



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:05 PM BST

PDB ID : 6NIG  
Title : Crystal structure of the human TLR2-Diprovocim complex  
Authors : Zhang, H.; Beutler, B.A.; Tomchick, D.R.; Su, L.  
Deposited on : 2018-12-27  
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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

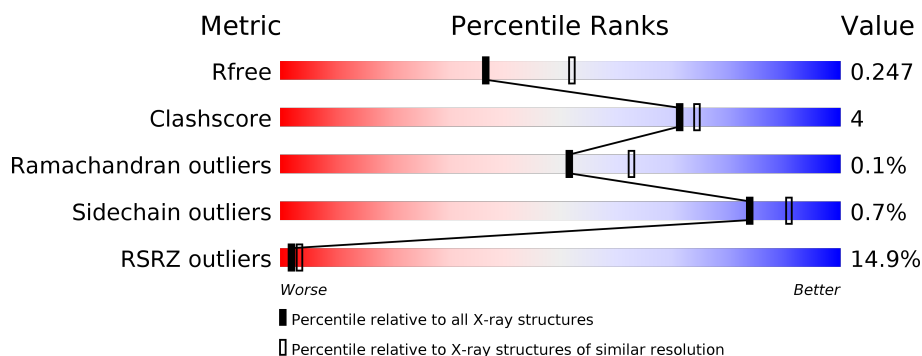
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	576	<div> <div>11%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	B	576	<div> <div>16%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	C	576	<div> <div>17%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
1	D	576	<div> <div>13%</div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
2	E	2	<div> <div>100%</div> </div>
2	F	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	H	2	 50%50%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 35983 atoms, of which 18046 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 Toll-like receptor 2, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	546	Total	C	H	N	O	S	0	0	0
			8745	2755	4400	732	837	21			
1	B	545	Total	C	H	N	O	S	0	0	0
			8716	2747	4385	727	836	21			
1	C	549	Total	C	H	N	O	S	0	0	0
			8784	2766	4419	735	843	21			
1	D	546	Total	C	H	N	O	S	0	2	0
			8750	2758	4402	731	838	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	ARG	-	linker	UNP O60603
B	508	ARG	-	linker	UNP O60603
C	508	ARG	-	linker	UNP O60603
D	508	ARG	-	linker	UNP O60603

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



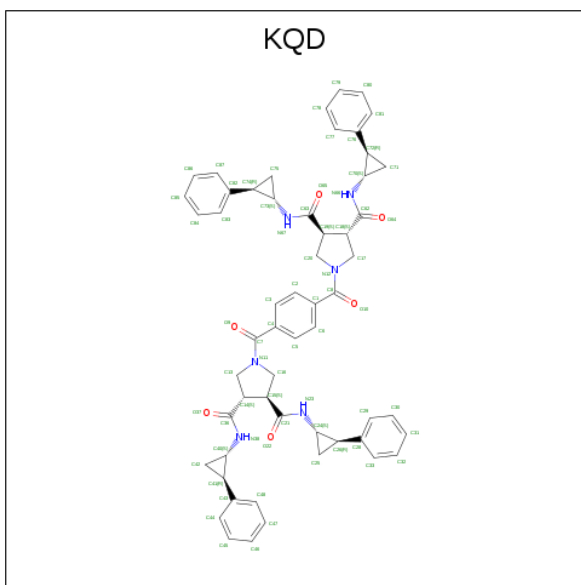
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				
2	F	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				
2	G	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 3 is (3S,4S,3'S,4'S)-1,1'-(1,4-phenylenedicarbonyl)bis{N 3 ,N 4 -bis[(1S,2R)-2-phenylcyclopropyl]pyrrolidine-3,4-dicarboxamide} (three-letter code: KQD) (formula: C<sub>56</sub>H<sub>56</sub>N<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			124	56	56	6	6		
3	B	1	Total	C	H	N	O	0	0
			124	56	56	6	6		
3	C	1	Total	C	H	N	O	0	0
			124	56	56	6	6		
3	D	1	Total	C	H	N	O	0	0
			124	56	56	6	6		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total	O	0	0
			14	14		
5	B	13	Total	O	0	0
			13	13		
5	C	4	Total	O	0	0
			4	4		

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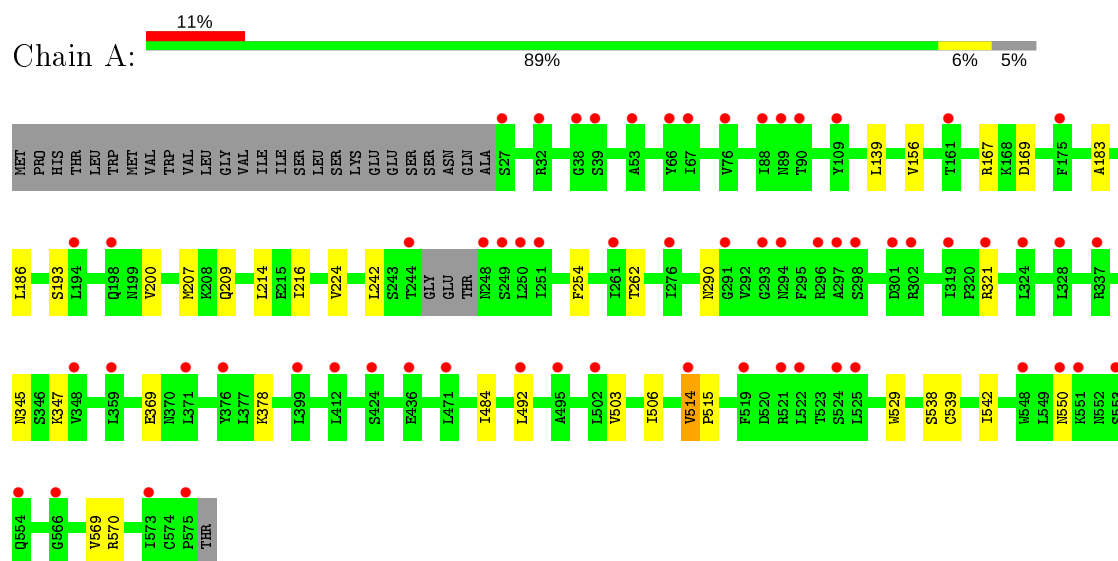
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	7	Total	O	0	0
			7	7		

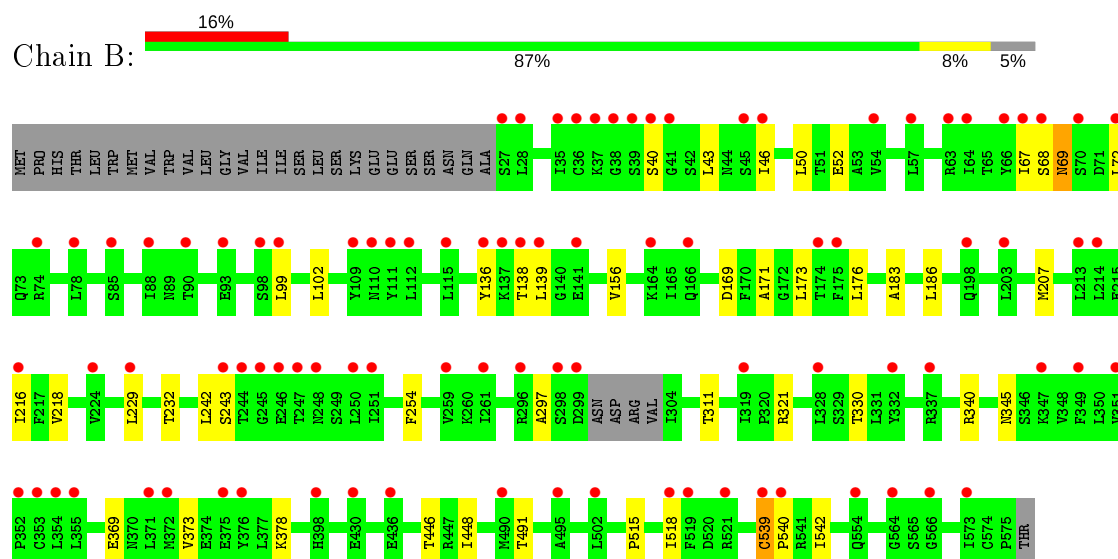
### 3 Residue-property plots [i](#)

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: Toll-like receptor 2,Variable lymphocyte receptor B




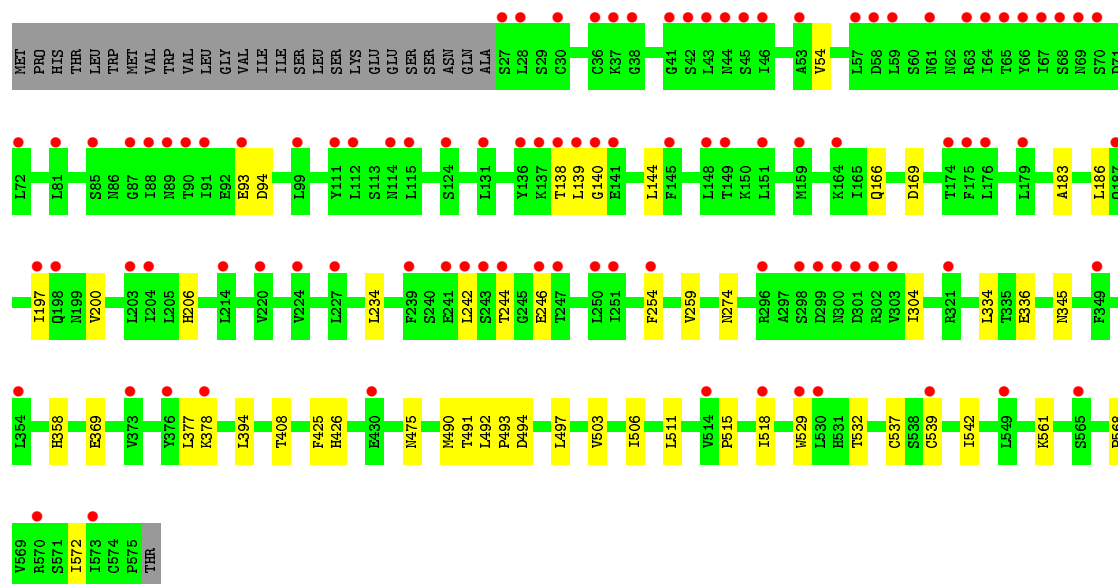
- Molecule 1: Toll-like receptor 2,Variable lymphocyte receptor B




- Molecule 1: Toll-like receptor 2,Variable lymphocyte receptor B

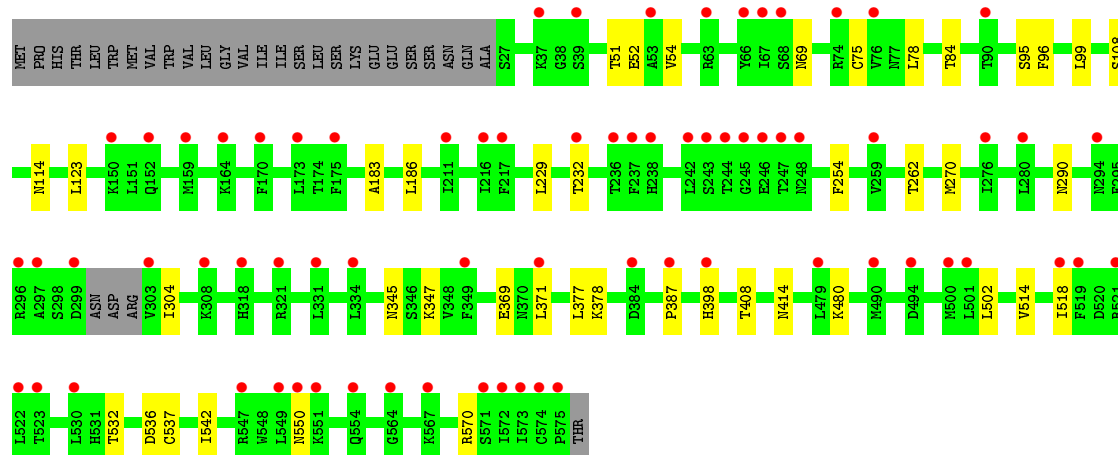


Chain C: 



- Molecule 1: Toll-like receptor 2, Variable lymphocyte receptor B

Chain D: 



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.10Å 201.25Å 109.36Å 90.00° 94.26° 90.00°	Depositor
Resolution (Å)	37.76 – 2.35 48.02 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.8 (37.76-2.35) 94.9 (48.02-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, $R_{free}$	0.210 , 0.236 0.224 , 0.247	Depositor DCC
$R_{free}$ test set	3364 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.8	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	35983	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.25	0/4420	0.46	0/5984
1	B	0.25	0/4406	0.46	0/5965
1	C	0.24	0/4441	0.45	0/6014
1	D	0.25	0/4436	0.45	0/6006
All	All	0.25	0/17703	0.46	0/23969

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4345	4400	4400	25	0
1	B	4331	4385	4385	34	0
1	C	4365	4419	4419	32	0
1	D	4348	4402	4392	29	0
2	E	28	25	25	0	0
2	F	28	25	25	0	0
2	G	28	25	25	3	0
2	H	28	25	25	0	0
3	A	68	56	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	68	56	0	0	0
3	C	68	56	0	0	0
3	D	68	56	0	1	0
4	A	56	51	51	1	0
4	B	28	26	26	2	0
4	C	14	13	13	1	0
4	D	28	26	26	1	0
5	A	14	0	0	0	0
5	B	13	0	0	1	0
5	C	4	0	0	0	0
5	D	7	0	0	0	0
All	All	17937	18046	17812	125	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 4.

