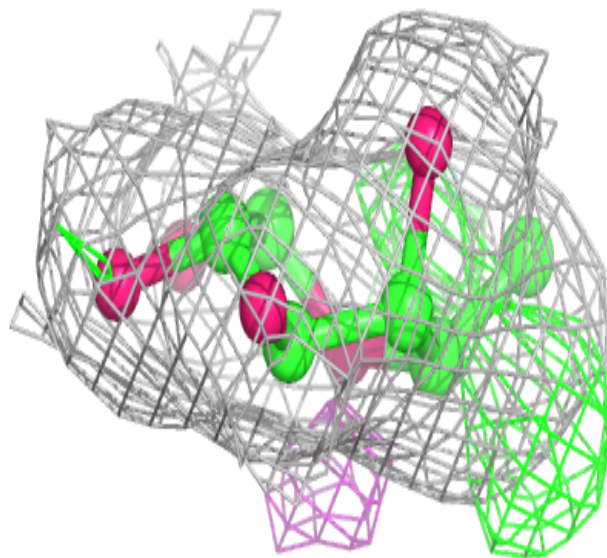
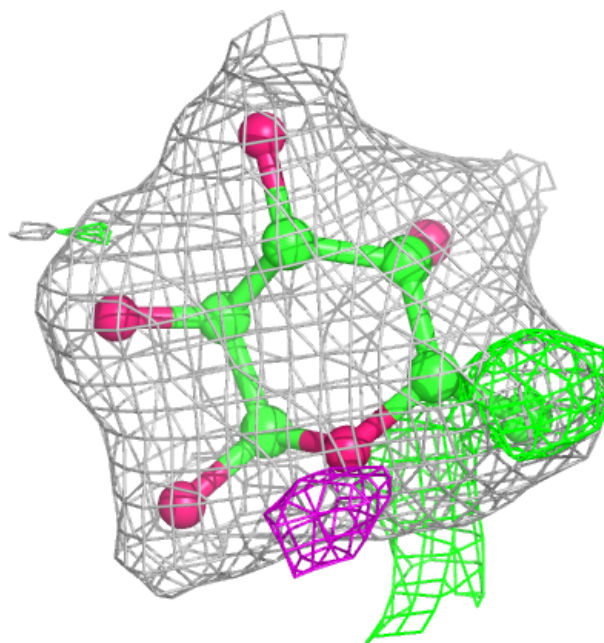
Electron density around FUC B 501:

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



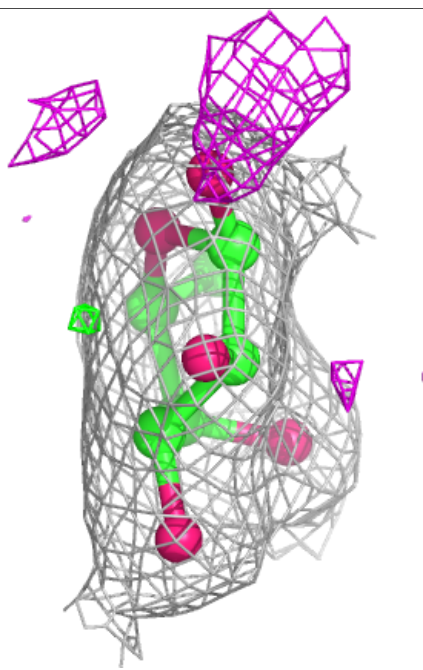
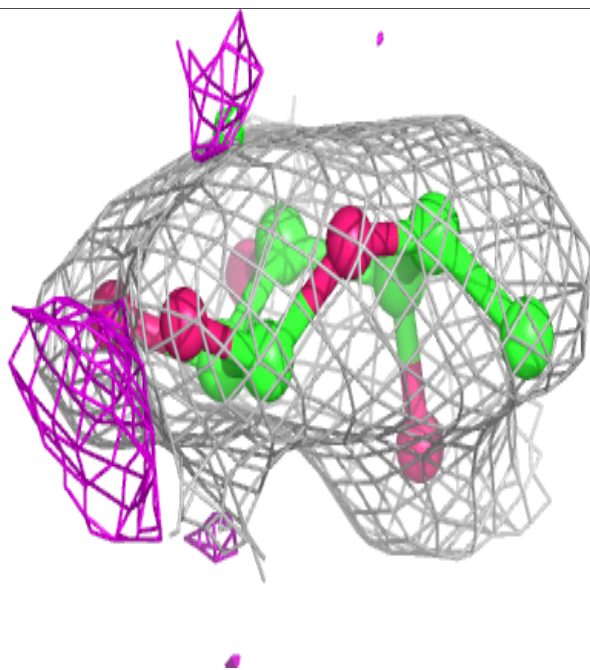
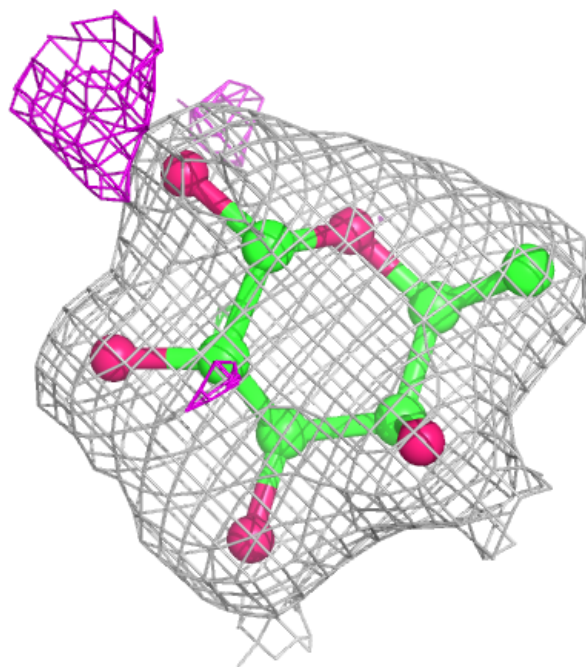
Electron density around FUC C 501:

