



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:42 AM UTC

PDB ID : 4FFG / pdb_00004ffg
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

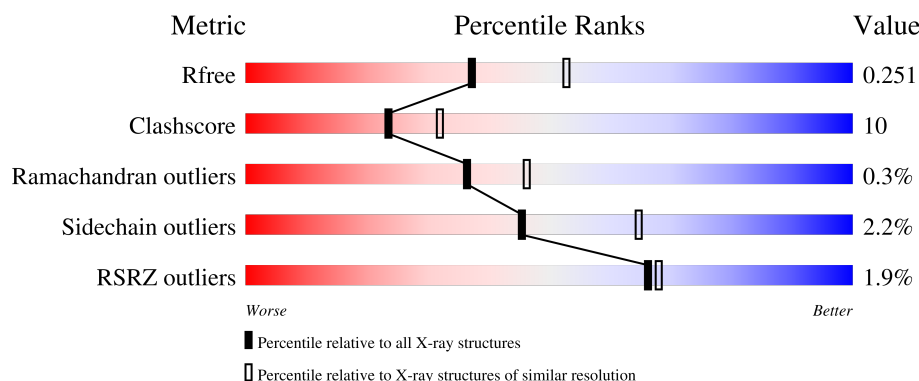
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

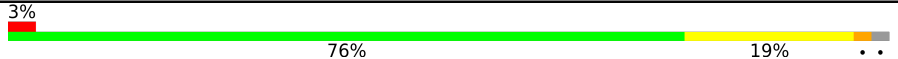
The reported resolution of this entry is 2.30 Å.

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.



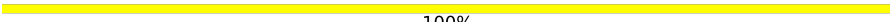
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	492	
1	B	492	
1	C	492	
1	D	492	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
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:

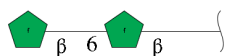
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	expression tag	UNP Q9KJD0
A	115	ASP	GLY	conflict	UNP Q9KJD0
A	522	LEU	-	expression tag	UNP Q9KJD0
A	523	GLU	-	expression tag	UNP Q9KJD0
A	524	HIS	-	expression tag	UNP Q9KJD0
A	525	HIS	-	expression tag	UNP Q9KJD0
A	526	HIS	-	expression tag	UNP 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.



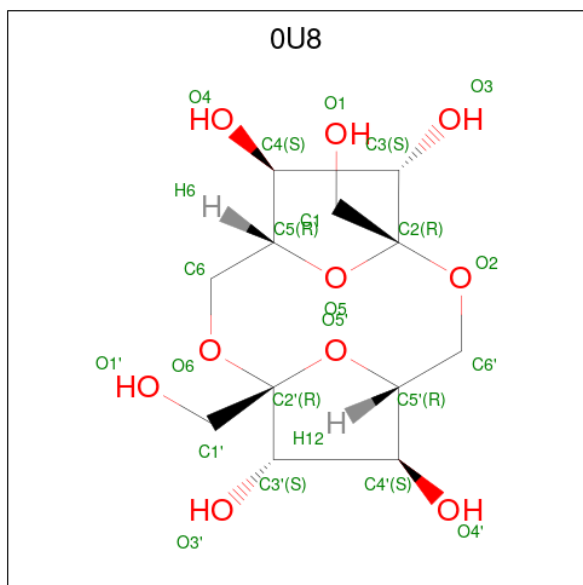
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			

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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 (CCD ID: 0U8) (formula: C₁₂H₂₀O₁₀).



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		

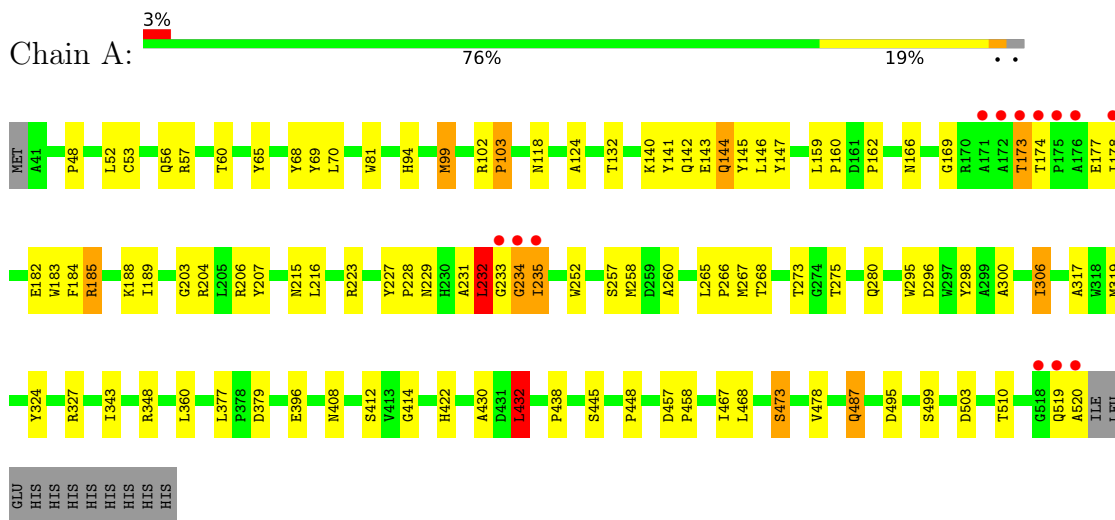
- Molecule 4 is water.

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		

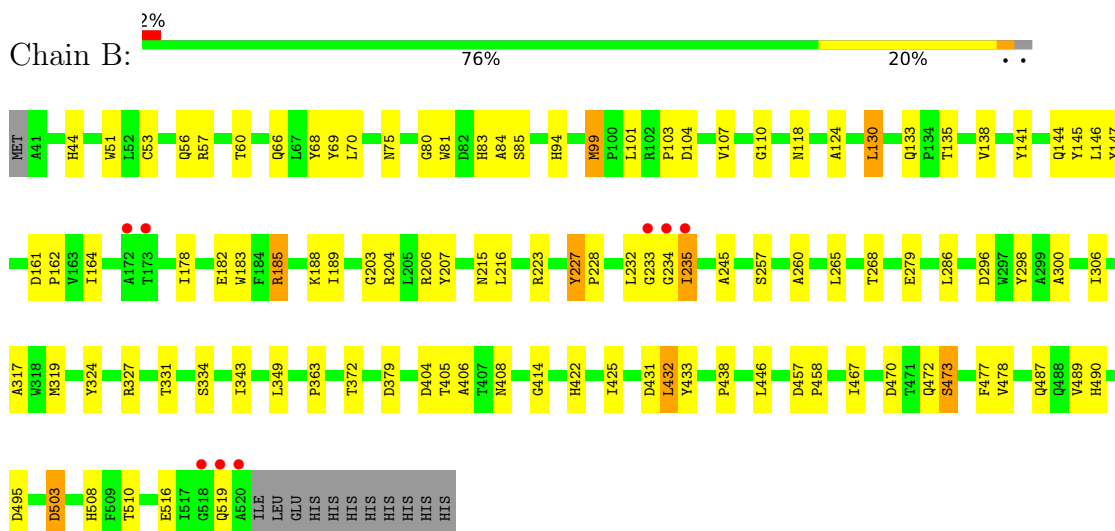
3 Residue-property plots [i](#)

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.

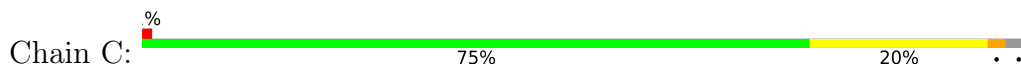
• Molecule 1: Levan fructotransferase



• Molecule 1: Levan fructotransferase



• Molecule 1: Levan fructotransferase





Chain H:

100%

FRU1
FRU2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.86Å 161.91Å 263.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.8 (50.00-2.30) 96.9 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.72 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.240 0.218 , 0.251	Depositor DCC
R_{free} test set	15480 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.757	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