All (125) 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:50:LEU:HD22	1:B:72:LEU:HD23	1.57	0.86
1:B:139:LEU:HD21	1:B:156:VAL:HG21	1.59	0.83
1:D:537:CYS:HA	1:D:542:ILE:HG21	1.69	0.73
1:D:229:LEU:HD21	1:D:232:THR:HG21	1.73	0.71
2:G:2:NAG:H83	2:G:2:NAG:H3	1.73	0.71
1:B:515:PRO:HG2	1:B:518:ILE:HD13	1.74	0.68
1:B:139:LEU:HD21	1:B:156:VAL:CG2	2.24	0.67
1:A:550:ASN:ND2	1:A:570:ARG:O	2.29	0.66
1:A:492:LEU:HD12	1:A:506:ILE:HD13	1.79	0.65
4:B:803:NAG:H3	4:B:803:NAG:H83	1.80	0.61
1:A:207:MET:HE1	1:A:216:ILE:HD12	1.83	0.60
1:A:139:LEU:HD21	1:A:156:VAL:CG2	2.32	0.60
1:C:537:CYS:HA	1:C:542:ILE:HG21	1.84	0.60
1:C:542:ILE:HD11	1:C:572:ILE:HG21	1.84	0.59
1:A:542:ILE:HD11	1:A:569:VAL:HG13	1.84	0.59
1:C:138:THR:HG21	1:C:166:GLN:NE2	2.18	0.58
1:C:139:LEU:HD12	1:C:169:ASP:HB3	1.84	0.58
1:A:542:ILE:HD11	1:A:569:VAL:CG1	2.34	0.58
1:D:270:MET:CE	1:D:304:ILE:HD13	2.34	0.58
1:A:207:MET:CE	1:A:216:ILE:HD12	2.34	0.57
1:B:229:LEU:HD11	1:B:232:THR:OG1	2.04	0.57
1:D:183:ALA:HB1	1:D:186:LEU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:LEU:HB3	1:D:408:THR:HG21	1.86	0.57
1:B:207:MET:CE	1:B:216:ILE:HD12	2.35	0.56
1:B:207:MET:HE1	1:B:216:ILE:HD12	1.87	0.56
1:B:242:LEU:HD23	1:B:243:SER:N	2.20	0.56
1:D:69:ASN:HA	1:D:95:SER:HA	1.87	0.56
1:B:40:SER:O	1:B:43:LEU:HD13	2.06	0.55
1:D:550:ASN:ND2	1:D:570:ARG:O	2.41	0.54
1:C:490:MET:HG3	1:C:491:THR:HG23	1.89	0.53
1:C:242:LEU:HB3	1:C:244:THR:HG22	1.88	0.53
1:B:218:VAL:HG11	1:B:242:LEU:HD13	1.91	0.53
1:A:183:ALA:HB1	1:A:186:LEU:HB2	1.91	0.53
1:C:304:ILE:HG21	1:C:334:LEU:HD11	1.91	0.52
4:C:802:NAG:H3	4:C:802:NAG:O7	2.10	0.52
1:B:99:LEU:HD13	1:B:102:LEU:HD22	1.92	0.51
1:C:304:ILE:HG21	1:C:334:LEU:CD1	2.40	0.51
1:A:542:ILE:HG13	1:A:542:ILE:O	2.10	0.51
1:C:506:ILE:CD1	1:C:511:LEU:HD11	2.41	0.50
1:A:538:SER:O	1:A:542:ILE:HG22	2.11	0.50
1:B:139:LEU:HD12	1:B:169:ASP:HB3	1.93	0.50
4:D:603:NAG:H3	4:D:603:NAG:O7	2.12	0.50
1:A:492:LEU:HD22	1:A:514:VAL:CG2	2.42	0.49
1:D:378:LYS:HG2	1:D:408:THR:HG23	1.94	0.49
1:C:542:ILE:CD1	1:C:572:ILE:HG21	2.42	0.49
1:D:270:MET:HE3	1:D:304:ILE:HD13	1.93	0.49
1:A:321:ARG:HD2	1:B:378:LYS:CG	2.43	0.49
1:B:311:THR:HG22	1:B:340:ARG:HB3	1.94	0.49
1:C:532:THR:O	1:C:532:THR:HG22	2.13	0.49
1:B:515:PRO:CG	1:B:518:ILE:HD13	2.40	0.49
1:C:139:LEU:O	1:C:144:LEU:HD11	2.13	0.48
1:A:514:VAL:HG22	1:A:515:PRO:HD2	1.94	0.48
1:A:321:ARG:HD2	1:B:378:LYS:HG2	1.95	0.48
4:B:803:NAG:C1	4:B:803:NAG:H82	2.44	0.48
1:B:171:ALA:N	5:B:901:HOH:O	2.44	0.48
1:C:515:PRO:HG2	1:C:518:ILE:HD13	1.94	0.48
1:C:377:LEU:HD21	1:C:394:LEU:CD1	2.43	0.48
1:D:51:THR:O	1:D:54:VAL:HG12	2.13	0.48
1:A:139:LEU:HD21	1:A:156:VAL:HG21	1.96	0.47
1:C:183:ALA:HB1	1:C:186:LEU:HB2	1.96	0.47
1:B:446:THR:HG23	1:B:448:ILE:HG23	1.96	0.47
1:D:270:MET:HE1	1:D:304:ILE:HD13	1.97	0.47
1:A:139:LEU:HD12	1:A:169:ASP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD22	1:B:72:LEU:CD2	2.39	0.47
1:C:503:VAL:HG13	1:C:529:TRP:HZ3	1.80	0.47
1:B:183:ALA:HB1	1:B:186:LEU:HB2	1.95	0.47
1:C:492:LEU:HD12	1:C:506:ILE:HD13	1.95	0.47
1:B:69:ASN:OD1	1:B:69:ASN:N	2.47	0.47
1:B:52:GLU:N	1:B:52:GLU:OE1	2.48	0.47
1:B:138:THR:HG22	1:B:139:LEU:N	2.31	0.46
1:C:537:CYS:HA	1:C:542:ILE:HD13	1.97	0.46
2:G:2:NAG:C8	2:G:2:NAG:H3	2.45	0.46
1:C:493:PRO:CD	1:C:506:ILE:HD12	2.45	0.46
1:D:347:LYS:O	3:D:601:KQD:N67	2.48	0.46
1:D:537:CYS:HA	1:D:542:ILE:HD13	1.97	0.46
1:A:214:LEU:HD22	1:A:242:LEU:HD21	1.98	0.46
1:C:244:THR:HG23	1:C:246:GLU:H	1.81	0.46
1:D:536:ASP:O	1:D:542:ILE:CG2	2.64	0.46
1:C:336:GLU:HA	1:C:358:HIS:O	2.16	0.45
1:D:52:GLU:OE1	1:D:52:GLU:N	2.41	0.45
1:A:503:VAL:HG13	1:A:529:TRP:HZ3	1.82	0.45
1:D:75:CYS:HB3	1:D:78:LEU:HB2	1.99	0.45
1:B:173:LEU:HD13	1:B:176:LEU:HD11	1.98	0.45
1:B:229:LEU:HD11	1:B:232:THR:CB	2.47	0.45
1:C:475:ASN:HA	1:C:497:LEU:HB3	1.98	0.45
1:A:347:LYS:O	3:A:601:KQD:N67	2.50	0.44
1:D:54:VAL:HG13	1:D:54:VAL:O	2.17	0.44
1:D:96:PHE:HB3	1:D:123:LEU:HD21	1.98	0.44
4:A:605:NAG:C1	4:A:605:NAG:O7	2.65	0.44
1:B:46:ILE:HD12	1:B:67:ILE:HG12	2.00	0.44
1:A:200:VAL:O	1:A:224:VAL:HA	2.18	0.43
1:A:378:LYS:HG2	1:B:321:ARG:HD3	2.00	0.43
1:C:377:LEU:HD21	1:C:394:LEU:HD11	1.99	0.43
1:C:425:PHE:O	1:C:426:HIS:HB2	2.18	0.43
1:B:297:ALA:CB	1:B:330:THR:HG21	2.48	0.43
1:D:387:PRO:O	1:D:414:ASN:ND2	2.47	0.43
1:B:542:ILE:HG12	1:B:542:ILE:O	2.19	0.43
1:D:229:LEU:CD2	1:D:232:THR:HG21	2.44	0.43
1:D:345:ASN:HA	1:D:369:GLU:O	2.19	0.43
1:C:138:THR:HG22	1:C:140:GLY:H	1.84	0.43
1:D:514:VAL:CG2	1:D:518:ILE:HG21	2.48	0.43
1:B:373:VAL:O	1:B:373:VAL:HG23	2.19	0.42
1:D:262:THR:HA	1:D:290:ASN:O	2.19	0.42
1:B:345:ASN:HA	1:B:369:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:CYS:N	1:B:540:PRO:HD2	2.35	0.42
1:B:136:TYR:OH	1:B:156:VAL:HG23	2.20	0.42
1:A:207:MET:HG2	1:A:209:GLN:O	2.20	0.42
1:B:218:VAL:HG21	1:B:242:LEU:HD13	2.02	0.42
1:C:197:ILE:HG21	1:C:200:VAL:HG23	2.01	0.42
1:D:532:THR:HG22	1:D:532:THR:O	2.20	0.42
1:D:371:LEU:HD22	1:D:398:HIS:NE2	2.35	0.41
1:D:480:LYS:O	1:D:502:LEU:N	2.45	0.41
1:C:345:ASN:HA	1:C:369:GLU:O	2.20	0.41
1:D:84:THR:HG23	1:D:108:SER:HB2	2.02	0.41
2:G:1:NAG:H62	2:G:2:NAG:H82	2.02	0.41
1:C:234:LEU:HD12	1:C:259:VAL:HG11	2.03	0.41
1:A:345:ASN:HA	1:A:369:GLU:O	2.21	0.41
1:C:378:LYS:HA	1:C:408:THR:HG23	2.01	0.41
1:D:96:PHE:CD1	1:D:99:LEU:HD12	2.56	0.41
1:A:167:ARG:HA	1:A:193:SER:HA	2.03	0.41
1:D:378:LYS:CG	1:D:408:THR:HG23	2.51	0.41
1:A:262:THR:HA	1:A:290:ASN:O	2.20	0.40
1:C:561:LYS:HD3	1:C:568:PRO:HA	2.03	0.40
1:C:54:VAL:O	1:C:54:VAL:HG13	2.20	0.40
1:C:93:GLU:O	1:C:94:ASP:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	542/576 (94%)	510 (94%)	31 (6%)	1 (0%)	47	56
1	B	541/576 (94%)	502 (93%)	39 (7%)	0	100	100
1	C	547/576 (95%)	512 (94%)	34 (6%)	1 (0%)	47	56
1	D	544/576 (94%)	512 (94%)	32 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2174/2304 (94%)	2036 (94%)	136 (6%)	2 (0%)	51 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	494	ASP
1	A	484	ILE

### 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	516/543 (95%)	513 (99%)	3 (1%)	86 93
1	B	514/543 (95%)	509 (99%)	5 (1%)	76 85
1	C	518/543 (95%)	514 (99%)	4 (1%)	81 89
1	D	517/543 (95%)	515 (100%)	2 (0%)	91 95
All	All	2065/2172 (95%)	2051 (99%)	14 (1%)	84 91

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	PHE
1	A	514	VAL
1	A	539	CYS
1	B	68	SER
1	B	69	ASN
1	B	254	PHE
1	B	491	THR
1	B	539	CYS
1	C	206	HIS
1	C	254	PHE
1	C	274	ASN
1	C	539	CYS
1	D	114	ASN

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Mol	Chain	Res	Type
1	D	254	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	E	1	1,2	14,14,15	0.15	0	17,19,21	0.48	0
2	NAG	E	2	2	14,14,15	0.18	0	17,19,21	0.44	0
2	NAG	F	1	1,2	14,14,15	0.29	0	17,19,21	0.47	0
2	NAG	F	2	2	14,14,15	0.30	0	17,19,21	0.35	0
2	NAG	G	1	1,2	14,14,15	0.21	0	17,19,21	0.49	0
2	NAG	G	2	2	14,14,15	0.18	0	17,19,21	1.13	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	H	2	2	14,14,15	0.30	0	17,19,21	0.86	1 (5%)

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	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	5/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C2-N2-C7	2.86	126.97	122.90
2	H	2	NAG	C1-O5-C5	2.56	115.66	112.19
2	G	2	NAG	C1-O5-C5	2.47	115.54	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

