



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:20 AM UTC

PDB ID : 6NIG / pdb_00006nig
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

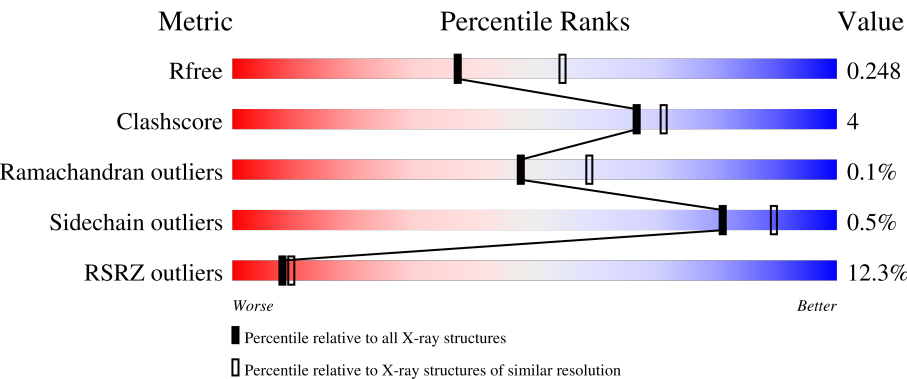
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 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	576	8% 89%6%5%
1	B	576	14% 86%8%5%
1	C	576	14% 86%10%5%
1	D	576	11% 87%7%5%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	100%
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.



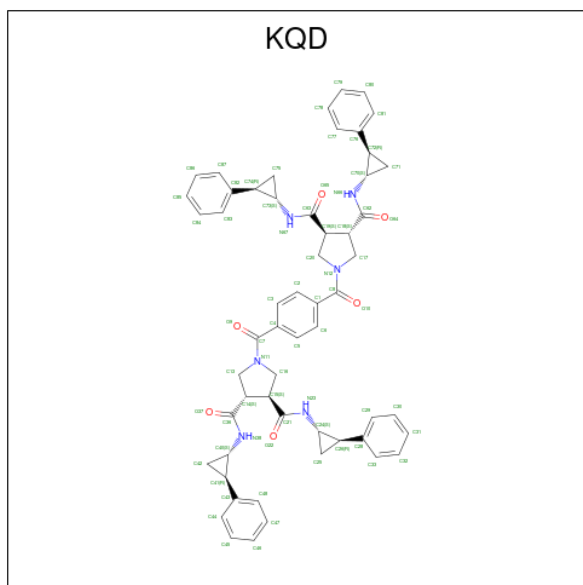
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				
2	F	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				
2	G	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				

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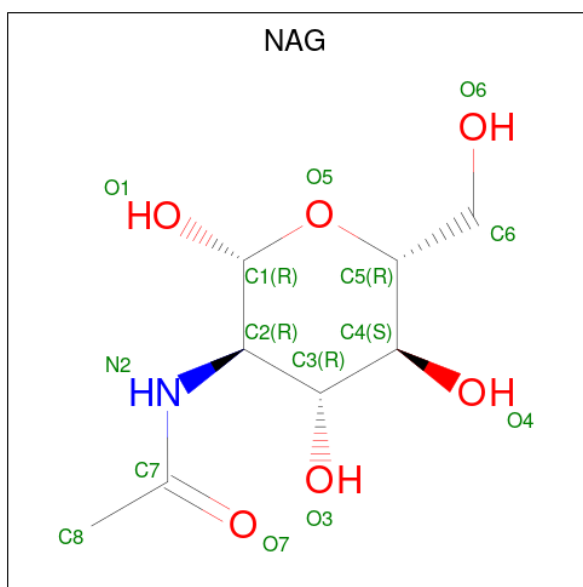
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- 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-dicarboxami de} (CCD ID: KQD) (formula: C₅₆H₅₆N₆O₆).



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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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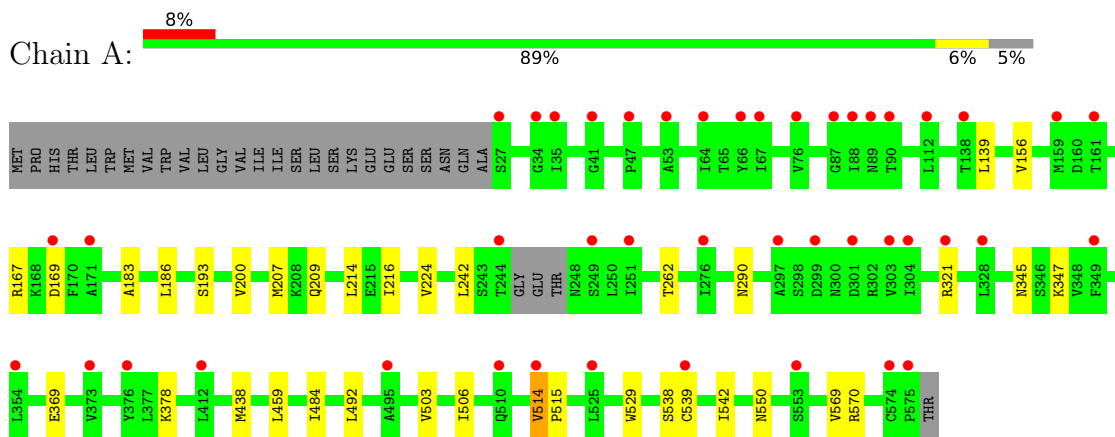
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	7	Total	O	0	0
			7	7		