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and green (positive)



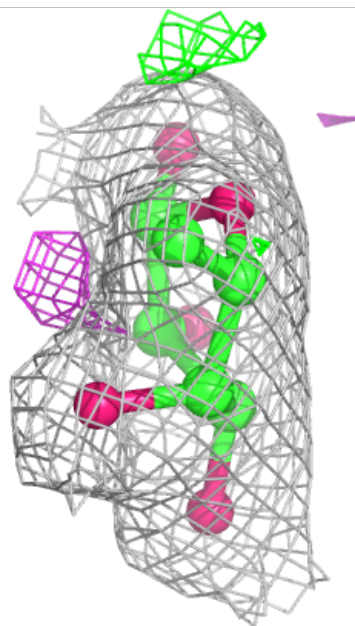
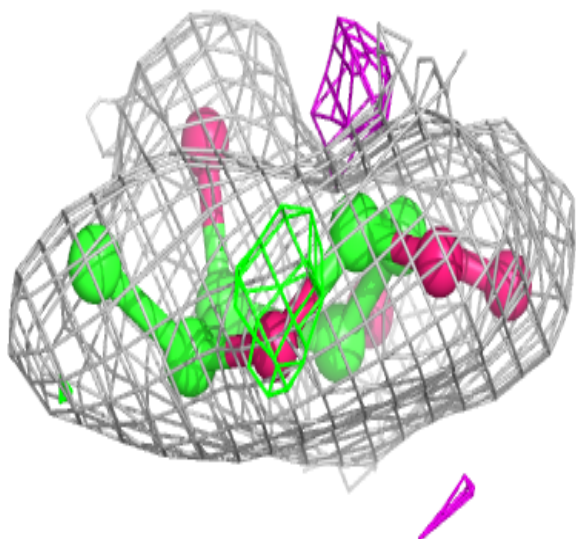
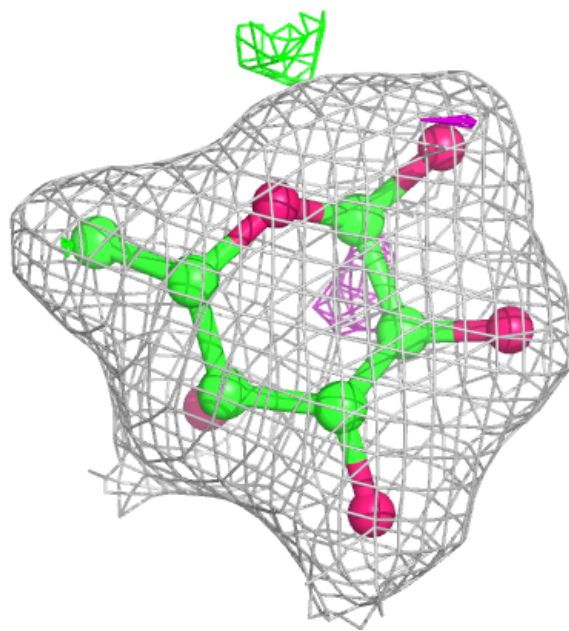
Electron density around FUC E 501:

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and green (positive)