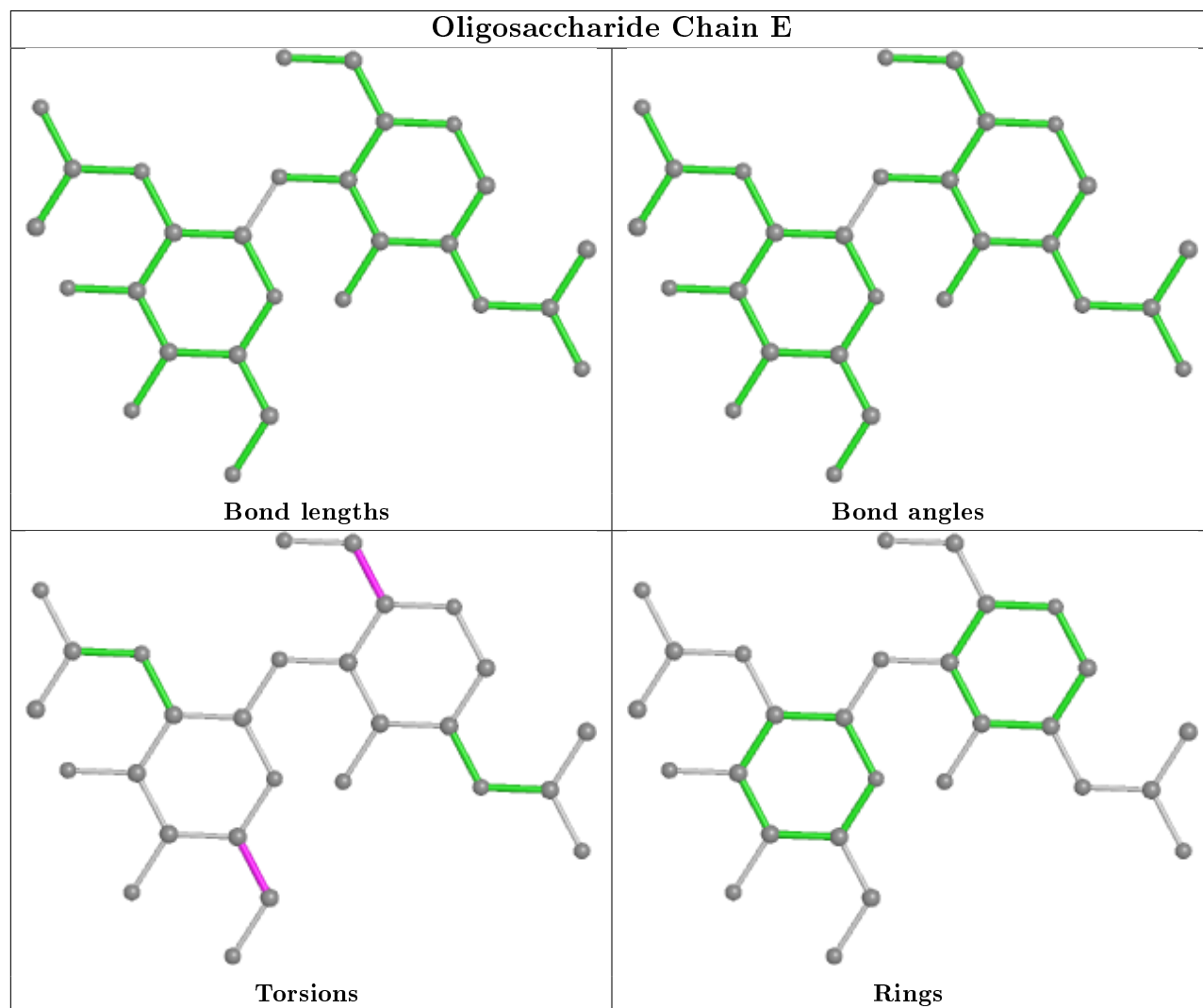
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C3-C2-N2-C7

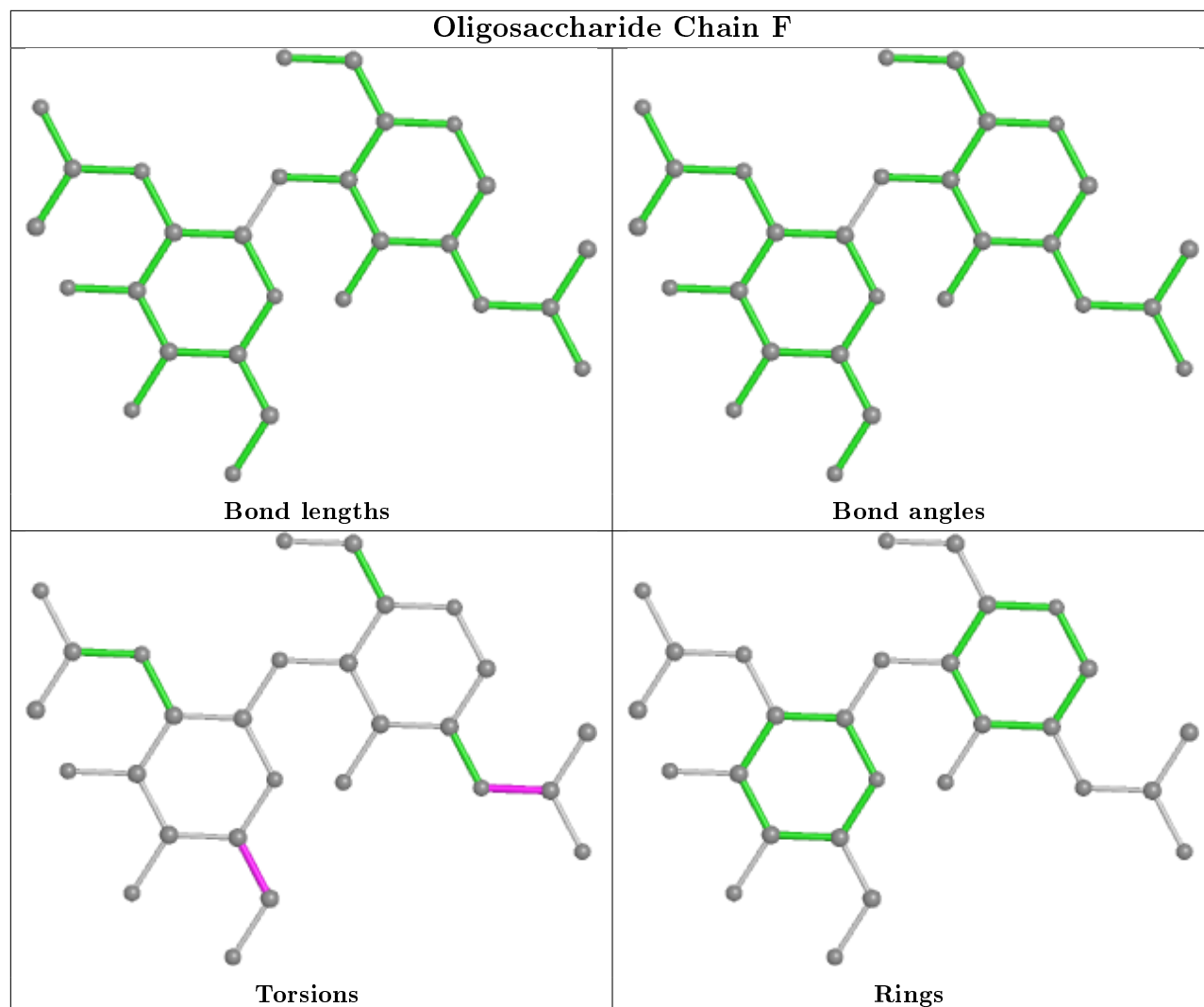
There are no ring outliers.

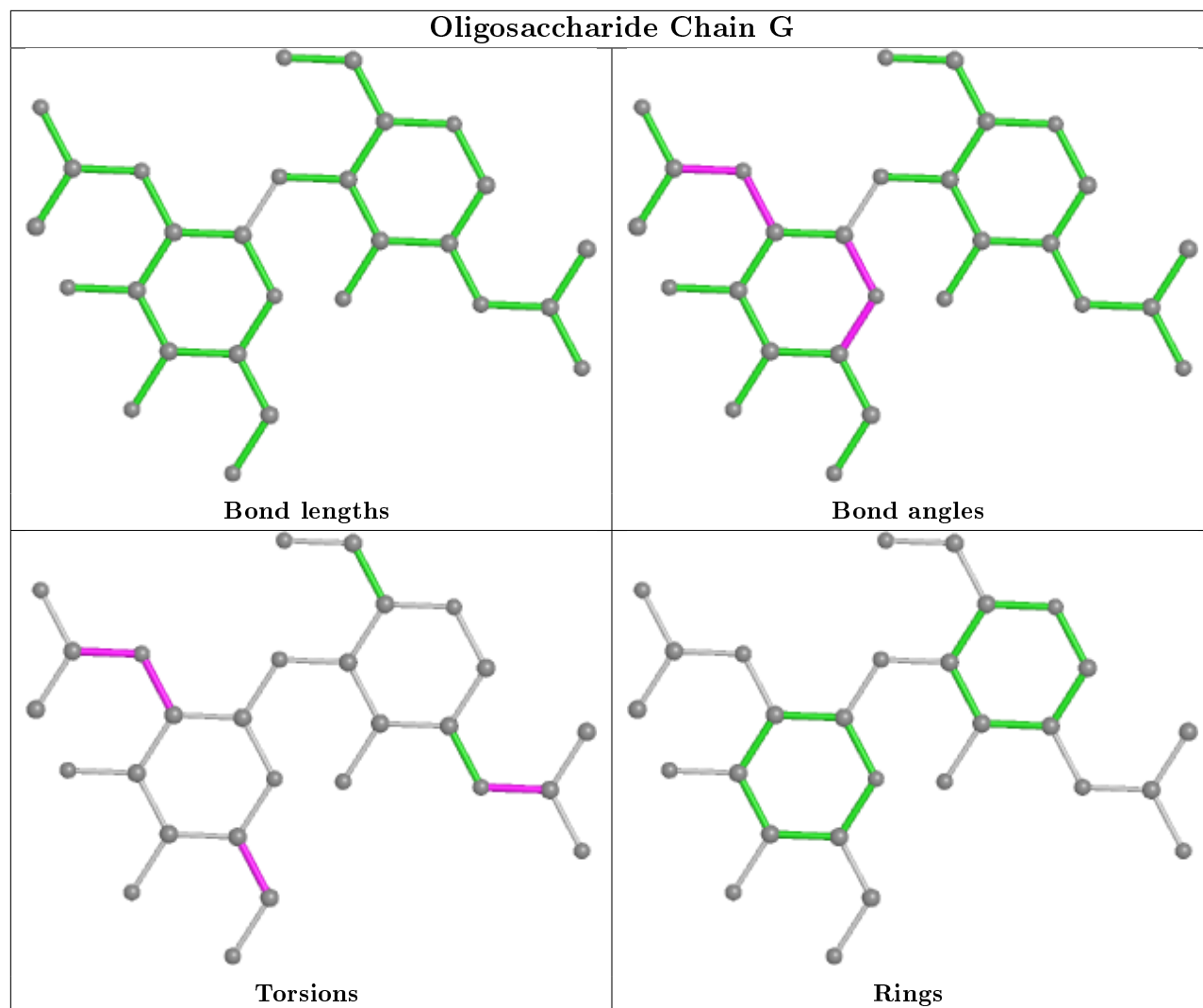
2 monomers are involved in 3 short contacts:

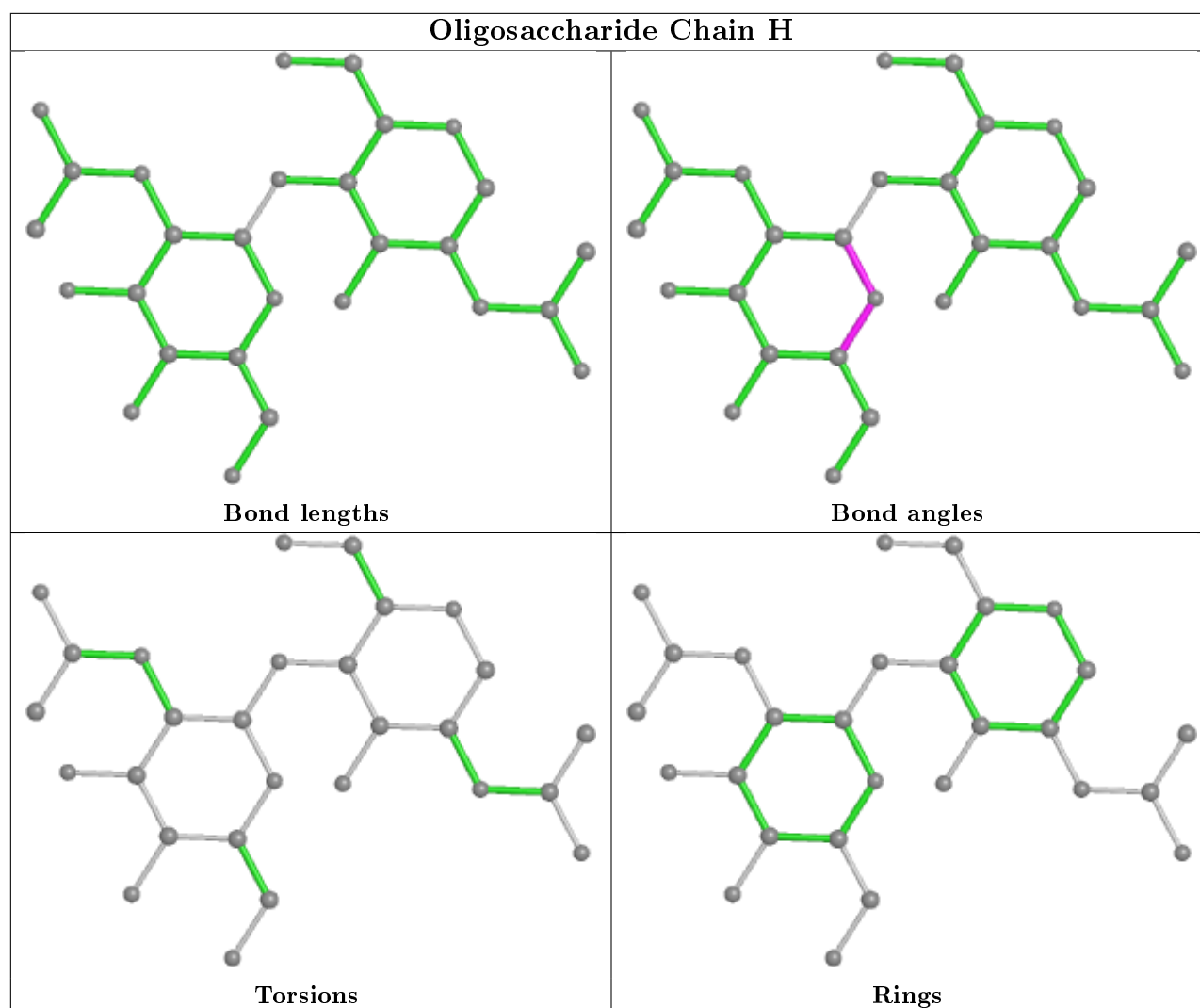
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	3	0
2	G	1	NAG	1	0

