



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 01:47 PM BST

PDB ID : 6JBR
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

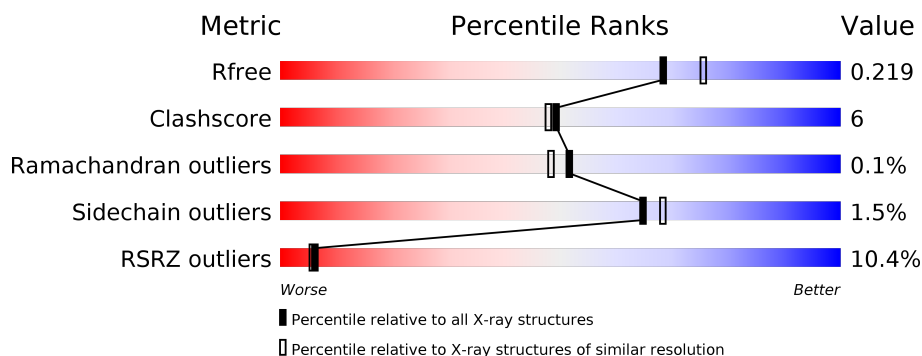
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (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 on 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	<div> <div>5%</div> <div>91%</div> <div>9%</div> </div>
1	B	465	<div> <div>4%</div> <div>92%</div> <div>7%</div> </div>
1	D	465	<div> <div>5%</div> <div>91%</div> <div>8%</div> </div>
1	F	465	<div> <div>13%</div> <div>84%</div> <div>14%</div> </div>
1	H	465	<div> <div>17%</div> <div>86%</div> <div>13%</div> </div>
1	K	465	<div> <div>22%</div> <div>86%</div> <div>13%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	C	1	-	-	-	X
2	GLC	G	1	-	-	-	X
2	GLC	I	1	-	-	-	X
2	GLC	J	1	-	-	-	X
2	GLC	L	1	-	-	-	X
2	GLC	N	1	-	-	-	X
2	GLC	P	1	-	-	-	X

2 Entry composition [i](#)

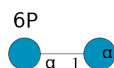
There are 4 unique types of molecules in this entry. The entry contains 32016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.



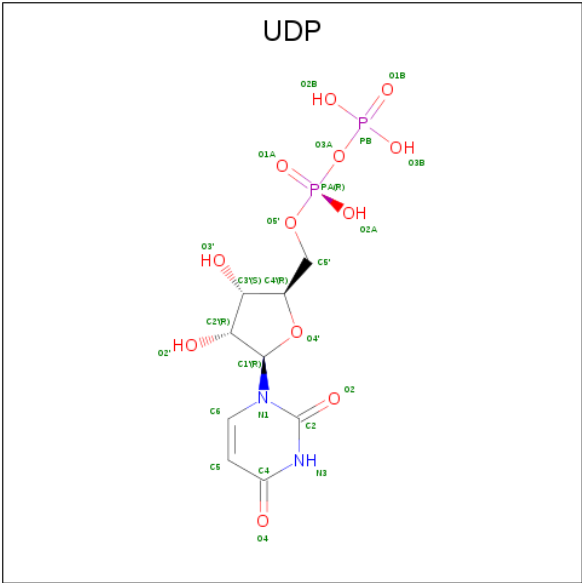
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	P	0	0	0
			27	12	14	1			
2	E	2	Total	C	O	P	0	0	0
			27	12	14	1			
2	G	2	Total	C	O	P	0	0	0
			27	12	14	1			
2	I	2	Total	C	O	P	0	0	0
			27	12	14	1			

Continued on next page...

Continued from previous page...

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 (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	H	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	K	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	M	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

Continued on next page...

Continued from previous page...

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

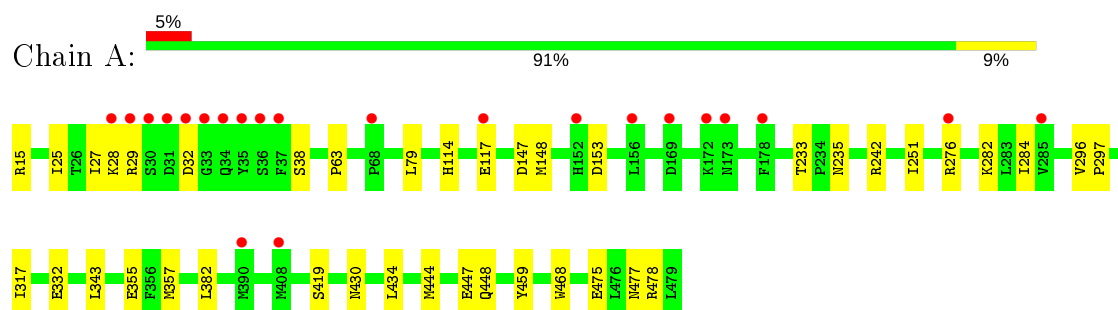
- Molecule 4 is water.

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		

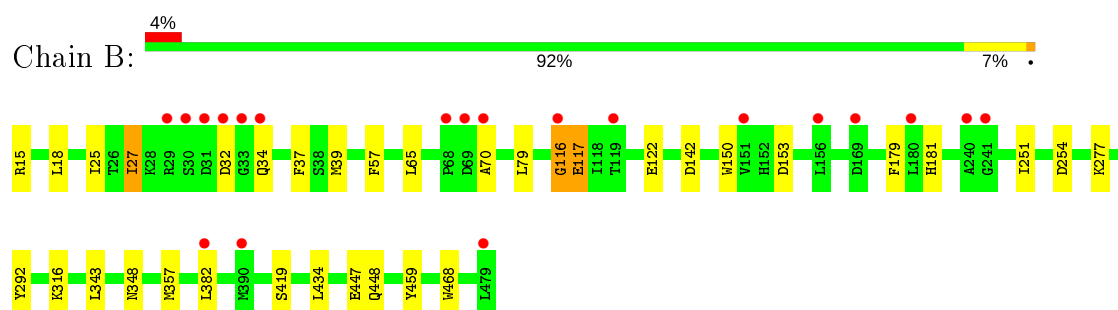
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

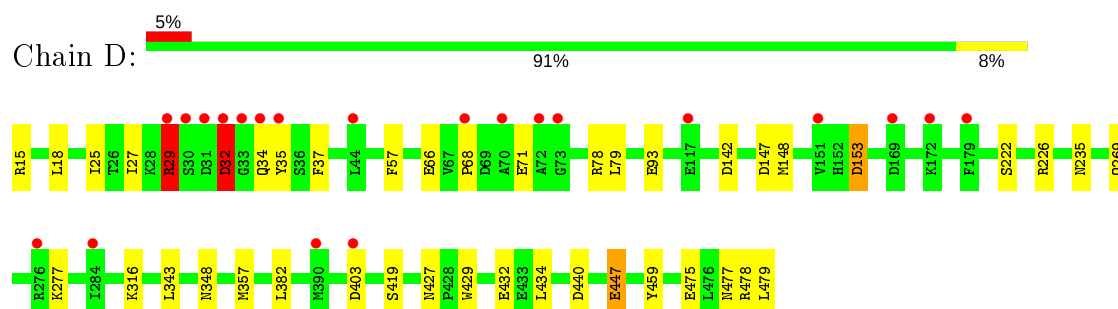
- Molecule 1: Trehalose-6-phosphate synthase



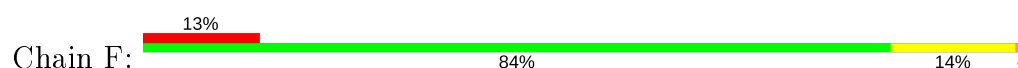
- Molecule 1: Trehalose-6-phosphate synthase

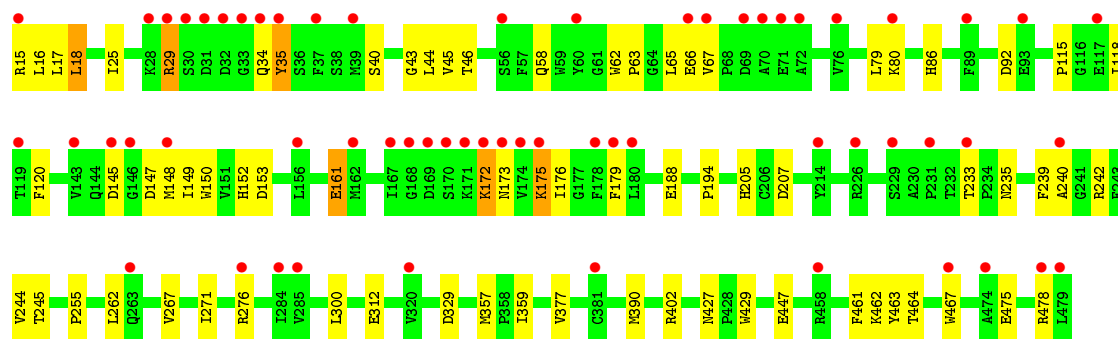


- Molecule 1: Trehalose-6-phosphate synthase

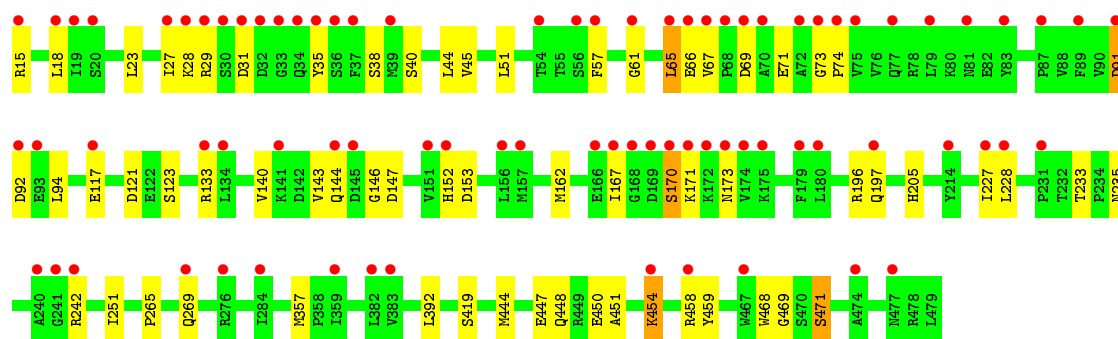
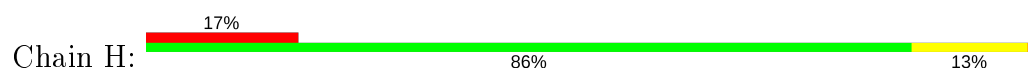


- Molecule 1: Trehalose-6-phosphate synthase

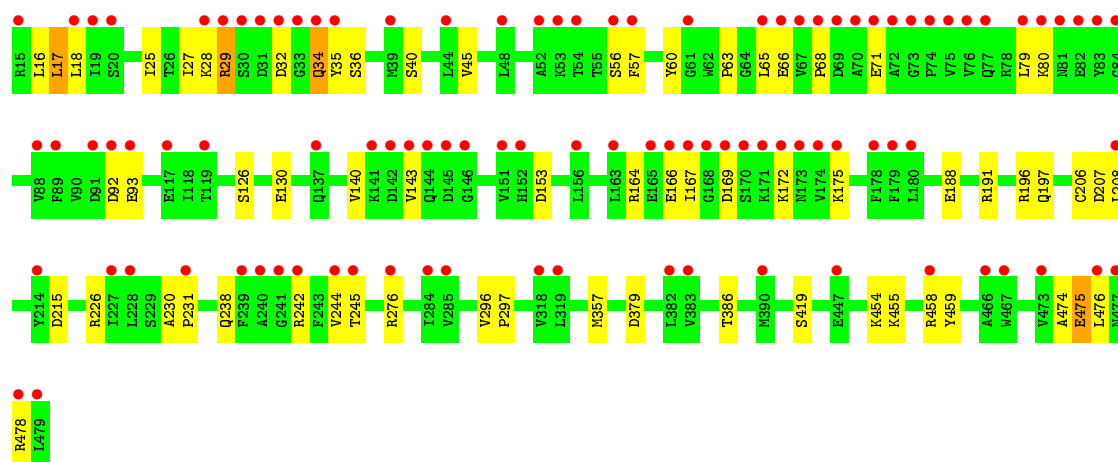
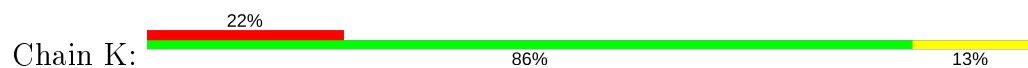




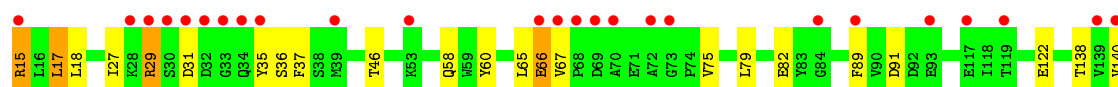
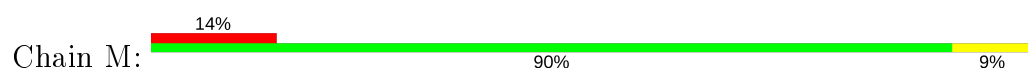
• Molecule 1: Trehalose-6-phosphate synthase

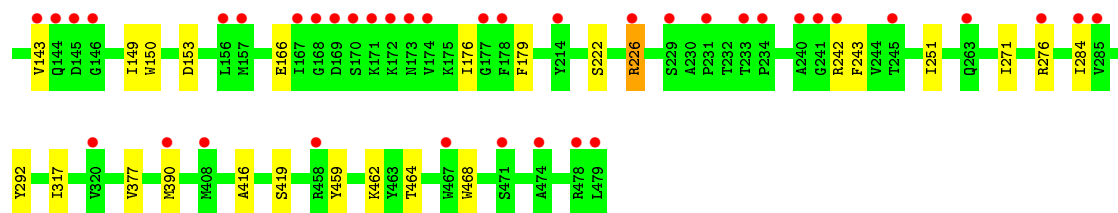


• Molecule 1: Trehalose-6-phosphate synthase

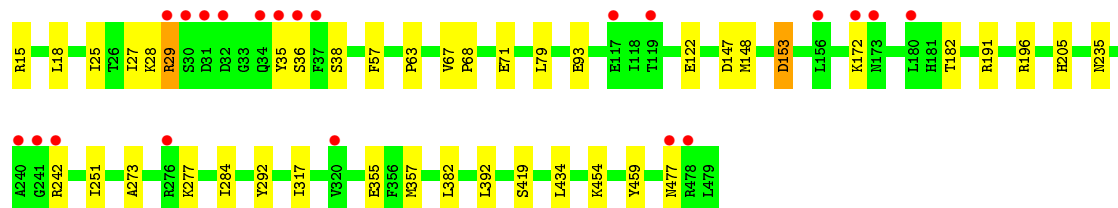


• Molecule 1: Trehalose-6-phosphate synthase





- Molecule 1: Trehalose-6-phosphate synthase



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



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



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



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



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

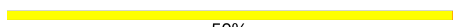



- Molecule 2: 6-O-phosphono-alpha-D-glucopyranose-(1-1)-alpha-D-glucopyranose

Chain L:  100%

GLC1
G6P2

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

Chain N:  50%  50%

GLC1
G6P2

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

Chain P:  100%

GLC1
G6P2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.28 Å 172.49 Å 141.70 Å 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) 99.6 (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 2.03 Å)	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	14918 reflections (4.88%)	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 , 51.6	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, GLC, G6P