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: 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	0.39	0/3863	0.94	19/5312 (0.4%)
1	B	0.40	0/3863	0.94	14/5312 (0.3%)
1	C	0.40	0/3858	0.93	14/5305 (0.3%)
1	D	0.42	0/3863	0.93	20/5312 (0.4%)
All	All	0.40	0/15447	0.94	67/21241 (0.3%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	GLY	N-CA-C	10.54	125.40	112.64
1	A	234	GLY	N-CA-C	8.69	127.83	112.53
1	B	232	LEU	N-CA-C	-8.03	102.94	112.89
1	C	227	TYR	CA-C-N	7.99	127.28	118.97
1	C	227	TYR	C-N-CA	7.99	127.28	118.97
1	A	343	ILE	N-CA-C	-7.93	101.25	110.21
1	A	228	PRO	N-CA-C	7.86	123.68	113.86
1	B	185	ARG	N-CA-C	7.81	120.27	109.18
1	A	432	LEU	N-CA-C	-7.76	94.25	107.99
1	A	232	LEU	N-CA-C	-7.53	103.55	112.89
1	C	432	LEU	N-CA-C	-7.33	93.18	107.62
1	A	185	ARG	N-CA-C	7.17	118.97	108.86
1	C	185	ARG	N-CA-C	7.14	118.60	108.74
1	A	99	MET	CA-C-N	7.10	127.09	119.78
1	A	99	MET	C-N-CA	7.10	127.09	119.78
1	B	99	MET	CA-C-N	7.10	127.06	120.03
1	B	99	MET	C-N-CA	7.10	127.06	120.03
1	D	144	GLN	N-CA-C	6.86	119.91	108.73
1	B	234	GLY	N-CA-C	6.69	126.61	112.17
1	D	99	MET	CA-C-N	6.64	126.61	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99	MET	C-N-CA	6.64	126.61	120.03
1	C	467	ILE	N-CA-C	6.59	117.36	107.80
1	D	432	LEU	N-CA-C	-6.58	94.66	107.62
1	A	227	TYR	CA-C-N	6.58	126.20	119.56
1	A	227	TYR	C-N-CA	6.58	126.20	119.56
1	A	231	ALA	N-CA-C	-6.38	105.35	113.01
1	A	267	MET	N-CA-C	-6.36	102.21	111.30
1	B	227	TYR	CA-C-N	6.20	125.93	119.05
1	B	227	TYR	C-N-CA	6.20	125.93	119.05
1	D	476	VAL	N-CA-C	6.17	116.74	107.80
1	C	267	MET	N-CA-C	-6.13	102.53	111.30
1	B	432	LEU	N-CA-C	-6.11	95.40	107.69
1	C	99	MET	CA-C-N	6.11	126.07	119.78
1	C	99	MET	C-N-CA	6.11	126.07	119.78
1	A	467	ILE	N-CA-C	6.08	116.62	107.75
1	B	343	ILE	N-CA-C	-6.07	101.73	109.80
1	D	343	ILE	N-CA-C	-6.01	101.81	109.80
1	C	144	GLN	N-CA-C	5.97	118.46	108.96
1	A	473	SER	N-CA-C	5.89	117.80	108.79
1	A	144	GLN	N-CA-C	5.84	118.25	108.96
1	D	234	GLY	N-CA-C	5.82	126.98	113.18
1	B	467	ILE	N-CA-C	5.81	116.23	107.80
1	C	296	ASP	N-CA-C	5.78	118.69	107.71
1	D	185	ARG	N-CA-C	5.77	116.71	108.74
1	D	227	TYR	CA-C-N	5.76	125.44	119.05
1	D	227	TYR	C-N-CA	5.76	125.44	119.05
1	D	433	TYR	N-CA-C	5.51	118.97	110.42
1	D	235	ILE	N-CA-C	5.49	120.75	109.34
1	C	473	SER	N-CA-C	5.48	117.18	108.79
1	D	467	ILE	N-CA-C	5.45	115.71	107.75
1	D	161	ASP	N-CA-C	5.45	116.94	110.07
1	D	165	VAL	N-CA-C	5.41	116.78	108.71
1	C	169	GLY	N-CA-C	5.39	118.75	112.50
1	B	473	SER	N-CA-C	5.39	117.04	108.79
1	D	268	THR	CB-CA-C	-5.32	108.77	116.54
1	A	296	ASP	N-CA-C	5.25	118.82	107.49
1	A	432	LEU	CA-CB-CG	-5.24	97.97	116.30
1	A	266	PRO	N-CA-C	5.23	118.81	111.33
1	D	109	SER	N-CA-C	5.23	117.43	110.53
1	B	296	ASP	N-CA-C	5.23	118.78	107.49
1	A	273	THR	N-CA-C	-5.22	103.50	110.55
1	B	431	ASP	N-CA-C	5.13	117.75	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	268	THR	N-CA-C	5.06	115.77	108.34
1	B	161	ASP	N-CA-C	5.05	116.03	109.72
1	D	231	ALA	N-CA-C	-5.03	107.16	113.15
1	C	165	VAL	N-CA-C	5.03	116.52	108.87
1	D	100	PRO	N-CA-C	5.00	118.92	111.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	73	0
1	B	3739	0	3489	68	0
1	C	3734	0	3484	83	0
1	D	3739	0	3489	63	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	297	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 (297) 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:OU8:H11	3:C:602:OU8:H19	1.34	1.07
1:D:267:MET:HE1	1:D:323:LYS:HD3	1.41	1.00
3:C:602:OU8:H11	3:C:602:OU8: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:D:223:ARG:HD2	1:D:280:GLN:CD	2.10	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:OU8:H7	1.88	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
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:A:146:LEU:C	1:A:146:LEU:HD23	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:166:ASN:C	1:A:166:ASN:HD22	2.11	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:C:57:ARG:HH12	1:C:188:LYS:HZ1	1.51	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
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:51:TRP:HB2	1:B:75:ASN:HD22	1.72	0.55
1:B:145:TYR:CE1	1:B:162:PRO:HG3	2.41	0.55
1:A:188:LYS:HE2	1:A:189:ILE:O	2.06	0.55
1:C:204:ARG:HH21	2:G:1:FRU:H3	1.71	0.55
1:D:323:LYS:HG2	1:D:449:TYR:CZ	2.42	0.55
1:B:44:HIS:HD2	1:B:470:ASP:OD2	1.88	0.55
1:C:146:LEU:C	1:C:146:LEU:HD23	2.32	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:146:LEU:HD23	1:D:146:LEU:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:146:LEU:HD23	1:B:146:LEU:C	2.34	0.53
1:C:510:THR:HG22	1:C:511:GLY:N	2.23	0.53
3:B:602:OU8:H11	3:B:602:OU8:O3	2.09	0.53
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: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
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:215:ASN:O	1:B:216:LEU:HB2	2.10	0.50
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:D:257:SER:HB3	1:D:298:TYR:CE2	2.47	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:66:GLN:NE2	1:D:85:SER:HB3	2.26	0.50
1:D:139:ARG:HG2	1:D:182:GLU:HG2	1.94	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:D:99:MET:HE3	1:D:147:TYR:CD2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:319:MET:HE1	1:A:473:SER:HB2	1.95	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: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:306:ILE:HD13	1:A:306:ILE:C	2.38	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
1:A:260:ALA:CB	1:A:265:LEU:HB2	2.45	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:D:267:MET:CE	1:D:323:LYS:HD3	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:425:ILE:HD12	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:56:GLN:HB2	1:A:68:TYR:HB2	1.98	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:379:ASP:CG	1:A:510:THR:HG22	2.42	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
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:83:HIS:HD2	1:C:84:ALA:N	2.13	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:D:230:HIS:C	1:D:232:LEU:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:166:ASN:C	1:A:166:ASN:ND2	2.75	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:O1	3:A:602:OU8:H10	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: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
1:A:412:SER:HB2	1:A:499:SER:OG	2.19	0.43
1:B:319:MET:HE1	1:B:473:SER:HB2	2.01	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: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:146:LEU:HD23	1:D:147:TYR:N	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:NH1	1:B:223:ARG:HG2	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:500:LEU:HD13	1:C:509:PHE:CG	2.54	0.41
1:C:508:HIS:HB2	4:C:868:HOH:O	2.20	0.41
1:D:363:PRO:O	1:D:364:VAL:C	2.63	0.41
1:B:327:ARG:NH2	1:B:446:LEU:HD21	2.35	0.41
1:A:102:ARG:O	1:A:103:PRO:C	2.63	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:83:HIS:CD2	1:D:84:ALA:N	2.89	0.41
1:D:206:ARG:NH1	1:D:234:GLY:N	2.69	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:56:GLN:HB2	1:B:68:TYR:HB2	2.03	0.41
1:B:432:LEU:HD13	1:B:478:VAL:HG11	2.02	0.41
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:227:TYR:CE2	1:B:235:ILE:HD11	2.56	0.41
1:B:245:ALA:HB2	1:B:349:LEU:HD23	2.03	0.41
1:C:223:ARG:HB2	1:C:280:GLN:HB3	2.03	0.41
1:D:223:ARG:HD2	1:D:280:GLN:CG	2.50	0.41
1:D:291:LEU:HD12	1:D:291:LEU:HA	1.92	0.41
1:D:432:LEU:HD22	1:D:432:LEU:HA	1.96	0.41
1:C:84:ALA:HA	1:C:93:THR:O	2.20	0.41
1:B:405:THR:O	1:B:406:ALA:C	2.63	0.40
1:C:174:THR:O	1:C:178:ILE:HG13	2.21	0.40
1:C:433:TYR:CD1	1:C:433:TYR:C	2.99	0.40
1:A:144:GLN:CD	1:A:144:GLN:N	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	478/492 (97%)	449 (94%)	27 (6%)	2 (0%)	30	38
1	B	478/492 (97%)	452 (95%)	24 (5%)	2 (0%)	30	38
1	C	477/492 (97%)	452 (95%)	24 (5%)	1 (0%)	43	55
1	D	478/492 (97%)	450 (94%)	27 (6%)	1 (0%)	43	55
All	All	1911/1968 (97%)	1803 (94%)	102 (5%)	6 (0%)	36	46

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%)	373 (98%)	8 (2%)	47	66
1	B	381/393 (97%)	373 (98%)	8 (2%)	47	66
1	C	381/393 (97%)	372 (98%)	9 (2%)	43	62
1	D	381/393 (97%)	373 (98%)	8 (2%)	47	66
All	All	1524/1572 (97%)	1491 (98%)	33 (2%)	45	65

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLU
1	A	173	THR
1	A	232	LEU
1	A	258	MET
1	A	306	ILE
1	A	432	LEU
1	A	448	PRO
1	A	487	GLN
1	B	101	LEU
1	B	104	ASP
1	B	130	LEU
1	B	279	GLU
1	B	372	THR
1	B	487	GLN
1	B	503	ASP
1	B	516	GLU
1	C	98	VAL
1	C	99	MET
1	C	223	ARG
1	C	232	LEU
1	C	279	GLU
1	C	329	VAL
1	C	382	VAL
1	C	432	LEU

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Mol	Chain	Res	Type
1	C	446	LEU
1	D	98	VAL
1	D	101	LEU
1	D	144	GLN
1	D	232	LEU
1	D	340	GLN
1	D	382	VAL
1	D	446	LEU
1	D	487	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	142	GLN
1	A	144	GLN
1	A	166	ASN
1	A	229	ASN
1	A	230	HIS
1	A	280	GLN
1	A	391	ASN
1	B	44	HIS
1	B	75	ASN
1	B	94	HIS
1	B	289	GLN
1	B	369	ASN
1	B	490	HIS
1	C	76	ASN
1	C	94	HIS
1	C	118	ASN
1	C	282	HIS
1	C	289	GLN
1	C	340	GLN
1	C	341	ASN
1	C	479	ASN
1	C	508	HIS
1	D	66	GLN
1	D	71	HIS
1	D	144	GLN
1	D	251	HIS
1	D	280	GLN
1	D	289	GLN