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









## 5.6 Ligand geometry [i](#)

13 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	$\# Z  > 2$
4	NAG	D	603	1	14,14,15	0.20	0	17,19,21	0.73	0
4	NAG	C	802	1	14,14,15	0.51	0	17,19,21	0.45	0
4	NAG	A	604	1	14,14,15	0.23	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	KQD	C	801	-	74,78,78	3.00	27 (36%)	86,114,114	1.87	14 (16%)
4	NAG	B	803	1	14,14,15	0.28	0	17,19,21	0.87	1 (5%)
4	NAG	A	607	-	14,14,15	0.30	0	17,19,21	0.47	0
3	KQD	D	601	-	74,78,78	2.99	27 (36%)	86,114,114	1.94	20 (23%)
4	NAG	A	605	1	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	D	602	1	14,14,15	0.21	0	17,19,21	0.45	0
3	KQD	A	601	-	74,78,78	3.00	23 (31%)	86,114,114	1.89	19 (22%)
3	KQD	B	801	-	74,78,78	3.02	25 (33%)	86,114,114	1.75	8 (9%)
4	NAG	B	802	1	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
4	NAG	A	606	1	14,14,15	0.29	0	17,19,21	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	603	1	-	1/6/23/26	0/1/1/1
4	NAG	C	802	1	-	3/6/23/26	0/1/1/1
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
3	KQD	C	801	-	-	21/64/108/108	0/11/11/11
4	NAG	B	803	1	-	6/6/23/26	0/1/1/1
4	NAG	A	607	-	-	2/6/23/26	0/1/1/1
3	KQD	D	601	-	-	5/64/108/108	0/11/11/11
4	NAG	A	605	1	-	3/6/23/26	0/1/1/1
4	NAG	D	602	1	-	0/6/23/26	0/1/1/1
3	KQD	A	601	-	-	5/64/108/108	0/11/11/11
3	KQD	B	801	-	-	22/64/108/108	0/11/11/11
4	NAG	B	802	1	-	2/6/23/26	0/1/1/1
4	NAG	A	606	1	-	2/6/23/26	0/1/1/1

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	KQD	C17-C18	-9.85	1.35	1.53
3	D	601	KQD	C17-C18	-9.80	1.35	1.53
3	B	801	KQD	C17-C18	-9.29	1.36	1.53
3	C	801	KQD	C17-C18	-9.28	1.36	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	KQD	C15-C14	-8.62	1.33	1.54
3	A	601	KQD	C15-C14	-8.57	1.33	1.54
3	D	601	KQD	C15-C14	-8.50	1.33	1.54
3	B	801	KQD	C15-C14	-8.49	1.33	1.54
3	B	801	KQD	C17-N12	7.64	1.62	1.46
3	C	801	KQD	C17-N12	7.47	1.62	1.46
3	D	601	KQD	C17-N12	7.34	1.61	1.46
3	A	601	KQD	C17-N12	7.30	1.61	1.46
3	B	801	KQD	C20-N12	-6.39	1.33	1.46
3	A	601	KQD	C21-N23	6.31	1.47	1.34
3	A	601	KQD	C36-N38	6.28	1.47	1.34
3	D	601	KQD	C36-N38	6.27	1.47	1.34
3	D	601	KQD	C21-N23	6.27	1.47	1.34
3	A	601	KQD	C13-N11	-6.27	1.33	1.46
3	D	601	KQD	C13-N11	-6.24	1.33	1.46
3	B	801	KQD	C21-N23	6.21	1.47	1.34
3	C	801	KQD	C13-C14	6.20	1.64	1.53
3	B	801	KQD	C36-N38	6.15	1.47	1.34
3	C	801	KQD	C21-N23	6.14	1.47	1.34
3	A	601	KQD	C63-N67	6.13	1.47	1.34
3	D	601	KQD	C63-N67	6.12	1.47	1.34
3	C	801	KQD	C13-N11	-6.12	1.33	1.46
3	B	801	KQD	C13-C14	6.08	1.64	1.53
3	C	801	KQD	C36-N38	6.08	1.47	1.34
3	B	801	KQD	C13-N11	-5.99	1.34	1.46
3	D	601	KQD	C20-N12	-5.95	1.34	1.46
3	C	801	KQD	C20-N12	-5.87	1.34	1.46
3	A	601	KQD	C20-N12	-5.87	1.34	1.46
3	B	801	KQD	C62-N66	5.82	1.46	1.34
3	A	601	KQD	C13-C14	5.75	1.63	1.53
3	D	601	KQD	C13-C14	5.69	1.63	1.53
3	C	801	KQD	C63-N67	5.68	1.46	1.34
3	C	801	KQD	C8-N12	5.25	1.46	1.34
3	B	801	KQD	C63-N67	5.24	1.45	1.34
3	C	801	KQD	C16-N11	5.12	1.57	1.46
3	C	801	KQD	C7-N11	5.05	1.46	1.34
3	C	801	KQD	C62-N66	4.97	1.45	1.34
3	A	601	KQD	C8-N12	4.96	1.45	1.34
3	B	801	KQD	C7-N11	4.93	1.45	1.34
3	A	601	KQD	C62-N66	4.91	1.44	1.34
3	D	601	KQD	C8-N12	4.91	1.45	1.34
3	A	601	KQD	C16-N11	4.90	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	KQD	C16-N11	4.89	1.56	1.46
3	B	801	KQD	C8-N12	4.84	1.45	1.34
3	D	601	KQD	C62-N66	4.83	1.44	1.34
3	B	801	KQD	C16-N11	4.78	1.56	1.46
3	A	601	KQD	C7-N11	4.49	1.44	1.34
3	D	601	KQD	C7-N11	4.30	1.44	1.34
3	B	801	KQD	C42-C40	3.34	1.54	1.49
3	C	801	KQD	C42-C40	3.28	1.54	1.49
3	C	801	KQD	C16-C15	3.07	1.59	1.53
3	D	601	KQD	C20-C19	3.00	1.58	1.53
3	A	601	KQD	C20-C19	2.99	1.58	1.53
3	B	801	KQD	C16-C15	2.98	1.58	1.53
3	D	601	KQD	C16-C15	2.91	1.58	1.53
3	A	601	KQD	C16-C15	2.88	1.58	1.53
3	B	801	KQD	C71-C70	2.85	1.53	1.49
3	C	801	KQD	C25-C24	2.81	1.53	1.49
3	B	801	KQD	C4-C7	2.81	1.54	1.50
3	D	601	KQD	C42-C40	2.80	1.53	1.49
3	A	601	KQD	C42-C40	2.79	1.53	1.49
3	A	601	KQD	C4-C7	2.77	1.54	1.50
3	A	601	KQD	C25-C24	2.73	1.53	1.49
3	B	801	KQD	C25-C24	2.72	1.53	1.49
3	B	801	KQD	C75-C73	2.71	1.53	1.49
3	D	601	KQD	C25-C24	2.71	1.53	1.49
3	D	601	KQD	C4-C7	2.68	1.54	1.50
3	C	801	KQD	C4-C7	2.64	1.54	1.50
3	C	801	KQD	C20-C19	2.63	1.58	1.53
3	C	801	KQD	C43-C41	2.62	1.55	1.51
3	D	601	KQD	C75-C73	2.59	1.53	1.49
3	B	801	KQD	C43-C41	2.57	1.55	1.51
3	B	801	KQD	C20-C19	2.56	1.58	1.53
3	A	601	KQD	C75-C73	2.55	1.53	1.49
3	A	601	KQD	C28-C26	2.54	1.55	1.51
3	C	801	KQD	C75-C73	2.53	1.53	1.49
3	B	801	KQD	O9-C7	-2.48	1.17	1.22
3	C	801	KQD	C71-C70	2.38	1.52	1.49
3	B	801	KQD	C1-C8	2.35	1.53	1.50
3	D	601	KQD	C1-C8	2.32	1.53	1.50
3	D	601	KQD	O22-C21	-2.31	1.18	1.23
3	B	801	KQD	O10-C8	-2.29	1.18	1.22
3	B	801	KQD	C15-C21	2.27	1.55	1.51
3	A	601	KQD	O22-C21	-2.26	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	KQD	O9-C7	-2.21	1.18	1.22
3	C	801	KQD	C15-C21	2.21	1.55	1.51
3	D	601	KQD	C71-C70	2.17	1.52	1.49
3	D	601	KQD	O9-C7	-2.17	1.18	1.22
3	A	601	KQD	C71-C70	2.15	1.52	1.49
3	A	601	KQD	O9-C7	-2.13	1.18	1.22
3	D	601	KQD	C28-C26	2.08	1.55	1.51
3	C	801	KQD	C1-C8	2.05	1.53	1.50
3	D	601	KQD	O65-C63	-2.05	1.19	1.23
3	C	801	KQD	O10-C8	-2.03	1.18	1.22
3	D	601	KQD	C15-C21	2.03	1.55	1.51
3	C	801	KQD	O64-C62	-2.02	1.19	1.23
3	D	601	KQD	C71-C72	2.00	1.53	1.50
3	C	801	KQD	C28-C26	2.00	1.54	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	KQD	C25-C26-C28	7.69	137.04	122.24
3	C	801	KQD	C42-C41-C43	7.66	136.97	122.24
3	B	801	KQD	C42-C41-C43	7.55	136.77	122.24
3	D	601	KQD	C42-C41-C43	7.36	136.41	122.24
3	A	601	KQD	C25-C26-C28	7.15	135.99	122.24
3	A	601	KQD	C42-C41-C43	7.13	135.97	122.24
3	B	801	KQD	C25-C26-C28	6.67	135.09	122.24
3	C	801	KQD	C25-C26-C28	6.45	134.65	122.24
3	B	801	KQD	C25-C24-N23	-5.52	106.74	117.50
3	C	801	KQD	C25-C24-N23	-5.43	106.91	117.50
3	A	601	KQD	C15-C21-N23	5.10	122.08	116.00
3	D	601	KQD	C15-C21-N23	5.08	122.05	116.00
3	D	601	KQD	C70-N66-C62	-4.59	114.96	123.07
3	C	801	KQD	C42-C40-N38	-4.14	109.42	117.50
3	C	801	KQD	C70-N66-C62	-4.03	115.96	123.07
3	C	801	KQD	C40-N38-C36	-3.93	116.13	123.07
3	B	801	KQD	C42-C40-N38	-3.87	109.96	117.50
3	A	601	KQD	C42-C40-N38	-3.73	110.23	117.50
3	D	601	KQD	C42-C40-N38	-3.63	110.43	117.50
3	B	801	KQD	C40-N38-C36	-3.62	116.67	123.07
3	A	601	KQD	C70-N66-C62	-3.62	116.68	123.07
3	A	601	KQD	C25-C24-N23	-3.47	110.74	117.50
3	B	801	KQD	C73-N67-C63	-3.33	117.19	123.07
3	D	601	KQD	C19-C63-N67	3.27	119.89	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	KQD	C29-C28-C26	-3.21	115.00	121.08
3	B	801	KQD	C29-C28-C26	-3.12	115.17	121.08
3	C	801	KQD	C1-C8-N12	-3.10	114.77	118.72
3	D	601	KQD	O22-C21-N23	-3.09	117.21	122.93
3	A	601	KQD	C19-C63-N67	3.05	119.64	116.00
3	C	801	KQD	C81-C76-C72	-3.00	115.41	121.08
3	D	601	KQD	O9-C7-N11	-2.95	117.46	122.34
3	A	601	KQD	O9-C7-N11	-2.89	117.56	122.34
3	A	601	KQD	C40-N38-C36	-2.87	118.00	123.07
3	D	601	KQD	C40-N38-C36	-2.87	118.00	123.07
3	A	601	KQD	O22-C21-N23	-2.77	117.80	122.93
4	B	803	NAG	C2-N2-C7	2.75	126.81	122.90
3	A	601	KQD	C2-C1-C6	2.62	122.31	118.59
3	A	601	KQD	O65-C63-N67	-2.57	118.16	122.93
3	D	601	KQD	O10-C8-N12	-2.57	118.09	122.34
3	D	601	KQD	C75-C73-N67	2.56	122.50	117.50
3	D	601	KQD	C25-C24-N23	-2.52	112.60	117.50
3	D	601	KQD	C81-C76-C72	-2.48	116.39	121.08
3	D	601	KQD	C81-C76-C77	2.48	121.38	118.29
3	B	801	KQD	C87-C82-C74	-2.47	116.41	121.08
3	D	601	KQD	O65-C63-N67	-2.44	118.42	122.93
3	D	601	KQD	C4-C7-N11	2.37	121.73	118.72
3	D	601	KQD	C2-C1-C6	2.36	121.95	118.59
3	C	801	KQD	C4-C7-N11	-2.36	115.72	118.72
3	A	601	KQD	C4-C7-N11	2.34	121.68	118.72
3	C	801	KQD	C73-N67-C63	-2.30	119.01	123.07
3	A	601	KQD	C17-C18-C19	2.26	108.13	104.05
3	A	601	KQD	C81-C76-C77	2.21	121.05	118.29
3	A	601	KQD	C81-C76-C72	-2.16	116.98	121.08
4	B	802	NAG	C1-O5-C5	2.13	115.08	112.19
3	C	801	KQD	C81-C76-C77	2.12	120.94	118.29
3	D	601	KQD	C3-C4-C5	2.10	121.58	118.59
3	A	601	KQD	O10-C8-N12	-2.09	118.88	122.34
3	A	601	KQD	C3-C4-C5	2.04	121.49	118.59
3	C	801	KQD	C33-C28-C26	2.03	124.93	121.08
3	A	601	KQD	C75-C73-N67	2.03	121.46	117.50
3	D	601	KQD	C17-C18-C19	2.01	107.69	104.05
3	C	801	KQD	C3-C4-C7	-2.01	115.20	120.29
3	D	601	KQD	C75-C74-C82	2.00	126.10	122.24

