



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:11 AM BST

PDB ID : 4FFG  
Title : Crystal Structure of Levan Fructotransferase from *Arthrobacter ureafaciens* in complex with DFA-IV  
Authors : Park, J.; Rhee, S.  
Deposited on : 2012-06-01  
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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

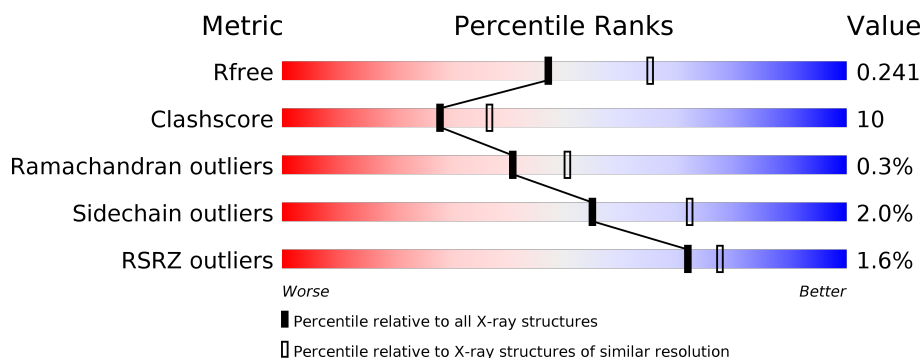
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on 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	492	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	492	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>
1	C	492	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>..</div> </div> </div>
1	D	492	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15976 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 Levan fructotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3739	2375	645	711	8			
1	B	480	Total	C	N	O	S	0	0	0
			3739	2375	645	711	8			
1	C	479	Total	C	N	O	S	0	0	0
			3734	2372	644	710	8			
1	D	480	Total	C	N	O	S	0	0	0
			3739	2375	645	711	8			

There are 48 discrepancies between the modelled and reference sequences:

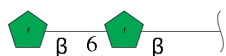
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	expression tag	UNP Q9KJD0
A	115	ASP	GLY	conflict	UNP Q9KJD0
A	522	LEU	-	expression tag	UNP Q9KJD0
A	523	GLU	-	expression tag	UNP Q9KJD0
A	524	HIS	-	expression tag	UNP Q9KJD0
A	525	HIS	-	expression tag	UNP Q9KJD0
A	526	HIS	-	expression tag	UNP Q9KJD0
A	527	HIS	-	expression tag	UNP Q9KJD0
A	528	HIS	-	expression tag	UNP Q9KJD0
A	529	HIS	-	expression tag	UNP Q9KJD0
A	530	HIS	-	expression tag	UNP Q9KJD0
A	531	HIS	-	expression tag	UNP Q9KJD0
B	40	MET	-	expression tag	UNP Q9KJD0
B	115	ASP	GLY	conflict	UNP Q9KJD0
B	522	LEU	-	expression tag	UNP Q9KJD0
B	523	GLU	-	expression tag	UNP Q9KJD0
B	524	HIS	-	expression tag	UNP Q9KJD0
B	525	HIS	-	expression tag	UNP Q9KJD0
B	526	HIS	-	expression tag	UNP Q9KJD0
B	527	HIS	-	expression tag	UNP Q9KJD0
B	528	HIS	-	expression tag	UNP Q9KJD0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	529	HIS	-	expression tag	UNP Q9KJD0
B	530	HIS	-	expression tag	UNP Q9KJD0
B	531	HIS	-	expression tag	UNP Q9KJD0
C	40	MET	-	expression tag	UNP Q9KJD0
C	115	ASP	GLY	conflict	UNP Q9KJD0
C	522	LEU	-	expression tag	UNP Q9KJD0
C	523	GLU	-	expression tag	UNP Q9KJD0
C	524	HIS	-	expression tag	UNP Q9KJD0
C	525	HIS	-	expression tag	UNP Q9KJD0
C	526	HIS	-	expression tag	UNP Q9KJD0
C	527	HIS	-	expression tag	UNP Q9KJD0
C	528	HIS	-	expression tag	UNP Q9KJD0
C	529	HIS	-	expression tag	UNP Q9KJD0
C	530	HIS	-	expression tag	UNP Q9KJD0
C	531	HIS	-	expression tag	UNP Q9KJD0
D	40	MET	-	expression tag	UNP Q9KJD0
D	115	ASP	GLY	conflict	UNP Q9KJD0
D	522	LEU	-	expression tag	UNP Q9KJD0
D	523	GLU	-	expression tag	UNP Q9KJD0
D	524	HIS	-	expression tag	UNP Q9KJD0
D	525	HIS	-	expression tag	UNP Q9KJD0
D	526	HIS	-	expression tag	UNP Q9KJD0
D	527	HIS	-	expression tag	UNP Q9KJD0
D	528	HIS	-	expression tag	UNP Q9KJD0
D	529	HIS	-	expression tag	UNP Q9KJD0
D	530	HIS	-	expression tag	UNP Q9KJD0
D	531	HIS	-	expression tag	UNP Q9KJD0

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



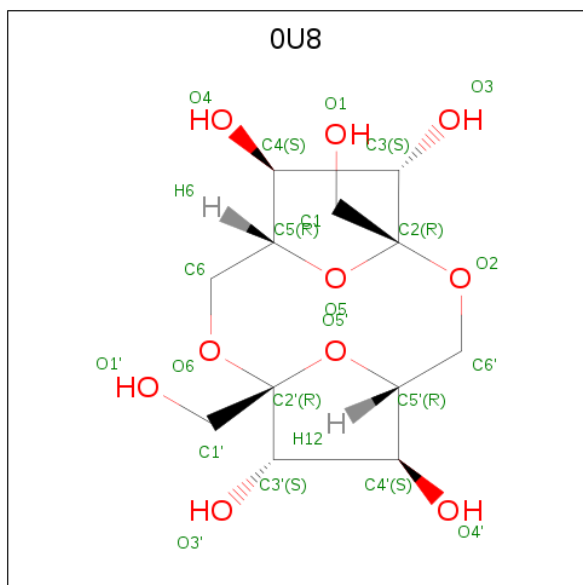
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is (1R,4R,5S,6S,7R,10R,11S,12S)-1,7-bis(hydroxymethyl)-2,8,13,14-tetraoxatricyclo[8.2.1.1.4,7]tetradecane-5,6,11,12-tetrol (three-letter code: 0U8) (formula: C<sub>12</sub>H<sub>20</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	12	10		
3	B	1	Total	C	O	0	0
			22	12	10		
3	C	1	Total	C	O	0	0
			22	12	10		
3	D	1	Total	C	O	0	0
			22	12	10		

- Molecule 4 is water.

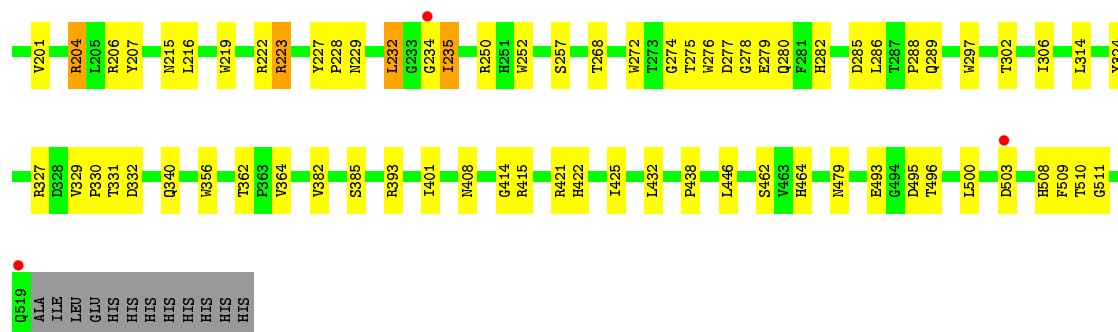
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	184	Total	O	0	0
			184	184		
4	C	240	Total	O	0	0
			240	240		
4	D	228	Total	O	0	0
			228	228		

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.

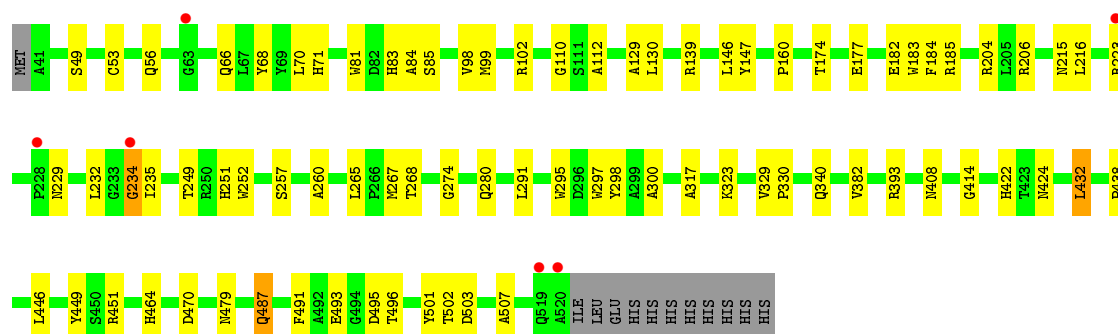
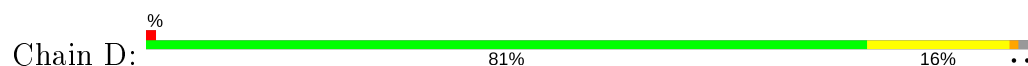
- Chain A:
- 
- 2% 79% 17%
- W183 F184 R185 K188 I189 G203 R204 L205 R206 Y207 N215 L216 R223 N229 L232 G233 G234 T235 W252 S257 W258 D259 A260 L265 T268 T275 Q280 K295 D296 W297 Y298 A299 A300 T306 A317 Y324 R327 R348 L360 L377
- MET A41 P48 L52 G53 Q56 R57 T60 Y65 Y68 Y69 L70 W81 H94 H99 P103 N118 A124 T132 K140 Y141 Q142 Y145 L146 Y147 L159 P160 D161 P162 H166 G169 R170 A171 A172 T173 T174 P175 A176 E177 L178 F182

- [illegible]

- Chain C:



- Molecule 1: Levan fructotransferase



- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose



- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose



- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose



- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose





FRU1  
FRU2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.86Å 161.91Å 263.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.8 (50.00-2.30) 96.9 (50.04-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.72 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.205 , 0.240 0.209 , 0.241	Depositor DCC
$R_{free}$ test set	15480 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.757	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15976	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.43% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0U8, FRU

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	0.31	0/3863	0.65	3/5312 (0.1%)
1	B	0.33	0/3863	0.65	2/5312 (0.0%)
1	C	0.33	0/3858	0.64	1/5305 (0.0%)
1	D	0.33	0/3863	0.65	2/5312 (0.0%)
All	All	0.32	0/15447	0.64	8/21241 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	LEU	CA-CB-CG	-7.53	97.97	115.30
1	C	432	LEU	N-CA-C	-6.60	93.18	111.00
1	A	432	LEU	N-CA-C	-6.20	94.25	111.00
1	D	432	LEU	N-CA-C	-6.05	94.66	111.00
1	A	234	GLY	N-CA-C	5.89	127.83	113.10
1	B	432	LEU	N-CA-C	-5.78	95.40	111.00
1	D	234	GLY	N-CA-C	5.55	126.98	113.10
1	B	234	GLY	N-CA-C	5.41	126.61	113.10

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	3739	0	3489	69	0
1	B	3739	0	3489	66	0
1	C	3734	0	3484	82	0
1	D	3739	0	3489	61	0
2	E	23	0	22	1	0
2	F	23	0	22	0	0
2	G	23	0	22	3	0
2	H	23	0	22	3	0
3	A	22	0	19	1	0
3	B	22	0	19	6	0
3	C	22	0	19	3	0
3	D	22	0	19	1	0
4	A	193	0	0	2	0
4	B	184	0	0	3	0
4	C	240	0	0	6	0
4	D	228	0	0	4	0
All	All	15976	0	14115	288	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 10.