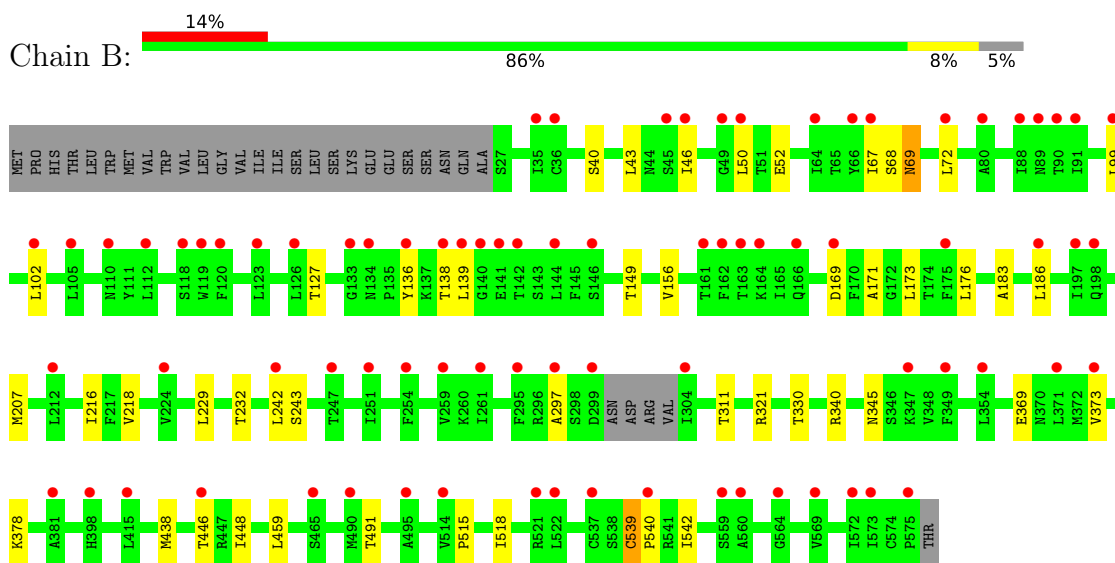
3 Residue-property plots [i](#)

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.

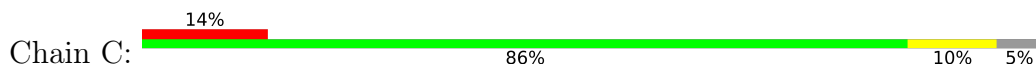
- Molecule 1: Toll-like receptor 2, Variable lymphocyte receptor B