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	603	NAG	C3-C2-N2-C7
3	B	801	KQD	C72-C70-N66-C62
3	D	601	KQD	C15-C21-N23-C24
3	D	601	KQD	C19-C63-N67-C73
3	A	601	KQD	C15-C21-N23-C24
3	A	601	KQD	C19-C63-N67-C73
4	A	604	NAG	O5-C5-C6-O6
4	A	605	NAG	C1-C2-N2-C7
4	A	605	NAG	C4-C5-C6-O6
4	B	803	NAG	C8-C7-N2-C2
4	B	803	NAG	O7-C7-N2-C2
4	A	607	NAG	C8-C7-N2-C2
4	A	607	NAG	O7-C7-N2-C2
4	A	606	NAG	C8-C7-N2-C2
4	A	606	NAG	O7-C7-N2-C2
4	B	802	NAG	O5-C5-C6-O6
4	B	803	NAG	C4-C5-C6-O6
4	B	802	NAG	C4-C5-C6-O6
3	D	601	KQD	O22-C21-N23-C24
3	A	601	KQD	O22-C21-N23-C24
3	D	601	KQD	O65-C63-N67-C73
3	A	601	KQD	O65-C63-N67-C73
4	A	605	NAG	O5-C5-C6-O6
4	B	803	NAG	O5-C5-C6-O6
4	A	604	NAG	C4-C5-C6-O6
3	C	801	KQD	C15-C14-C36-N38
3	C	801	KQD	C19-C18-C62-N66
3	C	801	KQD	C18-C19-C63-N67
3	B	801	KQD	C15-C14-C36-N38
3	B	801	KQD	C18-C19-C63-N67
3	C	801	KQD	C13-C14-C36-N38
3	C	801	KQD	C17-C18-C62-N66
3	B	801	KQD	C13-C14-C36-N38
3	C	801	KQD	C15-C14-C36-O37
3	C	801	KQD	C19-C18-C62-O64
3	C	801	KQD	C18-C19-C63-O65
3	B	801	KQD	C15-C14-C36-O37
3	B	801	KQD	C18-C19-C63-O65
3	B	801	KQD	C75-C74-C82-C87
3	C	801	KQD	C14-C15-C21-N23
3	B	801	KQD	C14-C15-C21-N23
4	C	802	NAG	C3-C2-N2-C7
3	C	801	KQD	C13-C14-C36-O37

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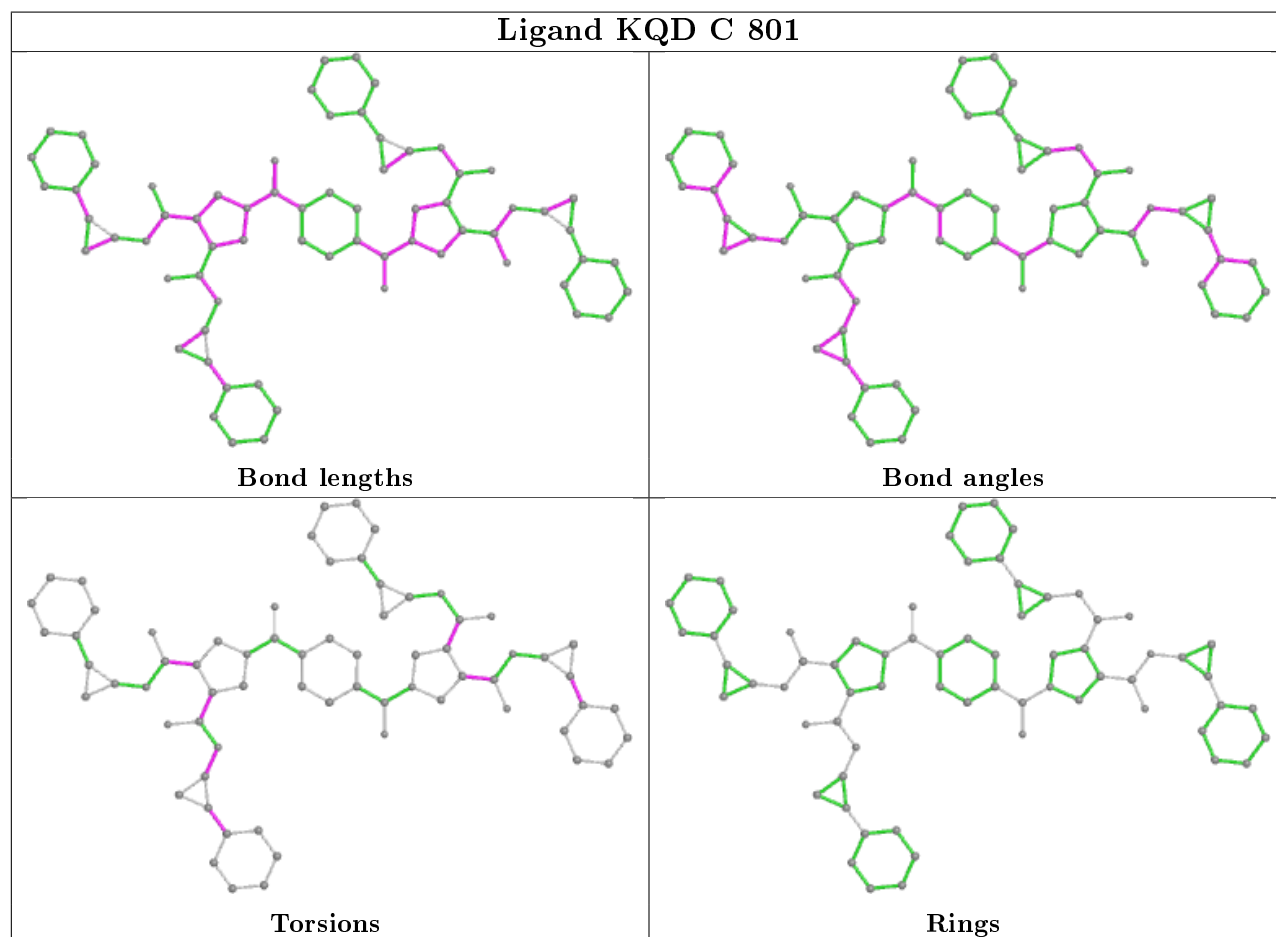
Mol	Chain	Res	Type	Atoms
3	C	801	KQD	C17-C18-C62-O64
3	B	801	KQD	C13-C14-C36-O37
3	B	801	KQD	C20-C19-C63-N67
4	C	802	NAG	C4-C5-C6-O6
3	C	801	KQD	C71-C72-C76-C81
4	C	802	NAG	O5-C5-C6-O6
3	B	801	KQD	C20-C19-C63-O65
3	C	801	KQD	C14-C15-C21-O22
3	B	801	KQD	C14-C15-C21-O22
3	C	801	KQD	C42-C41-C43-C48
3	B	801	KQD	C42-C41-C43-C48
3	B	801	KQD	C75-C74-C82-C83
3	C	801	KQD	C16-C15-C21-O22
3	B	801	KQD	C16-C15-C21-O22
3	B	801	KQD	C17-C18-C62-O64
3	C	801	KQD	C16-C15-C21-N23
3	C	801	KQD	C20-C19-C63-N67
3	B	801	KQD	C16-C15-C21-N23
3	C	801	KQD	C42-C41-C43-C44
3	B	801	KQD	C42-C41-C43-C44
3	C	801	KQD	C20-C19-C63-O65
3	B	801	KQD	C19-C18-C62-O64
3	C	801	KQD	C71-C72-C76-C77
3	B	801	KQD	C19-C18-C62-N66
3	C	801	KQD	C41-C40-N38-C36
3	D	601	KQD	C41-C40-N38-C36
3	A	601	KQD	C41-C40-N38-C36
3	B	801	KQD	C41-C40-N38-C36
3	B	801	KQD	C17-C18-C62-N66
4	B	803	NAG	C1-C2-N2-C7
4	B	803	NAG	C3-C2-N2-C7

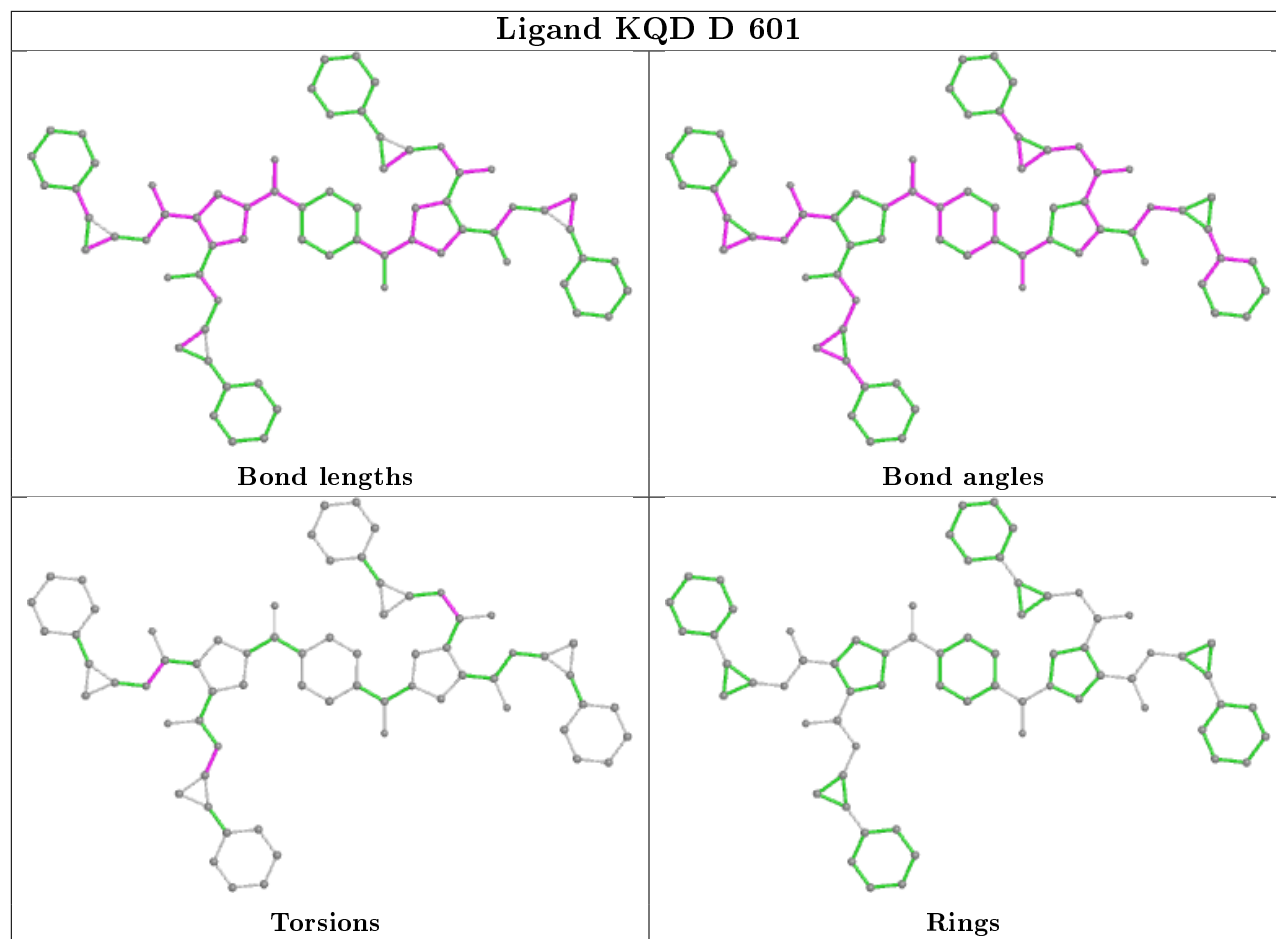
There are no ring outliers.