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	0.32	0/3808	0.49	1/5173 (0.0%)
1	B	0.35	0/3808	0.51	0/5173
1	D	0.32	0/3808	0.50	2/5173 (0.0%)
1	F	0.48	0/3808	0.59	2/5173 (0.0%)
1	H	0.38	0/3808	0.57	1/5173 (0.0%)
1	K	0.42	1/3808 (0.0%)	0.57	4/5173 (0.1%)
1	M	0.33	0/3808	0.54	1/5173 (0.0%)
1	O	0.35	0/3808	0.50	0/5173
All	All	0.37	1/30464 (0.0%)	0.53	11/41384 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	475	GLU	CB-CG	5.20	1.62	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	ASP	CB-CG-OD1	6.75	124.37	118.30
1	F	18	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	K	226	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	29	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	H	91	ASP	CB-CA-C	-5.39	99.62	110.40
1	D	29	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	K	197	GLN	CB-CA-C	-5.15	100.10	110.40
1	K	17	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	K	226	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	M	226	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	F	18	LEU	CB-CG-CD1	5.01	119.51	111.00

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	26	0
1	B	3710	0	3659	27	0
1	D	3710	0	3659	40	0
1	F	3710	0	3659	68	0
1	H	3710	0	3659	56	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	0	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	2	0
2	L	27	0	19	2	0
2	N	27	0	20	2	0
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	353	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 (353) 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:780: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
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:502: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:602: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:618: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:502: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:F:145:ASP:OD1	1:F:172:LYS:N	2.22	0.70
1:H:451:ALA:HA	1:H:454:LYS:HE3	1.73	0.70
1:D:269:GLN:NE2	4:D:608: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:621:HOH:O	2.50	0.70
1:F:29:ARG:HG2	1:F:29:ARG:HH11	1.56	0.69
1:M:35:TYR:HD1	1:M:35:TYR:H	1.38	0.69
1:O:36:SER:OG	4:O:602:HOH:O	2.07	0.69
1:K:357:MET:SD	4:K:614:HOH:O	2.50	0.68
1:B:277:LYS:NZ	4:B:606: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:502:UDP:O3B	2:G:1:GLC:O2	2.13	0.64
1:K:230:ALA:O	4:K:603:HOH:O	2.14	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:355:GLU:HB2	1:B:277:LYS:HG2	1.84	0.60
1:O:15:ARG:NH1	1:O:147:ASP:OD1	2.35	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
1:O:172:LYS:NZ	4:O:608:HOH:O	2.33	0.59
4:K:601: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:O:148:MET:SD	1:O:477:ASN:ND2	2.64	0.59
1:A:282:LYS:NZ	4:A:608: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:612: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:H:27:ILE:HB	1:H:65:LEU:CD2	2.34	0.57
1:M:390:MET:HE3	1:M:416:ALA:HA	1.85	0.57
1:D:71:GLU:N	1:D:71:GLU:OE1	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:222:SER:O	1:M:226:ARG:HG3	2.05	0.57
1:F:16:LEU:C	1:F:17:LEU:HD12	2.25	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
1:F:35:TYR:C	1:F:35:TYR:HD1	2.10	0.55
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:625:HOH:O	2.59	0.54
1:F:15:ARG:NH2	1:F:147:ASP:OD2	2.40	0.54
1:H:23:LEU:HD21	1:H:61:GLY:C	2.27	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: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:612:HOH:O	2.41	0.54
1:H:197:GLN:HB2	1:H:228:LEU:CD2	2.38	0.53
1:O:153:ASP:OD2	2:P:2:G6P:O2	2.20	0.53
1:F:240:ALA:HB3	1:F:242:ARG:NH2	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:TYR:C	1:F:35:TYR:CD1	2.82	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:D:382:LEU:HD11	1:D:434:LEU:HD11	1.92	0.52
1:F:17:LEU:CD1	1:F:17:LEU:N	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:H:140:VAL:O	1:H:143:VAL:HG12	2.10	0.51
1:K:379:ASP:OD1	4:K:605: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:636:HOH:O	2.10	0.51
1:K:140:VAL:O	1:K:143:VAL:HG12	2.10	0.50
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: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:447:GLU:CD	1:F:447:GLU:H	2.15	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:15:ARG:HH12	1:O:147:ASP:CG	2.14	0.49
1:O:25:ILE:HD11	1:O:79:LEU:HD21	1.94	0.49
1:B:70:ALA:N	4:B:620:HOH:O	2.46	0.48
1:K:419:SER:HB3	1:K:459:TYR:CZ	2.48	0.48
3:F:502: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:606: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:M:390:MET:HE3	1:M:416:ALA:CA	2.44	0.48
1:D:35:TYR:CD1	1:D:35:TYR:C	2.87	0.48
1:A:447:GLU:OE1	4:A:604:HOH:O	2.20	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:208:LEU:HD12	1:K:245:THR:O	2.14	0.47
1:K:276:ARG:NH2	4:K:611:HOH:O	2.36	0.47
1:K:18:LEU:HD13	1:K:57:PHE:CG	2.50	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:D:93:GLU:HG3	4:D:619:HOH:O	2.14	0.47
1:H:35:TYR:CE1	1:H:71:GLU:CD	2.86	0.47
1:K:35:TYR:CD2	1:K:71:GLU:HG3	2.49	0.47
1:K:35:TYR:CD1	1:K:35:TYR:N	2.72	0.47
1:B:448:GLN:NE2	4:B:608:HOH:O	2.26	0.47
1:H:265:PRO:O	1:H:269:GLN:NE2	2.48	0.47
1:D:277:LYS:HG2	1:O:355:GLU:HB2	1.95	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:35:TYR:OH	1:O:68:PRO:HD2	2.15	0.47
1:O:27:ILE:HG12	1:O:63:PRO:HB2	1.96	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:255:PRO:HB2	1:F:461:PHE:CE2	2.50	0.46
1:F:66:GLU:HB2	1:F:92:ASP:OD1	2.14	0.46
1:F:115:PRO:HA	1:F:118:ILE:HD12	1.97	0.46
1:D:447:GLU:H	1:D:447:GLU:CD	2.19	0.46
1:H:133:ARG:HG2	1:H:162:MET:SD	2.55	0.46
1:K:34:GLN:CA	1:K:34:GLN:HE21	2.20	0.46
1:F:29:ARG:HH11	1:F:29:ARG:HA	1.81	0.46
1:K:143:VAL:HG11	1:K:167:ILE:HG12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:386:THR:O	4:K:606:HOH:O	2.20	0.46
1:K:29:ARG:NH1	1:K:68:PRO:CD	2.63	0.46
1:M:242:ARG:HD2	1:M:243:PHE:N	2.31	0.46
1:F:18:LEU:HD22	1:F:152:HIS:NE2	2.31	0.46
1:H:67:VAL:HG23	1:H:67:VAL:O	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:615: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:701:HOH:O	2.15	0.45
2:J:1:GLC:HO2	2:J:2:G6P:HO2	1.61	0.45
1:D:148:MET:SD	1:D:477:ASN:ND2	2.82	0.45
1:D:35:TYR:O	1:D:35:TYR:CG	2.70	0.45
1:O:35:TYR:HE2	1:O:71:GLU:HG3	1.75	0.45
1:A:355:GLU:CB	1:B:277:LYS:HG2	2.46	0.45
1:D:316:LYS:HE3	4:D:749: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: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:F:44:LEU:CB	2:I:1:GLC:H61	2.47	0.44
1:O:191:ARG:O	1:O:196:ARG:NH1	2.45	0.44
1:O:235:ASN:HB2	4:O:768: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: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:765: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:H:471:SER:OG	4:H:601:HOH:O	1.89	0.43
1:K:29:ARG:CG	1:K:65:LEU:HD13	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:1:GLC:O2	2:L:2:G6P:H1	2.18	0.43
1:O:29:ARG:HB2	1:O:29:ARG:HE	1.46	0.43
1:A:382:LEU:HD11	1:A:434:LEU:HD11	1.99	0.43
1:H:121:ASP:OD1	1:H:123:SER:HB3	2.18	0.43
1:B:316:LYS:CE	1:H:269:GLN:OE1	2.67	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:A:419:SER:HB3	1:A:459:TYR:CZ	2.54	0.43
1:F:245:THR:N	4:F:605:HOH:O	2.05	0.43
1:H:451:ALA:O	1:H:454:LYS:HD2	2.18	0.43
1:H:66:GLU:N	1:H:92:ASP:OD1	2.46	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:150:TRP:HE1	1:B:179:PHE:HB2	1.83	0.43
1:B:27:ILE:HG22	1:B:65:LEU:HD23	2.01	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:D:348:ASN:HB3	1:D:357:MET:CE	2.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:GLN:HE22	1:F:80:LYS:NZ	2.17	0.42
1:M:138:THR:OG1	4:M:606:HOH:O	2.22	0.42
1:D:348:ASN:HB3	1:D:357:MET:HE3	2.02	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:O:15:ARG:NH1	1:O:147:ASP:CG	2.73	0.42
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
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:HA	1:K:476:LEU:HD12	1.51	0.41
1:D:153:ASP:OD2	2:G:2:G6P:O2	2.32	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
2:E:1:GLC:O2	2:E:2:G6P:H1	2.20	0.41
1:M:35:TYR:CG	1:M:35:TYR:O	2.74	0.41
1:O:205:HIS:HA	1:O:242:ARG:CZ	2.52	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

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:777: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:608: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%)	34	28
1	D	463/465 (100%)	458 (99%)	5 (1%)	0	100	100
1	F	463/465 (100%)	456 (98%)	7 (2%)	0	100	100
1	H	463/465 (100%)	457 (99%)	5 (1%)	1 (0%)	47	43
1	K	463/465 (100%)	457 (99%)	6 (1%)	0	100	100
1	M	463/465 (100%)	458 (99%)	4 (1%)	1 (0%)	47	43
1	O	463/465 (100%)	458 (99%)	5 (1%)	0	100	100
All	All	3704/3720 (100%)	3657 (99%)	43 (1%)	4 (0%)	51	48

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%)	397 (99%)	3 (1%)	81	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	400/400 (100%)	396 (99%)	4 (1%)	76	80
1	D	400/400 (100%)	395 (99%)	5 (1%)	69	72
1	F	400/400 (100%)	391 (98%)	9 (2%)	50	51
1	H	400/400 (100%)	394 (98%)	6 (2%)	65	68
1	K	400/400 (100%)	390 (98%)	10 (2%)	47	48
1	M	400/400 (100%)	394 (98%)	6 (2%)	65	68
1	O	400/400 (100%)	396 (99%)	4 (1%)	76	80
All	All	3200/3200 (100%)	3153 (98%)	47 (2%)	65	68

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	GLU
1	A	153	ASP
1	A	343	LEU
1	B	27	ILE
1	B	153	ASP
1	B	343	LEU
1	B	447	GLU
1	D	29	ARG
1	D	32	ASP
1	D	153	ASP
1	D	343	LEU
1	D	447	GLU
1	F	29	ARG
1	F	34	GLN
1	F	35	TYR
1	F	67	VAL
1	F	153	ASP
1	F	161	GLU
1	F	172	LYS
1	F	175	LYS
1	F	276	ARG
1	H	65	LEU
1	H	153	ASP
1	H	170	SER
1	H	447	GLU
1	H	454	LYS
1	H	471	SER
1	K	28	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	153	ASP
1	K	166	GLU
1	K	215	ASP
1	M	15	ARG
1	M	17	LEU
1	M	29	ARG
1	M	31	ASP
1	M	36	SER
1	M	153	ASP
1	O	29	ARG
1	O	67	VAL
1	O	93	GLU
1	O	153	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	197	GLN
1	A	448	GLN
1	B	34	GLN
1	D	34	GLN
1	F	58	GLN
1	F	477	ASN
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	448	GLN
1	K	477	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 ⓘ

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	2.15	3 (27%)	15,15,17	2.25	4 (26%)
2	G6P	C	2	2	16,16,16	2.02	6 (37%)	24,24,24	1.39	3 (12%)
2	GLC	E	1	2	11,11,12	1.98	3 (27%)	15,15,17	1.98	3 (20%)
2	G6P	E	2	2	16,16,16	1.98	6 (37%)	24,24,24	1.24	2 (8%)
2	GLC	G	1	2	11,11,12	1.92	2 (18%)	15,15,17	2.47	5 (33%)
2	G6P	G	2	2	16,16,16	2.01	6 (37%)	24,24,24	1.37	4 (16%)
2	GLC	I	1	2	11,11,12	1.26	1 (9%)	15,15,17	3.45	6 (40%)
2	G6P	I	2	2	16,16,16	1.95	6 (37%)	24,24,24	0.97	1 (4%)
2	GLC	J	1	1,2	11,11,12	1.67	2 (18%)	15,15,17	2.00	2 (13%)
2	G6P	J	2	2	16,16,16	2.05	6 (37%)	24,24,24	1.52	3 (12%)
2	GLC	L	1	2	11,11,12	2.40	3 (27%)	15,15,17	2.49	5 (33%)
2	G6P	L	2	2	16,16,16	2.02	6 (37%)	24,24,24	1.19	3 (12%)
2	GLC	N	1	2	11,11,12	1.87	2 (18%)	15,15,17	2.19	3 (20%)
2	G6P	N	2	2	16,16,16	2.00	6 (37%)	24,24,24	1.27	3 (12%)
2	GLC	P	1	2	11,11,12	2.20	3 (27%)	15,15,17	2.19	6 (40%)
2	G6P	P	2	2	16,16,16	2.03	6 (37%)	24,24,24	1.34	3 (12%)

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	-	0/6/26/26	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	-	2/6/26/26	0/1/1/1
2	GLC	J	1	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
2	G6P	P	2	2	-	0/6/26/26	0/1/1/1

