



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2026 – 12:16 PM EDT

PDB ID : 9P3K / pdb\_00009p3k  
Title : Crystal Structure of Xyloglucan Xylosyltransferase 2 and Xyloglucan Xylosyltransferase 5 Heterodimer Bound to UDP and Cellohexaose  
Authors : Jordan, D.J.; Stewart Jr, C.E.; Alan, T.C.; Zabolina, A.O.  
Deposited on : 2025-06-14  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
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

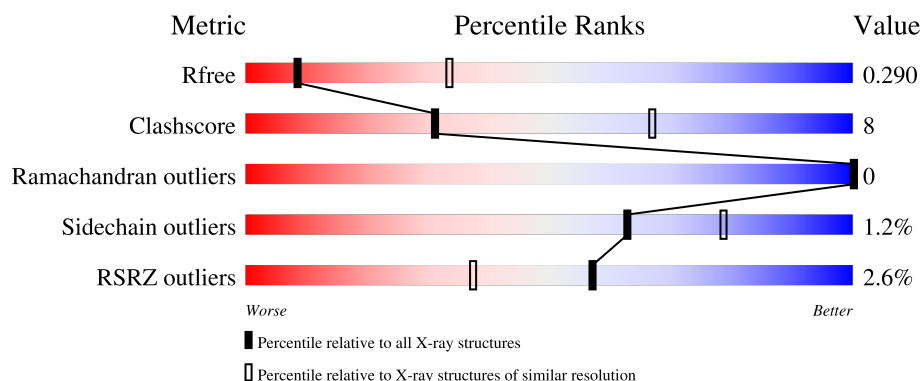
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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.



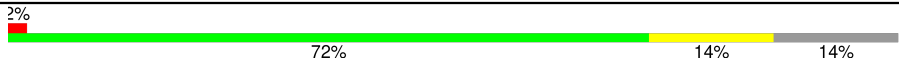

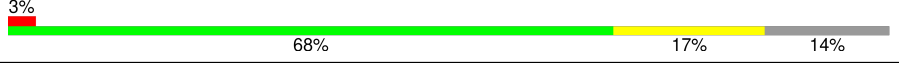
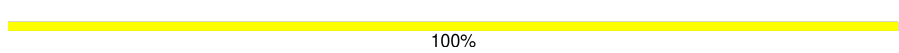
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	420	 2% 69% 15% 15%
1	C	420	 2% 70% 16% 15%
1	E	420	 3% 69% 17% 14%
1	G	420	 2% 70% 17% 13%
2	B	387	 2% 68% 18% 14%

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Mol	Chain	Length	Quality of chain
2	D	387	 2% 72% 14% 14%
2	F	387	 2% 71% 14% 14%
2	H	387	 3% 68% 17% 14%
3	K	6	 100%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 45479 atoms, of which 22412 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 Xyloglucan 6-xylosyltransferase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	358	Total	C	H	N	O	S	0	0	0
			5785	1898	2848	497	525	17			
1	C	358	Total	C	H	N	O	S	0	0	0
			5793	1897	2854	499	526	17			
1	E	363	Total	C	H	N	O	S	0	0	0
			5866	1923	2885	504	537	17			
1	G	365	Total	C	H	N	O	S	0	0	0
			5898	1933	2903	506	539	17			

- Molecule 2 is a protein called Xyloglucan 6-xylosyltransferase 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	332	Total	C	H	N	O	S	0	0	0
			5432	1779	2696	464	479	14			
2	D	331	Total	C	H	N	O	S	0	0	0
			5411	1770	2687	463	477	14			
2	F	331	Total	C	H	N	O	S	0	0	0
			5410	1770	2686	463	477	14			
2	H	331	Total	C	H	N	O	S	0	0	0
			5411	1770	2687	463	477	14			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	6	Total	C	H	O	0	0	0
			129	36	62	31			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



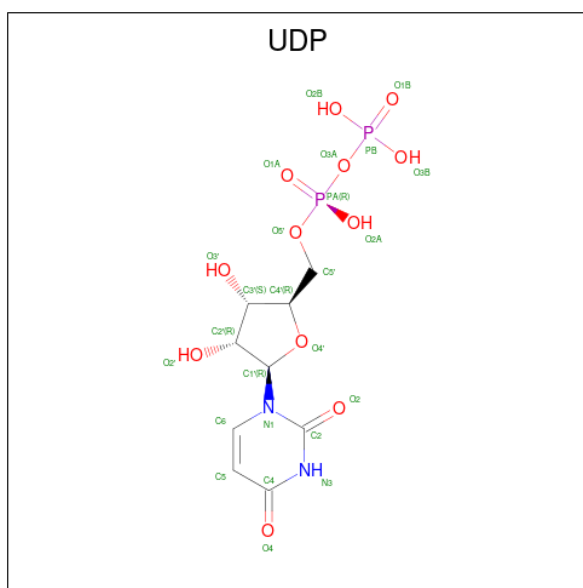
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	B	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		
5	E	1	Total	Mn	0	0
			1	1		
5	F	1	Total	Mn	0	0
			1	1		
5	G	1	Total	Mn	0	0
			1	1		
5	H	1	Total	Mn	0	0
			1	1		

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ )

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
6	B	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
6	C	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
6	D	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
6	E	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
6	F	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
6	G	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		
6	H	1	Total	C	H	N	O	P	0	0
			36	9	11	2	12	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total 3 O 3	0	0
7	B	2	Total 2 O 2	0	0
7	C	3	Total 3 O 3	0	0

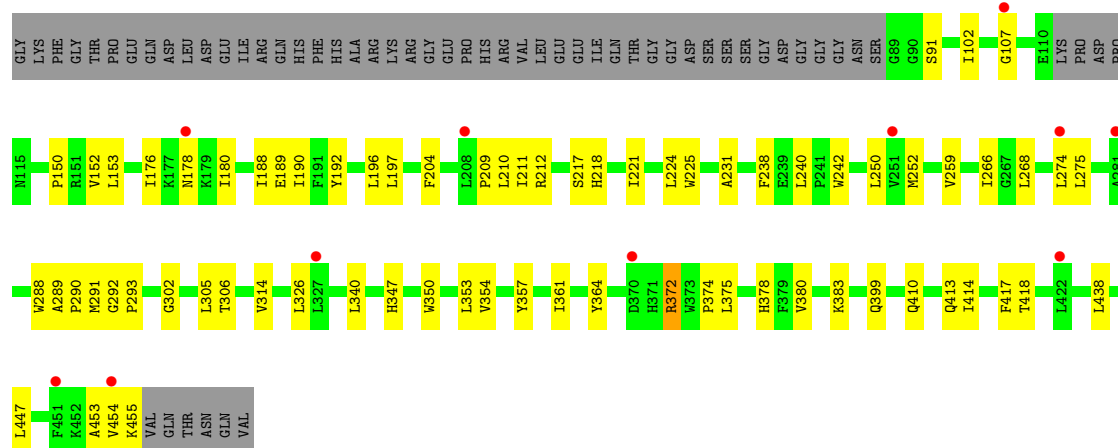
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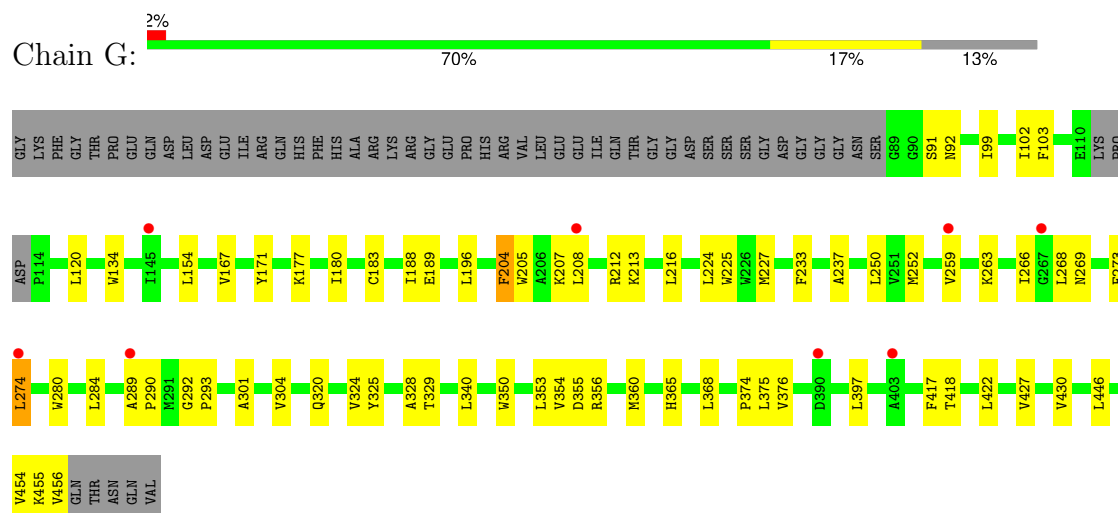
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total 1	O 1	0	0
7	E	3	Total 3	O 3	0	0
7	F	2	Total 2	O 2	0	0
7	G	5	Total 5	O 5	0	0
7	H	1	Total 1	O 1	0	0



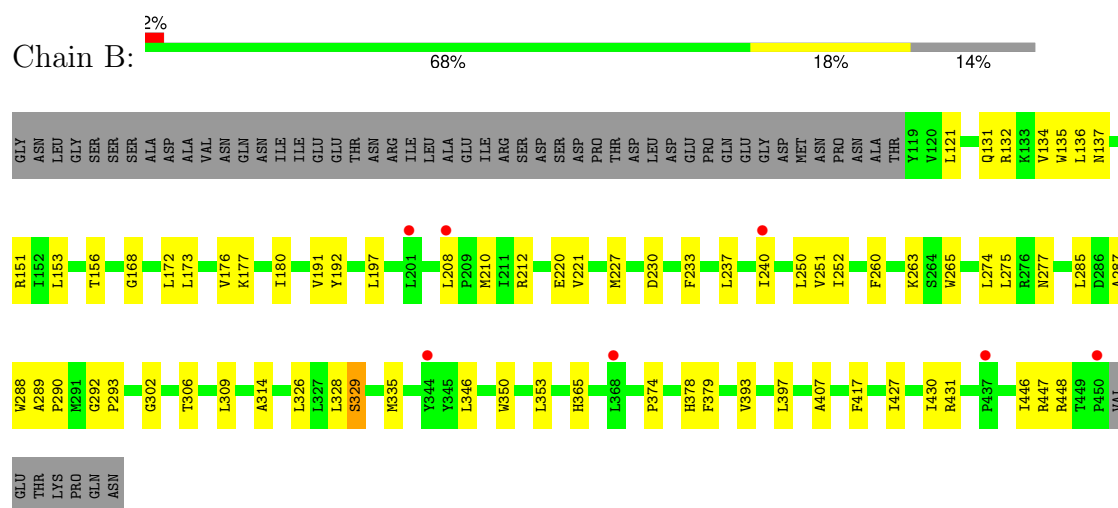




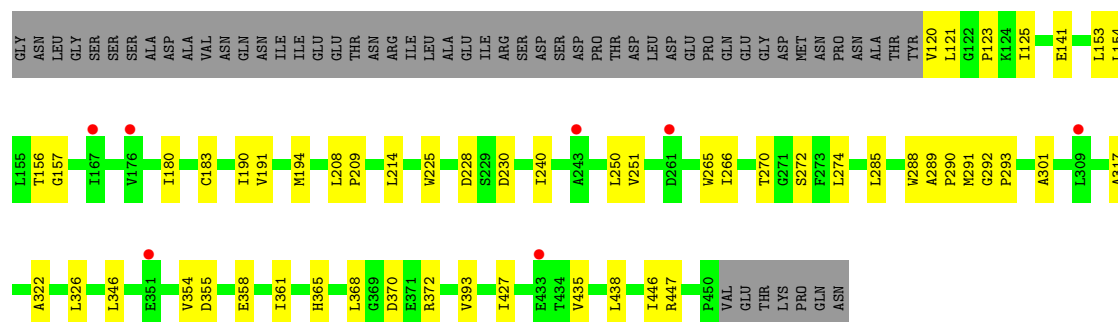
• Molecule 1: Xyloglucan 6-xylosyltransferase 2



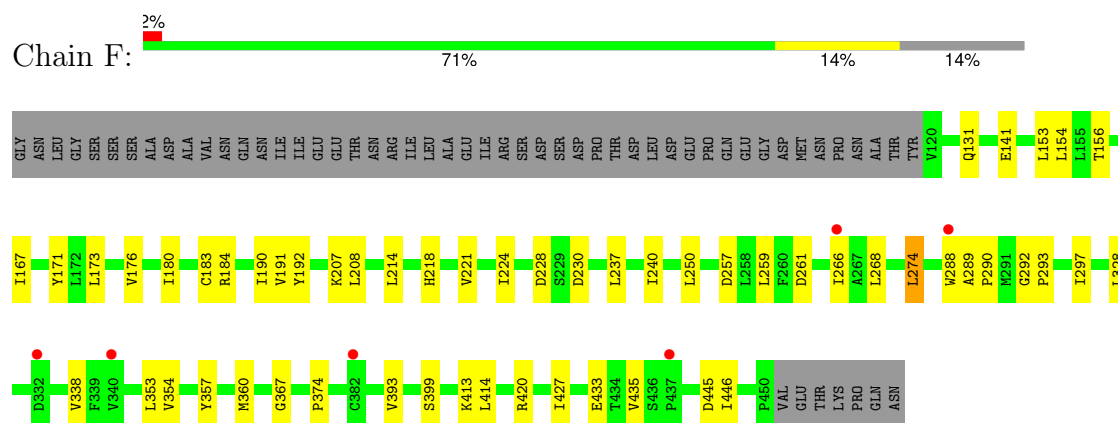
• Molecule 2: Xyloglucan 6-xylosyltransferase 5