6 monomers are involved in 7 short contacts:

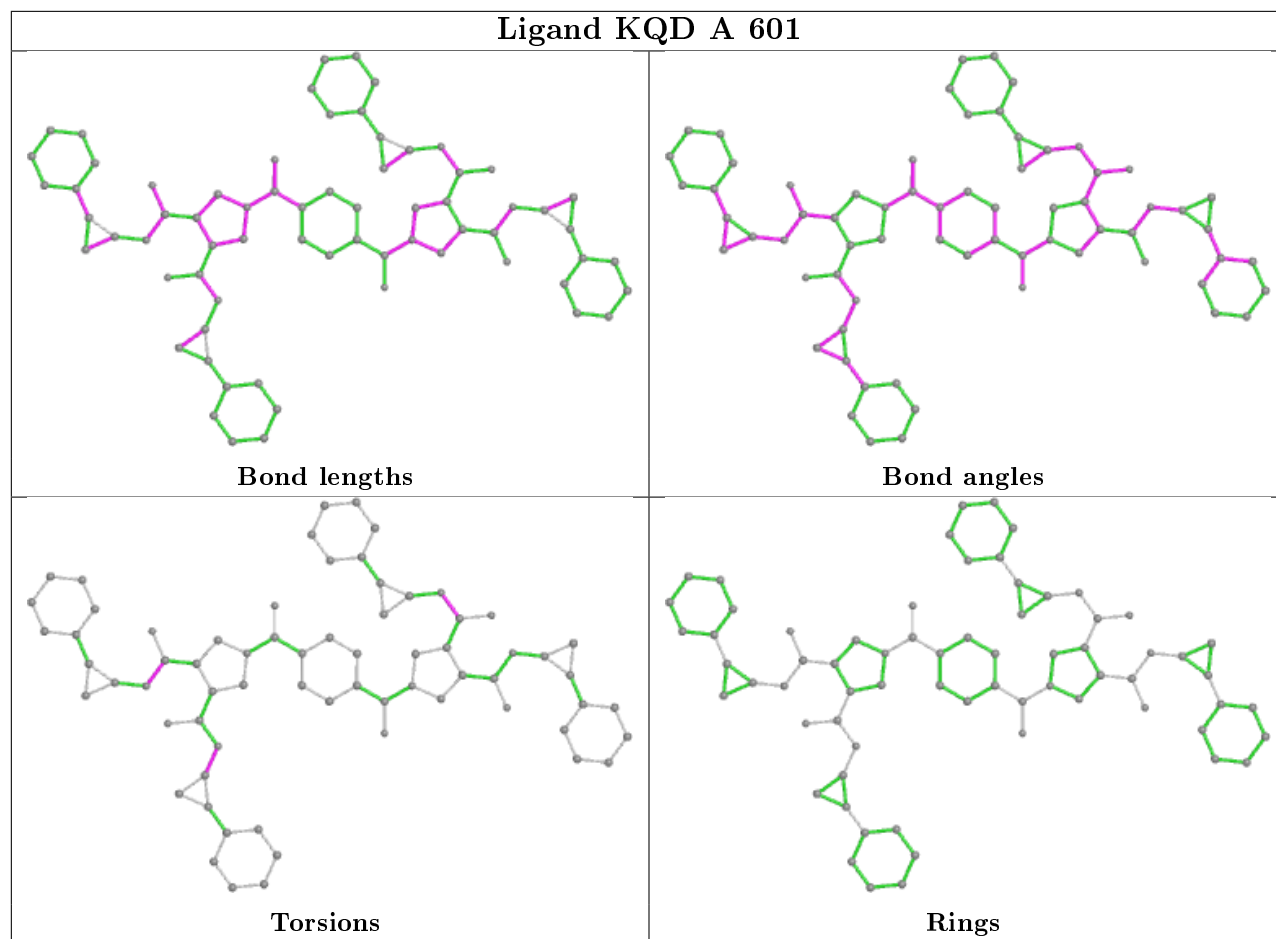
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	NAG	1	0
4	C	802	NAG	1	0
4	B	803	NAG	2	0
3	D	601	KQD	1	0
4	A	605	NAG	1	0
3	A	601	KQD	1	0

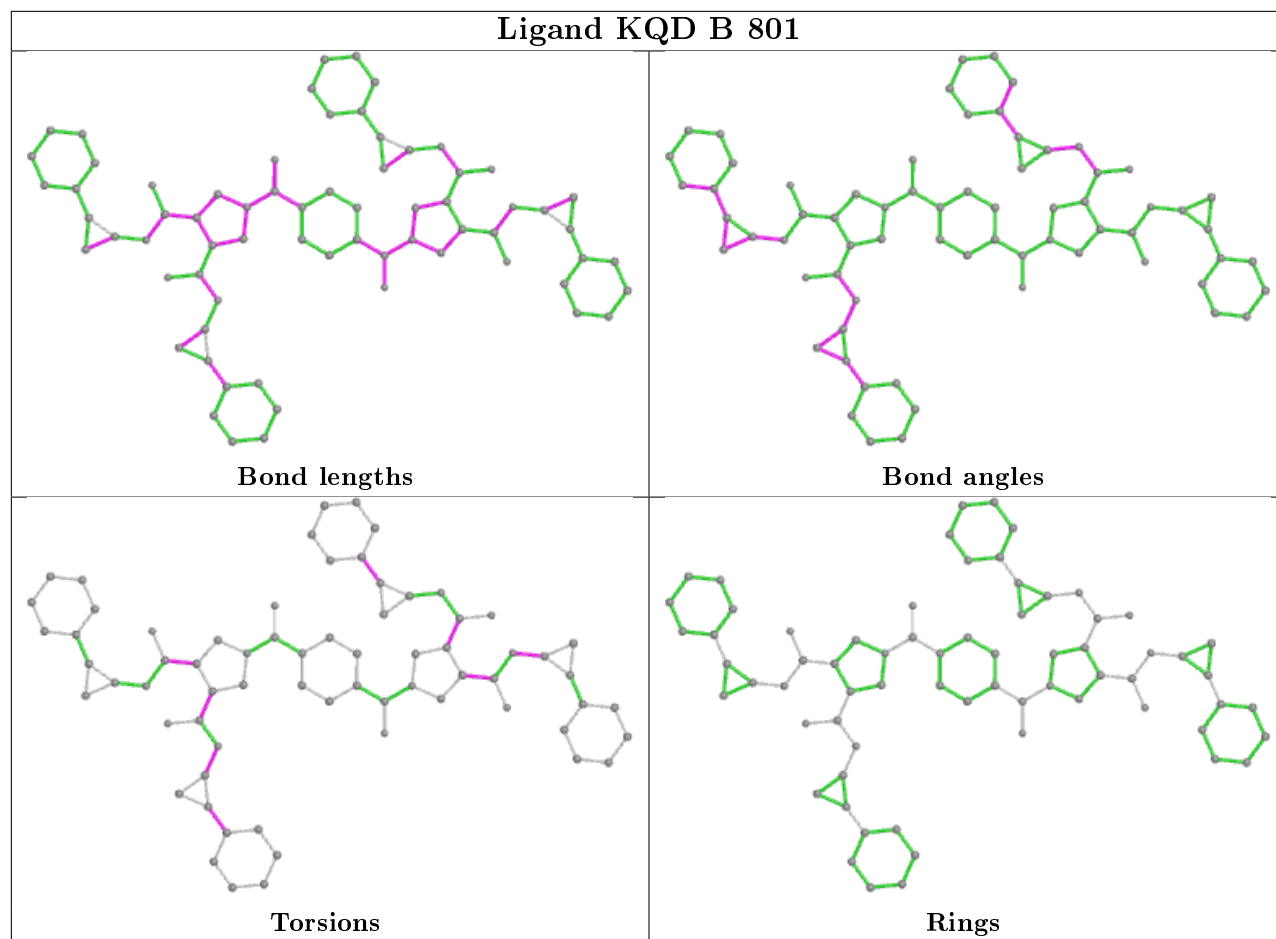
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	546/576 (94%)	0.86	62 (11%) <b>5</b> <b>7</b>	50, 74, 117, 203	0
1	B	545/576 (94%)	1.09	92 (16%) <b>1</b> <b>2</b>	48, 82, 148, 188	0
1	C	549/576 (95%)	1.17	99 (18%) <b>1</b> <b>2</b>	53, 86, 147, 209	0
1	D	546/576 (94%)	0.96	72 (13%) <b>3</b> <b>5</b>	53, 76, 133, 206	0
All	All	2186/2304 (94%)	1.02	325 (14%) <b>2</b> <b>3</b>	48, 79, 142, 209	0

All (325) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	245	GLY	14.5
1	C	302	ARG	14.3
1	B	66	TYR	13.0
1	C	243	SER	11.9
1	A	66	TYR	11.3
1	C	66	TYR	11.1
1	D	573	ILE	10.6
1	B	243	SER	9.9
1	C	27	SER	8.8
1	B	99	LEU	8.0
1	C	573	ILE	7.9
1	C	300	ASN	7.7
1	C	37	LYS	7.3
1	B	46	ILE	7.0
1	B	244	THR	6.7
1	B	245	GLY	6.5
1	B	246	GLU	6.4
1	C	303	VAL	6.2
1	C	64	ILE	6.0
1	D	521	ARG	5.9
1	C	67	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	553	SER	5.9
1	C	138	THR	5.8
1	B	67	ILE	5.7
1	A	550	ASN	5.6
1	D	66	TYR	5.5
1	B	112	LEU	5.5
1	B	247	THR	5.4
1	D	522	LEU	5.2
1	C	41	GLY	5.1
1	A	302	ARG	5.0
1	C	140	GLY	5.0
1	B	109	TYR	4.9
1	B	35	ILE	4.9
1	A	27	SER	4.8
1	C	141	GLU	4.8
1	A	90	THR	4.7
1	A	298	SER	4.6
1	B	39	SER	4.6
1	A	519	PHE	4.5
1	C	93	GLU	4.5
1	A	67	ILE	4.5
1	B	45	SER	4.5
1	B	137	LYS	4.4
1	B	27	SER	4.4
1	C	251	ILE	4.4
1	D	551	LYS	4.4
1	D	518	ILE	4.3
1	A	495	ALA	4.3
1	C	175	PHE	4.3
1	B	521	ARG	4.2
1	C	246	GLU	4.2
1	D	321	ARG	4.1
1	C	242	LEU	4.1
1	C	227	LEU	4.0
1	C	115	LEU	4.0
1	D	303	VAL	4.0
1	A	573	ILE	3.9
1	C	299	ASP	3.9
1	C	539	CYS	3.9
1	B	28	LEU	3.9
1	B	164	LYS	3.9
1	C	28	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	63	ARG	3.9
1	C	296	ARG	3.8
1	D	152	GLN	3.8
1	B	98	SER	3.8
1	B	141	GLU	3.8
1	D	247	THR	3.8
1	C	112	LEU	3.7
1	D	550	ASN	3.7
1	C	61	ASN	3.7
1	C	65	THR	3.7
1	A	376	TYR	3.7
1	B	371	LEU	3.6
1	D	243	SER	3.6
1	C	44	ASN	3.6
1	B	63	ARG	3.6
1	C	139	LEU	3.6
1	C	164	LYS	3.6
1	D	564	GLY	3.6
1	B	64	ILE	3.6
1	B	74	ARG	3.6
1	C	174	THR	3.6
1	B	349	PHE	3.5
1	B	354	LEU	3.5
1	C	247	THR	3.5
1	D	150	LYS	3.5
1	B	90	THR	3.5
1	A	297	ALA	3.5
1	C	376	TYR	3.5
1	D	349	PHE	3.5
1	D	248	ASN	3.5
1	C	90	THR	3.4
1	C	570	ARG	3.4
1	A	502	LEU	3.4
1	A	521	ARG	3.4
1	D	68	SER	3.3
1	A	244	THR	3.3
1	D	500	MET	3.3
1	C	68	SER	3.3
1	D	242	LEU	3.3
1	C	91	ILE	3.3
1	B	436	GLU	3.3
1	D	244	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	248	ASN	3.2
1	C	530	LEU	3.2
1	D	572	ILE	3.2
1	B	88	ILE	3.2
1	C	254	PHE	3.2
1	C	244	THR	3.2
1	B	214	LEU	3.2
1	C	43	LEU	3.2
1	B	224	VAL	3.2
1	B	502	LEU	3.2
1	B	251	ILE	3.2
1	C	88	ILE	3.2
1	C	518	ILE	3.2
1	B	40	SER	3.1
1	C	159	MET	3.1
1	D	173	LEU	3.1
1	C	301	ASP	3.1
1	B	540	PRO	3.1
1	C	136	TYR	3.1
1	A	436	GLU	3.1
1	C	354	LEU	3.1
1	B	296	ARG	3.1
1	B	138	THR	3.1
1	B	353	CYS	3.0
1	B	37	LYS	3.0
1	C	57	LEU	3.0
1	D	294	ASN	3.0
1	C	46	ILE	3.0
1	D	523	THR	3.0
1	A	424	SER	3.0
1	B	136	TYR	2.9
1	B	166	GLN	2.9
1	B	337	ARG	2.9
1	D	575	PRO	2.9
1	C	198	GLN	2.9
1	D	159	MET	2.9
1	C	70	SER	2.9
1	C	239	PHE	2.9
1	B	203	LEU	2.9
1	C	250	LEU	2.9
1	B	539	CYS	2.8
1	B	139	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	203	LEU	2.8
1	D	238[A]	HIS	2.8
1	D	296	ARG	2.8
1	B	198	GLN	2.8
1	C	187	GLN	2.8
1	B	490	MET	2.8
1	A	524	SER	2.8
1	A	88	ILE	2.8
1	B	111	TYR	2.8
1	B	372	MET	2.7
1	D	90	THR	2.7
1	D	67	ILE	2.7
1	A	38	GLY	2.7
1	D	490	MET	2.7
1	A	109	TYR	2.7
1	C	30	CYS	2.7
1	A	319	ILE	2.7
1	B	85	SER	2.7
1	D	74	ARG	2.7
1	D	211	ILE	2.7
1	C	349	PHE	2.7
1	B	78	LEU	2.7
1	A	39	SER	2.6
1	D	236	THR	2.6
1	A	514	VAL	2.6
1	A	525	LEU	2.6
1	C	214	LEU	2.6
1	A	522	LEU	2.6
1	C	298	SER	2.6
1	C	549	LEU	2.6
1	D	308	LYS	2.6
1	B	68	SER	2.6
1	C	45	SER	2.6
1	C	430	GLU	2.6
1	A	554	GLN	2.6
1	C	529	TRP	2.6
1	C	137	LYS	2.6
1	B	328	LEU	2.6
1	D	53	ALA	2.6
1	B	229	LEU	2.5
1	D	554	GLN	2.5
1	C	111	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	334	LEU	2.5
1	C	38	GLY	2.5
1	C	373	VAL	2.5
1	D	170	PHE	2.5
1	A	359	LEU	2.5
1	A	89	ASN	2.5
1	C	89	ASN	2.5
1	D	276	ILE	2.5
1	D	63	ARG	2.5
1	A	291	GLY	2.5
1	D	384	ASP	2.5
1	D	519	PHE	2.5
1	D	318	HIS	2.5
1	B	573	ILE	2.5
1	C	197	ILE	2.5
1	C	42	SER	2.4
1	B	54	VAL	2.4
1	B	519	PHE	2.4
1	D	574	CYS	2.4
1	D	547	ARG	2.4
1	C	176	LEU	2.4
1	B	319	ILE	2.4
1	B	250	LEU	2.4
1	B	430	GLU	2.4
1	C	378	LYS	2.4
1	A	399	LEU	2.4
1	A	293	GLY	2.4
1	B	93	GLU	2.4
1	C	87	GLY	2.4
1	B	174	THR	2.4
1	C	124	SER	2.4
1	D	331	LEU	2.4
1	D	299	ASP	2.4
1	C	36	CYS	2.4
1	C	149	THR	2.4
1	D	217	PHE	2.4
1	D	232	THR	2.4
1	C	85	SER	2.4
1	B	347	LYS	2.4
1	B	38	GLY	2.4
1	A	276	ILE	2.3
1	B	332	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	575	PRO	2.3
1	C	220	VAL	2.3
1	C	224	VAL	2.3
1	D	175	PHE	2.3
1	A	471	LEU	2.3
1	D	501	LEU	2.3
1	A	248	ASN	2.3
1	B	351	VAL	2.3
1	D	259	VAL	2.3
1	A	551	LYS	2.3
1	B	398	HIS	2.3
1	B	352	PRO	2.3
1	C	72	LEU	2.3
1	C	99	LEU	2.3
1	D	237	PHE	2.3
1	D	398	HIS	2.3
1	C	321	ARG	2.3
1	C	53	ALA	2.3
1	B	213	LEU	2.3
1	D	371	LEU	2.3
1	A	294	ASN	2.3
1	D	494	ASP	2.3
1	C	59	LEU	2.3
1	A	321	ARG	2.3
1	B	298	SER	2.3
1	C	131	LEU	2.2
1	C	145	PHE	2.2
1	B	518	ILE	2.2
1	D	216	ILE	2.2
1	D	164	LYS	2.2
1	D	280	LEU	2.2
1	D	549	LEU	2.2
1	A	337	ARG	2.2
1	A	548	TRP	2.2
1	A	194	LEU	2.2
1	A	250	LEU	2.2
1	B	72	LEU	2.2
1	C	81	LEU	2.2
1	A	53	ALA	2.2
1	B	261	ILE	2.2
1	A	324	LEU	2.2
1	B	115	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	355	LEU	2.2
1	B	376	TYR	2.2
1	D	387	PRO	2.2
1	C	114	ASN	2.2
1	D	530	LEU	2.2
1	A	76	VAL	2.2
1	A	175	PHE	2.2
1	C	514	VAL	2.1
1	C	151	LEU	2.1
1	D	479	LEU	2.1
1	B	259	VAL	2.1
1	A	301	ASP	2.1
1	A	198	GLN	2.1
1	A	251	ILE	2.1
1	A	249	SER	2.1
1	B	36	CYS	2.1
1	B	41	GLY	2.1
1	A	161	THR	2.1
1	B	299	ASP	2.1
1	B	564	GLY	2.1
1	C	148	LEU	2.1
1	D	37	LYS	2.1
1	C	69	ASN	2.1
1	D	246	GLU	2.1
1	B	70	SER	2.1
1	B	566	GLY	2.1
1	C	565	SER	2.1
1	D	567	LYS	2.1
1	B	554	GLN	2.1
1	D	76	VAL	2.1
1	A	328	LEU	2.1
1	A	492	LEU	2.1
1	A	348	VAL	2.1
1	D	39	SER	2.1
1	B	175	PHE	2.1
1	A	261	ILE	2.0
1	A	296	ARG	2.0
1	A	412	LEU	2.0
1	C	179	LEU	2.0
1	B	110	ASN	2.0
1	B	375	GLU	2.0
1	D	571	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	58	ASP	2.0
1	A	32	ARG	2.0
1	B	216	ILE	2.0
1	C	204	ILE	2.0
1	C	241	GLU	2.0
1	A	566	GLY	2.0
1	B	495	ALA	2.0
1	D	297	ALA	2.0
1	A	371	LEU	2.0
1	B	57	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