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1	GLC	O5-C1	6.00	1.53	1.43
2	P	1	GLC	O5-C1	5.46	1.52	1.43
2	C	1	GLC	O5-C1	5.45	1.52	1.43
2	G	1	GLC	O5-C1	5.18	1.52	1.43
2	N	1	GLC	O5-C1	5.06	1.51	1.43
2	E	1	GLC	O5-C1	5.04	1.51	1.43
2	J	2	G6P	O5-C5	4.65	1.55	1.44
2	C	2	G6P	O5-C5	4.55	1.55	1.44
2	G	2	G6P	O5-C5	4.52	1.55	1.44
2	J	1	GLC	O5-C1	4.50	1.50	1.43
2	L	2	G6P	O5-C5	4.46	1.55	1.44
2	N	2	G6P	O5-C5	4.45	1.55	1.44
2	E	2	G6P	O5-C5	4.45	1.55	1.44
2	P	2	G6P	O5-C5	4.45	1.55	1.44
2	I	2	G6P	O5-C5	4.32	1.54	1.44
2	L	1	GLC	C2-C3	-3.44	1.47	1.52
2	L	1	GLC	O5-C5	3.32	1.50	1.43
2	P	1	GLC	C2-C3	-3.25	1.47	1.52
2	I	1	GLC	O5-C1	3.24	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	2	G6P	C6-C5	-3.03	1.42	1.51
2	I	2	G6P	C6-C5	-3.00	1.42	1.51
2	N	2	G6P	C6-C5	-2.99	1.42	1.51
2	C	1	GLC	O5-C5	2.99	1.49	1.43
2	L	2	G6P	C6-C5	-2.98	1.42	1.51
2	P	1	GLC	O5-C5	2.89	1.49	1.43
2	E	2	G6P	C6-C5	-2.88	1.42	1.51
2	G	2	G6P	C6-C5	-2.88	1.42	1.51
2	C	2	G6P	C6-C5	-2.87	1.42	1.51
2	J	2	G6P	C6-C5	-2.84	1.42	1.51
2	L	2	G6P	C3-C2	-2.77	1.45	1.52
2	P	2	G6P	C3-C2	-2.76	1.45	1.52
2	E	1	GLC	O5-C5	2.72	1.49	1.43
2	J	2	G6P	C3-C2	-2.67	1.45	1.52
2	J	2	G6P	O5-C1	2.60	1.49	1.42
2	G	2	G6P	O5-C1	2.58	1.49	1.42
2	C	2	G6P	O5-C1	2.57	1.49	1.42
2	N	2	G6P	C3-C2	-2.57	1.45	1.52
2	N	2	G6P	O2-C2	2.53	1.48	1.43
2	C	1	GLC	C2-C3	-2.50	1.48	1.52
2	I	2	G6P	C3-C2	-2.48	1.46	1.52
2	E	2	G6P	O5-C1	2.48	1.49	1.42
2	C	2	G6P	O2-C2	2.47	1.48	1.43
2	G	2	G6P	C3-C2	-2.46	1.46	1.52
2	C	2	G6P	C3-C2	-2.46	1.46	1.52
2	E	2	G6P	C3-C2	-2.46	1.46	1.52
2	L	2	G6P	O2-C2	2.44	1.48	1.43
2	P	2	G6P	O2-C2	2.44	1.48	1.43
2	G	2	G6P	O2-C2	2.44	1.48	1.43
2	P	2	G6P	O5-C1	2.42	1.49	1.42
2	N	2	G6P	O5-C1	2.42	1.48	1.42
2	E	2	G6P	O2-C2	2.37	1.48	1.43
2	I	2	G6P	O2-C2	2.35	1.48	1.43
2	L	2	G6P	O5-C1	2.33	1.48	1.42
2	I	2	G6P	O3-C3	2.33	1.48	1.43
2	C	2	G6P	O3-C3	2.32	1.48	1.43
2	J	2	G6P	O3-C3	2.32	1.48	1.43
2	G	2	G6P	O3-C3	2.30	1.48	1.43
2	E	1	GLC	C2-C3	-2.28	1.49	1.52
2	E	2	G6P	O3-C3	2.27	1.48	1.43
2	P	2	G6P	O3-C3	2.27	1.48	1.43
2	J	2	G6P	O2-C2	2.26	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	GLC	O5-C5	2.26	1.48	1.43
2	L	2	G6P	O3-C3	2.23	1.48	1.43
2	N	2	G6P	O3-C3	2.23	1.48	1.43
2	I	2	G6P	O5-C1	2.21	1.48	1.42
2	J	1	GLC	O5-C5	2.11	1.47	1.43
2	N	1	GLC	C2-C3	-2.09	1.49	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	GLC	C1-C2-C3	9.29	121.08	109.67
2	G	1	GLC	C1-C2-C3	6.94	118.20	109.67
2	I	1	GLC	C1-O5-C5	-6.79	102.99	112.19
2	J	1	GLC	C1-C2-C3	6.55	117.72	109.67
2	C	1	GLC	C1-O5-C5	6.37	120.82	112.19
2	N	1	GLC	C1-C2-C3	6.18	117.26	109.67
2	E	1	GLC	C1-O5-C5	5.98	120.30	112.19
2	P	1	GLC	C1-O5-C5	5.30	119.37	112.19
2	L	1	GLC	C1-O5-C5	5.18	119.21	112.19
2	L	1	GLC	C2-C3-C4	-4.77	102.64	110.89
2	L	1	GLC	O2-C2-C1	4.26	117.87	109.15
2	G	1	GLC	C1-O5-C5	4.08	117.72	112.19
2	J	2	G6P	O5-C1-C2	3.89	117.23	110.28
2	C	2	G6P	O1-C1-C2	3.84	119.85	109.03
2	N	1	GLC	O5-C1-C2	3.73	116.53	110.77
2	J	2	G6P	C1-O5-C5	3.65	120.56	113.66
2	I	1	GLC	C3-C4-C5	-3.59	103.83	110.24
2	P	1	GLC	C1-C2-C3	3.58	114.07	109.67
2	P	2	G6P	O1-C1-C2	3.52	118.93	109.03
2	C	1	GLC	C1-C2-C3	3.46	113.91	109.67
2	G	2	G6P	O1-C1-C2	3.22	118.10	109.03
2	P	1	GLC	O2-C2-C1	3.18	115.67	109.15
2	I	1	GLC	O2-C2-C1	-3.17	102.67	109.15
2	L	1	GLC	O5-C5-C6	3.17	112.17	107.20
2	E	1	GLC	O2-C2-C1	3.16	115.63	109.15
2	G	1	GLC	O5-C1-C2	3.06	115.50	110.77
2	E	2	G6P	O1-C1-C2	3.04	117.60	109.03
2	N	2	G6P	O1-C1-C2	2.96	117.36	109.03
2	C	2	G6P	O5-C5-C6	2.96	112.63	106.67
2	N	2	G6P	O2-C2-C1	2.94	115.97	109.16
2	G	2	G6P	O5-C5-C6	2.93	112.58	106.67
2	I	1	GLC	O5-C5-C4	-2.92	103.73	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	O5-C5-C4	2.91	117.92	110.83
2	E	2	G6P	O5-C5-C6	2.83	112.39	106.67
2	P	2	G6P	O2-C2-C1	2.78	115.60	109.16
2	J	1	GLC	C2-C3-C4	2.77	115.69	110.89
2	J	2	G6P	O5-C5-C6	2.72	112.15	106.67
2	L	2	G6P	O1-C1-C2	2.71	116.67	109.03
2	G	2	G6P	O2-C2-C1	2.60	115.20	109.16
2	C	2	G6P	O2-C2-C1	2.54	115.06	109.16
2	P	1	GLC	C6-C5-C4	-2.52	107.11	113.00
2	N	2	G6P	O5-C5-C6	2.50	111.72	106.67
2	L	2	G6P	O2-C2-C1	2.50	114.96	109.16
2	N	1	GLC	C6-C5-C4	-2.50	107.16	113.00
2	C	1	GLC	C6-C5-C4	-2.37	107.45	113.00
2	P	1	GLC	O5-C5-C4	2.37	116.59	110.83
2	G	1	GLC	C2-C3-C4	2.33	114.93	110.89
2	L	1	GLC	C6-C5-C4	-2.31	107.59	113.00
2	P	1	GLC	C2-C3-C4	-2.26	106.98	110.89
2	I	2	G6P	O5-C5-C6	2.24	111.19	106.67
2	L	2	G6P	O5-C5-C6	2.23	111.16	106.67
2	P	2	G6P	O5-C5-C6	2.18	111.07	106.67
2	I	1	GLC	O2-C2-C3	-2.17	105.79	110.14
2	G	2	G6P	C1-C2-C3	2.12	114.72	110.31
2	E	1	GLC	C1-C2-C3	2.04	112.17	109.67
2	G	1	GLC	C6-C5-C4	-2.01	108.30	113.00

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	J	2	G6P	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

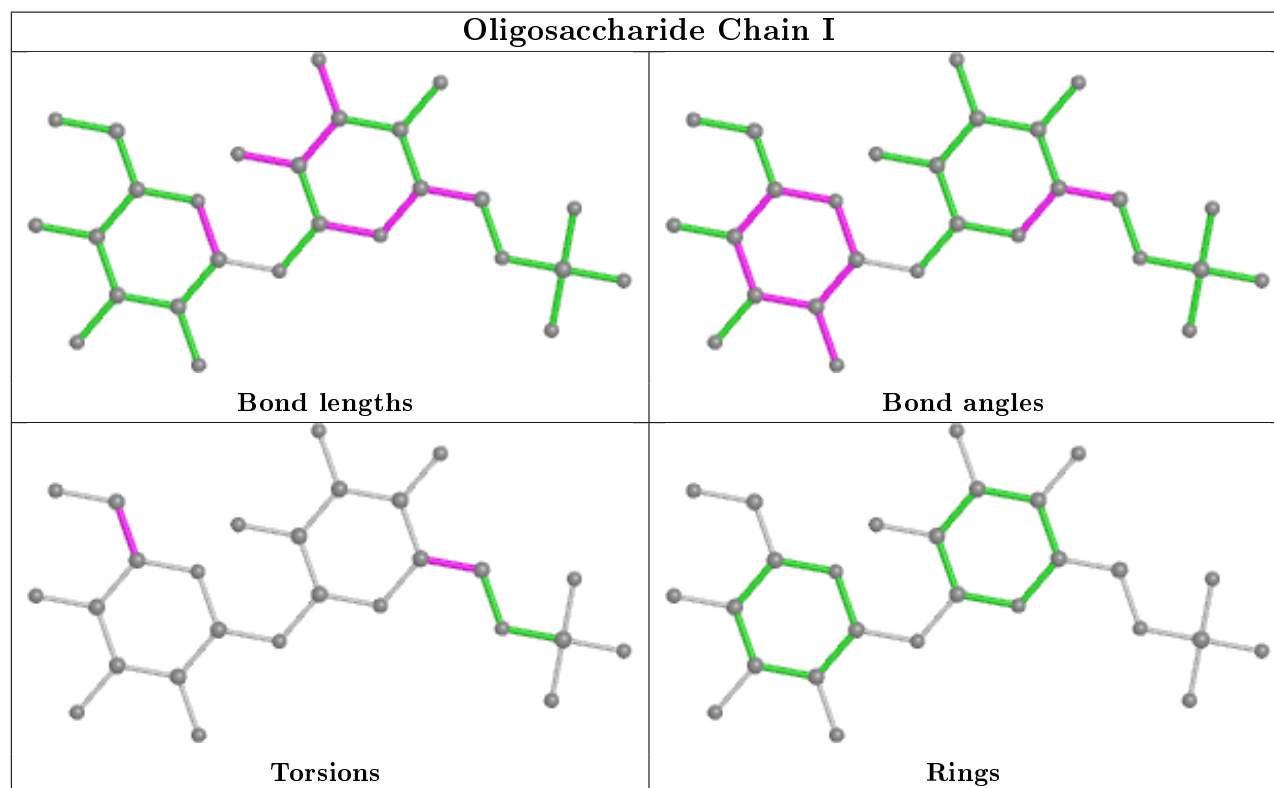
Mol	Chain	Res	Type	Atoms
2	I	2	G6P	C4-C5-C6-O6
2	I	2	G6P	O5-C5-C6-O6

There are no ring outliers.

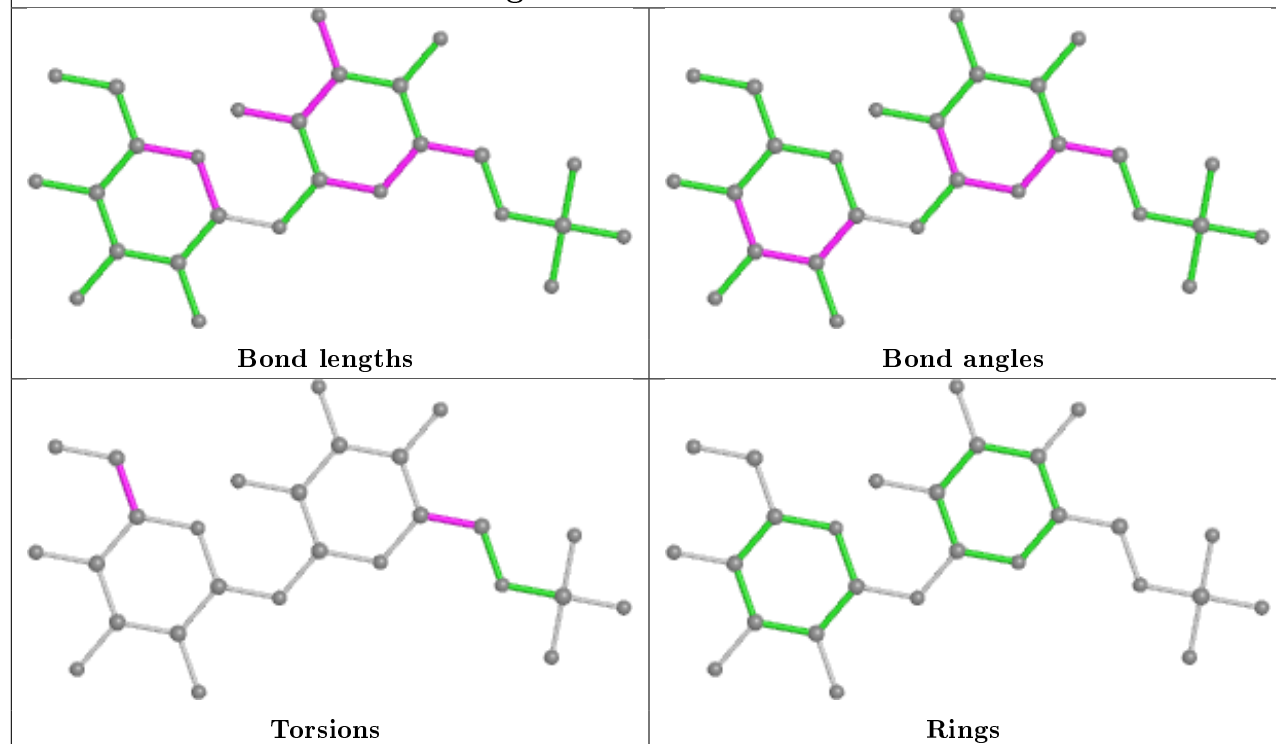
12 monomers are involved in 17 short contacts:

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

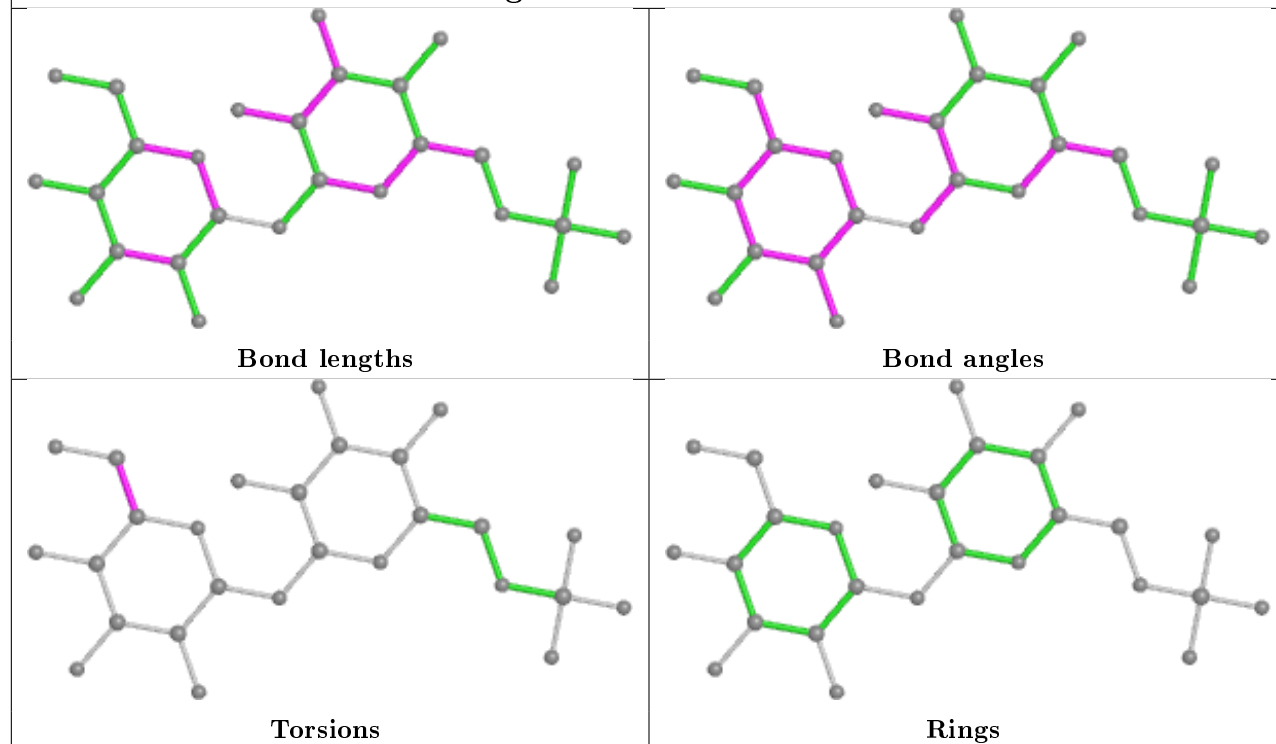
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

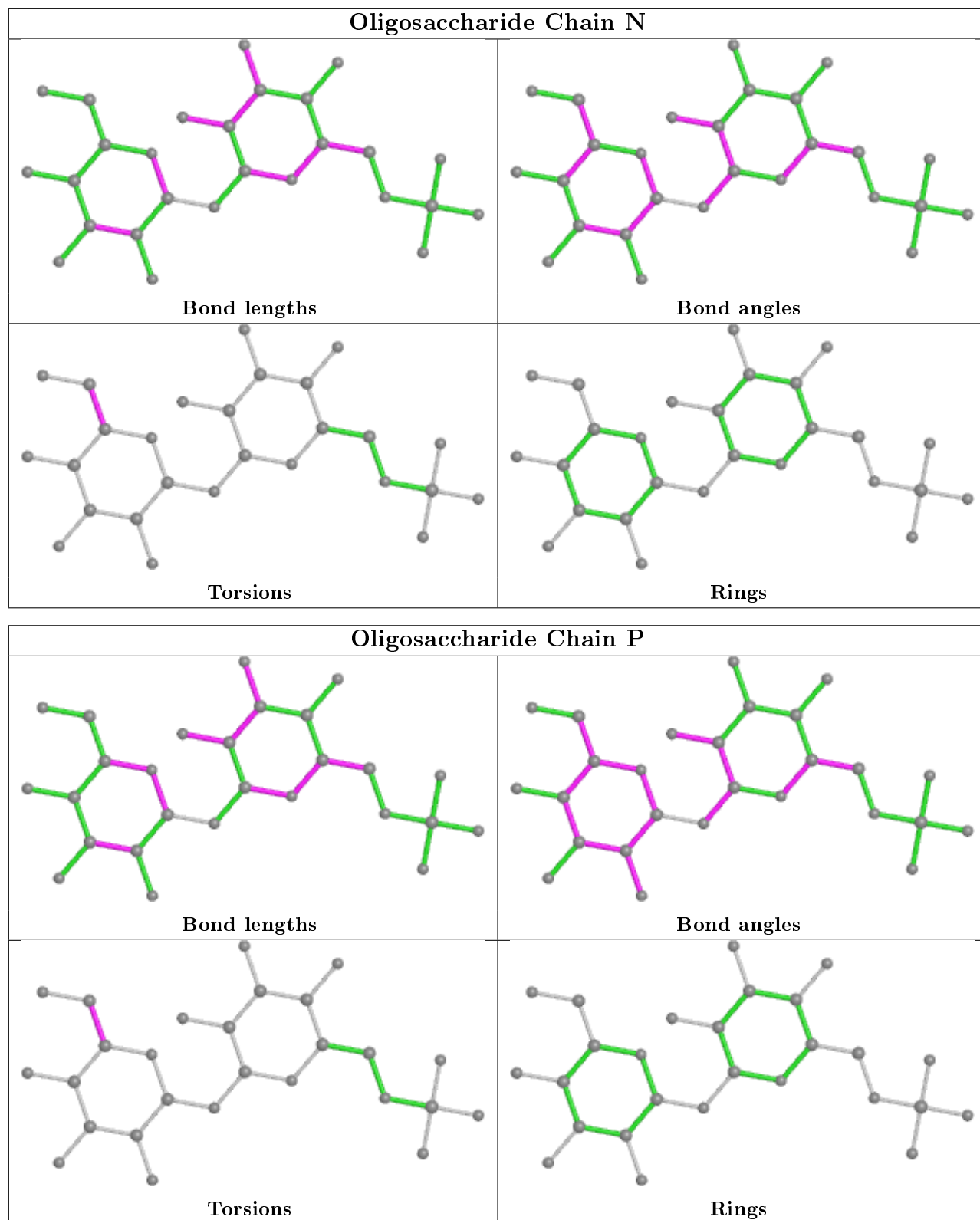


Oligosaccharide Chain J



Oligosaccharide Chain L





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	O	502	-	20,26,26	1.13	1 (5%)	25,40,40	0.94	1 (4%)
3	UDP	H	502	-	20,26,26	1.13	1 (5%)	25,40,40	0.95	1 (4%)
3	UDP	F	502	-	20,26,26	1.13	1 (5%)	25,40,40	1.01	2 (8%)
3	UDP	K	502	-	20,26,26	1.13	1 (5%)	25,40,40	0.91	1 (4%)
3	UDP	D	502	-	20,26,26	1.14	1 (5%)	25,40,40	0.92	1 (4%)
3	UDP	A	502	-	20,26,26	1.12	1 (5%)	25,40,40	1.03	1 (4%)
3	UDP	B	502	-	20,26,26	1.12	1 (5%)	25,40,40	0.96	1 (4%)
3	UDP	M	502	-	20,26,26	1.12	1 (5%)	25,40,40	0.97	1 (4%)

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	O	502	-	-	6/14/32/32	0/2/2/2
3	UDP	H	502	-	-	6/14/32/32	0/2/2/2
3	UDP	F	502	-	-	7/14/32/32	0/2/2/2
3	UDP	K	502	-	-	6/14/32/32	0/2/2/2
3	UDP	D	502	-	-	5/14/32/32	0/2/2/2
3	UDP	A	502	-	-	5/14/32/32	0/2/2/2
3	UDP	B	502	-	-	7/14/32/32	0/2/2/2
3	UDP	M	502	-	-	6/14/32/32	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	UDP	C4-N3	3.07	1.38	1.33
3	M	502	UDP	C4-N3	3.06	1.38	1.33
3	K	502	UDP	C4-N3	3.06	1.38	1.33
3	H	502	UDP	C4-N3	3.04	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	UDP	C4-N3	3.03	1.38	1.33
3	O	502	UDP	C4-N3	3.02	1.38	1.33
3	F	502	UDP	C4-N3	3.01	1.38	1.33
3	A	502	UDP	C4-N3	3.01	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	UDP	PA-O3A-PB	-3.40	121.17	132.83
3	B	502	UDP	PA-O3A-PB	-3.27	121.61	132.83
3	M	502	UDP	PA-O3A-PB	-3.21	121.80	132.83
3	H	502	UDP	PA-O3A-PB	-2.99	122.55	132.83
3	O	502	UDP	PA-O3A-PB	-2.89	122.90	132.83
3	K	502	UDP	PA-O3A-PB	-2.74	123.42	132.83
3	D	502	UDP	PA-O3A-PB	-2.48	124.31	132.83
3	F	502	UDP	O2B-PB-O3A	2.18	111.95	104.64
3	F	502	UDP	PA-O3A-PB	-2.08	125.69	132.83

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	502	UDP	O4'-C1'-N1-C6
3	O	502	UDP	PB-O3A-PA-O5'
3	H	502	UDP	O4'-C1'-N1-C6
3	H	502	UDP	PB-O3A-PA-O5'
3	H	502	UDP	PA-O3A-PB-O2B
3	F	502	UDP	O4'-C1'-N1-C6
3	F	502	UDP	PB-O3A-PA-O5'
3	F	502	UDP	PA-O3A-PB-O2B
3	F	502	UDP	PA-O3A-PB-O3B
3	K	502	UDP	O4'-C1'-N1-C6
3	K	502	UDP	PB-O3A-PA-O5'
3	K	502	UDP	PA-O3A-PB-O2B
3	D	502	UDP	O4'-C1'-N1-C6
3	D	502	UDP	PB-O3A-PA-O5'
3	A	502	UDP	O4'-C1'-N1-C6
3	A	502	UDP	PB-O3A-PA-O5'
3	B	502	UDP	O4'-C1'-N1-C6
3	B	502	UDP	PB-O3A-PA-O5'
3	M	502	UDP	O4'-C1'-N1-C6
3	M	502	UDP	PB-O3A-PA-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	M	502	UDP	PA-O3A-PB-O2B
3	H	502	UDP	O4'-C4'-C5'-O5'
3	F	502	UDP	O4'-C4'-C5'-O5'
3	B	502	UDP	O4'-C4'-C5'-O5'
3	M	502	UDP	O4'-C4'-C5'-O5'
3	O	502	UDP	O4'-C4'-C5'-O5'
3	K	502	UDP	O4'-C4'-C5'-O5'
3	A	502	UDP	O4'-C4'-C5'-O5'
3	H	502	UDP	C3'-C4'-C5'-O5'
3	F	502	UDP	C3'-C4'-C5'-O5'
3	B	502	UDP	C3'-C4'-C5'-O5'
3	M	502	UDP	C3'-C4'-C5'-O5'
3	O	502	UDP	PA-O3A-PB-O1B
3	K	502	UDP	PA-O3A-PB-O1B
3	B	502	UDP	PA-O3A-PB-O1B
3	M	502	UDP	PA-O3A-PB-O1B
3	D	502	UDP	O4'-C4'-C5'-O5'
3	A	502	UDP	C3'-C4'-C5'-O5'
3	O	502	UDP	PA-O3A-PB-O3B
3	D	502	UDP	PA-O3A-PB-O3B
3	A	502	UDP	PA-O3A-PB-O2B
3	B	502	UDP	PA-O3A-PB-O2B
3	O	502	UDP	C3'-C4'-C5'-O5'
3	K	502	UDP	C3'-C4'-C5'-O5'
3	D	502	UDP	C3'-C4'-C5'-O5'
3	H	502	UDP	PA-O3A-PB-O3B
3	B	502	UDP	C5'-O5'-PA-O1A
3	F	502	UDP	PA-O3A-PB-O1B

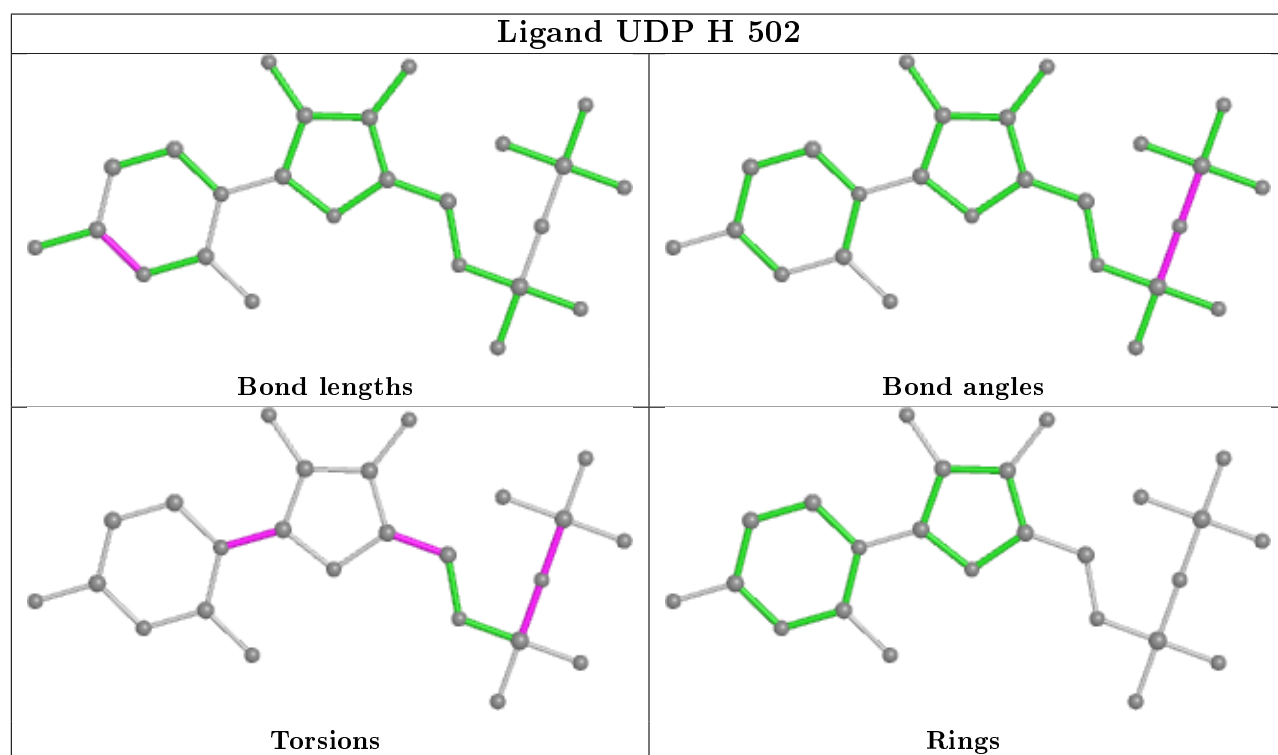
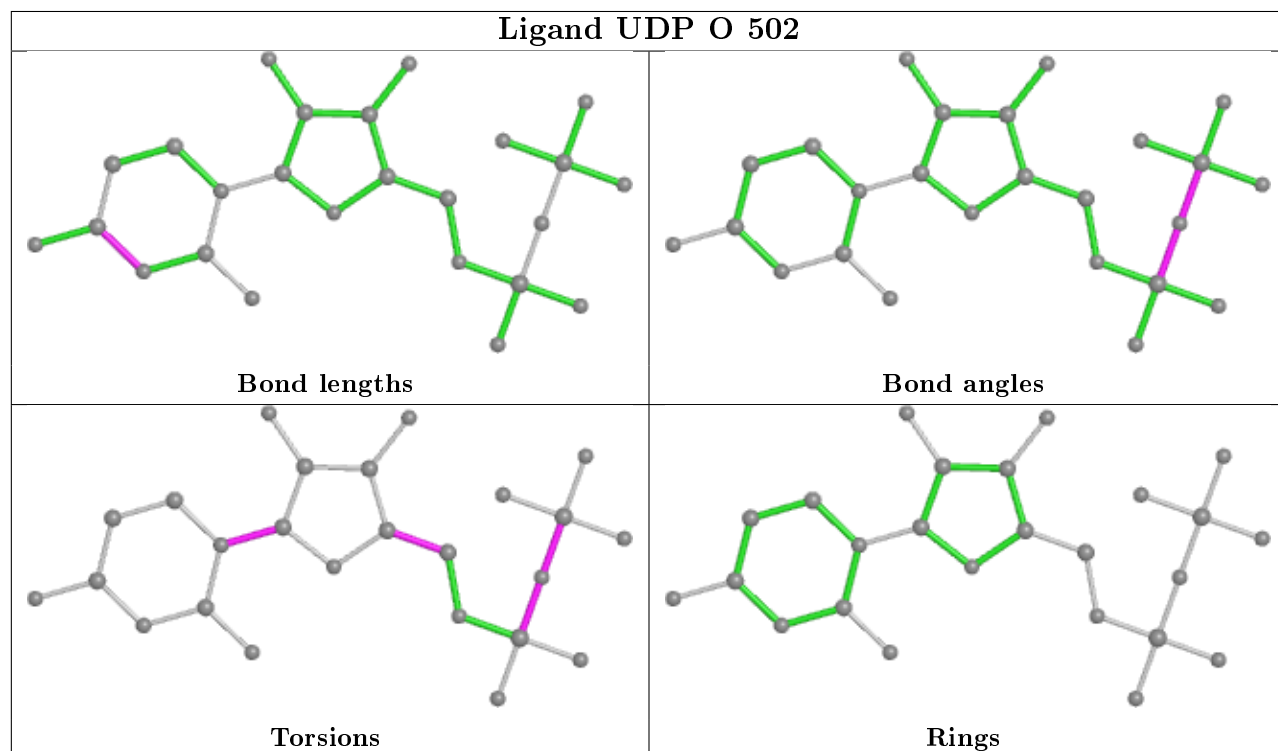
There are no ring outliers.