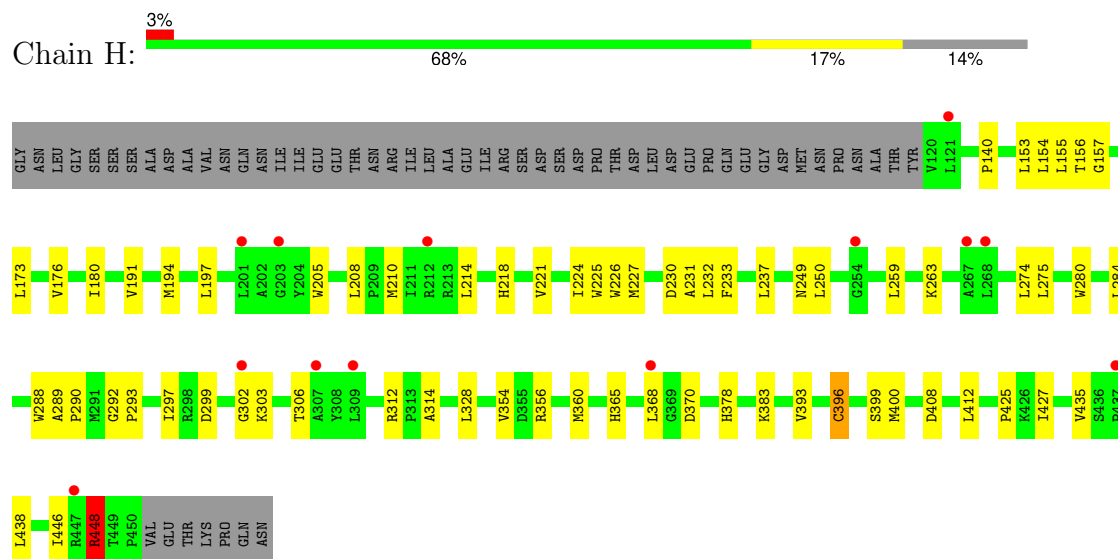
• Molecule 2: Xyloglucan 6-xylosyltransferase 5



• Molecule 2: Xyloglucan 6-xylosyltransferase 5



• Molecule 2: Xyloglucan 6-xylosyltransferase 5



• Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.72Å 111.85Å 115.67Å 89.34° 70.44° 80.92°	Depositor
Resolution (Å)	48.36 – 3.20 48.36 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.36-3.20) 87.3 (48.36-3.20)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.229 , 0.290 0.229 , 0.290	Depositor DCC
$R_{free}$ test set	1590 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.832	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,-h+l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	45479	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN, UDP, BGC

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	0.12	0/3026	0.29	0/4100
1	C	0.11	0/3026	0.28	0/4098
1	E	0.12	0/3070	0.30	0/4158
1	G	0.11	0/3085	0.28	0/4179
2	B	0.12	0/2821	0.29	0/3830
2	D	0.12	0/2808	0.29	0/3812
2	F	0.13	0/2808	0.31	0/3812
2	H	0.12	0/2808	0.32	0/3812
All	All	0.12	0/23452	0.30	0/31801

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
2	H	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	ARG	Sidechain
1	E	372	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	H	448	ARG	Sidechain

## 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	2937	2848	2848	52	0
1	C	2939	2854	2854	49	0
1	E	2981	2885	2885	52	0
1	G	2995	2903	2902	55	0
2	B	2736	2696	2695	52	0
2	D	2724	2687	2686	42	0
2	F	2724	2686	2686	48	0
2	H	2724	2687	2686	56	0
3	K	67	62	57	0	0
4	A	6	8	8	0	0
4	G	6	8	8	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	25	11	11	2	0
6	B	25	11	11	0	0
6	C	25	11	11	0	0
6	D	25	11	11	1	0
6	E	25	11	11	1	0
6	F	25	11	11	0	0
6	G	25	11	11	1	0
6	H	25	11	11	0	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
7	C	3	0	0	0	0
7	D	1	0	0	0	0
7	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	2	0	0	0	0
7	G	5	0	0	0	0
7	H	1	0	0	0	0
All	All	23067	22412	22403	372	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 8.

