



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:34 PM UTC

PDB ID : 8KB7 / pdb_00008kb7
Title : Crystal structure of UDP/mannose-bound AGO61/beta-1,4-N-Acetylglucosaminyltransferase 2 (POMGNT2)
Authors : Satoh, T.; Umezawa, F.; Yagi, H.; Kato, K.
Deposited on : 2023-08-04
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

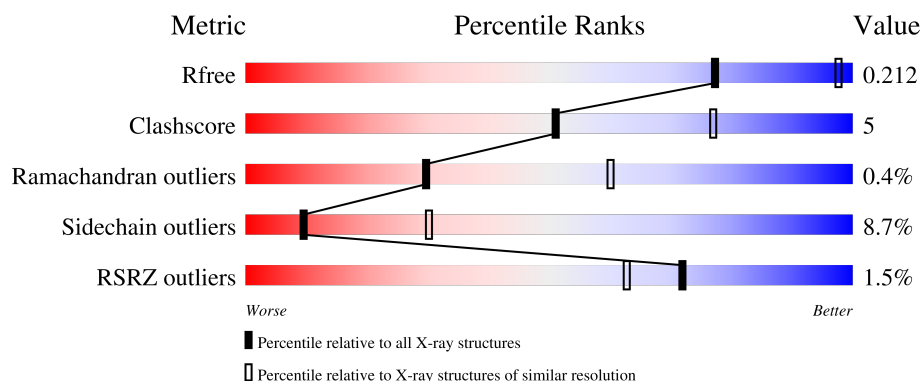
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

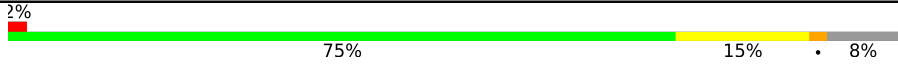
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	558	
1	B	558	
1	C	558	
1	D	558	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16869 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.

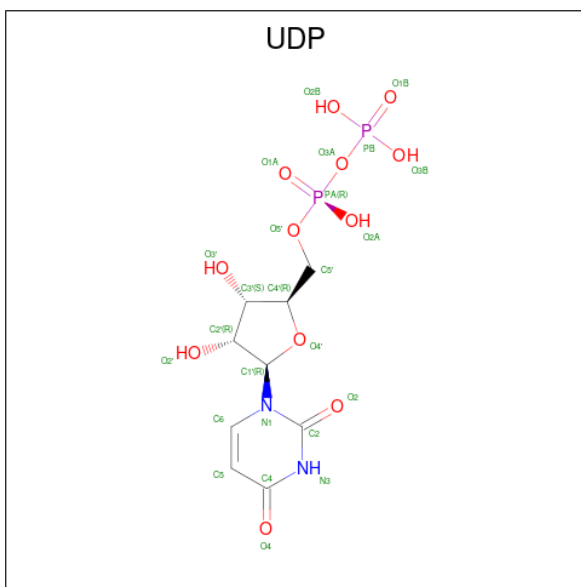
- Molecule 1 is a protein called Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4192	2712	724	733	23			
1	B	505	Total	C	N	O	S	0	0	0
			4121	2671	711	716	23			
1	C	511	Total	C	N	O	S	0	0	0
			4163	2695	720	725	23			
1	D	510	Total	C	N	O	S	0	0	0
			4157	2692	719	723	23			

There are 12 discrepancies between the modelled and reference sequences:

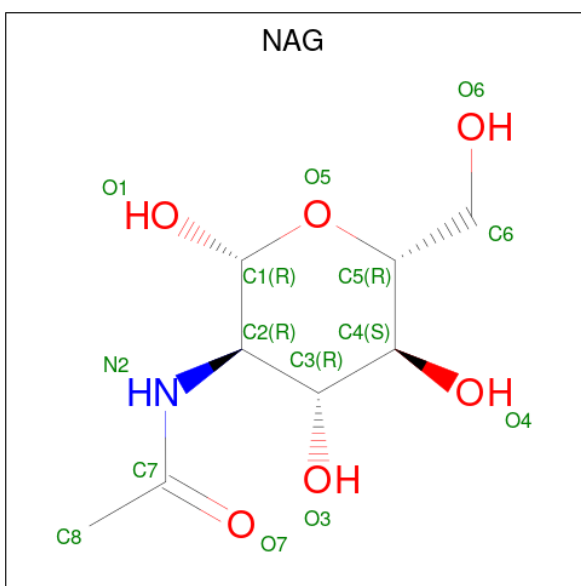
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP Q8NAT1
A	24	GLU	-	expression tag	UNP Q8NAT1
A	25	PHE	-	expression tag	UNP Q8NAT1
B	23	GLY	-	expression tag	UNP Q8NAT1
B	24	GLU	-	expression tag	UNP Q8NAT1
B	25	PHE	-	expression tag	UNP Q8NAT1
C	23	GLY	-	expression tag	UNP Q8NAT1
C	24	GLU	-	expression tag	UNP Q8NAT1
C	25	PHE	-	expression tag	UNP Q8NAT1
D	23	GLY	-	expression tag	UNP Q8NAT1
D	24	GLU	-	expression tag	UNP Q8NAT1
D	25	PHE	-	expression tag	UNP Q8NAT1

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



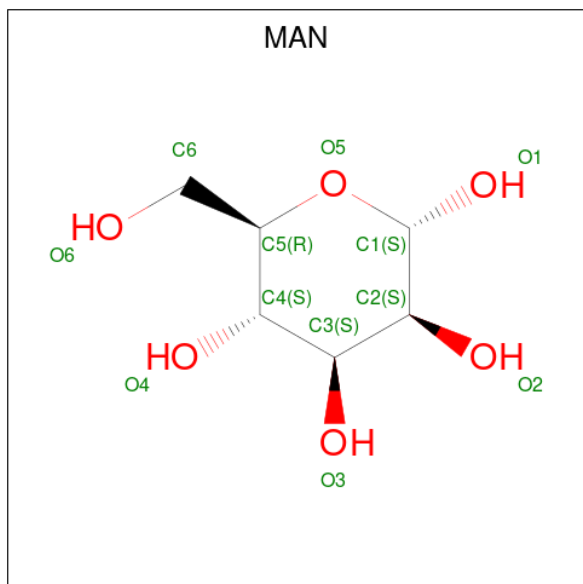
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		
4	D	1	Total	C	O	0	0
			12	6	6		

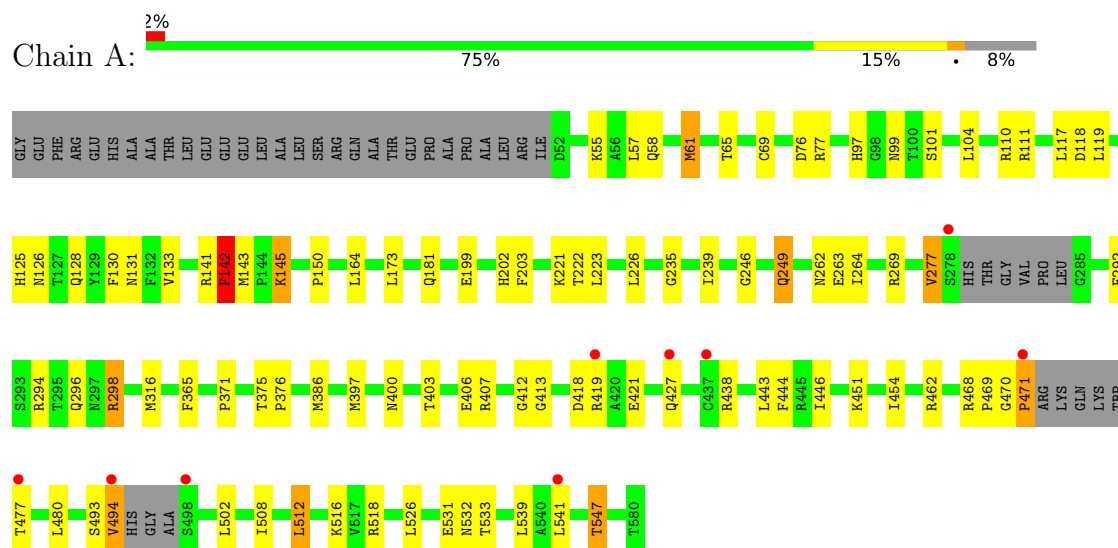
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0
5	C	1	Total 1	Cl 1	0	0
5	D	1	Total 1	Cl 1	0	0

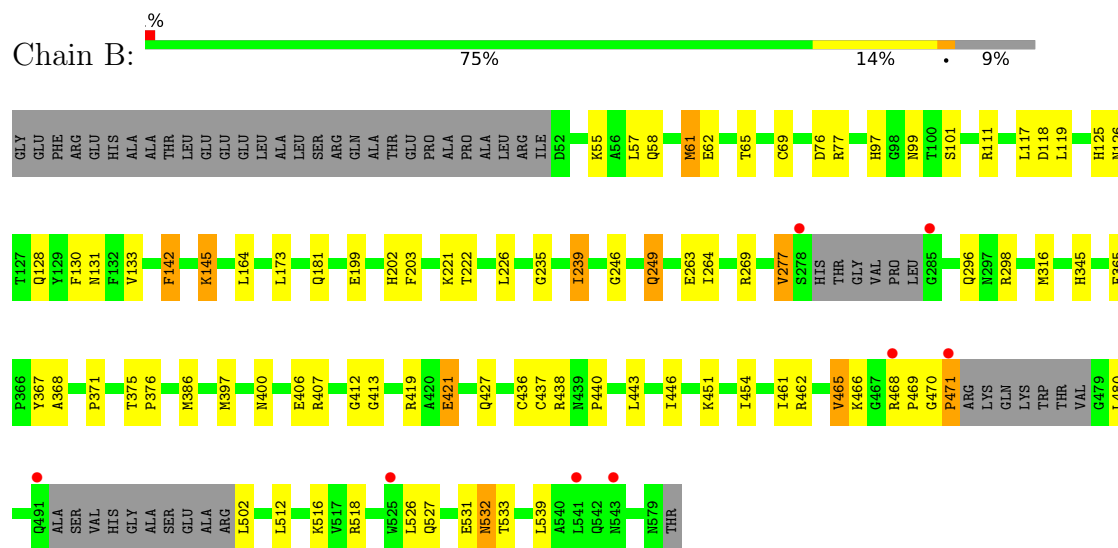
3 Residue-property plots [i](#)

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.

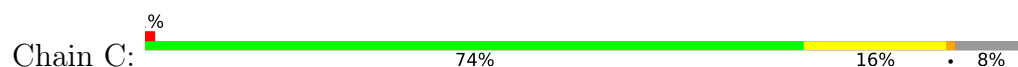
- Molecule 1: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

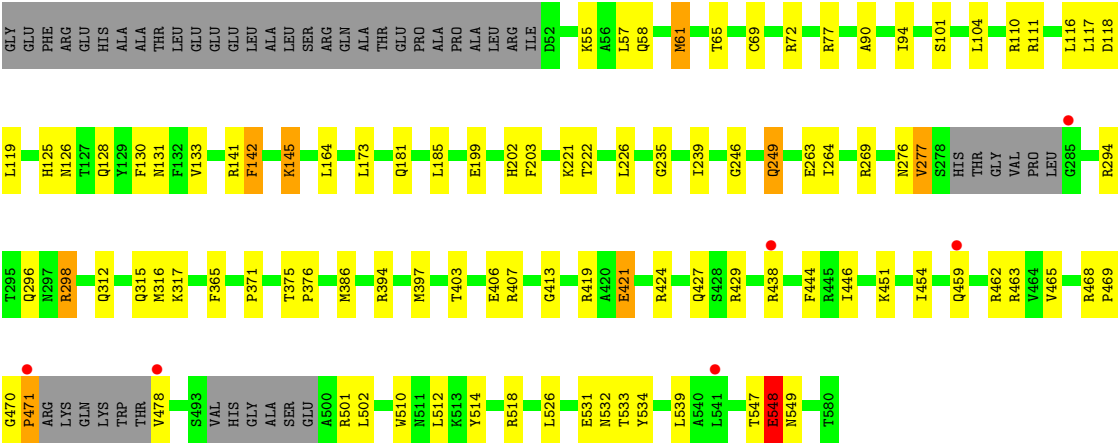


- Molecule 1: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2

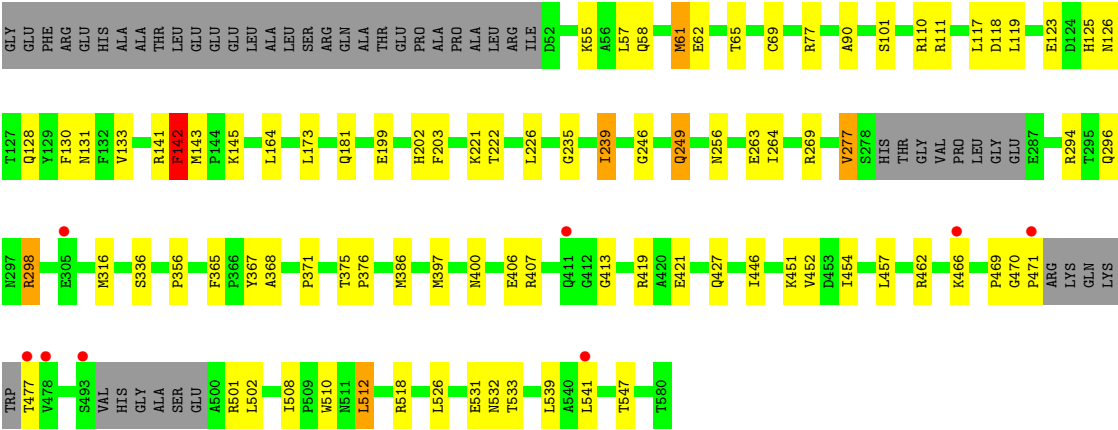
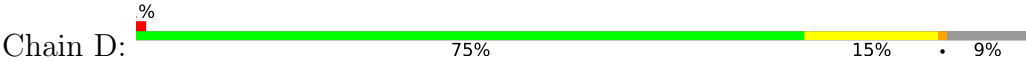