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Mol	Chain	Res	Type
1	D	340	GLN
1	D	341	ASN
1	D	422	HIS
1	D	479	ASN
1	D	487	GLN
1	D	508	HIS
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	1.40	2 (18%)	10,18,18	1.57	3 (30%)
2	FRU	E	2	2	11,11,12	1.52	1 (9%)	15,15,18	1.14	2 (13%)
2	FRU	F	1	2	11,12,12	1.35	2 (18%)	10,18,18	1.29	2 (20%)
2	FRU	F	2	2	11,11,12	1.51	1 (9%)	15,15,18	1.16	0
2	FRU	G	1	2	11,12,12	1.32	1 (9%)	10,18,18	1.68	1 (10%)
2	FRU	G	2	2	11,11,12	1.43	1 (9%)	15,15,18	1.05	0
2	FRU	H	1	2	11,12,12	1.26	2 (18%)	10,18,18	1.57	2 (20%)
2	FRU	H	2	2	11,11,12	1.50	1 (9%)	15,15,18	1.26	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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	FRU	C4-C3	-3.56	1.43	1.53
2	H	2	FRU	C4-C3	-3.29	1.44	1.53
2	G	2	FRU	C4-C3	-3.19	1.44	1.53
2	E	2	FRU	C4-C3	-3.08	1.45	1.53
2	F	1	FRU	O3-C3	-2.36	1.38	1.42
2	E	1	FRU	O3-C3	-2.27	1.38	1.42
2	E	1	FRU	C4-C3	-2.15	1.44	1.53
2	H	1	FRU	O3-C3	-2.12	1.38	1.42
2	F	1	FRU	C4-C3	-2.06	1.44	1.53
2	H	1	FRU	C4-C3	-2.01	1.45	1.53
2	G	1	FRU	O3-C3	-2.01	1.38	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	FRU	O1-C1-C2	4.44	121.50	111.67
2	H	1	FRU	O1-C1-C2	3.39	119.17	111.67
2	E	1	FRU	O1-C1-C2	3.12	118.57	111.67
2	H	1	FRU	O6-C6-C5	2.55	120.02	111.33
2	E	1	FRU	O6-C6-C5	2.51	119.89	111.33
2	F	1	FRU	O1-C1-C2	2.43	117.05	111.67
2	H	2	FRU	C1-C2-C3	-2.25	109.78	115.10
2	H	2	FRU	O1-C1-C2	2.22	118.88	111.33
2	F	1	FRU	O6-C6-C5	2.19	118.78	111.33
2	E	1	FRU	O5-C5-C6	2.14	114.73	108.89
2	E	2	FRU	O6-C6-C5	2.03	118.25	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	FRU	C1-C2-C3	-2.02	110.32	115.10

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	E	1	FRU	O5-C5-C6-O6
2	F	1	FRU	O5-C5-C6-O6
2	G	1	FRU	O1-C1-C2-O5
2	E	1	FRU	C4-C5-C6-O6
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	G	1	FRU	C4-C5-C6-O6
2	G	2	FRU	O1-C1-C2-O5
2	E	1	FRU	O1-C1-C2-C3
2	E	1	FRU	O1-C1-C2-O5
2	E	2	FRU	O1-C1-C2-C3

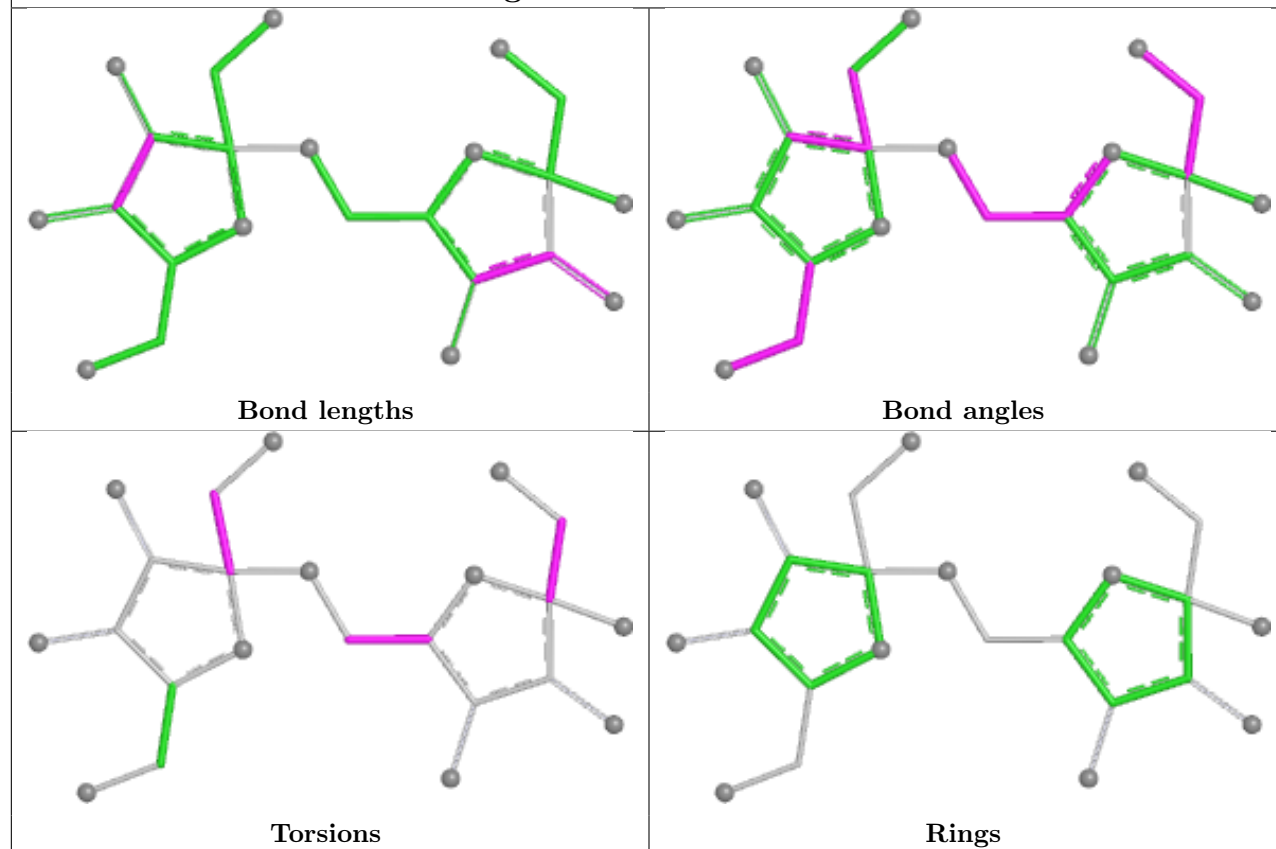
There are no ring outliers.

5 monomers are involved in 7 short contacts:

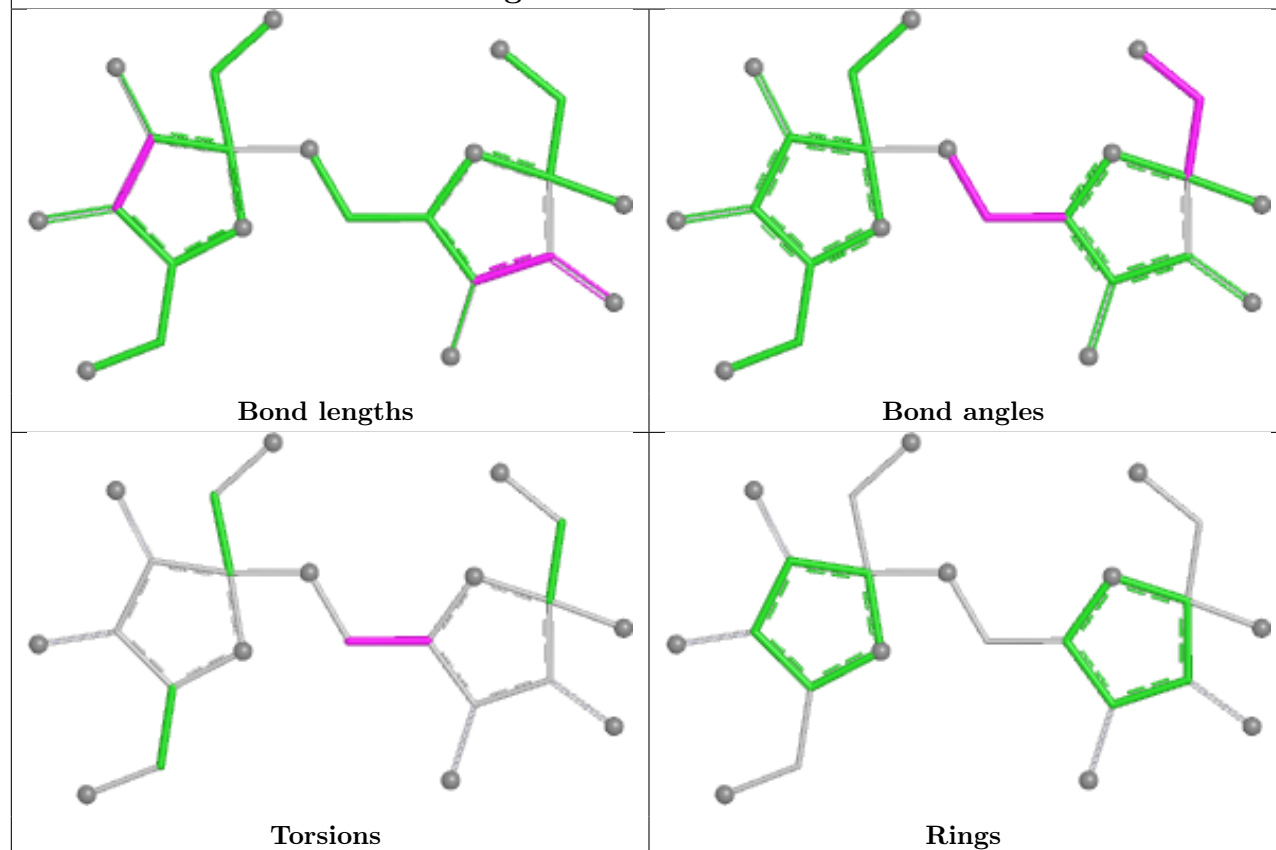
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	FRU	1	0
2	H	1	FRU	3	0
2	G	1	FRU	3	0
2	G	2	FRU	2	0
2	H	2	FRU	3	0