All (372) 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)
2:D:153:LEU:HD11	2:D:191:VAL:HG23	1.42	1.00
1:G:427:VAL:HG21	2:H:197:LEU:HD23	1.53	0.89
1:E:302:GLY:O	1:E:306:THR:HG23	1.84	0.76
1:E:252:MET:HE1	1:E:268:LEU:HD13	1.67	0.76
1:C:352:ILE:HG23	1:C:353:LEU:HD22	1.66	0.76
2:B:287:ALA:HB1	2:B:326:LEU:HD11	1.66	0.75
1:C:306:THR:HG21	1:C:314:VAL:HG23	1.67	0.74
2:H:218:HIS:O	2:H:221:VAL:HG12	1.87	0.74
2:B:227:MET:HE1	2:B:233:PHE:CZ	2.25	0.71
1:C:291:MET:HE1	1:C:305:LEU:CD1	2.20	0.70
2:F:259:LEU:O	2:F:328:LEU:HD21	1.92	0.70
1:E:306:THR:HG21	1:E:314:VAL:HA	1.75	0.67
1:A:414:ILE:HG23	1:A:447:LEU:HD21	1.75	0.67
2:D:120:VAL:HG12	2:D:121:LEU:H	1.58	0.67
2:F:266:ILE:HG22	2:F:266:ILE:O	1.94	0.67
2:F:208:LEU:HD21	2:F:288:TRP:CD2	2.31	0.65
2:H:354:VAL:HG21	2:H:399:SER:HB3	1.79	0.65
1:E:176:ILE:HD11	2:F:180:ILE:CD1	2.27	0.65
2:H:154:LEU:HD12	2:H:225:TRP:O	1.96	0.65
2:B:153:LEU:HD11	2:B:191:VAL:HG23	1.79	0.64
1:C:171:TYR:CE2	1:C:397:LEU:HD22	2.32	0.64
1:G:325:TYR:O	1:G:329:THR:HG22	1.97	0.64
1:A:259:VAL:HG21	1:A:340:LEU:HD21	1.78	0.64
2:D:365:HIS:O	2:D:368:LEU:HD13	1.99	0.62
1:G:171:TYR:CE2	1:G:397:LEU:HD22	2.33	0.62
1:G:252:MET:HE1	1:G:268:LEU:HD13	1.81	0.62
1:E:176:ILE:HD12	1:E:192:TYR:CD2	2.34	0.62
2:B:430:ILE:HD12	2:B:431:ARG:HG3	1.81	0.62
1:G:180:ILE:HD11	2:H:180:ILE:HD11	1.81	0.61
1:C:305:LEU:HD22	1:C:309:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:MET:HE1	1:E:305:LEU:HD21	1.83	0.60
1:E:414:ILE:HG23	1:E:447:LEU:HD21	1.83	0.60
2:H:153:LEU:HD11	2:H:191:VAL:HG23	1.83	0.60
1:G:154:LEU:HD23	1:G:183:CYS:SG	2.42	0.60
2:H:155:LEU:HD22	2:H:226:TRP:CZ3	2.37	0.60
1:E:217:SER:HB3	2:F:414:LEU:HD21	1.84	0.60
1:E:218:HIS:HB2	1:E:221:ILE:HD12	1.84	0.59
2:F:292:GLY:N	2:F:293:PRO:HD2	2.17	0.59
1:A:197:LEU:HA	2:B:427:ILE:HD11	1.84	0.59
2:H:249:ASN:O	2:H:275:LEU:HD12	2.01	0.59
2:F:259:LEU:HD22	2:F:268:LEU:HD11	1.85	0.59
1:C:352:ILE:HG23	1:C:353:LEU:CD2	2.32	0.58
2:F:208:LEU:HD21	2:F:288:TRP:CG	2.39	0.57
1:A:434:THR:HG22	1:A:440:MET:HE2	1.86	0.57
2:F:237:LEU:HD23	2:F:237:LEU:O	2.04	0.57
2:D:153:LEU:CD2	2:D:214:LEU:HD23	2.34	0.57
1:G:154:LEU:HD12	1:G:225:TRP:O	2.04	0.57
1:A:268:LEU:HD11	1:A:327:LEU:HD12	1.87	0.57
1:C:305:LEU:HD21	1:C:325:TYR:HB2	1.85	0.57
2:H:155:LEU:HD23	2:H:156:THR:N	2.18	0.57
1:C:256:ASN:HA	1:C:340:LEU:HD12	1.86	0.56
2:B:208:LEU:HD21	2:B:288:TRP:CD2	2.40	0.56
1:A:171:TYR:CE2	1:A:397:LEU:HD22	2.39	0.56
1:G:356:ARG:HB2	1:G:360:MET:HE3	1.87	0.56
1:A:227:MET:HE1	1:A:233:PHE:CZ	2.41	0.56
2:D:208:LEU:HD11	2:D:288:TRP:CE3	2.41	0.56
2:H:227:MET:HE1	2:H:233:PHE:CZ	2.41	0.56
1:C:306:THR:HG21	1:C:314:VAL:CG2	2.34	0.56
1:A:417:PHE:CG	2:B:197:LEU:HD22	2.41	0.55
1:C:91:SER:O	2:D:393:VAL:HG22	2.06	0.55
1:C:216:LEU:HD21	1:C:282:LEU:HD21	1.88	0.55
1:E:414:ILE:HG23	1:E:447:LEU:HD11	1.88	0.55
2:B:302:GLY:O	2:B:306:THR:HG23	2.08	0.54
1:A:171:TYR:CD2	1:A:397:LEU:HD22	2.41	0.54
2:D:123:PRO:O	2:D:125:ILE:HD12	2.07	0.54
2:F:237:LEU:HD22	2:F:367:GLY:HA3	1.89	0.54
2:H:231:ALA:C	2:H:232:LEU:HD12	2.32	0.54
2:B:306:THR:HG21	2:B:314:ALA:HA	1.89	0.54
1:A:185:LEU:O	1:A:185:LEU:HD23	2.08	0.54
2:D:228:ASP:HB3	2:D:230:ASP:OD1	2.08	0.54
1:G:259:VAL:HG21	1:G:340:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:TRP:HB2	2:H:438:LEU:HD23	1.90	0.53
1:C:230:ASP:OD1	1:C:378:HIS:CD2	2.61	0.53
1:A:167:VAL:HG11	1:A:397:LEU:HD13	1.91	0.53
1:E:292:GLY:N	1:E:293:PRO:CD	2.72	0.53
1:G:227:MET:HE1	1:G:233:PHE:CZ	2.42	0.53
1:A:173:LEU:O	1:A:176:ILE:HG22	2.09	0.53
2:B:292:GLY:N	2:B:293:PRO:CD	2.71	0.53
1:C:350:TRP:O	1:C:354:VAL:HG22	2.07	0.53
2:H:302:GLY:O	2:H:306:THR:HG23	2.08	0.53
2:B:265:TRP:HA	2:B:309:LEU:HD23	1.90	0.53
1:A:326:LEU:C	1:A:326:LEU:HD23	2.33	0.53
1:C:266:ILE:O	1:C:266:ILE:HG22	2.08	0.53
2:H:306:THR:HG21	2:H:314:ALA:HA	1.91	0.53
1:G:204:PHE:HA	6:G:503:UDP:H5'1	1.89	0.52
2:F:154:LEU:C	2:F:154:LEU:HD23	2.34	0.52
2:F:414:LEU:HD12	2:F:445:ASP:HB3	1.91	0.52
2:H:230:ASP:OD1	2:H:378:HIS:CD2	2.63	0.52
2:F:224:ILE:N	2:F:224:ILE:HD12	2.24	0.52
1:G:418:THR:HG22	1:G:430:VAL:HG23	1.90	0.52
2:H:259:LEU:O	2:H:328:LEU:HD21	2.10	0.52
1:C:250:LEU:C	1:C:250:LEU:HD23	2.34	0.52
2:D:153:LEU:HD21	2:D:214:LEU:HD23	1.91	0.52
2:D:250:LEU:HD23	2:D:251:VAL:N	2.24	0.52
1:E:354:VAL:HG21	1:E:399:GLN:HG2	1.91	0.52
1:E:204:PHE:HA	6:E:502:UDP:H5'1	1.92	0.52
1:G:196:LEU:O	2:H:427:ILE:HD11	2.10	0.52
1:G:273:PHE:C	1:G:274:LEU:HD23	2.35	0.52
1:A:250:LEU:HD21	1:A:252:MET:HG3	1.91	0.52
1:A:427:VAL:HG21	2:B:197:LEU:HD23	1.92	0.52
2:H:237:LEU:HD23	2:H:237:LEU:O	2.09	0.52
2:F:218:HIS:O	2:F:221:VAL:HG12	2.10	0.52
1:A:414:ILE:HG23	1:A:447:LEU:CD2	2.40	0.51
1:G:292:GLY:N	1:G:293:PRO:CD	2.74	0.51
2:F:153:LEU:HD23	2:F:214:LEU:HD23	1.92	0.51
1:A:274:LEU:HD12	1:A:274:LEU:N	2.26	0.51
2:B:135:TRP:CZ3	2:B:136:LEU:HD23	2.46	0.51
2:H:197:LEU:HD12	2:H:210:MET:SD	2.51	0.51
2:D:291:MET:HE3	2:D:322:ALA:HB1	1.92	0.51
1:E:438:LEU:HD12	2:F:131:GLN:HG2	1.93	0.51
2:H:280:TRP:CH2	2:H:284:LEU:HD22	2.45	0.51
2:F:228:ASP:HB3	2:F:230:ASP:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:THR:HG22	2:H:157:GLY:H	1.76	0.51
1:G:266:ILE:HG22	1:G:266:ILE:O	2.11	0.50
2:F:207:LYS:HG3	2:F:208:LEU:HD12	1.92	0.50
1:C:417:PHE:O	1:C:418:THR:HG23	2.12	0.50
1:G:280:TRP:CH2	1:G:284:LEU:HD22	2.46	0.50
1:C:291:MET:HE1	1:C:305:LEU:HD12	1.92	0.50
1:E:453:ALA:HB1	2:F:141:GLU:HB3	1.93	0.50
1:E:153:LEU:HD12	1:E:221:ILE:HD11	1.94	0.50
1:C:438:LEU:HD23	1:C:438:LEU:H	1.77	0.50
2:D:292:GLY:N	2:D:293:PRO:CD	2.75	0.50
1:E:266:ILE:O	1:E:266:ILE:HG22	2.12	0.49
2:H:156:THR:HG22	2:H:157:GLY:N	2.27	0.49
2:H:263:LYS:HG2	2:H:328:LEU:HD13	1.94	0.49
1:C:292:GLY:N	1:C:293:PRO:CD	2.75	0.49
1:A:275:LEU:HD21	1:A:281:ALA:HB1	1.92	0.49
1:E:150:PRO:O	1:E:152:VAL:HG23	2.11	0.49
1:E:224:LEU:C	1:E:224:LEU:HD23	2.37	0.49
1:G:224:LEU:C	1:G:224:LEU:HD23	2.38	0.49
1:A:292:GLY:N	1:A:293:PRO:CD	2.76	0.49
2:D:358:GLU:O	2:D:361:ILE:HG12	2.12	0.49
1:G:171:TYR:CD2	1:G:397:LEU:HD22	2.48	0.49
2:H:224:ILE:HD12	2:H:224:ILE:N	2.28	0.49
1:C:150:PRO:O	1:C:152:VAL:HG23	2.12	0.49
1:C:327:LEU:HD22	1:C:338:VAL:HG21	1.94	0.49
1:A:291:MET:HE2	1:A:301:ALA:HB1	1.93	0.49
2:B:250:LEU:HD23	2:B:251:VAL:N	2.27	0.49
2:D:289:ALA:N	2:D:290:PRO:CD	2.76	0.49
1:E:353:LEU:HD22	1:E:374:PRO:HG3	1.93	0.49
1:E:289:ALA:N	1:E:290:PRO:CD	2.76	0.49
2:B:208:LEU:HD21	2:B:288:TRP:CG	2.47	0.48
2:F:289:ALA:N	2:F:290:PRO:CD	2.76	0.48
1:E:196:LEU:O	2:F:427:ILE:HD11	2.13	0.48
1:E:252:MET:CE	1:E:268:LEU:HD13	2.38	0.48
1:G:103:PHE:HB3	2:H:425:PRO:HD3	1.94	0.48
1:C:289:ALA:N	1:C:290:PRO:CD	2.77	0.48
2:D:208:LEU:HD13	2:D:285:LEU:HD23	1.95	0.48
1:E:180:ILE:HD11	2:F:180:ILE:HG12	1.96	0.48
2:D:438:LEU:HD12	2:D:438:LEU:H	1.78	0.48
1:E:188:ILE:HG22	1:E:189:GLU:O	2.14	0.48
2:F:250:LEU:HD12	2:F:338:VAL:HG13	1.95	0.48
1:A:180:ILE:HD13	1:A:190:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:446:ILE:N	2:D:446:ILE:HD12	2.28	0.48
2:F:167:ILE:HD12	2:F:167:ILE:H	1.78	0.48
2:F:266:ILE:O	2:F:266:ILE:CG2	2.62	0.48
1:G:177:LYS:HD2	2:H:194:MET:HE3	1.96	0.48
1:G:188:ILE:HG22	1:G:189:GLU:O	2.14	0.48
2:B:417:PHE:CD1	2:B:427:ILE:HD13	2.49	0.48
1:C:156:THR:HG23	1:C:192:TYR:CD1	2.49	0.48
1:E:414:ILE:CG2	1:E:447:LEU:HD11	2.43	0.48
2:F:237:LEU:HD23	2:F:237:LEU:C	2.38	0.48
1:G:456:VAL:HG11	2:H:140:PRO:HB2	1.96	0.48
2:B:237:LEU:O	2:B:237:LEU:HD23	2.14	0.48
1:C:172:LEU:O	1:C:176:ILE:HG12	2.13	0.48
1:G:205:TRP:CD2	1:G:292:GLY:HA3	2.48	0.48
1:A:154:LEU:HD21	1:A:227:MET:HB3	1.96	0.47
1:C:221:ILE:C	1:C:221:ILE:HD12	2.39	0.47
2:D:208:LEU:HD11	2:D:288:TRP:CD2	2.48	0.47
2:H:448:ARG:HG3	2:H:448:ARG:HH11	1.79	0.47
2:F:414:LEU:C	2:F:414:LEU:HD23	2.39	0.47
1:A:350:TRP:O	1:A:354:VAL:HG13	2.15	0.47
1:E:225:TRP:HA	1:E:274:LEU:HD23	1.96	0.47
1:E:153:LEU:C	1:E:153:LEU:HD23	2.39	0.47
2:H:154:LEU:HD11	2:H:227:MET:HB3	1.97	0.47
1:C:291:MET:HE3	1:C:301:ALA:HB1	1.97	0.47
1:G:268:LEU:O	1:G:268:LEU:HD12	2.13	0.47
2:H:289:ALA:N	2:H:290:PRO:CD	2.78	0.47
1:A:118:TYR:CZ	1:A:201:MET:HE2	2.50	0.47
2:B:197:LEU:HD12	2:B:210:MET:SD	2.54	0.47
2:B:230:ASP:OD1	2:B:378:HIS:CD2	2.67	0.47
1:E:91:SER:O	2:F:393:VAL:HG22	2.15	0.47
1:E:102:ILE:HG21	2:F:171:TYR:OH	2.13	0.47
1:G:92:ASN:HA	2:H:393:VAL:HG13	1.96	0.47
1:G:207:LYS:HG3	1:G:208:LEU:HD12	1.97	0.47
1:A:250:LEU:C	1:A:250:LEU:HD23	2.40	0.47
2:D:270:THR:HG22	2:D:270:THR:O	2.15	0.47
1:A:289:ALA:N	1:A:290:PRO:HD3	2.30	0.47
2:H:250:LEU:HD12	2:H:274:LEU:O	2.14	0.47
1:A:182:TYR:HB2	1:A:236:MET:HE1	1.96	0.47
1:A:289:ALA:N	1:A:290:PRO:CD	2.77	0.47
1:G:268:LEU:HG	1:G:324:VAL:HG22	1.96	0.47
2:B:233:PHE:O	2:B:407:ALA:HB2	2.15	0.46
2:H:356:ARG:O	2:H:360:MET:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:448:ARG:HH11	2:H:448:ARG:CG	2.29	0.46
1:C:127:TRP:HZ3	2:D:438:LEU:HD11	1.78	0.46
1:G:353:LEU:HD22	1:G:374:PRO:HG3	1.98	0.46
1:G:350:TRP:O	1:G:354:VAL:HG22	2.16	0.46
1:C:196:LEU:HD22	1:C:206:ALA:HB2	1.98	0.46
2:F:357:TYR:HA	2:F:360:MET:HE3	1.97	0.46
1:G:99:ILE:HG23	1:G:102:ILE:HD12	1.97	0.46
1:G:252:MET:CE	1:G:268:LEU:HD13	2.44	0.46
1:A:284:LEU:C	1:A:284:LEU:HD23	2.41	0.46
2:B:250:LEU:HD12	2:B:275:LEU:HD13	1.97	0.46
1:E:268:LEU:C	1:E:268:LEU:HD12	2.41	0.46
2:H:191:VAL:HG21	2:H:214:LEU:HD13	1.96	0.46
1:A:314:VAL:HG13	1:A:314:VAL:O	2.15	0.46
1:C:167:VAL:O	1:C:167:VAL:HG22	2.15	0.46
2:D:365:HIS:CE1	2:D:368:LEU:HD11	2.50	0.46
2:F:292:GLY:N	2:F:293:PRO:CD	2.79	0.46
1:A:266:ILE:HG22	1:A:266:ILE:O	2.16	0.46
1:G:320:GLN:O	1:G:324:VAL:HG23	2.15	0.46
1:G:350:TRP:O	1:G:354:VAL:HG13	2.16	0.46
1:E:250:LEU:HD12	1:E:275:LEU:HD13	1.98	0.45
2:F:250:LEU:HD13	2:F:250:LEU:C	2.41	0.45
1:G:177:LYS:CD	2:H:194:MET:HE3	2.46	0.45
1:G:417:PHE:CG	2:H:197:LEU:HD22	2.51	0.45
2:D:121:LEU:HD22	2:D:209:PRO:HA	1.97	0.45
1:C:124:ILE:HG12	2:D:435:VAL:HG13	1.98	0.45
1:C:154:LEU:C	1:C:154:LEU:HD23	2.41	0.45
1:C:334:TRP:O	1:C:338:VAL:HG23	2.16	0.45
1:E:259:VAL:HG11	1:E:340:LEU:HD21	1.97	0.45
2:H:427:ILE:HD12	2:H:427:ILE:C	2.41	0.45
1:A:226:TRP:HH2	6:A:503:UDP:H1'	1.81	0.45
2:B:346:LEU:O	2:B:346:LEU:HD23	2.17	0.45
1:C:431:ARG:NH1	1:C:440:MET:HE1	2.32	0.45
2:H:292:GLY:N	2:H:293:PRO:CD	2.79	0.45
1:E:240:LEU:HD12	1:E:242:TRP:CZ2	2.52	0.45
1:E:454:VAL:O	1:E:455:LYS:C	2.59	0.45
1:A:150:PRO:O	1:A:152:VAL:HG23	2.17	0.45
2:D:326:LEU:C	2:D:326:LEU:HD13	2.42	0.45
2:F:435:VAL:HG12	2:F:435:VAL:O	2.17	0.45
1:G:250:LEU:HD21	1:G:252:MET:SD	2.55	0.45
1:A:202:ALA:H	1:A:298:ARG:HH22	1.65	0.45
2:B:237:LEU:HD23	2:B:237:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:VAL:HG22	1:G:167:VAL:O	2.17	0.45
1:A:354:VAL:HG23	1:A:355:ASP:N	2.32	0.45
2:B:250:LEU:HD23	2:B:250:LEU:C	2.41	0.45
1:E:153:LEU:CD1	1:E:221:ILE:HD11	2.47	0.45
2:H:205:TRP:CE2	2:H:292:GLY:HA2	2.52	0.45
2:H:208:LEU:HD11	2:H:288:TRP:CE3	2.52	0.45
2:B:353:LEU:HD13	2:B:374:PRO:HB3	1.98	0.44
1:C:96:THR:O	1:C:96:THR:HG22	2.16	0.44
1:E:231:ALA:HA	1:E:378:HIS:HA	1.98	0.44
1:E:350:TRP:O	1:E:354:VAL:HG22	2.17	0.44
2:H:435:VAL:HG12	2:H:435:VAL:O	2.17	0.44
2:B:287:ALA:CB	2:B:326:LEU:HD11	2.43	0.44
2:B:326:LEU:HD23	2:B:326:LEU:C	2.43	0.44
2:H:173:LEU:O	2:H:176:VAL:HG12	2.17	0.44
2:H:263:LYS:CG	2:H:328:LEU:HD13	2.46	0.44
1:C:253:HIS:HB2	1:C:346:LEU:HB3	1.98	0.44
2:B:156:THR:HG23	2:B:192:TYR:CD2	2.53	0.44
1:C:314:VAL:HG13	1:C:314:VAL:O	2.18	0.44
2:F:413:LYS:HE2	2:F:446:ILE:HD11	2.00	0.44
2:D:365:HIS:NE2	2:D:368:LEU:HD11	2.32	0.44
1:G:375:LEU:HG	1:G:376:VAL:HG23	2.00	0.44
2:H:365:HIS:NE2	2:H:368:LEU:HD21	2.32	0.44
2:H:237:LEU:HD23	2:H:237:LEU:C	2.43	0.44
2:B:446:ILE:HD12	2:B:447:ARG:N	2.32	0.44
2:B:260:PHE:HZ	2:B:335:MET:HE2	1.82	0.43
2:F:153:LEU:HD11	2:F:191:VAL:HG23	1.99	0.43
1:A:185:LEU:HD11	1:A:446:LEU:HB3	2.00	0.43
1:C:291:MET:HE1	1:C:305:LEU:HD11	1.98	0.43
1:C:427:VAL:HG12	1:C:428:LYS:N	2.33	0.43
2:D:153:LEU:HD11	2:D:191:VAL:CG2	2.30	0.43
2:D:228:ASP:CB	2:D:230:ASP:OD1	2.66	0.43
2:D:354:VAL:HG23	2:D:355:ASP:N	2.33	0.43
2:D:346:LEU:O	2:D:346:LEU:HD23	2.18	0.43
2:D:368:LEU:HD23	2:D:372:ARG:CZ	2.48	0.43
2:F:240:ILE:HD13	2:F:274:LEU:HD11	1.99	0.43
1:G:289:ALA:N	1:G:290:PRO:CD	2.82	0.43
2:H:289:ALA:N	2:H:290:PRO:HD3	2.33	0.43
1:A:102:ILE:HD11	2:B:397:LEU:HD13	2.00	0.43
2:B:447:ARG:HG3	2:B:448:ARG:HG3	2.00	0.43
1:C:284:LEU:C	1:C:284:LEU:HD23	2.44	0.43
2:D:156:THR:HG22	2:D:157:GLY:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:250:LEU:HD22	2:F:274:LEU:O	2.18	0.43
2:B:168:GLY:O	2:B:172:LEU:HD13	2.18	0.43
2:D:183:CYS:HB2	2:D:190:ILE:HD11	1.99	0.43
2:B:289:ALA:N	2:B:290:PRO:CD	2.82	0.43
1:G:454:VAL:HG12	1:G:455:LYS:N	2.33	0.43
1:A:180:ILE:HD11	2:B:180:ILE:HG12	2.01	0.43
1:C:453:ALA:HB1	2:D:141:GLU:HB2	2.01	0.43
2:D:265:TRP:NE1	2:D:266:ILE:HG23	2.34	0.43
2:F:353:LEU:HD13	2:F:374:PRO:HB3	2.00	0.43
2:F:427:ILE:HD12	2:F:427:ILE:C	2.44	0.43
1:E:107:GLY:H	2:F:420:ARG:HB3	1.84	0.43
1:G:213:LYS:O	1:G:216:LEU:HG	2.19	0.43
1:A:204:PHE:HA	6:A:503:UDP:H5'1	2.00	0.42
2:B:240:ILE:HD13	2:B:274:LEU:HD11	2.00	0.42
1:C:171:TYR:CD2	1:C:397:LEU:HD22	2.54	0.42
2:H:408:ASP:O	2:H:412:LEU:HG	2.18	0.42
2:B:173:LEU:O	2:B:176:VAL:HG12	2.19	0.42
2:B:350:TRP:CD1	2:B:379:PHE:HA	2.55	0.42
1:A:375:LEU:HG	1:A:376:VAL:HG23	2.00	0.42
2:B:132:ARG:NH1	2:B:277:ASN:O	2.52	0.42
1:C:250:LEU:HD22	1:C:338:VAL:HG13	2.00	0.42
6:D:502:UDP:O1A	6:D:502:UDP:O1B	2.36	0.42
1:E:364:TYR:CG	1:E:372:ARG:HG2	2.55	0.42
2:F:446:ILE:N	2:F:446:ILE:HD12	2.35	0.42
1:G:91:SER:O	2:H:393:VAL:HG22	2.19	0.42
1:E:357:TYR:O	1:E:361:ILE:HG23	2.20	0.42
2:F:297:ILE:HD12	2:F:297:ILE:H	1.83	0.42
1:G:120:LEU:HD23	1:G:212:ARG:HD2	2.01	0.42
2:B:121:LEU:HD11	2:B:285:LEU:O	2.20	0.42
2:F:183:CYS:SG	2:F:190:ILE:HD11	2.59	0.42
2:B:326:LEU:O	2:B:329:SER:O	2.37	0.42
2:H:155:LEU:HD22	2:H:226:TRP:HZ3	1.85	0.42
2:B:135:TRP:HZ3	2:B:136:LEU:HD23	1.84	0.42
2:B:151:ARG:HG2	2:B:221:VAL:HA	2.02	0.42
1:C:180:ILE:HD11	2:D:180:ILE:HD11	2.02	0.42
2:B:250:LEU:HD21	2:B:252:ILE:HB	2.02	0.42
2:D:301:ALA:HB3	2:D:317:ALA:HB2	2.01	0.42
1:E:225:TRP:CZ3	1:E:240:LEU:HD11	2.55	0.42
2:F:156:THR:HG23	2:F:192:TYR:CD2	2.55	0.42
2:F:173:LEU:O	2:F:176:VAL:HG12	2.20	0.42
2:F:354:VAL:HG11	2:F:399:SER:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422:LEU:N	1:G:422:LEU:HD22	2.35	0.42
2:H:396:CYS:O	2:H:400:MET:HG2	2.19	0.42
2:H:297:ILE:H	2:H:297:ILE:HD12	1.85	0.42
2:B:263:LYS:HD3	2:B:328:LEU:HD13	2.01	0.41
2:D:272:SER:O	2:D:346:LEU:HD22	2.20	0.41
1:C:224:LEU:C	1:C:224:LEU:HD23	2.45	0.41
1:G:354:VAL:HG23	1:G:355:ASP:N	2.35	0.41
1:G:365:HIS:NE2	1:G:368:LEU:HD21	2.35	0.41
2:H:299:ASP:O	2:H:303:LYS:HG2	2.20	0.41
1:A:120:LEU:HD23	1:A:201:MET:HE1	2.03	0.41
1:C:188:ILE:HG22	1:C:189:GLU:O	2.21	0.41
1:A:181:ASP:O	1:A:182:TYR:C	2.64	0.41
1:C:250:LEU:HD22	1:C:338:VAL:HG22	2.03	0.41
2:D:154:LEU:HD12	2:D:225:TRP:CG	2.56	0.41
1:E:417:PHE:O	1:E:418:THR:HG23	2.21	0.41
2:H:214:LEU:HD23	2:H:214:LEU:N	2.35	0.41
2:H:237:LEU:HA	2:H:446:ILE:HD13	2.02	0.41
1:A:153:LEU:CB	1:A:221:ILE:HD13	2.51	0.41
1:G:120:LEU:HB3	1:G:212:ARG:HD2	2.03	0.41
1:A:192:TYR:HB3	2:B:177:LYS:HG2	2.02	0.41
1:A:284:LEU:HD21	1:A:323:MET:HE1	2.02	0.41
1:A:350:TRP:O	1:A:354:VAL:HG22	2.21	0.41
1:C:391:TYR:HB3	1:C:392:PRO:HD2	2.01	0.41
2:D:225:TRP:CG	2:D:274:LEU:CD2	3.04	0.41
1:E:238:PHE:HD2	1:E:375:LEU:HD13	1.85	0.41
1:E:288:TRP:HA	1:E:326:LEU:HD11	2.03	0.41
1:A:153:LEU:HB2	1:A:221:ILE:HD13	2.03	0.41
1:A:197:LEU:HD23	2:B:417:PHE:CE2	2.55	0.41
1:A:438:LEU:HD11	2:B:131:GLN:OE1	2.21	0.41
2:D:427:ILE:C	2:D:427:ILE:HD12	2.46	0.41
1:E:197:LEU:H	1:E:197:LEU:HD12	1.86	0.41
1:G:237:ALA:HA	1:G:446:LEU:HD21	2.03	0.41
1:C:266:ILE:O	1:C:266:ILE:CG2	2.68	0.41
1:E:209:PRO:O	1:E:210:LEU:C	2.64	0.41
1:E:210:LEU:O	1:E:211:ILE:C	2.63	0.41
2:B:287:ALA:O	2:B:290:PRO:HD2	2.21	0.40
1:E:378:HIS:CG	1:E:380:VAL:HG13	2.56	0.40
1:E:454:VAL:HG12	1:E:455:LYS:HG2	2.03	0.40
2:H:306:THR:HG22	2:H:312:ARG:HG2	2.03	0.40
1:A:211:ILE:O	1:A:212:ARG:C	2.64	0.40
2:D:240:ILE:HD13	2:D:274:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:257:ASP:O	2:F:261:ASP:HB3	2.21	0.40
1:G:263:LYS:HE3	1:G:328:ALA:HB1	2.04	0.40
1:G:268:LEU:HD12	1:G:268:LEU:C	2.46	0.40
2:B:212:ARG:HB2	2:B:285:LEU:HD13	2.04	0.40
2:D:194:MET:HG2	2:D:194:MET:O	2.22	0.40
2:B:134:VAL:O	2:B:137:ASN:OD1	2.40	0.40
1:E:190:ILE:O	2:F:184:ARG:HD3	2.21	0.40
1:G:227:MET:HE1	1:G:233:PHE:CE1	2.56	0.40
1:G:301:ALA:HA	1:G:304:VAL:HG22	2.03	0.40
1:A:92:ASN:HA	2:B:393:VAL:HG13	2.02	0.40
1:A:210:LEU:O	1:A:211:ILE:C	2.64	0.40
1:C:414:ILE:CG2	1:C:447:LEU:HD21	2.52	0.40
1:E:211:ILE:O	1:E:212:ARG:C	2.65	0.40
1:G:216:LEU:HD12	1:G:216:LEU:C	2.47	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	354/420 (84%)	338 (96%)	16 (4%)	0	100	100
1	C	352/420 (84%)	340 (97%)	12 (3%)	0	100	100
1	E	359/420 (86%)	347 (97%)	12 (3%)	0	100	100
1	G	361/420 (86%)	353 (98%)	8 (2%)	0	100	100
2	B	330/387 (85%)	321 (97%)	9 (3%)	0	100	100
2	D	329/387 (85%)	323 (98%)	6 (2%)	0	100	100
2	F	329/387 (85%)	323 (98%)	6 (2%)	0	100	100
2	H	329/387 (85%)	318 (97%)	11 (3%)	0	100	100
All	All	2743/3228 (85%)	2663 (97%)	80 (3%)	0	100	100