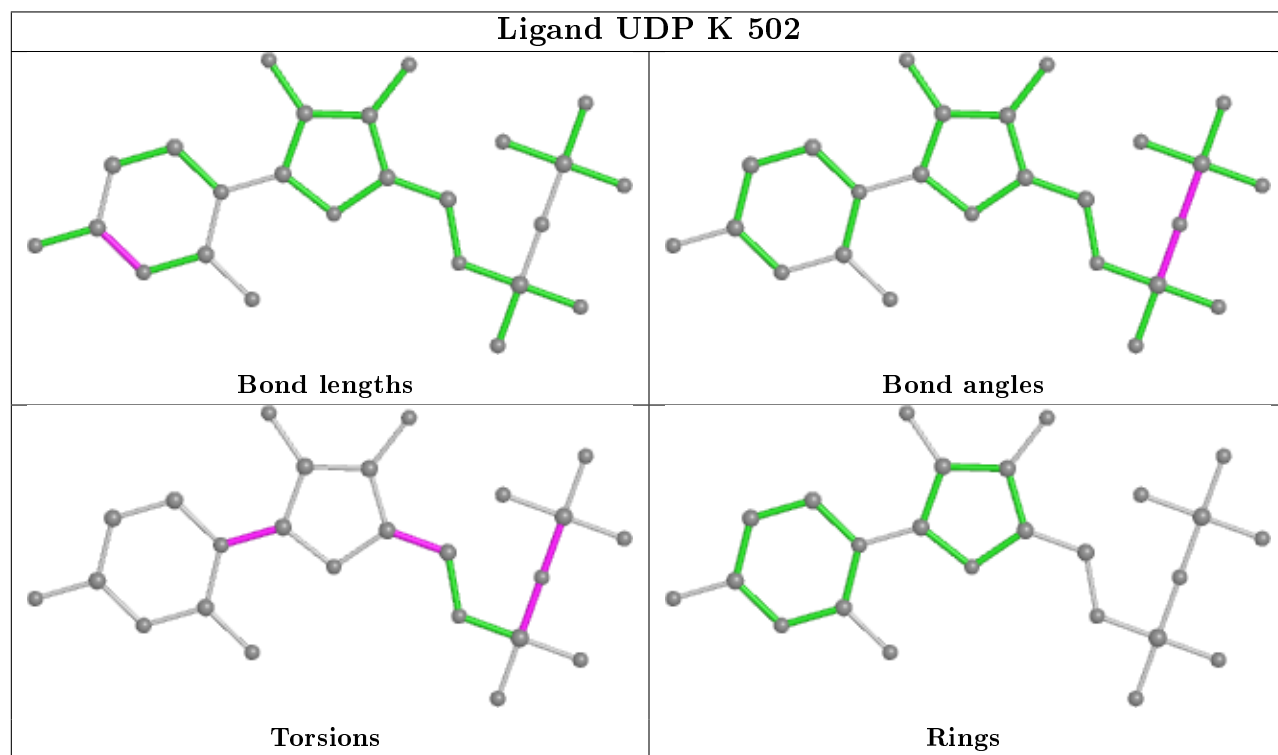
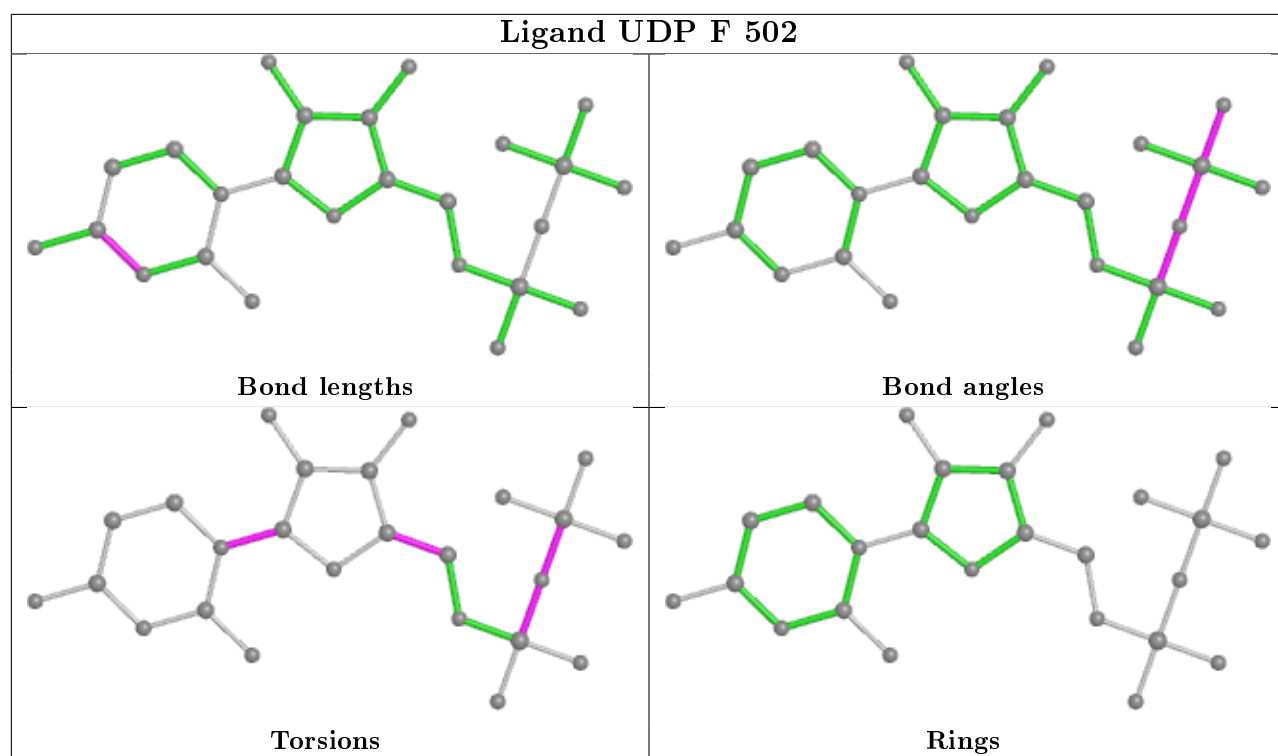
3 monomers are involved in 4 short contacts:

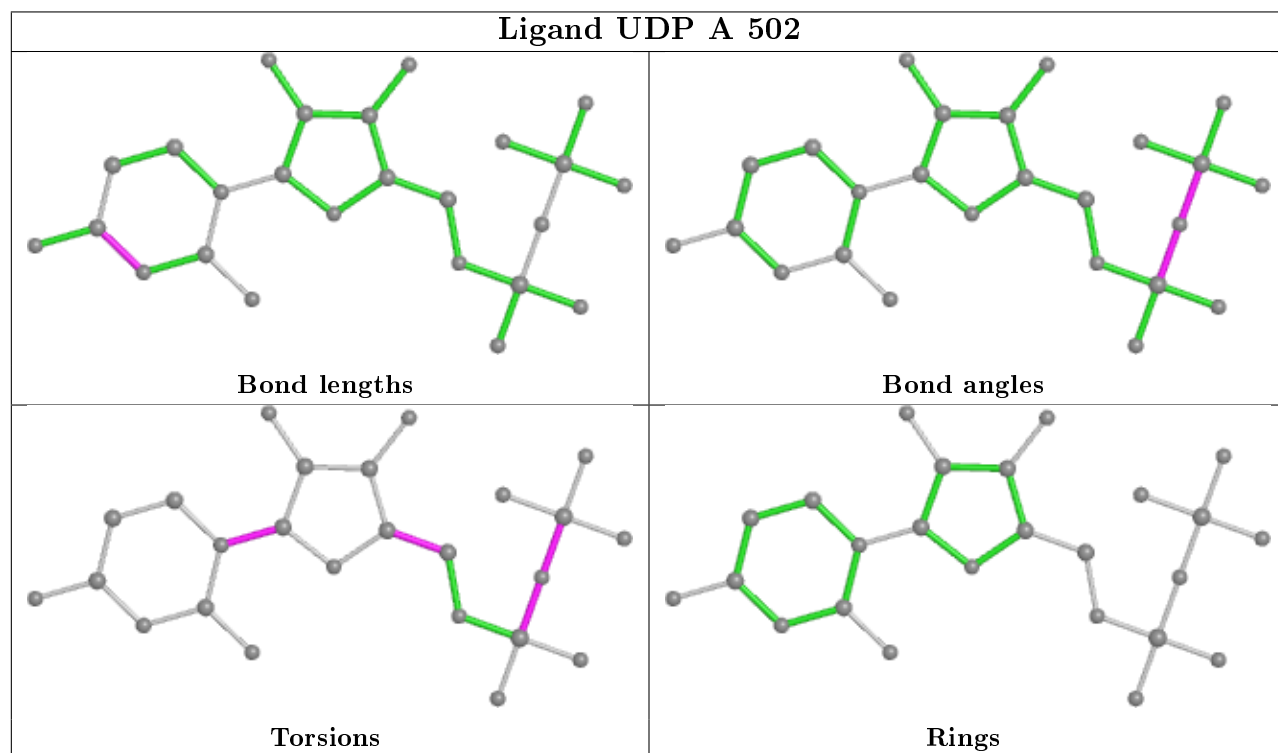
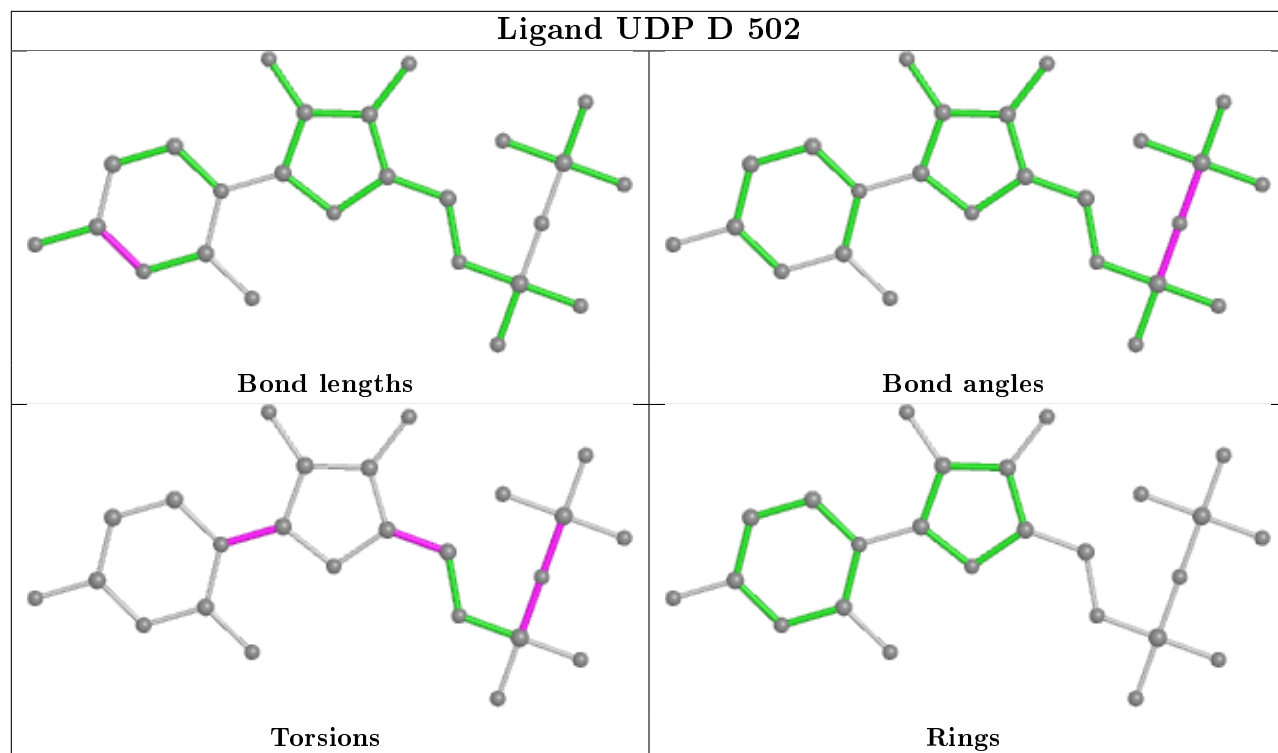
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	502	UDP	1	0
3	F	502	UDP	2	0
3	D	502	UDP	1	0