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

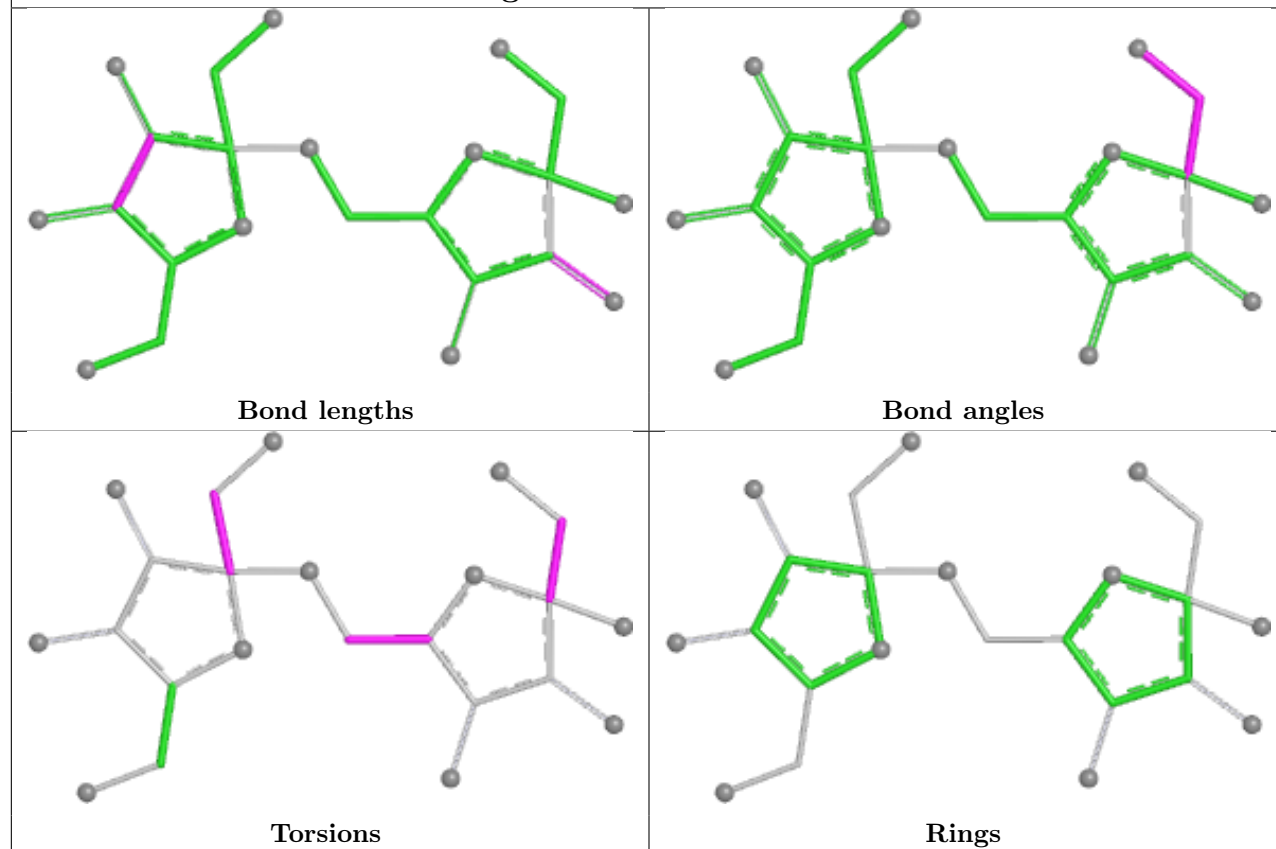
Oligosaccharide Chain E



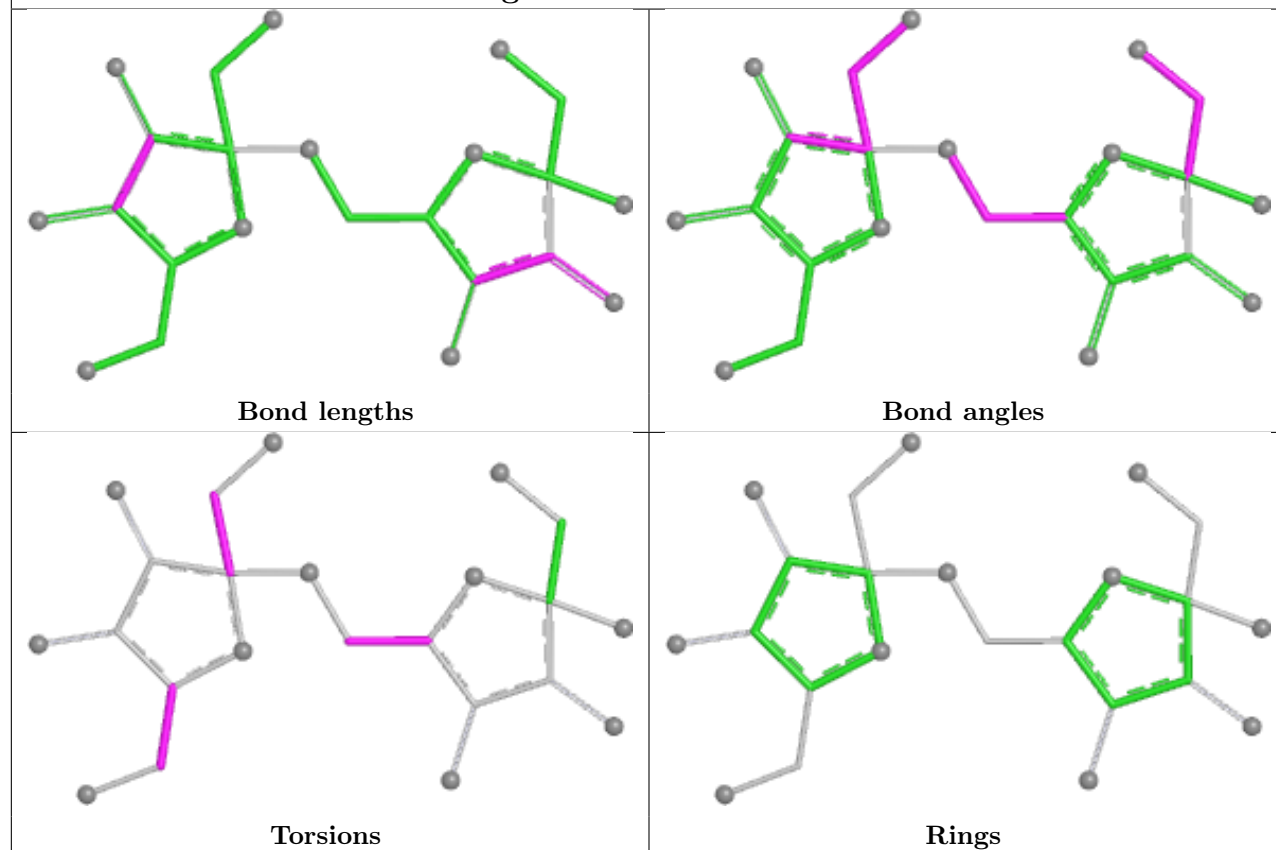
Oligosaccharide Chain F



Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry

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	C	602	-	24,24,24	2.22	6 (25%)	36,38,38	2.16	12 (33%)
3	0U8	B	602	-	24,24,24	1.94	6 (25%)	36,38,38	2.06	10 (27%)
3	0U8	A	602	-	24,24,24	2.06	7 (29%)	36,38,38	2.06	11 (30%)
3	0U8	D	602	-	24,24,24	2.09	6 (25%)	36,38,38	2.64	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	C	602	-	-	7/18/56/56	0/2/3/3
3	0U8	B	602	-	-	11/18/56/56	0/2/3/3
3	0U8	A	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'	7.56	1.51	1.41
3	A	602	0U8	O6-C2'	6.67	1.50	1.41
3	D	602	0U8	O6-C2'	6.60	1.50	1.41
3	B	602	0U8	O6-C2'	5.87	1.49	1.41
3	A	602	0U8	O5'-C2'	3.56	1.50	1.42
3	B	602	0U8	O5'-C2'	3.36	1.49	1.42
3	C	602	0U8	O5'-C2'	3.27	1.49	1.42
3	D	602	0U8	O3-C3	-3.13	1.36	1.42
3	D	602	0U8	O5'-C2'	3.12	1.49	1.42
3	A	602	0U8	O3-C3	-3.06	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	0U8	O3-C3	-3.06	1.36	1.42
3	C	602	0U8	O4'-C4'	-2.90	1.35	1.43
3	C	602	0U8	O3-C3	-2.83	1.37	1.42
3	C	602	0U8	O5-C5	2.79	1.49	1.43
3	D	602	0U8	O5-C5	2.78	1.49	1.43
3	B	602	0U8	O5-C5	2.63	1.49	1.43
3	B	602	0U8	O4'-C4'	-2.42	1.37	1.43
3	D	602	0U8	O4'-C4'	-2.40	1.37	1.43
3	C	602	0U8	O5'-C5'	-2.32	1.38	1.43
3	A	602	0U8	O4'-C4'	-2.18	1.37	1.43
3	A	602	0U8	O5-C5	2.17	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'	2.07	1.58	1.53
3	A	602	0U8	O5'-C5'	-2.00	1.39	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	0U8	C1'-C2'-C3'	-6.47	95.82	114.83
3	D	602	0U8	O5'-C2'-C1'	6.27	123.21	107.94
3	C	602	0U8	C1'-C2'-C3'	-6.06	97.01	114.83
3	D	602	0U8	O6-C2'-C1'	-6.05	92.39	109.63
3	D	602	0U8	O6-C2'-C3'	5.96	127.26	108.19
3	A	602	0U8	C1'-C2'-C3'	-5.84	97.65	114.83
3	B	602	0U8	C1'-C2'-C3'	-5.22	99.48	114.83
3	B	602	0U8	O6-C2'-C1'	-4.83	95.85	109.63
3	A	602	0U8	O6-C2'-C3'	4.76	123.43	108.19
3	C	602	0U8	O6-C2'-C3'	4.55	122.75	108.19
3	D	602	0U8	C6-O6-C2'	-4.46	108.74	116.31
3	B	602	0U8	O6-C2'-C3'	4.44	122.40	108.19
3	A	602	0U8	O6-C2'-C1'	-3.94	98.38	109.63
3	C	602	0U8	O6-C6-C5	3.87	116.05	107.69
3	A	602	0U8	C2'-C3'-C4'	-3.74	93.85	102.19
3	B	602	0U8	O5'-C2'-C1'	3.61	116.73	107.94
3	A	602	0U8	O5'-C2'-C1'	3.61	116.72	107.94
3	C	602	0U8	O5'-C2'-C1'	3.58	116.67	107.94
3	D	602	0U8	C2'-C3'-C4'	-3.36	94.69	102.19
3	C	602	0U8	O6-C2'-C1'	-3.31	100.19	109.63
3	B	602	0U8	O1'-C1'-C2'	3.29	122.49	111.54
3	D	602	0U8	O5-C5-C6	3.29	117.24	109.50
3	B	602	0U8	O2-C2-C3	3.02	117.87	108.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	0U8	O2-C6'-C5'	2.98	114.13	107.69
3	C	602	0U8	O5-C5-C6	2.87	116.25	109.50
3	C	602	0U8	O1'-C1'-C2'	2.86	121.07	111.54
3	C	602	0U8	C6'-O2-C2	-2.85	111.47	116.31
3	C	602	0U8	C2'-C3'-C4'	-2.79	95.96	102.19
3	C	602	0U8	O2-C6'-C5'	2.76	113.64	107.69
3	B	602	0U8	O5'-C2'-C3'	2.68	110.79	105.42
3	A	602	0U8	O6-C6-C5	2.60	113.30	107.69
3	D	602	0U8	C2'-O5'-C5'	-2.51	101.21	108.14
3	C	602	0U8	C2'-O5'-C5'	-2.45	101.38	108.14
3	A	602	0U8	O1'-C1'-C2'	2.44	119.68	111.54
3	B	602	0U8	C1-C2-C3	-2.44	107.65	114.83
3	D	602	0U8	O5'-C2'-C3'	2.41	110.26	105.42
3	B	602	0U8	C2'-O5'-C5'	-2.41	101.49	108.14
3	A	602	0U8	O5'-C2'-C3'	2.35	110.14	105.42
3	B	602	0U8	C2'-C3'-C4'	-2.31	97.04	102.19
3	D	602	0U8	O1-C1-C2	2.30	119.20	111.54
3	A	602	0U8	O2-C6'-C5'	2.18	112.39	107.69
3	D	602	0U8	O6-C6-C5	2.17	112.38	107.69
3	D	602	0U8	O5-C2-C3	-2.16	101.08	105.42
3	A	602	0U8	O4'-C4'-C5'	2.13	117.21	111.08
3	C	602	0U8	C1-C2-C3	-2.09	108.69	114.83
3	A	602	0U8	O5-C5-C6	2.05	114.33	109.50