- Molecule 1: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2





● Molecule 1: Protein O-linked-mannose beta-1,4-N-acetylglucosaminyltransferase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.02Å 150.00Å 191.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 2.80 47.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.92-2.80) 99.9 (47.92-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.228 (Not available) , 0.212	Depositor DCC
R_{free} test set	5042 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	89.1	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16869	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MAN, UDP, NAG

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	1.01	1/4306 (0.0%)	1.36	4/5854 (0.1%)
1	B	1.00	0/4235	1.35	4/5758 (0.1%)
1	C	1.01	0/4277	1.34	5/5814 (0.1%)
1	D	0.99	0/4271	1.34	5/5807 (0.1%)
All	All	1.00	1/17089 (0.0%)	1.35	18/23233 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	MET	N-CA	5.05	1.50	1.45

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	GLY	CA-C-O	-6.73	117.61	122.45
1	C	235	GLY	CA-C-O	-6.32	117.90	122.45
1	A	235	GLY	CA-C-O	-6.12	118.04	122.45
1	C	534	TYR	CB-CA-C	5.85	119.45	109.80
1	D	235	GLY	CA-C-O	-5.68	118.03	122.52
1	B	99	ASN	CB-CA-C	5.46	119.15	109.65
1	A	418	ASP	CA-C-O	-5.30	115.72	121.44
1	D	62	GLU	CA-C-N	5.27	125.69	119.94
1	D	62	GLU	C-N-CA	5.27	125.69	119.94
1	A	99	ASN	CB-CA-C	5.22	118.73	109.65
1	A	142	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	548	GLU	N-CA-C	-5.18	103.69	110.53
1	D	123	GLU	CA-C-O	-5.08	116.28	122.64
1	B	62	GLU	CA-C-N	5.04	125.44	119.94
1	B	62	GLU	C-N-CA	5.04	125.44	119.94
1	C	438	ARG	CB-CG-CD	5.04	122.90	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	PHE	CA-CB-CG	5.04	118.84	113.80
1	C	465	VAL	CA-C-O	-5.01	118.28	122.63

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	4192	0	4168	49	0
1	B	4121	0	4098	52	0
1	C	4163	0	4141	48	0
1	D	4157	0	4140	47	0
2	A	25	0	11	0	0
2	B	25	0	11	3	0
2	C	25	0	11	0	0
2	D	25	0	11	0	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
3	C	28	0	26	2	0
3	D	14	0	13	0	0
4	A	12	0	12	0	0
4	B	12	0	12	0	0
4	C	12	0	12	0	0
4	D	12	0	12	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
All	All	16869	0	16717	174	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 5.

All (174) 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:B:421:GLU:HG3	1:D:547:THR:HG21	1.68	0.76
1:B:440:PRO:HG2	1:D:501:ARG:HH12	1.51	0.75
1:B:277:VAL:CG1	1:B:277:VAL:O	2.39	0.70
1:A:547:THR:HG21	1:C:421:GLU:HG3	1.76	0.68
1:A:277:VAL:CG1	1:A:277:VAL:O	2.43	0.67
1:B:264:ILE:HB	1:B:386:MET:HE2	1.78	0.65
1:A:76:ASP:OD2	1:B:76:ASP:OD2	2.15	0.65
1:B:277:VAL:O	1:B:277:VAL:HG12	1.96	0.65
1:A:397:MET:HE2	1:A:400:ASN:ND2	2.11	0.64
1:A:277:VAL:O	1:A:277:VAL:HG12	1.97	0.64
1:C:277:VAL:CG1	1:C:277:VAL:O	2.45	0.64
1:C:264:ILE:HB	1:C:386:MET:HE2	1.79	0.64
1:D:277:VAL:CG1	1:D:277:VAL:O	2.45	0.64
1:A:493:SER:O	1:A:494:VAL:HG23	1.98	0.63
1:B:298:ARG:NH2	1:B:345:HIS:O	2.31	0.63
1:A:264:ILE:HB	1:A:386:MET:HE2	1.80	0.63
1:C:276:ASN:HD22	3:C:603:NAG:H83	1.64	0.62
1:D:125:HIS:H	1:D:128:GLN:HE21	1.48	0.62
1:B:397:MET:HE2	1:B:400:ASN:ND2	2.15	0.61
1:C:57:LEU:O	1:C:61:MET:HG3	2.00	0.61
1:C:119:LEU:HG	1:C:130:PHE:HB2	1.83	0.61
1:B:57:LEU:O	1:B:61:MET:HG3	2.01	0.60
1:D:277:VAL:O	1:D:277:VAL:HG12	2.00	0.60
1:C:277:VAL:O	1:C:277:VAL:HG12	2.01	0.60
1:C:125:HIS:H	1:C:128:GLN:HE21	1.50	0.59
2:B:601:UDP:H2'	2:B:601:UDP:O5'	2.02	0.59
1:D:119:LEU:HG	1:D:130:PHE:HB2	1.84	0.59
1:A:119:LEU:HG	1:A:130:PHE:HB2	1.85	0.59
1:B:421:GLU:OE1	1:D:501:ARG:NH2	2.35	0.59
1:B:125:HIS:H	1:B:128:GLN:HE21	1.51	0.58
1:A:125:HIS:H	1:A:128:GLN:HE21	1.50	0.58
1:C:65:THR:O	1:C:101:SER:HB2	2.04	0.58
1:D:57:LEU:O	1:D:61:MET:HG3	2.03	0.58
1:B:119:LEU:HG	1:B:130:PHE:HB2	1.86	0.57
1:C:421:GLU:HG2	1:C:424:ARG:NH2	2.20	0.57
1:D:264:ILE:HB	1:D:386:MET:HE2	1.86	0.56
1:A:57:LEU:O	1:A:61:MET:HG3	2.06	0.56
1:A:480:LEU:CD2	1:B:97:HIS:CD2	2.89	0.56
1:C:514:TYR:CE2	1:D:143:MET:HG3	2.41	0.55
1:A:65:THR:O	1:A:101:SER:HB2	2.07	0.55
1:B:65:THR:O	1:B:101:SER:HB2	2.08	0.54
1:D:65:THR:O	1:D:101:SER:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:MET:HE2	1:D:400:ASN:ND2	2.22	0.54
1:A:316:MET:HE1	1:A:469:PRO:HG2	1.92	0.52
1:B:465:VAL:O	1:B:465:VAL:HG23	2.09	0.52
1:A:118:ASP:HA	1:A:128:GLN:O	2.10	0.52
1:C:118:ASP:HA	1:C:128:GLN:O	2.11	0.51
1:A:97:HIS:CD2	1:B:480:LEU:CD2	2.95	0.50
1:D:118:ASP:HA	1:D:128:GLN:O	2.10	0.50
1:C:77:ARG:HB3	1:C:117:LEU:HD23	1.94	0.49
1:B:118:ASP:HA	1:B:128:GLN:O	2.11	0.49
1:A:480:LEU:HD22	1:B:97:HIS:CD2	2.48	0.49
1:D:77:ARG:HB3	1:D:117:LEU:HD23	1.94	0.49
1:C:145:LYS:HA	1:C:145:LYS:HE2	1.95	0.48
1:A:145:LYS:HA	1:A:145:LYS:HE2	1.95	0.48
1:C:119:LEU:N	1:C:128:GLN:O	2.41	0.48
1:A:480:LEU:HD21	1:B:97:HIS:CD2	2.48	0.48
1:B:298:ARG:NH1	2:B:601:UDP:O3B	2.46	0.48
1:C:510:TRP:CE2	1:D:90:ALA:HB2	2.48	0.48
1:B:465:VAL:O	1:B:465:VAL:CG2	2.61	0.48
2:B:601:UDP:O5'	2:B:601:UDP:C2'	2.62	0.48
1:D:316:MET:HE1	1:D:469:PRO:HG2	1.96	0.47
1:C:90:ALA:HB2	1:D:510:TRP:CD1	2.50	0.47
1:A:119:LEU:N	1:A:128:GLN:O	2.41	0.47
1:A:77:ARG:HB3	1:A:117:LEU:HD23	1.97	0.47
1:D:77:ARG:O	1:D:117:LEU:CD2	2.63	0.47
1:A:61:MET:HE1	1:A:141:ARG:HG3	1.96	0.47
1:D:119:LEU:N	1:D:128:GLN:O	2.43	0.47
1:B:117:LEU:HB2	1:B:130:PHE:HB3	1.96	0.46
1:B:264:ILE:HG21	1:B:386:MET:CE	2.45	0.46
1:C:459:GLN:HB3	1:C:463:ARG:NH2	2.30	0.46
1:D:375:THR:N	1:D:376:PRO:CD	2.78	0.46
1:A:470:GLY:O	1:A:471:PRO:C	2.58	0.46
1:A:77:ARG:O	1:A:117:LEU:CD2	2.62	0.46
1:B:199:GLU:HB3	1:B:203:PHE:CG	2.51	0.46
1:A:375:THR:N	1:A:376:PRO:CD	2.79	0.46
1:C:77:ARG:O	1:C:117:LEU:CD2	2.64	0.46
1:D:117:LEU:HB2	1:D:130:PHE:HB3	1.98	0.46
1:B:77:ARG:HB3	1:B:117:LEU:HD23	1.96	0.46
1:B:119:LEU:N	1:B:128:GLN:O	2.43	0.46
1:D:470:GLY:O	1:D:471:PRO:C	2.58	0.46
1:A:117:LEU:HB2	1:A:130:PHE:HB3	1.99	0.45
1:B:440:PRO:CG	1:D:501:ARG:HH12	2.23	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:HIS:CD2	1:B:480:LEU:HD22	2.52	0.45
1:A:264:ILE:HG21	1:A:386:MET:CE	2.47	0.45
1:B:77:ARG:O	1:B:117:LEU:CD2	2.64	0.45
1:C:199:GLU:HB3	1:C:203:PHE:HB2	1.96	0.45
1:B:470:GLY:O	1:B:471:PRO:C	2.59	0.45
1:C:375:THR:N	1:C:376:PRO:CD	2.80	0.45
1:A:164:LEU:HD13	1:A:202:HIS:CE1	2.52	0.45
1:B:199:GLU:HB3	1:B:203:PHE:HB2	1.98	0.45
1:C:470:GLY:O	1:C:471:PRO:C	2.59	0.45
1:A:264:ILE:CB	1:A:386:MET:HE2	2.47	0.45
1:B:264:ILE:CB	1:B:386:MET:HE2	2.46	0.45
1:C:104:LEU:HG	1:D:239:ILE:HG21	1.98	0.45
1:D:199:GLU:HB3	1:D:203:PHE:HB2	1.98	0.45
1:D:446:ILE:HD12	1:D:446:ILE:HA	1.91	0.45
1:C:117:LEU:HB2	1:C:130:PHE:HB3	1.98	0.45
1:A:412:GLY:HA2	1:A:443:LEU:HB3	1.99	0.44
1:B:145:LYS:HA	1:B:145:LYS:HE2	1.98	0.44
1:B:246:GLY:HA2	1:B:249:GLN:O	2.17	0.44
1:B:375:THR:N	1:B:376:PRO:CD	2.80	0.44
1:C:61:MET:HE2	1:C:61:MET:HB3	1.89	0.44
1:A:199:GLU:HB3	1:A:203:PHE:HB2	1.98	0.44
1:B:316:MET:HE1	1:B:469:PRO:HG2	2.00	0.44
1:C:371:PRO:CD	1:C:394:ARG:HD2	2.47	0.44
1:A:403:THR:HB	1:A:444:PHE:CZ	2.53	0.44
1:C:164:LEU:HD13	1:C:202:HIS:CE1	2.53	0.44
1:D:111:ARG:HD2	1:D:131:ASN:OD1	2.18	0.44
1:C:298:ARG:HG3	1:C:446:ILE:O	2.18	0.43
1:C:264:ILE:HG21	1:C:386:MET:CE	2.48	0.43
1:D:199:GLU:HB3	1:D:203:PHE:CG	2.53	0.43
1:D:298:ARG:HG3	1:D:446:ILE:O	2.18	0.43
1:A:298:ARG:HG3	1:A:446:ILE:O	2.18	0.43
1:C:181:GLN:HE22	1:D:69:CYS:C	2.25	0.43
1:C:199:GLU:HB3	1:C:203:PHE:CG	2.53	0.43
1:C:365:PHE:CD1	1:C:371:PRO:HG3	2.53	0.43
1:D:508:ILE:HD12	1:D:512:LEU:HB3	2.01	0.43
1:C:547:THR:OG1	1:C:548:GLU:N	2.51	0.43
1:D:164:LEU:HD13	1:D:202:HIS:CE1	2.53	0.43
1:A:446:ILE:HD12	1:A:446:ILE:HA	1.91	0.43
1:B:412:GLY:HA2	1:B:443:LEU:HB3	2.01	0.43
1:C:316:MET:HE1	1:C:469:PRO:HG2	2.00	0.43
1:A:199:GLU:HB3	1:A:203:PHE:CG	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ARG:O	1:B:413:GLY:HA3	2.18	0.43
1:D:365:PHE:CD1	1:D:371:PRO:HG3	2.54	0.43
1:A:294:ARG:NH2	1:A:298:ARG:NH1	2.67	0.43
1:B:436:CYS:HA	1:B:437:CYS:HA	1.73	0.43
1:D:407:ARG:O	1:D:413:GLY:HA3	2.19	0.42
1:A:111:ARG:HD2	1:A:131:ASN:OD1	2.19	0.42
1:A:104:LEU:HG	1:B:239:ILE:HG21	2.01	0.42
1:A:508:ILE:HD12	1:A:512:LEU:HB3	2.00	0.42
1:C:94:ILE:HD11	1:D:510:TRP:CH2	2.54	0.42
1:B:111:ARG:HD2	1:B:131:ASN:OD1	2.19	0.42
1:A:365:PHE:CD1	1:A:371:PRO:HG3	2.54	0.42
1:B:164:LEU:HD13	1:B:202:HIS:CE1	2.55	0.42
1:B:527:GLN:HE21	1:B:532:ASN:HA	1.85	0.42
1:C:69:CYS:C	1:D:181:GLN:HE22	2.28	0.42
1:B:142:PHE:CD1	1:B:142:PHE:N	2.88	0.42
1:C:72:ARG:NH2	1:D:256:ASN:HB2	2.35	0.42
1:C:514:TYR:CE2	1:D:143:MET:CG	3.02	0.42
1:C:407:ARG:O	1:C:413:GLY:HA3	2.20	0.42
1:A:142:PHE:CD1	1:A:142:PHE:N	2.87	0.42
1:B:365:PHE:CD1	1:B:371:PRO:HG3	2.54	0.42
1:D:61:MET:HE1	1:D:141:ARG:HG3	2.00	0.42
1:C:199:GLU:HB3	1:C:203:PHE:CB	2.50	0.41
1:D:142:PHE:N	1:D:142:PHE:CD1	2.88	0.41
1:D:264:ILE:HG21	1:D:386:MET:CE	2.50	0.41
1:A:181:GLN:HE22	1:B:69:CYS:C	2.28	0.41
1:A:246:GLY:HA2	1:A:249:GLN:O	2.21	0.41
1:B:367:TYR:O	1:B:368:ALA:HB3	2.19	0.41
1:C:294:ARG:NH2	1:C:298:ARG:NH1	2.68	0.41
1:C:111:ARG:HD2	1:C:131:ASN:OD1	2.19	0.41
1:A:97:HIS:CD2	1:B:480:LEU:HD21	2.56	0.41
1:D:294:ARG:NH2	1:D:298:ARG:NH1	2.68	0.41
1:D:367:TYR:O	1:D:368:ALA:HB3	2.20	0.41
1:A:199:GLU:HB3	1:A:203:PHE:CB	2.51	0.41
1:A:407:ARG:O	1:A:413:GLY:HA3	2.21	0.41
1:C:77:ARG:HD2	1:C:116:LEU:O	2.21	0.41
1:D:336:SER:O	1:D:356:PRO:HD3	2.21	0.41
1:A:69:CYS:C	1:B:181:GLN:HE22	2.29	0.41
1:D:199:GLU:HB3	1:D:203:PHE:CB	2.51	0.41
1:B:461:ILE:HG22	1:B:465:VAL:HG22	2.03	0.41
1:C:246:GLY:HA2	1:C:249:GLN:O	2.20	0.41
1:C:276:ASN:HD22	3:C:603:NAG:C8	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:GLY:HA2	1:D:249:GLN:O	2.21	0.41
1:A:223:LEU:HD23	1:A:223:LEU:HA	1.92	0.40
1:B:298:ARG:HG2	1:B:446:ILE:O	2.21	0.40
1:D:452:VAL:HG11	1:D:457:LEU:HD22	2.03	0.40
1:C:61:MET:HE1	1:C:141:ARG:HG3	2.01	0.40
1:C:142:PHE:CD1	1:C:142:PHE:N	2.89	0.40
1:A:494:VAL:O	1:A:494:VAL:CG1	2.68	0.40
1:B:199:GLU:HB3	1:B:203:PHE:CB	2.51	0.40
1:C:403:THR:HB	1:C:444:PHE:CZ	2.56	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	507/558 (91%)	475 (94%)	30 (6%)	2 (0%)	30	60
1	B	497/558 (89%)	467 (94%)	28 (6%)	2 (0%)	30	60
1	C	503/558 (90%)	470 (93%)	30 (6%)	3 (1%)	21	51
1	D	502/558 (90%)	472 (94%)	28 (6%)	2 (0%)	30	60
All	All	2009/2232 (90%)	1884 (94%)	116 (6%)	9 (0%)	30	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	B	126	ASN
1	C	126	ASN
1	D	126	ASN
1	B	518	ARG
1	C	518	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	518	ARG
1	C	185	LEU
1	A	150	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	457/490 (93%)	414 (91%)	43 (9%)	8	27
1	B	449/490 (92%)	413 (92%)	36 (8%)	11	34
1	C	453/490 (92%)	410 (90%)	43 (10%)	8	26
1	D	453/490 (92%)	418 (92%)	35 (8%)	12	36
All	All	1812/1960 (92%)	1655 (91%)	157 (9%)	9	30