There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/364 (86%)	307 (98%)	5 (2%)	55	75
1	C	313/364 (86%)	309 (99%)	4 (1%)	61	78
1	E	317/364 (87%)	312 (98%)	5 (2%)	55	75
1	G	319/364 (88%)	316 (99%)	3 (1%)	70	81
2	B	294/342 (86%)	291 (99%)	3 (1%)	68	80
2	D	293/342 (86%)	291 (99%)	2 (1%)	76	83
2	F	293/342 (86%)	291 (99%)	2 (1%)	76	83
2	H	293/342 (86%)	289 (99%)	4 (1%)	59	77
All	All	2434/2824 (86%)	2406 (99%)	28 (1%)	63	79

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	PHE
1	A	294	LYS
1	A	299	GLU
1	A	326	LEU
1	A	332	ASP
2	B	220	GLU
2	B	329	SER
2	B	365	HIS
1	C	115	ASN
1	C	204	PHE
1	C	315	PHE
1	C	370	ASP
2	D	370	ASP
2	D	447	ARG
1	E	178	ASN
1	E	347	HIS

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Mol	Chain	Res	Type
1	E	383	LYS
1	E	410	GLN
1	E	413	GLN
2	F	274	LEU
2	F	433	GLU
1	G	204	PHE
1	G	269	ASN
1	G	274	LEU
2	H	370	ASP
2	H	383	LYS
2	H	396	CYS
2	H	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	448	HIS
2	B	419	HIS
1	C	413	GLN
2	D	131	GLN
1	E	115	ASN
1	E	279	GLN
1	G	249	ASN
1	G	269	ASN

### 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 ⓘ

6 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$
3	BGC	K	1	3	12,12,12	2.09	4 (33%)	17,17,17	0.71	0
3	BGC	K	2	3	11,11,12	2.71	5 (45%)	15,15,17	1.95	3 (20%)
3	BGC	K	3	3	11,11,12	1.81	2 (18%)	15,15,17	1.51	3 (20%)
3	BGC	K	4	3	11,11,12	1.61	3 (27%)	15,15,17	1.69	2 (13%)
3	BGC	K	5	3	11,11,12	1.84	4 (36%)	15,15,17	1.98	3 (20%)
3	BGC	K	6	3	11,11,12	1.47	2 (18%)	15,15,17	1.66	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	K	1	3	-	2/2/22/22	0/1/1/1
3	BGC	K	2	3	-	0/2/19/22	0/1/1/1
3	BGC	K	3	3	-	0/2/19/22	0/1/1/1
3	BGC	K	4	3	-	2/2/19/22	0/1/1/1
3	BGC	K	5	3	-	0/2/19/22	0/1/1/1
3	BGC	K	6	3	-	0/2/19/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2	BGC	O5-C5	6.34	1.55	1.43
3	K	3	BGC	O5-C1	4.49	1.51	1.43
3	K	1	BGC	O5-C5	4.12	1.54	1.44
3	K	4	BGC	O5-C1	3.71	1.49	1.43
3	K	6	BGC	O5-C1	3.41	1.49	1.43
3	K	5	BGC	O5-C1	3.38	1.49	1.43
3	K	2	BGC	C2-C3	-3.37	1.47	1.52
3	K	1	BGC	C6-C5	-3.19	1.41	1.51
3	K	3	BGC	O5-C5	2.91	1.49	1.43
3	K	5	BGC	O5-C5	2.86	1.49	1.43
3	K	2	BGC	O2-C2	2.43	1.48	1.43
3	K	5	BGC	C2-C3	-2.41	1.48	1.52
3	K	6	BGC	O5-C5	2.30	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2	BGC	O3-C3	2.23	1.48	1.43
3	K	1	BGC	C4-C5	2.22	1.57	1.53
3	K	4	BGC	O5-C5	2.19	1.47	1.43
3	K	2	BGC	C6-C5	-2.13	1.44	1.51
3	K	5	BGC	O3-C3	2.13	1.48	1.43
3	K	1	BGC	O3-C3	2.12	1.48	1.43
3	K	4	BGC	C2-C3	-2.04	1.49	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	5	BGC	C1-O5-C5	6.13	120.40	112.19
3	K	2	BGC	C1-O5-C5	5.51	119.57	112.19
3	K	4	BGC	C1-C2-C3	4.67	116.44	109.64
3	K	3	BGC	C1-C2-C3	4.06	115.55	109.64
3	K	6	BGC	C3-C4-C5	3.81	117.14	110.23
3	K	2	BGC	C3-C4-C5	3.26	116.15	110.23
3	K	4	BGC	C2-C3-C4	2.92	115.99	110.86
3	K	2	BGC	O4-C4-C3	-2.62	104.19	110.38
3	K	3	BGC	C1-O5-C5	2.60	115.68	112.19
3	K	6	BGC	C1-O5-C5	-2.54	108.78	112.19
3	K	6	BGC	C2-C3-C4	2.51	115.28	110.86
3	K	3	BGC	O5-C1-C2	2.48	116.69	110.79
3	K	6	BGC	C1-C2-C3	2.41	113.15	109.64
3	K	5	BGC	O5-C1-C2	2.31	116.29	110.79
3	K	5	BGC	O5-C5-C4	2.29	116.40	110.83

There are no chirality outliers.

