



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:09 PM UTC

PDB ID : 6JBR / pdb_00006jbr
Title : Tps1/UDP/T6P complex
Authors : Wang, S.; Zhao, Y.; Wang, D.; Liu, J.
Deposited on : 2019-01-26
Resolution : 2.03 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:

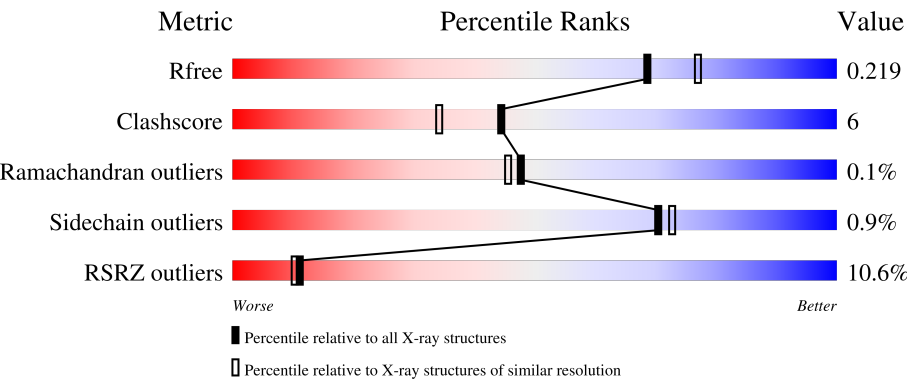
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	465	3% 92% 8%
1	B	465	4% 93% 6%
1	D	465	5% 91% 9%
1	F	465	15% 83% 15%
1	H	465	18% 85% 14%

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Mol	Chain	Length	Quality of chain
1	K	465	
1	M	465	
1	O	465	
2	C	2	
2	E	2	
2	G	2	
2	I	2	
2	J	2	
2	L	2	
2	N	2	
2	P	2	

2 Entry composition [i](#)

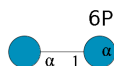
There are 4 unique types of molecules in this entry. The entry contains 32016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Trehalose-6-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3710	2391	633	675	11			
1	B	465	Total	C	N	O	S	0	0	0
			3710	2391	633	675	11			
1	D	465	Total	C	N	O	S	0	0	0
			3710	2391	633	675	11			
1	F	465	Total	C	N	O	S	0	0	0
			3710	2391	633	675	11			
1	H	465	Total	C	N	O	S	0	0	0
			3710	2391	633	675	11			
1	K	465	Total	C	N	O	S	0	0	0
			3710	2391	633	675	11			
1	M	465	Total	C	N	O	S	0	0	0
			3710	2391	633	675	11			
1	O	465	Total	C	N	O	S	0	0	0
			3710	2391	633	675	11			

- Molecule 2 is an oligosaccharide called 6-O-phosphono-alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose.



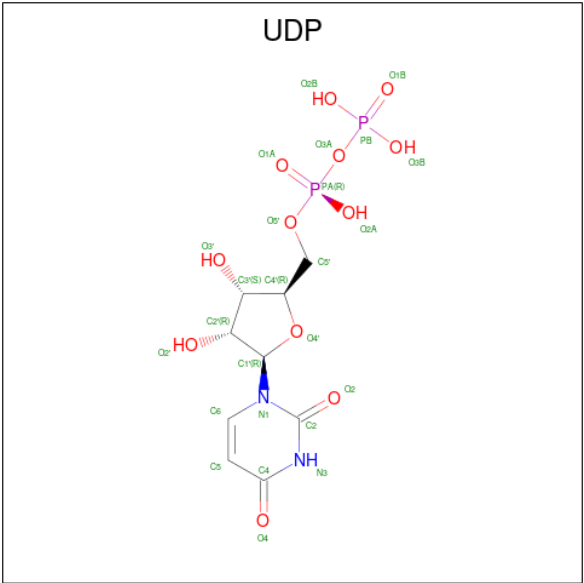
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	P	0	0	0
			27	12	14	1			
2	E	2	Total	C	O	P	0	0	0
			27	12	14	1			
2	G	2	Total	C	O	P	0	0	0
			27	12	14	1			
2	I	2	Total	C	O	P	0	0	0
			27	12	14	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	2	Total	C	O	P	0	0	0
			27	12	14	1			
2	L	2	Total	C	O	P	0	0	0
			27	12	14	1			
2	N	2	Total	C	O	P	0	0	0
			27	12	14	1			
2	P	2	Total	C	O	P	0	0	0
			27	12	14	1			

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

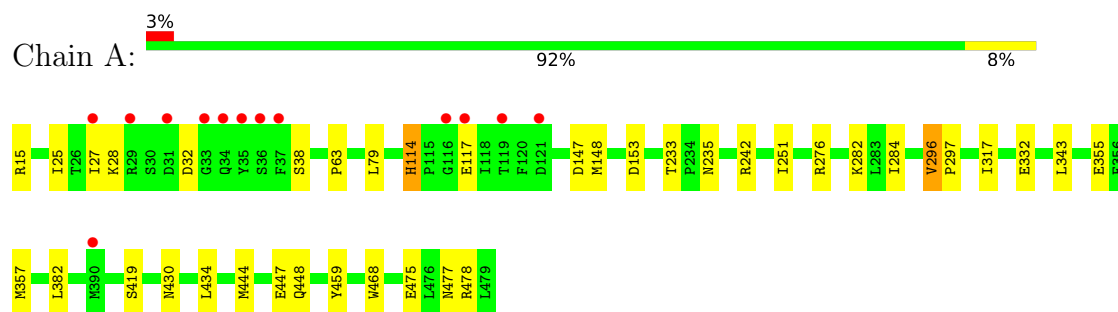
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	305	Total	O	0	0
			305	305		
4	B	330	Total	O	0	0
			330	330		
4	D	312	Total	O	0	0
			312	312		
4	F	178	Total	O	0	0
			178	178		
4	H	177	Total	O	0	0
			177	177		
4	K	154	Total	O	0	0
			154	154		
4	M	171	Total	O	0	0
			171	171		
4	O	293	Total	O	0	0
			293	293		

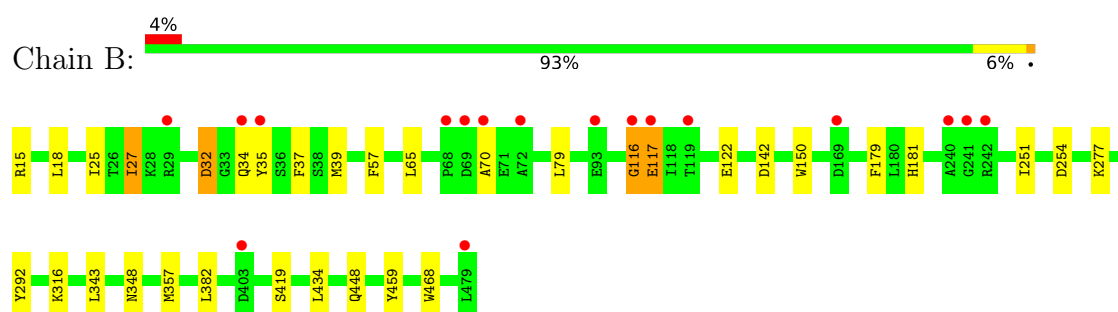
3 Residue-property plots

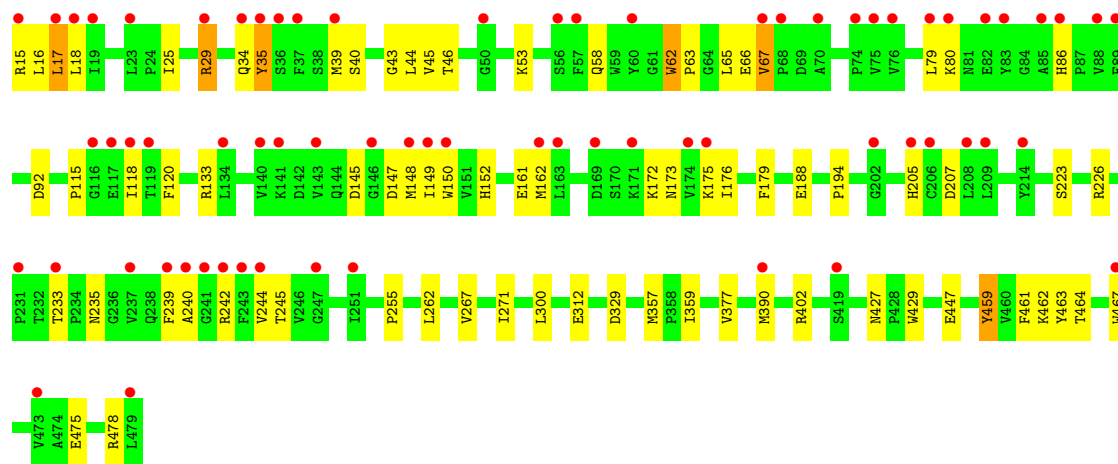
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Trehalose-6-phosphate synthase

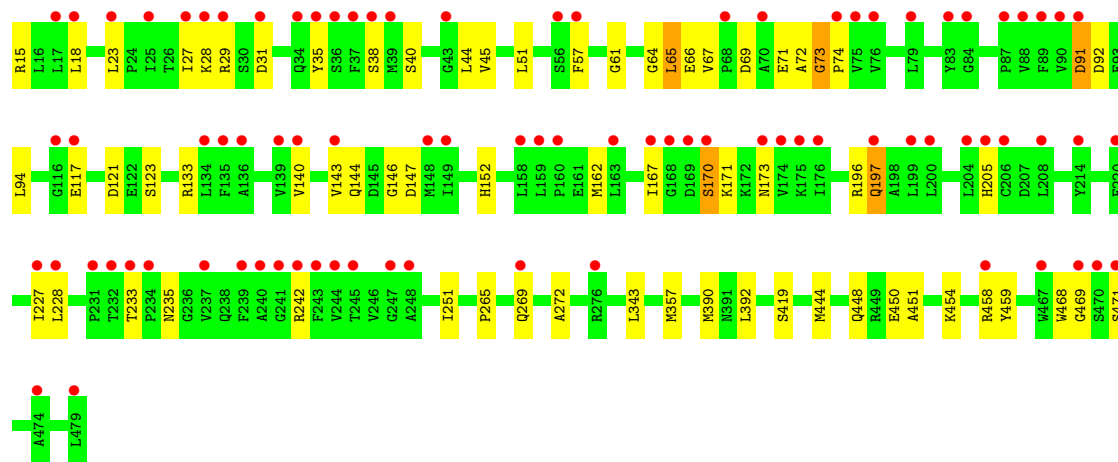
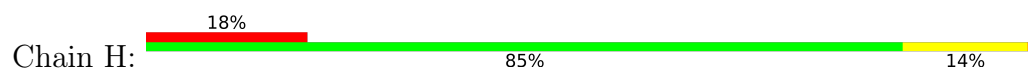


- Molecule 1: Trehalose-6-phosphate synthase

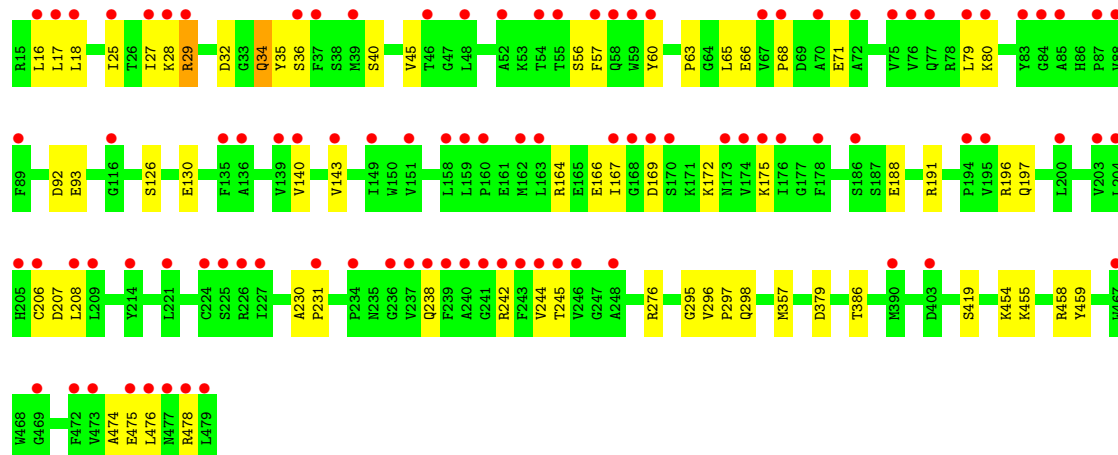
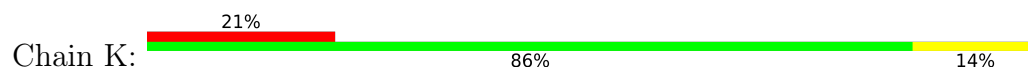




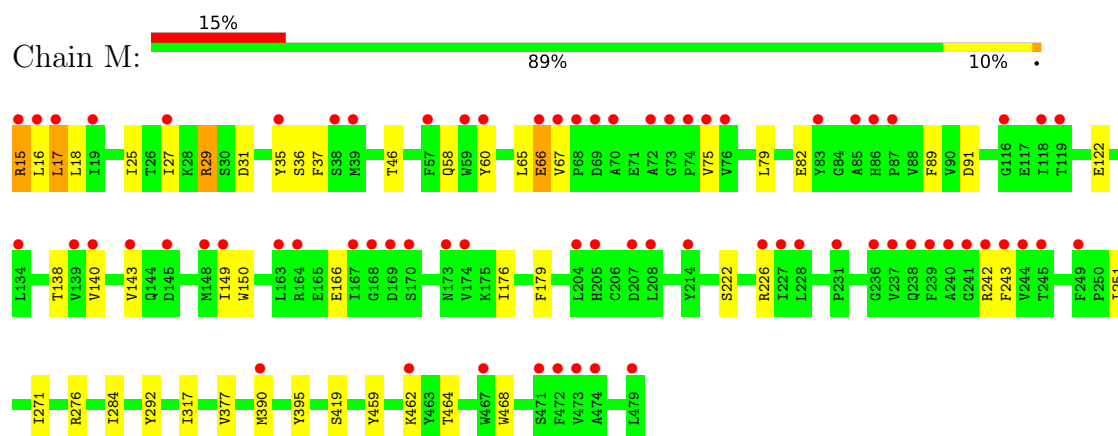
• Molecule 1: Trehalose-6-phosphate synthase



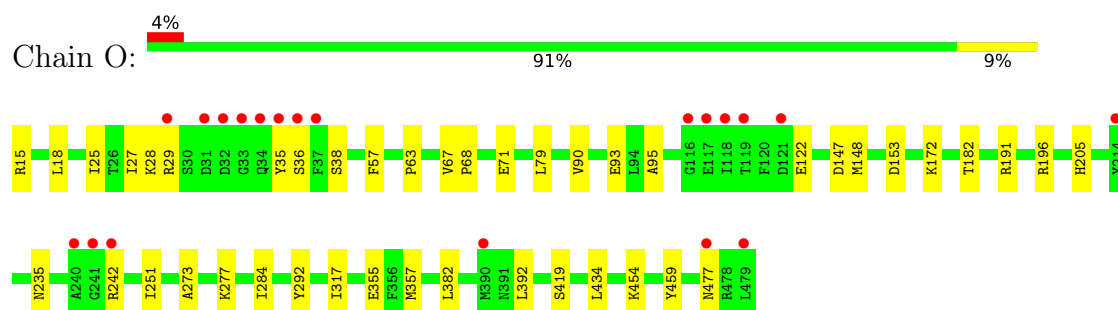
• Molecule 1: Trehalose-6-phosphate synthase



- Molecule 1: Trehalose-6-phosphate synthase



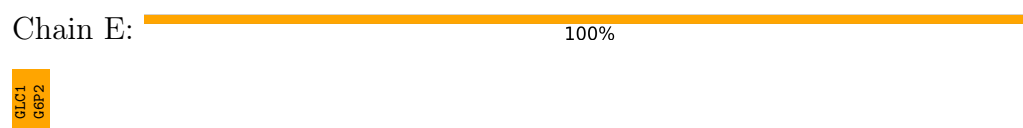
- Molecule 1: Trehalose-6-phosphate synthase



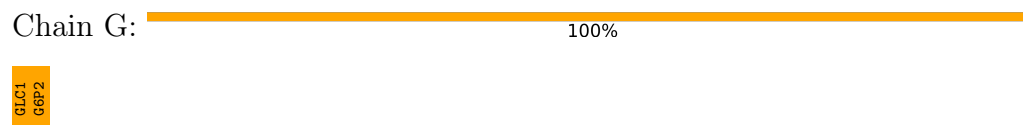
- Molecule 2: 6-O-phosphono-alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose



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- Molecule 2: 6-O-phosphono-alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain J:  100%



- Molecule 2: 6-O-phosphono-alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain L:  100%



- Molecule 2: 6-O-phosphono-alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain N:  50% 50%



- Molecule 2: 6-O-phosphono-alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain P:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.28Å 172.49Å 141.70Å 90.00° 90.92° 90.00°	Depositor
Resolution (Å)	29.80 – 2.03 29.80 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.80-2.03) 99.7 (29.80-2.03)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.211 , 0.234 0.200 , 0.219	Depositor DCC
R_{free} test set	14921 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32016	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.07% 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: G6P, GLC, UDP

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	0.33	2/3808 (0.1%)	0.48	2/5173 (0.0%)
1	B	0.34	0/3808	0.47	2/5173 (0.0%)
1	D	0.29	0/3808	0.43	0/5173
1	F	0.59	3/3808 (0.1%)	0.70	6/5173 (0.1%)
1	H	0.42	1/3808 (0.0%)	0.59	5/5173 (0.1%)
1	K	0.47	2/3808 (0.1%)	0.58	1/5173 (0.0%)
1	M	0.33	0/3808	0.54	1/5173 (0.0%)
1	O	0.34	2/3808 (0.1%)	0.44	0/5173
All	All	0.40	10/30464 (0.0%)	0.53	17/41384 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	90	VAL	C-O	-7.00	1.17	1.24
1	A	114	HIS	C-O	-6.16	1.17	1.24
1	A	296	VAL	C-O	-5.88	1.17	1.24
1	O	95	ALA	C-O	-5.81	1.17	1.24
1	F	53	LYS	C-O	-5.54	1.17	1.24
1	F	223	SER	C-O	-5.51	1.17	1.24
1	H	272	ALA	C-O	-5.38	1.17	1.24
1	F	459	TYR	C-O	-5.17	1.18	1.24
1	K	295	GLY	C-O	-5.13	1.18	1.24
1	K	298	GLN	C-O	-5.12	1.18	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	67	VAL	CA-C-N	11.91	132.66	119.92
1	F	67	VAL	C-N-CA	11.91	132.66	119.92
1	A	114	HIS	CA-C-N	11.25	131.12	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	HIS	C-N-CA	11.25	131.12	119.19
1	F	62	TRP	CA-C-N	10.75	131.05	119.87
1	F	62	TRP	C-N-CA	10.75	131.05	119.87
1	H	72	ALA	N-CA-C	7.70	119.67	111.28
1	F	226	ARG	N-CA-C	7.01	119.00	111.36
1	K	197	GLN	CB-CA-C	-6.32	100.10	110.85
1	H	64	GLY	N-CA-C	5.84	122.52	114.92
1	B	35	TYR	N-CA-C	5.72	117.84	108.52
1	B	32	ASP	CB-CA-C	-5.69	101.94	110.88
1	H	91	ASP	CB-CA-C	-5.66	99.62	109.64
1	F	67	VAL	N-CA-C	5.35	113.72	107.89
1	M	16	LEU	N-CA-C	5.13	116.89	108.52
1	H	197	GLN	CA-CB-CG	5.12	124.34	114.10
1	H	73	GLY	O-C-N	5.09	122.90	121.07

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	3710	0	3659	27	0
1	B	3710	0	3659	27	0
1	D	3710	0	3659	40	0
1	F	3710	0	3659	71	0
1	H	3710	0	3659	57	0
1	K	3710	0	3659	53	0
1	M	3710	0	3659	43	0
1	O	3710	0	3659	37	0
2	C	27	0	19	1	0
2	E	27	0	19	2	0
2	G	27	0	19	3	0
2	I	27	0	19	4	0
2	J	27	0	19	3	0
2	L	27	0	19	2	0
2	N	27	0	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	27	0	19	2	0
3	A	25	0	11	0	0
3	B	25	0	11	0	0
3	D	25	0	11	1	0
3	F	25	0	11	2	0
3	H	25	0	11	1	0
3	K	25	0	11	0	0
3	M	25	0	11	0	0
3	O	25	0	11	0	0
4	A	305	0	0	8	1
4	B	330	0	0	8	1
4	D	312	0	0	11	2
4	F	178	0	0	14	1
4	H	177	0	0	5	0
4	K	154	0	0	7	1
4	M	171	0	0	6	1
4	O	293	0	0	9	1
All	All	32016	0	29513	358	4

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 6.