All (288) 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)
3:C:602:0U8:H11	3:C:602:0U8:H19	1.34	1.07
3:C:602:0U8:H11	3:C:602:0U8:C4	1.91	0.99
1:A:57:ARG:HD2	1:A:188:LYS:HE3	1.56	0.86
1:D:329:VAL:HG13	1:D:330:PRO:HD2	1.58	0.86
1:D:206:ARG:HH11	1:D:234:GLY:HA3	1.44	0.82
1:B:57:ARG:HD2	1:B:188:LYS:HE2	1.61	0.80
1:C:329:VAL:HG13	1:C:330:PRO:HD2	1.65	0.79
1:C:206:ARG:HD3	1:C:234:GLY:HA2	1.66	0.77
1:D:464:HIS:H	1:D:479:ASN:ND2	1.83	0.76
1:B:327:ARG:HH22	1:B:490:HIS:HE1	1.36	0.73
1:B:53:CYS:HB3	1:B:70:LEU:HB2	1.70	0.73
1:C:503:ASP:OD2	3:C:602:0U8:H7	1.88	0.72
1:D:223:ARG:HD2	1:D:280:GLN:CD	2.10	0.72
1:B:331:THR:HA	1:B:334:SER:HB3	1.70	0.72
1:C:234:GLY:O	1:C:235:ILE:HG12	1.89	0.71
1:A:81:TRP:HB2	1:A:99:MET:HB2	1.73	0.71
2:G:1:FRU:H62	2:G:2:FRU:H61	1.72	0.70
1:C:229:ASN:HB3	1:C:232:LEU:HD22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:HH12	1:C:188:LYS:NZ	1.91	0.69
1:C:206:ARG:HH11	1:C:234:GLY:CA	2.07	0.68
1:C:414:GLY:O	1:C:495:ASP:HB3	1.92	0.68
1:A:142:GLN:HE22	1:A:185:ARG:HH11	1.41	0.67
1:C:53:CYS:HB3	1:C:70:LEU:HB2	1.77	0.67
1:D:464:HIS:H	1:D:479:ASN:HD21	1.42	0.67
1:A:53:CYS:HB3	1:A:70:LEU:HB2	1.78	0.66
1:B:145:TYR:CZ	1:B:162:PRO:HG3	2.30	0.66
1:B:146:LEU:HD23	1:B:147:TYR:N	2.11	0.65
1:A:432:LEU:HD22	1:A:478:VAL:CG2	2.28	0.64
1:D:53:CYS:HB3	1:D:70:LEU:HB2	1.78	0.64
1:C:464:HIS:H	1:C:479:ASN:ND2	1.95	0.63
2:H:1:FRU:H62	2:H:2:FRU:C6	2.29	0.63
1:A:206:ARG:NE	1:A:233:GLY:HA2	2.14	0.63
1:A:229:ASN:O	1:A:232:LEU:HB2	1.99	0.62
1:B:408:ASN:HB3	1:B:503:ASP:HB2	1.82	0.62
1:D:267:MET:CE	1:D:323:LYS:HD3	2.30	0.62
1:C:285:ASP:HB3	4:C:754:HOH:O	1.98	0.61
1:D:249:THR:OG1	1:D:251:HIS:HE1	1.83	0.61
1:C:422:HIS:O	1:C:438:PRO:HB2	2.01	0.61
1:D:229:ASN:O	1:D:232:LEU:HB2	1.99	0.60
1:D:329:VAL:CG1	1:D:330:PRO:HD2	2.30	0.60
1:A:174:THR:HG23	1:A:177:GLU:OE1	2.01	0.60
1:A:324:TYR:O	1:A:327:ARG:HG2	2.02	0.60
1:B:203:GLY:HA2	1:B:235:ILE:HG22	1.82	0.60
1:A:223:ARG:HB2	1:A:280:GLN:HB3	1.84	0.59
1:B:324:TYR:O	1:B:327:ARG:HG2	2.02	0.59
1:D:66:GLN:HE22	1:D:85:SER:HB3	1.68	0.59
1:B:327:ARG:HH22	1:B:490:HIS:CE1	2.20	0.59
1:A:229:ASN:ND2	1:A:232:LEU:HD13	2.18	0.58
1:A:422:HIS:O	1:A:438:PRO:HB2	2.03	0.58
1:B:206:ARG:NE	1:B:233:GLY:HA2	2.18	0.58
1:A:306:ILE:HD13	1:A:306:ILE:O	2.04	0.58
1:C:64:ALA:HB2	1:C:87:THR:HG22	1.85	0.58
1:A:203:GLY:HA2	1:A:235:ILE:HG22	1.85	0.58
1:C:329:VAL:HG13	1:C:330:PRO:CD	2.33	0.58
3:B:602:OU8:H19	3:B:602:OU8:H11	1.86	0.57
1:D:329:VAL:HG13	1:D:330:PRO:CD	2.33	0.57
1:D:267:MET:HE1	1:D:323:LYS:HD3	1.86	0.57
1:D:184:PHE:HD1	1:D:204:ARG:HD3	1.69	0.57
1:A:204:ARG:HD3	1:A:207:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:C	1:A:146:LEU:HD23	2.25	0.57
1:C:329:VAL:HG12	1:C:331:THR:H	1.69	0.57
1:D:206:ARG:HH11	1:D:234:GLY:CA	2.14	0.56
1:D:215:ASN:O	1:D:216:LEU:HB2	2.06	0.56
1:D:422:HIS:O	1:D:438:PRO:HB2	2.05	0.55
1:D:257:SER:HA	1:D:268:THR:O	2.06	0.55
1:B:145:TYR:CE1	1:B:162:PRO:HG3	2.41	0.55
1:B:51:TRP:HB2	1:B:75:ASN:HD22	1.72	0.55
1:A:188:LYS:HE2	1:A:189:ILE:O	2.06	0.55
1:D:323:LYS:HG2	1:D:449:TYR:CZ	2.42	0.55
1:C:204:ARG:HH21	2:G:1:FRU:H3	1.71	0.55
1:B:44:HIS:HD2	1:B:470:ASP:OD2	1.88	0.55
1:C:83:HIS:CD2	1:C:84:ALA:N	2.75	0.55
1:A:432:LEU:HD22	1:A:478:VAL:HG21	1.87	0.54
2:H:1:FRU:H62	2:H:2:FRU:H61	1.89	0.54
1:B:130:LEU:HB2	1:B:189:ILE:HD11	1.89	0.54
1:B:327:ARG:NH2	1:B:490:HIS:HE1	2.03	0.54
1:D:206:ARG:NH1	1:D:234:GLY:HA3	2.19	0.54
1:C:215:ASN:O	1:C:216:LEU:HB2	2.07	0.54
1:C:229:ASN:O	1:C:232:LEU:HB2	2.07	0.54
3:B:602:OU8:H11	3:B:602:OU8:C4	2.35	0.53
1:A:166:ASN:HD22	1:A:166:ASN:C	2.11	0.53
1:D:251:HIS:HD2	4:D:749:HOH:O	1.91	0.53
1:C:183:TRP:O	1:C:204:ARG:HD2	2.09	0.53
1:A:145:TYR:CE1	1:A:162:PRO:HD3	2.43	0.53
1:C:510:THR:HG22	1:C:511:GLY:N	2.23	0.53
3:B:602:OU8:O3	3:B:602:OU8:H11	2.09	0.53
1:B:215:ASN:O	1:B:216:LEU:HB2	2.10	0.52
1:C:393:ARG:HD3	1:C:496:THR:HG22	1.91	0.52
1:B:508:HIS:HB2	4:B:861:HOH:O	2.08	0.52
1:A:60:THR:HG22	1:A:65:TYR:HD1	1.73	0.52
1:C:57:ARG:HH12	1:C:188:LYS:HZ1	1.56	0.52
1:D:393:ARG:HD3	1:D:496:THR:HG22	1.92	0.52
1:C:324:TYR:O	1:C:327:ARG:HG2	2.10	0.52
1:A:142:GLN:NE2	1:A:184:PHE:H	2.08	0.51
1:B:118:ASN:HB2	1:B:124:ALA:HA	1.92	0.51
1:B:519:GLN:N	1:B:519:GLN:OE1	2.41	0.51
1:A:432:LEU:HD22	1:A:478:VAL:HG22	1.91	0.51
1:B:178:ILE:O	1:B:182:GLU:HG3	2.10	0.51
1:A:408:ASN:HB3	1:A:503:ASP:HB2	1.92	0.51
1:D:252:TRP:HB2	1:D:274:GLY:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:NH1	1:C:188:LYS:HE2	2.26	0.51
1:D:56:GLN:HB2	1:D:68:TYR:HB2	1.92	0.51
1:C:252:TRP:HB2	1:C:274:GLY:O	2.11	0.51
1:C:329:VAL:O	1:C:332:ASP:HB2	2.11	0.51
1:B:257:SER:HB3	1:B:298:TYR:CE1	2.46	0.50
1:B:69:TYR:OH	1:B:94:HIS:HD2	1.94	0.50
2:G:1:FRU:H62	2:G:2:FRU:C6	2.41	0.50
1:C:146:LEU:HD23	1:C:146:LEU:C	2.32	0.50
1:D:257:SER:HB3	1:D:298:TYR:CE2	2.47	0.50
1:D:146:LEU:HD23	1:D:146:LEU:C	2.32	0.50
1:D:295:TRP:H	1:D:487:GLN:HG3	1.77	0.50
1:B:363:PRO:HG3	1:B:477:PHE:CE2	2.46	0.50
1:D:139:ARG:HG2	1:D:182:GLU:HG2	1.94	0.50
1:D:66:GLN:NE2	1:D:85:SER:HB3	2.26	0.50
1:C:81:TRP:HB2	1:C:99:MET:HB2	1.93	0.50
1:A:257:SER:HB3	1:A:298:TYR:CE1	2.47	0.49
1:A:379:ASP:HB3	1:A:510:THR:HG22	1.93	0.49
1:B:404:ASP:HB3	4:B:850:HOH:O	2.12	0.49
1:A:295:TRP:HD1	1:A:487:GLN:HG2	1.77	0.49
1:C:234:GLY:O	1:C:235:ILE:CG1	2.60	0.49
1:A:178:ILE:O	1:A:182:GLU:HG3	2.12	0.49
1:C:57:ARG:NH1	1:C:188:LYS:NZ	2.58	0.49
1:D:174:THR:OG1	1:D:177:GLU:HG3	2.13	0.49
1:A:207:TYR:CE2	2:E:2:FRU:H61	2.47	0.49
1:C:393:ARG:CD	1:C:496:THR:HG22	2.42	0.49
1:B:118:ASN:HB2	1:B:124:ALA:CA	2.42	0.49
1:C:464:HIS:H	1:C:479:ASN:HD21	1.58	0.49
1:B:138:VAL:HB	1:B:141:TYR:CD2	2.48	0.49
1:A:48:PRO:HD3	1:A:94:HIS:CD2	2.48	0.48
1:C:276:TRP:NE1	1:C:278:GLY:HA2	2.28	0.48
1:C:510:THR:CG2	1:C:511:GLY:N	2.75	0.48
1:B:146:LEU:HD23	1:B:146:LEU:C	2.34	0.48
1:B:260:ALA:CB	1:B:265:LEU:HB2	2.43	0.48
1:B:432:LEU:HD13	1:B:478:VAL:HG21	1.95	0.48
1:C:408:ASN:HB3	1:C:503:ASP:HB2	1.94	0.48
1:A:146:LEU:HD23	1:A:147:TYR:N	2.29	0.48
1:C:165:VAL:HG22	4:C:886:HOH:O	2.13	0.48
1:B:81:TRP:HB2	1:B:99:MET:HB2	1.95	0.48
1:A:396:GLU:HG3	1:A:468:LEU:HD12	1.96	0.48
1:C:204:ARG:HB2	1:C:207:TYR:O	2.13	0.47
1:A:140:LYS:HG3	1:A:141:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ALA:CB	1:A:265:LEU:HB2	2.45	0.47
1:D:267:MET:HE3	1:D:323:LYS:HD3	1.96	0.47
1:D:300:ALA:HB2	1:D:317:ALA:HB2	1.96	0.47
1:D:329:VAL:CG1	1:D:330:PRO:CD	2.92	0.47
1:B:183:TRP:HA	1:B:185:ARG:NH1	2.30	0.47
1:C:206:ARG:HD3	1:C:234:GLY:CA	2.41	0.47
1:B:83:HIS:CD2	1:B:84:ALA:N	2.82	0.47
1:C:252:TRP:HB2	1:C:275:THR:HA	1.97	0.47
1:C:206:ARG:H	1:C:234:GLY:HA2	1.80	0.47
1:D:204:ARG:O	1:D:234:GLY:O	2.33	0.47
1:D:408:ASN:HB3	1:D:503:ASP:HB2	1.97	0.47
1:B:433:TYR:CZ	3:B:602:OU8:H2	2.50	0.47
1:C:493:GLU:HG2	1:D:493:GLU:HG2	1.95	0.47
1:A:118:ASN:HB2	1:A:124:ALA:HA	1.97	0.47
1:C:206:ARG:NH1	1:C:234:GLY:CA	2.78	0.47
1:A:300:ALA:HB2	1:A:317:ALA:HB2	1.97	0.46
1:C:206:ARG:NH1	1:C:234:GLY:N	2.63	0.46
1:B:257:SER:HA	1:B:268:THR:O	2.15	0.46
1:B:300:ALA:HB2	1:B:317:ALA:HB2	1.98	0.46
1:D:81:TRP:HB2	1:D:99:MET:HB2	1.97	0.46
1:B:60:THR:HG21	1:B:306:ILE:HD13	1.97	0.46
1:C:133:GLN:HB2	1:C:145:TYR:CD2	2.51	0.46
1:D:102:ARG:HD3	4:D:780:HOH:O	2.16	0.46
1:D:414:GLY:O	1:D:495:ASP:HB3	2.16	0.46
1:A:252:TRP:HB2	1:A:275:THR:HA	1.98	0.46
1:C:234:GLY:O	1:C:235:ILE:CB	2.63	0.46
1:A:118:ASN:HB2	1:A:124:ALA:CA	2.45	0.46
1:B:432:LEU:HD13	1:B:478:VAL:CG2	2.46	0.46
1:B:433:TYR:CE2	3:B:602:OU8:H2	2.50	0.46
1:C:160:PRO:HG2	4:C:772:HOH:O	2.16	0.46
1:A:174:THR:O	1:A:178:ILE:HG12	2.15	0.46
1:B:425:ILE:HD12	1:B:425:ILE:N	2.31	0.46
1:B:470:ASP:HB3	4:B:708:HOH:O	2.15	0.45
1:B:472:GLN:OE1	1:B:490:HIS:HD2	1.99	0.45
1:C:302:THR:HA	1:C:314:LEU:O	2.16	0.45
1:A:203:GLY:CA	1:A:235:ILE:HG22	2.47	0.45
1:A:166:ASN:ND2	1:A:169:GLY:H	2.14	0.45
1:A:215:ASN:O	1:A:216:LEU:HB2	2.16	0.45
1:A:56:GLN:HB2	1:A:68:TYR:HB2	1.98	0.45
1:A:60:THR:HG22	1:A:65:TYR:CD1	2.52	0.45
1:B:80:GLY:HA2	1:B:107:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:PRO:CG	1:C:286:LEU:HD13	2.47	0.45
1:D:260:ALA:HB1	1:D:265:LEU:HB2	1.98	0.45
1:A:183:TRP:CD1	1:A:204:ARG:HA	2.52	0.45
1:B:422:HIS:O	1:B:438:PRO:HB2	2.17	0.45
1:C:118:ASN:HB2	1:C:124:ALA:CA	2.47	0.45
1:B:457:ASP:HA	1:B:458:PRO:HD3	1.89	0.45
1:C:60:THR:HG21	1:C:306:ILE:HD13	1.99	0.45
1:A:173:THR:HG23	1:A:177:GLU:OE1	2.16	0.44
1:A:234:GLY:HA2	4:A:866:HOH:O	2.17	0.44
1:C:98:VAL:HG13	1:C:156:PHE:CD2	2.52	0.44
1:D:183:TRP:HA	1:D:185:ARG:NH1	2.32	0.44
1:D:424:ASN:HB3	1:D:501:TYR:OH	2.17	0.44
1:A:295:TRP:H	1:A:487:GLN:HG3	1.82	0.44
1:A:257:SER:HA	1:A:268:THR:O	2.16	0.44
1:B:203:GLY:CA	1:B:235:ILE:HG22	2.46	0.44
1:A:260:ALA:HB1	1:A:265:LEU:HB2	1.99	0.44
1:A:377:LEU:N	1:A:377:LEU:HD12	2.33	0.44
1:C:206:ARG:HH11	1:C:234:GLY:HA2	1.83	0.44
1:C:425:ILE:HD12	1:C:425:ILE:N	2.33	0.44
1:C:83:HIS:HD2	1:C:84:ALA:N	2.13	0.44
1:B:228:PRO:HD3	1:B:286:LEU:HD13	2.00	0.44
1:D:451:ARG:HE	3:D:602:OU8:H3	1.82	0.44
1:B:433:TYR:CE1	3:B:602:OU8:H15	2.52	0.44
1:C:216:LEU:HA	1:C:219:TRP:CZ2	2.53	0.44
3:A:602:OU8:H10	3:A:602:OU8:O1	2.18	0.44
1:B:183:TRP:CD1	1:B:204:ARG:HA	2.53	0.44
1:C:146:LEU:HD23	1:C:147:TYR:N	2.34	0.43
1:C:401:ILE:O	1:C:462:SER:HA	2.17	0.43
1:A:142:GLN:HE21	1:A:184:PHE:H	1.66	0.43
1:A:445:SER:HA	4:A:836:HOH:O	2.17	0.43
1:B:110:GLY:HA3	1:B:130:LEU:O	2.18	0.43
1:C:188:LYS:HB3	1:C:201:VAL:CG1	2.49	0.43
1:D:206:ARG:HA	1:D:234:GLY:HA2	1.99	0.43
1:B:107:VAL:HA	1:B:133:GLN:HG2	2.00	0.43
1:C:250:ARG:HH11	1:C:250:ARG:HG2	1.83	0.43
1:C:362:THR:HG22	4:C:897:HOH:O	2.18	0.43
1:D:112:ALA:HB2	1:D:129:ALA:HB2	2.00	0.43
1:D:260:ALA:CB	1:D:265:LEU:HB2	2.49	0.43
1:A:306:ILE:C	1:A:306:ILE:HD13	2.38	0.43
1:B:66:GLN:OE1	1:B:85:SER:HB3	2.19	0.43
1:D:110:GLY:HA3	1:D:130:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:SER:HB2	1:A:499:SER:OG	2.19	0.43
1:A:229:ASN:HB3	1:A:232:LEU:HD22	2.01	0.43
1:A:414:GLY:O	1:A:495:ASP:HB3	2.19	0.43
1:C:415:ARG:HA	1:C:421:ARG:O	2.19	0.43
1:B:207:TYR:O	1:B:235:ILE:HG21	2.19	0.42
1:B:414:GLY:O	1:B:495:ASP:HB3	2.19	0.42
1:D:414:GLY:HA3	1:D:491:PHE:CE1	2.54	0.42
1:D:502:THR:HG21	1:D:507:ALA:HB3	2.01	0.42
1:C:110:GLY:HA3	1:C:130:LEU:O	2.19	0.42
1:B:472:GLN:HA	1:B:489:VAL:O	2.19	0.42
1:C:272:TRP:CE2	1:C:288:PRO:HB3	2.54	0.42
1:C:277:ASP:OD1	1:C:282:HIS:HE1	2.02	0.42
1:D:146:LEU:HD23	1:D:147:TYR:N	2.34	0.42
1:A:295:TRP:CD1	1:A:487:GLN:HG2	2.54	0.42
1:A:430:ALA:HB2	1:A:458:PRO:HG3	2.01	0.42
1:B:144:GLN:HB2	1:B:164:ILE:HB	2.02	0.42
1:C:222:ARG:HA	1:C:222:ARG:HD3	1.86	0.42
1:D:160:PRO:HG2	4:D:835:HOH:O	2.20	0.42
1:B:135:THR:HB	1:B:141:TYR:HB3	2.02	0.42
1:B:223:ARG:HG2	1:B:223:ARG:NH1	2.35	0.42
1:C:118:ASN:HB2	1:C:124:ALA:HA	2.01	0.42
1:D:470:ASP:HB3	4:D:777:HOH:O	2.20	0.42
2:H:1:FRU:H62	2:H:2:FRU:C5	2.49	0.42
1:C:159:LEU:HD12	1:C:160:PRO:HD2	2.02	0.41
1:C:227:TYR:HA	1:C:228:PRO:HD3	1.85	0.41
1:C:508:HIS:HB2	4:C:868:HOH:O	2.20	0.41
1:C:500:LEU:HD13	1:C:509:PHE:CG	2.54	0.41
1:B:327:ARG:NH2	1:B:446:LEU:HD21	2.35	0.41
1:A:203:GLY:HA2	1:A:235:ILE:CG2	2.50	0.41
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.85	0.41
1:C:159:LEU:HA	1:C:160:PRO:HD2	1.82	0.41
1:C:184:PHE:HD1	1:C:204:ARG:HD3	1.85	0.41
1:B:379:ASP:HB3	1:B:510:THR:HG22	2.01	0.41
1:C:107:VAL:HA	1:C:133:GLN:HG2	2.02	0.41
1:D:206:ARG:NH1	1:D:234:GLY:N	2.69	0.41
1:D:83:HIS:CD2	1:D:84:ALA:N	2.89	0.41
1:A:159:LEU:HA	1:A:160:PRO:HD2	1.85	0.41
1:A:457:ASP:HA	1:A:458:PRO:HD3	1.95	0.41
1:A:519:GLN:O	1:A:520:ALA:HB2	2.21	0.41
1:B:432:LEU:HD13	1:B:478:VAL:HG11	2.02	0.41
1:B:56:GLN:HB2	1:B:68:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:SER:HA	1:C:500:LEU:O	2.21	0.41
1:C:57:ARG:HA	1:C:58:PRO:HD3	1.89	0.41
1:A:132:THR:HG21	1:A:185:ARG:HB3	2.03	0.41
1:A:140:LYS:O	1:A:169:GLY:HA3	2.21	0.41
1:B:245:ALA:HB2	1:B:349:LEU:HD23	2.03	0.41
1:D:223:ARG:HD2	1:D:280:GLN:CG	2.50	0.41
1:D:291:LEU:HA	1:D:291:LEU:HD12	1.92	0.41
1:B:227:TYR:CE2	1:B:235:ILE:HD11	2.56	0.41
1:C:223:ARG:HB2	1:C:280:GLN:HB3	2.03	0.41
1:D:432:LEU:HA	1:D:432:LEU:HD22	1.96	0.41
1:C:84:ALA:HA	1:C:93:THR:O	2.20	0.41
1:C:174:THR:O	1:C:178:ILE:HG13	2.21	0.40
1:A:379:ASP:CG	1:A:510:THR:HG22	2.42	0.40
1:C:257:SER:HA	1:C:268:THR:O	2.21	0.40
1:D:99:MET:HG2	1:D:147:TYR:CD1	2.56	0.40
1:A:52:LEU:HD12	1:A:69:TYR:CD1	2.56	0.40
1:B:260:ALA:HB3	1:B:265:LEU:HB2	2.03	0.40
1:C:364:VAL:HG22	4:C:871:HOH:O	2.21	0.40
1:A:348:ARG:NH2	1:A:360:LEU:HD13	2.36	0.40
1:C:289:GLN:NE2	1:C:356:TRP:HZ3	2.19	0.40
1:D:49:SER:O	1:D:71:HIS:HE1	2.05	0.40
1:A:69:TYR:OH	1:A:94:HIS:HD2	2.04	0.40
1:D:183:TRP:O	1:D:204:ARG:HD2	2.21	0.40
1:D:295:TRP:HD1	1:D:487:GLN:HG2	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	478/492 (97%)	449 (94%)	27 (6%)	2 (0%)	34 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	478/492 (97%)	452 (95%)	24 (5%)	2 (0%)	34	42
1	C	477/492 (97%)	452 (95%)	24 (5%)	1 (0%)	47	58
1	D	478/492 (97%)	450 (94%)	27 (6%)	1 (0%)	47	58
All	All	1911/1968 (97%)	1803 (94%)	102 (5%)	6 (0%)	41	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ILE
1	B	235	ILE
1	C	235	ILE
1	D	235	ILE
1	A	103	PRO
1	B	103	PRO