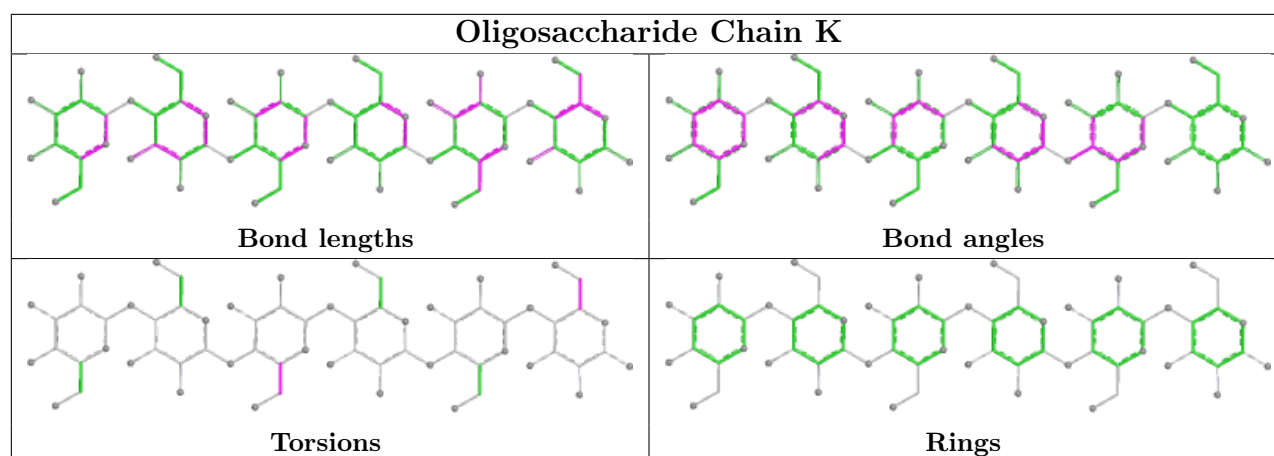
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	4	BGC	O5-C5-C6-O6
3	K	4	BGC	C4-C5-C6-O6
3	K	1	BGC	O5-C5-C6-O6
3	K	1	BGC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

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	$\# Z  > 2$
4	GOL	G	501	-	5,5,5	0.36	0	5,5,5	0.39	0
6	UDP	H	502	5	25,26,26	0.47	0	38,40,40	0.62	1 (2%)
6	UDP	G	503	5	25,26,26	0.49	0	38,40,40	0.62	1 (2%)
6	UDP	F	502	5	25,26,26	0.47	0	38,40,40	0.61	1 (2%)
6	UDP	C	502	5	25,26,26	0.36	0	38,40,40	0.62	1 (2%)
6	UDP	D	502	5	25,26,26	0.45	0	38,40,40	0.61	1 (2%)
6	UDP	A	503	5	25,26,26	0.43	0	38,40,40	0.64	1 (2%)
6	UDP	B	502	5	25,26,26	0.42	0	38,40,40	0.60	1 (2%)
4	GOL	A	501	-	5,5,5	0.35	0	5,5,5	0.57	0
6	UDP	E	502	5	25,26,26	0.40	0	38,40,40	0.62	1 (2%)

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
4	GOL	G	501	-	-	0/4/4/4	-
6	UDP	H	502	5	-	9/16/32/32	0/2/2/2
6	UDP	G	503	5	-	0/16/32/32	0/2/2/2
6	UDP	F	502	5	-	5/16/32/32	0/2/2/2
6	UDP	C	502	5	-	4/16/32/32	0/2/2/2
6	UDP	D	502	5	-	3/16/32/32	0/2/2/2
6	UDP	A	503	5	-	2/16/32/32	0/2/2/2
6	UDP	B	502	5	-	6/16/32/32	0/2/2/2
4	GOL	A	501	-	-	0/4/4/4	-
6	UDP	E	502	5	-	5/16/32/32	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	503	UDP	O3B-PB-O3A	2.23	112.11	104.64
6	E	502	UDP	O3B-PB-O3A	2.23	112.10	104.64
6	H	502	UDP	O3B-PB-O3A	2.22	112.07	104.64
6	D	502	UDP	O3B-PB-O3A	2.22	112.07	104.64
6	C	502	UDP	O3B-PB-O3A	2.21	112.06	104.64
6	F	502	UDP	O3B-PB-O3A	2.20	112.01	104.64
6	B	502	UDP	O3B-PB-O3A	2.20	112.01	104.64
6	G	503	UDP	O3B-PB-O3A	2.19	111.99	104.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	503	UDP	PB-O3A-PA-O5'
6	B	502	UDP	C3'-C4'-C5'-O5'
6	B	502	UDP	O4'-C4'-C5'-O5'
6	B	502	UDP	C5'-O5'-PA-O2A
6	B	502	UDP	C5'-O5'-PA-O3A
6	E	502	UDP	C4'-C5'-O5'-PA
6	E	502	UDP	C5'-O5'-PA-O3A
6	F	502	UDP	C5'-O5'-PA-O2A
6	F	502	UDP	C5'-O5'-PA-O3A
6	H	502	UDP	C5'-O5'-PA-O1A
6	H	502	UDP	C5'-O5'-PA-O2A
6	H	502	UDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
6	C	502	UDP	C3'-C4'-C5'-O5'
6	C	502	UDP	O4'-C4'-C5'-O5'
6	D	502	UDP	O4'-C4'-C5'-O5'
6	E	502	UDP	O4'-C4'-C5'-O5'
6	F	502	UDP	O4'-C4'-C5'-O5'
6	E	502	UDP	C3'-C4'-C5'-O5'
6	F	502	UDP	C3'-C4'-C5'-O5'
6	D	502	UDP	C3'-C4'-C5'-O5'
6	B	502	UDP	C4'-C5'-O5'-PA
6	F	502	UDP	C4'-C5'-O5'-PA
6	H	502	UDP	C3'-C4'-C5'-O5'
6	D	502	UDP	PA-O3A-PB-O2B
6	H	502	UDP	O4'-C4'-C5'-O5'
6	C	502	UDP	C5'-O5'-PA-O1A
6	E	502	UDP	C5'-O5'-PA-O1A
6	H	502	UDP	C4'-C5'-O5'-PA
6	H	502	UDP	C2'-C1'-N1-C6
6	A	503	UDP	O4'-C4'-C5'-O5'
6	H	502	UDP	O4'-C1'-N1-C6
6	C	502	UDP	C4'-C5'-O5'-PA
6	H	502	UDP	O4'-C1'-N1-C2
6	B	502	UDP	PB-O3A-PA-O1A

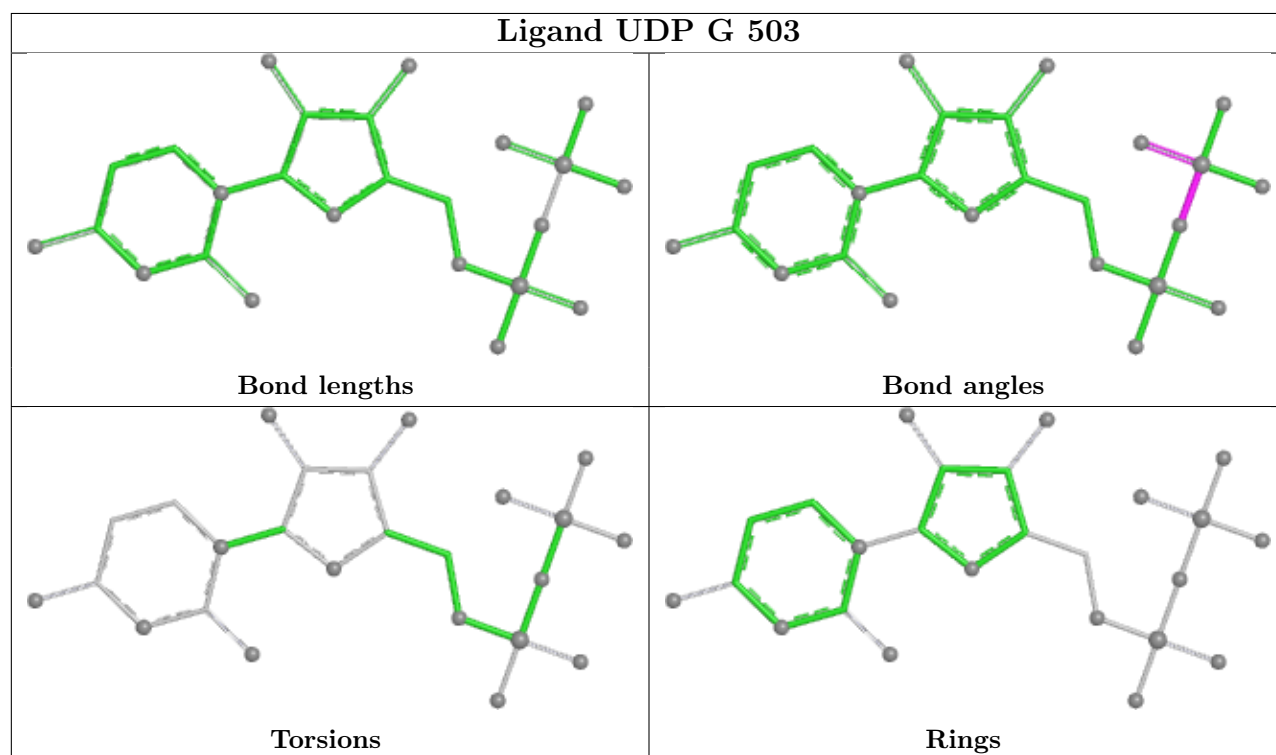
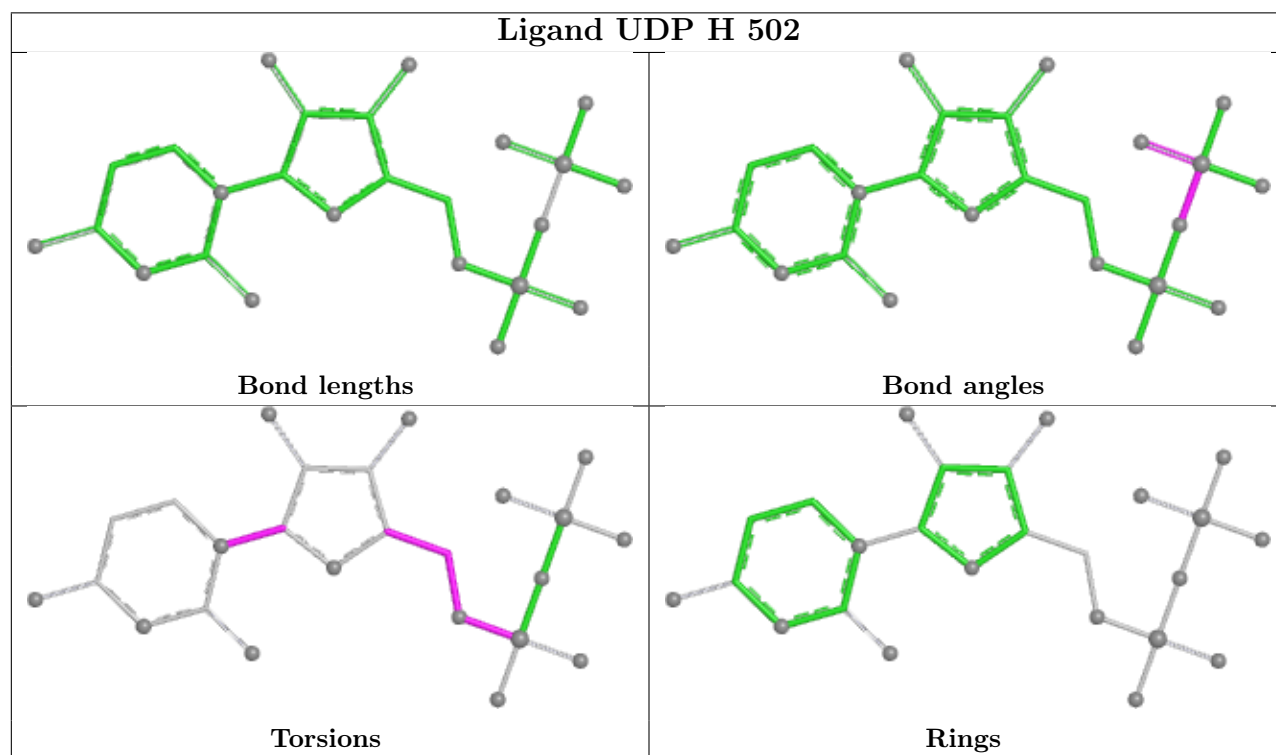
There are no ring outliers.