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:35:TYR:CE2	1:O:71:GLU:HG2	1.54	1.43
1:K:29:ARG:HH12	1:K:68:PRO:HD3	1.04	1.18
1:H:35:TYR:CE1	1:H:71:GLU:OE2	2.08	1.06
1:O:35:TYR:CE2	1:O:71:GLU:CG	2.37	1.06
1:A:357:MET:SD	4:A:779:HOH:O	2.15	1.05
1:M:82:GLU:OE1	4:M:601:HOH:O	1.73	1.04
1:F:240:ALA:HB3	1:F:242:ARG:HH21	1.30	0.96
1:O:35:TYR:HE2	1:O:71:GLU:HG2	1.21	0.95
1:K:29:ARG:HH12	1:K:68:PRO:CD	1.78	0.95
1:O:35:TYR:CZ	1:O:71:GLU:HG2	2.00	0.94
1:M:15:ARG:HH22	1:M:58:GLN:H	1.09	0.94
1:H:196:ARG:NH1	4:H:602:HOH:O	2.01	0.93
1:K:29:ARG:NH1	1:K:68:PRO:HD3	1.85	0.91
1:B:254:ASP:OD2	4:B:601:HOH:O	1.88	0.91
1:F:16:LEU:O	4:F:601:HOH:O	1.86	0.91
1:F:188:GLU:OE2	4:F:602:HOH:O	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:471:SER:OG	4:H:601:HOH:O	1.89	0.90
1:O:292:TYR:O	4:O:601:HOH:O	1.89	0.88
1:K:231:PRO:HG2	1:K:238:GLN:HB3	1.56	0.88
1:F:464:THR:OG1	4:F:603:HOH:O	1.93	0.86
1:K:34:GLN:HA	1:K:34:GLN:HE21	1.39	0.85
1:M:15:ARG:HH12	1:M:58:GLN:HG2	1.42	0.85
1:O:35:TYR:HE2	1:O:71:GLU:CG	1.82	0.84
1:M:18:LEU:CD2	1:M:150:TRP:HB3	2.08	0.82
1:M:292:TYR:O	4:M:602:HOH:O	1.97	0.82
1:M:390:MET:O	2:N:1:GLC:O4	1.98	0.82
1:F:464:THR:HG23	1:F:467:TRP:H	1.44	0.81
1:M:91:ASP:OD1	4:M:603:HOH:O	1.99	0.81
1:K:27:ILE:HD13	1:K:63:PRO:HB2	1.62	0.80
1:F:207:ASP:O	4:F:605:HOH:O	1.99	0.80
1:A:32:ASP:OD1	4:A:601:HOH:O	1.99	0.79
1:M:122:GLU:OE2	4:M:604:HOH:O	2.00	0.78
1:H:18:LEU:HD13	1:H:57:PHE:CG	2.19	0.78
3:F:501:UDP:O2B	2:I:1:GLC:O2	2.01	0.78
1:D:440:ASP:OD2	4:D:601:HOH:O	2.01	0.77
1:D:29:ARG:NH1	1:D:35:TYR:HB3	2.00	0.77
1:F:148:MET:CG	1:F:175:LYS:HE2	2.15	0.76
1:F:29:ARG:CG	1:F:29:ARG:HH11	1.98	0.76
1:D:432:GLU:OE2	4:D:602:HOH:O	2.03	0.76
1:F:161:GLU:HB2	1:F:205:HIS:ND1	2.01	0.76
1:H:35:TYR:HE1	1:H:71:GLU:OE2	1.62	0.76
1:A:233:THR:HG23	1:A:235:ASN:H	1.51	0.75
1:M:242:ARG:NH1	1:M:243:PHE:O	2.19	0.75
1:O:242:ARG:NH1	4:O:603:HOH:O	2.18	0.75
1:M:15:ARG:NH1	1:M:58:GLN:HG2	2.03	0.74
1:F:233:THR:HG23	1:F:235:ASN:H	1.52	0.74
1:K:188:GLU:OE2	4:K:601:HOH:O	2.05	0.73
1:K:143:VAL:HG21	1:K:167:ILE:HD11	1.70	0.73
1:O:357:MET:SD	4:O:617:HOH:O	2.46	0.73
1:F:18:LEU:CD2	1:F:150:TRP:HB3	2.19	0.72
1:M:15:ARG:NH2	1:M:58:GLN:H	1.86	0.72
1:D:479:LEU:O	4:D:603:HOH:O	2.07	0.71
3:H:501:UDP:O3B	4:H:603:HOH:O	2.08	0.71
1:H:167:ILE:O	1:H:170:SER:HB3	1.90	0.71
1:H:69:ASP:O	4:H:604:HOH:O	2.09	0.71
1:O:36:SER:OG	4:O:602:HOH:O	2.07	0.71
1:F:145:ASP:OD1	1:F:172:LYS:N	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:451:ALA:HA	1:H:454:LYS:HE3	1.73	0.70
1:D:269:GLN:NE2	4:D:607:HOH:O	2.24	0.70
1:F:148:MET:HG2	1:F:175:LYS:HE2	1.71	0.70
1:D:66:GLU:OE2	4:D:604:HOH:O	2.10	0.70
1:F:357:MET:SD	4:F:620:HOH:O	2.50	0.70
1:F:29:ARG:HH11	1:F:29:ARG:HG2	1.56	0.69
1:M:35:TYR:HD1	1:M:35:TYR:H	1.38	0.69
1:K:357:MET:SD	4:K:613:HOH:O	2.50	0.68
1:B:277:LYS:NZ	4:B:605:HOH:O	2.26	0.68
1:M:15:ARG:HH22	1:M:58:GLN:N	1.86	0.68
1:H:35:TYR:CZ	1:H:71:GLU:OE2	2.47	0.68
1:M:276:ARG:HA	1:M:276:ARG:NE	2.09	0.67
1:M:17:LEU:HD23	1:M:60:TYR:CE1	2.28	0.67
1:H:18:LEU:HD13	1:H:57:PHE:CD1	2.30	0.67
1:F:17:LEU:N	1:F:17:LEU:HD12	2.11	0.66
1:F:18:LEU:HD21	1:F:150:TRP:HB3	1.77	0.66
1:O:273:ALA:O	1:O:277:LYS:HG3	1.95	0.66
1:F:29:ARG:HH12	1:F:35:TYR:HA	1.59	0.66
1:D:29:ARG:NH1	1:D:35:TYR:CB	2.60	0.65
1:D:427:ASN:OD1	1:D:429:TRP:HD1	1.79	0.65
3:D:501:UDP:O3B	2:G:1:GLC:O2	2.13	0.64
1:K:230:ALA:O	4:K:602:HOH:O	2.14	0.64
1:D:403:ASP:OD1	4:D:605:HOH:O	2.14	0.64
1:F:312:GLU:OE1	4:F:606:HOH:O	2.15	0.64
1:H:144:GLN:HA	1:H:171:LYS:HE2	1.80	0.64
1:H:454:LYS:HD3	1:H:458:ARG:NH2	2.13	0.63
1:K:164:ARG:HH21	1:K:242:ARG:HH12	1.45	0.63
1:A:15:ARG:NH2	1:A:147:ASP:OD2	2.31	0.63
1:K:25:ILE:HD11	1:K:79:LEU:HD21	1.80	0.63
1:K:208:LEU:HD22	1:K:475:GLU:HG2	1.81	0.62
1:M:46:THR:OG1	4:M:605:HOH:O	2.16	0.62
1:F:16:LEU:C	1:F:17:LEU:HD12	2.25	0.62
1:K:169:ASP:O	1:K:172:LYS:NZ	2.33	0.61
1:K:66:GLU:CB	1:K:92:ASP:OD1	2.48	0.61
1:K:474:ALA:O	1:K:478:ARG:HG2	2.00	0.61
1:H:44:LEU:HB2	2:J:1:GLC:H2	1.82	0.61
1:F:148:MET:HG3	1:F:175:LYS:HE2	1.82	0.60
1:H:233:THR:HG23	1:H:235:ASN:H	1.66	0.60
1:K:245:THR:HG21	1:K:475:GLU:OE2	2.00	0.60
1:M:18:LEU:HD22	1:M:150:TRP:HB3	1.83	0.60
1:K:207:ASP:HB2	1:K:476:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLU:HB2	1:B:277:LYS:HG2	1.84	0.60
1:O:172:LYS:NZ	4:O:608:HOH:O	2.33	0.60
1:O:15:ARG:NH1	1:O:147:ASP:OD1	2.35	0.60
1:F:35:TYR:HD1	1:F:35:TYR:C	2.10	0.60
1:H:197:GLN:NE2	1:H:228:LEU:HD22	2.17	0.60
1:K:454:LYS:O	1:K:458:ARG:HG3	2.02	0.59
1:D:37:PHE:CE2	1:D:78:ARG:HG2	2.38	0.59
1:H:29:ARG:HG3	1:H:65:LEU:HD11	1.84	0.59
4:K:673:HOH:O	2:L:1:GLC:O3	1.99	0.59
1:F:44:LEU:HB2	2:I:1:GLC:H61	1.85	0.59
1:F:25:ILE:HD11	1:F:79:LEU:HD21	1.85	0.59
1:H:23:LEU:HD21	1:H:61:GLY:C	2.27	0.59
1:O:153:ASP:OD2	2:P:2:G6P:O2	2.20	0.59
1:O:148:MET:SD	1:O:477:ASN:ND2	2.64	0.59
1:A:282:LYS:NZ	4:A:607:HOH:O	2.36	0.59
1:M:17:LEU:HD13	1:M:149:ILE:HG12	1.85	0.58
1:K:126:SER:O	1:K:130:GLU:HG3	2.02	0.58
1:F:58:GLN:HB2	4:F:601:HOH:O	2.04	0.58
1:H:27:ILE:HB	1:H:65:LEU:HD21	1.87	0.57
1:A:242:ARG:CZ	4:A:611:HOH:O	2.53	0.57
1:F:29:ARG:HG2	1:F:29:ARG:NH1	2.20	0.57
1:M:29:ARG:O	1:M:29:ARG:HG3	1.98	0.57
1:F:29:ARG:HG3	1:F:65:LEU:HD21	1.87	0.57
1:F:35:TYR:C	1:F:35:TYR:CD1	2.82	0.57
1:H:27:ILE:HB	1:H:65:LEU:CD2	2.34	0.57
1:D:71:GLU:N	1:D:71:GLU:OE1	2.38	0.57
1:M:222:SER:O	1:M:226:ARG:HG3	2.05	0.57
1:K:29:ARG:HG3	1:K:65:LEU:HD11	1.87	0.57
1:K:66:GLU:HB2	1:K:92:ASP:OD1	2.04	0.57
1:O:454:LYS:NZ	4:O:614:HOH:O	2.37	0.57
1:B:292:TYR:O	4:B:603:HOH:O	2.18	0.57
1:F:29:ARG:HH11	1:F:29:ARG:CB	2.17	0.57
1:A:355:GLU:HB2	1:B:277:LYS:HE3	1.86	0.57
1:D:475:GLU:OE2	1:D:478:ARG:NH2	2.37	0.57
1:F:402:ARG:NH1	4:F:614:HOH:O	2.27	0.56
1:F:475:GLU:OE2	1:F:478:ARG:NH2	2.38	0.56
1:K:18:LEU:HB2	1:K:57:PHE:CE1	2.40	0.56
1:M:251:ILE:HG22	1:M:390:MET:HG2	1.87	0.56
1:A:475:GLU:OE2	1:A:478:ARG:NH2	2.31	0.56
1:K:16:LEU:HD23	1:K:57:PHE:HB3	1.88	0.56
1:H:73:GLY:N	1:H:74:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ASP:OD1	1:D:34:GLN:NE2	2.40	0.55
1:F:262:LEU:HA	1:F:267:VAL:HG11	1.87	0.55
1:F:271:ILE:HG23	1:F:377:VAL:HG12	1.87	0.55
1:B:25:ILE:HD11	1:B:79:LEU:HD21	1.87	0.55
1:K:475:GLU:OE1	1:K:478:ARG:NH1	2.38	0.55
1:B:116:GLY:O	1:B:117:GLU:HB3	2.06	0.55
1:O:196:ARG:NH2	4:O:605:HOH:O	2.27	0.55
1:K:34:GLN:HA	1:K:34:GLN:NE2	2.18	0.55
1:B:357:MET:SD	4:B:623:HOH:O	2.59	0.54
1:F:15:ARG:NH2	1:F:147:ASP:OD2	2.40	0.54
1:M:462:LYS:O	1:M:464:THR:HG23	2.08	0.54
1:A:430:ASN:OD1	4:A:603:HOH:O	2.18	0.54
1:F:18:LEU:HD23	1:F:150:TRP:HB3	1.90	0.54
1:F:447:GLU:CD	1:F:447:GLU:H	2.15	0.54
1:H:66:GLU:HB2	1:H:92:ASP:OD1	2.08	0.54
1:H:31:ASP:OD1	1:H:31:ASP:N	2.38	0.54
1:A:242:ARG:NH1	4:A:611:HOH:O	2.41	0.54
1:H:197:GLN:HB2	1:H:228:LEU:CD2	2.38	0.53
1:O:15:ARG:HH12	1:O:147:ASP:CG	2.14	0.53
1:F:240:ALA:HB3	1:F:242:ARG:NH2	2.13	0.53
1:M:390:MET:HE2	1:M:395:TYR:OH	2.09	0.53
1:B:27:ILE:HD11	1:B:37:PHE:CE1	2.44	0.53
1:F:427:ASN:OD1	1:F:429:TRP:HD1	1.92	0.53
1:F:149:ILE:O	1:F:176:ILE:HA	2.08	0.53
1:H:40:SER:HB2	1:H:45:VAL:HG21	1.91	0.52
1:D:35:TYR:CD1	1:D:35:TYR:C	2.87	0.52
1:H:146:GLY:HA2	1:H:173:ASN:HB3	1.91	0.52
1:A:114:HIS:HE1	1:A:332:GLU:OE2	1.91	0.52
1:H:29:ARG:NH2	1:H:71:GLU:HG2	2.25	0.52
1:H:35:TYR:CE1	1:H:71:GLU:CD	2.86	0.52
1:D:382:LEU:HD11	1:D:434:LEU:HD11	1.92	0.52
1:F:17:LEU:N	1:F:17:LEU:CD1	2.73	0.52
1:D:27:ILE:CD1	1:D:37:PHE:CE1	2.93	0.51
1:D:29:ARG:HH11	1:D:35:TYR:CB	2.23	0.51
1:D:447:GLU:CD	1:D:447:GLU:H	2.19	0.51
1:H:140:VAL:O	1:H:143:VAL:HG12	2.10	0.51
1:K:379:ASP:OD1	4:K:604:HOH:O	2.19	0.51
1:M:419:SER:HB3	1:M:459:TYR:CZ	2.45	0.51
1:A:276:ARG:HG3	4:A:635:HOH:O	2.10	0.51
1:D:348:ASN:HB3	1:D:357:MET:HE3	1.93	0.50
1:K:140:VAL:O	1:K:143:VAL:HG12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:GLU:CB	1:H:92:ASP:OD1	2.59	0.50
1:O:28:LYS:HD3	1:O:38:SER:OG	2.11	0.50
1:H:29:ARG:NH1	1:H:35:TYR:HB3	2.26	0.50
1:K:80:LYS:HD2	1:K:80:LYS:O	2.11	0.50
1:F:329:ASP:OD2	4:F:607:HOH:O	2.18	0.50
1:H:390:MET:O	2:J:1:GLC:O6	2.23	0.50
1:K:17:LEU:HD23	1:K:60:TYR:CE1	2.46	0.50
1:F:462:LYS:HD3	1:F:463:TYR:CE2	2.46	0.50
1:H:450:GLU:O	1:H:454:LYS:HG3	2.12	0.50
1:M:149:ILE:O	1:M:176:ILE:HA	2.12	0.49
1:M:150:TRP:HE1	1:M:179:PHE:HB2	1.77	0.49
1:F:18:LEU:HD22	1:F:152:HIS:HE2	1.78	0.49
1:A:148:MET:SD	1:A:477:ASN:ND2	2.74	0.49
1:B:32:ASP:HB3	1:B:34:GLN:HE21	1.78	0.49
1:O:25:ILE:HD11	1:O:79:LEU:HD21	1.94	0.49
1:B:70:ALA:N	4:B:618:HOH:O	2.46	0.48
1:K:419:SER:HB3	1:K:459:TYR:CZ	2.48	0.48
3:F:501:UDP:O1B	4:F:608:HOH:O	2.20	0.48
2:N:1:GLC:O4	2:N:1:GLC:O6	2.22	0.48
1:K:191:ARG:O	1:K:196:ARG:NH1	2.44	0.48
1:B:15:ARG:NH2	1:B:142:ASP:O	2.47	0.48
4:D:650:HOH:O	2:G:2:G6P:O2P	2.20	0.48
1:K:455:LYS:HG2	1:K:458:ARG:NH2	2.28	0.48
1:F:40:SER:HB2	1:F:45:VAL:HG21	1.96	0.48
1:A:447:GLU:OE1	4:A:604:HOH:O	2.20	0.47
1:D:235:ASN:HB3	4:D:654:HOH:O	2.13	0.47
1:K:175:LYS:HD2	1:K:207:ASP:OD2	2.14	0.47
1:B:316:LYS:NZ	1:H:269:GLN:OE1	2.46	0.47
1:A:28:LYS:HD2	1:A:38:SER:OG	2.14	0.47
1:D:25:ILE:HD11	1:D:79:LEU:HD21	1.94	0.47
1:F:239:PHE:HD2	1:F:242:ARG:HH22	1.62	0.47
1:K:18:LEU:HD13	1:K:57:PHE:CG	2.50	0.47
1:K:208:LEU:HD12	1:K:245:THR:O	2.14	0.47
1:K:276:ARG:NH2	4:K:610:HOH:O	2.36	0.47
1:M:140:VAL:HG21	1:M:166:GLU:HB3	1.95	0.47
1:H:419:SER:HB3	1:H:459:TYR:CZ	2.50	0.47
1:K:35:TYR:CE2	1:K:71:GLU:HG3	2.49	0.47
1:A:444:MET:HG3	1:A:448:GLN:NE2	2.29	0.47
1:M:251:ILE:HG13	1:M:468:TRP:CD2	2.50	0.47
1:O:382:LEU:HD11	1:O:434:LEU:HD11	1.96	0.47
1:B:448:GLN:NE2	4:B:607:HOH:O	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:GLU:HG3	4:D:618:HOH:O	2.14	0.47
1:D:277:LYS:HG2	1:O:355:GLU:HB2	1.95	0.47
1:H:265:PRO:O	1:H:269:GLN:NE2	2.48	0.47
1:K:35:TYR:CD2	1:K:71:GLU:HG3	2.49	0.47
1:K:35:TYR:N	1:K:35:TYR:CD1	2.72	0.47
1:A:284:ILE:HD11	1:A:317:ILE:HD11	1.97	0.47
1:F:86:HIS:CG	4:F:618:HOH:O	2.67	0.47
1:H:15:ARG:NH2	1:H:147:ASP:OD2	2.47	0.47
1:H:197:GLN:HE21	1:H:228:LEU:HD22	1.79	0.47
1:M:15:ARG:O	1:M:15:ARG:HG3	2.07	0.47
1:M:15:ARG:NH2	1:M:58:GLN:HB2	2.30	0.47
1:O:27:ILE:HG12	1:O:63:PRO:HB2	1.96	0.47
1:O:35:TYR:OH	1:O:68:PRO:HD2	2.15	0.47
1:F:150:TRP:HE1	1:F:179:PHE:HB2	1.78	0.46
1:M:18:LEU:HD23	1:M:150:TRP:HB3	1.93	0.46
1:M:67:VAL:HG21	1:M:89:PHE:CD1	2.50	0.46
1:F:66:GLU:HB2	1:F:92:ASP:OD1	2.14	0.46
1:F:255:PRO:HB2	1:F:461:PHE:CE2	2.50	0.46
1:F:115:PRO:HA	1:F:118:ILE:HD12	1.97	0.46
1:H:133:ARG:HG2	1:H:162:MET:SD	2.55	0.46
1:K:34:GLN:HE21	1:K:34:GLN:CA	2.20	0.46
1:F:29:ARG:HH11	1:F:29:ARG:HA	1.81	0.46
1:K:29:ARG:NH1	1:K:68:PRO:CD	2.63	0.46
1:K:143:VAL:HG11	1:K:167:ILE:HG12	1.98	0.46
1:K:386:THR:O	4:K:605:HOH:O	2.20	0.46
1:M:242:ARG:HD2	1:M:243:PHE:N	2.31	0.46
1:O:15:ARG:NH1	1:O:147:ASP:CG	2.73	0.46
1:F:18:LEU:HD22	1:F:152:HIS:NE2	2.31	0.46
1:H:67:VAL:O	1:H:67:VAL:HG23	2.16	0.46
1:H:227:ILE:HG22	1:H:228:LEU:HD23	1.97	0.46
1:H:251:ILE:HG23	1:H:392:LEU:HD21	1.98	0.46
1:K:29:ARG:HG3	1:K:65:LEU:CD1	2.46	0.46
1:D:35:TYR:CD1	1:D:35:TYR:O	2.69	0.46
1:D:15:ARG:NH2	1:D:142:ASP:O	2.48	0.45
1:D:357:MET:SD	4:D:614:HOH:O	2.61	0.45
1:K:29:ARG:CG	1:K:65:LEU:CD1	2.94	0.45
1:O:122:GLU:HG2	4:O:700:HOH:O	2.15	0.45
2:J:1:GLC:HO2	2:J:2:G6P:HO2	1.61	0.45
1:D:35:TYR:O	1:D:35:TYR:CG	2.70	0.45
1:D:148:MET:SD	1:D:477:ASN:ND2	2.82	0.45
1:O:35:TYR:HE2	1:O:71:GLU:HG3	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLU:CB	1:B:277:LYS:HG2	2.46	0.45
1:D:316:LYS:HE3	4:D:748:HOH:O	2.16	0.45
1:M:27:ILE:CD1	1:M:37:PHE:CE1	2.99	0.45
1:D:222:SER:OG	1:D:226:ARG:NH2	2.50	0.45
1:H:18:LEU:HD23	1:H:152:HIS:NE2	2.32	0.45
1:F:44:LEU:CB	2:I:1:GLC:H61	2.47	0.44
1:F:133:ARG:CZ	1:F:162:MET:HE3	2.46	0.44
1:F:244:VAL:HA	4:F:605:HOH:O	2.17	0.44
1:H:73:GLY:N	1:H:74:PRO:HD2	2.31	0.44
1:O:191:ARG:O	1:O:196:ARG:NH1	2.45	0.44
1:O:235:ASN:HB2	4:O:766:HOH:O	2.16	0.44
1:B:122:GLU:HG3	1:D:432:GLU:HG3	2.00	0.44
1:F:29:ARG:HG3	1:F:65:LEU:CD2	2.47	0.44
1:F:390:MET:O	2:I:1:GLC:O3	2.36	0.44
1:F:459:TYR:CD1	1:F:459:TYR:C	2.95	0.44
1:F:43:GLY:HA2	1:F:46:THR:HB	1.99	0.44
1:B:419:SER:HB3	1:B:459:TYR:CZ	2.53	0.44
1:M:284:ILE:HD11	1:M:317:ILE:HD11	1.99	0.44
1:A:25:ILE:HD11	1:A:79:LEU:HD21	2.00	0.44
1:B:316:LYS:HE2	4:B:764:HOH:O	2.17	0.44
1:D:427:ASN:OD1	1:D:429:TRP:CD1	2.65	0.44
1:H:51:LEU:HD13	1:H:469:GLY:HA3	1.99	0.43
1:A:114:HIS:CE1	1:A:332:GLU:OE2	2.71	0.43
1:F:29:ARG:HH11	1:F:29:ARG:CA	2.31	0.43
1:K:29:ARG:CG	1:K:65:LEU:HD13	2.48	0.43
1:M:271:ILE:HG23	1:M:377:VAL:HG12	2.00	0.43
1:A:251:ILE:HG13	1:A:468:TRP:CD2	2.53	0.43
1:F:18:LEU:HD22	1:F:152:HIS:CD2	2.54	0.43
1:M:65:LEU:HG	1:M:66:GLU:N	2.33	0.43
1:A:27:ILE:HG12	1:A:63:PRO:HB2	2.00	0.43
1:O:29:ARG:HE	1:O:29:ARG:HB2	1.46	0.43
2:L:1:GLC:O2	2:L:2:G6P:H1	2.18	0.43
1:A:382:LEU:HD11	1:A:434:LEU:HD11	1.99	0.43
1:B:316:LYS:CE	1:H:269:GLN:OE1	2.67	0.43
1:H:121:ASP:OD1	1:H:123:SER:HB3	2.18	0.43
1:H:444:MET:HG3	1:H:448:GLN:NE2	2.34	0.43
1:K:206:CYS:O	1:K:244:VAL:HG22	2.18	0.43
1:M:15:ARG:HH21	1:M:17:LEU:HA	1.84	0.43
1:M:75:VAL:O	1:M:79:LEU:HD23	2.18	0.43
1:O:35:TYR:CD2	1:O:71:GLU:OE1	2.72	0.43
1:F:39:MET:HE3	1:F:39:MET:HB3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:HB3	1:A:459:TYR:CZ	2.54	0.43
1:D:153:ASP:OD2	2:G:2:G6P:O2	2.32	0.43
1:F:245:THR:N	4:F:605:HOH:O	2.05	0.43
1:H:66:GLU:N	1:H:92:ASP:OD1	2.46	0.43
1:H:451:ALA:O	1:H:454:LYS:HD2	2.18	0.43
1:D:419:SER:HB3	1:D:459:TYR:CZ	2.54	0.43
1:H:29:ARG:CZ	1:H:35:TYR:HB3	2.48	0.43
1:O:419:SER:HB3	1:O:459:TYR:CZ	2.53	0.43
1:B:27:ILE:HG22	1:B:65:LEU:HD23	2.01	0.43
1:B:150:TRP:HE1	1:B:179:PHE:HB2	1.83	0.43
1:B:251:ILE:HG13	1:B:468:TRP:CD2	2.53	0.43
1:H:205:HIS:CG	1:H:242:ARG:HH22	2.36	0.43
1:M:140:VAL:O	1:M:143:VAL:HG12	2.18	0.42
1:D:27:ILE:HD11	1:D:37:PHE:CE1	2.53	0.42
1:F:271:ILE:HG23	1:F:377:VAL:CG1	2.49	0.42
1:F:239:PHE:O	1:F:242:ARG:NH2	2.53	0.42
1:F:300:LEU:HD22	1:F:359:ILE:HD13	2.02	0.42
1:O:18:LEU:HD13	1:O:57:PHE:CG	2.54	0.42
1:F:172:LYS:HD3	1:F:173:ASN:H	1.84	0.42
1:H:15:ARG:NE	1:H:147:ASP:OD2	2.52	0.42
1:H:357:MET:SD	4:H:613:HOH:O	2.62	0.42
1:K:27:ILE:HD13	1:K:63:PRO:CB	2.41	0.42
1:F:62:TRP:HA	1:F:63:PRO:HD2	1.71	0.42
1:O:35:TYR:N	1:O:35:TYR:CD1	2.88	0.42
1:A:153:ASP:OD2	2:C:2:G6P:O2	2.32	0.42
1:K:40:SER:HB2	1:K:45:VAL:HG21	2.02	0.42
1:O:251:ILE:HG23	1:O:392:LEU:HD21	2.01	0.42
1:F:58:GLN:HE22	1:F:80:LYS:NZ	2.17	0.42
1:B:348:ASN:HB3	1:B:357:MET:CE	2.49	0.42
1:F:120:PHE:CG	1:F:194:PRO:HG2	2.55	0.42
1:M:25:ILE:HD12	1:M:25:ILE:C	2.45	0.42
1:D:348:ASN:HB3	1:D:357:MET:CE	2.50	0.41
1:A:296:VAL:HB	1:A:297:PRO:HD3	2.01	0.41
1:B:181:HIS:HB3	2:E:1:GLC:H2	2.01	0.41
1:D:29:ARG:HH21	1:D:68:PRO:HD2	1.85	0.41
1:H:28:LYS:HE3	1:H:38:SER:OG	2.20	0.41
1:H:91:ASP:HB3	1:H:94:LEU:H	1.85	0.41
1:B:18:LEU:HD13	1:B:57:PHE:CG	2.55	0.41
1:D:18:LEU:HD13	1:D:57:PHE:CG	2.55	0.41
1:O:182:THR:HG22	2:P:1:GLC:O2	2.20	0.41
1:B:382:LEU:HD11	1:B:434:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:251:ILE:HG13	1:H:468:TRP:CD2	2.55	0.41
1:K:164:ARG:NH2	1:K:242:ARG:HH12	2.13	0.41
1:D:15:ARG:NH2	1:D:147:ASP:OD2	2.52	0.41
1:K:476:LEU:HD12	1:K:476:LEU:HA	1.51	0.41
1:O:284:ILE:HD11	1:O:317:ILE:HD11	2.03	0.41
1:H:29:ARG:HH22	1:H:71:GLU:HG2	1.85	0.41
1:B:39:MET:HE3	4:B:870:HOH:O	2.21	0.41
1:M:35:TYR:O	1:M:35:TYR:CG	2.74	0.41
1:O:205:HIS:HA	1:O:242:ARG:CZ	2.52	0.41
2:E:1:GLC:O2	2:E:2:G6P:H1	2.20	0.41
1:D:29:ARG:NH2	1:D:68:PRO:HD2	2.36	0.40
1:K:296:VAL:HB	1:K:297:PRO:HD3	2.03	0.40
1:F:86:HIS:CE1	4:F:618:HOH:O	2.74	0.40
1:M:138:THR:OG1	4:M:606:HOH:O	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:766:HOH:O	4:M:754:HOH:O[2_455]	1.86	0.34
4:D:776:HOH:O	4:K:741:HOH:O[2_445]	2.06	0.14
4:B:916:HOH:O	4:O:890:HOH:O[1_455]	2.09	0.11
4:A:874:HOH:O	4:D:607:HOH:O[2_455]	2.11	0.09