### 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	381/393 (97%)	372 (98%)	9 (2%)	49	66
1	B	381/393 (97%)	375 (98%)	6 (2%)	62	78
1	C	381/393 (97%)	371 (97%)	10 (3%)	46	63
1	D	381/393 (97%)	375 (98%)	6 (2%)	62	78
All	All	1524/1572 (97%)	1493 (98%)	31 (2%)	55	72

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	173	THR
1	A	232	LEU
1	A	258	MET
1	A	297	TRP

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Mol	Chain	Res	Type
1	A	306	ILE
1	A	432	LEU
1	A	448	PRO
1	A	487	GLN
1	B	104	ASP
1	B	130	LEU
1	B	279	GLU
1	B	297	TRP
1	B	487	GLN
1	B	503	ASP
1	C	99	MET
1	C	118	ASN
1	C	204	ARG
1	C	223	ARG
1	C	232	LEU
1	C	279	GLU
1	C	297	TRP
1	C	340	GLN
1	C	382	VAL
1	C	446	LEU
1	D	98	VAL
1	D	297	TRP
1	D	340	GLN
1	D	382	VAL
1	D	446	LEU
1	D	487	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	133	GLN
1	A	142	GLN
1	A	144	GLN
1	A	166	ASN
1	A	229	ASN
1	A	280	GLN
1	B	44	HIS
1	B	75	ASN
1	B	94	HIS
1	B	369	ASN
1	B	490	HIS