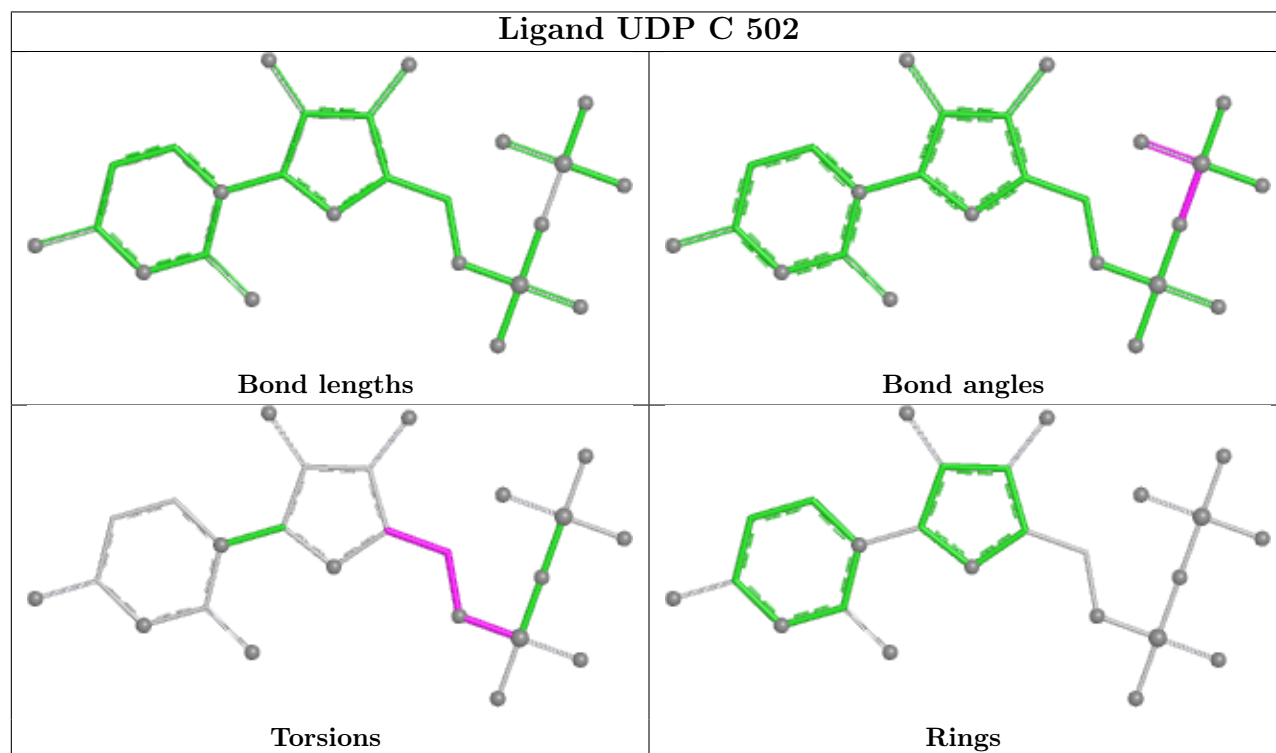
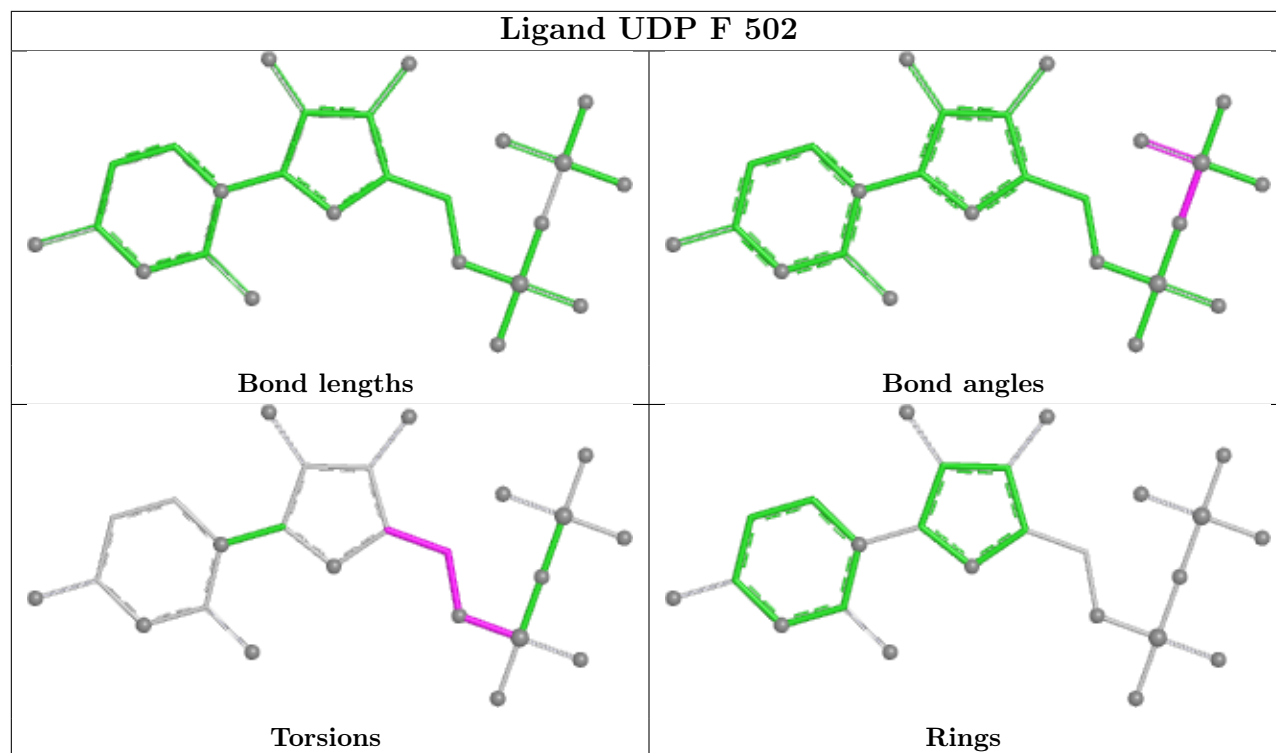
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	503	UDP	1	0
6	D	502	UDP	1	0
6	A	503	UDP	2	0
6	E	502	UDP	1	0

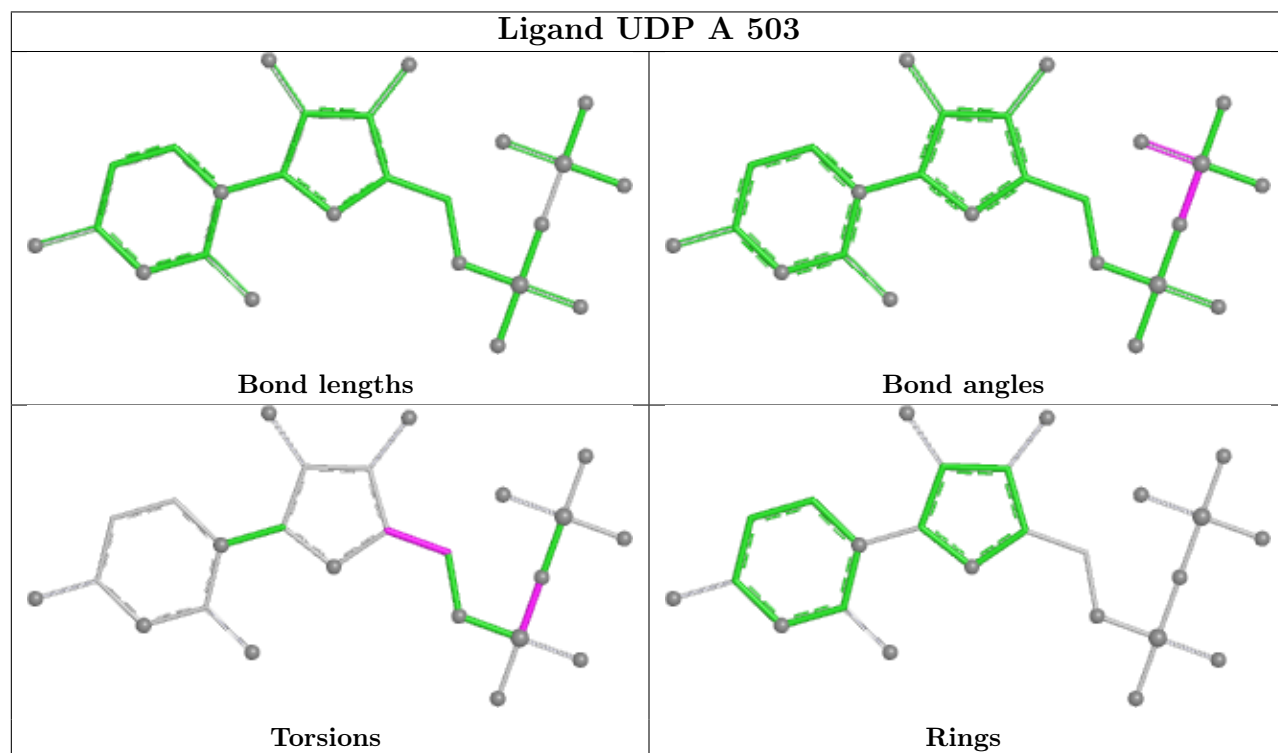
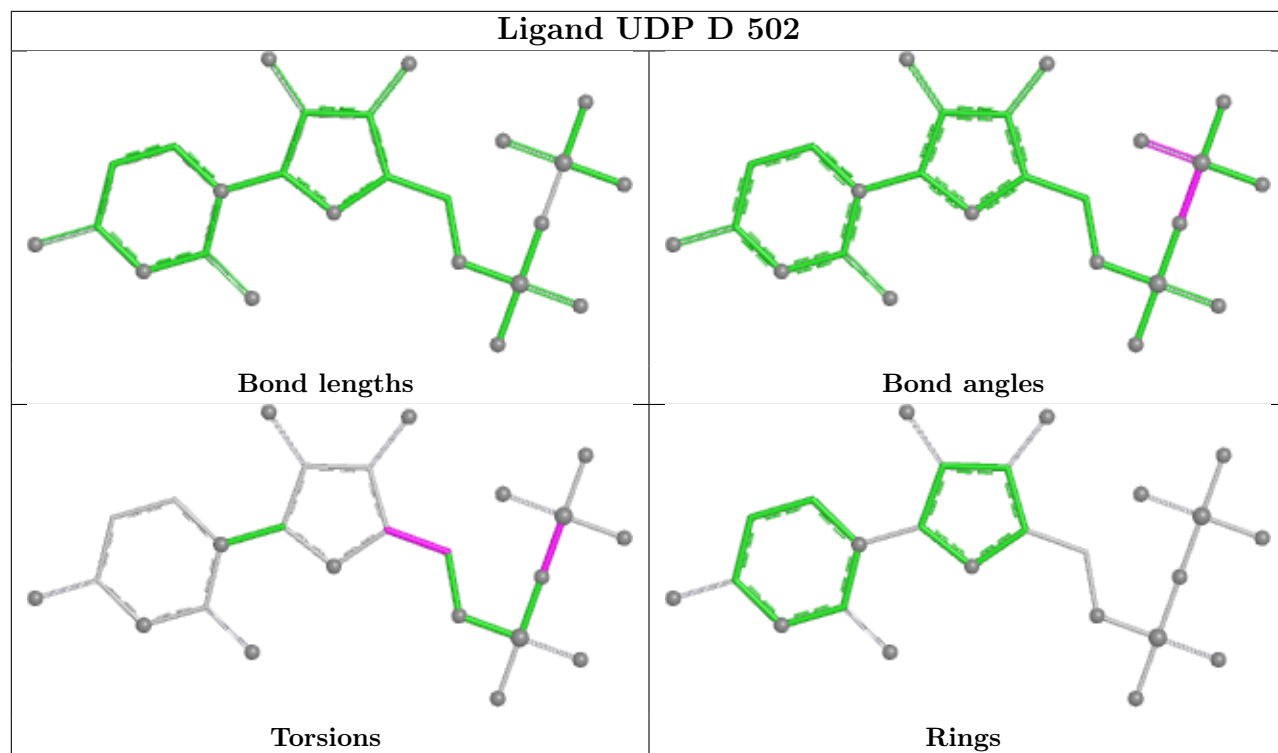
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