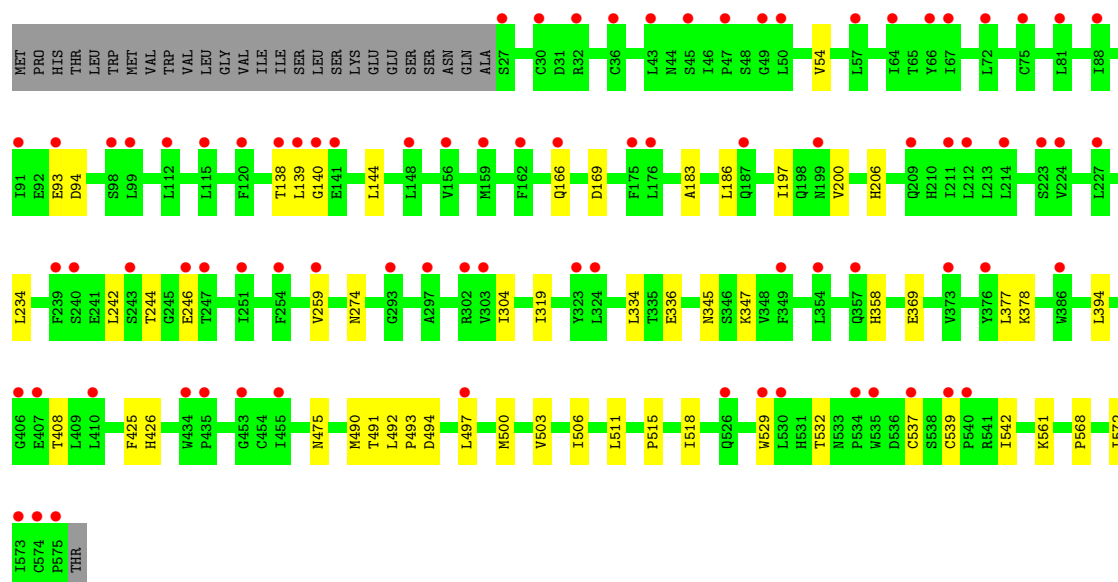


- Molecule 1: Toll-like receptor 2, Variable lymphocyte receptor B

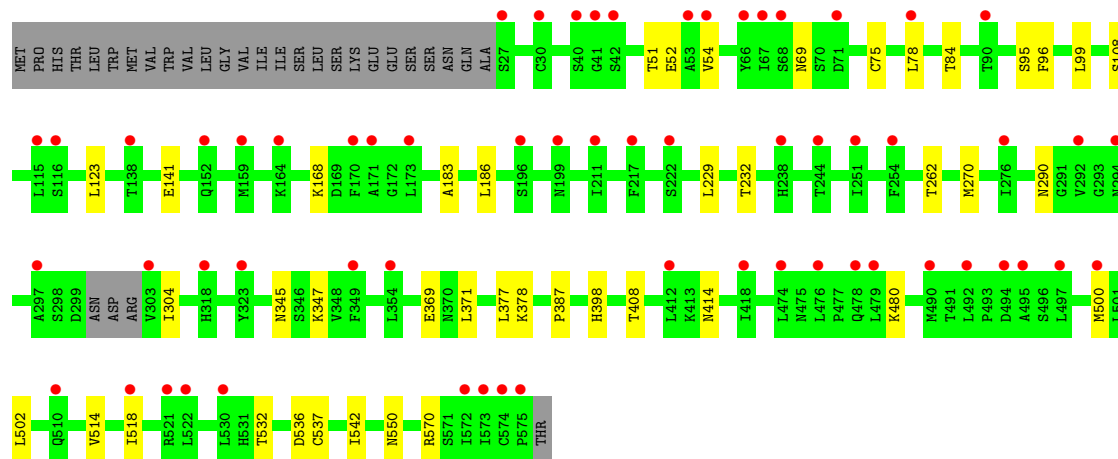
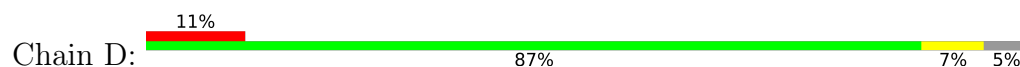


- Molecule 1: Toll-like receptor 2, Variable lymphocyte receptor B





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



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



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



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

Chain G:  50% 50%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.10Å 201.25Å 109.36Å 90.00° 94.26° 90.00°	Depositor
Resolution (Å)	37.76 – 2.35 37.76 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.8 (37.76-2.35) 94.8 (37.76-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.210 , 0.236 0.225 , 0.248	Depositor DCC
R_{free} test set	3364 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.13	0/4420	0.31	0/5984
1	B	0.11	0/4406	0.31	0/5965
1	C	0.11	0/4441	0.30	0/6014
1	D	0.11	0/4436	0.31	0/6006
All	All	0.11	0/17703	0.31	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	26	0
1	B	4331	4385	4385	36	0
1	C	4365	4419	4419	34	0
1	D	4348	4402	4392	30	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	131	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 (131) 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:207:MET:HE1	1:B:216:ILE:HD12	1.56	0.85
1:B:139:LEU:HD21	1:B:156:VAL:HG21	1.59	0.83
1:A:207:MET:HE1	1:A:216:ILE:HD12	1.66	0.76
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:H83	4:B:803:NAG:H3	1.80	0.61
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:500:MET:HA	1:C:500:MET:HE2	1.83	0.60
1:D:500:MET:HA	1:D:500:MET:HE2	1.83	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:HE1	1:D:304:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:MET:CE	1:D:304:ILE:HD13	2.34	0.58
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
1:D:377:LEU:HB3	1:D:408:THR:HG21	1.86	0.57
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:A:207:MET:CE	1:A:216:ILE:HD12	2.34	0.54
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:B:438:MET:HE3	1:B:459:LEU:HD21	1.90	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:O7	4:C:802:NAG:H3	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:O7	4:D:603:NAG:H3	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: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
1:B:207:MET:CE	1:B:216:ILE:HD12	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:THR:HG23	1:B:448:ILE:HG23	1.96	0.47
1:A:139:LEU:HD12	1:A:169:ASP:HB3	1.97	0.47
1:B:50:LEU:HD22	1:B:72:LEU:CD2	2.39	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:C:503:VAL:HG13	1:C:529:TRP:HZ3	1.80	0.47
1:B:69:ASN:N	1:B:69:ASN:OD1	2.47	0.47
1:B:52:GLU:OE1	1:B:52:GLU:N	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:H3	2:G:2:NAG:C8	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:D:141:GLU:O	1:D:168:LYS:NZ	2.45	0.45
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:O	1:D:54:VAL:HG13	2.17	0.44
1:D:96:PHE:HB3	1:D:123:LEU:HD21	1.98	0.44
4:A:605:NAG:O7	4:A:605:NAG:C1	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:A:438:MET:HE3	1:A:459:LEU:HD21	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:O	1:B:542:ILE:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ILE:H	1:C:347:LYS:HZ1	1.67	0.43
1:D:514:VAL:CG2	1:D:518:ILE:HG21	2.48	0.43
1:B:373:VAL:HG23	1:B:373:VAL:O	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
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:B:229:LEU:C	1:B:229:LEU:HD13	2.44	0.41
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 ⓘ

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	542/576 (94%)	510 (94%)	31 (6%)	1 (0%)	43	52
1	B	541/576 (94%)	502 (93%)	39 (7%)	0	100	100
1	C	547/576 (95%)	512 (94%)	34 (6%)	1 (0%)	43	52
1	D	544/576 (94%)	512 (94%)	32 (6%)	0	100	100
All	All	2174/2304 (94%)	2036 (94%)	136 (6%)	2 (0%)	48	59