There are no chirality outliers.

All (35) 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

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

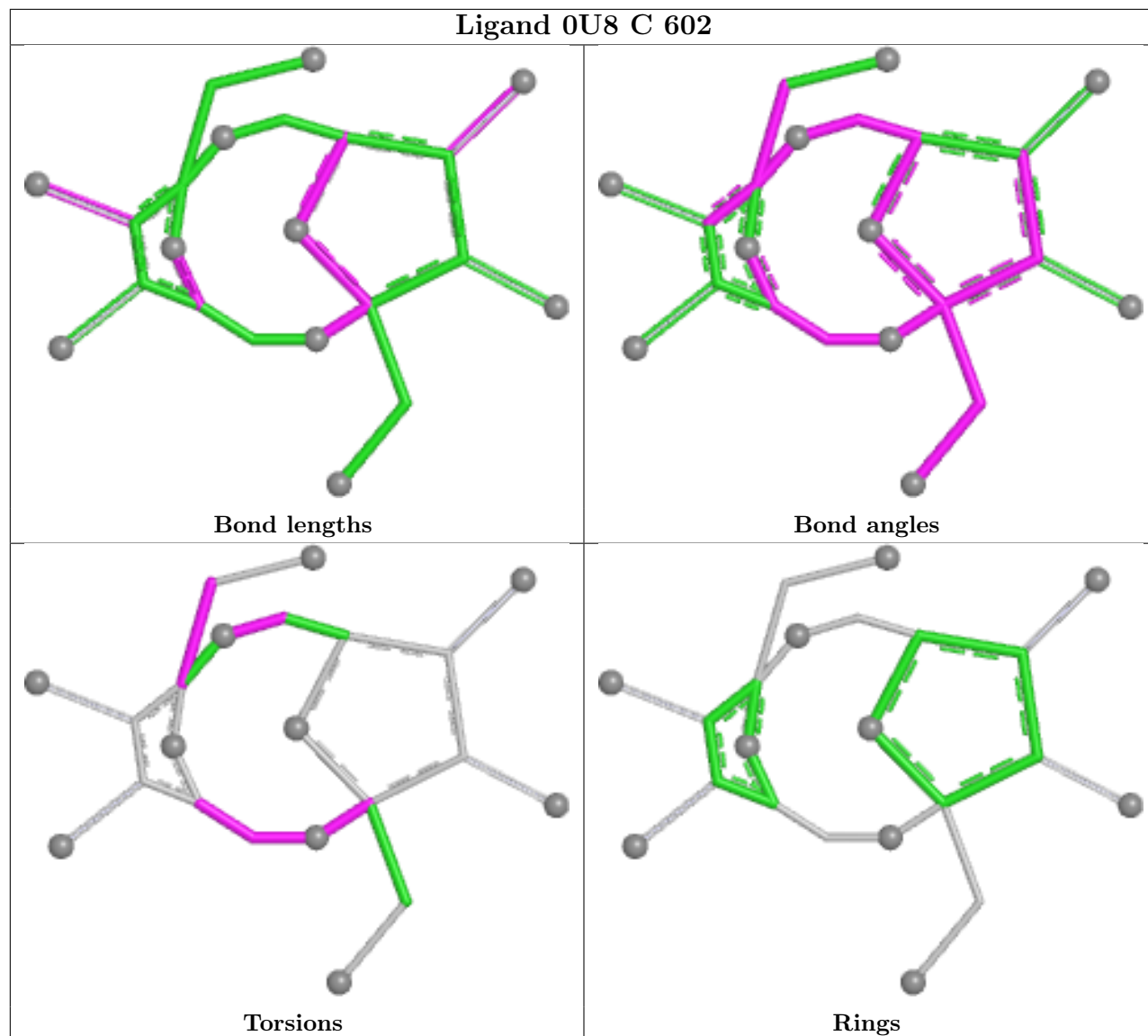
There are no ring outliers.

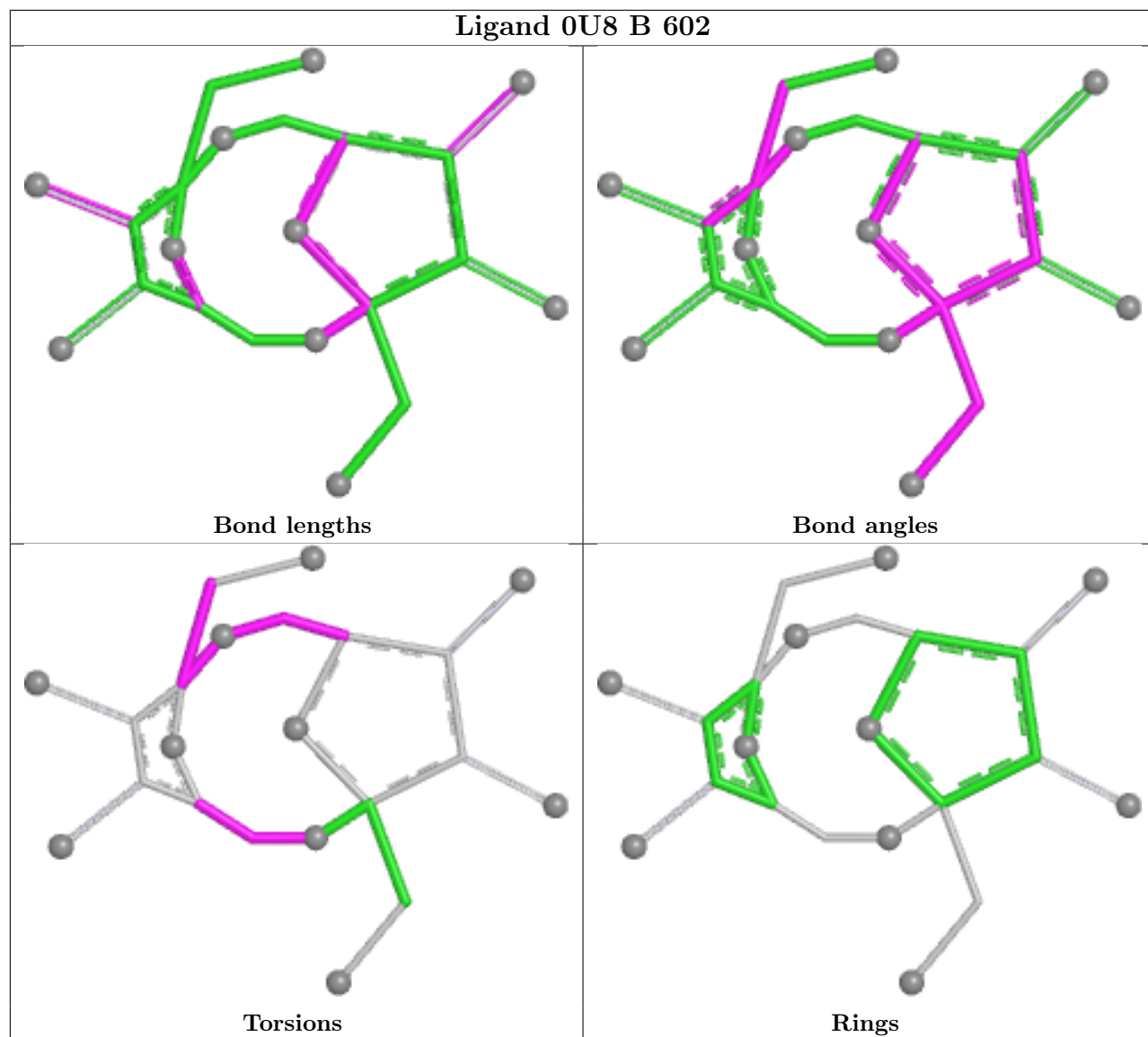
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	0U8	3	0
3	B	602	0U8	6	0
3	A	602	0U8	1	0
3	D	602	0U8	1	0