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Mol	Chain	Res	Type
1	C	94	HIS
1	C	118	ASN
1	C	282	HIS
1	C	289	GLN
1	C	341	ASN
1	C	479	ASN
1	D	66	GLN
1	D	71	HIS
1	D	144	GLN
1	D	251	HIS
1	D	280	GLN
1	D	289	GLN
1	D	341	ASN
1	D	391	ASN
1	D	422	HIS
1	D	479	ASN
1	D	519	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 ⓘ

8 monosaccharides 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	FRU	E	1	2	11,12,12	1.39	1 (9%)	10,18,18	1.56	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FRU	E	2	2	11,11,12	1.53	1 (9%)	15,15,18	1.13	1 (6%)
2	FRU	F	1	2	11,12,12	1.34	1 (9%)	10,18,18	1.29	2 (20%)
2	FRU	F	2	2	11,11,12	1.52	1 (9%)	15,15,18	1.15	0
2	FRU	G	1	2	11,12,12	1.31	0	10,18,18	1.69	1 (10%)
2	FRU	G	2	2	11,11,12	1.44	1 (9%)	15,15,18	1.04	0
2	FRU	H	1	2	11,12,12	1.25	1 (9%)	10,18,18	1.57	2 (20%)
2	FRU	H	2	2	11,11,12	1.51	1 (9%)	15,15,18	1.24	2 (13%)

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	FRU	E	1	2	-	5/5/24/24	0/1/1/1
2	FRU	E	2	2	-	2/4/20/24	0/1/1/1
2	FRU	F	1	2	-	2/5/24/24	0/1/1/1
2	FRU	F	2	2	-	0/4/20/24	0/1/1/1
2	FRU	G	1	2	-	5/5/24/24	0/1/1/1
2	FRU	G	2	2	-	1/4/20/24	0/1/1/1
2	FRU	H	1	2	-	2/5/24/24	0/1/1/1
2	FRU	H	2	2	-	4/4/20/24	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	FRU	C4-C3	-3.52	1.43	1.53
2	H	2	FRU	C4-C3	-3.25	1.44	1.53
2	G	2	FRU	C4-C3	-3.15	1.44	1.53
2	E	2	FRU	C4-C3	-3.04	1.45	1.53
2	F	1	FRU	O3-C3	-2.33	1.38	1.42
2	E	1	FRU	O3-C3	-2.25	1.38	1.42
2	H	1	FRU	O3-C3	-2.10	1.38	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	FRU	O1-C1-C2	4.53	121.50	111.86
2	H	1	FRU	O1-C1-C2	3.43	119.17	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	FRU	O1-C1-C2	3.15	118.57	111.86
2	H	1	FRU	O6-C6-C5	2.54	120.02	111.29
2	E	1	FRU	O6-C6-C5	2.51	119.89	111.29
2	F	1	FRU	O1-C1-C2	2.44	117.05	111.86
2	H	2	FRU	O1-C1-C2	2.21	118.88	111.29
2	H	2	FRU	C1-C2-C3	-2.20	109.78	115.09
2	F	1	FRU	O6-C6-C5	2.18	118.78	111.29
2	E	1	FRU	O5-C5-C6	2.11	114.73	108.85
2	E	2	FRU	O6-C6-C5	2.03	118.25	111.29

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	FRU	O1-C1-C2-O2
2	G	1	FRU	O1-C1-C2-C3
2	G	1	FRU	O1-C1-C2-O2
2	H	2	FRU	O1-C1-C2-O5
2	H	1	FRU	C4-C5-C6-O6
2	H	2	FRU	O1-C1-C2-C3
2	E	2	FRU	O1-C1-C2-O5
2	H	1	FRU	O5-C5-C6-O6
2	F	1	FRU	O5-C5-C6-O6
2	E	1	FRU	O5-C5-C6-O6
2	E	1	FRU	C4-C5-C6-O6
2	G	1	FRU	O1-C1-C2-O5
2	G	1	FRU	O5-C5-C6-O6
2	F	1	FRU	C4-C5-C6-O6
2	H	2	FRU	O5-C5-C6-O6
2	H	2	FRU	C4-C5-C6-O6
2	E	1	FRU	O1-C1-C2-C3
2	G	1	FRU	C4-C5-C6-O6
2	G	2	FRU	O1-C1-C2-O5
2	E	1	FRU	O1-C1-C2-O5
2	E	2	FRU	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	FRU	2	0

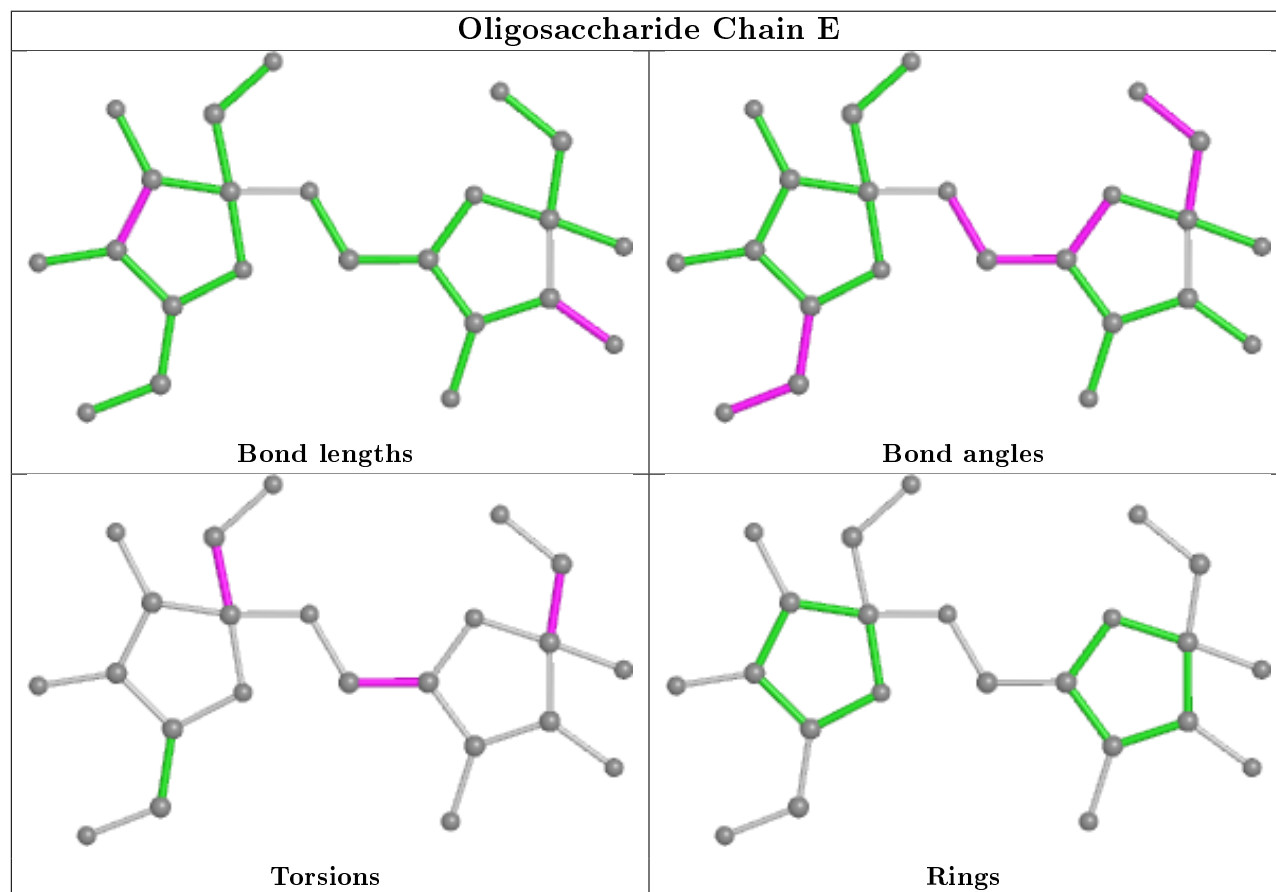
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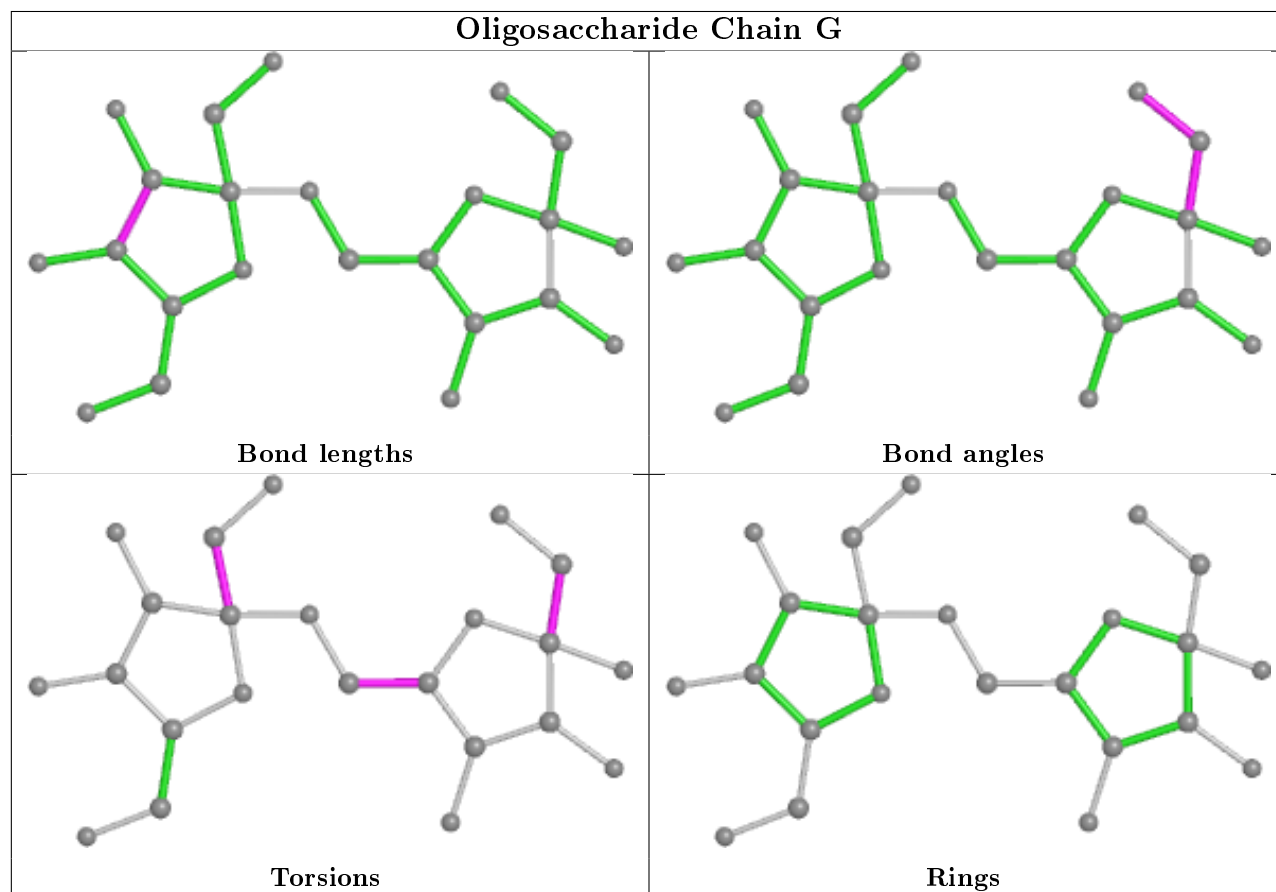
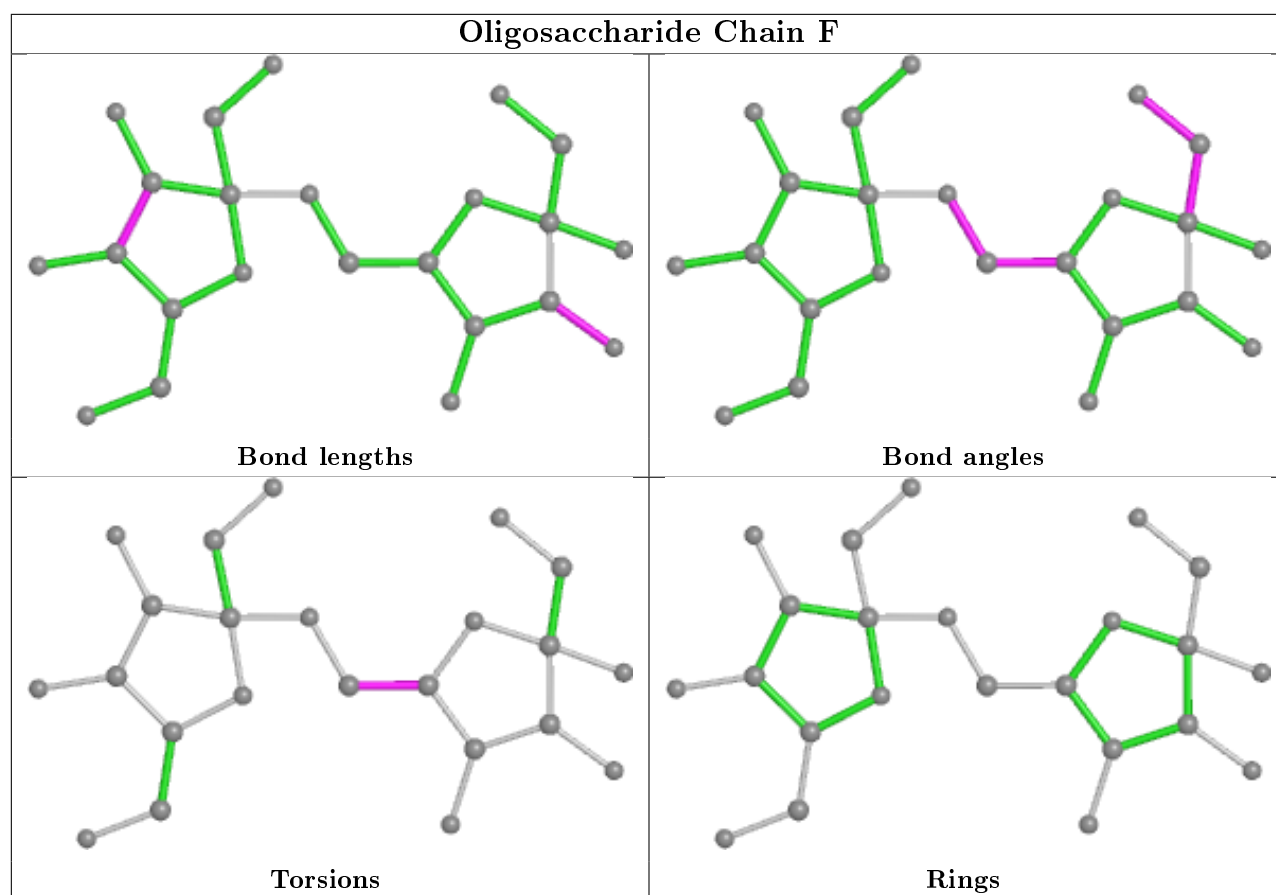