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	463/465 (100%)	458 (99%)	5 (1%)	0	100	100
1	B	463/465 (100%)	455 (98%)	6 (1%)	2 (0%)	30	22
1	D	463/465 (100%)	458 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	463/465 (100%)	456 (98%)	7 (2%)	0	100	100
1	H	463/465 (100%)	457 (99%)	5 (1%)	1 (0%)	43	40
1	K	463/465 (100%)	457 (99%)	6 (1%)	0	100	100
1	M	463/465 (100%)	458 (99%)	4 (1%)	1 (0%)	43	40
1	O	463/465 (100%)	458 (99%)	5 (1%)	0	100	100
All	All	3704/3720 (100%)	3657 (99%)	43 (1%)	4 (0%)	48	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	117	GLU
1	H	117	GLU
1	M	66	GLU
1	B	116	GLY

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	400/400 (100%)	398 (100%)	2 (0%)	81	81
1	B	400/400 (100%)	398 (100%)	2 (0%)	81	81
1	D	400/400 (100%)	397 (99%)	3 (1%)	73	75
1	F	400/400 (100%)	395 (99%)	5 (1%)	61	63
1	H	400/400 (100%)	397 (99%)	3 (1%)	73	75
1	K	400/400 (100%)	392 (98%)	8 (2%)	48	48
1	M	400/400 (100%)	395 (99%)	5 (1%)	61	63
1	O	400/400 (100%)	398 (100%)	2 (0%)	81	81
All	All	3200/3200 (100%)	3170 (99%)	30 (1%)	70	73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	GLU
1	A	343	LEU
1	B	27	ILE
1	B	343	LEU
1	D	32	ASP
1	D	34	GLN
1	D	343	LEU
1	F	17	LEU
1	F	29	ARG
1	F	34	GLN
1	F	35	TYR
1	F	67	VAL
1	H	65	LEU
1	H	170	SER
1	H	343	LEU
1	K	28	LYS
1	K	29	ARG
1	K	32	ASP
1	K	34	GLN
1	K	36	SER
1	K	56	SER
1	K	93	GLU
1	K	166	GLU
1	M	15	ARG
1	M	17	LEU
1	M	29	ARG
1	M	31	ASP
1	M	36	SER
1	O	67	VAL
1	O	93	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	114	HIS
1	A	197	GLN
1	A	448	GLN
1	B	34	GLN
1	B	77	GLN
1	B	81	ASN
1	B	197	GLN
1	B	263	GLN

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Mol	Chain	Res	Type
1	B	418	GLN
1	D	34	GLN
1	F	58	GLN
1	F	77	GLN
1	F	197	GLN
1	F	263	GLN
1	F	328	GLN
1	F	418	GLN
1	H	144	GLN
1	H	173	ASN
1	H	197	GLN
1	H	448	GLN
1	K	34	GLN
1	K	335	ASN
1	K	418	GLN
1	K	448	GLN
1	M	418	GLN
1	M	477	ASN
1	O	77	GLN
1	O	197	GLN
1	O	201	GLN
1	O	263	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 ⓘ

16 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	GLC	C	1	2	11,11,12	2.09	3 (27%)	15,15,17	2.19	4 (26%)
2	G6P	C	2	2	16,16,16	2.01	6 (37%)	23,24,24	1.41	3 (13%)
2	GLC	E	1	2	11,11,12	1.92	3 (27%)	15,15,17	1.91	2 (13%)
2	G6P	E	2	2	16,16,16	1.97	6 (37%)	23,24,24	1.25	2 (8%)
2	GLC	G	1	2	11,11,12	1.86	2 (18%)	15,15,17	2.19	3 (20%)
2	G6P	G	2	2	16,16,16	2.00	6 (37%)	23,24,24	1.39	4 (17%)
2	GLC	I	1	2	11,11,12	1.22	1 (9%)	15,15,17	3.16	6 (40%)
2	G6P	I	2	2	16,16,16	1.94	6 (37%)	23,24,24	0.99	1 (4%)
2	GLC	J	1	2	11,11,12	1.62	2 (18%)	15,15,17	1.74	2 (13%)
2	G6P	J	2	2	16,16,16	2.04	6 (37%)	23,24,24	1.55	3 (13%)
2	GLC	L	1	2	11,11,12	2.33	3 (27%)	15,15,17	2.35	5 (33%)
2	G6P	L	2	2	16,16,16	2.01	6 (37%)	23,24,24	1.20	3 (13%)
2	GLC	N	1	2	11,11,12	1.80	1 (9%)	15,15,17	1.83	3 (20%)
2	G6P	N	2	2	16,16,16	1.99	6 (37%)	23,24,24	1.29	3 (13%)
2	GLC	P	1	2	11,11,12	2.14	3 (27%)	15,15,17	2.09	6 (40%)
2	G6P	P	2	2	16,16,16	2.02	6 (37%)	23,24,24	1.36	3 (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	GLC	C	1	2	-	1/2/19/22	0/1/1/1
2	G6P	C	2	2	-	0/6/26/26	0/1/1/1
2	GLC	E	1	2	-	2/2/19/22	0/1/1/1
2	G6P	E	2	2	-	1/6/26/26	0/1/1/1
2	GLC	G	1	2	-	0/2/19/22	0/1/1/1
2	G6P	G	2	2	-	0/6/26/26	0/1/1/1
2	GLC	I	1	2	-	2/2/19/22	0/1/1/1
2	G6P	I	2	2	-	1/6/26/26	0/1/1/1
2	GLC	J	1	2	-	2/2/19/22	0/1/1/1
2	G6P	J	2	2	-	2/6/26/26	0/1/1/1
2	GLC	L	1	2	-	1/2/19/22	0/1/1/1
2	G6P	L	2	2	-	0/6/26/26	0/1/1/1
2	GLC	N	1	2	-	1/2/19/22	0/1/1/1
2	G6P	N	2	2	-	0/6/26/26	0/1/1/1
2	GLC	P	1	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G6P	P	2	2	-	0/6/26/26	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1	GLC	O5-C1	5.72	1.53	1.43
2	P	1	GLC	O5-C1	5.20	1.52	1.43
2	C	1	GLC	O5-C1	5.20	1.52	1.43
2	G	1	GLC	O5-C1	4.94	1.52	1.43
2	N	1	GLC	O5-C1	4.82	1.51	1.43
2	E	1	GLC	O5-C1	4.81	1.51	1.43
2	J	2	G6P	O5-C5	4.60	1.55	1.44
2	C	2	G6P	O5-C5	4.51	1.55	1.44
2	G	2	G6P	O5-C5	4.48	1.55	1.44
2	L	2	G6P	O5-C5	4.42	1.55	1.44
2	N	2	G6P	O5-C5	4.41	1.55	1.44
2	E	2	G6P	O5-C5	4.41	1.55	1.44
2	P	2	G6P	O5-C5	4.40	1.55	1.44
2	J	1	GLC	O5-C1	4.29	1.50	1.43
2	I	2	G6P	O5-C5	4.28	1.54	1.44
2	L	1	GLC	O5-C5	3.46	1.50	1.43
2	L	1	GLC	C2-C3	-3.29	1.47	1.52
2	P	2	G6P	C6-C5	-3.13	1.42	1.51
2	C	1	GLC	O5-C5	3.12	1.49	1.43
2	P	1	GLC	C2-C3	-3.11	1.47	1.52
2	I	2	G6P	C6-C5	-3.10	1.42	1.51
2	I	1	GLC	O5-C1	3.10	1.48	1.43
2	N	2	G6P	C6-C5	-3.09	1.42	1.51
2	L	2	G6P	C6-C5	-3.08	1.42	1.51
2	P	1	GLC	O5-C5	3.01	1.49	1.43
2	E	2	G6P	C6-C5	-2.97	1.42	1.51
2	G	2	G6P	C6-C5	-2.97	1.42	1.51
2	C	2	G6P	C6-C5	-2.97	1.42	1.51
2	J	2	G6P	C6-C5	-2.94	1.42	1.51
2	E	1	GLC	O5-C5	2.84	1.49	1.43
2	L	2	G6P	C3-C2	-2.72	1.45	1.52
2	P	2	G6P	C3-C2	-2.71	1.45	1.52
2	J	2	G6P	O5-C1	2.67	1.49	1.42
2	G	2	G6P	O5-C1	2.64	1.49	1.42
2	C	2	G6P	O5-C1	2.64	1.49	1.42
2	J	2	G6P	C3-C2	-2.63	1.45	1.52
2	E	2	G6P	O5-C1	2.54	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	2	G6P	C3-C2	-2.52	1.45	1.52
2	P	2	G6P	O5-C1	2.49	1.49	1.42
2	N	2	G6P	O5-C1	2.48	1.48	1.42
2	I	2	G6P	C3-C2	-2.44	1.46	1.52
2	G	2	G6P	C3-C2	-2.42	1.46	1.52
2	C	2	G6P	C3-C2	-2.42	1.46	1.52
2	E	2	G6P	C3-C2	-2.41	1.46	1.52
2	N	2	G6P	O2-C2	2.41	1.48	1.43
2	L	2	G6P	O5-C1	2.39	1.48	1.42
2	C	1	GLC	C2-C3	-2.38	1.48	1.52
2	C	2	G6P	O2-C2	2.36	1.48	1.43
2	G	1	GLC	O5-C5	2.35	1.48	1.43
2	L	2	G6P	O2-C2	2.33	1.48	1.43
2	P	2	G6P	O2-C2	2.33	1.48	1.43
2	G	2	G6P	O2-C2	2.33	1.48	1.43
2	I	2	G6P	O5-C1	2.27	1.48	1.42
2	E	2	G6P	O2-C2	2.26	1.48	1.43
2	I	2	G6P	O2-C2	2.24	1.48	1.43
2	I	2	G6P	O3-C3	2.23	1.48	1.43
2	C	2	G6P	O3-C3	2.22	1.48	1.43
2	J	2	G6P	O3-C3	2.21	1.48	1.43
2	J	1	GLC	O5-C5	2.20	1.47	1.43
2	G	2	G6P	O3-C3	2.20	1.48	1.43
2	E	1	GLC	C2-C3	-2.17	1.49	1.52
2	E	2	G6P	O3-C3	2.17	1.48	1.43
2	P	2	G6P	O3-C3	2.17	1.48	1.43
2	J	2	G6P	O2-C2	2.16	1.48	1.43
2	L	2	G6P	O3-C3	2.13	1.48	1.43
2	N	2	G6P	O3-C3	2.13	1.48	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	GLC	C1-C2-C3	7.86	121.08	109.64
2	I	1	GLC	C1-O5-C5	-6.86	102.99	112.19
2	C	1	GLC	C1-O5-C5	6.44	120.82	112.19
2	E	1	GLC	C1-O5-C5	6.05	120.30	112.19
2	G	1	GLC	C1-C2-C3	5.88	118.20	109.64
2	J	1	GLC	C1-C2-C3	5.55	117.72	109.64
2	P	1	GLC	C1-O5-C5	5.36	119.37	112.19
2	L	1	GLC	C1-O5-C5	5.24	119.21	112.19
2	N	1	GLC	C1-C2-C3	5.23	117.26	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	GLC	C2-C3-C4	-4.68	102.64	110.86
2	G	1	GLC	C1-O5-C5	4.13	117.72	112.19
2	J	2	G6P	O5-C1-C2	3.94	117.23	110.30
2	L	1	GLC	O2-C2-C1	3.78	117.87	109.22
2	C	2	G6P	O1-C1-C2	3.75	119.85	108.98
2	J	2	G6P	C1-O5-C5	3.57	120.56	113.65
2	I	1	GLC	C3-C4-C5	-3.53	103.83	110.23
2	P	2	G6P	O1-C1-C2	3.43	118.93	108.98
2	G	2	G6P	O1-C1-C2	3.14	118.10	108.98
2	P	1	GLC	C1-C2-C3	3.04	114.07	109.64
2	C	2	G6P	O5-C5-C6	2.99	112.63	106.69
2	E	2	G6P	O1-C1-C2	2.97	117.60	108.98
2	G	2	G6P	O5-C5-C6	2.97	112.58	106.69
2	C	1	GLC	C1-C2-C3	2.93	113.91	109.64
2	I	1	GLC	O5-C5-C4	-2.92	103.73	110.83
2	N	2	G6P	O2-C2-C1	2.92	115.97	109.25
2	C	1	GLC	O5-C5-C4	2.91	117.92	110.83
2	N	2	G6P	O1-C1-C2	2.89	117.36	108.98
2	E	2	G6P	O5-C5-C6	2.87	112.39	106.69
2	I	1	GLC	O2-C2-C1	-2.86	102.67	109.22
2	P	1	GLC	O2-C2-C1	2.81	115.67	109.22
2	E	1	GLC	O2-C2-C1	2.80	115.63	109.22
2	P	2	G6P	O2-C2-C1	2.75	115.60	109.25
2	J	2	G6P	O5-C5-C6	2.75	112.15	106.69
2	J	1	GLC	C2-C3-C4	2.75	115.69	110.86
2	L	2	G6P	O1-C1-C2	2.65	116.67	108.98
2	G	2	G6P	O2-C2-C1	2.58	115.20	109.25
2	N	2	G6P	O5-C5-C6	2.53	111.72	106.69
2	C	2	G6P	O2-C2-C1	2.52	115.06	109.25
2	L	2	G6P	O2-C2-C1	2.48	114.96	109.25
2	N	1	GLC	O5-C1-C2	2.41	116.53	110.79
2	P	1	GLC	C6-C5-C4	-2.41	107.11	113.02
2	N	1	GLC	C6-C5-C4	-2.39	107.16	113.02
2	P	1	GLC	O5-C5-C4	2.37	116.59	110.83
2	L	1	GLC	O5-C5-C6	2.32	112.17	107.66
2	G	1	GLC	C2-C3-C4	2.31	114.93	110.86
2	I	2	G6P	O5-C5-C6	2.27	111.19	106.69
2	C	1	GLC	C6-C5-C4	-2.27	107.45	113.02
2	L	2	G6P	O5-C5-C6	2.25	111.16	106.69
2	L	1	GLC	C6-C5-C4	-2.21	107.59	113.02
2	P	1	GLC	C2-C3-C4	-2.21	106.98	110.86
2	P	2	G6P	O5-C5-C6	2.21	111.07	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	G6P	C1-C2-C3	2.14	114.72	110.36
2	I	1	GLC	O2-C2-C3	-2.11	105.79	110.15

There are no chirality outliers.