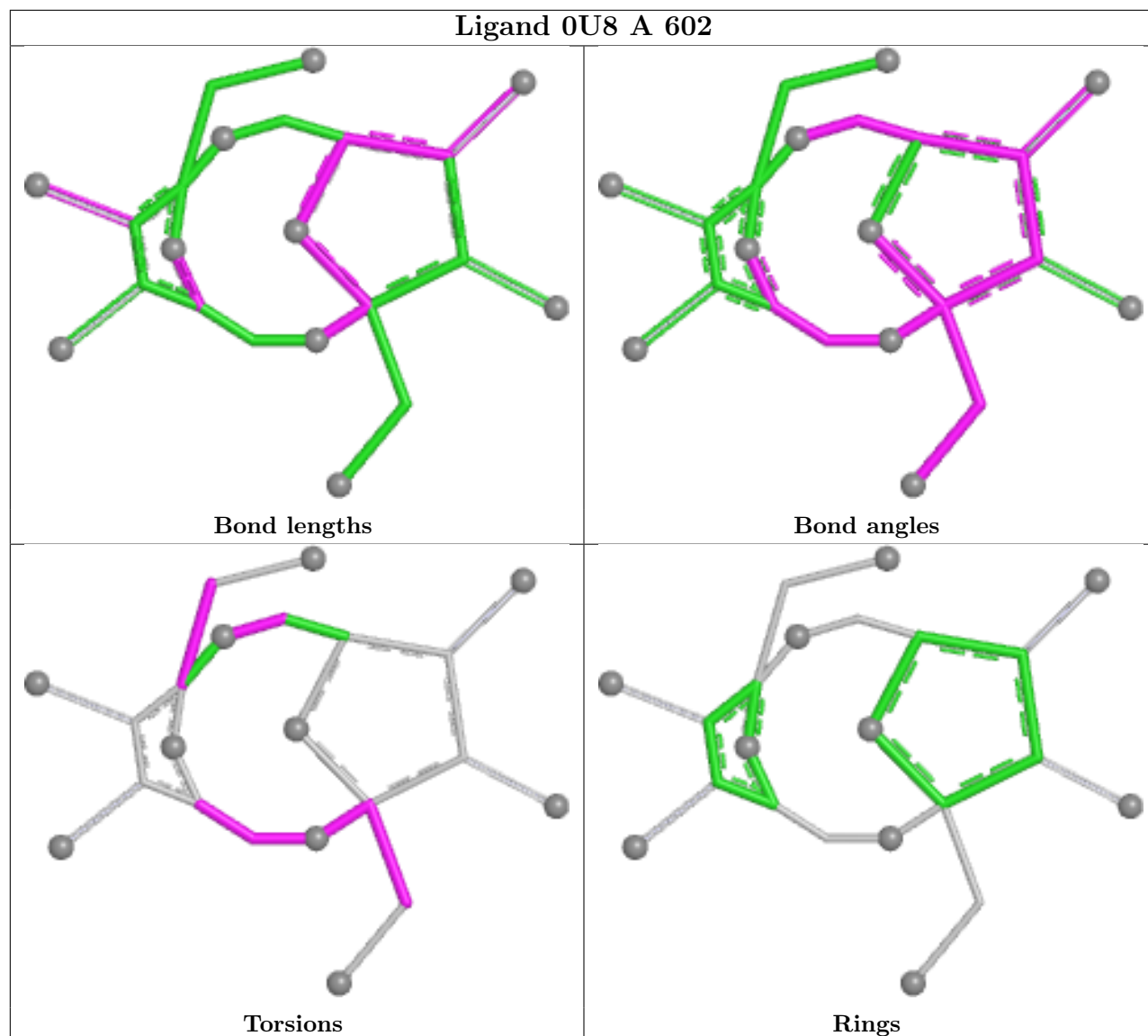
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

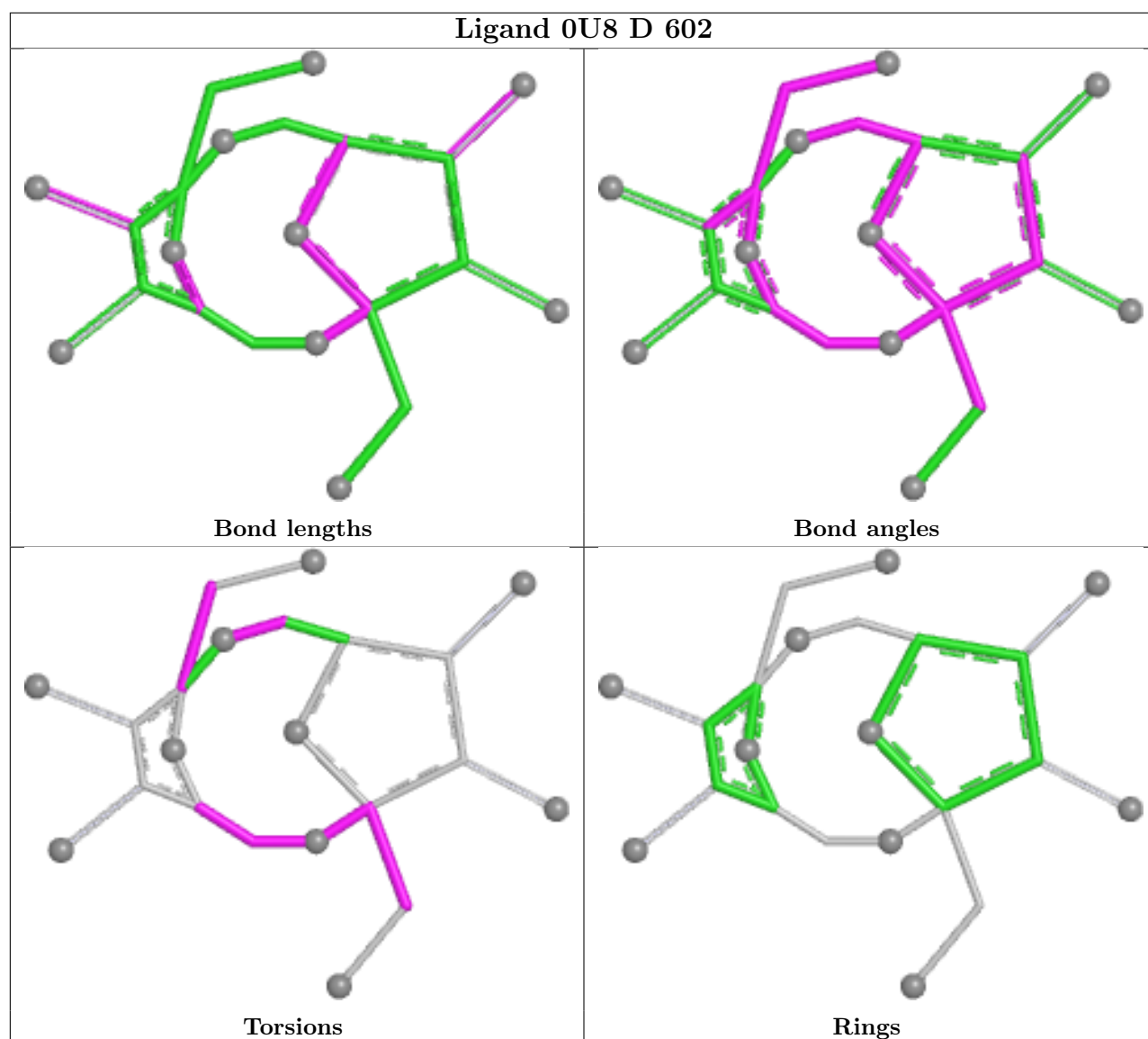
equivalents in the CSD to analyse the geometry.





Ligand 0U8 A 602





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	480/492 (97%)	0.02	13 (2%) 56 58	12, 27, 42, 64	0
1	B	480/492 (97%)	-0.03	8 (1%) 69 70	14, 27, 40, 65	0
1	C	479/492 (97%)	-0.04	7 (1%) 72 73	13, 24, 37, 55	0
1	D	480/492 (97%)	-0.17	8 (1%) 69 70	14, 23, 35, 59	0
All	All	1919/1968 (97%)	-0.05	36 (1%) 66 68	12, 25, 38, 65	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	520	ALA	8.7
1	C	234	GLY	7.6
1	A	520	ALA	6.1
1	D	520	ALA	6.1
1	D	234	GLY	5.0
1	A	235	ILE	4.1
1	A	173	THR	3.7
1	B	235	ILE	3.5
1	C	519	GLN	3.4
1	D	519	GLN	3.4
1	A	519	GLN	3.1
1	D	223	ARG	3.1
1	A	233	GLY	3.0
1	B	518	GLY	3.0
1	B	519	GLN	2.9
1	C	233	GLY	2.9
1	D	180	ASN	2.7
1	D	233	GLY	2.6
1	C	348	ARG	2.5
1	A	518	GLY	2.5
1	B	173	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	172	ALA	2.4
1	D	494	GLY	2.4
1	A	174	THR	2.4
1	A	175	PRO	2.3
1	B	234	GLY	2.3
1	D	518	GLY	2.3
1	C	155	THR	2.3
1	B	233	GLY	2.2
1	A	234	GLY	2.2
1	A	171	ALA	2.2
1	A	176	ALA	2.1
1	C	117	ALA	2.1
1	A	172	ALA	2.1
1	C	148	TRP	2.1
1	A	178	ILE	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](#)

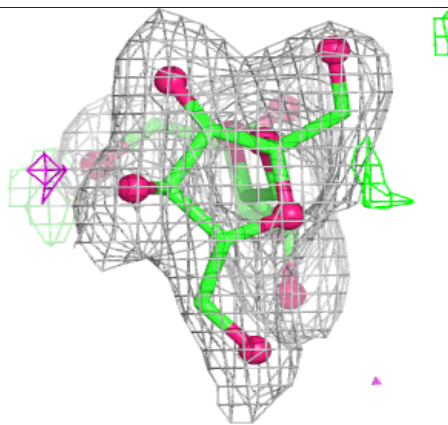
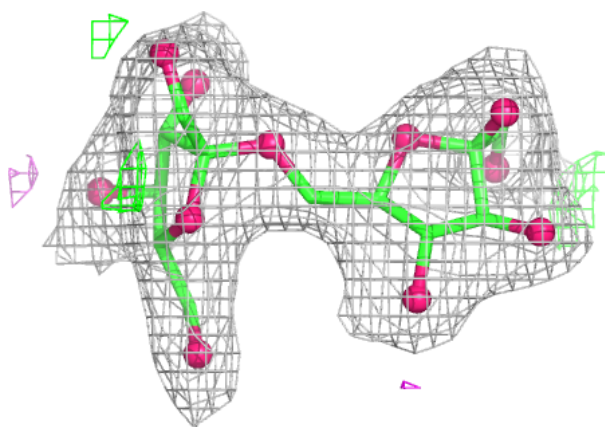
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	FRU	E	2	11/12	0.87	0.13	42,43,45,45	0
2	FRU	H	1	12/12	0.87	0.14	61,63,64,64	0
2	FRU	H	2	11/12	0.87	0.13	57,59,60,60	0
2	FRU	G	1	12/12	0.93	0.08	27,29,30,31	0
2	FRU	G	2	11/12	0.93	0.09	29,32,34,36	0
2	FRU	E	1	12/12	0.93	0.09	41,42,43,46	0
2	FRU	F	2	11/12	0.93	0.09	37,38,39,40	0
2	FRU	F	1	12/12	0.94	0.08	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.