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	58	GLN
1	A	61	MET
1	A	110	ARG
1	A	133	VAL
1	A	142	PHE
1	A	145	LYS
1	A	173	LEU
1	A	221	LYS
1	A	222	THR
1	A	226	LEU
1	A	239	ILE
1	A	249	GLN
1	A	262	ASN
1	A	263	GLU
1	A	269	ARG
1	A	277	VAL
1	A	292	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	296	GLN
1	A	298	ARG
1	A	406	GLU
1	A	419	ARG
1	A	421	GLU
1	A	427	GLN
1	A	438	ARG
1	A	451	LYS
1	A	454	ILE
1	A	462	ARG
1	A	468	ARG
1	A	471	PRO
1	A	477	THR
1	A	494	VAL
1	A	502	LEU
1	A	512	LEU
1	A	516	LYS
1	A	518	ARG
1	A	526	LEU
1	A	531	GLU
1	A	532	ASN
1	A	533	THR
1	A	539	LEU
1	A	541	LEU
1	A	547	THR
1	B	55	LYS
1	B	58	GLN
1	B	61	MET
1	B	133	VAL
1	B	142	PHE
1	B	145	LYS
1	B	173	LEU
1	B	221	LYS
1	B	222	THR
1	B	226	LEU
1	B	239	ILE
1	B	249	GLN
1	B	263	GLU
1	B	269	ARG
1	B	277	VAL
1	B	296	GLN
1	B	406	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	419	ARG
1	B	421	GLU
1	B	427	GLN
1	B	438	ARG
1	B	451	LYS
1	B	454	ILE
1	B	462	ARG
1	B	465	VAL
1	B	466	LYS
1	B	468	ARG
1	B	471	PRO
1	B	502	LEU
1	B	512	LEU
1	B	516	LYS
1	B	526	LEU
1	B	531	GLU
1	B	532	ASN
1	B	533	THR
1	B	539	LEU
1	C	55	LYS
1	C	58	GLN
1	C	61	MET
1	C	110	ARG
1	C	133	VAL
1	C	142	PHE
1	C	145	LYS
1	C	173	LEU
1	C	221	LYS
1	C	222	THR
1	C	226	LEU
1	C	239	ILE
1	C	249	GLN
1	C	263	GLU
1	C	269	ARG
1	C	277	VAL
1	C	296	GLN
1	C	298	ARG
1	C	312	GLN
1	C	315	GLN
1	C	317	LYS
1	C	397	MET
1	C	406	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	419	ARG
1	C	421	GLU
1	C	427	GLN
1	C	429	ARG
1	C	451	LYS
1	C	454	ILE
1	C	462	ARG
1	C	468	ARG
1	C	471	PRO
1	C	478	VAL
1	C	501	ARG
1	C	502	LEU
1	C	512	LEU
1	C	526	LEU
1	C	531	GLU
1	C	532	ASN
1	C	533	THR
1	C	539	LEU
1	C	548	GLU
1	C	549	ASN
1	D	55	LYS
1	D	58	GLN
1	D	61	MET
1	D	110	ARG
1	D	133	VAL
1	D	142	PHE
1	D	145	LYS
1	D	173	LEU
1	D	221	LYS
1	D	222	THR
1	D	226	LEU
1	D	239	ILE
1	D	249	GLN
1	D	263	GLU
1	D	269	ARG
1	D	277	VAL
1	D	296	GLN
1	D	298	ARG
1	D	406	GLU
1	D	419	ARG
1	D	421	GLU
1	D	427	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	451	LYS
1	D	454	ILE
1	D	462	ARG
1	D	466	LYS
1	D	477	THR
1	D	502	LEU
1	D	512	LEU
1	D	526	LEU
1	D	531	GLU
1	D	532	ASN
1	D	533	THR
1	D	539	LEU
1	D	541	LEU

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

Mol	Chain	Res	Type
1	A	125	HIS
1	A	181	GLN
1	A	202	HIS
1	A	219	GLN
1	A	251	GLN
1	A	256	ASN
1	A	262	ASN
1	A	315	GLN
1	A	400	ASN
1	A	527	GLN
1	B	125	HIS
1	B	181	GLN
1	B	202	HIS
1	B	219	GLN
1	B	251	GLN
1	B	315	GLN
1	B	400	ASN
1	B	527	GLN
1	B	579	ASN
1	C	125	HIS
1	C	181	GLN
1	C	202	HIS
1	C	251	GLN
1	C	256	ASN
1	C	262	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	400	ASN
1	C	579	ASN
1	D	125	HIS
1	D	128	GLN
1	D	181	GLN
1	D	202	HIS
1	D	251	GLN
1	D	315	GLN
1	D	400	ASN
1	D	527	GLN
1	D	579	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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
3	NAG	B	602	1	14,14,15	0.82	1 (7%)	17,19,21	1.50	3 (17%)
4	MAN	A	604	-	12,12,12	1.03	0	17,17,17	1.98	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	C	604	-	12,12,12	0.98	0	17,17,17	1.62	4 (23%)
3	NAG	A	603	1	14,14,15	1.19	1 (7%)	17,19,21	3.01	8 (47%)
4	MAN	D	603	-	12,12,12	1.06	0	17,17,17	2.80	10 (58%)
3	NAG	D	602	1	14,14,15	1.72	4 (28%)	17,19,21	2.85	11 (64%)
4	MAN	B	603	-	12,12,12	1.26	2 (16%)	17,17,17	1.97	5 (29%)
2	UDP	A	601	-	25,26,26	1.71	5 (20%)	38,40,40	1.53	6 (15%)
3	NAG	A	602	1	14,14,15	0.87	1 (7%)	17,19,21	1.47	2 (11%)
2	UDP	D	601	-	25,26,26	1.63	5 (20%)	38,40,40	1.53	7 (18%)
3	NAG	C	602	1	14,14,15	0.82	1 (7%)	17,19,21	1.39	3 (17%)
3	NAG	C	603	1	14,14,15	1.05	1 (7%)	17,19,21	2.48	4 (23%)
2	UDP	B	601	-	25,26,26	1.86	4 (16%)	38,40,40	2.20	15 (39%)
2	UDP	C	601	-	25,26,26	1.55	4 (16%)	38,40,40	1.68	12 (31%)