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%)	514 (100%)	2 (0%)	84	91
1	B	514/543 (95%)	508 (99%)	6 (1%)	63	77
1	C	518/543 (95%)	515 (99%)	3 (1%)	78	87
1	D	517/543 (95%)	517 (100%)	0	100	100
All	All	2065/2172 (95%)	2054 (100%)	11 (0%)	81	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	514	VAL
1	A	539	CYS
1	B	68	SER
1	B	69	ASN
1	B	127	THR
1	B	149	THR
1	B	491	THR
1	B	539	CYS
1	C	206	HIS

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Mol	Chain	Res	Type
1	C	274	ASN
1	C	539	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	238	HIS
1	A	318	HIS
1	A	552	ASN
1	B	238	HIS
1	B	475	ASN
1	B	557	GLN
1	C	318	HIS
1	C	510	GLN
1	D	77	ASN
1	D	433	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	F	1	1,2	14,14,15	0.30	0	17,19,21	0.49	0
2	NAG	F	2	2	14,14,15	0.30	0	17,19,21	0.36	0
2	NAG	G	1	1,2	14,14,15	0.22	0	17,19,21	0.51	0
2	NAG	G	2	2	14,14,15	0.18	0	17,19,21	1.18	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.88	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	-	6/6/23/26	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	3.04	126.97	122.90
2	H	2	NAG	C1-O5-C5	2.59	115.66	112.19
2	G	2	NAG	C1-O5-C5	2.50	115.54	112.19

There are no chirality outliers.

All (16) 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	E	2	NAG	O5-C5-C6-O6

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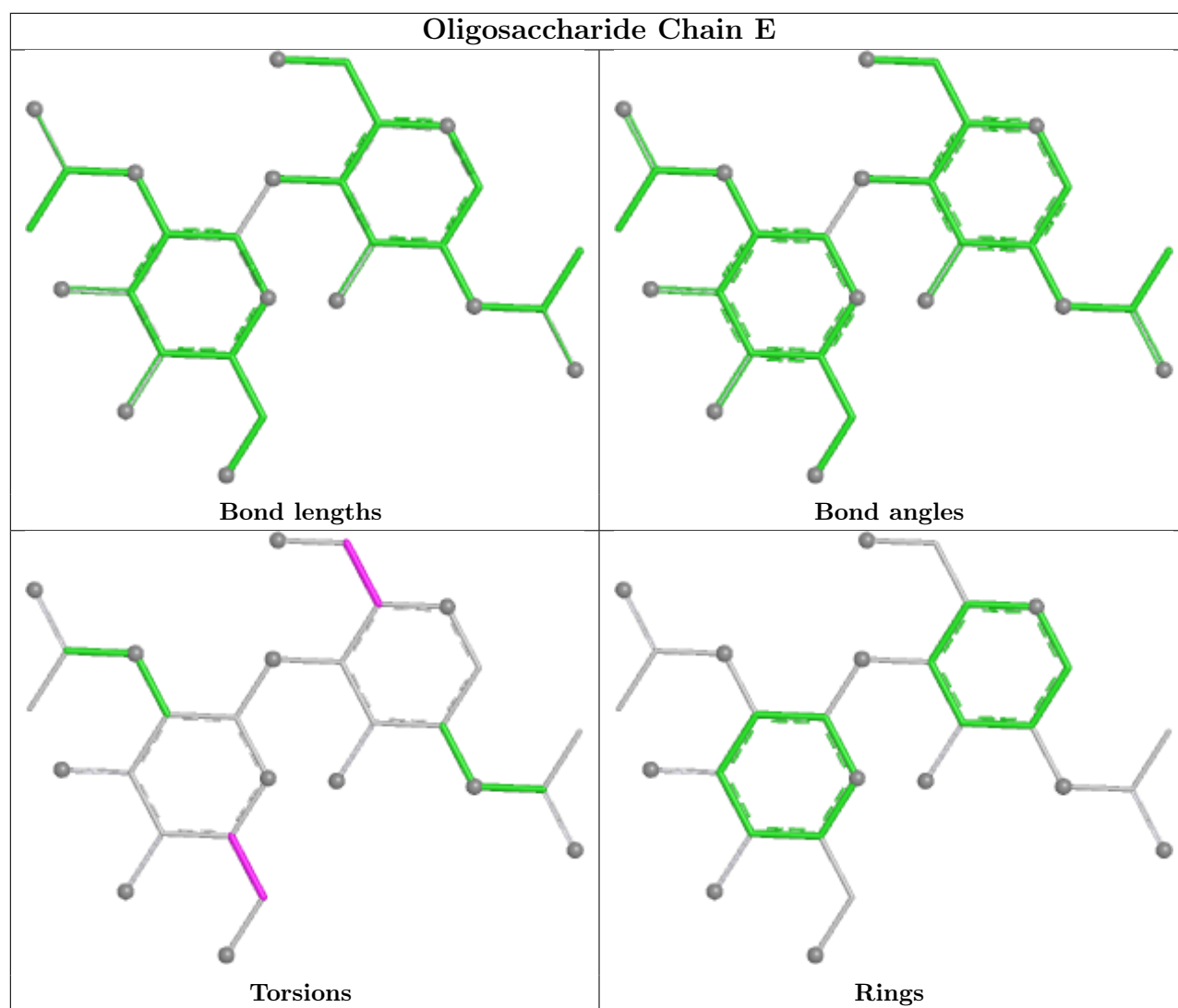
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7