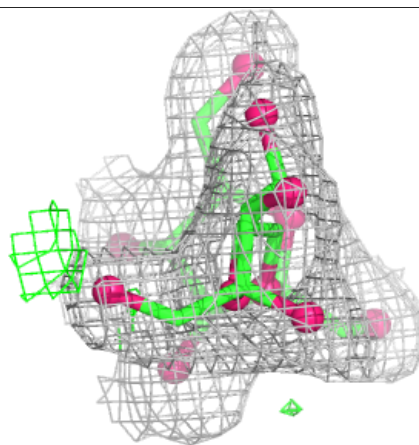
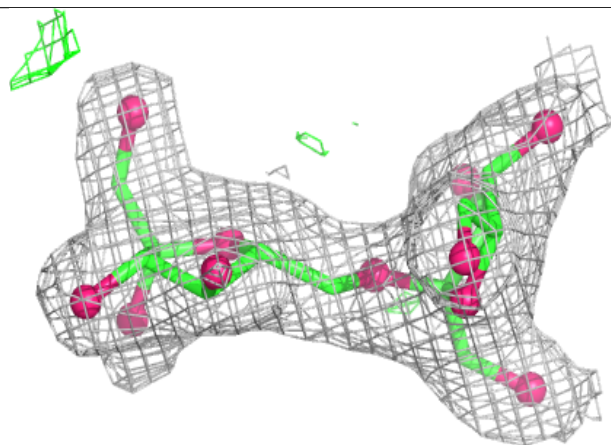
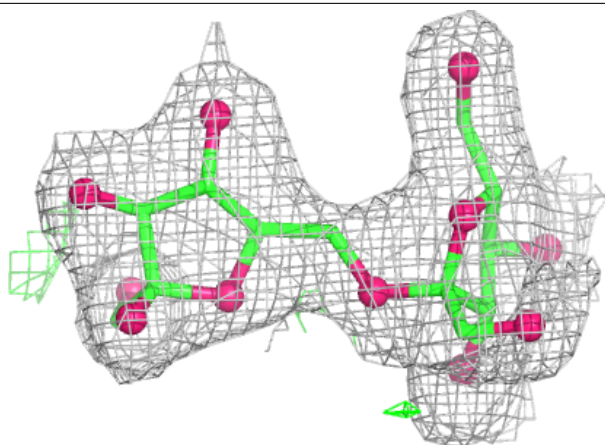
Electron density around Chain E:

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



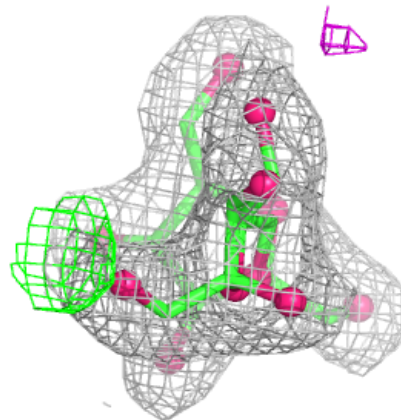
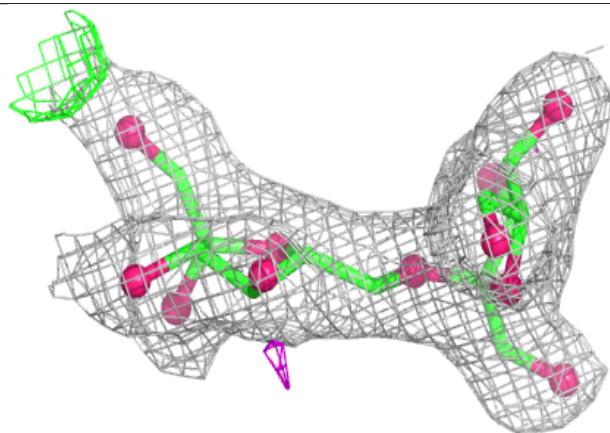
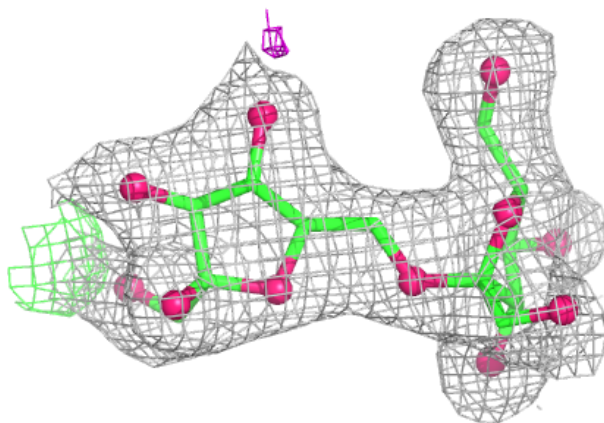
Electron density around Chain F:

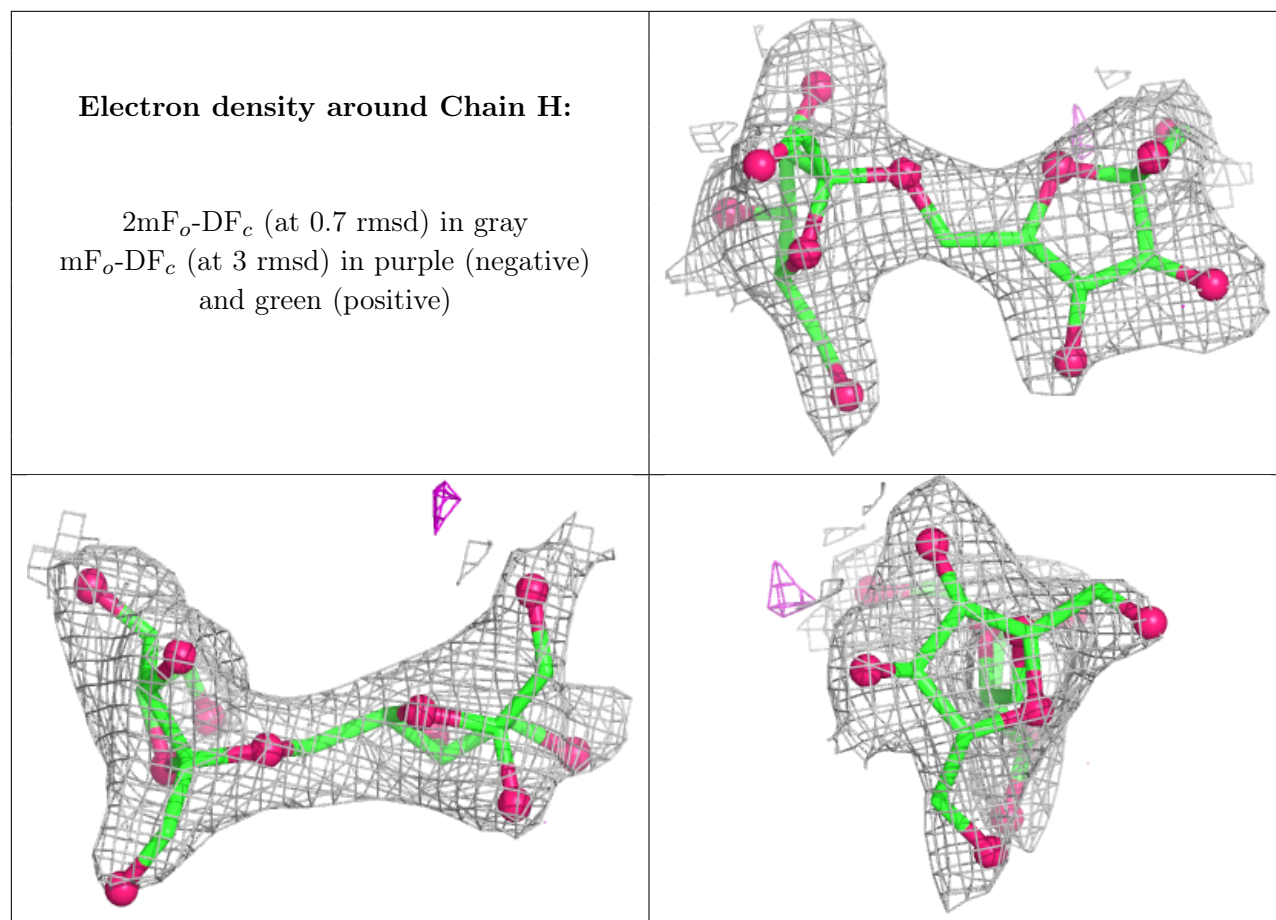
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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 [i](#)