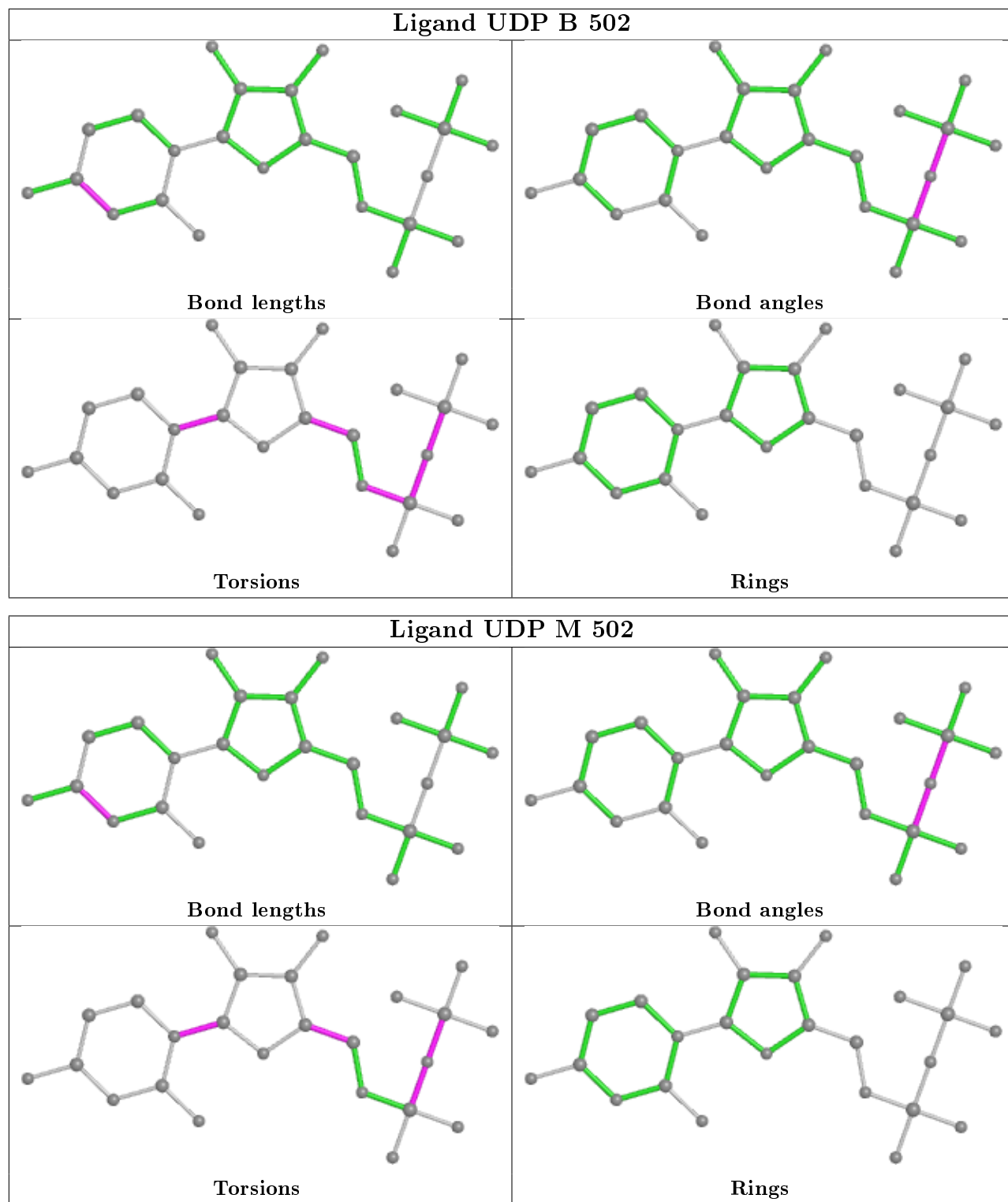
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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%)	0.12	22 (4%) 31 31	16, 27, 49, 88	0
1	B	465/465 (100%)	0.10	20 (4%) 35 34	16, 26, 48, 92	0
1	D	465/465 (100%)	0.09	21 (4%) 33 32	16, 26, 47, 91	0
1	F	465/465 (100%)	0.71	60 (12%) 3 3	24, 42, 68, 96	0
1	H	465/465 (100%)	0.88	80 (17%) 1 1	23, 40, 75, 99	0
1	K	465/465 (100%)	1.03	100 (21%) 0 0	23, 43, 78, 104	0
1	M	465/465 (100%)	0.72	64 (13%) 2 2	23, 43, 72, 94	0
1	O	465/465 (100%)	0.13	21 (4%) 33 32	17, 28, 52, 82	0
All	All	3720/3720 (100%)	0.47	388 (10%) 6 6	16, 33, 68, 104	0

All (388) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	TYR	10.9
1	K	241	GLY	9.9
1	K	167	ILE	9.5
1	K	70	ALA	9.3
1	M	241	GLY	8.8
1	H	75	VAL	8.4
1	H	35	TYR	8.2
1	M	170	SER	8.0
1	K	67	VAL	7.5
1	H	168	GLY	7.4
1	K	169	ASP	7.3
1	H	169	ASP	7.3
1	H	30	SER	7.2
1	F	169	ASP	7.2
1	O	35	TYR	7.2
1	F	35	TYR	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	32	ASP	6.8
1	K	32	ASP	6.8
1	H	31	ASP	6.8
1	H	33	GLY	6.8
1	K	240	ALA	6.7
1	M	30	SER	6.6
1	K	29	ARG	6.5
1	M	169	ASP	6.4
1	H	70	ALA	6.4
1	H	241	GLY	6.1
1	M	69	ASP	6.0
1	A	31	ASP	5.9
1	K	35	TYR	5.8
1	K	68	PRO	5.7
1	K	31	ASP	5.7
1	D	35	TYR	5.6
1	A	32	ASP	5.3
1	K	174	VAL	5.3
1	K	77	GLN	5.2
1	F	31	ASP	5.2
1	M	168	GLY	5.2
1	F	170	SER	5.1
1	K	173	ASN	5.1
1	A	390	MET	5.1
1	F	214	TYR	5.0
1	H	117	GLU	5.0
1	B	31	ASP	5.0
1	F	67	VAL	5.0
1	B	70	ALA	5.0
1	H	173	ASN	5.0
1	K	34	GLN	4.9
1	K	145	ASP	4.9
1	A	33	GLY	4.8
1	H	34	GLN	4.7
1	M	66	GLU	4.7
1	H	15	ARG	4.7
1	K	72	ALA	4.7
1	H	77	GLN	4.7
1	K	33	GLY	4.6
1	M	70	ALA	4.6
1	K	175	LYS	4.6
1	O	241	GLY	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	173	ASN	4.6
1	H	170	SER	4.6
1	D	70	ALA	4.6
1	F	70	ALA	4.6
1	M	31	ASP	4.5
1	H	167	ILE	4.5
1	H	89	PHE	4.5
1	K	89	PHE	4.5
1	H	242	ARG	4.5
1	K	69	ASP	4.4
1	K	75	VAL	4.4
1	F	30	SER	4.4
1	K	30	SER	4.4
1	H	68	PRO	4.4
1	K	168	GLY	4.3
1	B	33	GLY	4.3
1	K	172	LYS	4.3
1	A	34	GLN	4.3
1	O	31	ASP	4.3
1	K	146	GLY	4.3
1	M	35	TYR	4.3
1	H	28	LYS	4.2
1	M	72	ALA	4.2
1	M	32	ASP	4.2
1	M	15	ARG	4.2
1	H	144	GLN	4.1
1	M	29	ARG	4.1
1	H	56	SER	4.1
1	M	467	TRP	4.1
1	H	69	ASP	4.1
1	H	145	ASP	4.1
1	F	32	ASP	4.0
1	K	478	ARG	4.0
1	F	172	LYS	4.0
1	H	172	LYS	4.0
1	B	32	ASP	4.0
1	H	29	ARG	4.0
1	M	167	ILE	4.0
1	H	227	ILE	3.9
1	K	144	GLN	3.9
1	H	36	SER	3.9
1	M	156	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	30	SER	3.8
1	K	156	LEU	3.8
1	M	34	GLN	3.8
1	H	174	VAL	3.8
1	F	143	VAL	3.7
1	H	91	ASP	3.7
1	O	30	SER	3.7
1	H	81	ASN	3.7
1	D	34	GLN	3.7
1	D	31	ASP	3.6
1	O	34	GLN	3.6
1	K	170	SER	3.6
1	F	173	ASN	3.6
1	K	242	ARG	3.6
1	B	116	GLY	3.6
1	M	145	ASP	3.5
1	O	173	ASN	3.5
1	O	117	GLU	3.5
1	A	117	GLU	3.5
1	K	117	GLU	3.5
1	H	474	ALA	3.5
1	M	144	GLN	3.5
1	H	67	VAL	3.5
1	F	37	PHE	3.4
1	K	151	VAL	3.4
1	K	477	ASN	3.4
1	K	65	LEU	3.4
1	K	54	THR	3.4
1	D	72	ALA	3.4
1	H	228	LEU	3.4
1	M	39	MET	3.4
1	K	19	ILE	3.4
1	H	134	LEU	3.4
1	O	242	ARG	3.3
1	O	32	ASP	3.3
1	F	117	GLU	3.3
1	H	231	PRO	3.3
1	M	178	PHE	3.3
1	O	29	ARG	3.3
1	K	53	LYS	3.3
1	B	34	GLN	3.3
1	K	71	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	229	SER	3.3
1	H	74	PRO	3.3
1	K	81	ASN	3.3
1	F	29	ARG	3.3
1	A	169	ASP	3.3
1	K	208	LEU	3.3
1	M	458	ARG	3.2
1	H	37	PHE	3.2
1	K	15	ARG	3.2
1	M	390	MET	3.2
1	B	240	ALA	3.2
1	D	30	SER	3.2
1	F	69	ASP	3.2
1	K	74	PRO	3.2
1	K	152	HIS	3.2
1	M	117	GLU	3.2
1	D	32	ASP	3.2
1	K	466	ALA	3.1
1	M	172	LYS	3.1
1	H	214	TYR	3.1
1	F	39	MET	3.1
1	H	240	ALA	3.1
1	K	214	TYR	3.1
1	K	476	LEU	3.1
1	K	239	PHE	3.1
1	M	231	PRO	3.1
1	H	171	LYS	3.1
1	K	166	GLU	3.1
1	K	163	LEU	3.1
1	D	169	ASP	3.1
1	F	458	ARG	3.1
1	K	80	LYS	3.0
1	A	156	LEU	3.0
1	D	29	ARG	3.0
1	M	68	PRO	3.0
1	M	474	ALA	3.0
1	M	73	GLY	3.0
1	F	34	GLN	3.0
1	F	15	ARG	3.0
1	K	28	LYS	3.0
1	H	175	LYS	2.9
1	K	467	TRP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	36	SER	2.9
1	A	29	ARG	2.9
1	M	242	ARG	2.9
1	K	180	LEU	2.9
1	O	119	THR	2.9
1	F	76	VAL	2.9
1	F	284	ILE	2.9
1	H	27	ILE	2.9
1	H	284	ILE	2.9
1	K	178	PHE	2.9
1	M	226	ARG	2.9
1	O	180	LEU	2.9
1	A	68	PRO	2.9
1	F	28	LYS	2.9
1	H	19	ILE	2.8
1	K	179	PHE	2.8
1	K	141	LYS	2.8
1	M	245	THR	2.8
1	H	92	ASP	2.8
1	K	39	MET	2.8
1	H	73	GLY	2.8
1	M	67	VAL	2.8
1	F	240	ALA	2.8
1	H	93	GLU	2.8
1	F	146	GLY	2.8
1	H	57	PHE	2.8
1	H	382	LEU	2.8
1	F	178	PHE	2.7
1	B	382	LEU	2.7
1	K	276	ARG	2.7
1	D	68	PRO	2.7
1	K	52	ALA	2.7
1	A	36	SER	2.7
1	H	166	GLU	2.7
1	M	471	SER	2.7
1	M	119	THR	2.7
1	H	79	LEU	2.7
1	K	171	LYS	2.6
1	K	73	GLY	2.6
1	K	227	ILE	2.6
1	H	72	ALA	2.6
1	F	467	TRP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	143	VAL	2.6
1	H	197	GLN	2.6
1	F	276	ARG	2.6
1	M	263	GLN	2.6
1	M	84	GLY	2.6
1	H	180	LEU	2.6
1	M	139	VAL	2.6
1	H	83	TYR	2.6
1	M	146	GLY	2.6
1	B	479	LEU	2.6
1	M	214	TYR	2.6
1	M	171	LYS	2.6
1	K	284	ILE	2.6
1	B	169	ASP	2.5
1	O	156	LEU	2.6
1	D	276	ARG	2.5
1	K	20	SER	2.5
1	F	156	LEU	2.5
1	H	152	HIS	2.5
1	B	241	GLY	2.5
1	M	140	VAL	2.5
1	H	157	MET	2.5
1	F	80	LYS	2.5
1	K	57	PHE	2.5
1	B	156	LEU	2.5
1	H	276	ARG	2.5
1	F	233	THR	2.5
1	K	82	GLU	2.5
1	F	167	ILE	2.5
1	A	178	PHE	2.5
1	A	172	LYS	2.5
1	M	53	LYS	2.5
1	M	285	VAL	2.5
1	F	168	GLY	2.5
1	H	454	LYS	2.5
1	H	156	LEU	2.4
1	M	276	ARG	2.4
1	O	276	ARG	2.4
1	H	467	TRP	2.4
1	A	37	PHE	2.4
1	F	179	PHE	2.4
1	K	119	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	65	LEU	2.4
1	K	66	GLU	2.4
1	K	319	LEU	2.4
1	M	93	GLU	2.4
1	H	359	ILE	2.4
1	B	68	PRO	2.4
1	F	479	LEU	2.4
1	B	151	VAL	2.4
1	M	157	MET	2.4
1	K	61	GLY	2.4
1	K	93	GLU	2.4
1	M	320	VAL	2.4
1	H	54	THR	2.4
1	M	229	SER	2.4
1	M	233	THR	2.4
1	A	276	ARG	2.4
1	F	175	LYS	2.4
1	H	458	ARG	2.4
1	D	403	ASP	2.4
1	H	179	PHE	2.3
1	H	383	VAL	2.3
1	B	29	ARG	2.3
1	F	226	ARG	2.3
1	O	240	ALA	2.3
1	F	145	ASP	2.3
1	A	173	ASN	2.3
1	M	478	ARG	2.3
1	K	473	VAL	2.3
1	D	33	GLY	2.3
1	O	477	ASN	2.3
1	F	60	TYR	2.3
1	H	151	VAL	2.3
1	H	66	GLU	2.3
1	K	228	LEU	2.3
1	M	28	LYS	2.3
1	F	478	ARG	2.3
1	M	174	VAL	2.3
1	M	284	ILE	2.3
1	K	91	ASP	2.3
1	F	66	GLU	2.3
1	F	320	VAL	2.2
1	F	93	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	390	MET	2.2
1	K	244	VAL	2.2
1	D	73	GLY	2.2
1	K	84	GLY	2.2
1	B	69	ASP	2.2
1	F	72	ALA	2.2
1	H	39	MET	2.2
1	H	18	LEU	2.2
1	K	382	LEU	2.2
1	H	477	ASN	2.2
1	F	33	GLY	2.2
1	F	56	SER	2.2
1	K	318	VAL	2.2
1	M	33	GLY	2.2
1	A	408	MET	2.2
1	K	390	MET	2.2
1	K	245	THR	2.2
1	A	30	SER	2.2
1	F	71	GLU	2.2
1	K	76	VAL	2.2
1	F	171	LYS	2.2
1	O	172	LYS	2.2
1	D	117	GLU	2.2
1	D	44	LEU	2.2
1	K	79	LEU	2.2
1	K	137	GLN	2.2
1	A	285	VAL	2.2
1	F	174	VAL	2.2
1	O	320	VAL	2.2
1	M	240	ALA	2.2
1	K	56	SER	2.2
1	F	263	GLN	2.1
1	K	479	LEU	2.1
1	M	479	LEU	2.1
1	A	28	LYS	2.1
1	H	141	LYS	2.1
1	F	89	PHE	2.1
1	F	162	MET	2.1
1	F	474	ALA	2.1
1	H	20	SER	2.1
1	O	478	ARG	2.1
1	B	390	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	179	PHE	2.1
1	H	133	ARG	2.1
1	F	285	VAL	2.1
1	K	231	PRO	2.1
1	M	234	PRO	2.1
1	O	37	PHE	2.1
1	K	165	GLU	2.1
1	K	447	GLU	2.1
1	K	458	ARG	2.1
1	H	61	GLY	2.1
1	F	180	LEU	2.1
1	K	48	LEU	2.1
1	D	151	VAL	2.1
1	M	89	PHE	2.1
1	A	152	HIS	2.1
1	M	177	GLY	2.1
1	F	381	CYS	2.1
1	D	284	ILE	2.0
1	K	92	ASP	2.0
1	H	87	PRO	2.0
1	M	408	MET	2.0
1	K	88	VAL	2.0
1	K	143	VAL	2.0
1	K	383	VAL	2.0
1	K	83	TYR	2.0
1	B	180	LEU	2.0
1	K	18	LEU	2.0
1	B	119	THR	2.0
1	K	142	ASP	2.0
1	F	231	PRO	2.0
1	F	148	MET	2.0
1	F	119	THR	2.0
1	K	44	LEU	2.0
1	D	172	LYS	2.0
1	H	269	GLN	2.0
1	K	285	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