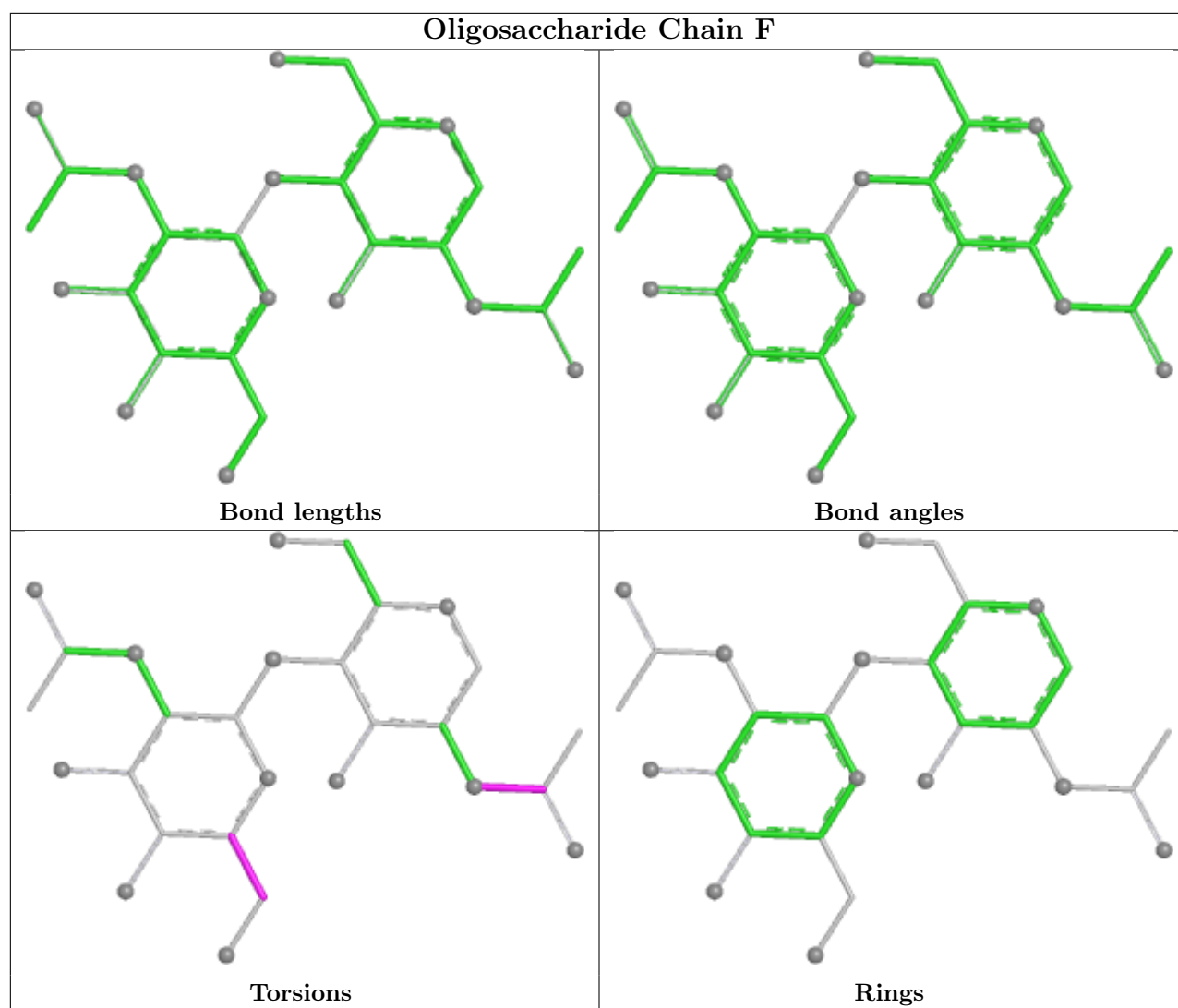
There are no ring outliers.