All (15) torsion outliers are listed below:

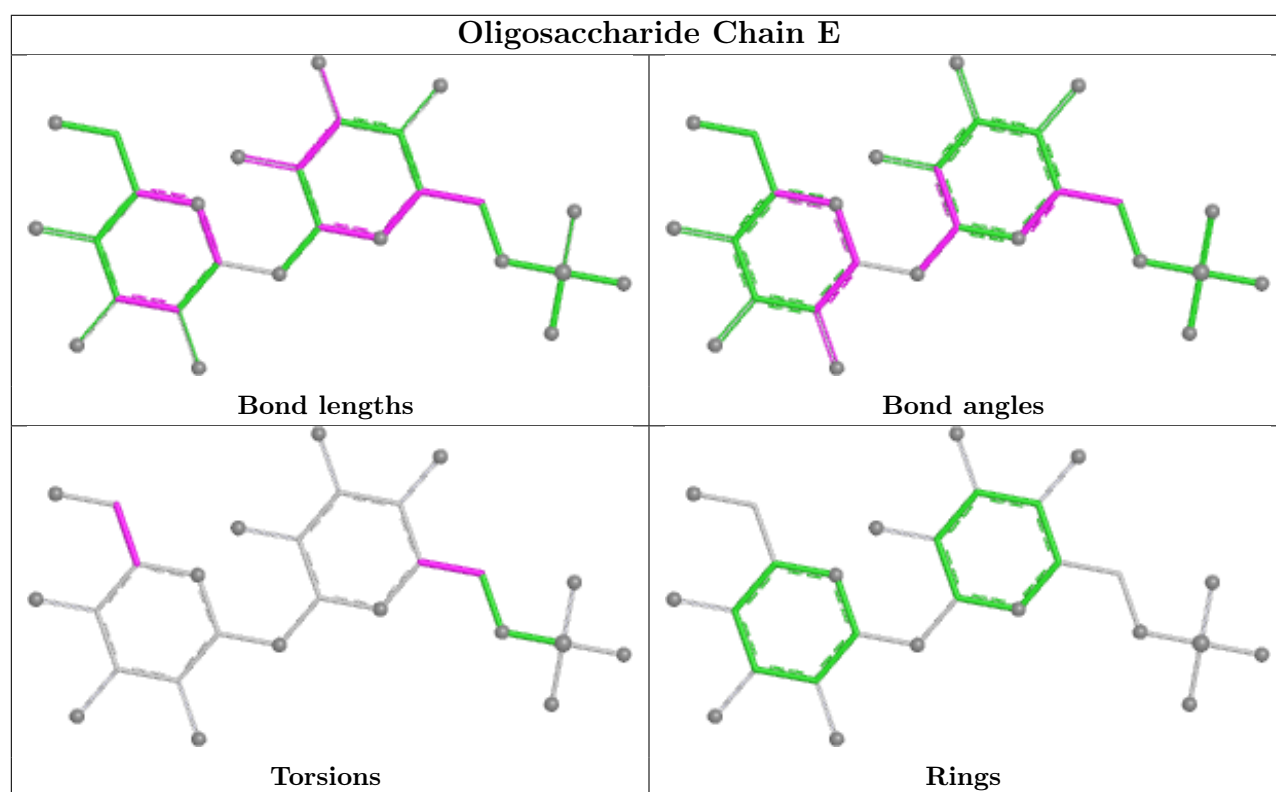
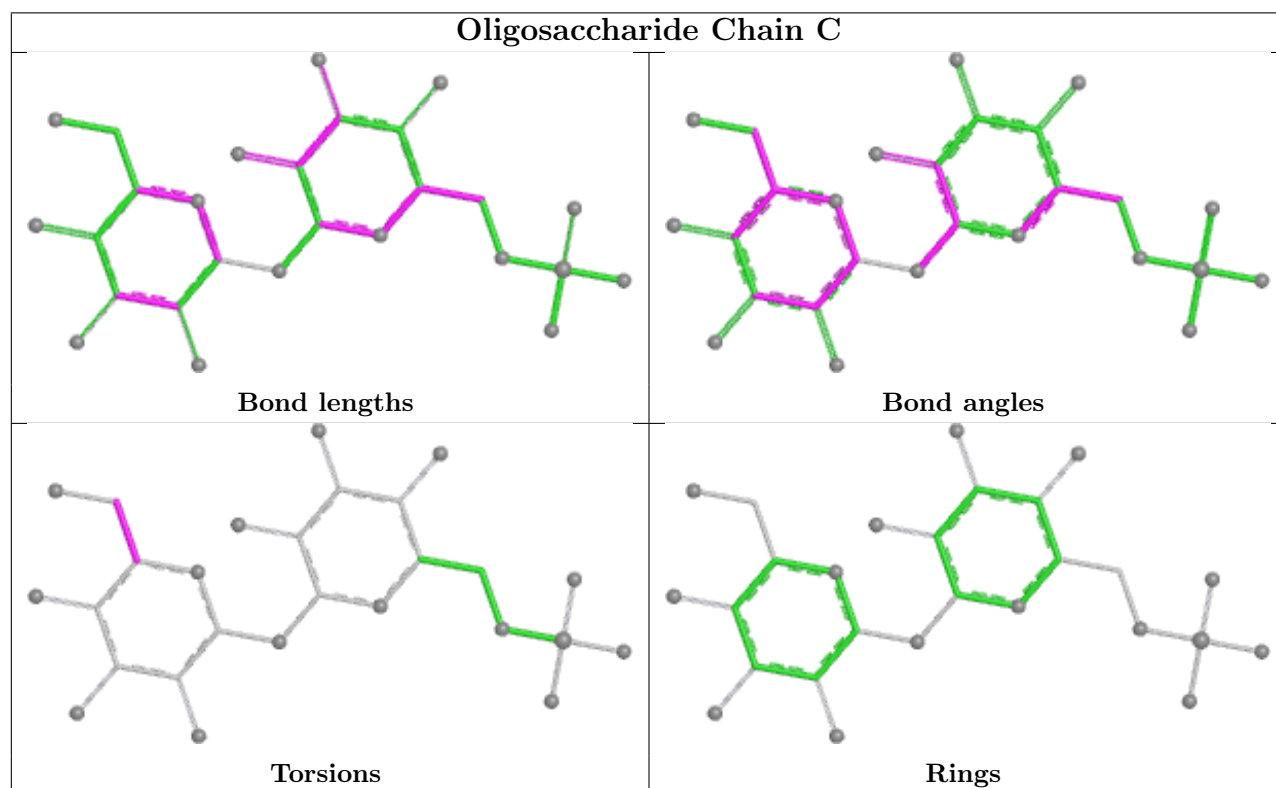
Mol	Chain	Res	Type	Atoms
2	J	2	G6P	O5-C5-C6-O6
2	J	1	GLC	C4-C5-C6-O6
2	J	1	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	P	1	GLC	O5-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	L	1	GLC	O5-C5-C6-O6
2	N	1	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	P	1	GLC	C4-C5-C6-O6
2	I	2	G6P	C4-C5-C6-O6
2	J	2	G6P	C4-C5-C6-O6
2	E	2	G6P	C4-C5-C6-O6

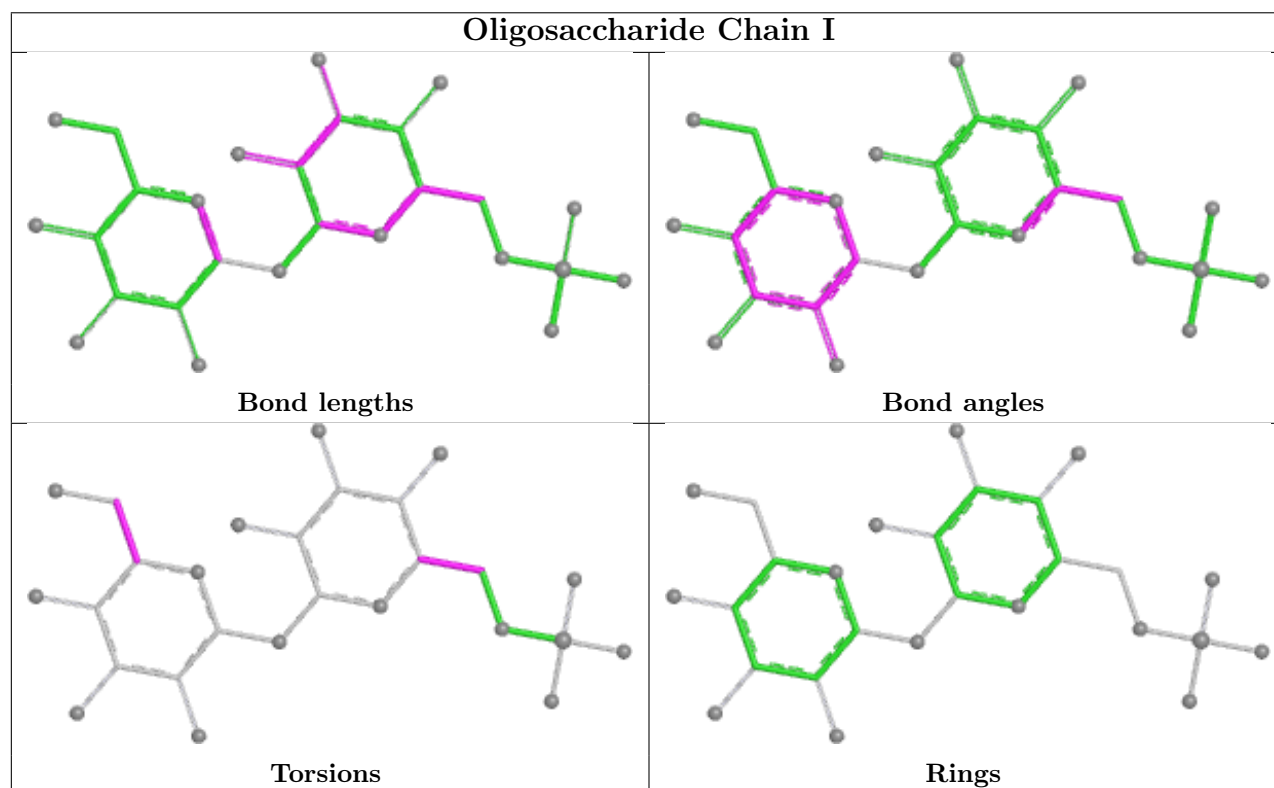
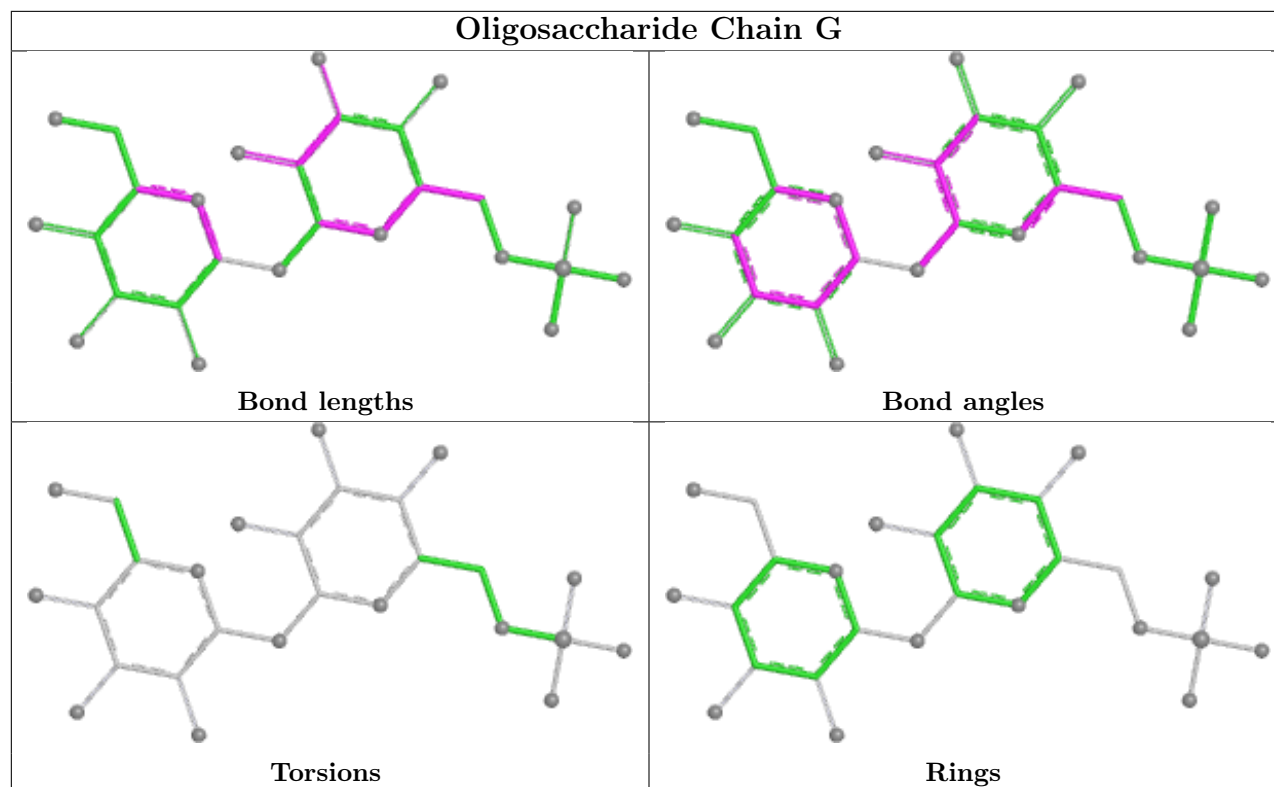
There are no ring outliers.

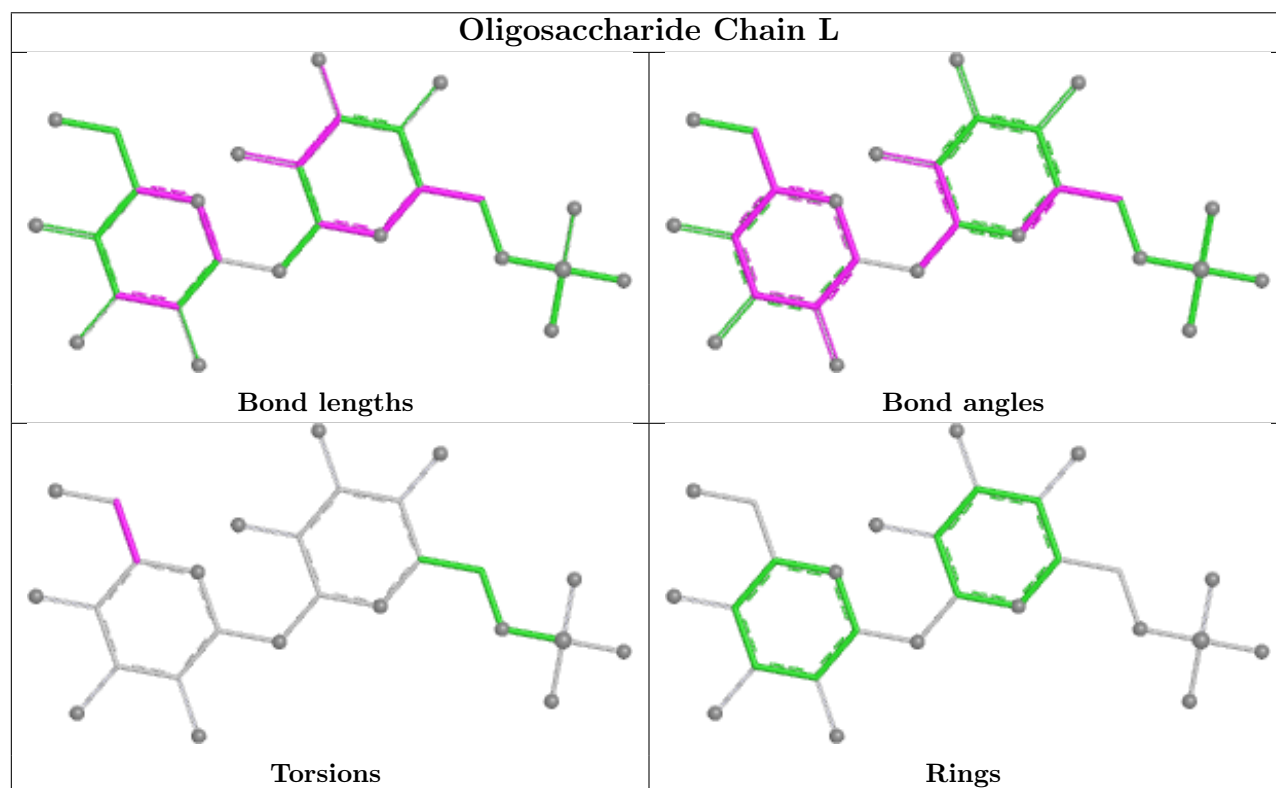
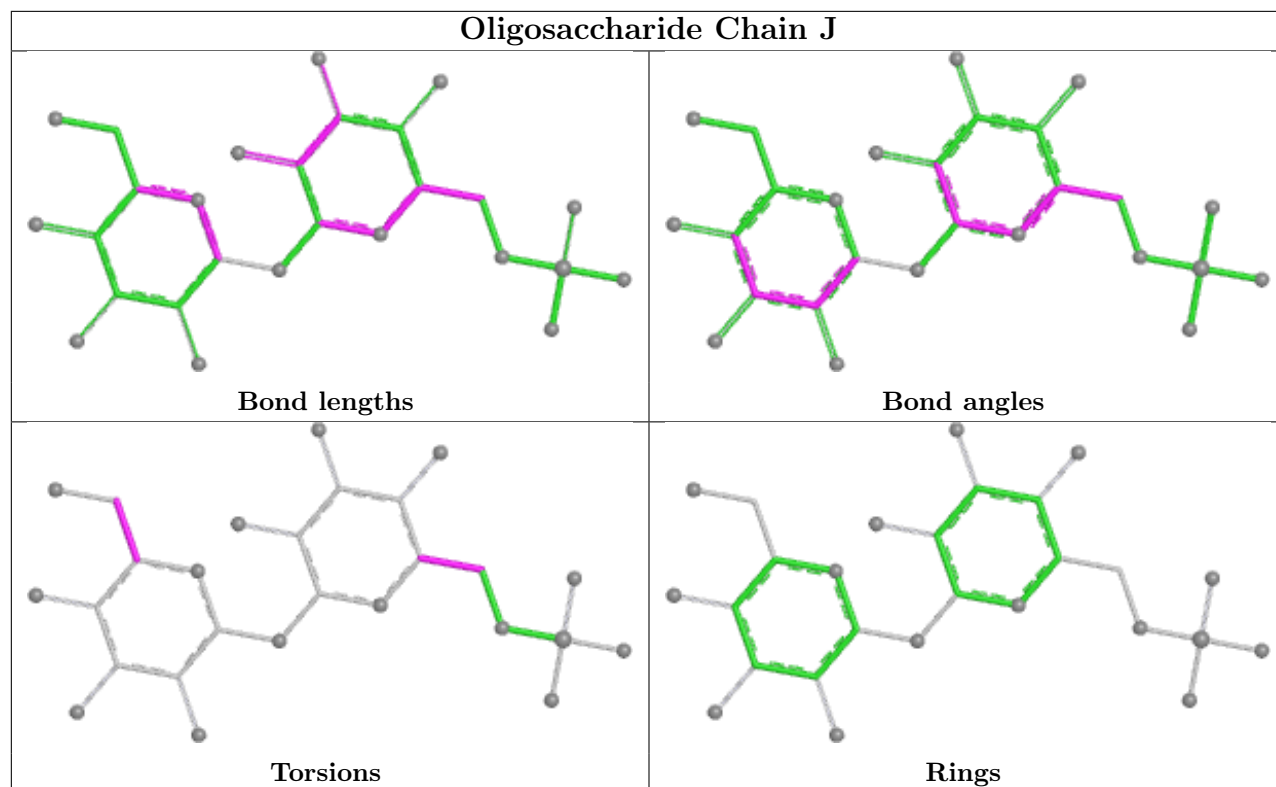
13 monomers are involved in 19 short contacts:

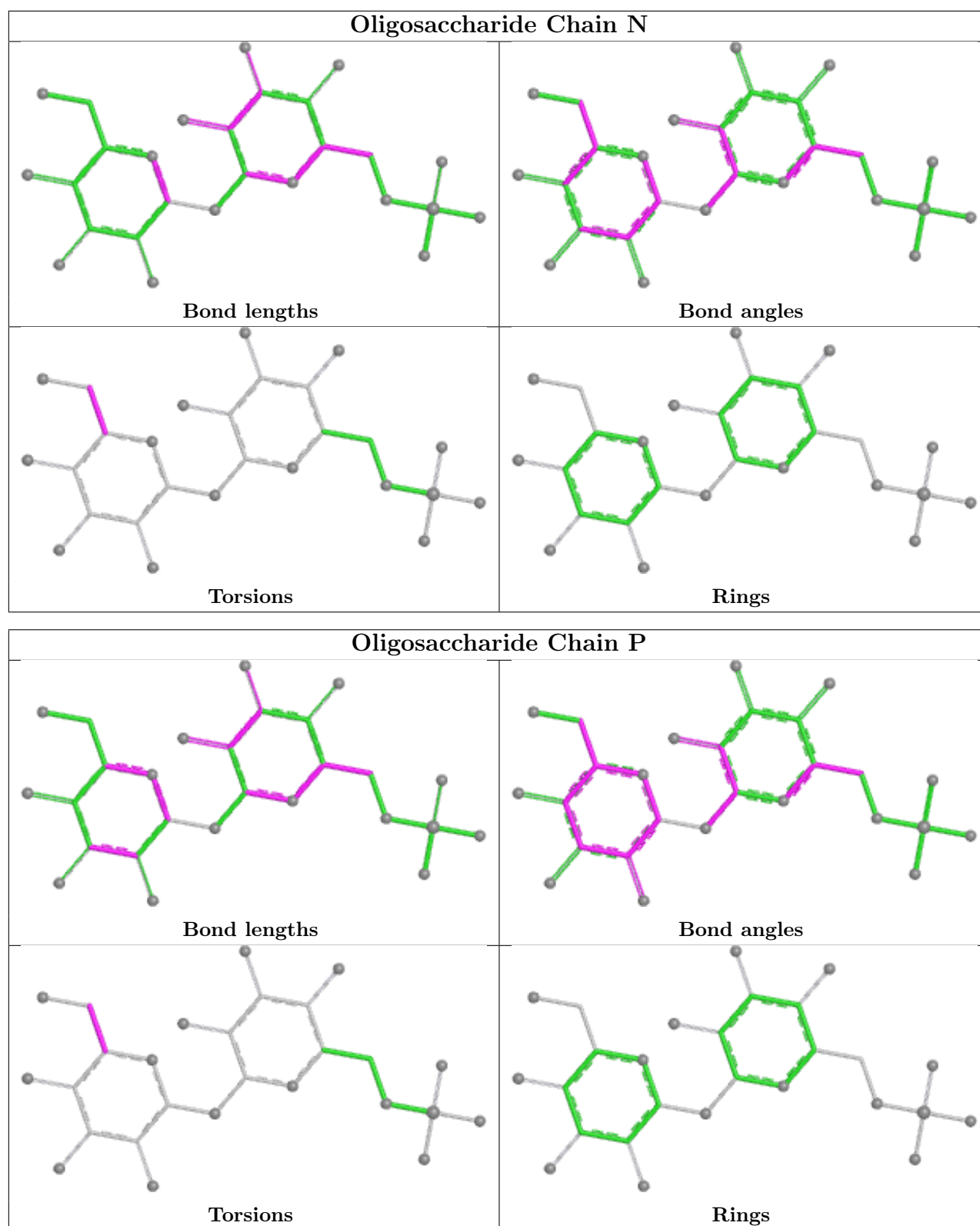
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	G6P	1	0
2	N	1	GLC	2	0
2	E	2	G6P	1	0
2	I	1	GLC	4	0
2	P	1	GLC	1	0
2	G	1	GLC	1	0
2	L	1	GLC	2	0
2	P	2	G6P	1	0
2	L	2	G6P	1	0
2	J	2	G6P	1	0
2	E	1	GLC	2	0
2	G	2	G6P	2	0
2	J	1	GLC	3	0

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](#)

8 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	UDP	H	501	-	25,26,26	1.06	1 (4%)	38,40,40	1.61	5 (13%)
3	UDP	D	501	-	25,26,26	1.03	1 (4%)	38,40,40	1.65	6 (15%)
3	UDP	M	501	-	25,26,26	1.01	1 (4%)	38,40,40	1.61	6 (15%)
3	UDP	A	501	-	25,26,26	1.00	0	38,40,40	1.61	6 (15%)
3	UDP	B	501	-	25,26,26	1.03	1 (4%)	38,40,40	1.60	5 (13%)
3	UDP	K	501	-	25,26,26	1.04	1 (4%)	38,40,40	1.61	6 (15%)
3	UDP	O	501	-	25,26,26	1.03	1 (4%)	38,40,40	1.62	5 (13%)
3	UDP	F	501	-	25,26,26	1.07	2 (8%)	38,40,40	1.68	7 (18%)

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	UDP	H	501	-	-	9/16/32/32	0/2/2/2
3	UDP	D	501	-	-	8/16/32/32	0/2/2/2
3	UDP	M	501	-	-	9/16/32/32	0/2/2/2
3	UDP	A	501	-	-	8/16/32/32	0/2/2/2
3	UDP	B	501	-	-	10/16/32/32	0/2/2/2
3	UDP	K	501	-	-	9/16/32/32	0/2/2/2
3	UDP	O	501	-	-	10/16/32/32	0/2/2/2
3	UDP	F	501	-	-	10/16/32/32	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	UDP	PA-O3A	2.40	1.62	1.59
3	H	501	UDP	PA-O3A	2.34	1.62	1.59
3	D	501	UDP	PA-O3A	2.24	1.61	1.59
3	K	501	UDP	PA-O3A	2.21	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	UDP	PA-O3A	2.15	1.61	1.59
3	O	501	UDP	PA-O3A	2.14	1.61	1.59
3	M	501	UDP	C5-C4	-2.02	1.39	1.43
3	F	501	UDP	C5-C4	-2.00	1.39	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	UDP	C4-N3-C2	-5.76	119.46	126.61
3	H	501	UDP	C4-N3-C2	-5.73	119.50	126.61
3	B	501	UDP	C4-N3-C2	-5.69	119.55	126.61
3	O	501	UDP	C4-N3-C2	-5.67	119.57	126.61
3	K	501	UDP	C4-N3-C2	-5.65	119.59	126.61
3	F	501	UDP	C4-N3-C2	-5.65	119.60	126.61
3	M	501	UDP	C4-N3-C2	-5.64	119.61	126.61
3	A	501	UDP	C4-N3-C2	-5.59	119.67	126.61
3	D	501	UDP	N3-C2-N1	4.43	120.66	114.89
3	B	501	UDP	N3-C2-N1	4.33	120.53	114.89
3	M	501	UDP	N3-C2-N1	4.26	120.44	114.89
3	O	501	UDP	N3-C2-N1	4.23	120.40	114.89
3	A	501	UDP	N3-C2-N1	4.22	120.38	114.89
3	K	501	UDP	N3-C2-N1	4.17	120.32	114.89
3	H	501	UDP	N3-C2-N1	4.12	120.25	114.89
3	F	501	UDP	N3-C2-N1	4.08	120.20	114.89
3	H	501	UDP	C5-C4-N3	3.79	120.10	114.80
3	F	501	UDP	C5-C4-N3	3.71	119.99	114.80
3	O	501	UDP	C5-C4-N3	3.70	119.98	114.80
3	K	501	UDP	C5-C4-N3	3.69	119.97	114.80
3	A	501	UDP	C5-C4-N3	3.62	119.88	114.80
3	D	501	UDP	C5-C4-N3	3.62	119.86	114.80
3	B	501	UDP	C5-C4-N3	3.60	119.84	114.80
3	M	501	UDP	C5-C4-N3	3.60	119.84	114.80
3	D	501	UDP	O2-C2-N1	-3.14	118.71	122.80
3	H	501	UDP	O4-C4-C5	-3.05	119.91	125.16
3	K	501	UDP	O4-C4-C5	-3.00	119.98	125.16
3	O	501	UDP	O4-C4-C5	-3.00	119.99	125.16
3	F	501	UDP	O4-C4-C5	-2.97	120.04	125.16
3	B	501	UDP	O4-C4-C5	-2.96	120.05	125.16
3	A	501	UDP	O4-C4-C5	-2.96	120.06	125.16
3	D	501	UDP	O4-C4-C5	-2.95	120.07	125.16
3	M	501	UDP	O4-C4-C5	-2.93	120.10	125.16
3	B	501	UDP	O2-C2-N1	-2.78	119.18	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	501	UDP	O2-C2-N1	-2.63	119.38	122.80
3	M	501	UDP	O2-C2-N1	-2.59	119.43	122.80
3	A	501	UDP	O2-C2-N1	-2.58	119.44	122.80
3	H	501	UDP	O2-C2-N1	-2.53	119.50	122.80
3	K	501	UDP	O2-C2-N1	-2.53	119.51	122.80
3	F	501	UDP	O2-C2-N1	-2.38	119.69	122.80
3	M	501	UDP	O4'-C1'-N1	2.19	113.32	108.36
3	F	501	UDP	O2B-PB-O3A	2.18	111.95	104.64
3	A	501	UDP	O4'-C1'-N1	2.13	113.20	108.36
3	F	501	UDP	O2A-PA-O3A	2.11	112.98	107.27
3	K	501	UDP	O4'-C1'-N1	2.07	113.04	108.36
3	D	501	UDP	O4'-C1'-N1	2.03	112.97	108.36

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	UDP	C2'-C1'-N1-C2
3	A	501	UDP	C2'-C1'-N1-C6
3	A	501	UDP	PB-O3A-PA-O5'
3	B	501	UDP	C2'-C1'-N1-C2
3	B	501	UDP	C2'-C1'-N1-C6
3	B	501	UDP	PB-O3A-PA-O5'
3	D	501	UDP	C2'-C1'-N1-C2
3	D	501	UDP	C2'-C1'-N1-C6
3	D	501	UDP	PB-O3A-PA-O5'
3	F	501	UDP	C2'-C1'-N1-C2
3	F	501	UDP	C2'-C1'-N1-C6
3	F	501	UDP	PB-O3A-PA-O5'
3	F	501	UDP	PA-O3A-PB-O2B
3	F	501	UDP	PA-O3A-PB-O3B
3	H	501	UDP	C2'-C1'-N1-C2
3	H	501	UDP	C2'-C1'-N1-C6
3	H	501	UDP	PB-O3A-PA-O5'
3	H	501	UDP	PA-O3A-PB-O2B
3	K	501	UDP	C2'-C1'-N1-C2
3	K	501	UDP	C2'-C1'-N1-C6
3	K	501	UDP	PB-O3A-PA-O5'
3	K	501	UDP	PA-O3A-PB-O2B
3	M	501	UDP	C2'-C1'-N1-C2
3	M	501	UDP	C2'-C1'-N1-C6
3	M	501	UDP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
3	M	501	UDP	PA-O3A-PB-O2B
3	O	501	UDP	C2'-C1'-N1-C2
3	O	501	UDP	C2'-C1'-N1-C6
3	O	501	UDP	PB-O3A-PA-O5'
3	B	501	UDP	O4'-C4'-C5'-O5'
3	F	501	UDP	O4'-C4'-C5'-O5'
3	H	501	UDP	O4'-C4'-C5'-O5'
3	B	501	UDP	PA-O3A-PB-O1B
3	K	501	UDP	PA-O3A-PB-O1B
3	M	501	UDP	PA-O3A-PB-O1B
3	O	501	UDP	PA-O3A-PB-O1B
3	M	501	UDP	O4'-C4'-C5'-O5'
3	A	501	UDP	O4'-C4'-C5'-O5'
3	K	501	UDP	O4'-C4'-C5'-O5'
3	O	501	UDP	O4'-C4'-C5'-O5'
3	B	501	UDP	C3'-C4'-C5'-O5'
3	F	501	UDP	C3'-C4'-C5'-O5'
3	H	501	UDP	C3'-C4'-C5'-O5'
3	M	501	UDP	C3'-C4'-C5'-O5'
3	A	501	UDP	PA-O3A-PB-O2B
3	B	501	UDP	PA-O3A-PB-O2B
3	D	501	UDP	PA-O3A-PB-O3B
3	O	501	UDP	PA-O3A-PB-O3B
3	A	501	UDP	C3'-C4'-C5'-O5'
3	B	501	UDP	C5'-O5'-PA-O1A
3	O	501	UDP	C5'-O5'-PA-O1A
3	K	501	UDP	C3'-C4'-C5'-O5'
3	O	501	UDP	C3'-C4'-C5'-O5'
3	D	501	UDP	O4'-C4'-C5'-O5'
3	B	501	UDP	O4'-C1'-N1-C6
3	D	501	UDP	O4'-C1'-N1-C6
3	F	501	UDP	O4'-C1'-N1-C6
3	H	501	UDP	O4'-C1'-N1-C6
3	K	501	UDP	O4'-C1'-N1-C6
3	A	501	UDP	O4'-C1'-N1-C6
3	M	501	UDP	O4'-C1'-N1-C6
3	O	501	UDP	O4'-C1'-N1-C6
3	H	501	UDP	PA-O3A-PB-O3B
3	D	501	UDP	C3'-C4'-C5'-O5'
3	F	501	UDP	PA-O3A-PB-O1B
3	A	501	UDP	O4'-C1'-N1-C2
3	B	501	UDP	O4'-C1'-N1-C2

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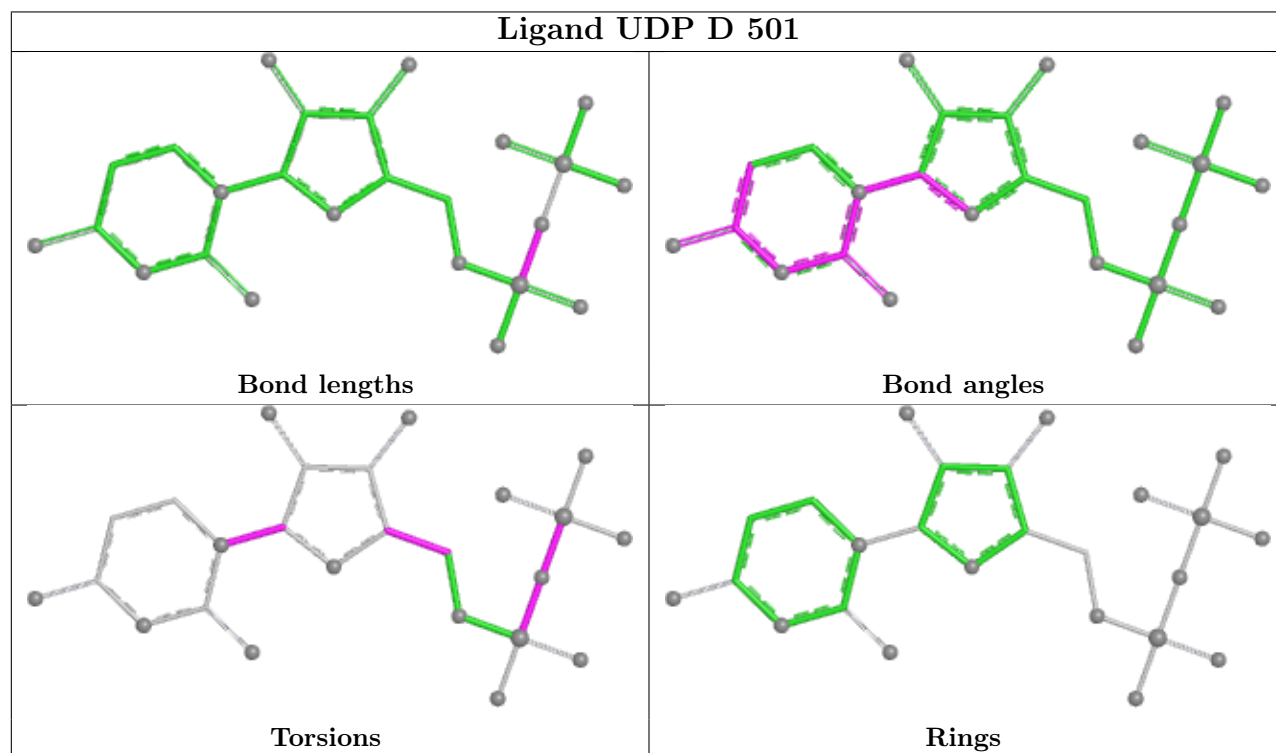
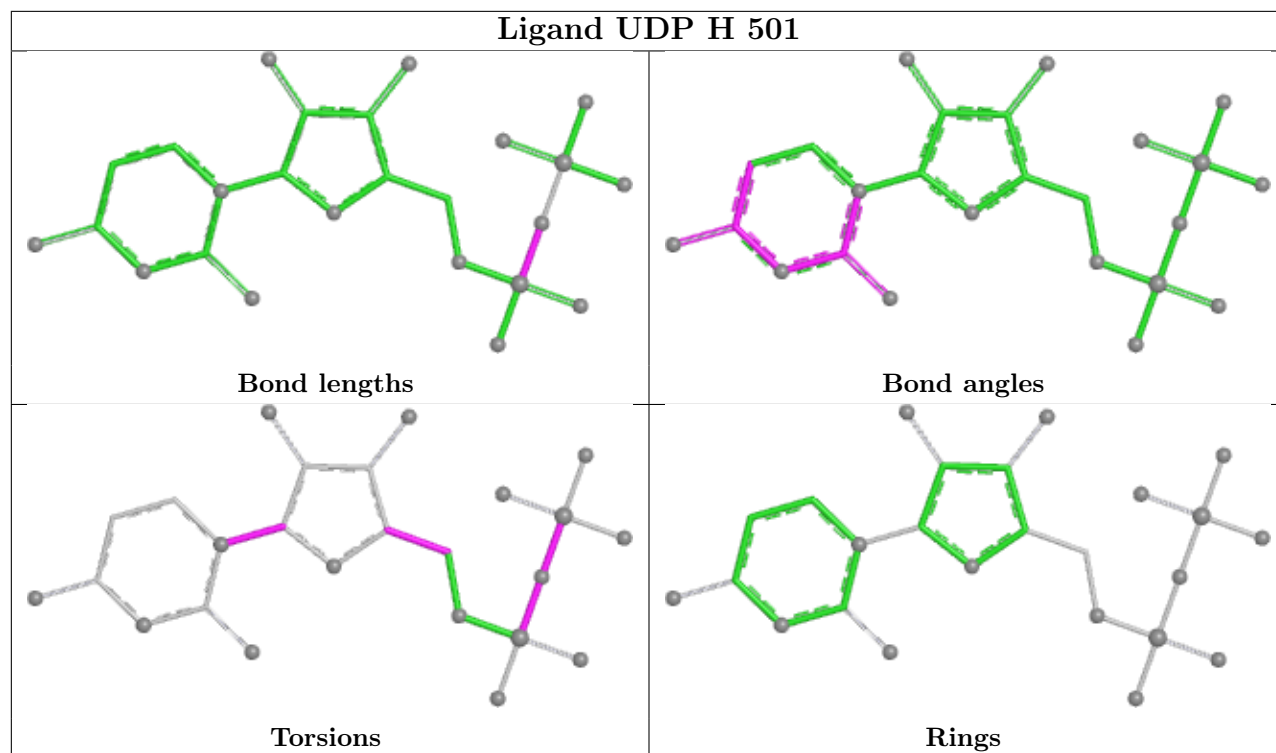
Mol	Chain	Res	Type	Atoms
3	D	501	UDP	O4'-C1'-N1-C2
3	F	501	UDP	O4'-C1'-N1-C2
3	K	501	UDP	O4'-C1'-N1-C2
3	M	501	UDP	O4'-C1'-N1-C2
3	O	501	UDP	O4'-C1'-N1-C2
3	H	501	UDP	O4'-C1'-N1-C2