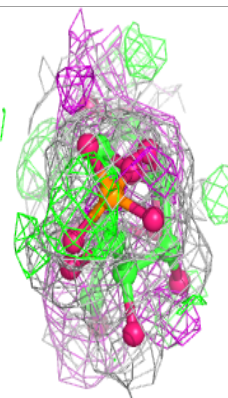
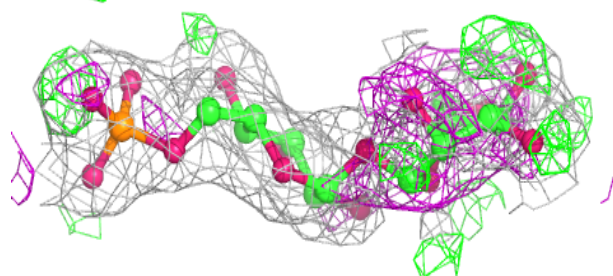
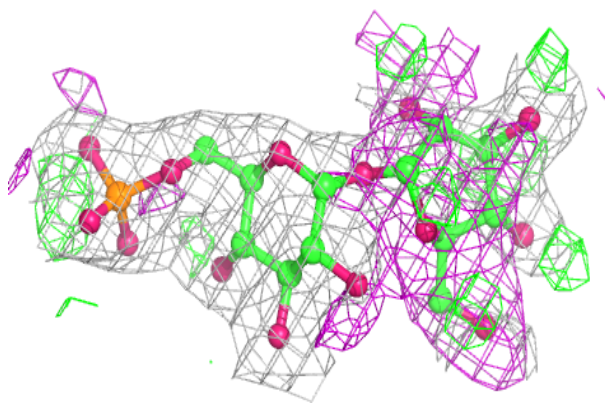
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	J	1	11/12	0.36	0.56	35,36,37,37	0
2	GLC	P	1	11/12	0.37	0.50	20,21,23,25	0
2	GLC	I	1	11/12	0.38	0.60	36,36,37,38	0
2	GLC	G	1	11/12	0.39	0.53	19,20,21,23	0
2	GLC	N	1	11/12	0.39	0.47	34,36,38,38	0
2	GLC	L	1	11/12	0.46	0.46	35,37,39,39	0
2	GLC	C	1	11/12	0.49	0.47	21,22,23,25	0
2	GLC	E	1	11/12	0.62	0.40	18,20,21,22	0
2	G6P	I	2	16/16	0.88	0.16	34,36,38,38	0
2	G6P	L	2	16/16	0.89	0.14	36,38,41,42	0
2	G6P	N	2	16/16	0.89	0.15	34,35,37,37	0
2	G6P	G	2	16/16	0.89	0.15	18,19,20,21	0
2	G6P	J	2	16/16	0.91	0.13	34,35,38,38	0
2	G6P	C	2	16/16	0.92	0.14	20,22,23,23	0
2	G6P	E	2	16/16	0.92	0.15	19,20,20,21	0
2	G6P	P	2	16/16	0.95	0.12	20,21,22,24	0

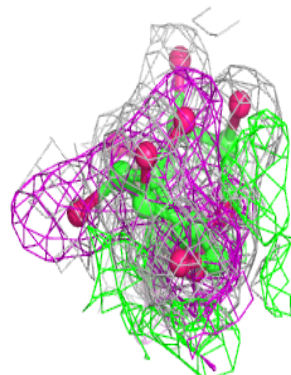
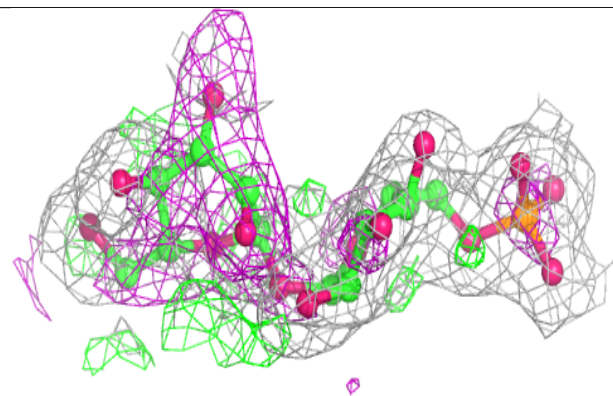
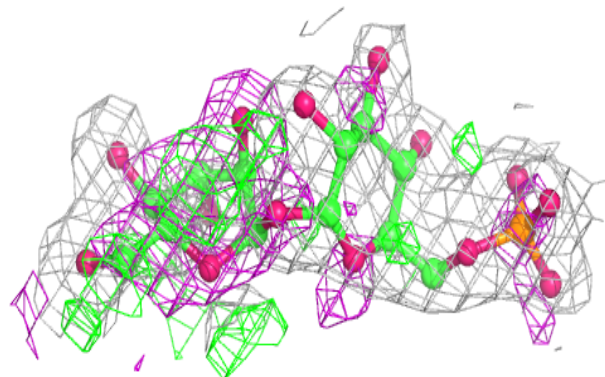
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

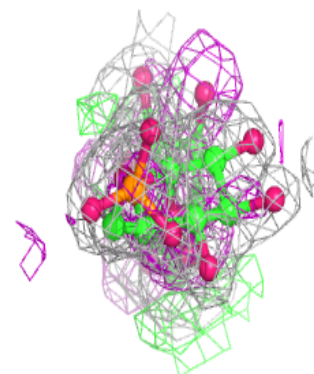
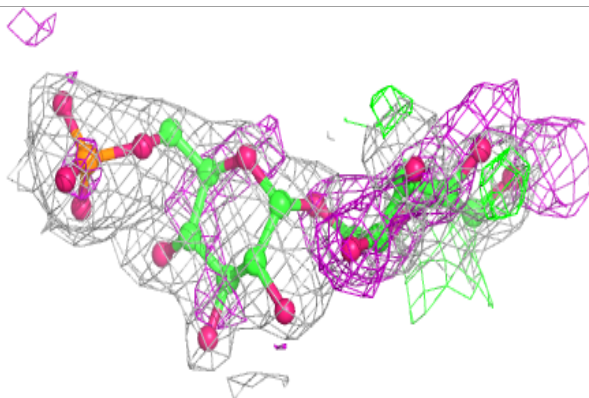
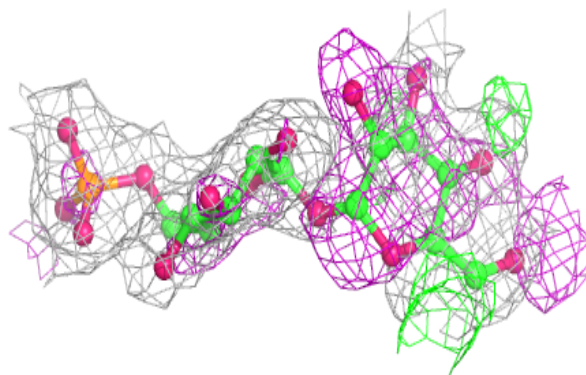
**Electron density around Chain J:**

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

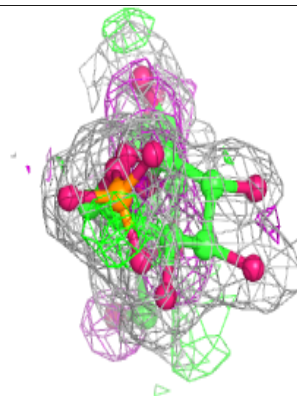
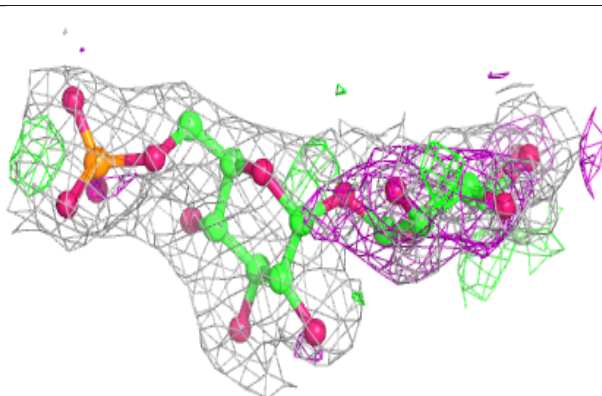
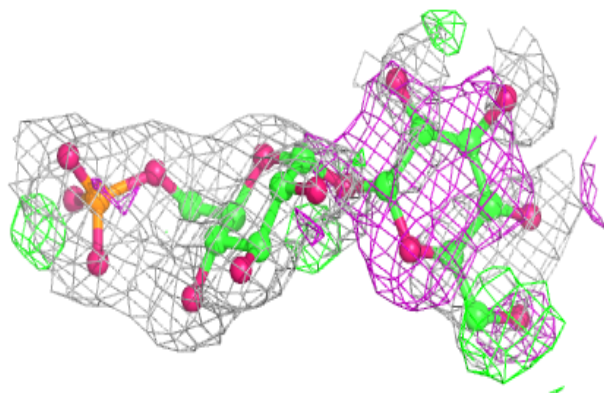


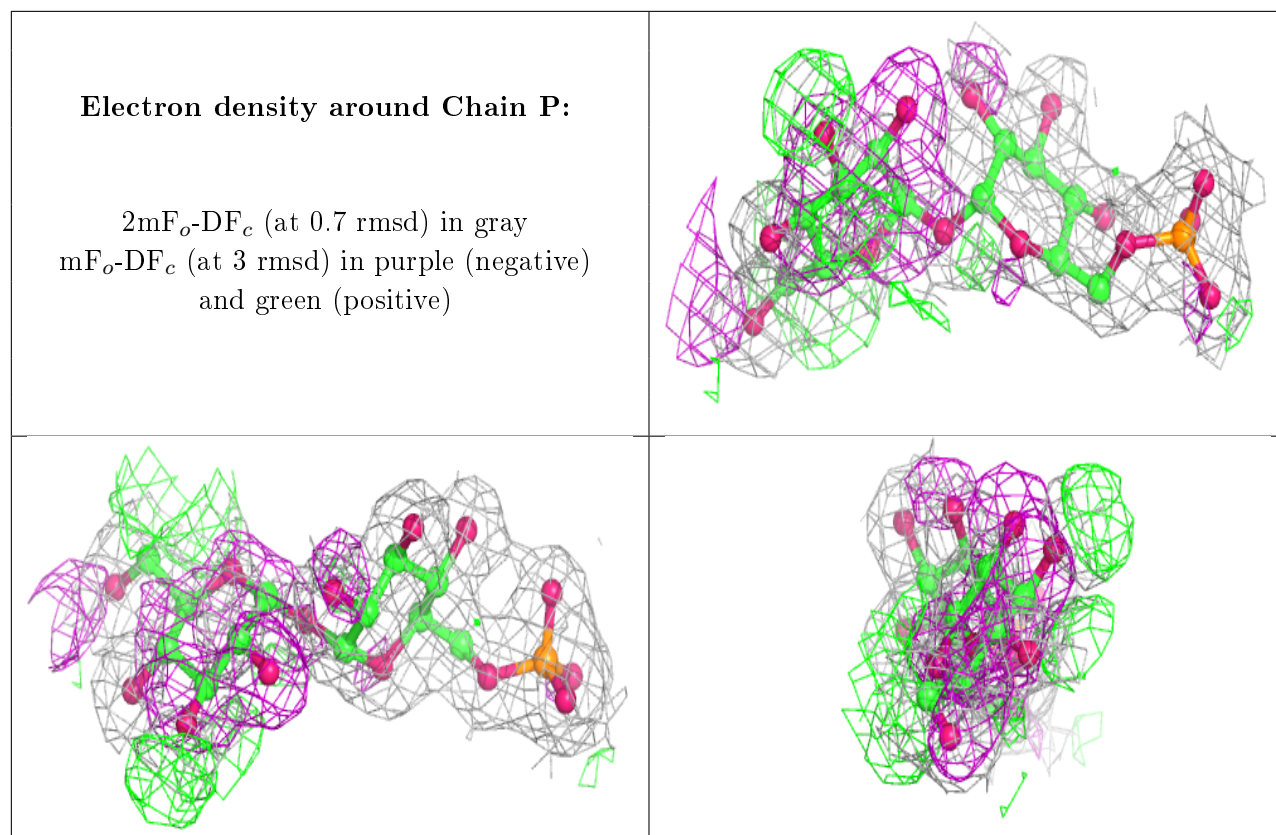
Electron density around Chain L:

$2mF_o-DF_c$ (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)