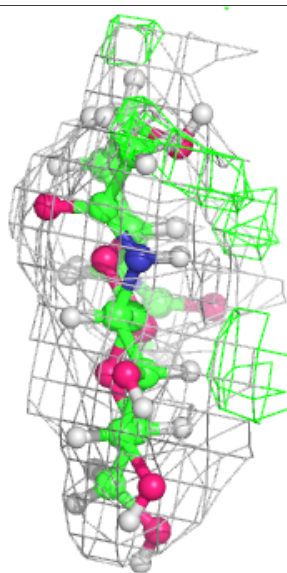
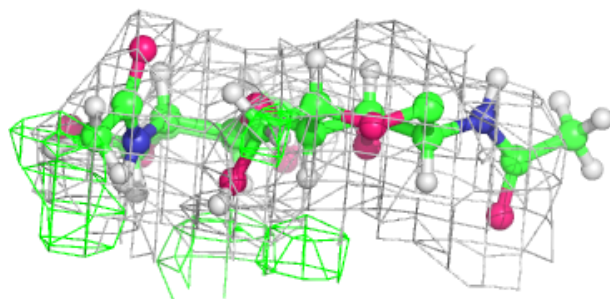
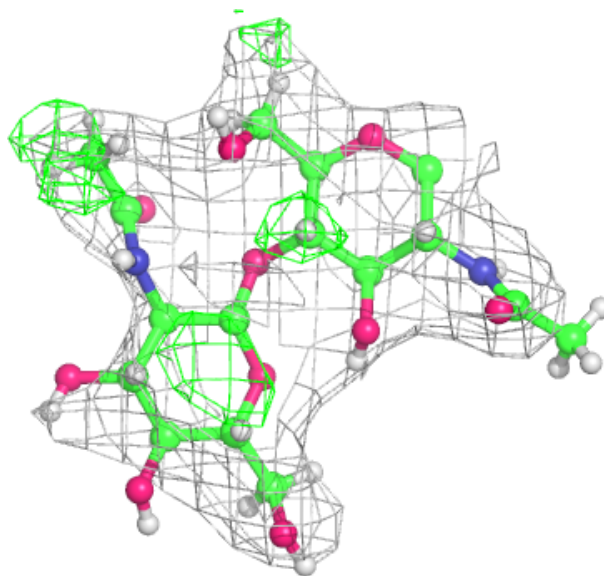
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	E	2	14/15	0.69	0.21	104,110,131,133	0
2	NAG	H	2	14/15	0.70	0.24	84,97,116,121	0
2	NAG	G	2	14/15	0.77	0.24	84,98,117,119	0
2	NAG	E	1	14/15	0.83	0.15	91,104,123,124	0
2	NAG	F	2	14/15	0.85	0.23	81,93,111,112	0
2	NAG	G	1	14/15	0.94	0.16	53,64,75,76	0
2	NAG	H	1	14/15	0.95	0.15	52,67,78,81	0
2	NAG	F	1	14/15	0.97	0.12	48,59,70,70	0

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

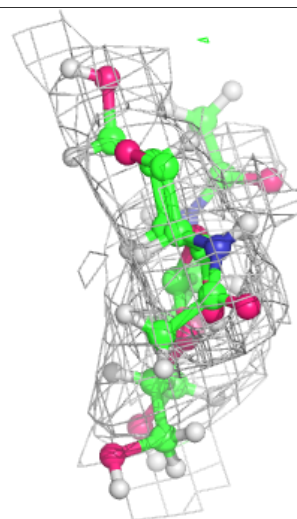
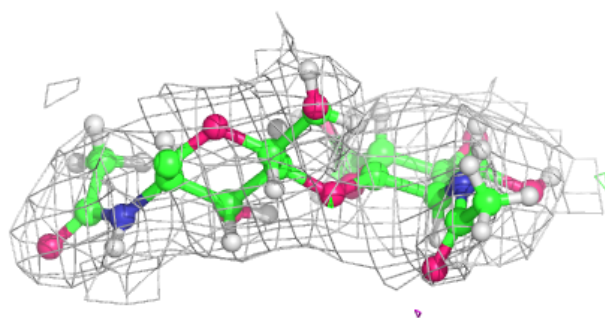
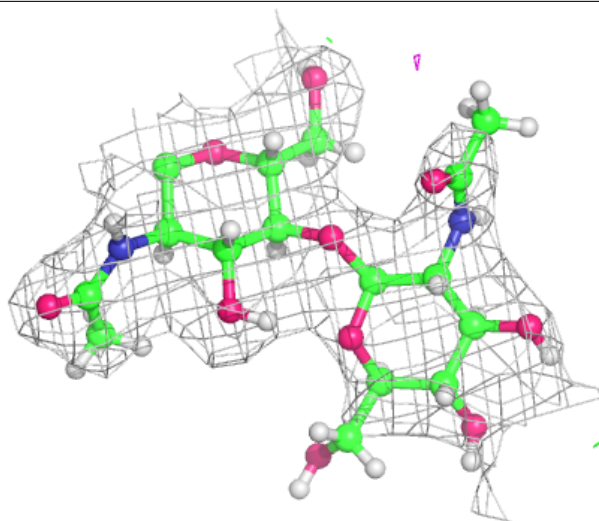
**Electron density around Chain E:**

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



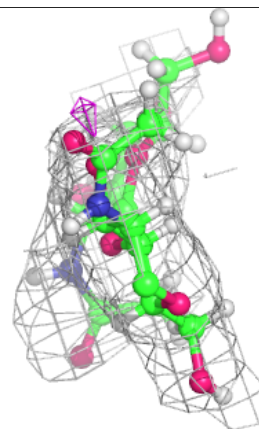
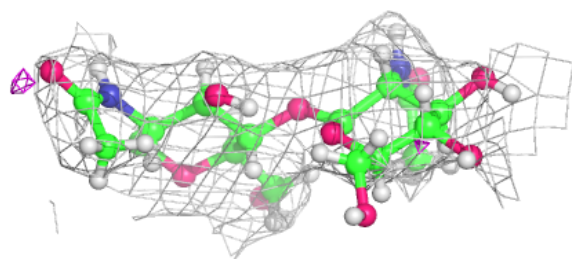
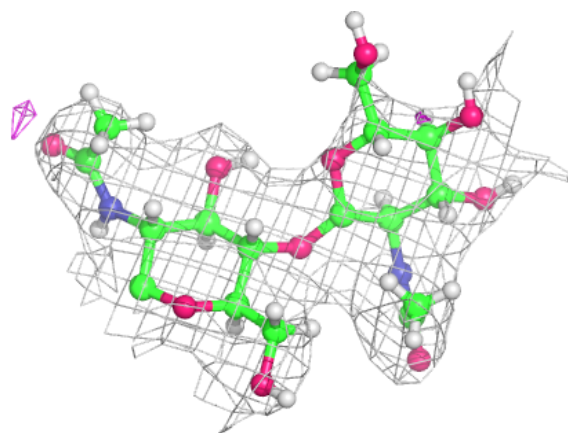
**Electron density around Chain F:**