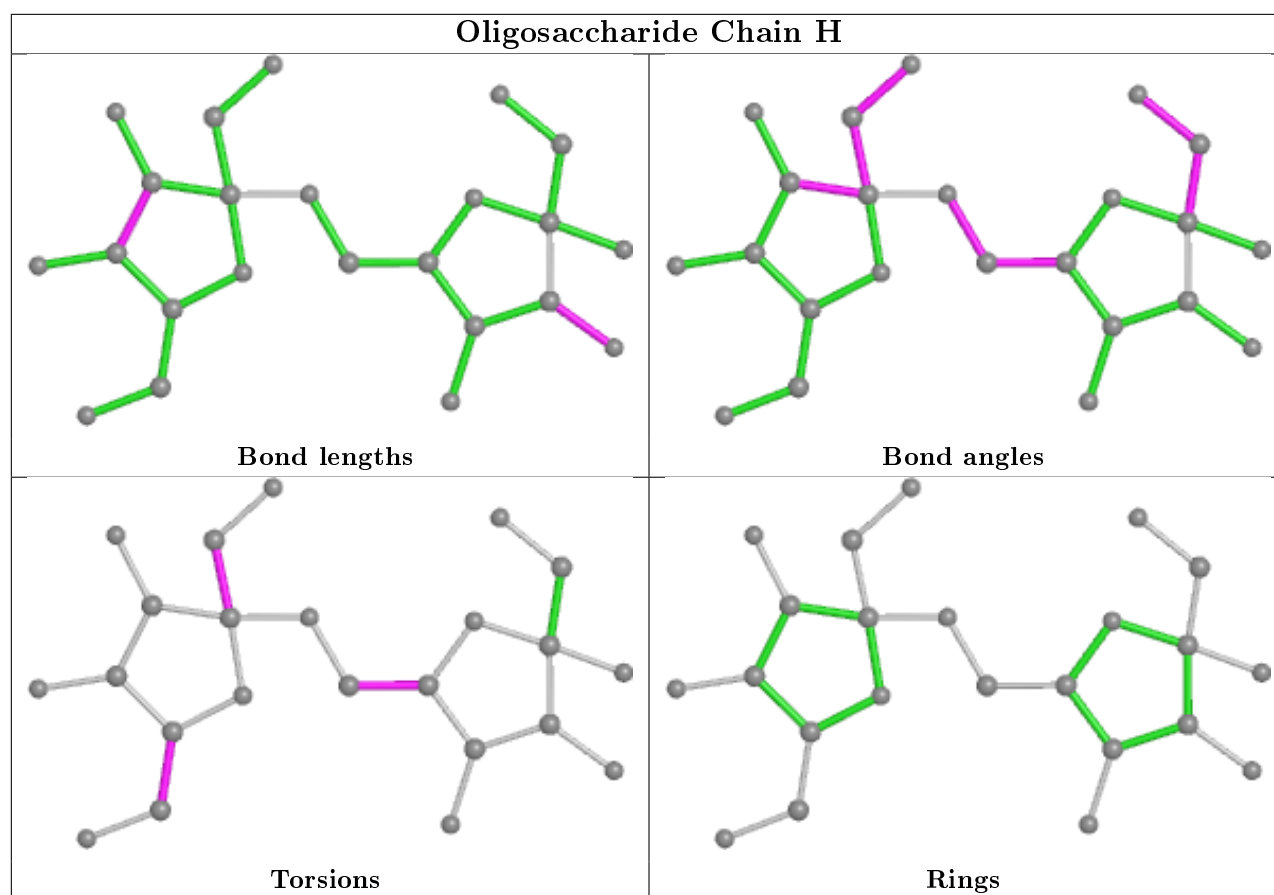
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	FRU	1	0
2	H	1	FRU	3	0
2	H	2	FRU	3	0
2	G	1	FRU	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







## 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	$\# Z  > 2$
3	0U8	A	602	-	24,24,24	2.05	7 (29%)	36,38,38	2.01	11 (30%)
3	0U8	B	602	-	24,24,24	1.93	6 (25%)	36,38,38	2.01	10 (27%)
3	0U8	C	602	-	24,24,24	2.22	6 (25%)	36,38,38	2.12	11 (30%)
3	0U8	D	602	-	24,24,24	2.08	6 (25%)	36,38,38	2.59	13 (36%)

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
3	0U8	A	602	-	-	7/18/56/56	0/2/3/3
3	0U8	B	602	-	-	10/18/56/56	0/2/3/3
3	0U8	C	602	-	-	7/18/56/56	0/2/3/3
3	0U8	D	602	-	-	10/18/56/56	0/2/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	0U8	O6-C2'	7.66	1.51	1.41
3	A	602	0U8	O6-C2'	6.76	1.50	1.41
3	D	602	0U8	O6-C2'	6.69	1.50	1.41
3	B	602	0U8	O6-C2'	5.96	1.49	1.41
3	A	602	0U8	O5'-C2'	3.43	1.50	1.42
3	B	602	0U8	O5'-C2'	3.24	1.49	1.42
3	C	602	0U8	O5'-C2'	3.15	1.49	1.42
3	D	602	0U8	O3-C3	-3.10	1.36	1.42
3	C	602	0U8	O4'-C4'	-3.05	1.35	1.43
3	A	602	0U8	O3-C3	-3.03	1.36	1.42
3	B	602	0U8	O3-C3	-3.03	1.36	1.42
3	D	602	0U8	O5'-C2'	3.01	1.49	1.42
3	C	602	0U8	O5-C5	2.81	1.49	1.43
3	D	602	0U8	O5-C5	2.81	1.49	1.43
3	C	602	0U8	O3-C3	-2.80	1.37	1.42
3	B	602	0U8	O5-C5	2.65	1.49	1.43
3	B	602	0U8	O4'-C4'	-2.56	1.37	1.43
3	D	602	0U8	O4'-C4'	-2.53	1.37	1.43
3	C	602	0U8	O5'-C5'	-2.33	1.38	1.43
3	A	602	0U8	O4'-C4'	-2.31	1.37	1.43
3	A	602	0U8	O5-C5	2.20	1.48	1.43
3	B	602	0U8	O5'-C5'	-2.16	1.39	1.43
3	D	602	0U8	O5'-C5'	-2.09	1.39	1.43
3	A	602	0U8	C4'-C5'	2.06	1.58	1.53
3	A	602	0U8	O5'-C5'	-2.00	1.39	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	0U8	C1'-C2'-C3'	-6.35	95.82	114.56
3	D	602	0U8	O5'-C2'-C1'	6.24	123.21	108.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	0U8	C1'-C2'-C3'	-5.95	97.01	114.56
3	D	602	0U8	O6-C2'-C3'	5.81	127.26	108.08
3	D	602	0U8	O6-C2'-C1'	-5.78	92.39	109.56
3	A	602	0U8	C1'-C2'-C3'	-5.73	97.65	114.56
3	B	602	0U8	C1'-C2'-C3'	-5.11	99.48	114.56
3	A	602	0U8	O6-C2'-C3'	4.65	123.43	108.08
3	B	602	0U8	O6-C2'-C1'	-4.62	95.85	109.56
3	C	602	0U8	O6-C2'-C3'	4.45	122.75	108.08
3	B	602	0U8	O6-C2'-C3'	4.34	122.40	108.08
3	D	602	0U8	C6-O6-C2'	-4.29	108.74	116.20
3	C	602	0U8	O6-C6-C5	3.79	116.05	107.68
3	A	602	0U8	O6-C2'-C1'	-3.76	98.38	109.56
3	A	602	0U8	C2'-C3'-C4'	-3.60	93.85	102.10
3	B	602	0U8	O5'-C2'-C1'	3.58	116.73	108.03
3	A	602	0U8	O5'-C2'-C1'	3.57	116.72	108.03
3	C	602	0U8	O5'-C2'-C1'	3.55	116.67	108.03
3	D	602	0U8	O5-C5-C6	3.53	117.24	109.45
3	D	602	0U8	C2'-C3'-C4'	-3.24	94.69	102.10
3	B	602	0U8	O1'-C1'-C2'	3.18	122.49	111.70
3	C	602	0U8	O6-C2'-C1'	-3.16	100.19	109.56
3	C	602	0U8	O5-C5-C6	3.09	116.25	109.45
3	B	602	0U8	O2-C2-C3	2.97	117.87	108.08
3	D	602	0U8	O2-C6'-C5'	2.92	114.13	107.68
3	C	602	0U8	O1'-C1'-C2'	2.76	121.07	111.70
3	C	602	0U8	C6'-O2-C2	-2.72	111.47	116.20
3	C	602	0U8	O2-C6'-C5'	2.70	113.64	107.68
3	C	602	0U8	C2'-C3'-C4'	-2.68	95.96	102.10
3	B	602	0U8	O5'-C2'-C3'	2.57	110.79	105.49
3	A	602	0U8	O6-C6-C5	2.55	113.30	107.68
3	D	602	0U8	C2'-O5'-C5'	-2.53	101.21	108.28
3	C	602	0U8	C2'-O5'-C5'	-2.47	101.38	108.28
3	B	602	0U8	C2'-O5'-C5'	-2.43	101.49	108.28
3	A	602	0U8	O1'-C1'-C2'	2.35	119.68	111.70
3	B	602	0U8	C1-C2-C3	-2.34	107.65	114.56
3	D	602	0U8	O5'-C2'-C3'	2.31	110.26	105.49
3	A	602	0U8	O5'-C2'-C3'	2.26	110.14	105.49
3	A	602	0U8	O5-C5-C6	2.21	114.33	109.45
3	B	602	0U8	C2'-C3'-C4'	-2.21	97.04	102.10
3	D	602	0U8	O1-C1-C2	2.21	119.20	111.70
3	D	602	0U8	O5-C2-C3	-2.14	101.08	105.49
3	A	602	0U8	O2-C6'-C5'	2.14	112.39	107.68
3	D	602	0U8	O6-C6-C5	2.13	112.38	107.68

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	602	0U8	O4'-C4'-C5'	2.13	117.21	111.05