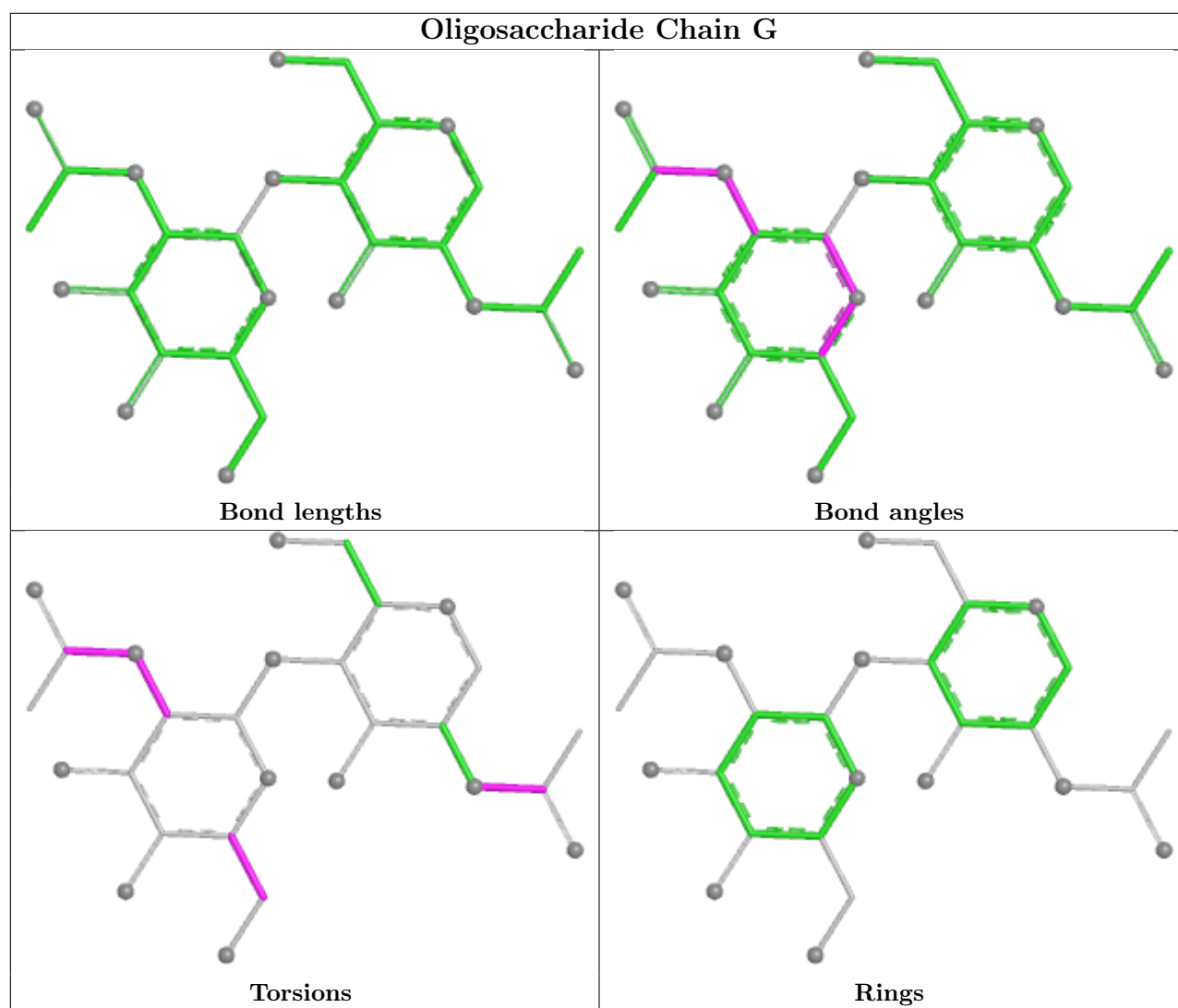
2 monomers are involved in 3 short contacts:

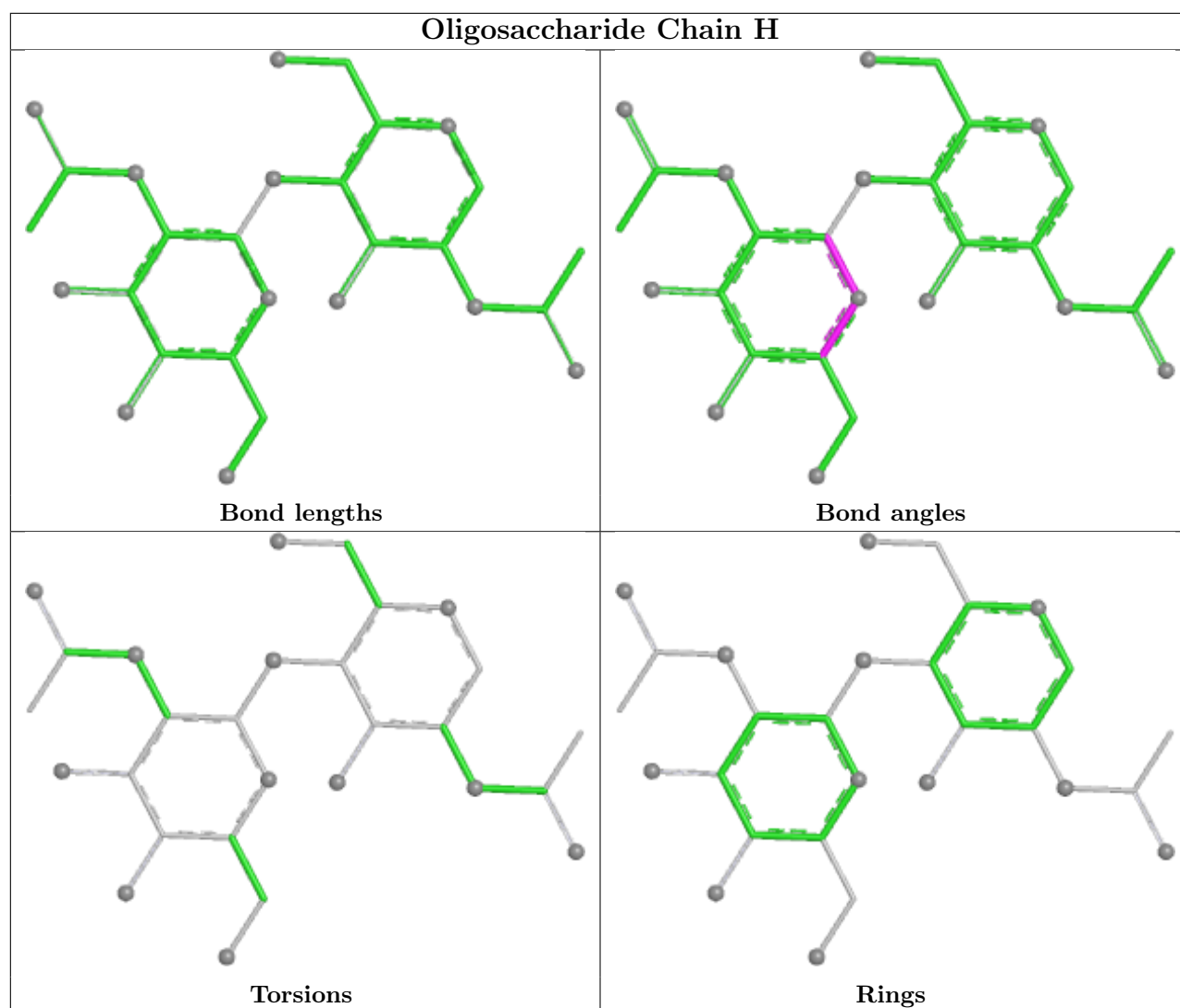
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	3	0
2	G	1	NAG	1	0