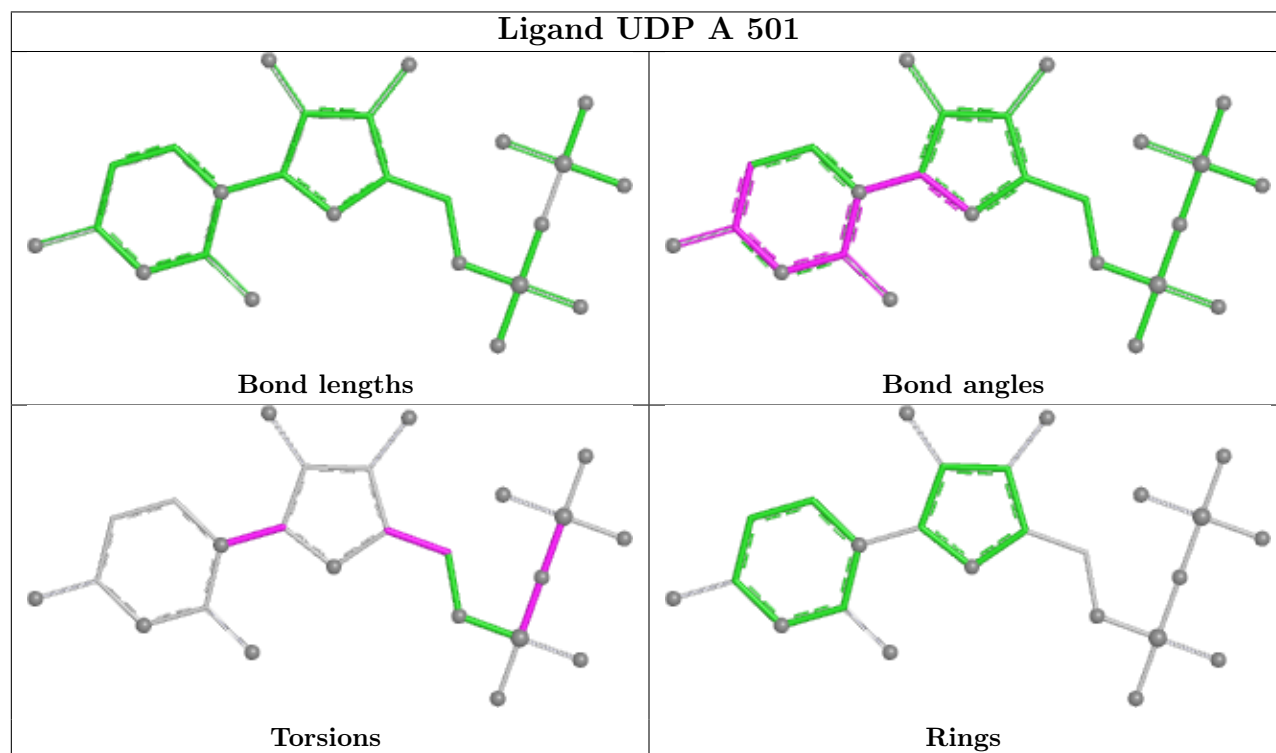
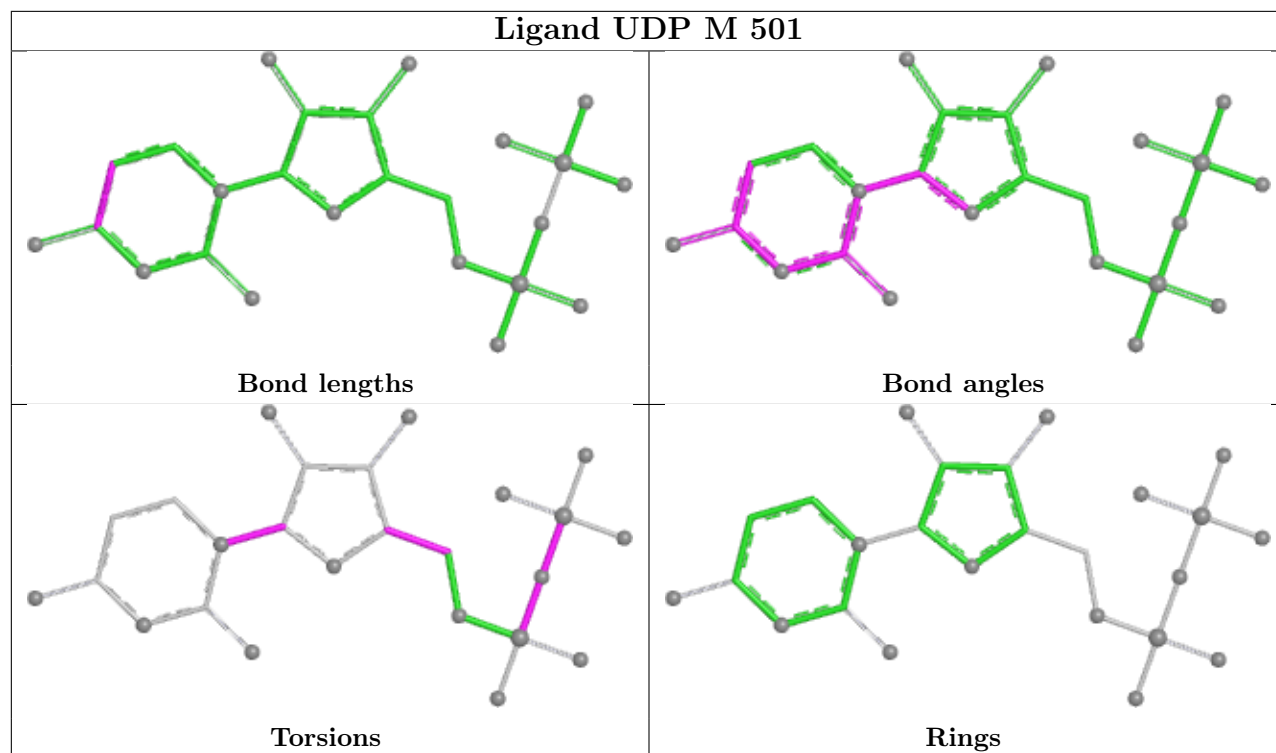
There are no ring outliers.

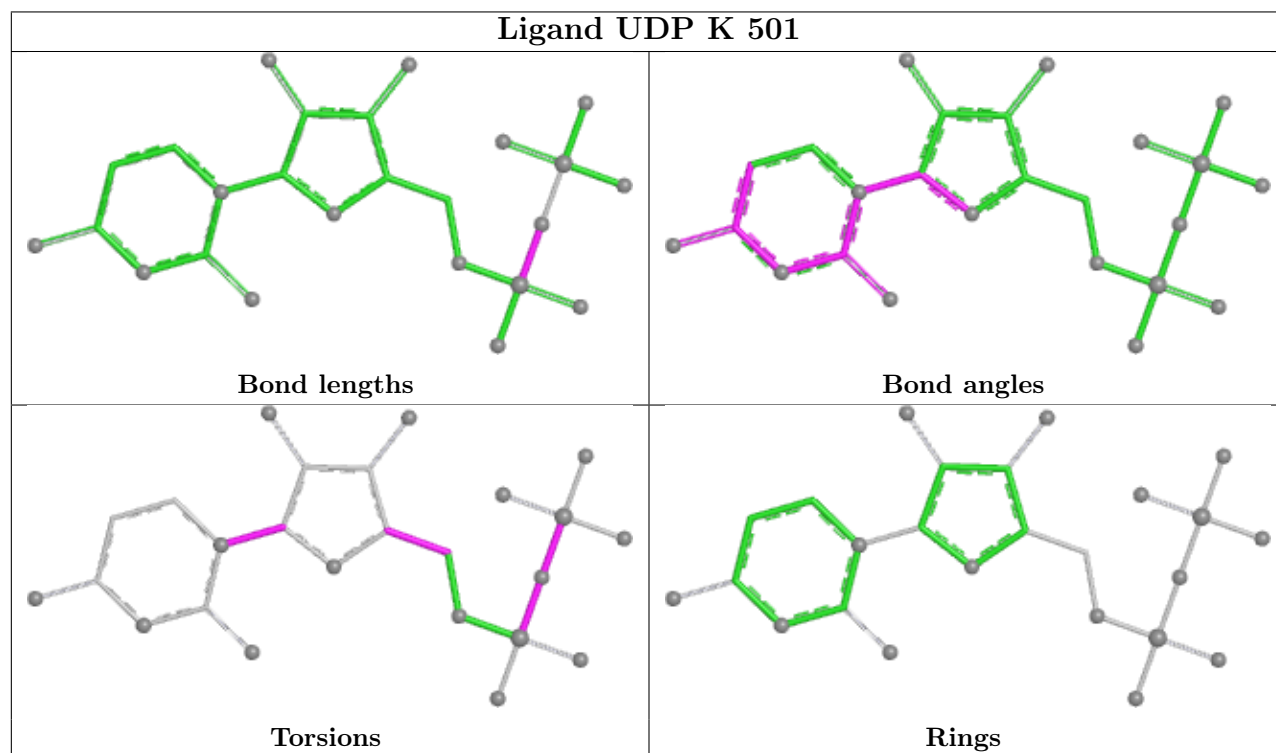
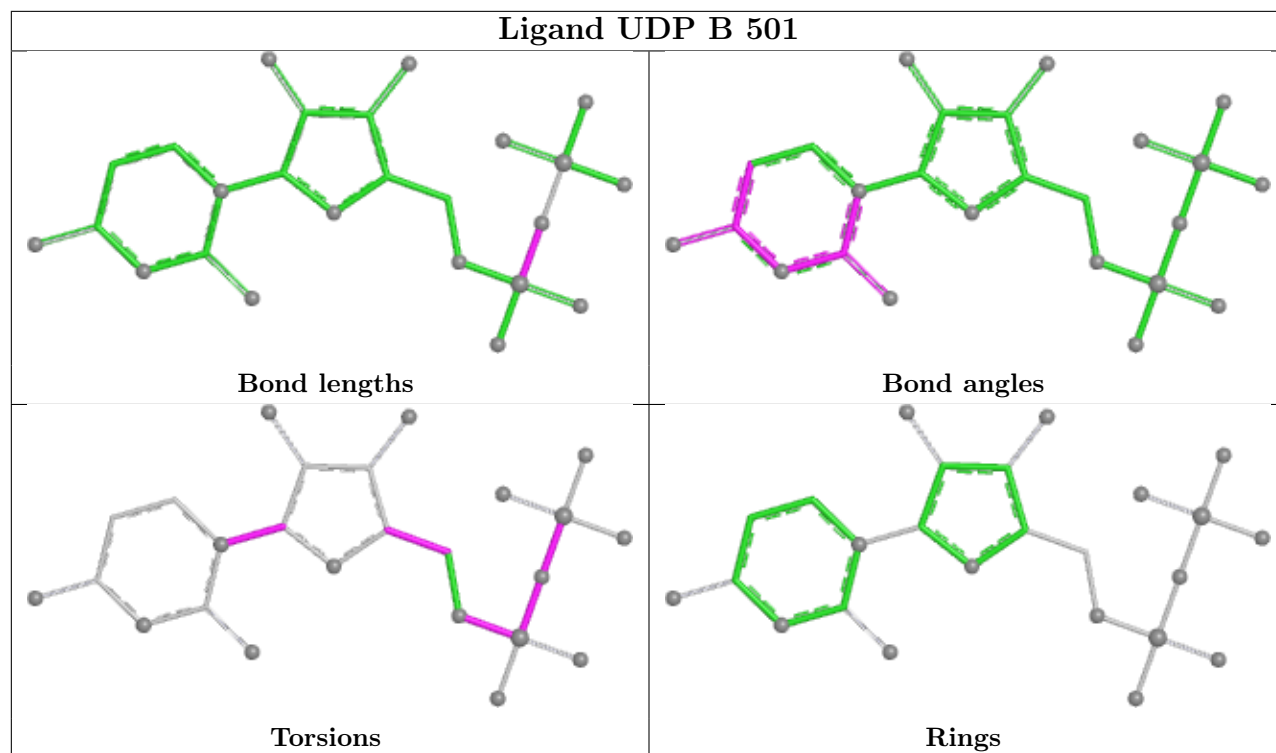
3 monomers are involved in 4 short contacts:

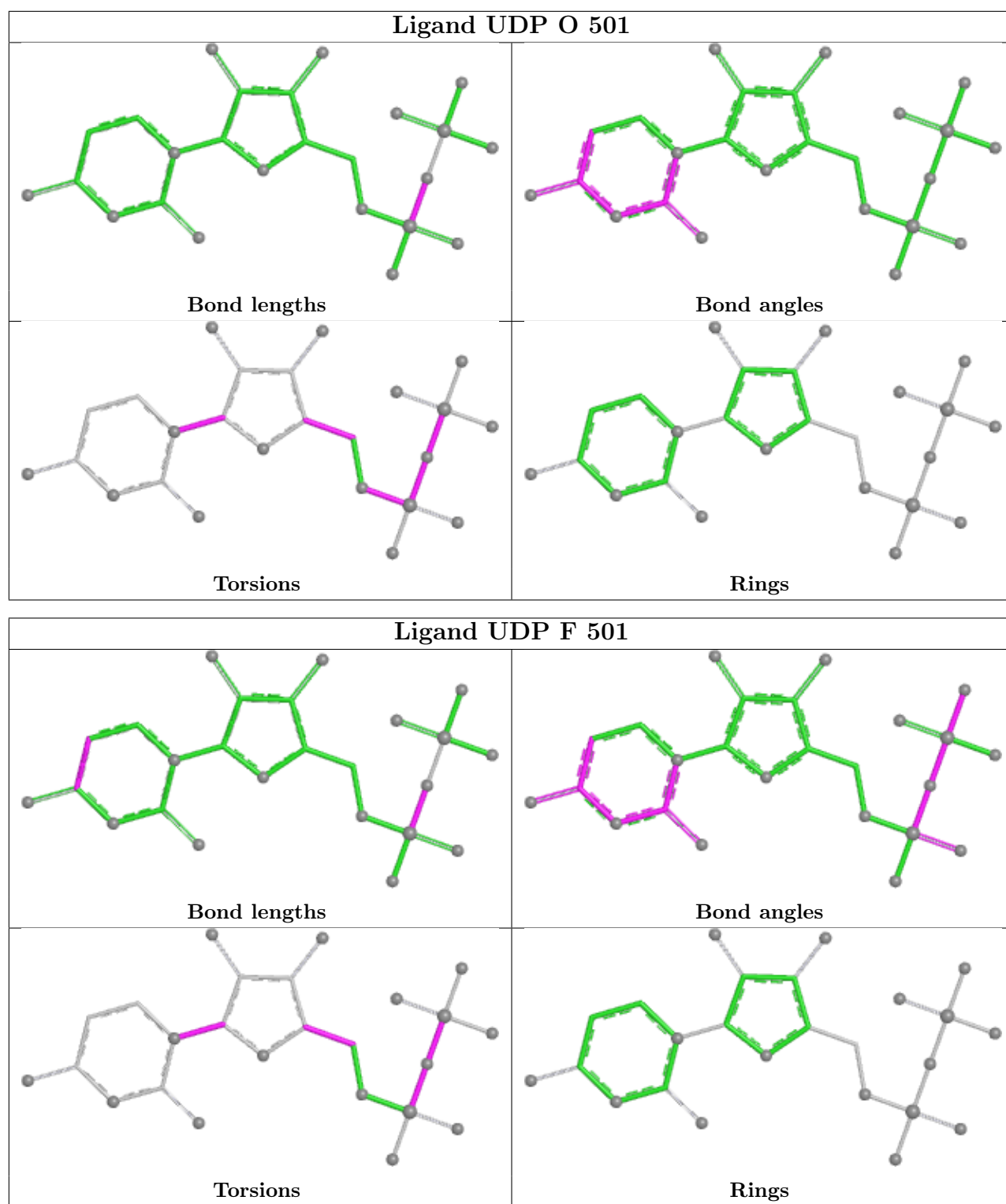
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	501	UDP	1	0
3	D	501	UDP	1	0
3	F	501	UDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	465/465 (100%)	0.03	13 (2%) 55 54	16, 27, 49, 88	0
1	B	465/465 (100%)	-0.02	17 (3%) 45 44	16, 26, 48, 92	0
1	D	465/465 (100%)	-0.02	23 (4%) 35 34	16, 26, 47, 91	0
1	F	465/465 (100%)	0.94	69 (14%) 5 5	24, 42, 68, 96	0
1	H	465/465 (100%)	0.93	86 (18%) 3 3	23, 40, 75, 99	0
1	K	465/465 (100%)	1.03	97 (20%) 2 2	23, 43, 78, 104	0
1	M	465/465 (100%)	0.87	71 (15%) 5 4	23, 43, 72, 94	0
1	O	465/465 (100%)	0.06	20 (4%) 40 39	17, 28, 52, 82	0
All	All	3720/3720 (100%)	0.48	396 (10%) 11 10	16, 33, 68, 104	0