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	0U8	C4-C5-C6-O6
3	B	602	0U8	O5-C2-O2-C6'
3	B	602	0U8	C1-C2-O2-C6'
3	B	602	0U8	C3-C2-O2-C6'
3	C	602	0U8	C5-C6-O6-C2'
3	C	602	0U8	O1-C1-C2-O5
3	C	602	0U8	O1-C1-C2-O2
3	C	602	0U8	O1-C1-C2-C3
3	D	602	0U8	O1'-C1'-C2'-O6
3	D	602	0U8	O1'-C1'-C2'-O5'
3	D	602	0U8	O1'-C1'-C2'-C3'
3	D	602	0U8	O1-C1-C2-O5
3	D	602	0U8	O1-C1-C2-O2
3	D	602	0U8	O1-C1-C2-C3
3	B	602	0U8	O5-C5-C6-O6
3	A	602	0U8	C5-C6-O6-C2'
3	B	602	0U8	C5'-C6'-O2-C2
3	B	602	0U8	O5'-C5'-C6'-O2
3	A	602	0U8	C5'-C6'-O2-C2
3	B	602	0U8	C5-C6-O6-C2'
3	C	602	0U8	C5'-C6'-O2-C2
3	D	602	0U8	C5-C6-O6-C2'
3	D	602	0U8	C5'-C6'-O2-C2
3	B	602	0U8	O1-C1-C2-O5
3	D	602	0U8	O5-C5-C6-O6
3	A	602	0U8	O5'-C2'-O6-C6
3	A	602	0U8	C1'-C2'-O6-C6
3	C	602	0U8	C1'-C2'-O6-C6
3	D	602	0U8	C1'-C2'-O6-C6
3	C	602	0U8	O5-C5-C6-O6
3	B	602	0U8	O1-C1-C2-C3
3	A	602	0U8	O1'-C1'-C2'-O5'
3	A	602	0U8	O5-C5-C6-O6
3	A	602	0U8	O1-C1-C2-C3

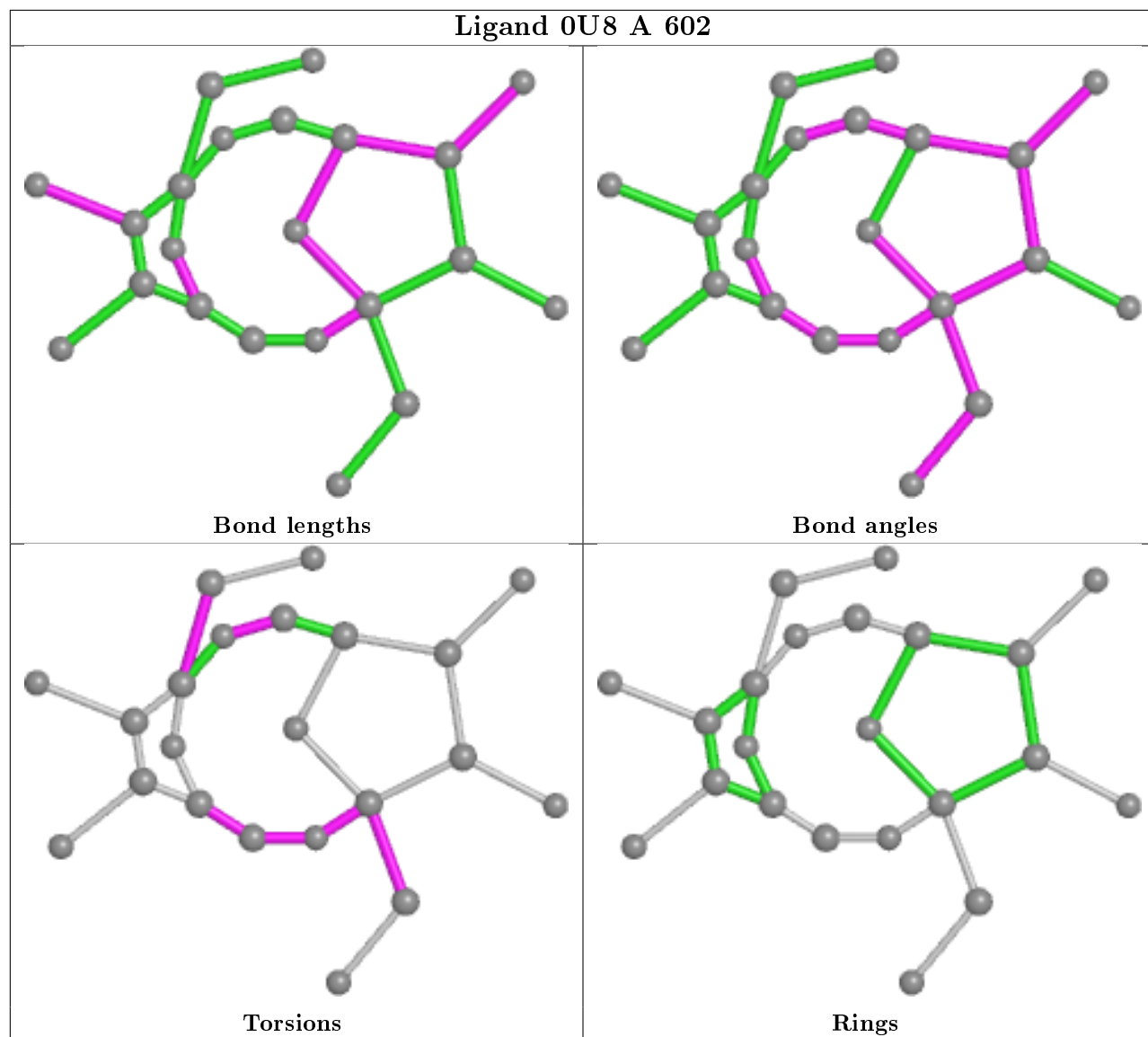
There are no ring outliers.

4 monomers are involved in 11 short contacts:

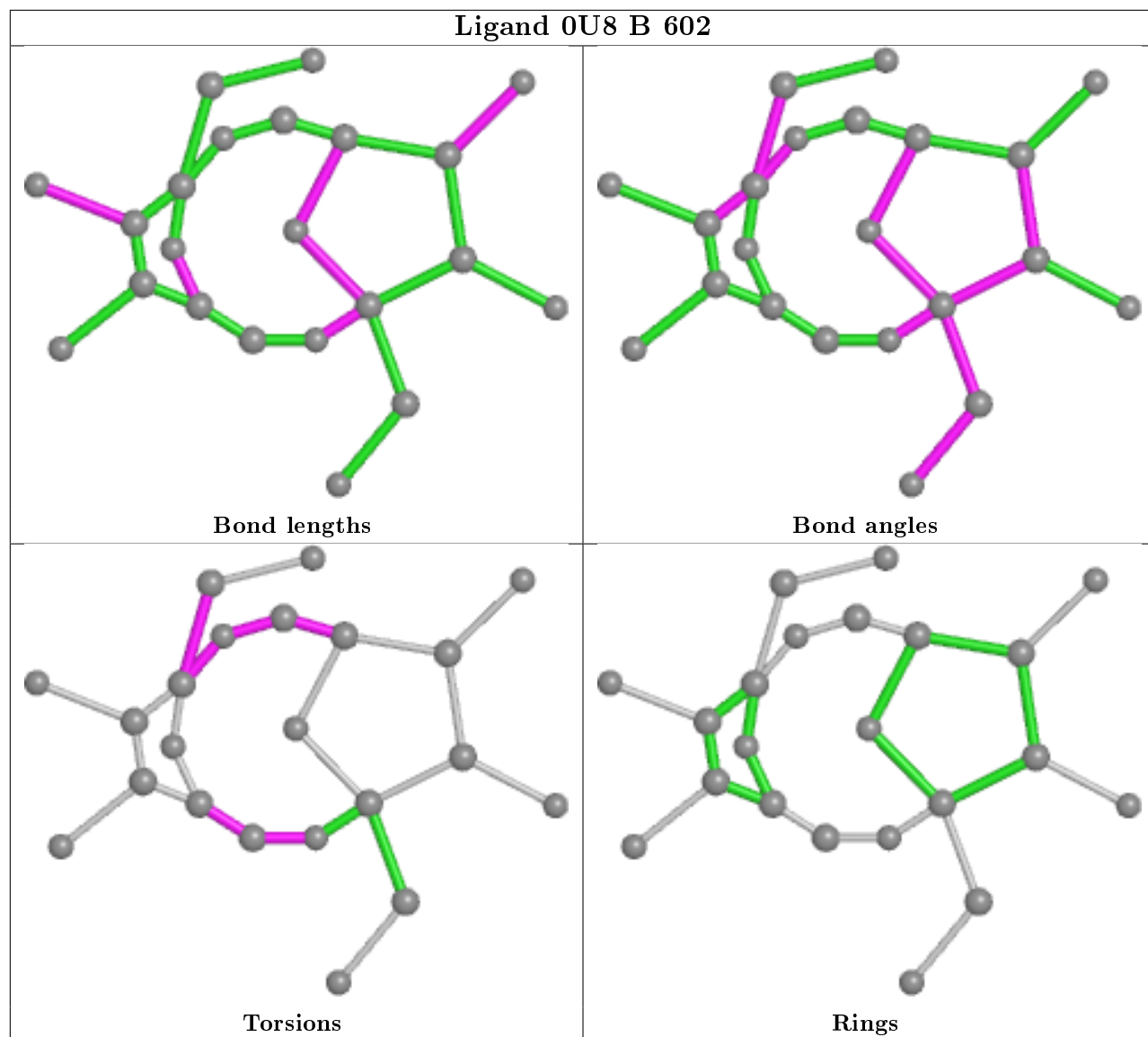
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	OU8	1	0
3	B	602	OU8	6	0
3	C	602	OU8	3	0
3	D	602	OU8	1	0

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.