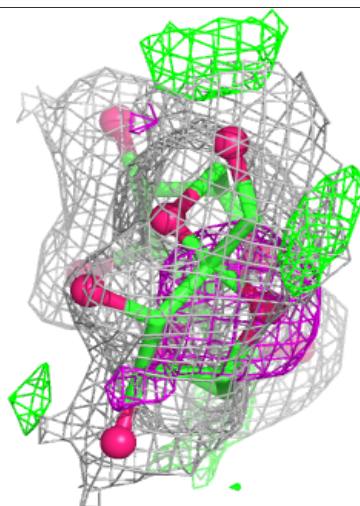
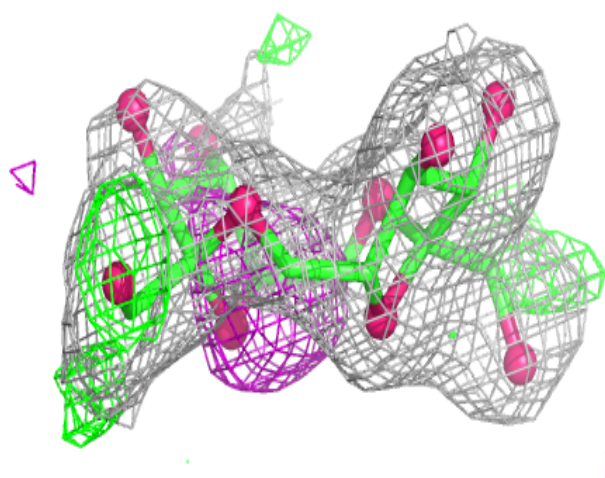
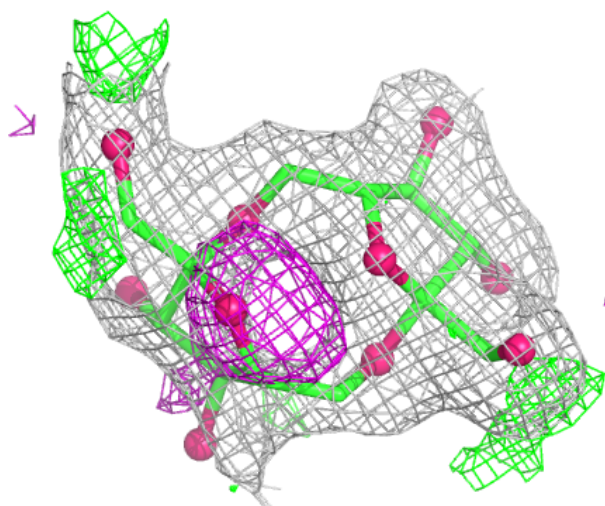
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	0U8	D	602	22/22	0.79	0.18	31,40,51,53	0
3	0U8	B	602	22/22	0.83	0.15	22,34,46,49	0
3	0U8	C	602	22/22	0.85	0.16	23,34,46,50	0
3	0U8	A	602	22/22	0.91	0.10	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.

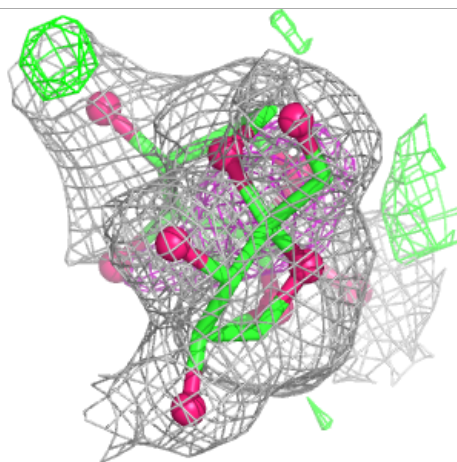
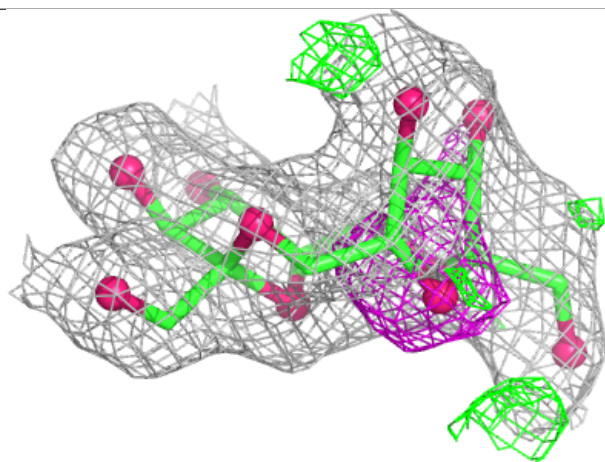
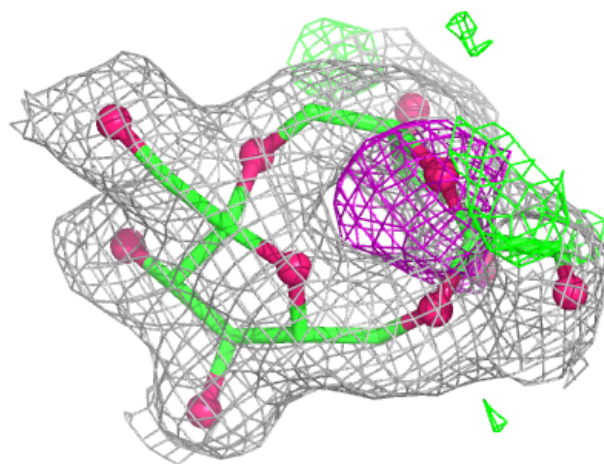
Electron density around 0U8 D 602:

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



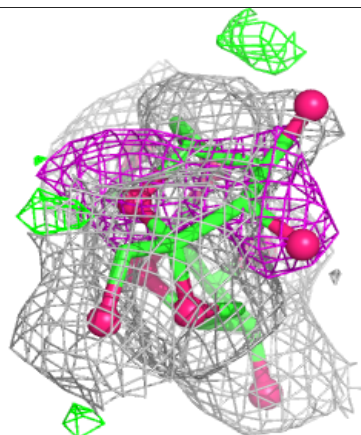
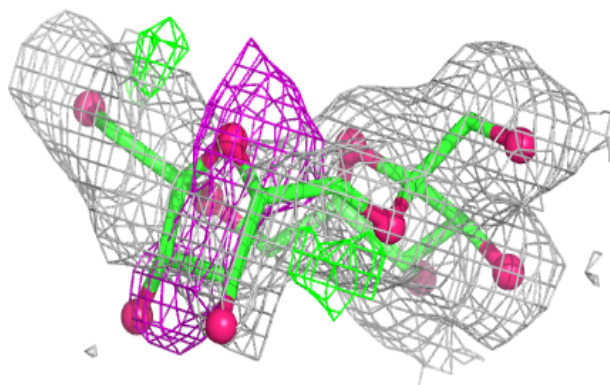
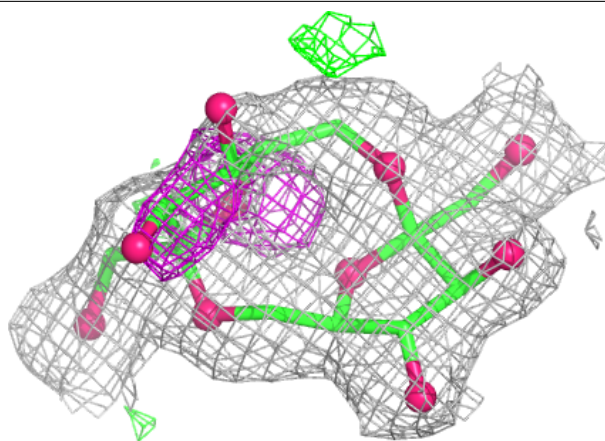
Electron density around 0U8 B 602:

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



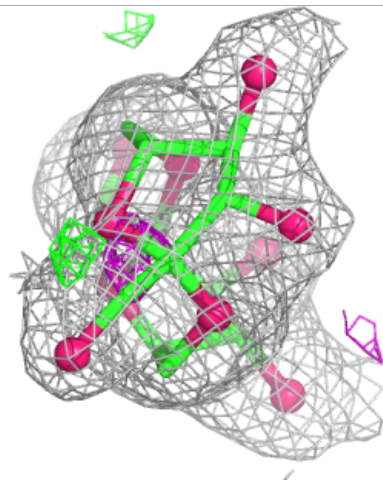
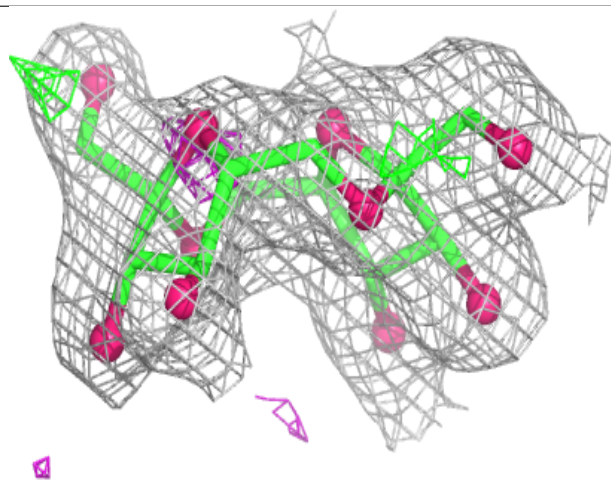
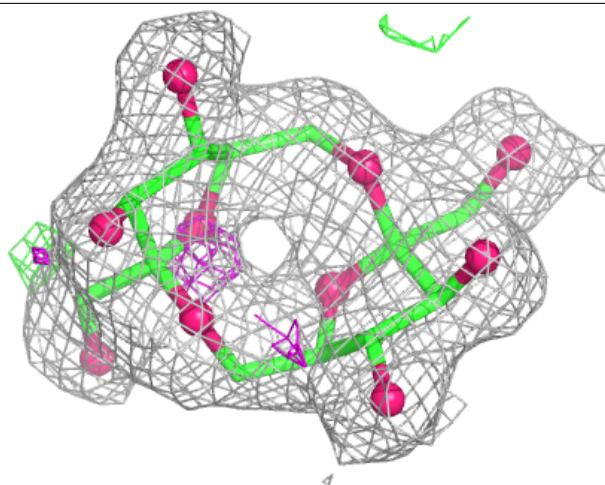
Electron density around 0U8 C 602:

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



Electron density around 0U8 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.