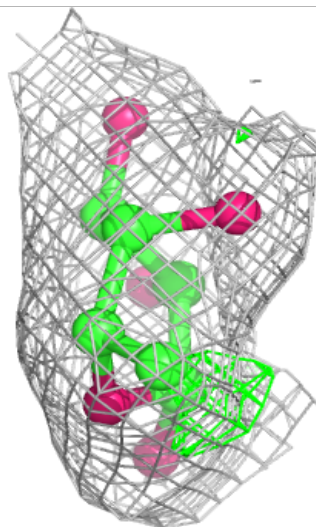
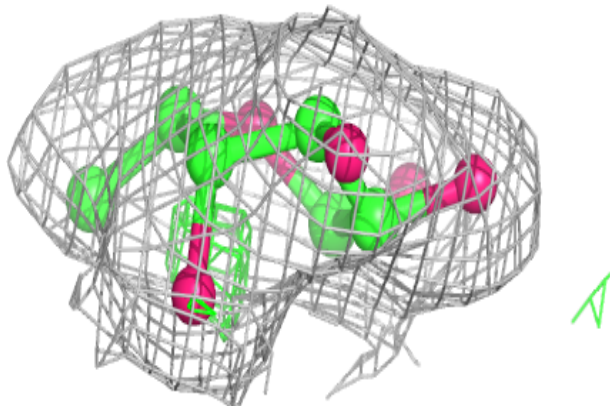
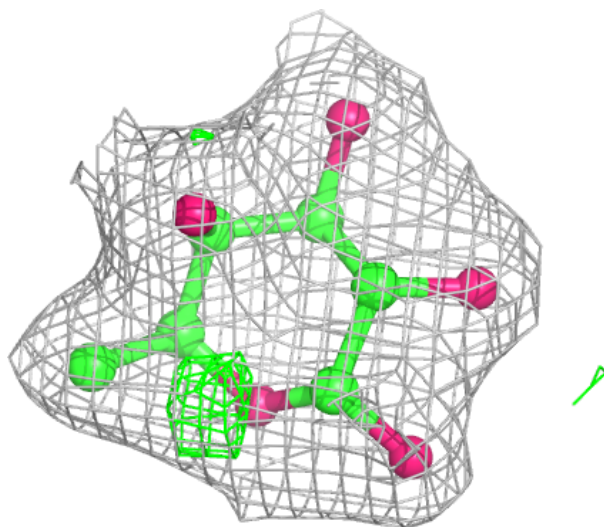
Electron density around FUC D 501:

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and green (positive)



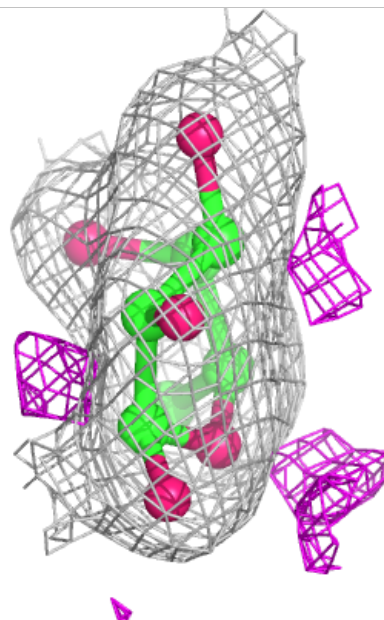
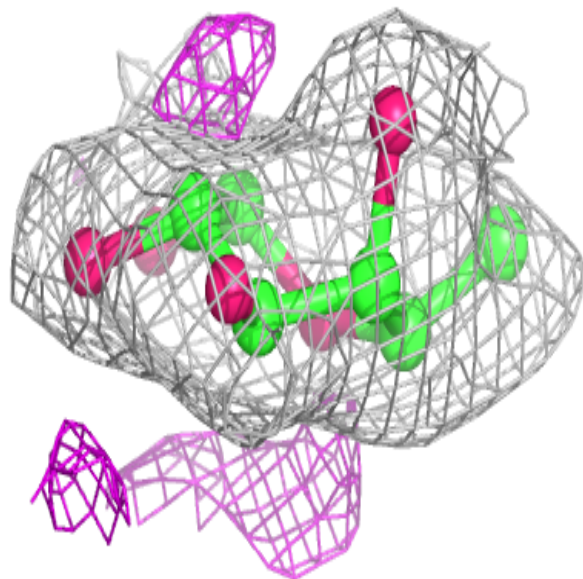
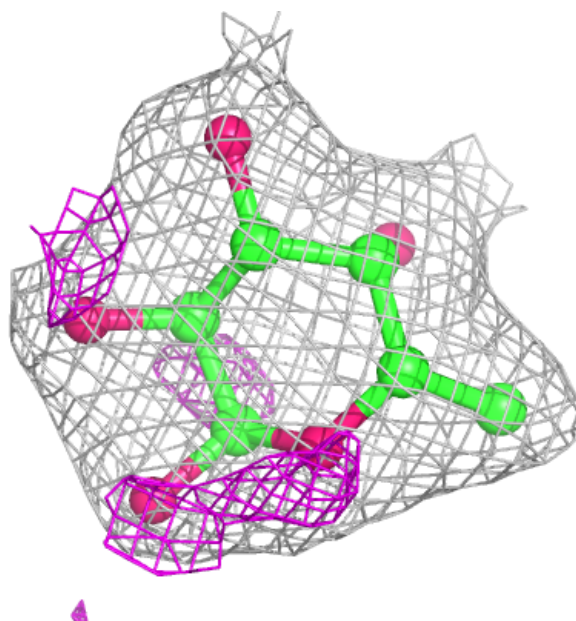
Electron density around FUC A 501:

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



Electron density around FUC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.