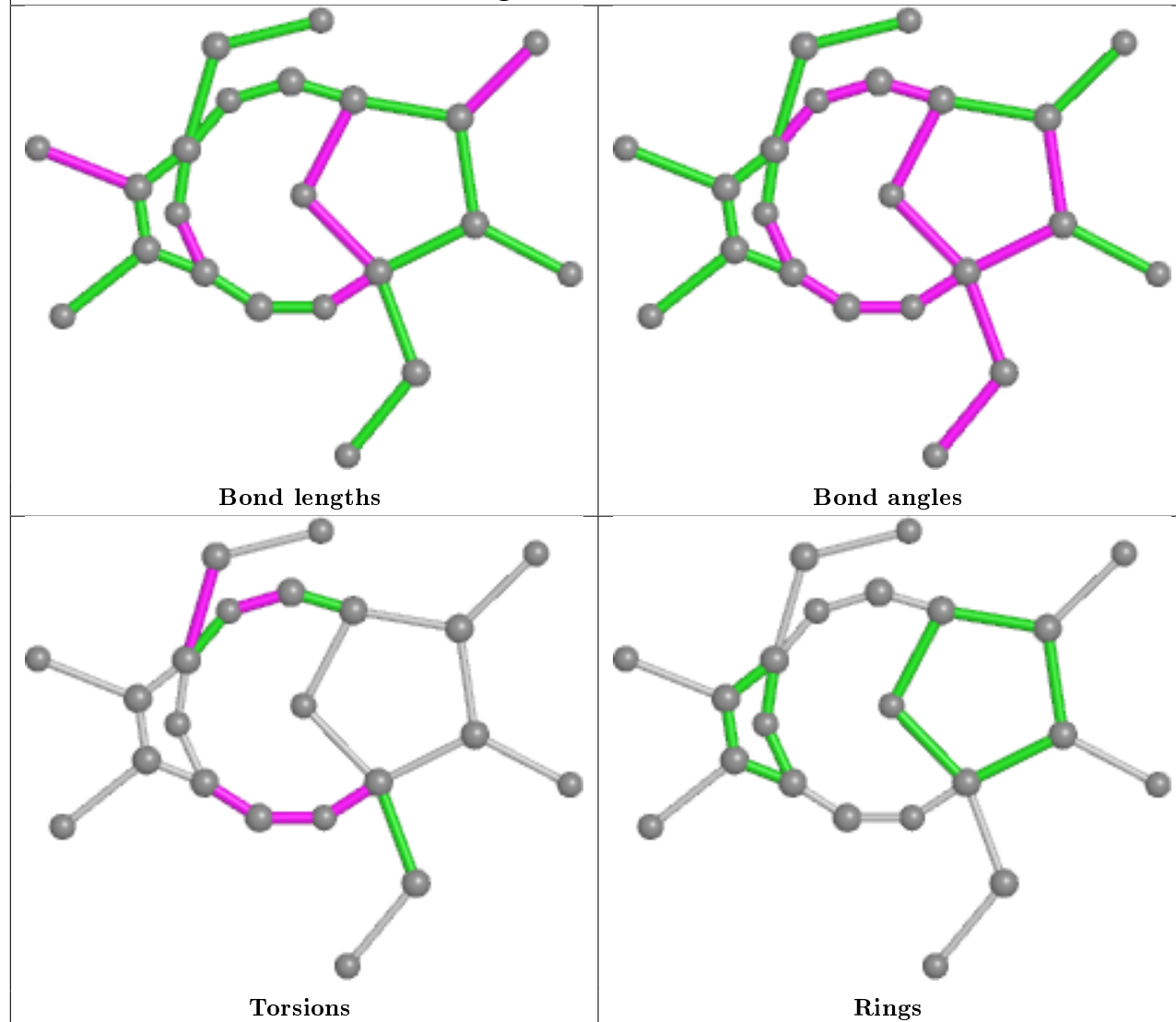
## Ligand 0U8 A 602

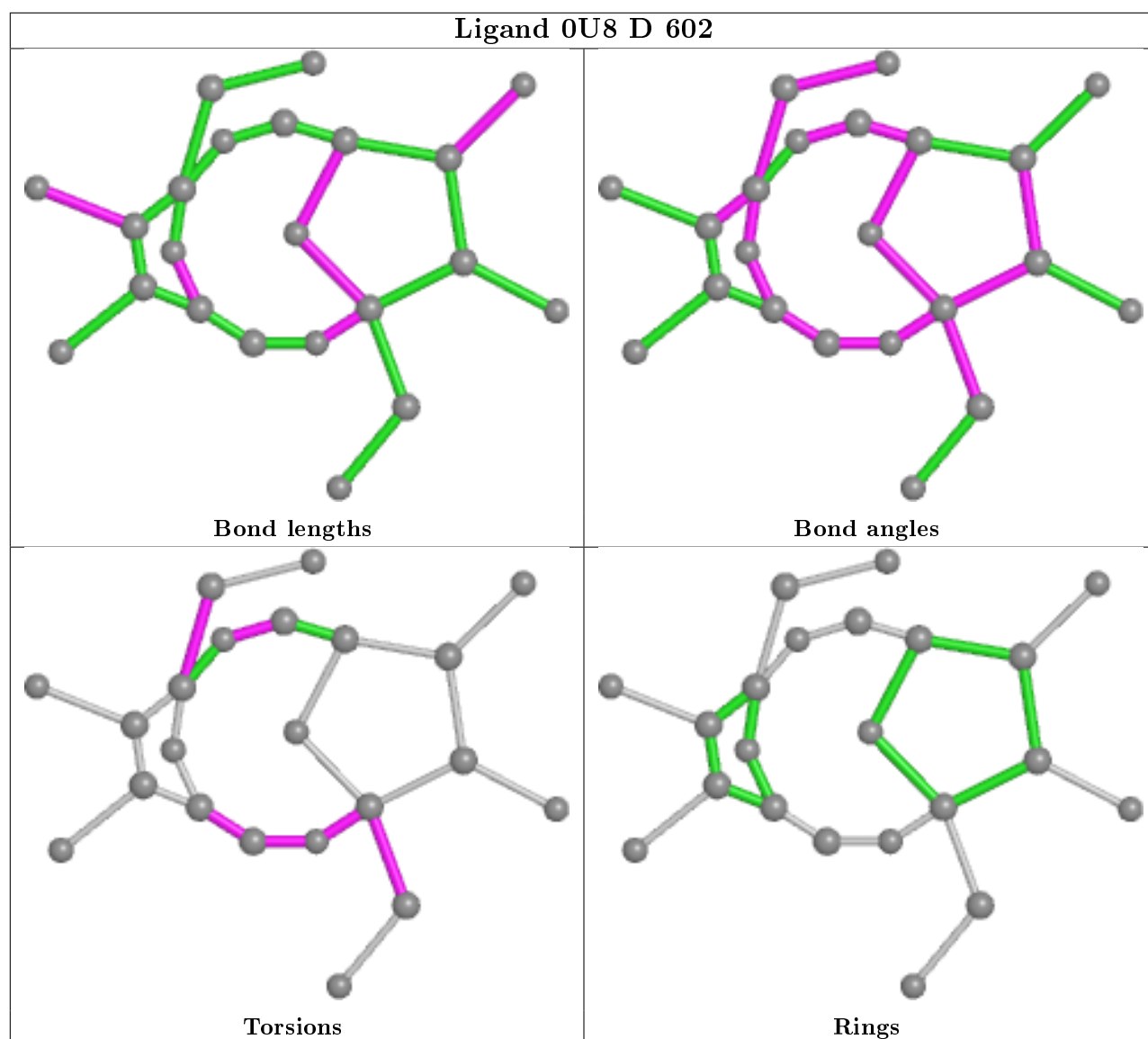






## Ligand 0U8 C 602





## 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	480/492 (97%)	-0.08	10 (2%) 63 70	12, 27, 42, 64	0
1	B	480/492 (97%)	-0.05	9 (1%) 66 73	14, 27, 40, 65	0
1	C	479/492 (97%)	-0.12	5 (1%) 82 86	13, 24, 37, 55	0
1	D	480/492 (97%)	-0.16	6 (1%) 77 81	14, 23, 35, 59	0
All	All	1919/1968 (97%)	-0.10	30 (1%) 72 77	12, 25, 38, 65	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	520	ALA	6.5
1	D	520	ALA	4.9
1	A	173	THR	4.8
1	C	234	GLY	4.6
1	B	174	THR	4.5
1	B	173	THR	4.2
1	B	172	ALA	3.7
1	A	520	ALA	3.6
1	A	174	THR	3.3
1	D	234	GLY	2.9
1	A	175	PRO	2.7
1	A	176	ALA	2.7
1	D	519	GLN	2.7
1	C	519	GLN	2.6
1	B	171	ALA	2.4
1	C	503	ASP	2.3
1	D	228	PRO	2.3
1	D	223	ARG	2.3
1	A	171	ALA	2.3
1	D	63	GLY	2.2
1	C	150	THR	2.2

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	381	THR	2.2
1	B	138	VAL	2.1
1	B	178	ILE	2.1
1	B	333	ALA	2.1
1	B	196	GLY	2.1
1	A	235	ILE	2.0
1	A	172	ALA	2.0
1	C	63	GLY	2.0
1	A	233	GLY	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](#)

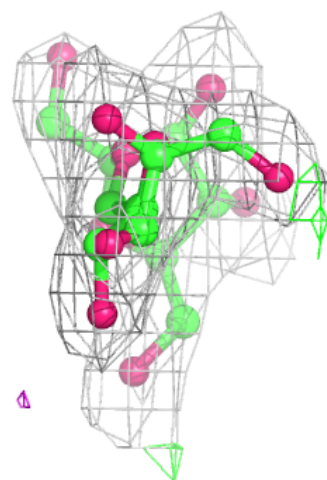
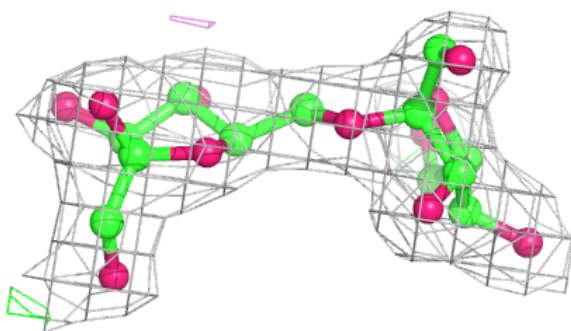
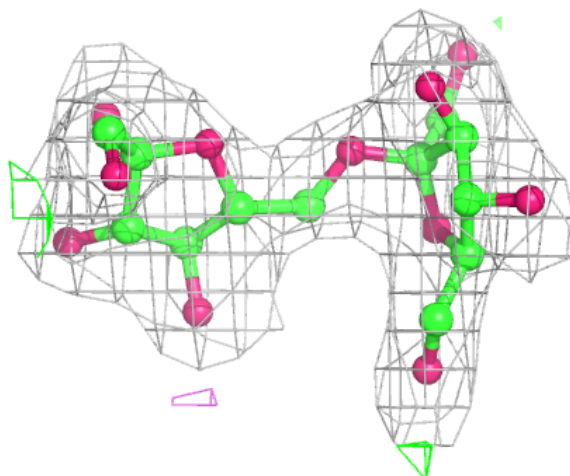
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	FRU	H	1	12/12	0.81	0.31	61,63,64,64	0
2	FRU	H	2	11/12	0.84	0.29	57,59,60,60	0
2	FRU	E	2	11/12	0.85	0.22	42,43,45,45	0
2	FRU	G	2	11/12	0.88	0.18	29,32,34,36	0
2	FRU	E	1	12/12	0.93	0.16	41,42,43,46	0
2	FRU	G	1	12/12	0.93	0.17	27,29,30,31	0
2	FRU	F	2	11/12	0.94	0.16	37,38,39,40	0
2	FRU	F	1	12/12	0.94	0.20	37,39,40,40	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

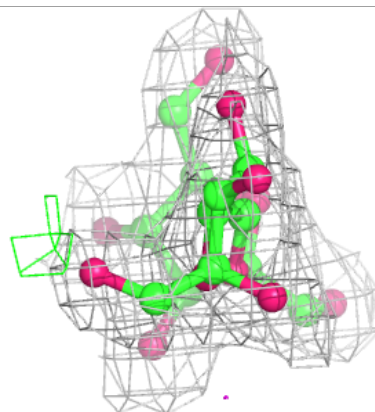
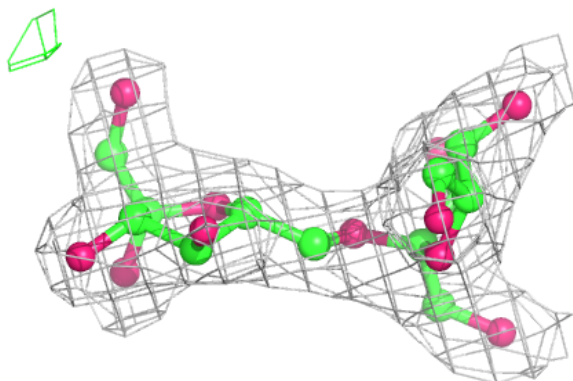
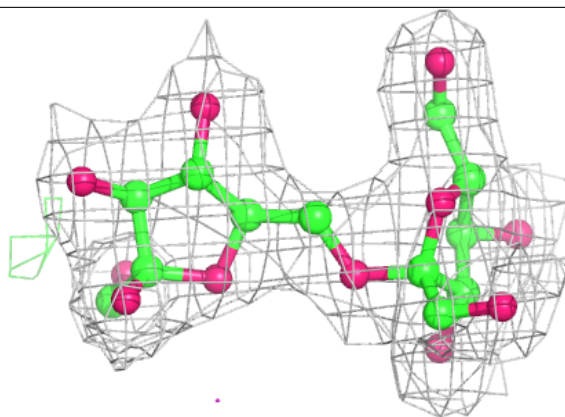
**Electron density around Chain E:**

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

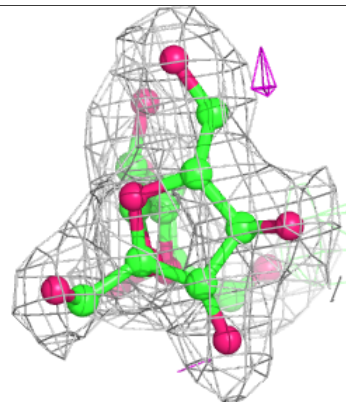
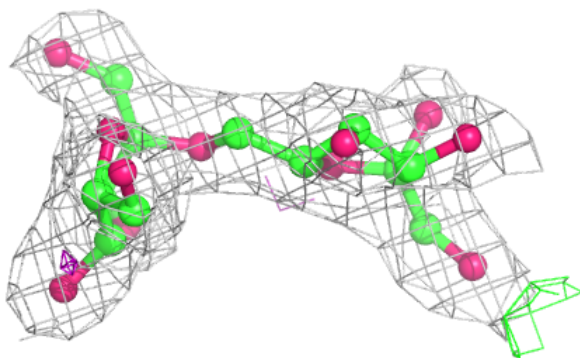
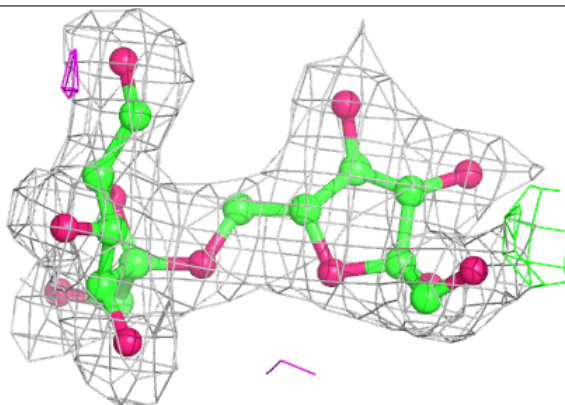