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	NAG	B	602	1	-	0/6/23/26	0/1/1/1
4	MAN	A	604	-	-	1/2/22/22	0/1/1/1
4	MAN	C	604	-	-	2/2/22/22	0/1/1/1
3	NAG	A	603	1	-	0/6/23/26	0/1/1/1
4	MAN	D	603	-	-	2/2/22/22	0/1/1/1
3	NAG	D	602	1	-	2/6/23/26	0/1/1/1
4	MAN	B	603	-	-	0/2/22/22	0/1/1/1
2	UDP	A	601	-	-	2/16/32/32	0/2/2/2
3	NAG	A	602	1	-	3/6/23/26	0/1/1/1
2	UDP	D	601	-	-	6/16/32/32	0/2/2/2
3	NAG	C	602	1	-	2/6/23/26	0/1/1/1
3	NAG	C	603	1	-	4/6/23/26	0/1/1/1
2	UDP	B	601	-	-	5/16/32/32	0/2/2/2
2	UDP	C	601	-	-	2/16/32/32	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	UDP	PA-O3A	6.44	1.66	1.59
2	A	601	UDP	PA-O3A	5.71	1.65	1.59
2	D	601	UDP	PA-O3A	5.02	1.64	1.59
2	C	601	UDP	PA-O3A	4.62	1.64	1.59
2	C	601	UDP	C2-N1	3.61	1.44	1.38
2	D	601	UDP	C2-N1	3.53	1.44	1.38
3	D	602	NAG	C1-C2	3.53	1.57	1.52
2	B	601	UDP	C2-N1	3.53	1.44	1.38
2	A	601	UDP	C2-N1	3.20	1.43	1.38
3	D	602	NAG	O5-C5	2.72	1.48	1.43
3	C	602	NAG	C1-C2	2.71	1.56	1.52
2	A	601	UDP	C4-N3	-2.62	1.34	1.38
3	B	602	NAG	C1-C2	2.58	1.55	1.52
2	C	601	UDP	C6-C5	2.46	1.40	1.35
3	D	602	NAG	C6-C5	2.45	1.60	1.51
3	A	603	NAG	O5-C5	2.41	1.48	1.43
4	B	603	MAN	O1-C1	2.35	1.47	1.39
3	D	602	NAG	O5-C1	2.31	1.47	1.43
2	D	601	UDP	O2-C2	2.25	1.27	1.23
3	A	602	NAG	C1-C2	2.23	1.55	1.52
4	B	603	MAN	O2-C2	2.17	1.48	1.43
2	A	601	UDP	C2-N3	-2.16	1.34	1.38
2	B	601	UDP	C6-C5	2.16	1.40	1.35
2	D	601	UDP	C4-N3	-2.15	1.34	1.38
2	D	601	UDP	C6-C5	2.09	1.39	1.35
3	C	603	NAG	O5-C1	2.08	1.47	1.43
2	A	601	UDP	C6-C5	2.04	1.39	1.35
2	B	601	UDP	C3'-C2'	2.03	1.58	1.53
2	C	601	UDP	C4-N3	-2.01	1.35	1.38

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	NAG	C1-O5-C5	9.17	124.48	112.19
3	C	603	NAG	C1-O5-C5	7.49	122.22	112.19
4	D	603	MAN	C3-C4-C5	7.06	123.03	110.23
3	D	602	NAG	C1-O5-C5	5.50	119.56	112.19
2	B	601	UDP	O3'-C3'-C2'	4.89	127.50	111.82
4	B	603	MAN	C3-C4-C5	4.51	118.40	110.23
2	C	601	UDP	N3-C2-N1	4.34	120.54	114.89
3	D	602	NAG	O4-C4-C3	-4.27	100.31	110.38
2	B	601	UDP	O3'-C3'-C4'	-4.17	99.10	111.08
3	D	602	NAG	C1-C2-N2	4.14	116.95	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	UDP	C4-N3-C2	-4.10	121.53	126.61
3	C	603	NAG	C8-C7-N2	3.93	122.64	116.12
2	A	601	UDP	N3-C2-N1	3.90	119.97	114.89
3	A	603	NAG	C6-C5-C4	-3.90	103.44	113.02
2	C	601	UDP	C4-N3-C2	-3.87	121.81	126.61
2	D	601	UDP	C4-N3-C2	-3.87	121.81	126.61
2	B	601	UDP	N3-C2-N1	3.82	119.86	114.89
4	A	604	MAN	C3-C4-C5	3.78	117.08	110.23
2	B	601	UDP	C4-N3-C2	-3.74	121.98	126.61
4	B	603	MAN	O2-C2-C1	3.72	117.82	109.25
3	A	603	NAG	O5-C5-C6	3.65	114.76	107.66
2	A	601	UDP	C5-C4-N3	3.60	119.84	114.80
2	B	601	UDP	O2'-C2'-C3'	3.59	123.33	111.82
4	A	604	MAN	C4-C3-C2	3.59	117.13	110.83
2	D	601	UDP	C5-C4-N3	3.50	119.70	114.80
4	A	604	MAN	O3-C3-C2	-3.47	102.19	110.38
4	C	604	MAN	C3-C4-C5	3.44	116.47	110.23
2	D	601	UDP	N3-C2-N1	3.41	119.34	114.89
3	D	602	NAG	C2-N2-C7	3.35	127.39	122.90
3	C	602	NAG	C4-C3-C2	-3.33	106.14	111.02
3	A	602	NAG	C1-O5-C5	3.31	116.62	112.19
2	B	601	UDP	O2B-PB-O1B	3.29	123.67	110.83
4	D	603	MAN	O3-C3-C2	-3.24	102.73	110.38
4	D	603	MAN	O5-C1-C2	3.23	115.98	110.30
2	B	601	UDP	O4'-C1'-C2'	-3.19	99.80	106.62
2	B	601	UDP	C5-C4-N3	3.17	119.25	114.80
3	D	602	NAG	O7-C7-N2	3.12	127.50	121.98
2	B	601	UDP	C2'-C1'-N1	3.09	121.85	113.25
3	B	602	NAG	C1-C2-N2	3.05	115.24	110.43
3	D	602	NAG	O7-C7-C8	-3.01	116.70	122.05
4	D	603	MAN	C6-C5-C4	3.00	120.39	113.02
4	D	603	MAN	O4-C4-C5	-3.00	101.95	109.32
2	B	601	UDP	O4-C4-C5	-2.99	120.00	125.16
3	A	603	NAG	O3-C3-C4	-2.97	103.38	110.38
3	D	602	NAG	O6-C6-C5	2.96	121.41	111.33
4	D	603	MAN	O5-C5-C6	2.90	113.64	106.44
4	C	604	MAN	O3-C3-C2	-2.90	103.54	110.38
4	D	603	MAN	O5-C5-C4	-2.88	104.51	109.70
4	C	604	MAN	O2-C2-C1	2.82	115.74	109.25
2	B	601	UDP	C2'-C3'-C4'	-2.79	97.21	102.61
4	D	603	MAN	O2-C2-C3	-2.78	103.82	110.38
3	A	603	NAG	C2-N2-C7	2.76	126.59	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	UDP	C5-C4-N3	2.68	118.56	114.80
2	B	601	UDP	C1'-N1-C2	2.66	122.36	117.59
3	A	603	NAG	C4-C3-C2	2.63	114.87	111.02
4	B	603	MAN	C4-C3-C2	2.63	115.45	110.83
3	A	602	NAG	O4-C4-C5	2.61	115.76	109.32
3	D	602	NAG	O4-C4-C5	2.61	115.74	109.32
4	A	604	MAN	O2-C2-C3	-2.58	104.28	110.38
2	A	601	UDP	O4-C4-C5	-2.57	120.73	125.16
3	D	602	NAG	O5-C1-C2	2.56	115.26	111.29
2	C	601	UDP	O2-C2-N3	-2.56	116.76	121.49
3	A	603	NAG	O5-C5-C4	2.54	117.01	110.83
2	A	601	UDP	O2-C2-N3	-2.49	116.90	121.49
2	A	601	UDP	O4'-C1'-N1	2.48	113.98	108.36
4	D	603	MAN	O3-C3-C4	2.48	116.22	110.38
2	D	601	UDP	O4-C4-C5	-2.36	121.10	125.16
2	B	601	UDP	O3B-PB-O3A	2.36	112.54	104.64
3	B	602	NAG	O4-C4-C5	2.36	115.13	109.32
3	C	602	NAG	C1-C2-N2	2.34	114.11	110.43
2	C	601	UDP	O4-C4-C5	-2.31	121.18	125.16
4	C	604	MAN	C4-C3-C2	2.31	114.88	110.83
4	B	603	MAN	O4-C4-C3	-2.30	104.95	110.38
2	C	601	UDP	C2'-C3'-C4'	-2.29	98.18	102.61
3	A	603	NAG	C3-C4-C5	2.28	114.36	110.23
2	C	601	UDP	O3'-C3'-C2'	2.26	119.06	111.82
3	D	602	NAG	C3-C4-C5	2.24	114.28	110.23
2	D	601	UDP	O4'-C1'-C2'	-2.23	101.84	106.62
3	C	603	NAG	C4-C3-C2	-2.23	107.75	111.02
3	B	602	NAG	C1-O5-C5	2.23	115.17	112.19
2	B	601	UDP	C6-N1-C2	-2.22	118.30	121.00
2	C	601	UDP	C1'-N1-C2	2.19	121.52	117.59
4	A	604	MAN	O1-C1-O5	-2.14	104.04	110.41
4	B	603	MAN	C1-C2-C3	-2.14	105.98	110.36
4	D	603	MAN	O4-C4-C3	-2.12	105.38	110.38
2	C	601	UDP	O4'-C1'-C2'	-2.12	102.08	106.62
3	C	603	NAG	O7-C7-C8	-2.10	118.32	122.05
2	D	601	UDP	O3B-PB-O1B	2.09	118.96	110.83
2	C	601	UDP	O3B-PB-O1B	2.07	118.88	110.83
2	B	601	UDP	O2-C2-N3	-2.06	117.70	121.49
3	C	602	NAG	C3-C4-C5	-2.06	106.50	110.23
2	C	601	UDP	C6-N1-C2	-2.05	118.50	121.00
2	C	601	UDP	O4'-C4'-C3'	2.02	109.17	105.15
3	D	602	NAG	C6-C5-C4	2.02	117.99	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	MAN	O1-C1-C2	2.02	114.85	108.98
2	D	601	UDP	O2-C2-N3	-2.01	117.77	121.49

There are no chirality outliers.