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	B	803	1	14,14,15	0.30	0	17,19,21	0.92	1 (5%)
3	KQD	C	801	-	74,78,78	3.08	27 (36%)	78,114,114	1.84	12 (15%)
4	NAG	D	603	1	14,14,15	0.20	0	17,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	KQD	B	801	-	74,78,78	3.10	26 (35%)	78,114,114	1.70	7 (8%)
4	NAG	A	607	-	14,14,15	0.31	0	17,19,21	0.50	0
3	KQD	D	601	-	74,78,78	3.07	27 (36%)	78,114,114	2.01	16 (20%)
4	NAG	C	802	1	14,14,15	0.53	0	17,19,21	0.45	0
4	NAG	A	606	1	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	D	602	1	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	B	802	1	14,14,15	0.24	0	17,19,21	0.73	1 (5%)
4	NAG	A	605	1	14,14,15	0.26	0	17,19,21	0.51	0
4	NAG	A	604	1	14,14,15	0.24	0	17,19,21	0.42	0
3	KQD	A	601	-	74,78,78	3.07	24 (32%)	78,114,114	1.94	17 (21%)

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	B	803	1	-	6/6/23/26	0/1/1/1
3	KQD	C	801	-	-	21/64/108/108	0/11/11/11
4	NAG	D	603	1	-	1/6/23/26	0/1/1/1
3	KQD	B	801	-	-	20/64/108/108	0/11/11/11
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	C	802	1	-	3/6/23/26	0/1/1/1
4	NAG	A	606	1	-	2/6/23/26	0/1/1/1
4	NAG	D	602	1	-	0/6/23/26	0/1/1/1
4	NAG	B	802	1	-	2/6/23/26	0/1/1/1
4	NAG	A	605	1	-	3/6/23/26	0/1/1/1
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
3	KQD	A	601	-	-	5/64/108/108	0/11/11/11