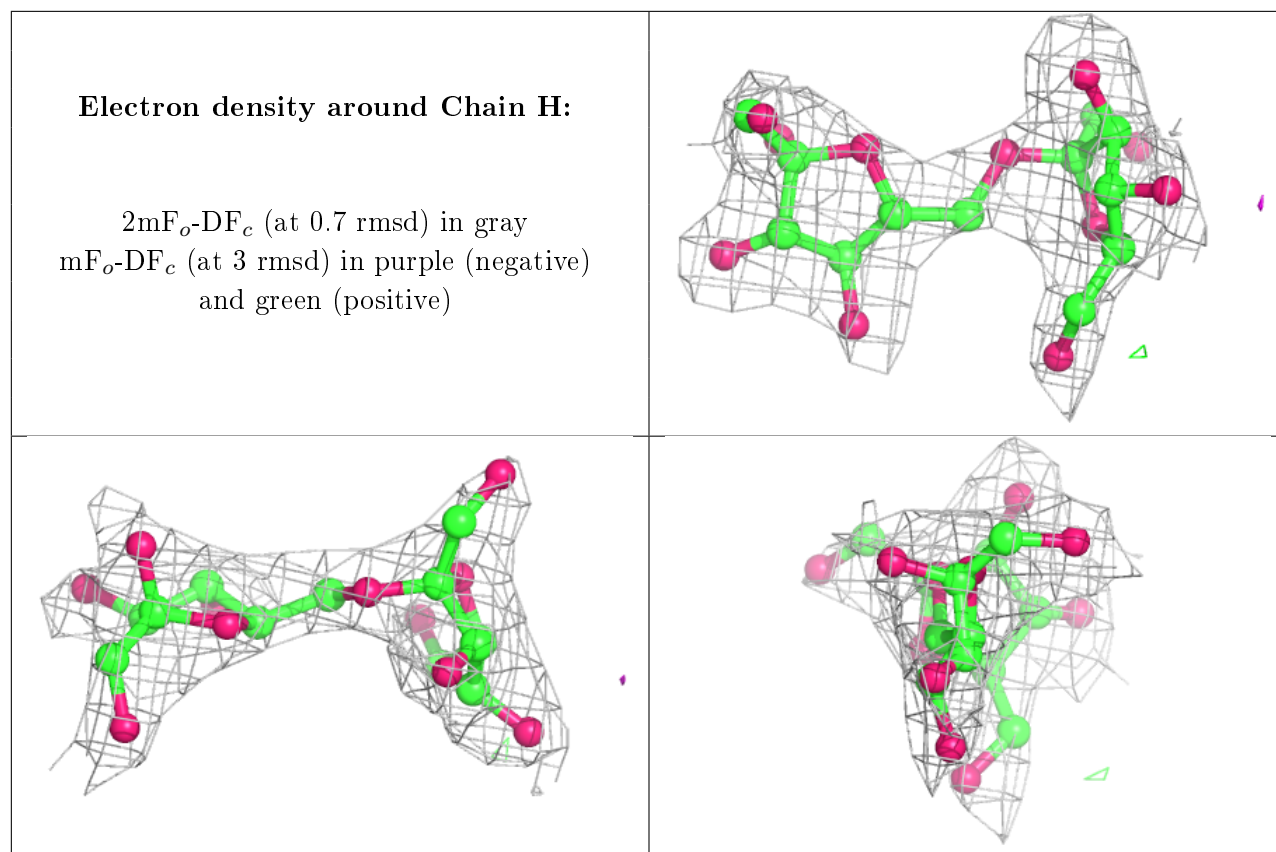
**Electron density around Chain F:**

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

**Electron density around Chain G:**

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





## 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, 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.

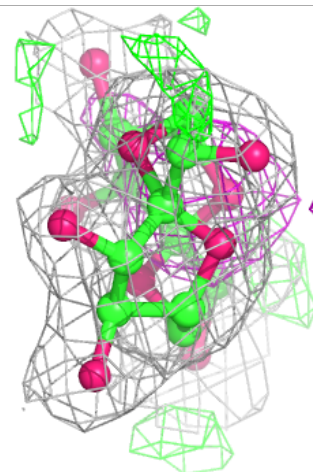
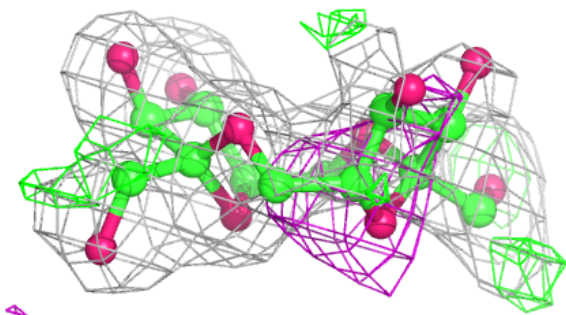
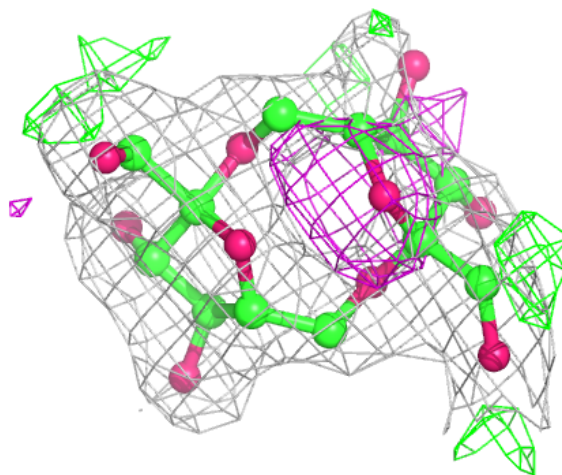
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	0U8	D	602	22/22	0.68	0.28	31,40,51,53	0
3	0U8	C	602	22/22	0.79	0.24	23,34,46,50	0
3	0U8	B	602	22/22	0.79	0.20	22,34,46,49	0
3	0U8	A	602	22/22	0.86	0.16	23,33,42,43	0

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.



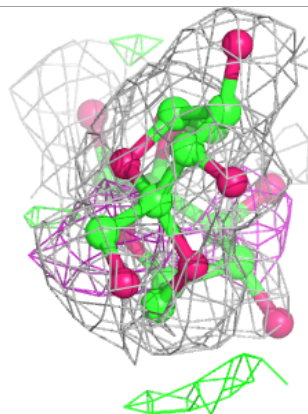
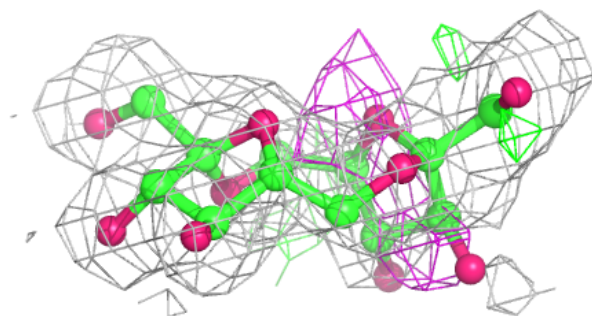
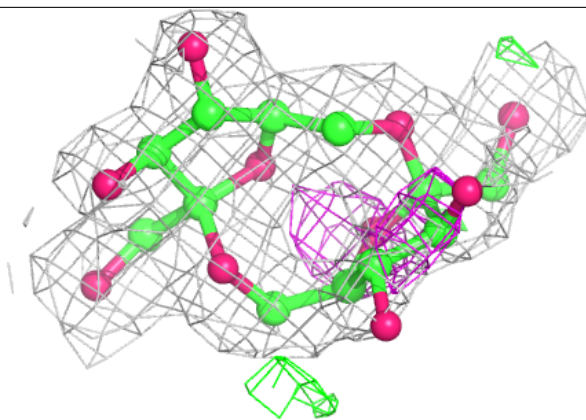
**Electron density around 0U8 D 602:**

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



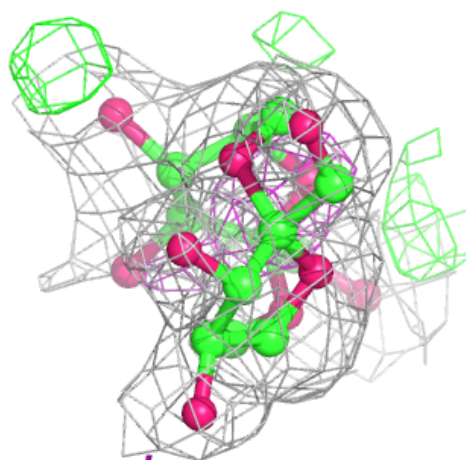
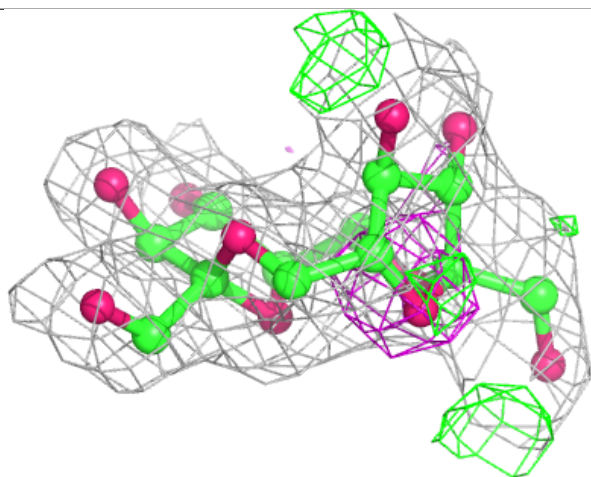
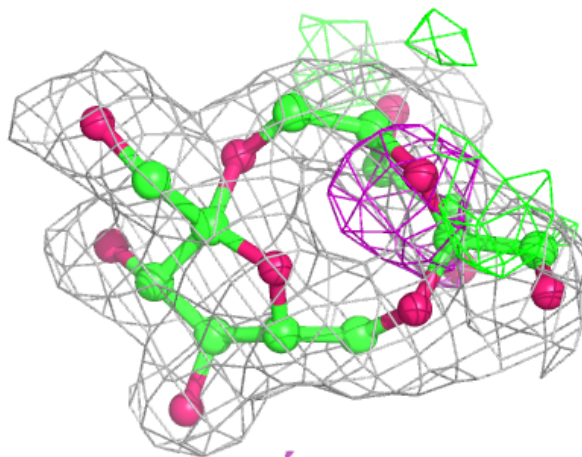
**Electron density around 0U8 C 602:**

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



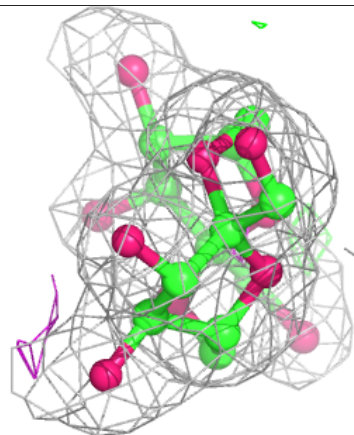
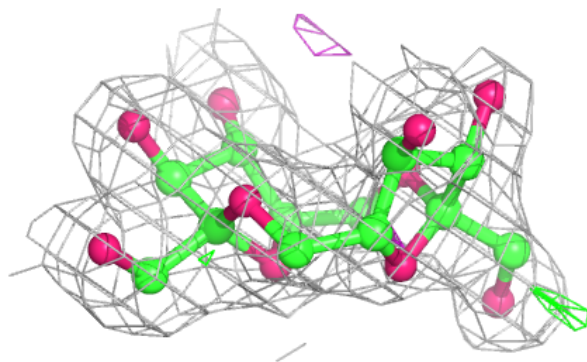
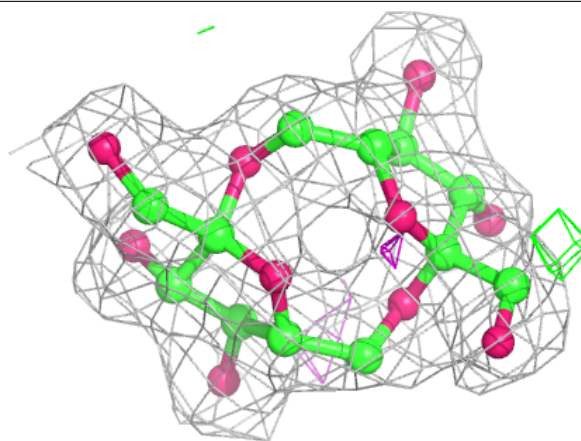
**Electron density around 0U8 B 602:**

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



**Electron density around 0U8 A 602:**

$2mF_o-DF_c$  (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.