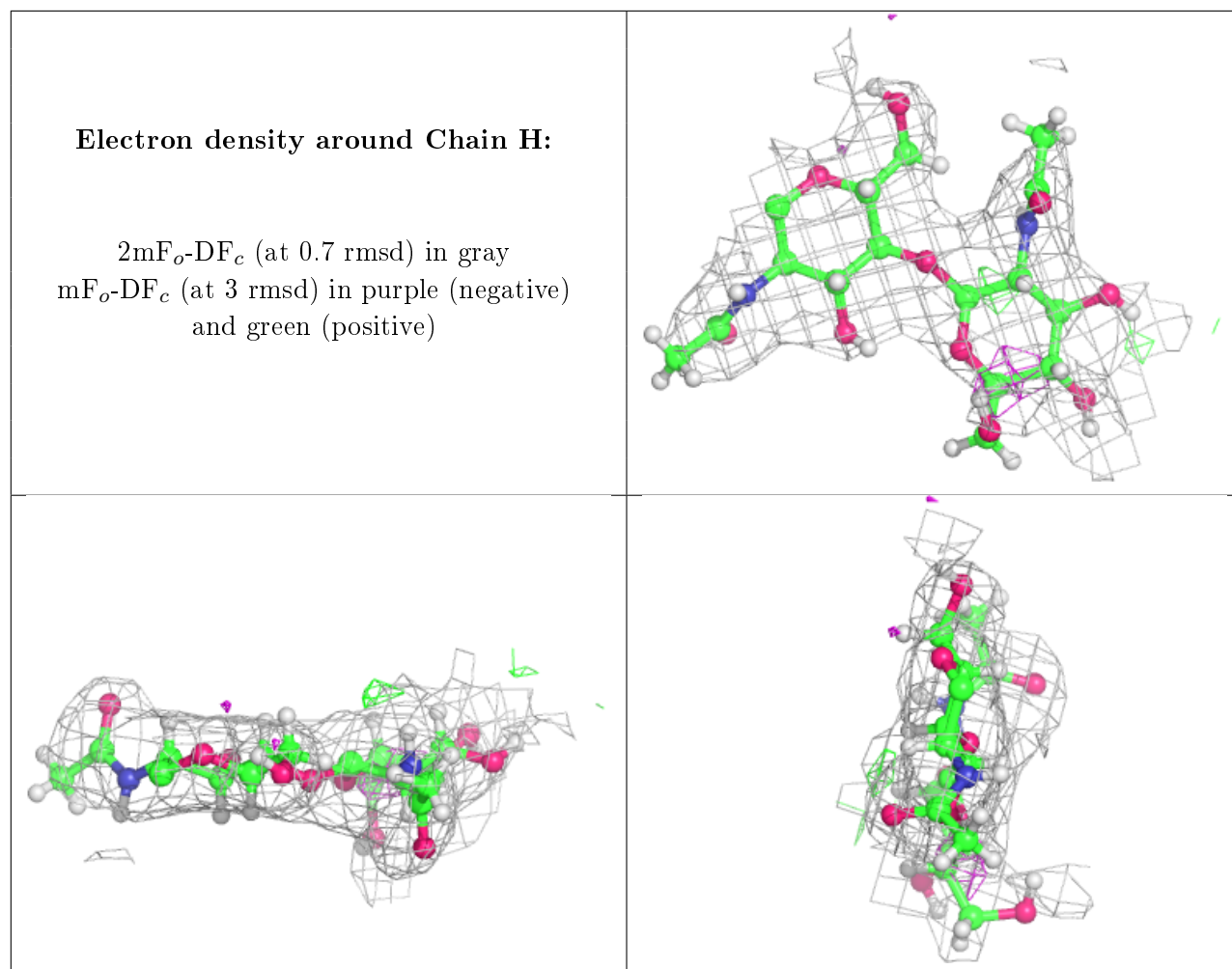
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain G:**

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





## 6.4 Ligands [i](#)

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

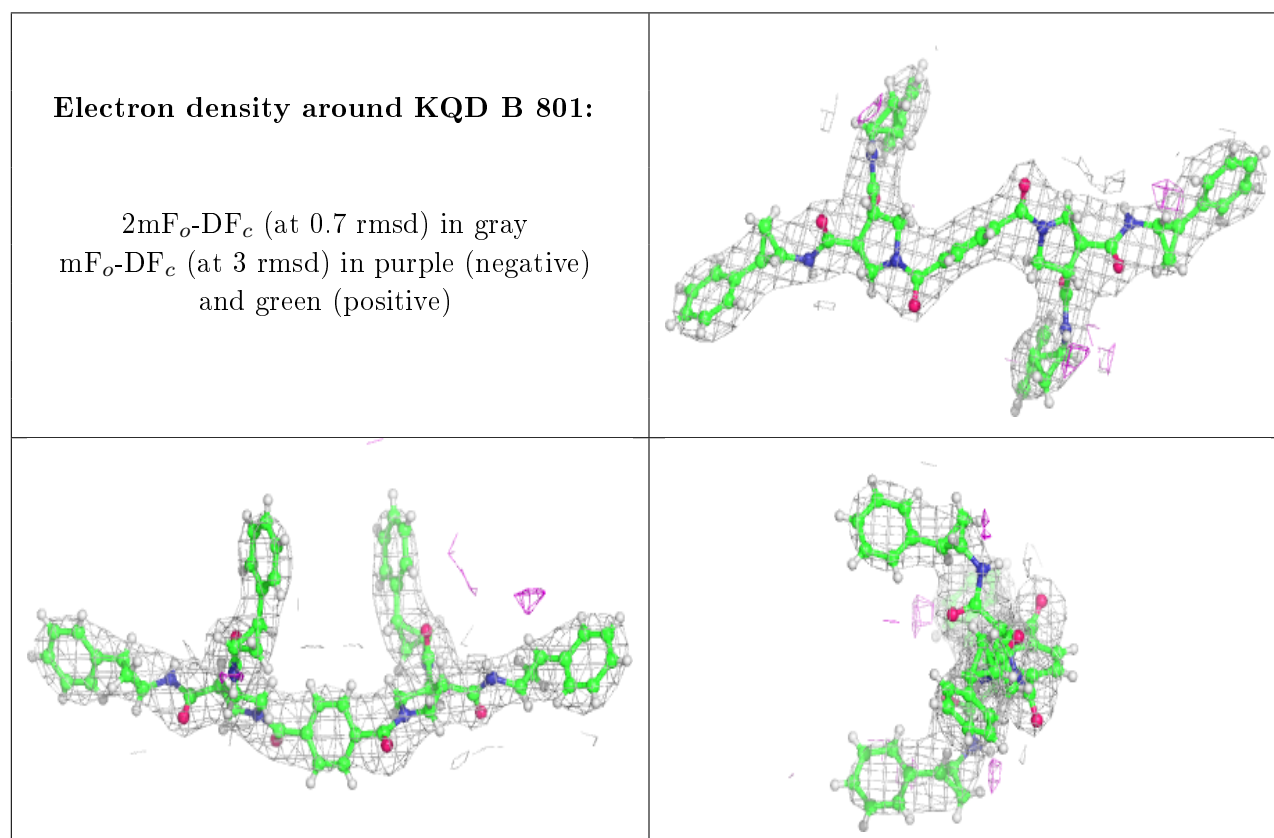
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	B	802	14/15	0.72	0.17	78,92,110,111	0
4	NAG	A	604	14/15	0.76	0.39	79,94,112,112	0
4	NAG	B	803	14/15	0.78	0.19	99,116,139,139	0
4	NAG	A	607	14/15	0.81	0.24	87,97,117,118	0
4	NAG	D	602	14/15	0.82	0.34	83,94,112,113	0
4	NAG	C	802	14/15	0.82	0.23	83,94,113,114	0
4	NAG	D	603	14/15	0.84	0.30	99,115,138,138	0
4	NAG	A	605	14/15	0.86	0.28	75,92,110,110	0
3	KQD	B	801	68/68	0.93	0.20	59,71,83,91	0
3	KQD	A	601	68/68	0.93	0.20	57,67,79,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	KQD	D	601	68/68	0.94	0.20	56,65,78,79	0
3	KQD	C	801	68/68	0.94	0.20	59,68,81,84	0
4	NAG	A	606	14/15	0.97	0.16	49,65,76,79	0

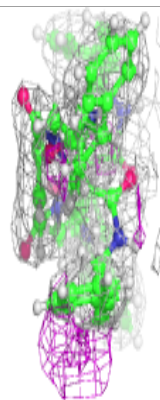
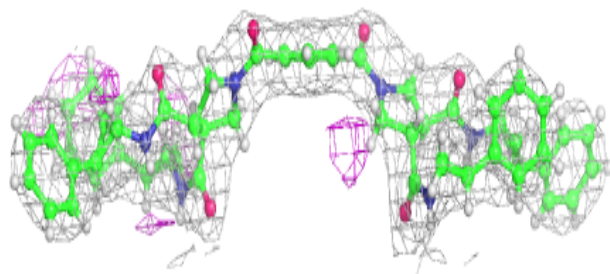
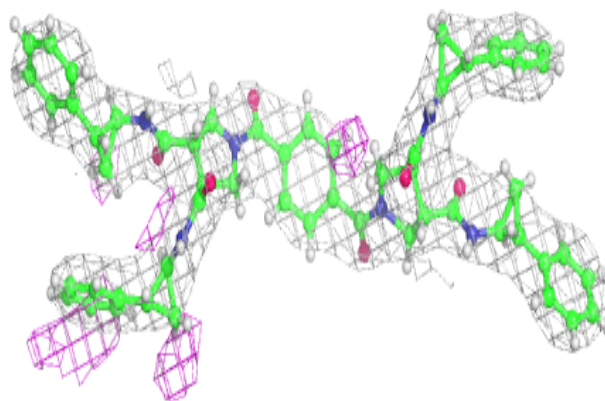
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



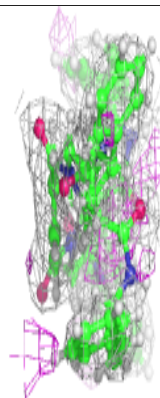
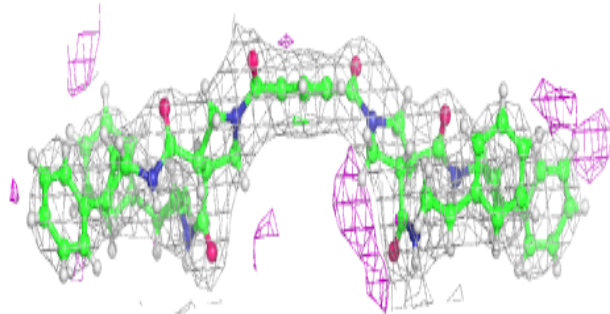
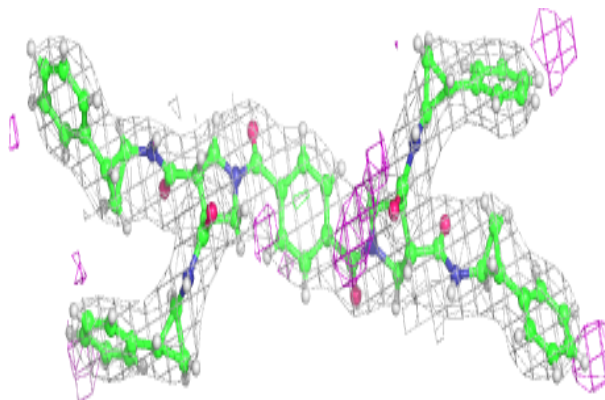


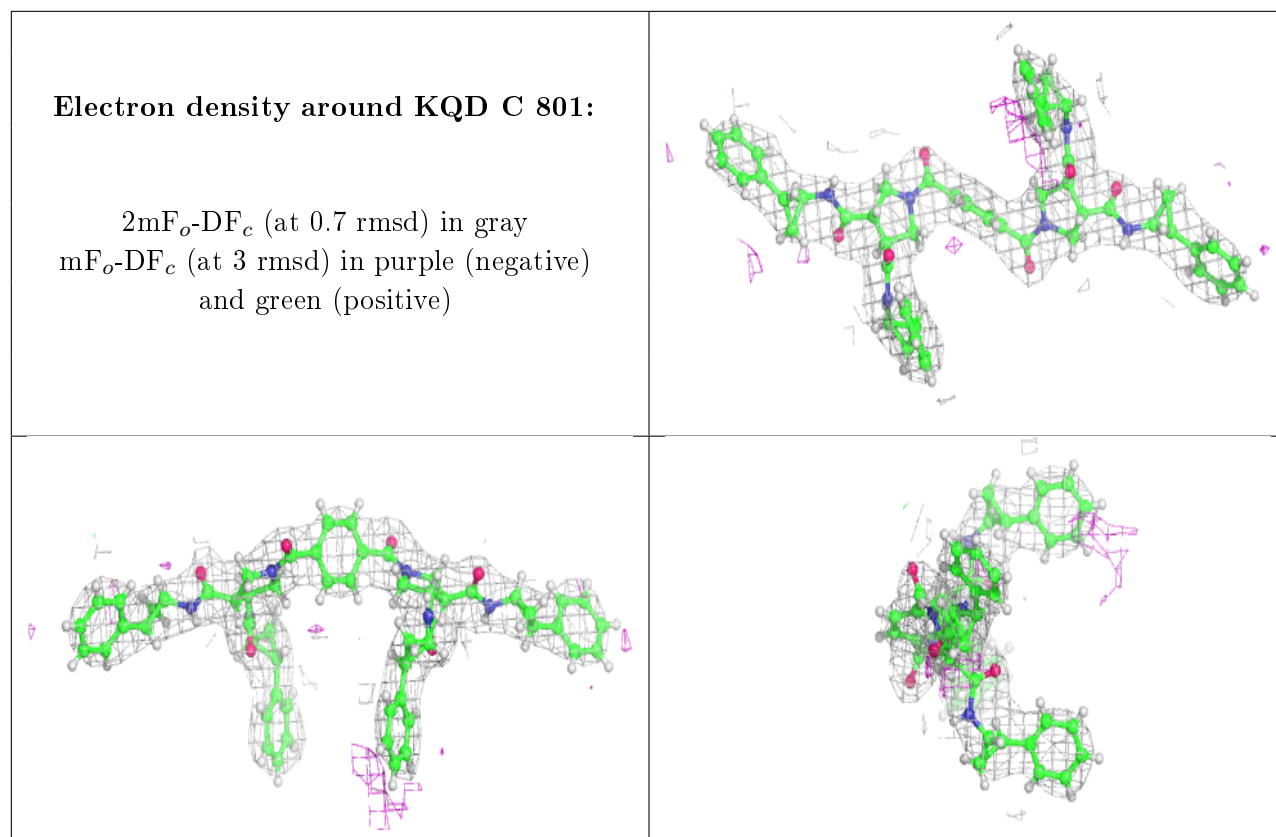
**Electron density around KQD A 601:**

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

**Electron density around KQD 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.