All (31) torsion outliers are listed below:

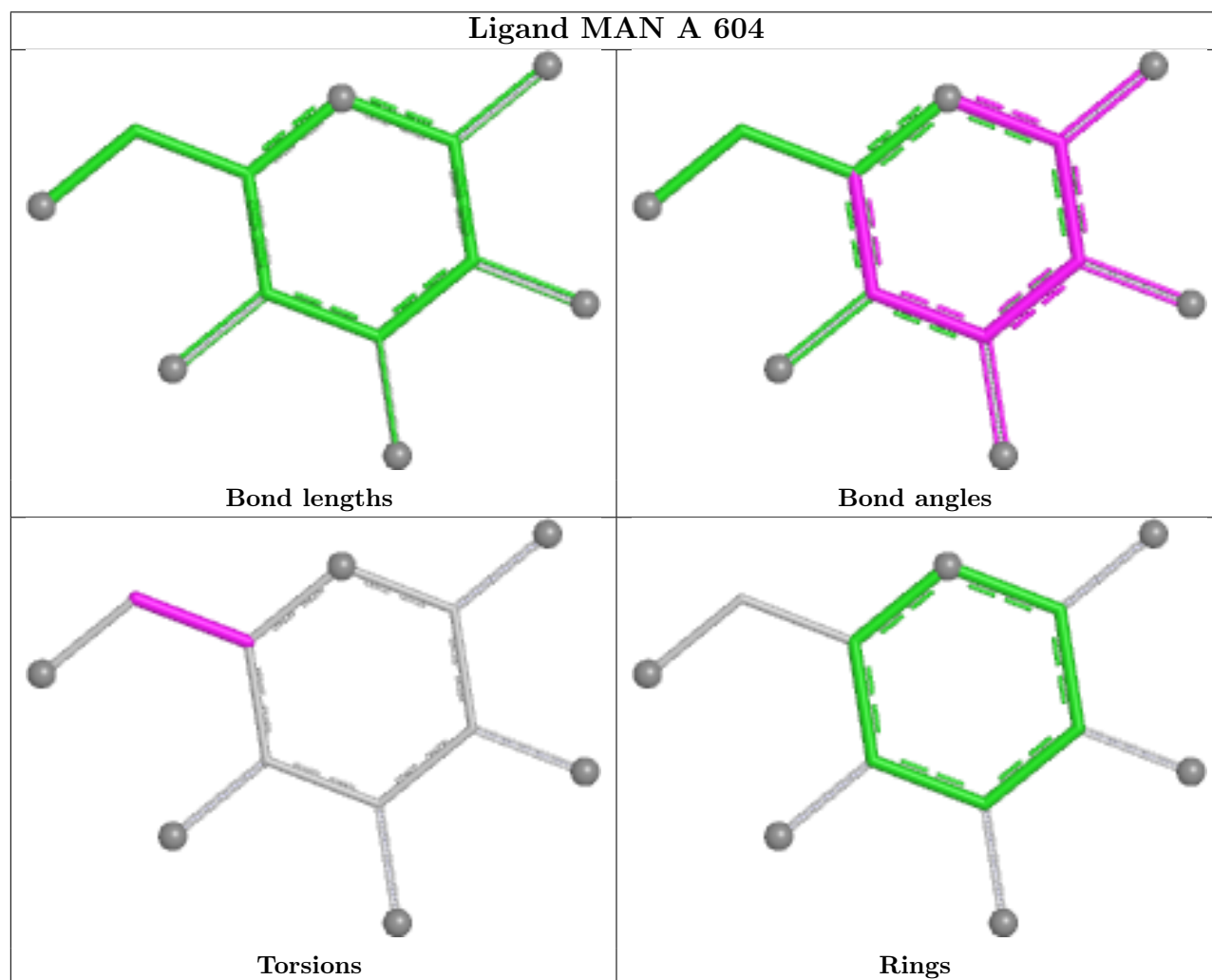
Mol	Chain	Res	Type	Atoms
2	A	601	UDP	C5'-O5'-PA-O2A
2	B	601	UDP	C5'-O5'-PA-O2A
2	B	601	UDP	C5'-O5'-PA-O3A
2	D	601	UDP	O4'-C4'-C5'-O5'
3	D	602	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
4	C	604	MAN	O5-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
2	D	601	UDP	C3'-C4'-C5'-O5'
4	C	604	MAN	C4-C5-C6-O6
3	D	602	NAG	C4-C5-C6-O6
3	C	602	NAG	O5-C5-C6-O6
3	C	603	NAG	C8-C7-N2-C2
3	C	603	NAG	O7-C7-N2-C2
3	C	603	NAG	O5-C5-C6-O6
4	D	603	MAN	C4-C5-C6-O6
3	C	602	NAG	C4-C5-C6-O6
3	C	603	NAG	C4-C5-C6-O6
4	A	604	MAN	O5-C5-C6-O6
4	D	603	MAN	O5-C5-C6-O6
2	D	601	UDP	PA-O3A-PB-O2B
2	C	601	UDP	O4'-C4'-C5'-O5'
2	A	601	UDP	C5'-O5'-PA-O3A
2	D	601	UDP	C5'-O5'-PA-O1A
2	D	601	UDP	C5'-O5'-PA-O2A
2	D	601	UDP	C5'-O5'-PA-O3A
2	B	601	UDP	PB-O3A-PA-O1A
3	A	602	NAG	C1-C2-N2-C7
2	B	601	UDP	PA-O3A-PB-O3B
2	C	601	UDP	C3'-C4'-C5'-O5'
2	B	601	UDP	PB-O3A-PA-O2A

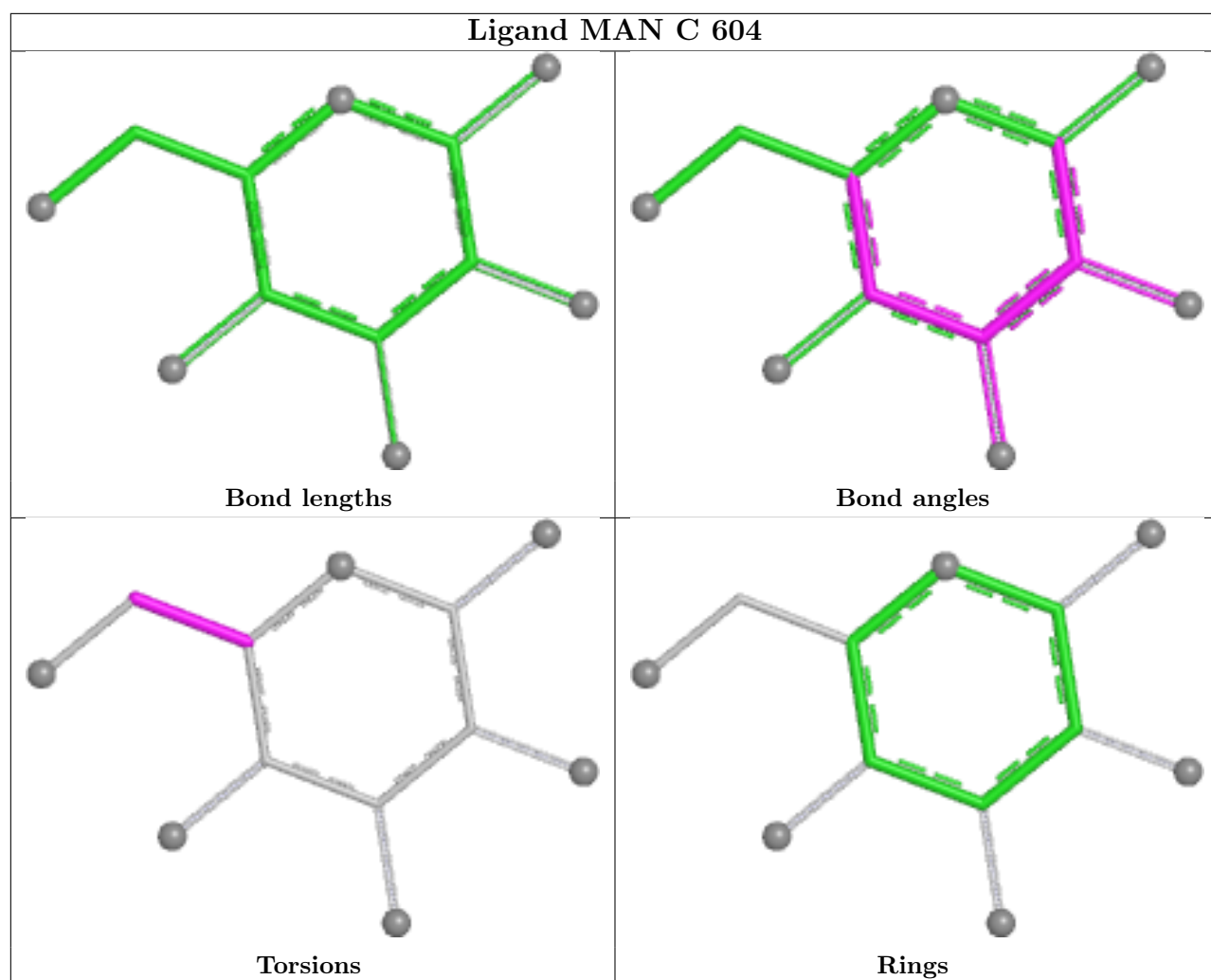
There are no ring outliers.

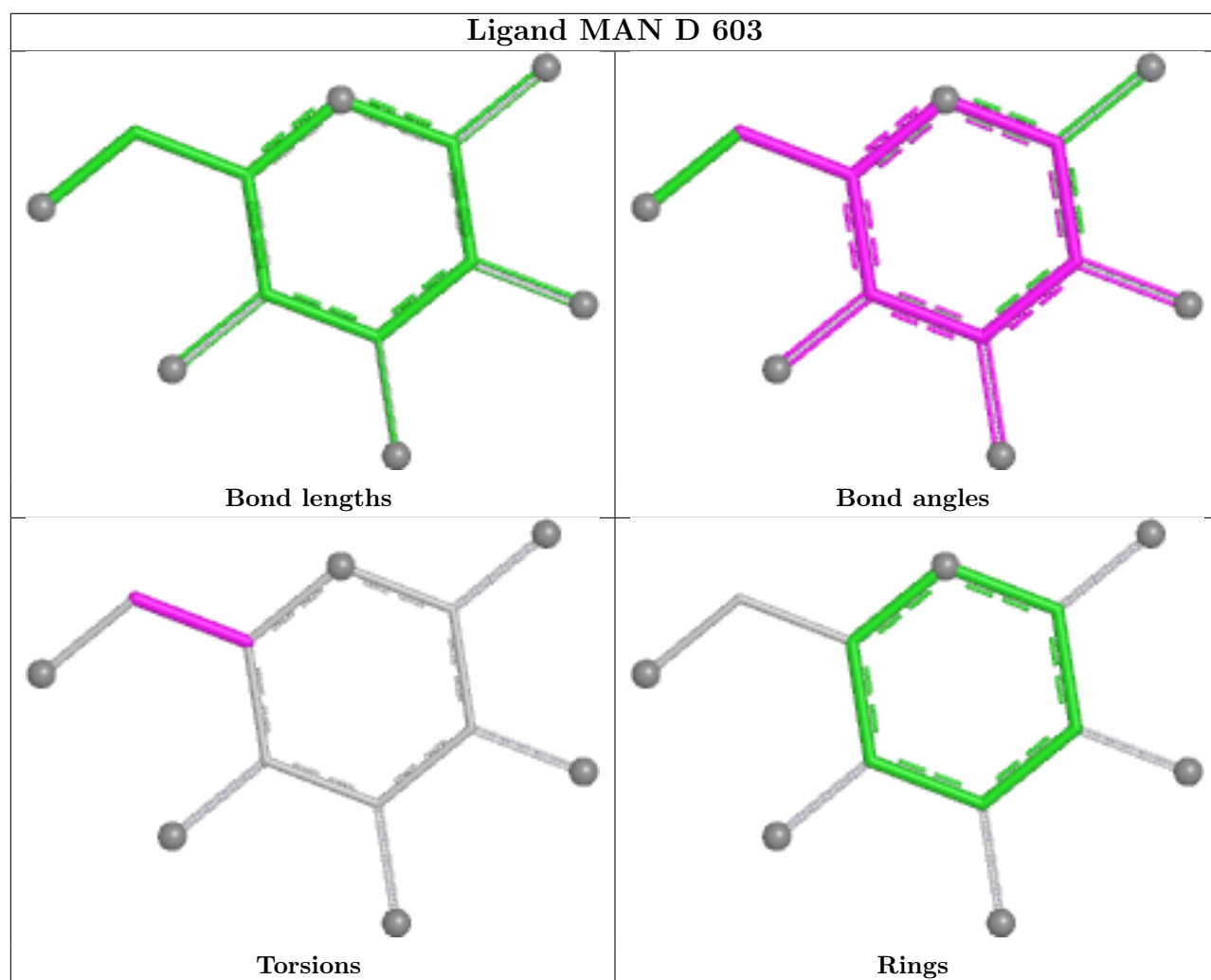
2 monomers are involved in 5 short contacts:

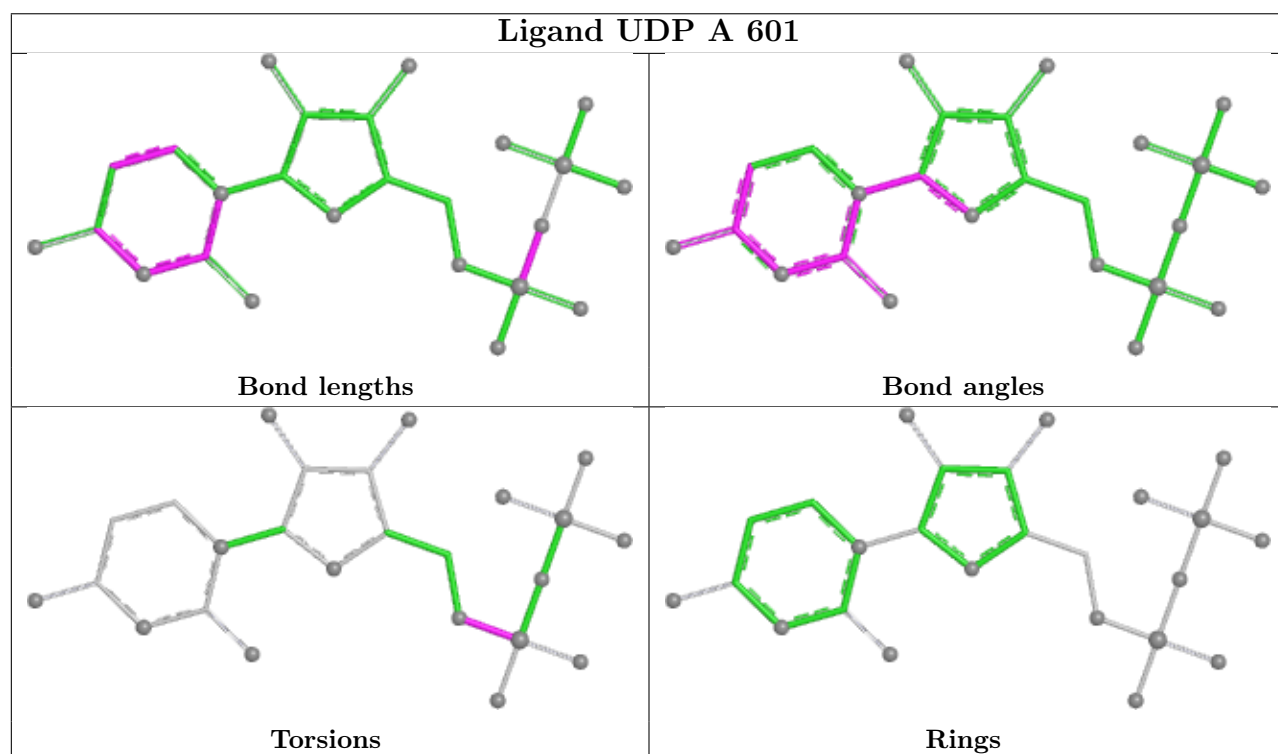
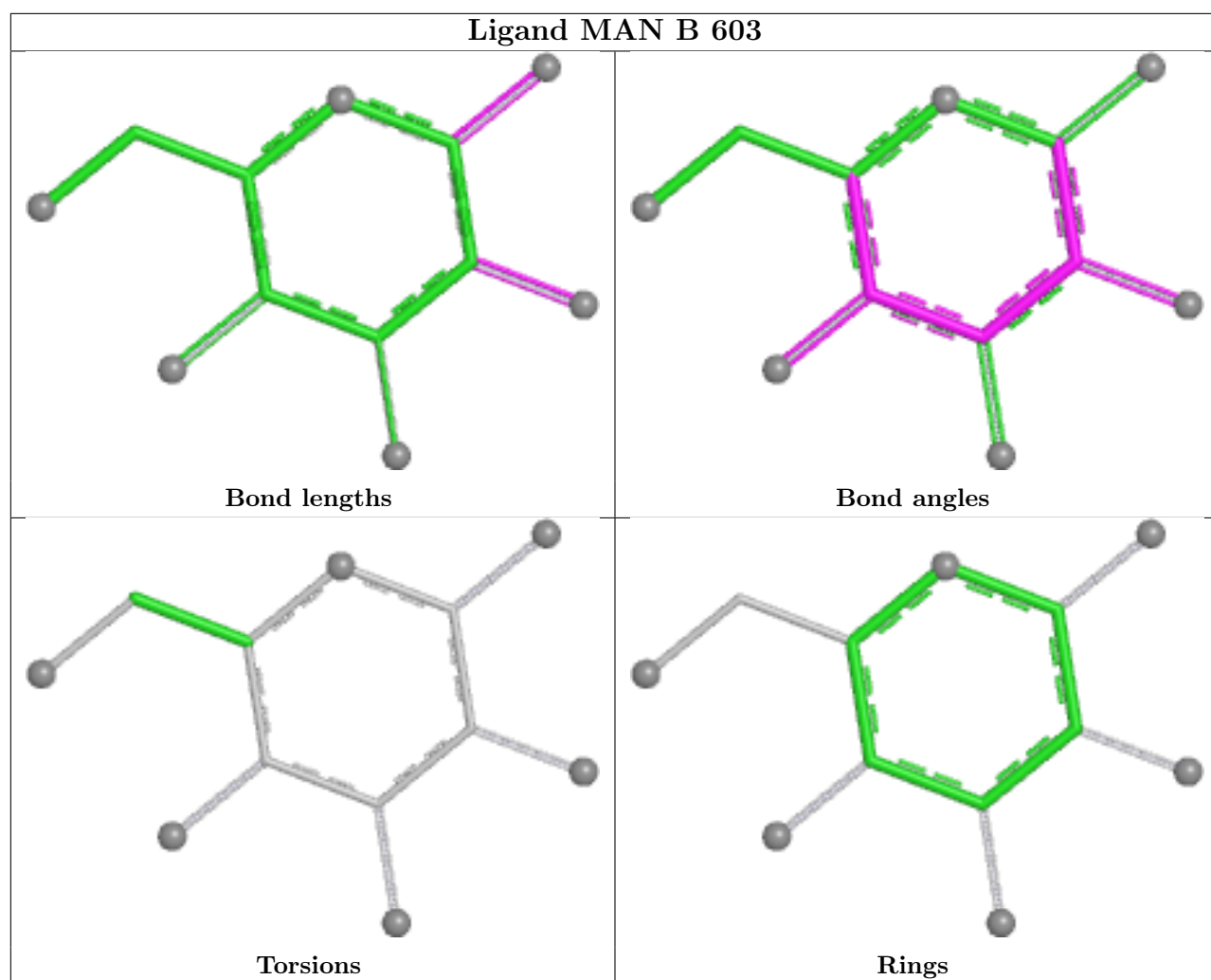
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	NAG	2	0
2	B	601	UDP	3	0

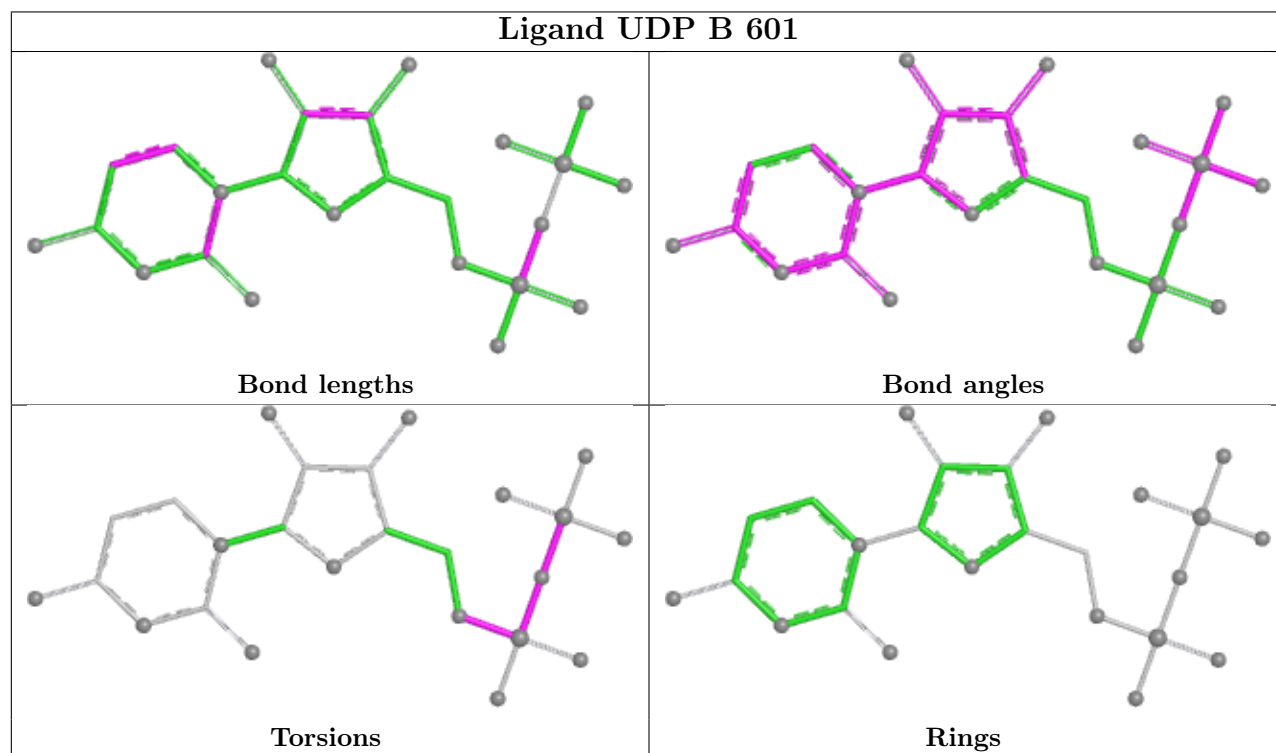
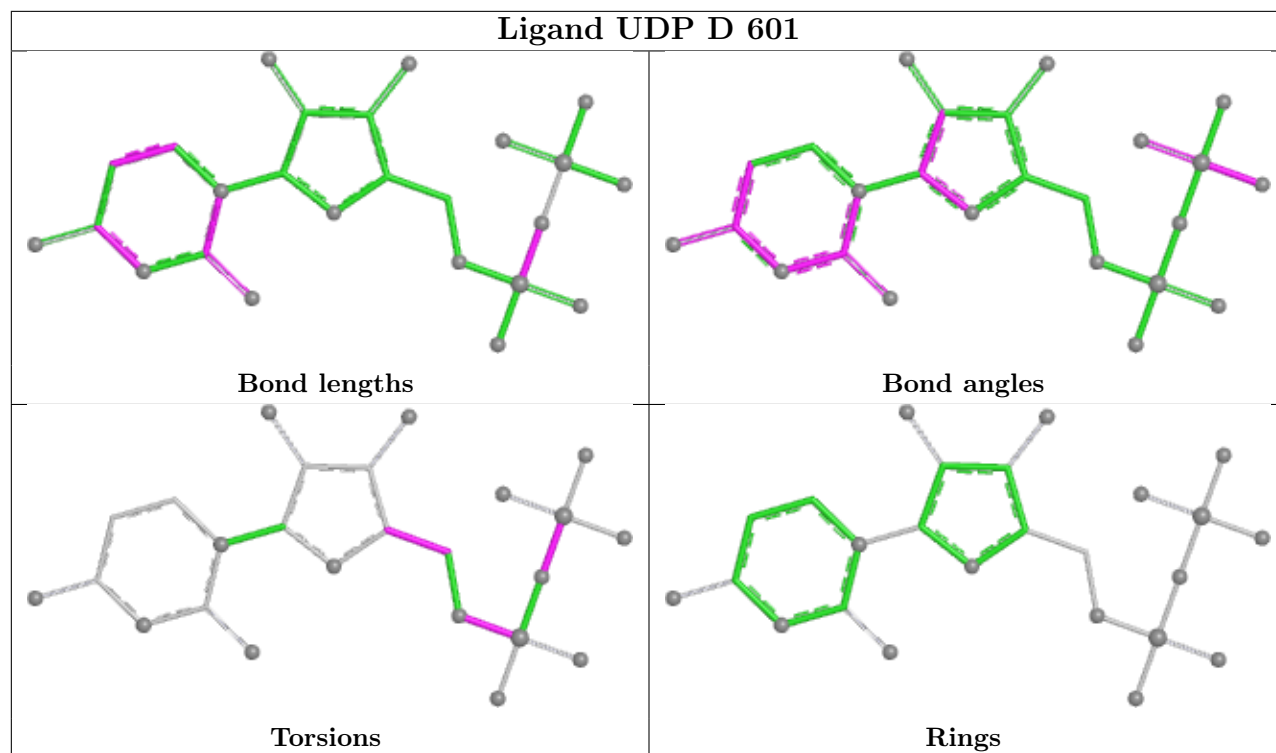
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