All (396) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	70	ALA	8.2
1	B	70	ALA	8.0
1	O	35	TYR	7.5
1	A	35	TYR	7.3
1	A	390	MET	6.1
1	D	35	TYR	6.0
1	D	72	ALA	5.9
1	K	241	GLY	5.6
1	M	241	GLY	5.3
1	D	68	PRO	5.3
1	B	116	GLY	5.3
1	K	167	ILE	5.0
1	K	208	LEU	4.9
1	O	242	ARG	4.9
1	B	68	PRO	4.8
1	O	240	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	117	GLU	4.8
1	O	241	GLY	4.7
1	K	240	ALA	4.6
1	M	390	MET	4.6
1	D	224	CYS	4.5
1	K	479	LEU	4.5
1	K	174	VAL	4.5
1	B	241	GLY	4.4
1	H	227	ILE	4.4
1	A	116	GLY	4.3
1	K	116	GLY	4.3
1	M	170	SER	4.3
1	F	35	TYR	4.2
1	K	476	LEU	4.2
1	O	36	SER	4.1
1	H	241	GLY	4.1
1	F	39	MET	4.1
1	H	27	ILE	4.1
1	H	168	GLY	4.1
1	M	39	MET	4.1
1	A	36	SER	4.0
1	H	37	PHE	4.0
1	D	69	ASP	4.0
1	D	73	GLY	4.0
1	H	479	LEU	3.9
1	M	245	THR	3.9
1	F	214	TYR	3.9
1	H	75	VAL	3.9
1	H	167	ILE	3.9
1	H	116	GLY	3.9
1	F	70	ALA	3.9
1	K	239	PHE	3.8
1	K	243	PHE	3.8
1	A	33	GLY	3.8
1	H	242	ARG	3.8
1	M	119	THR	3.8
1	M	35	TYR	3.8
1	M	240	ALA	3.8
1	B	479	LEU	3.8
1	H	35	TYR	3.7
1	H	206	CYS	3.7
1	K	244	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	76	VAL	3.7
1	H	117	GLU	3.7
1	B	240	ALA	3.7
1	H	143	VAL	3.6
1	K	57	PHE	3.6
1	M	15	ARG	3.6
1	F	143	VAL	3.5
1	H	231	PRO	3.5
1	H	17	LEU	3.5
1	F	67	VAL	3.5
1	F	17	LEU	3.5
1	B	35	TYR	3.5
1	K	139	VAL	3.5
1	A	34	GLN	3.5
1	K	67	VAL	3.5
1	M	116	GLY	3.4
1	K	204	LEU	3.4
1	K	206	CYS	3.4
1	K	88	VAL	3.4
1	K	52	ALA	3.4
1	K	245	THR	3.4
1	H	68	PRO	3.4
1	K	227	ILE	3.4
1	A	27	ILE	3.3
1	H	57	PHE	3.3
1	O	29	ARG	3.3
1	H	36	SER	3.3
1	H	175	LYS	3.3
1	K	175	LYS	3.3
1	B	119	THR	3.3
1	H	240	ALA	3.3
1	F	116	GLY	3.2
1	F	60	TYR	3.2
1	K	163	LEU	3.2
1	F	162	MET	3.2
1	B	72	ALA	3.2
1	M	479	LEU	3.2
1	F	74	PRO	3.2
1	H	39	MET	3.2
1	H	204	LEU	3.2
1	A	31	ASP	3.2
1	M	237	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	79	LEU	3.1
1	D	29	ARG	3.1
1	M	242	ARG	3.1
1	F	174	VAL	3.1
1	H	91	ASP	3.1
1	M	67	VAL	3.1
1	M	139	VAL	3.1
1	D	71	GLU	3.1
1	K	214	TYR	3.1
1	H	170	SER	3.1
1	B	69	ASP	3.1
1	H	79	LEU	3.1
1	K	17	LEU	3.1
1	K	149	ILE	3.1
1	B	242	ARG	3.1
1	F	233	THR	3.0
1	O	117	GLU	3.0
1	M	169	ASP	3.0
1	H	228	LEU	3.0
1	M	471	SER	3.0
1	D	116	GLY	3.0
1	M	168	GLY	3.0
1	O	33	GLY	3.0
1	O	119	THR	3.0
1	M	214	TYR	3.0
1	M	86	HIS	3.0
1	F	148	MET	3.0
1	M	66	GLU	3.0
1	K	390	MET	3.0
1	K	29	ARG	2.9
1	K	242	ARG	2.9
1	H	169	ASP	2.9
1	M	231	PRO	2.9
1	H	89	PHE	2.9
1	H	214	TYR	2.9
1	K	54	THR	2.9
1	K	68	PRO	2.9
1	H	199	LEU	2.9
1	M	149	ILE	2.9
1	K	84	GLY	2.9
1	H	134	LEU	2.8
1	H	158	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	169	ASP	2.8
1	F	88	VAL	2.8
1	H	174	VAL	2.8
1	M	473	VAL	2.8
1	F	68	PRO	2.8
1	H	197	GLN	2.8
1	K	238	GLN	2.8
1	O	32	ASP	2.8
1	F	75	VAL	2.8
1	M	244	VAL	2.8
1	M	173	ASN	2.8
1	K	469	GLY	2.8
1	O	116	GLY	2.8
1	H	70	ALA	2.8
1	O	479	LEU	2.8
1	F	467	TRP	2.8
1	K	231	PRO	2.8
1	B	34	GLN	2.8
1	K	70	ALA	2.8
1	K	176	ILE	2.8
1	M	226	ARG	2.7
1	K	173	ASN	2.7
1	F	146	GLY	2.7
1	H	248	ALA	2.7
1	K	158	LEU	2.7
1	M	76	VAL	2.7
1	K	72	ALA	2.7
1	F	119	THR	2.7
1	K	16	LEU	2.7
1	H	83	TYR	2.7
1	B	117	GLU	2.7
1	F	117	GLU	2.7
1	K	237	VAL	2.7
1	K	246	VAL	2.7
1	F	57	PHE	2.7
1	M	70	ALA	2.7
1	M	472	PHE	2.7
1	O	34	GLN	2.7
1	H	173	ASN	2.7
1	H	205	HIS	2.7
1	F	76	VAL	2.7
1	H	25	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	85	ALA	2.6
1	F	37	PHE	2.6
1	F	479	LEU	2.6
1	F	473	VAL	2.6
1	H	237	VAL	2.6
1	K	473	VAL	2.6
1	F	15	ARG	2.6
1	K	226	ARG	2.6
1	F	50	GLY	2.6
1	F	34	GLN	2.6
1	H	208	LEU	2.6
1	F	242	ARG	2.6
1	H	469	GLY	2.6
1	H	23	LEU	2.6
1	K	135	PHE	2.6
1	H	29	ARG	2.6
1	M	38	SER	2.6
1	H	139	VAL	2.6
1	K	80	LYS	2.6
1	K	478	ARG	2.6
1	A	37	PHE	2.5
1	F	149	ILE	2.5
1	K	76	VAL	2.5
1	F	205	HIS	2.5
1	A	29	ARG	2.5
1	F	169	ASP	2.5
1	M	69	ASP	2.5
1	D	240	ALA	2.5
1	M	72	ALA	2.5
1	F	163	LEU	2.5
1	H	18	LEU	2.5
1	H	269	GLN	2.5
1	M	17	LEU	2.5
1	O	37	PHE	2.5
1	H	148	MET	2.5
1	K	236	GLY	2.5
1	M	73	GLY	2.5
1	K	77	GLN	2.5
1	F	79	LEU	2.5
1	M	16	LEU	2.5
1	M	57	PHE	2.5
1	K	75	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	164	ARG	2.5
1	K	83	TYR	2.5
1	K	36	SER	2.5
1	H	136	ALA	2.5
1	M	228	LEU	2.5
1	F	29	ARG	2.5
1	F	89	PHE	2.5
1	K	89	PHE	2.5
1	K	178	PHE	2.5
1	D	33	GLY	2.5
1	M	59	TRP	2.5
1	M	238	GLN	2.4
1	K	224	CYS	2.4
1	F	18	LEU	2.4
1	H	84	GLY	2.4
1	H	239	PHE	2.4
1	H	176	ILE	2.4
1	H	467	TRP	2.4
1	K	143	VAL	2.4
1	M	467	TRP	2.4
1	M	60	TYR	2.4
1	M	83	TYR	2.4
1	M	68	PRO	2.4
1	B	29	ARG	2.4
1	M	474	ALA	2.4
1	K	205	HIS	2.4
1	B	403	ASP	2.4
1	F	83	TYR	2.4
1	H	87	PRO	2.4
1	K	18	LEU	2.4
1	D	117	GLU	2.4
1	O	477	ASN	2.4
1	H	220	PHE	2.4
1	F	118	ILE	2.4
1	F	244	VAL	2.4
1	M	174	VAL	2.4
1	F	175	LYS	2.4
1	F	150	TRP	2.4
1	H	245	THR	2.4
1	K	55	THR	2.4
1	K	160	PRO	2.4
1	H	474	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	209	LEU	2.3
1	M	236	GLY	2.3
1	D	39	MET	2.3
1	H	135	PHE	2.3
1	H	470	SER	2.3
1	K	225	SER	2.3
1	M	118	ILE	2.3
1	K	221	LEU	2.3
1	D	242	ARG	2.3
1	H	243	PHE	2.3
1	M	243	PHE	2.3
1	F	36	SER	2.3
1	F	86	HIS	2.3
1	M	167	ILE	2.3
1	M	227	ILE	2.3
1	H	88	VAL	2.3
1	H	90	VAL	2.3
1	F	240	ALA	2.3
1	D	429	TRP	2.3
1	H	43	GLY	2.3
1	H	163	LEU	2.3
1	M	145	ASP	2.3
1	D	390	MET	2.3
1	H	56	SER	2.3
1	H	471	SER	2.3
1	F	19	ILE	2.3
1	H	149	ILE	2.3
1	K	151	VAL	2.3
1	F	247	GLY	2.3
1	K	48	LEU	2.3
1	M	134	LEU	2.3
1	M	208	LEU	2.3
1	K	60	TYR	2.3
1	K	25	ILE	2.2
1	F	231	PRO	2.2
1	K	194	PRO	2.2
1	M	140	VAL	2.2
1	H	28	LYS	2.2
1	D	403	ASP	2.2
1	F	206	CYS	2.2
1	H	247	GLY	2.2
1	M	205	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	38	SER	2.2
1	F	239	PHE	2.2
1	F	140	VAL	2.2
1	F	237	VAL	2.2
1	H	160	PRO	2.2
1	K	477	ASN	2.2
1	K	195	VAL	2.2
1	K	162	MET	2.2
1	M	207	ASP	2.2
1	D	241	GLY	2.2
1	F	202	GLY	2.2
1	K	85	ALA	2.2
1	K	136	ALA	2.2
1	H	159	LEU	2.2
1	M	163	LEU	2.2
1	K	59	TRP	2.2
1	K	467	TRP	2.2
1	K	28	LYS	2.2
1	H	234	PRO	2.2
1	K	46	THR	2.2
1	M	87	PRO	2.2
1	O	121	ASP	2.2
1	K	58	GLN	2.2
1	K	200	LEU	2.2
1	F	56	SER	2.2
1	M	148	MET	2.2
1	B	169	ASP	2.2
1	B	93	GLU	2.1
1	K	27	ILE	2.1
1	H	140	VAL	2.1
1	H	244	VAL	2.1
1	M	143	VAL	2.1
1	H	34	GLN	2.1
1	F	134	LEU	2.1
1	F	209	LEU	2.1
1	M	204	LEU	2.1
1	F	171	LYS	2.1
1	A	119	THR	2.1
1	H	74	PRO	2.1
1	K	87	PRO	2.1
1	M	74	PRO	2.1
1	F	251	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	27	ILE	2.1
1	K	140	VAL	2.1
1	H	276	ARG	2.1
1	F	208	LEU	2.1
1	H	200	LEU	2.1
1	F	390	MET	2.1
1	K	39	MET	2.1
1	F	82	GLU	2.1
1	O	214	TYR	2.1
1	H	233	THR	2.1
1	M	19	ILE	2.1
1	M	249	PHE	2.1
1	M	75	VAL	2.1
1	M	462	LYS	2.1
1	K	248	ALA	2.1
1	D	30	SER	2.1
1	F	23	LEU	2.1
1	K	159	LEU	2.1
1	K	170	SER	2.1
1	K	186	SER	2.1
1	O	390	MET	2.1
1	D	169	ASP	2.1
1	H	31	ASP	2.1
1	K	403	ASP	2.1
1	O	31	ASP	2.1
1	K	234	PRO	2.1
1	K	168	GLY	2.1
1	D	75	VAL	2.1
1	K	37	PHE	2.1
1	K	472	PHE	2.1
1	F	85	ALA	2.1
1	K	475	GLU	2.0
1	A	121	ASP	2.0
1	H	458	ARG	2.0
1	H	232	THR	2.0
1	F	141	LYS	2.0
1	F	241	GLY	2.0
1	O	118	ILE	2.0
1	F	243	PHE	2.0
1	K	203	VAL	2.0
1	M	239	PHE	2.0
1	F	419	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	80	LYS	2.0
1	D	214	TYR	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](#)

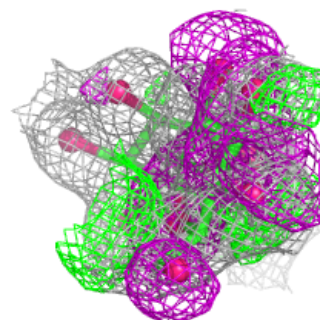
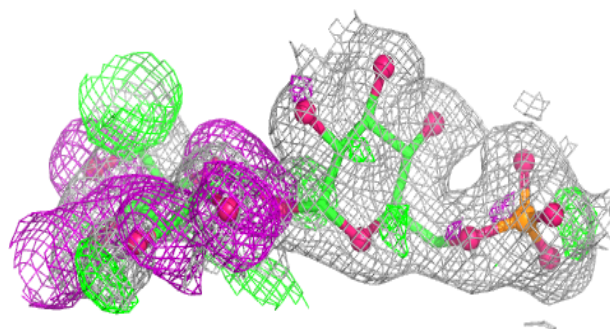
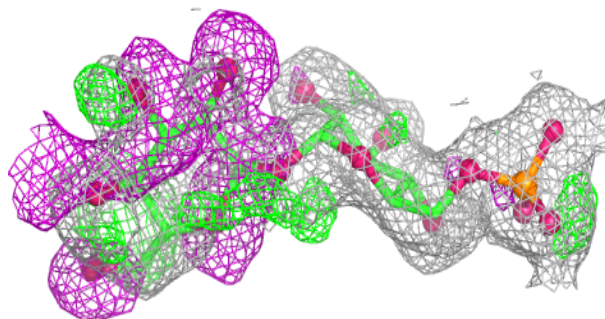
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	1	11/12	-	-	21,22,23,25	0
2	G6P	C	2	16/16	-	-	20,22,23,23	0
2	GLC	E	1	11/12	-	-	18,20,21,22	0
2	G6P	E	2	16/16	-	-	19,20,20,21	0
2	GLC	G	1	11/12	-	-	19,20,21,23	0
2	G6P	G	2	16/16	-	-	18,19,20,21	0
2	GLC	P	1	11/12	0.37	0.28	20,21,23,25	0
2	GLC	L	1	11/12	0.39	0.29	35,37,39,39	0
2	GLC	N	1	11/12	0.40	0.24	34,36,38,38	0
2	GLC	I	1	11/12	0.41	0.28	36,36,37,38	0
2	GLC	J	1	11/12	0.58	0.24	35,36,37,37	0
2	G6P	N	2	16/16	0.86	0.12	34,35,37,37	0
2	G6P	L	2	16/16	0.87	0.12	36,38,41,42	0
2	G6P	J	2	16/16	0.90	0.11	34,35,38,38	0
2	G6P	I	2	16/16	0.92	0.10	34,36,38,38	0
2	G6P	P	2	16/16	0.93	0.10	20,21,22,24	0

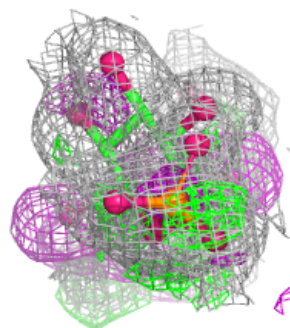
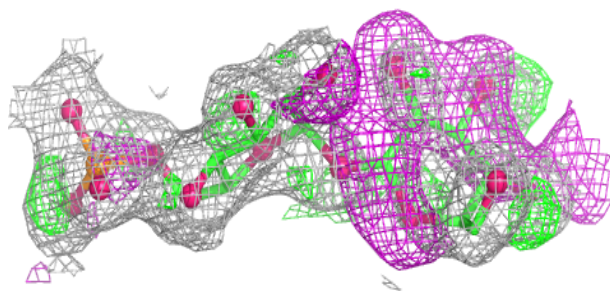
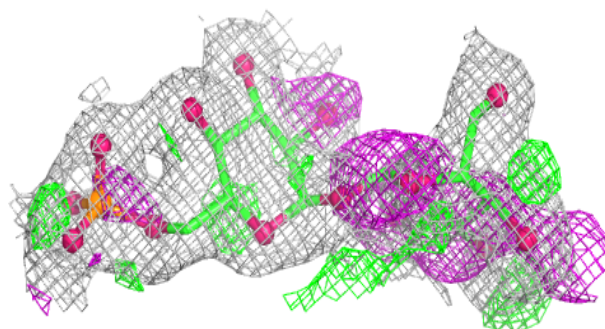
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

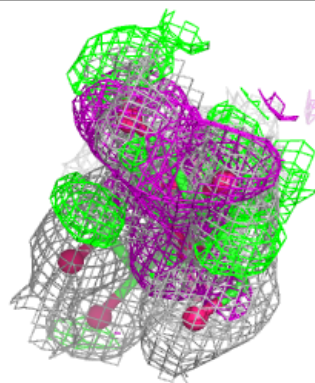
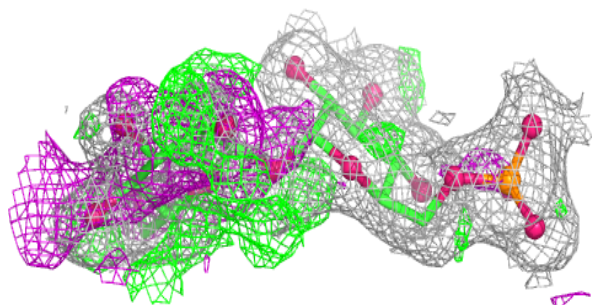
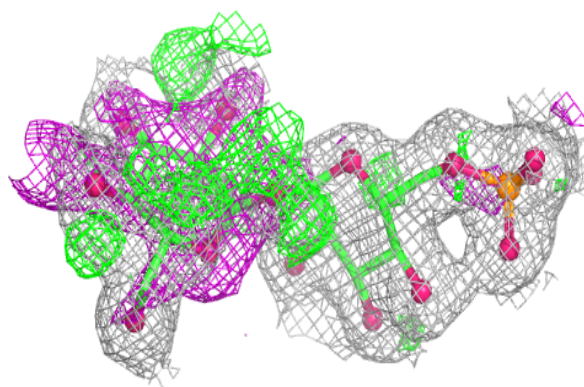
**Electron density around Chain E:**

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

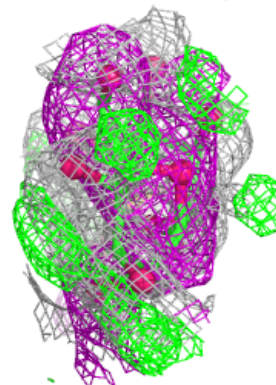
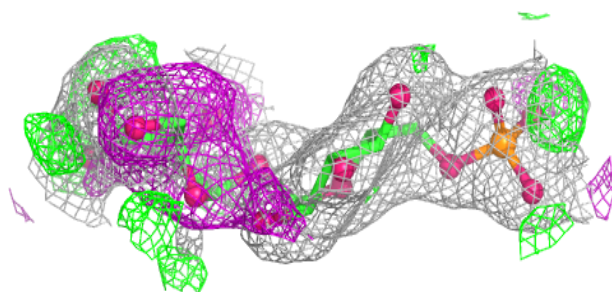
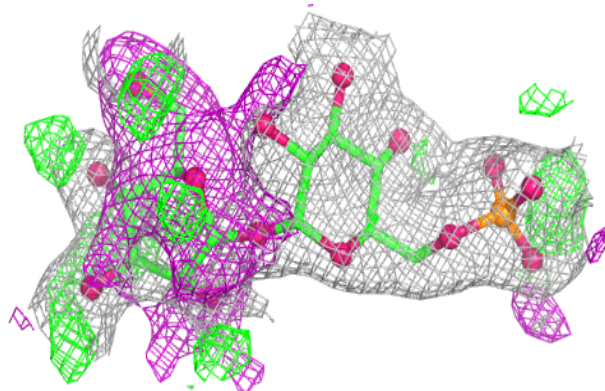


Electron density around Chain G:

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

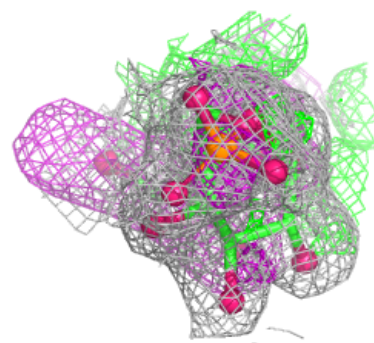
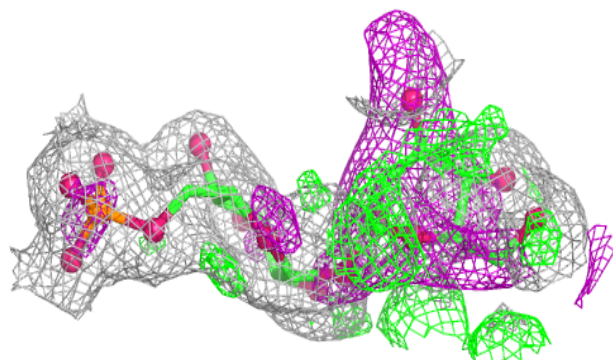
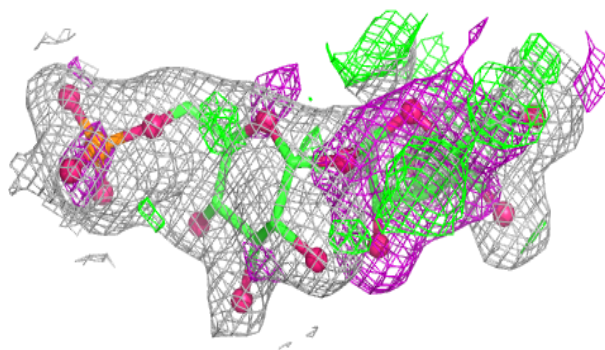
**Electron density around Chain I:**

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

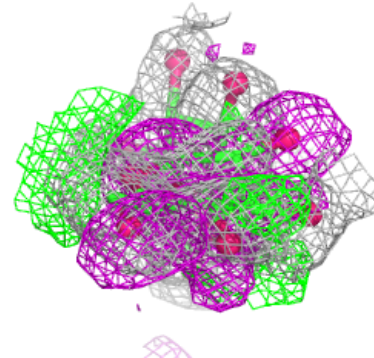
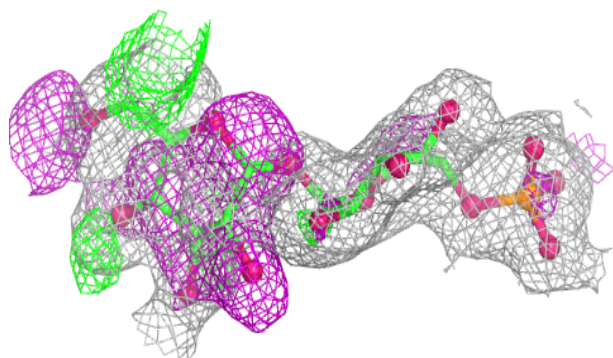
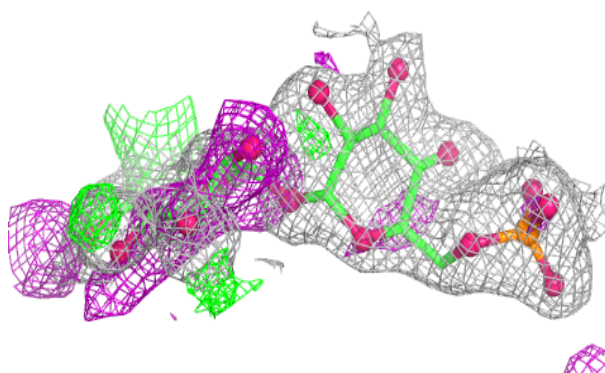


Electron density around Chain J:

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

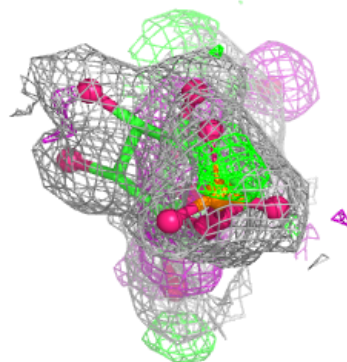
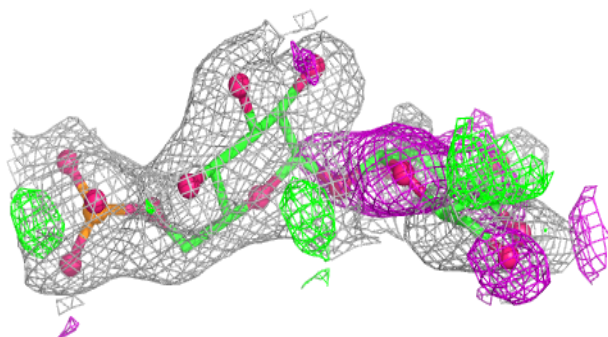
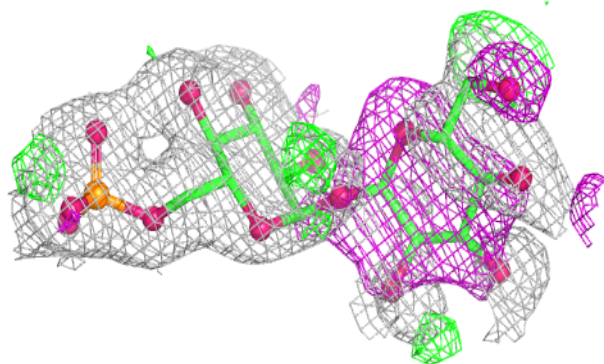
**Electron density around Chain L:**