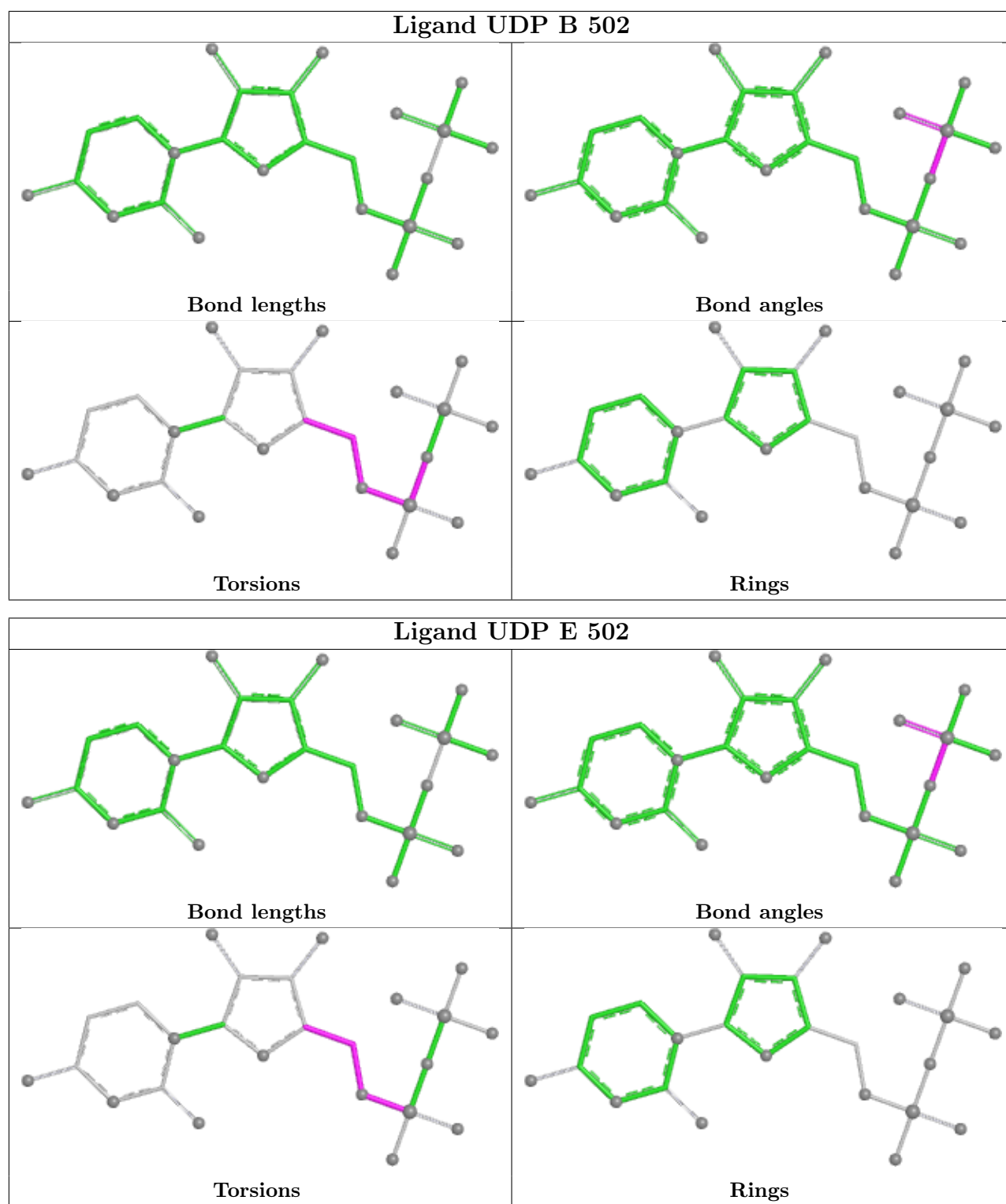
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	358/420 (85%)	0.34	9 (2%) 58 39	39, 72, 117, 173	0
1	C	358/420 (85%)	0.38	10 (2%) 55 35	44, 77, 125, 175	0
1	E	363/420 (86%)	0.40	11 (3%) 52 33	37, 78, 123, 145	0
1	G	365/420 (86%)	0.34	8 (2%) 62 42	38, 76, 126, 159	0
2	B	332/387 (85%)	0.36	7 (2%) 63 43	48, 80, 119, 172	0
2	D	331/387 (85%)	0.31	7 (2%) 63 43	46, 72, 108, 141	0
2	F	331/387 (85%)	0.25	6 (1%) 67 48	44, 71, 106, 149	0
2	H	331/387 (85%)	0.36	13 (3%) 43 27	48, 78, 114, 156	0
All	All	2769/3228 (85%)	0.34	71 (2%) 57 37	37, 76, 119, 175	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	GLY	7.1
2	B	208	LEU	4.8
2	H	267	ALA	4.7
1	C	254	GLY	4.5
1	A	264	ASN	3.7
2	D	243	ALA	3.4
1	A	327	LEU	3.3
2	D	261	ASP	3.2
2	H	212	ARG	3.2
1	E	281	ALA	3.2
2	H	201	LEU	3.1
2	B	201	LEU	3.0
1	G	259	VAL	3.0
2	B	368	LEU	3.0
1	A	285	LEU	3.0
2	F	266	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	332	ASP	2.9
1	G	403	ALA	2.9
1	A	124	ILE	2.8
2	B	450	PRO	2.8
1	C	208	LEU	2.8
1	E	370	ASP	2.7
1	A	417	PHE	2.7
2	B	240	ILE	2.7
1	G	208	LEU	2.7
2	D	167	ILE	2.7
1	E	178	ASN	2.7
1	E	422	LEU	2.6
2	F	340	VAL	2.6
1	C	327	LEU	2.6
2	D	351	GLU	2.6
1	E	327	LEU	2.5
1	G	390	ASP	2.5
2	H	368	LEU	2.5
1	E	251	VAL	2.5
2	H	437	PRO	2.5
1	A	259	VAL	2.5
1	C	289	ALA	2.4
2	B	437	PRO	2.4
1	G	274	LEU	2.4
2	H	268	LEU	2.4
2	D	433	GLU	2.3
1	E	107	GLY	2.3
1	C	107	GLY	2.2
2	H	254	GLY	2.2
2	H	309	LEU	2.2
1	A	388	PHE	2.2
1	C	105	ASP	2.2
1	E	451	PHE	2.2
2	H	447	ARG	2.2
2	F	382	CYS	2.2
2	H	302	GLY	2.2
1	C	251	VAL	2.2
1	E	208	LEU	2.1
2	D	309	LEU	2.1
1	E	274	LEU	2.1
2	H	203	GLY	2.1
2	B	344	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	254	GLY	2.1
2	F	288	TRP	2.1
2	H	307	ALA	2.1
2	F	437	PRO	2.1
1	C	447	LEU	2.1
1	G	289	ALA	2.1
1	G	267	GLY	2.1
1	E	454	VAL	2.0
1	C	425	ARG	2.0
2	H	121	LEU	2.0
1	G	145	ILE	2.0
2	D	176	VAL	2.0
1	C	274	LEU	2.0

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

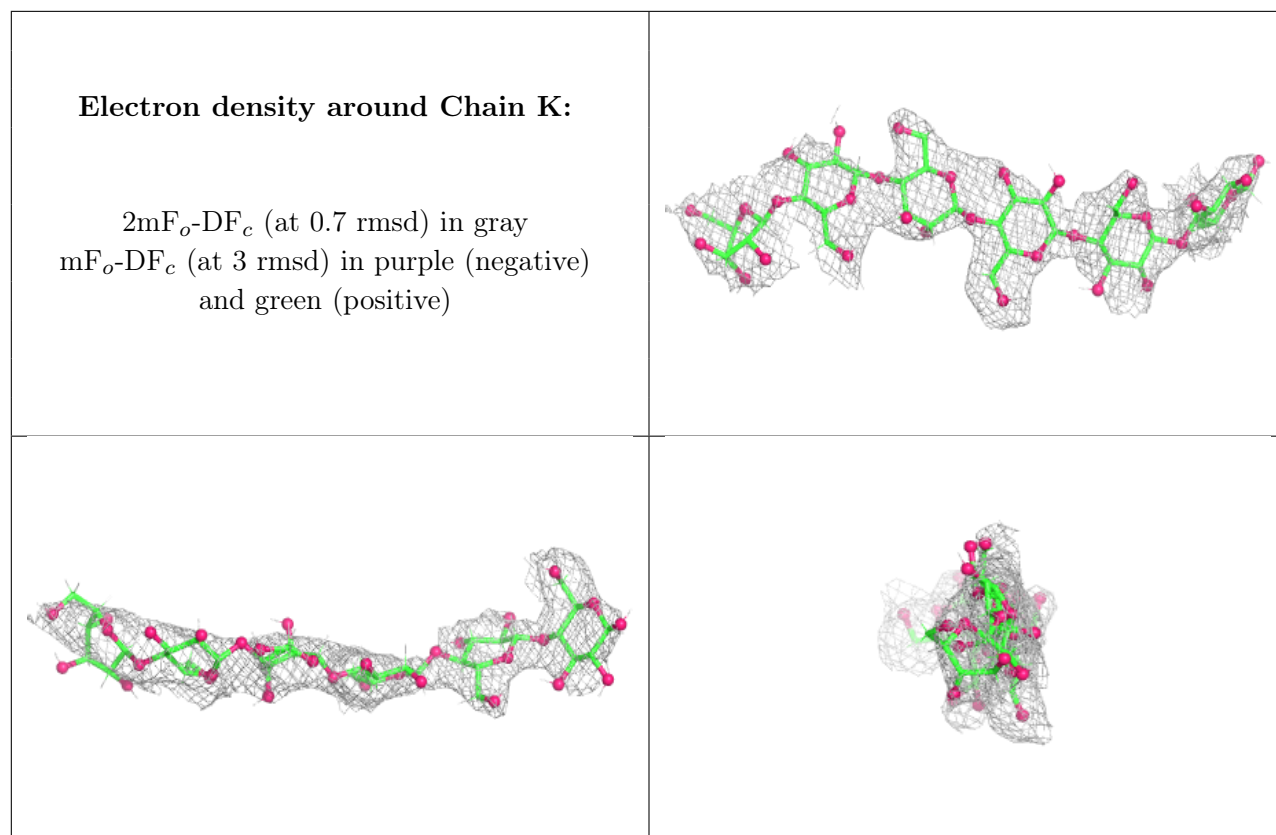
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BGC	K	1	12/12	-	-	59,87,109,120	23
3	BGC	K	2	11/12	-	-	51,82,99,108	21
3	BGC	K	3	11/12	-	-	45,77,96,116	21
3	BGC	K	4	11/12	-	-	73,93,114,138	21
3	BGC	K	5	11/12	-	-	81,97,113,118	21
3	BGC	K	6	11/12	-	-	80,107,134,137	22

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.



## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	UDP	D	502	25/25	0.77	0.16	115,128,155,166	0
6	UDP	H	502	25/25	0.77	0.18	94,114,148,167	0
6	UDP	F	502	25/25	0.83	0.13	77,93,126,142	0
6	UDP	B	502	25/25	0.85	0.15	94,109,141,162	0
6	UDP	A	503	25/25	0.86	0.15	90,104,141,160	0
6	UDP	E	502	25/25	0.86	0.13	69,82,101,114	0
4	GOL	A	501	6/6	0.90	0.10	34,59,77,77	0
4	GOL	G	501	6/6	0.92	0.12	47,60,100,100	0
6	UDP	G	503	25/25	0.92	0.12	85,103,125,136	0
5	MN	H	501	1/1	0.92	0.19	246,246,246,246	0
6	UDP	C	502	25/25	0.93	0.10	74,80,107,116	0
5	MN	A	502	1/1	0.98	0.03	46,46,46,46	0
5	MN	D	501	1/1	0.98	0.04	49,49,49,49	0
5	MN	F	501	1/1	0.98	0.04	77,77,77,77	0

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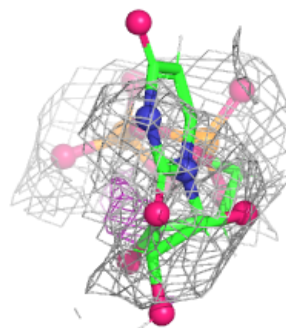
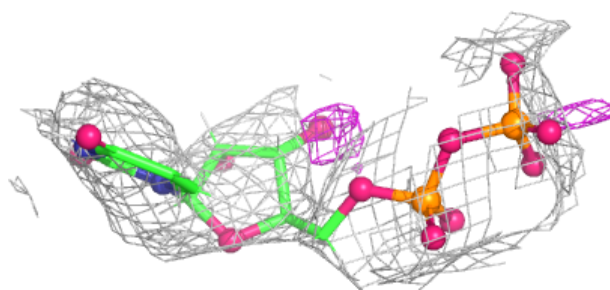
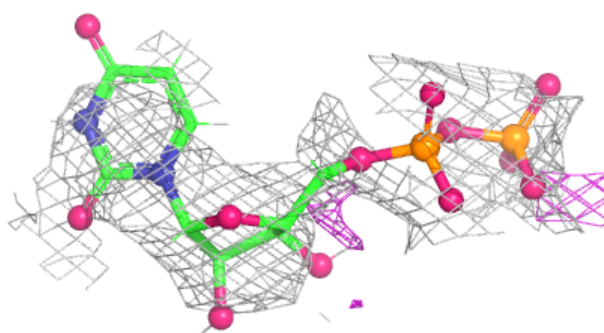
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MN	B	501	1/1	0.99	0.07	66,66,66,66	0
5	MN	E	501	1/1	0.99	0.03	57,57,57,57	0
5	MN	C	501	1/1	0.99	0.04	43,43,43,43	0
5	MN	G	502	1/1	1.00	0.08	60,60,60,60	0