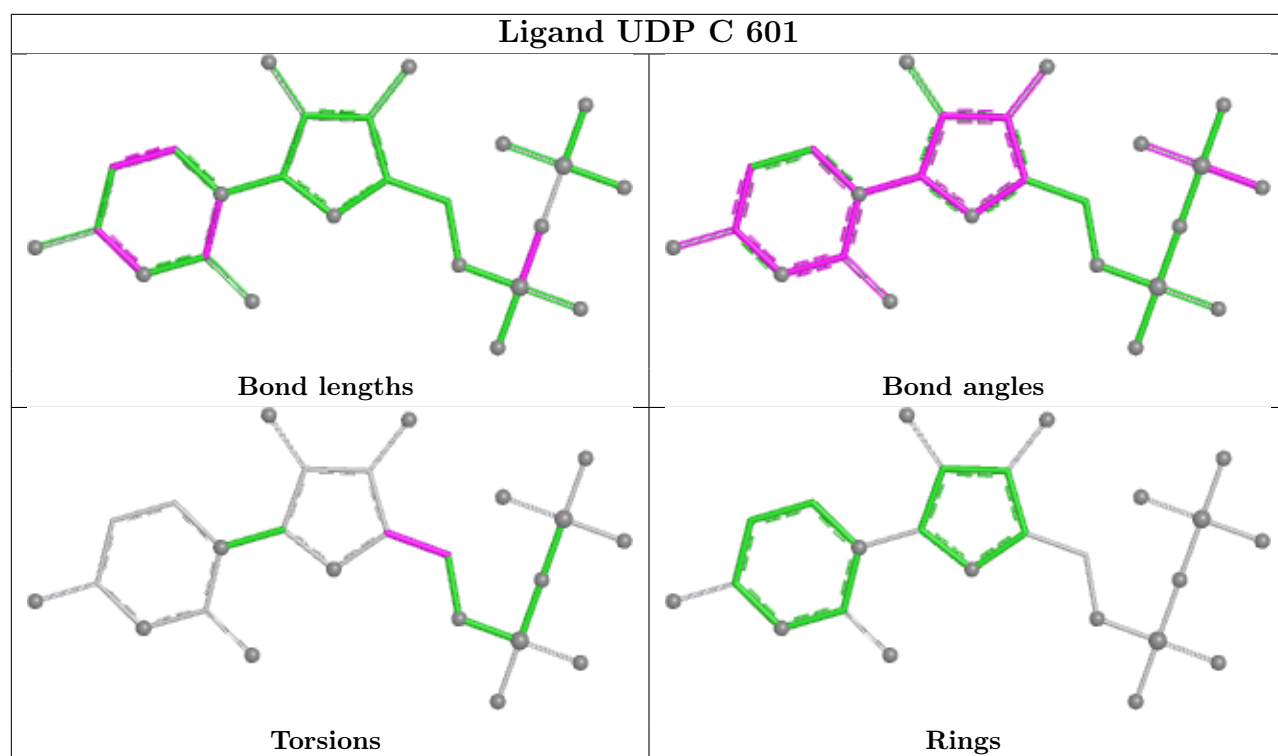












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	515/558 (92%)	-0.16	9 (1%) 69 60	52, 83, 127, 159	0
1	B	505/558 (90%)	-0.09	8 (1%) 70 61	57, 80, 148, 187	0
1	C	511/558 (91%)	-0.06	6 (1%) 76 68	58, 89, 137, 162	0
1	D	510/558 (91%)	0.09	8 (1%) 70 61	65, 98, 141, 175	0
All	All	2041/2232 (91%)	-0.06	31 (1%) 72 63	52, 88, 139, 187	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	478	VAL	5.4
1	D	471	PRO	4.7
1	C	471	PRO	3.7
1	A	437	CYS	3.4
1	A	494	VAL	3.4
1	D	541	LEU	3.3
1	B	471	PRO	3.2
1	B	468	ARG	2.8
1	A	471	PRO	2.8
1	C	438	ARG	2.8
1	D	411	GLN	2.7
1	D	477	THR	2.7
1	A	419	ARG	2.7
1	A	498	SER	2.7
1	D	493	SER	2.7
1	A	477	THR	2.6
1	B	541	LEU	2.6
1	B	491	GLN	2.5
1	D	478	VAL	2.5
1	D	305	GLU	2.4
1	D	466	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	278	SER	2.3
1	B	285	GLY	2.2
1	A	427	GLN	2.2
1	C	459	GLN	2.2
1	C	285	GLY	2.1
1	A	541	LEU	2.1
1	B	525	TRP	2.1
1	B	278	SER	2.0
1	C	541	LEU	2.0
1	B	543	ASN	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	603	14/15	0.68	0.13	117,148,167,168	0
3	NAG	B	602	14/15	0.69	0.11	109,161,167,167	0
3	NAG	C	602	14/15	0.74	0.11	111,152,171,177	0
3	NAG	D	602	14/15	0.77	0.17	90,113,156,169	0
3	NAG	A	603	14/15	0.78	0.14	116,135,147,150	0
5	CL	A	605	1/1	0.84	0.24	108,108,108,108	0
3	NAG	A	602	14/15	0.85	0.09	117,150,161,172	0
4	MAN	B	603	12/12	0.86	0.13	77,111,128,133	0
2	UDP	B	601	25/25	0.86	0.14	78,136,210,226	0
4	MAN	D	603	12/12	0.88	0.13	84,120,127,127	0
5	CL	C	605	1/1	0.89	0.21	112,112,112,112	0
2	UDP	C	601	25/25	0.90	0.10	93,135,145,169	0
2	UDP	D	601	25/25	0.90	0.11	108,147,171,174	0

Continued on next page...

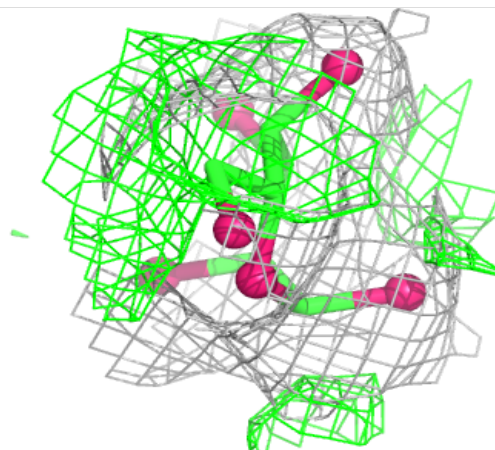
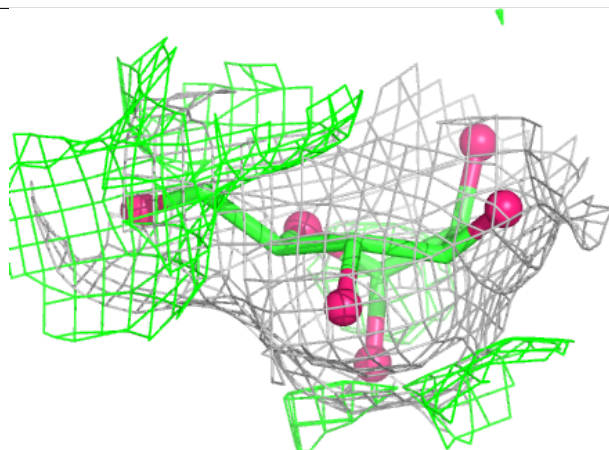
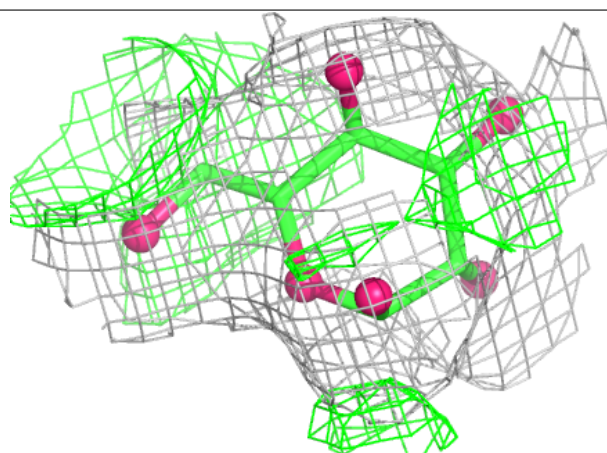
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	D	604	1/1	0.90	0.27	105,105,105,105	0
4	MAN	C	604	12/12	0.92	0.11	82,112,122,126	0
5	CL	B	604	1/1	0.92	0.20	100,100,100,100	0
4	MAN	A	604	12/12	0.94	0.09	78,100,114,122	0
2	UDP	A	601	25/25	0.96	0.08	73,99,126,141	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.

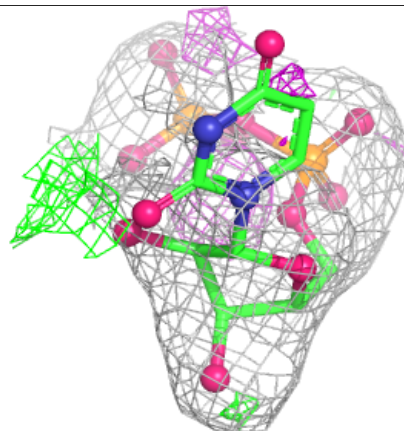
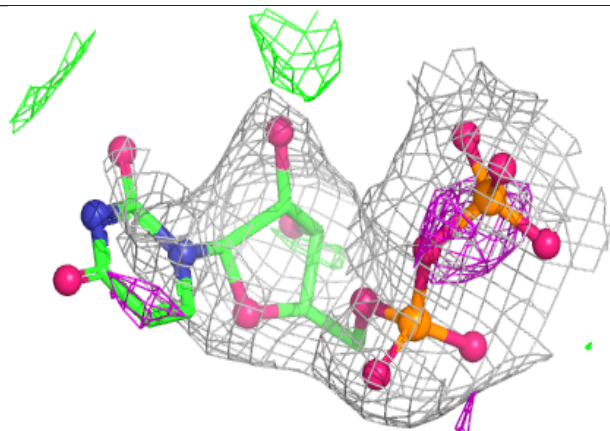
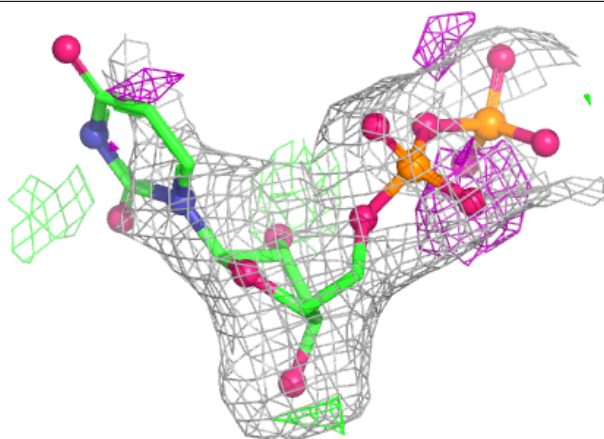
Electron density around MAN B 603:

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

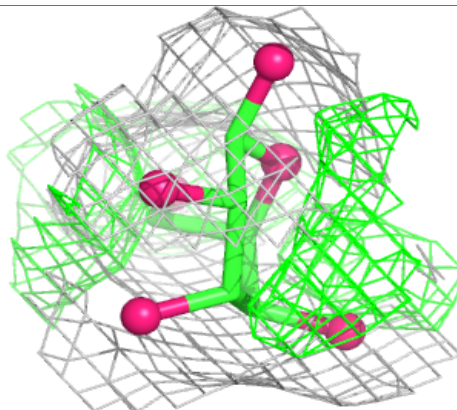
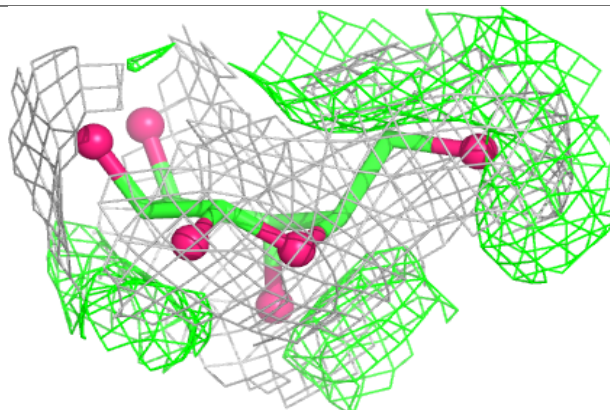
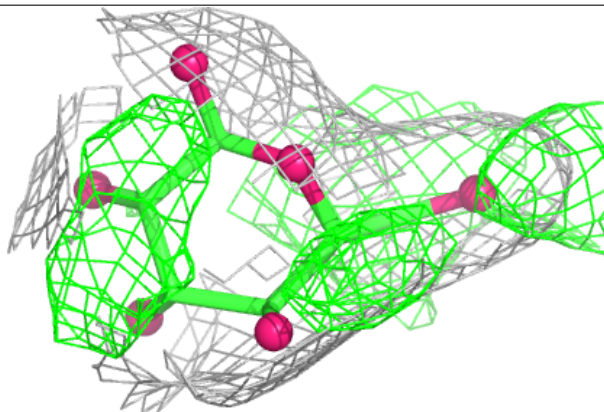


Electron density around UDP B 601:

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

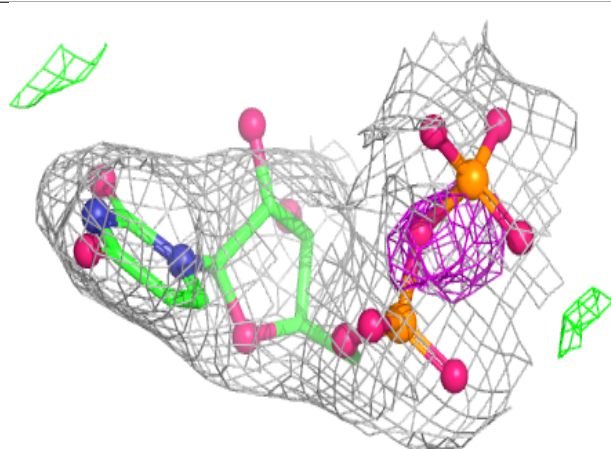
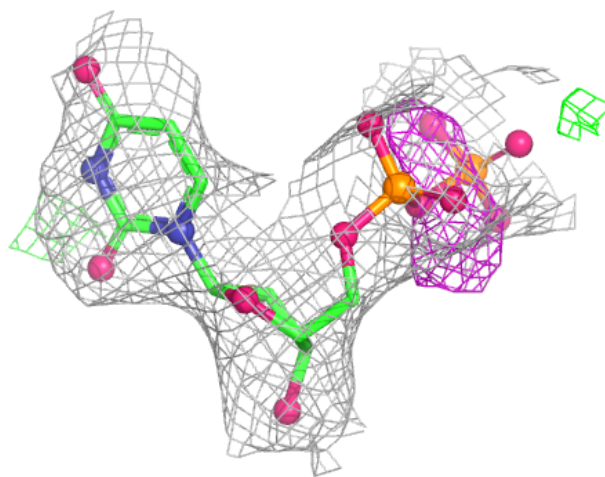
**Electron density around MAN D 603:**

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



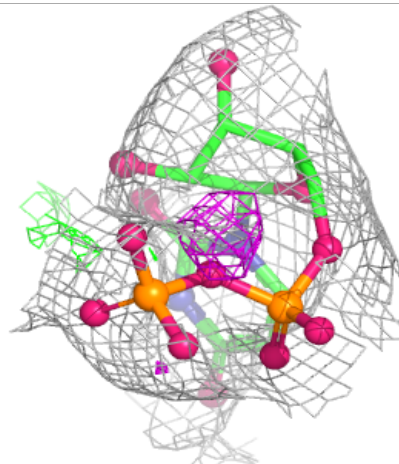
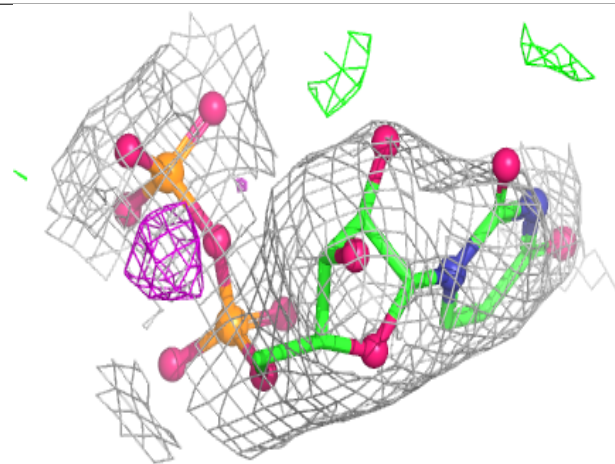
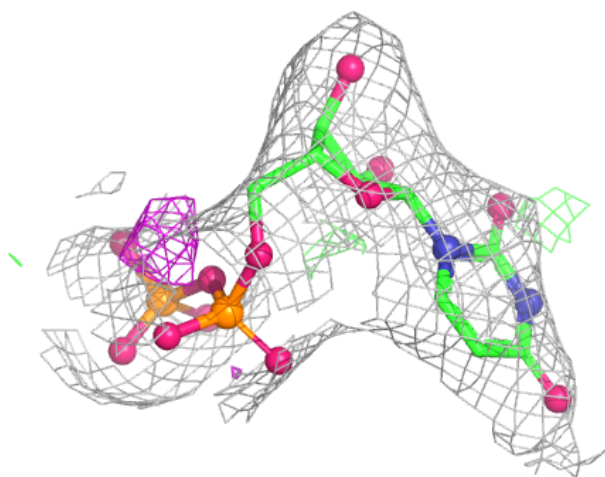
Electron density around UDP C 601:

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



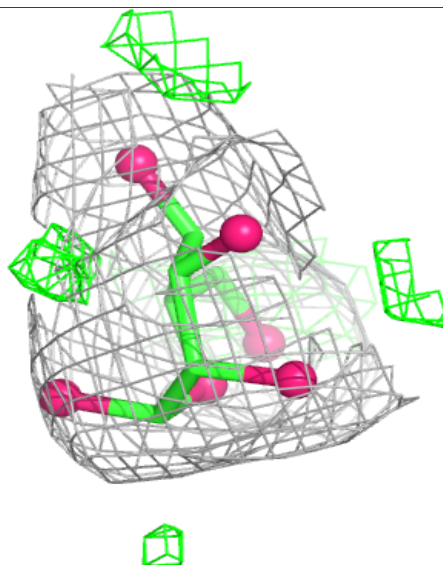
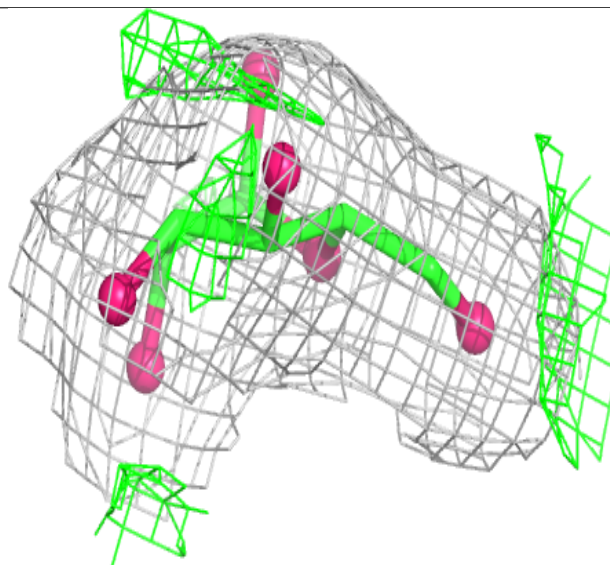
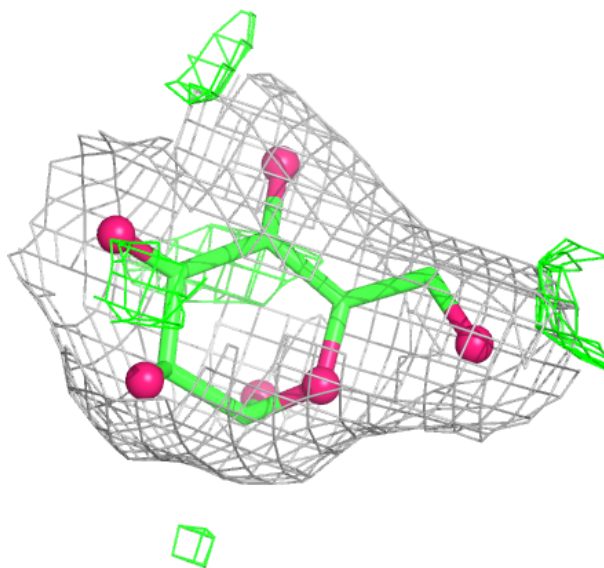
Electron density around UDP D 601:

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



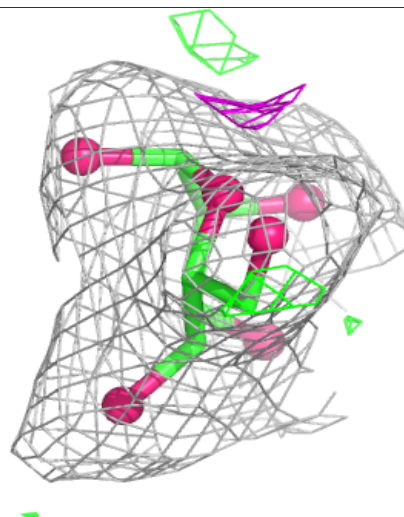
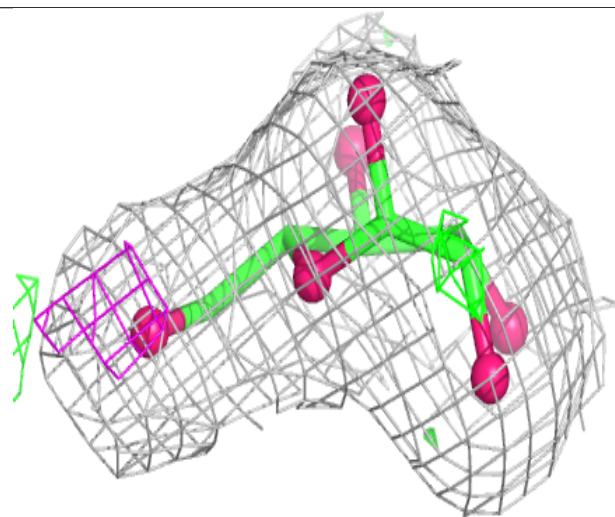
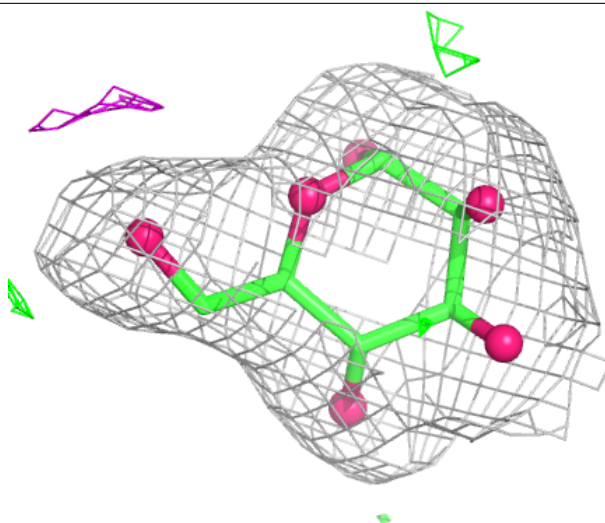
Electron density around MAN C 604:

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



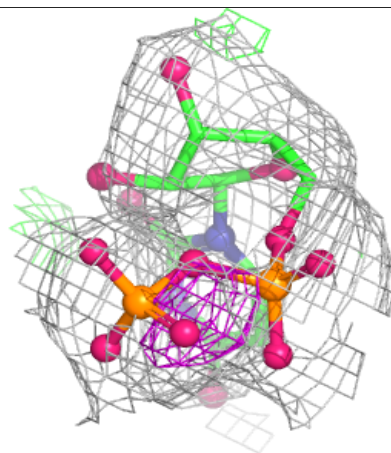
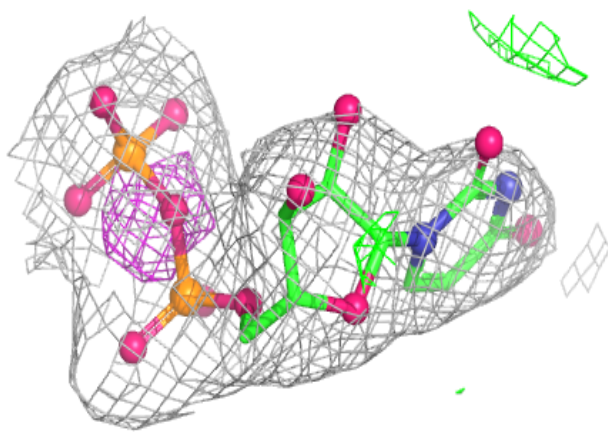
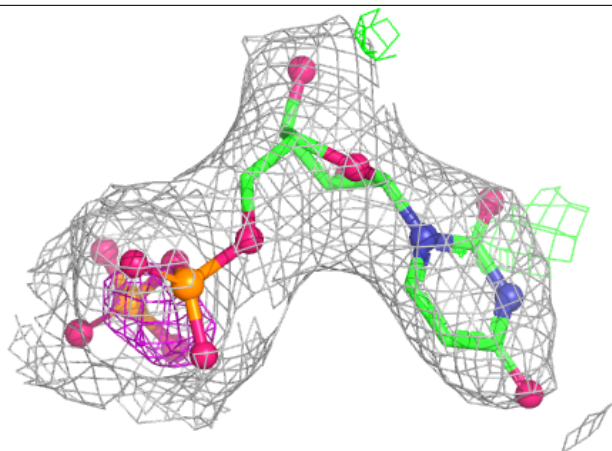
Electron density around MAN A 604:

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



Electron density around UDP A 601:

$2mF_o-DF_c$ (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.