6.4 Ligands ⓘ

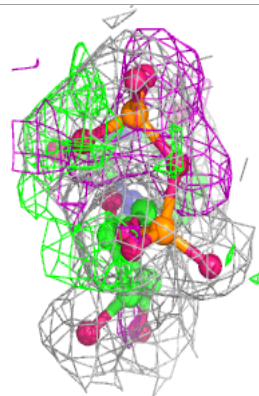
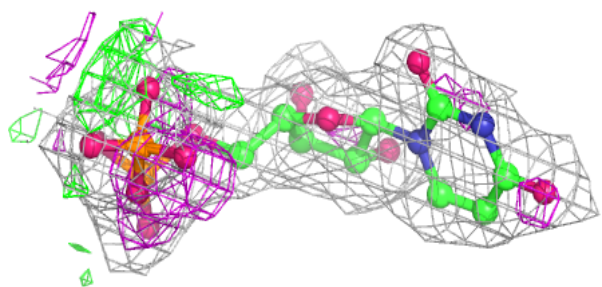
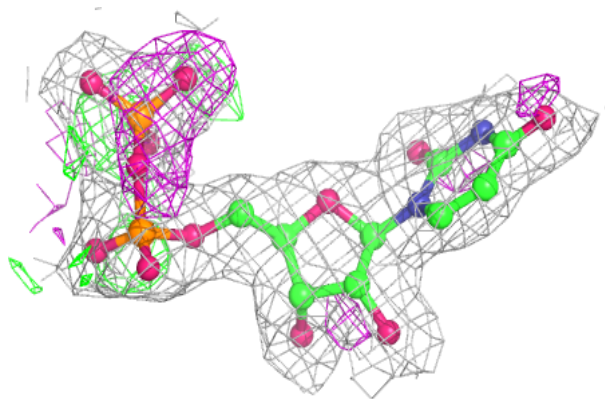
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UDP	H	502	25/25	0.83	0.17	29,31,33,36	0
3	UDP	F	502	25/25	0.89	0.13	31,34,35,35	0
3	UDP	D	502	25/25	0.91	0.14	18,21,22,22	0
3	UDP	M	502	25/25	0.92	0.14	32,34,36,36	0
3	UDP	K	502	25/25	0.94	0.12	33,35,36,38	0
3	UDP	A	502	25/25	0.95	0.11	20,23,24,24	0
3	UDP	B	502	25/25	0.95	0.12	18,20,21,22	0
3	UDP	O	502	25/25	0.95	0.13	20,22,24,25	0

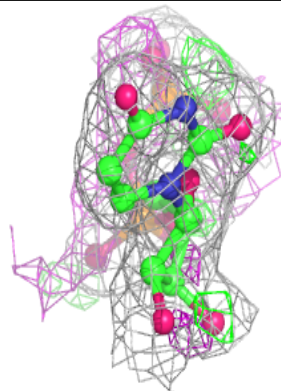
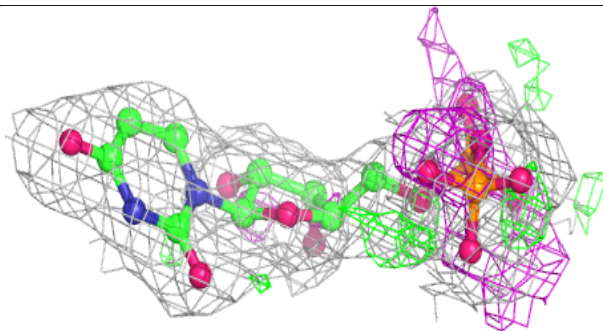
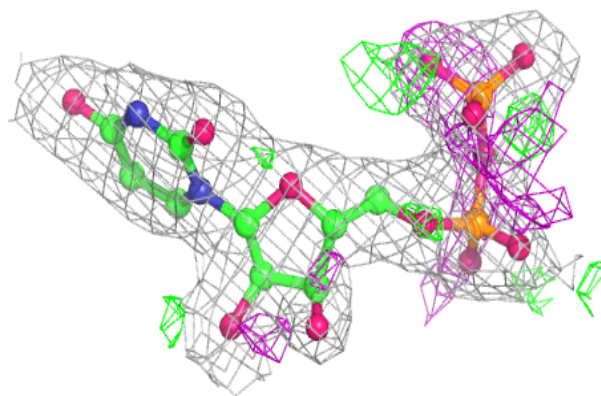
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UDP 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)

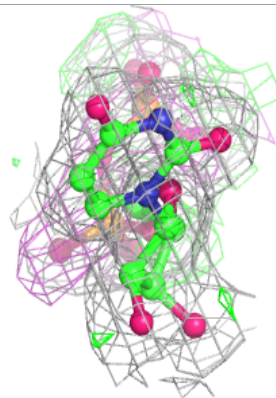
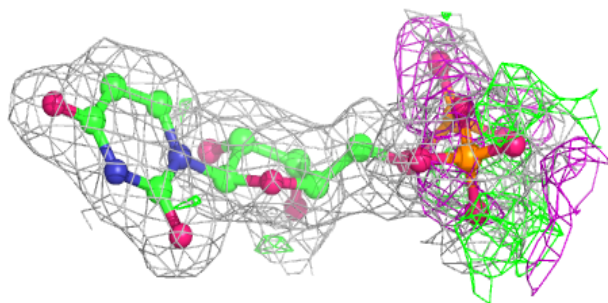
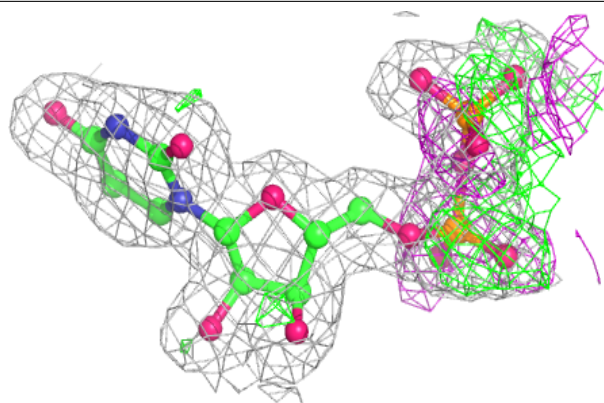
**Electron density around UDP F 502:**

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

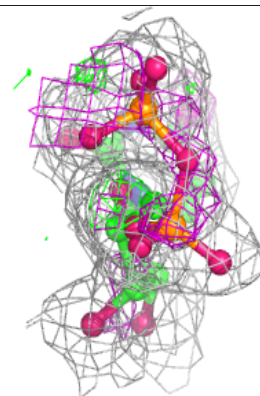
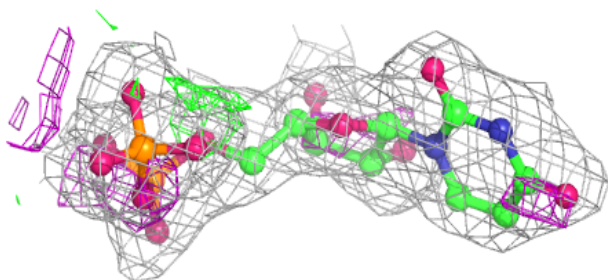
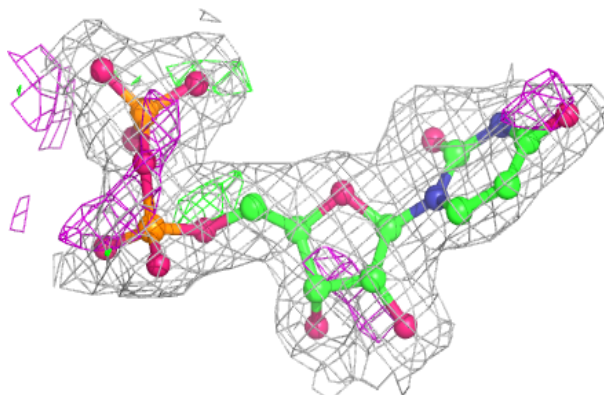


Electron density around UDP D 502:

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

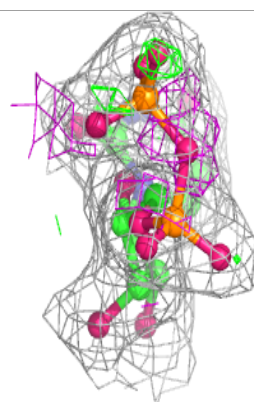
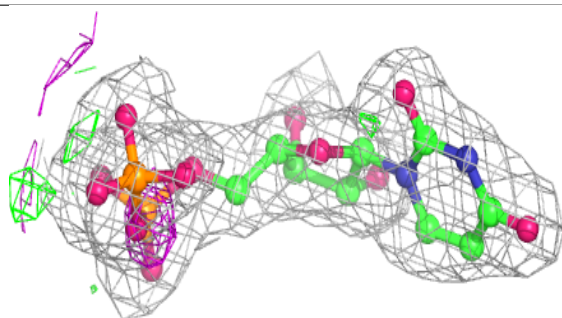
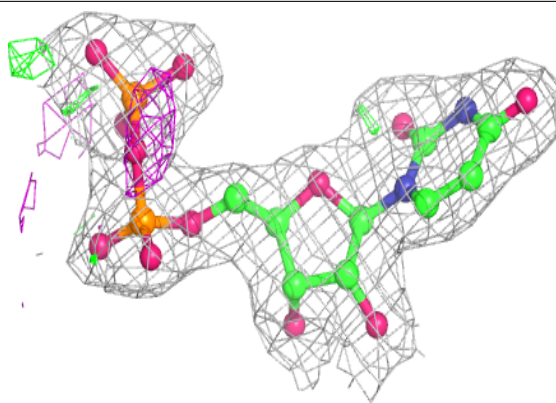
**Electron density around UDP M 502:**

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

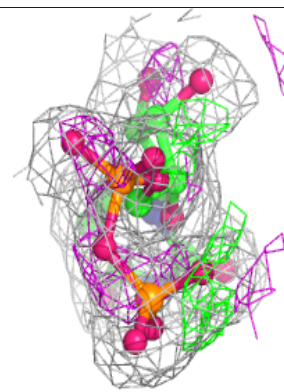
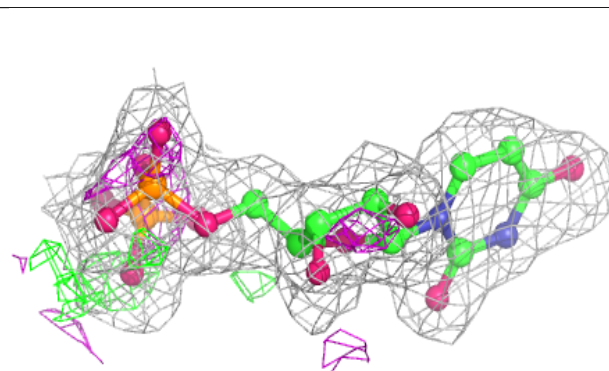
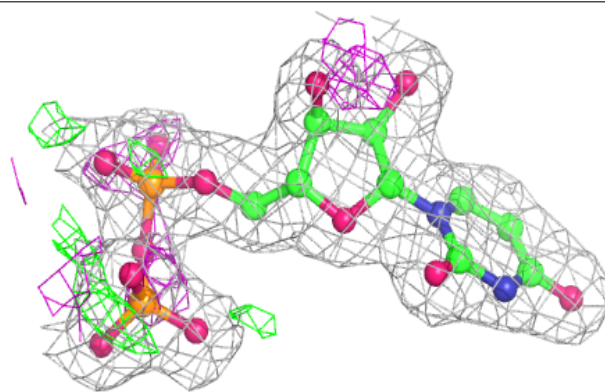


Electron density around UDP K 502:

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

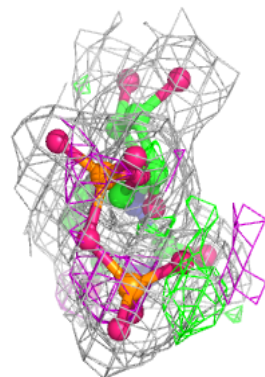
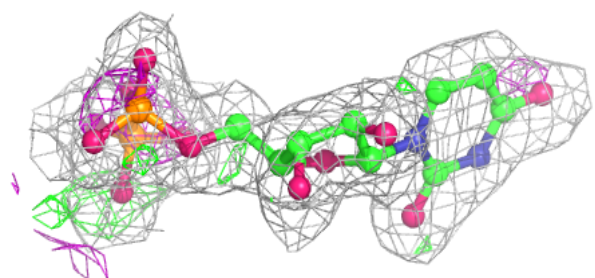
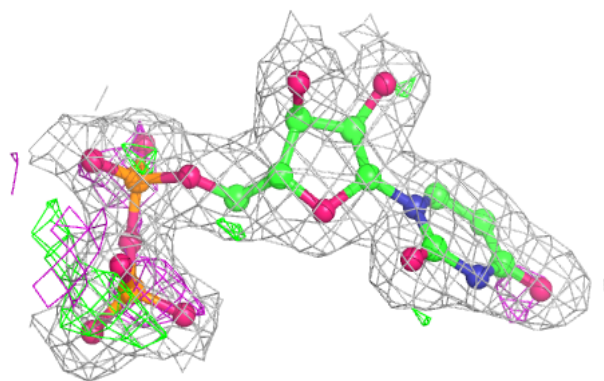
**Electron density around UDP A 502:**

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

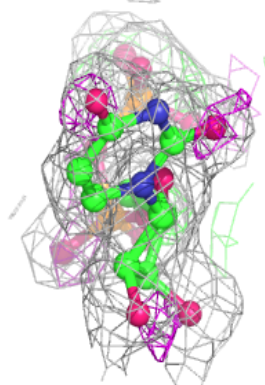
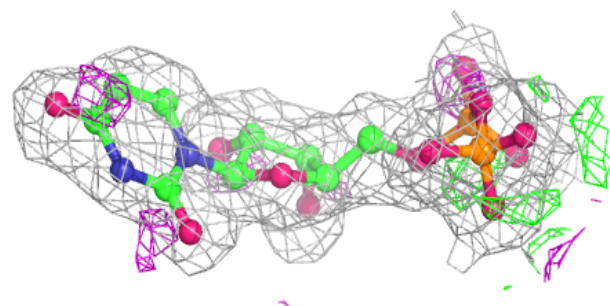
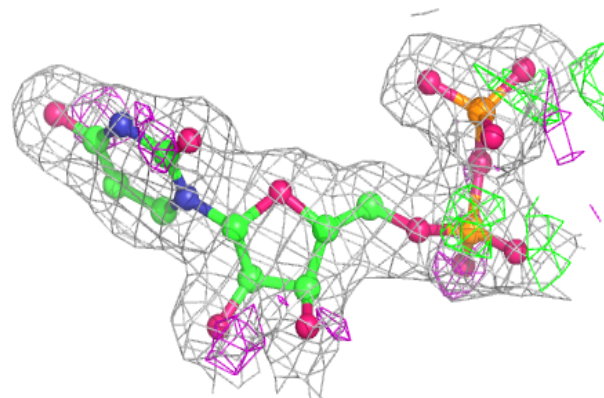


Electron density around UDP B 502:

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

**Electron density around UDP O 502:**

$2mF_o-DF_c$ (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.