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 D 502:**

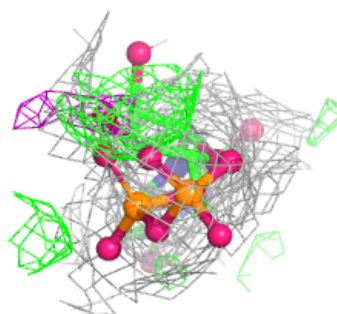
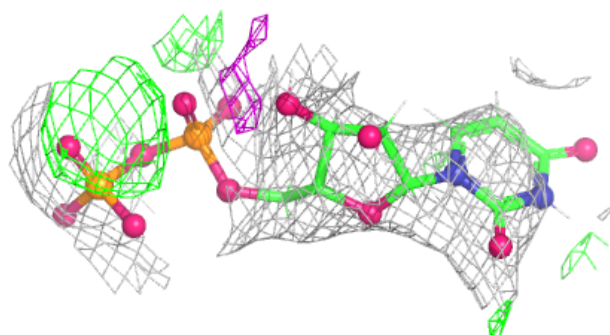
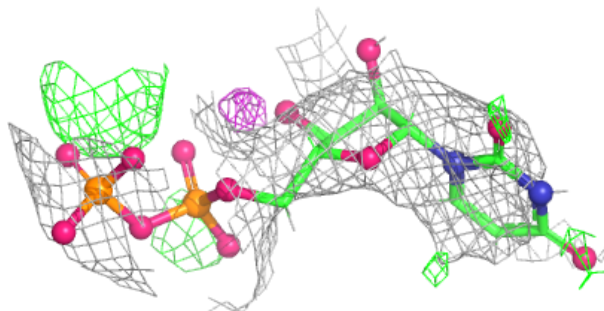
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



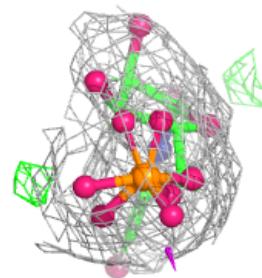
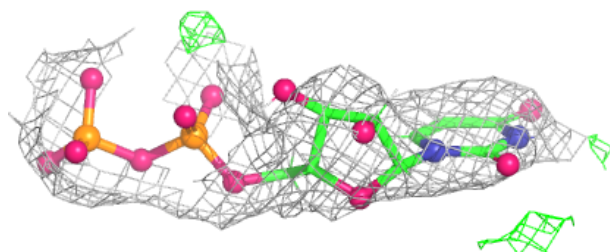
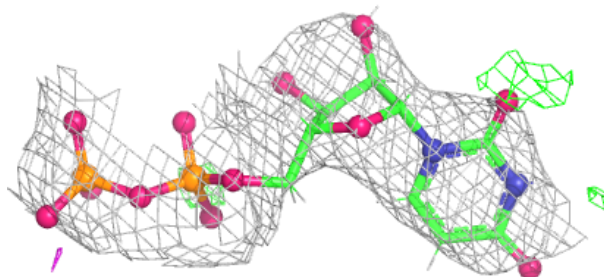


**Electron density around UDP H 502:**

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

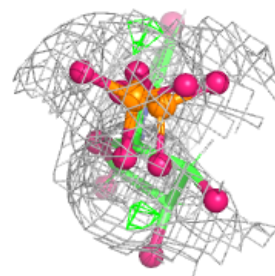
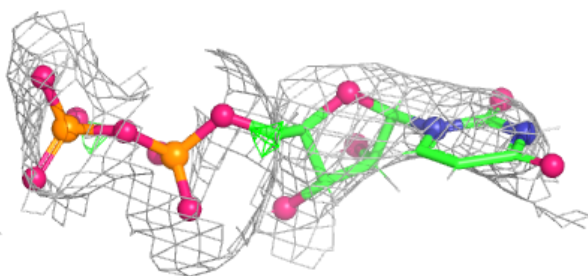
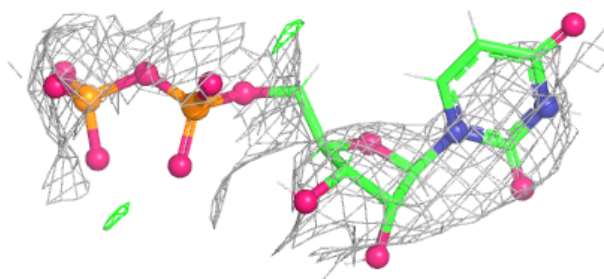
**Electron density around UDP F 502:**

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

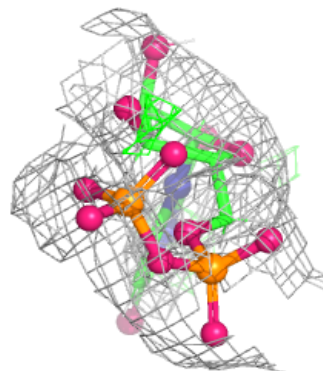
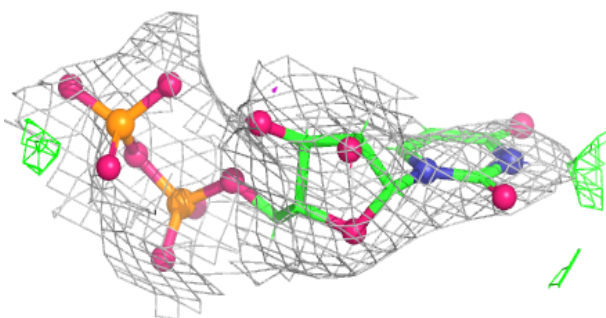
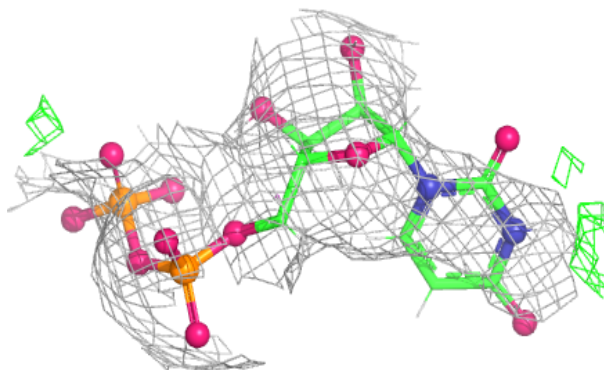


**Electron density around UDP B 502:**

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

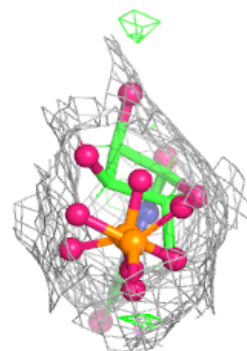
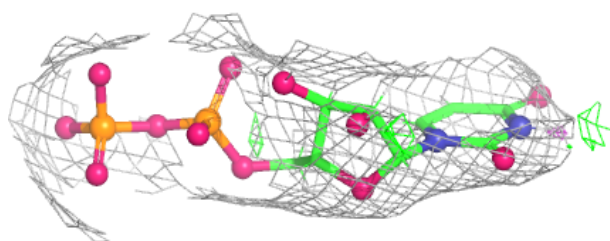
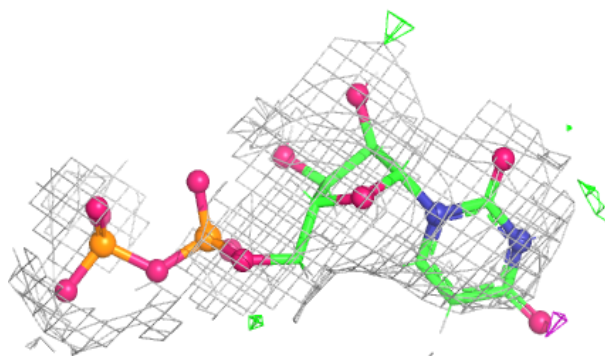
**Electron density around UDP A 503:**

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

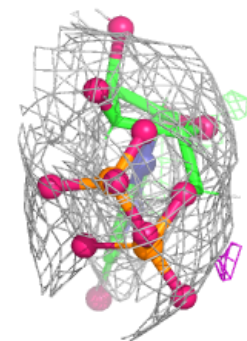
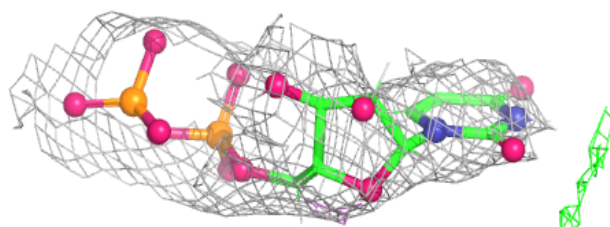
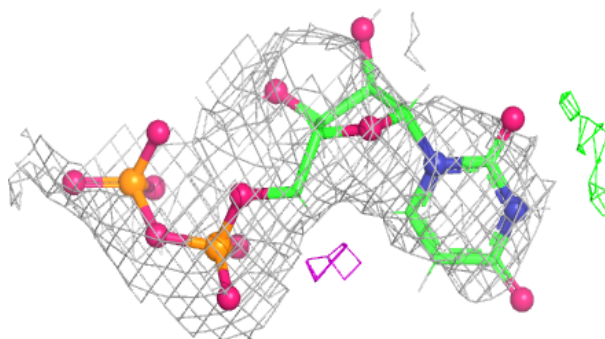


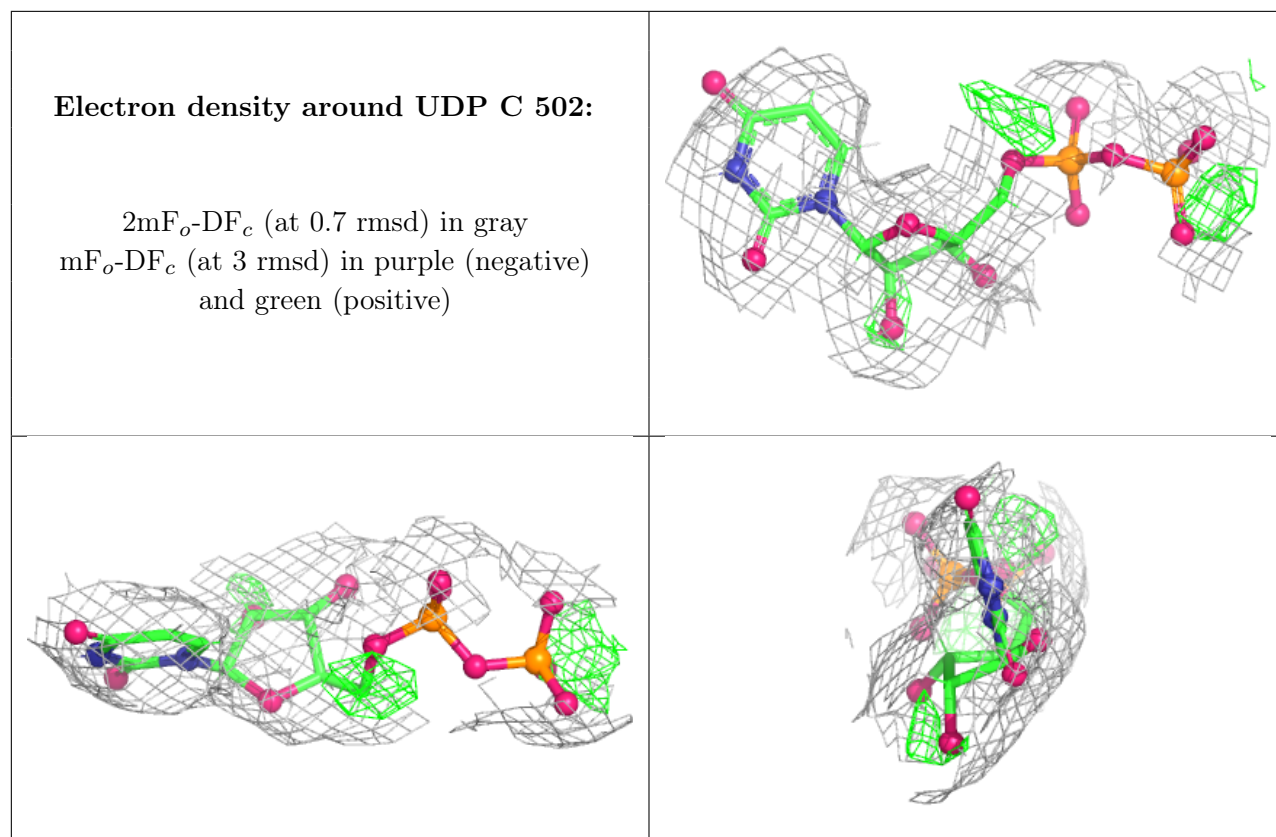
**Electron density around UDP E 502:**

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

**Electron density around UDP G 503:**

$2mF_o - DF_c$  (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.