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

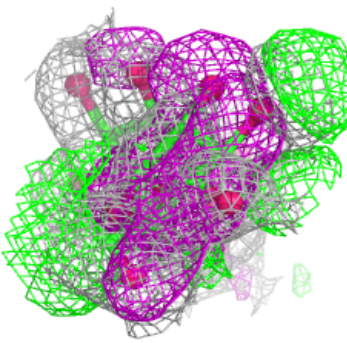
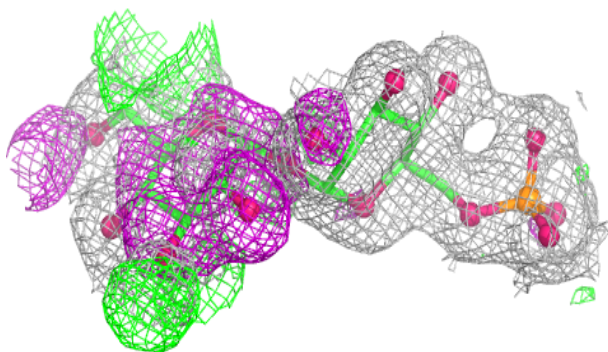
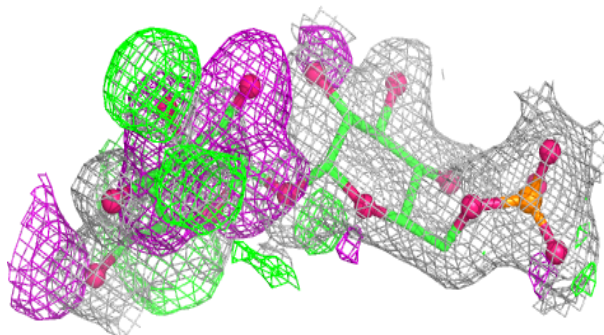


Electron density around Chain N:

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

**Electron density around Chain P:**

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

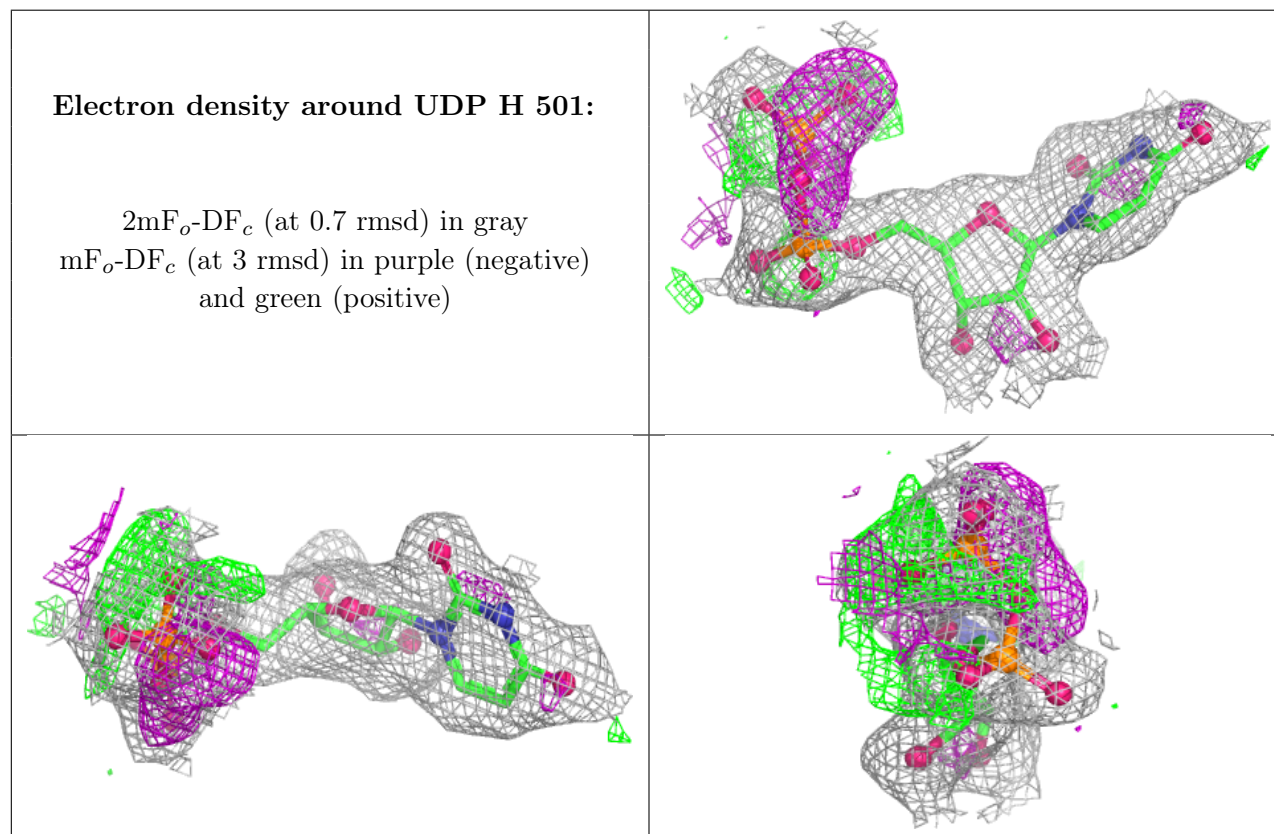


6.4 Ligands ⓘ

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, 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.

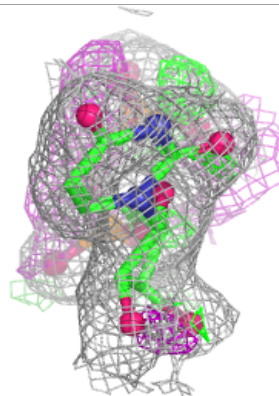
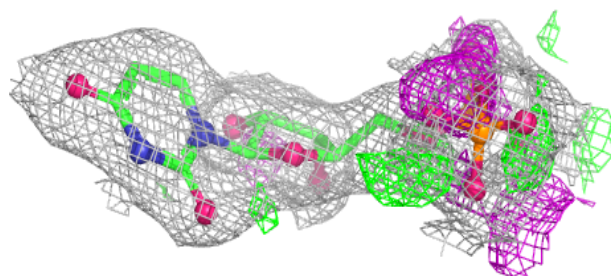
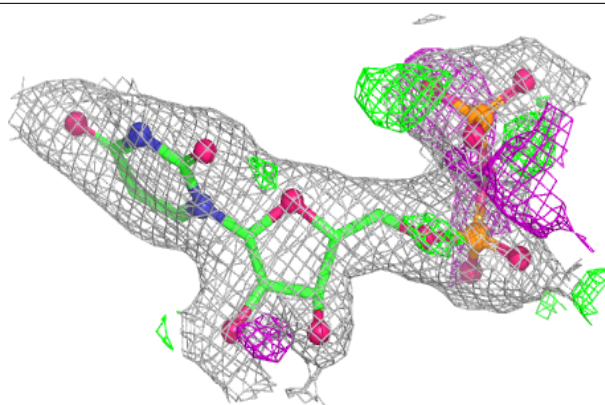
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	UDP	H	501	25/25	0.85	0.13	29,31,33,36	0
3	UDP	F	501	25/25	0.89	0.11	31,34,35,35	0
3	UDP	D	501	25/25	0.90	0.11	18,21,22,22	0
3	UDP	M	501	25/25	0.91	0.11	32,34,36,36	0
3	UDP	K	501	25/25	0.94	0.09	33,35,36,38	0
3	UDP	B	501	25/25	0.95	0.08	18,20,21,22	0
3	UDP	A	501	25/25	0.95	0.08	20,23,24,24	0
3	UDP	O	501	25/25	0.96	0.08	20,22,24,25	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.

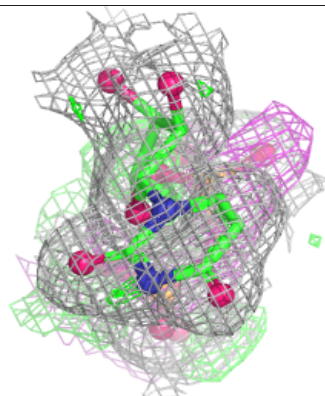
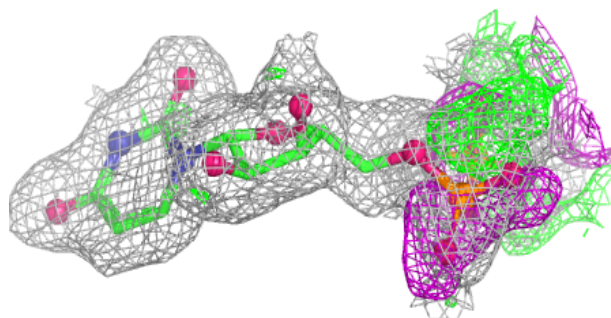
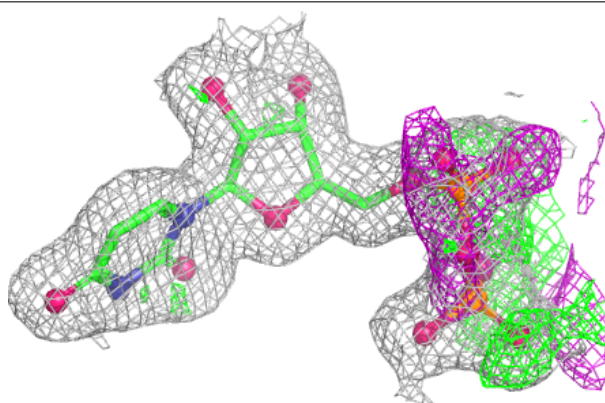


Electron density around UDP F 501:

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

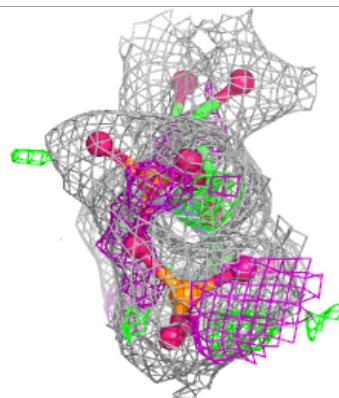
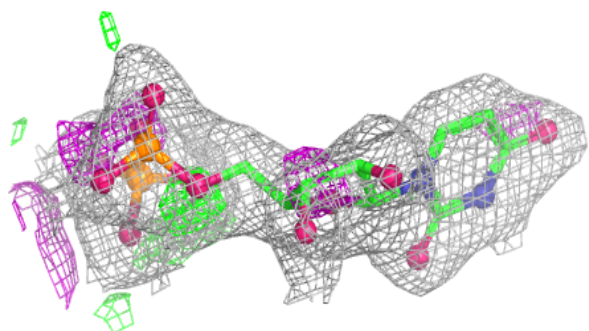
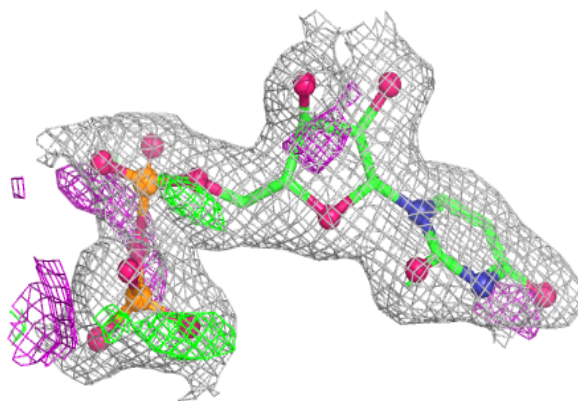
**Electron density around UDP D 501:**

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

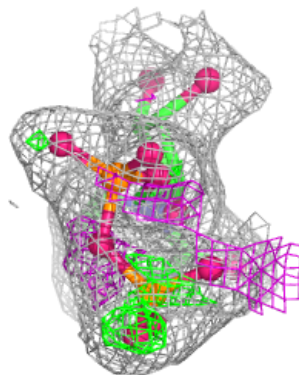
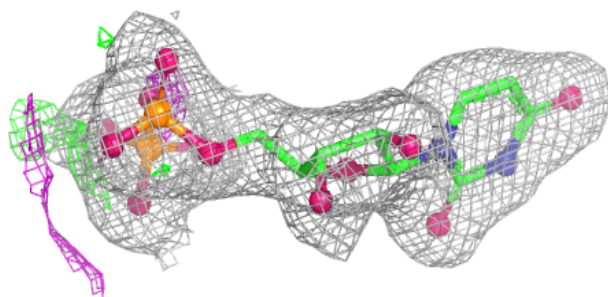
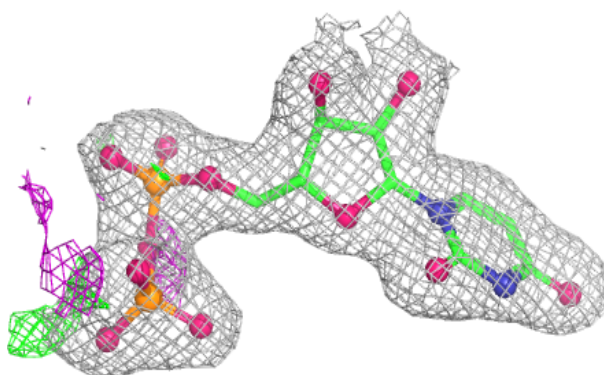


Electron density around UDP M 501:

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

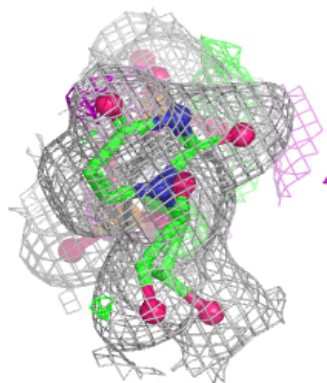
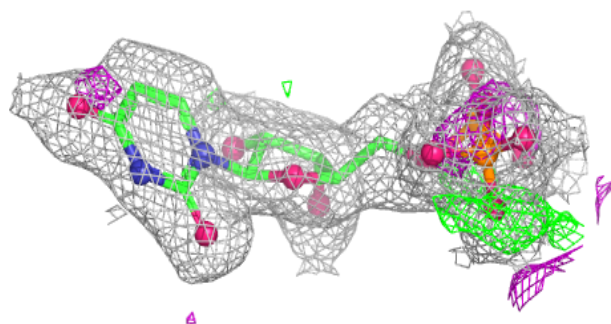
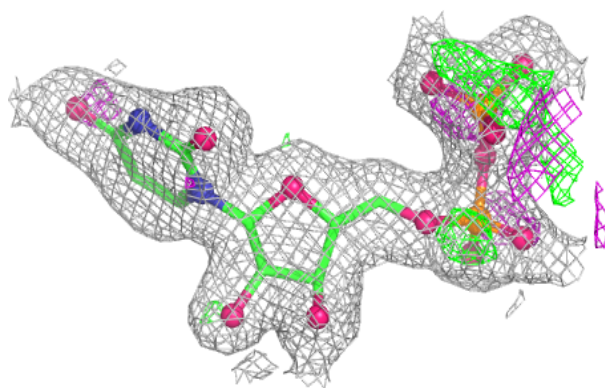
**Electron density around UDP K 501:**

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

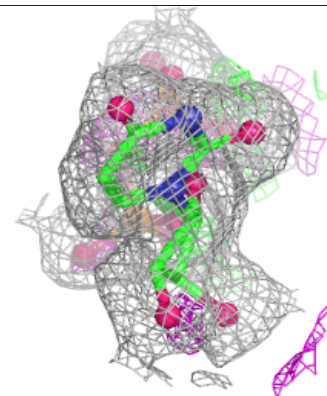
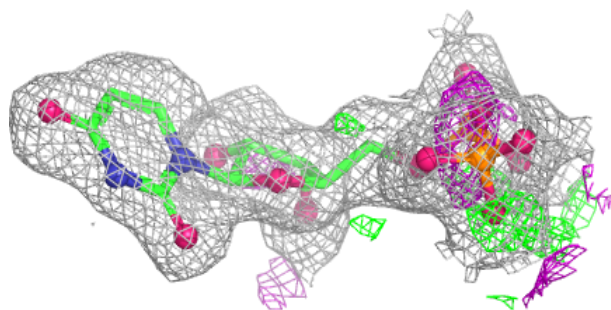
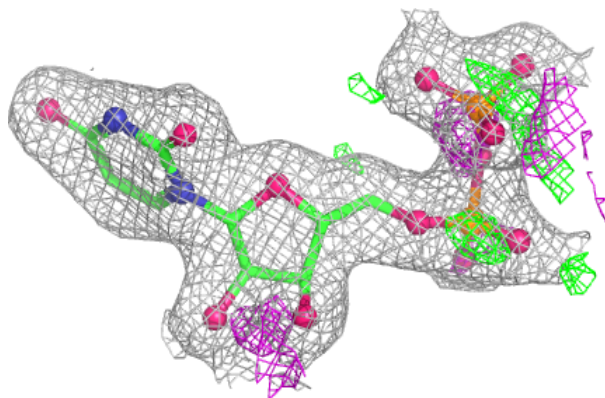


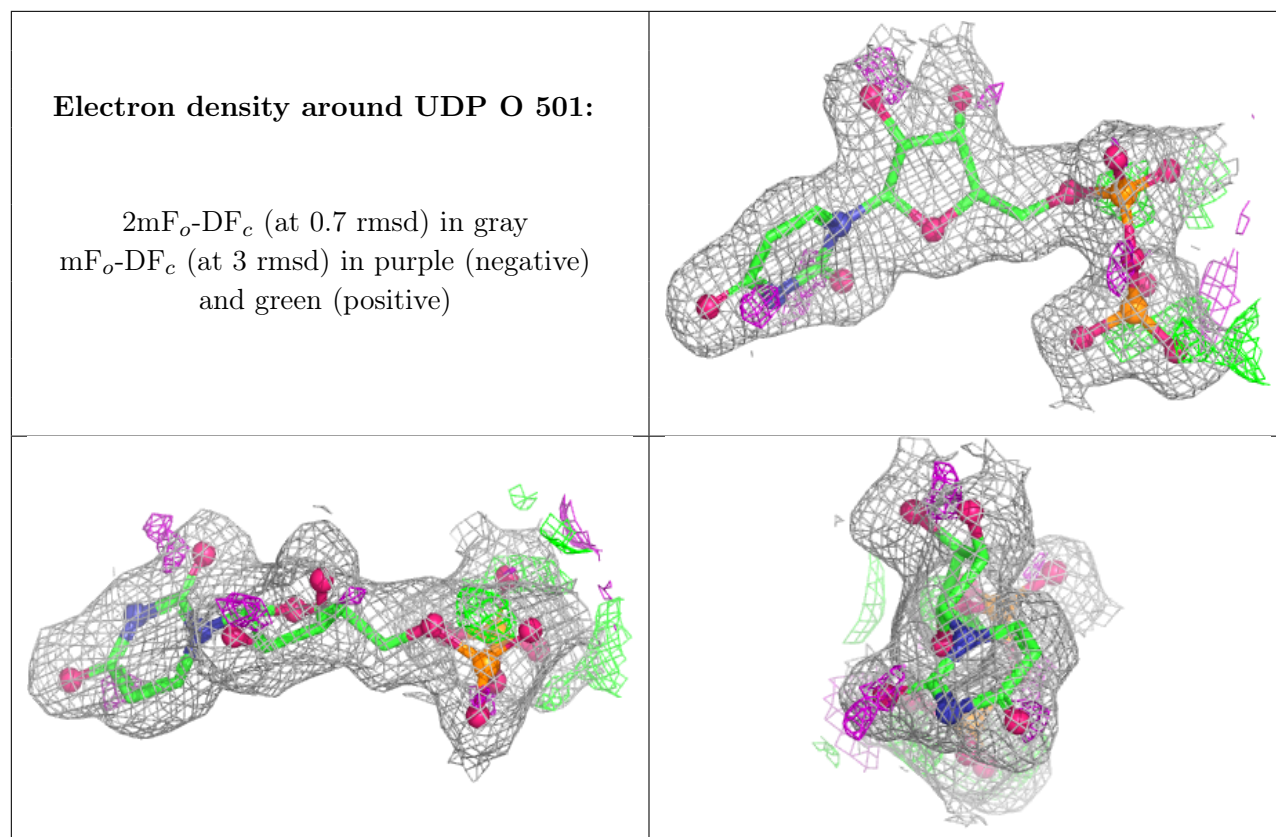
Electron density around UDP B 501:

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

**Electron density around UDP A 501:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.