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	KQD	C17-C18	-9.77	1.35	1.53
3	D	601	KQD	C17-C18	-9.73	1.35	1.53
3	B	801	KQD	C17-C18	-9.22	1.36	1.53
3	C	801	KQD	C17-C18	-9.21	1.36	1.53
3	B	801	KQD	C17-N12	8.26	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	KQD	C15-C14	-8.21	1.33	1.54
3	A	601	KQD	C15-C14	-8.17	1.33	1.54
3	D	601	KQD	C15-C14	-8.10	1.33	1.54
3	B	801	KQD	C15-C14	-8.09	1.33	1.54
3	C	801	KQD	C17-N12	8.07	1.62	1.46
3	D	601	KQD	C17-N12	7.93	1.61	1.46
3	A	601	KQD	C17-N12	7.88	1.61	1.46
3	B	801	KQD	C20-N12	-6.93	1.33	1.46
3	A	601	KQD	C13-N11	-6.79	1.33	1.46
3	D	601	KQD	C13-N11	-6.77	1.33	1.46
3	C	801	KQD	C13-N11	-6.64	1.33	1.46
3	B	801	KQD	C13-N11	-6.49	1.34	1.46
3	A	601	KQD	C21-N23	6.48	1.47	1.34
3	D	601	KQD	C20-N12	-6.46	1.34	1.46
3	A	601	KQD	C36-N38	6.45	1.47	1.34
3	D	601	KQD	C36-N38	6.44	1.47	1.34
3	D	601	KQD	C21-N23	6.44	1.47	1.34
3	B	801	KQD	C21-N23	6.37	1.47	1.34
3	C	801	KQD	C20-N12	-6.37	1.34	1.46
3	A	601	KQD	C20-N12	-6.37	1.34	1.46
3	B	801	KQD	C36-N38	6.31	1.47	1.34
3	C	801	KQD	C21-N23	6.30	1.47	1.34
3	A	601	KQD	C63-N67	6.29	1.47	1.34
3	D	601	KQD	C63-N67	6.29	1.47	1.34
3	C	801	KQD	C36-N38	6.24	1.47	1.34
3	C	801	KQD	C13-C14	6.15	1.64	1.53
3	B	801	KQD	C13-C14	6.04	1.64	1.53
3	B	801	KQD	C62-N66	5.97	1.46	1.34
3	C	801	KQD	C63-N67	5.83	1.46	1.34
3	A	601	KQD	C13-C14	5.70	1.63	1.53
3	D	601	KQD	C13-C14	5.64	1.63	1.53
3	C	801	KQD	C8-N12	5.55	1.46	1.34
3	C	801	KQD	C16-N11	5.52	1.57	1.46
3	B	801	KQD	C63-N67	5.38	1.45	1.34
3	C	801	KQD	C7-N11	5.34	1.46	1.34
3	A	601	KQD	C16-N11	5.28	1.56	1.46
3	D	601	KQD	C16-N11	5.28	1.56	1.46
3	A	601	KQD	C8-N12	5.23	1.45	1.34
3	B	801	KQD	C7-N11	5.20	1.45	1.34
3	D	601	KQD	C8-N12	5.18	1.45	1.34
3	B	801	KQD	C16-N11	5.16	1.56	1.46
3	B	801	KQD	C8-N12	5.11	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	KQD	C62-N66	5.10	1.45	1.34
3	A	601	KQD	C62-N66	5.04	1.44	1.34
3	D	601	KQD	C62-N66	4.96	1.44	1.34
3	A	601	KQD	C7-N11	4.74	1.44	1.34
3	D	601	KQD	C7-N11	4.54	1.44	1.34
3	B	801	KQD	C42-C40	3.59	1.54	1.49
3	C	801	KQD	C42-C40	3.53	1.54	1.49
3	B	801	KQD	C71-C70	3.07	1.53	1.49
3	C	801	KQD	C16-C15	3.05	1.59	1.53
3	C	801	KQD	C25-C24	3.04	1.53	1.49
3	D	601	KQD	C42-C40	3.02	1.53	1.49
3	A	601	KQD	C42-C40	3.02	1.53	1.49
3	D	601	KQD	C20-C19	2.98	1.58	1.53
3	A	601	KQD	C20-C19	2.96	1.58	1.53
3	B	801	KQD	C16-C15	2.96	1.58	1.53
3	A	601	KQD	C25-C24	2.95	1.53	1.49
3	B	801	KQD	C25-C24	2.94	1.53	1.49
3	B	801	KQD	C75-C73	2.93	1.53	1.49
3	D	601	KQD	C25-C24	2.92	1.53	1.49
3	D	601	KQD	C16-C15	2.89	1.58	1.53
3	A	601	KQD	C16-C15	2.86	1.58	1.53
3	D	601	KQD	C75-C73	2.80	1.53	1.49
3	A	601	KQD	C75-C73	2.76	1.53	1.49
3	C	801	KQD	C75-C73	2.74	1.53	1.49
3	B	801	KQD	C4-C7	2.74	1.54	1.50
3	A	601	KQD	C4-C7	2.71	1.54	1.50
3	D	601	KQD	C4-C7	2.61	1.54	1.50
3	C	801	KQD	C20-C19	2.61	1.58	1.53
3	C	801	KQD	C43-C41	2.60	1.55	1.51
3	C	801	KQD	C71-C70	2.58	1.52	1.49
3	C	801	KQD	C4-C7	2.58	1.54	1.50
3	B	801	KQD	C43-C41	2.55	1.55	1.51
3	B	801	KQD	C20-C19	2.54	1.58	1.53
3	A	601	KQD	C28-C26	2.52	1.55	1.51
3	D	601	KQD	O22-C21	-2.39	1.18	1.23
3	B	801	KQD	O9-C7	-2.36	1.17	1.22
3	D	601	KQD	C71-C70	2.36	1.52	1.49
3	A	601	KQD	O22-C21	-2.35	1.18	1.23
3	A	601	KQD	C71-C70	2.33	1.52	1.49
3	B	801	KQD	C1-C8	2.30	1.53	1.50
3	D	601	KQD	C1-C8	2.27	1.53	1.50
3	B	801	KQD	C15-C21	2.25	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	KQD	C15-C21	2.19	1.55	1.51
3	B	801	KQD	O10-C8	-2.19	1.18	1.22
3	D	601	KQD	O65-C63	-2.12	1.19	1.23
3	C	801	KQD	O9-C7	-2.10	1.18	1.22
3	C	801	KQD	O64-C62	-2.10	1.19	1.23
3	C	801	KQD	O22-C21	-2.07	1.19	1.23
3	D	601	KQD	C28-C26	2.07	1.55	1.51
3	D	601	KQD	O9-C7	-2.06	1.18	1.22
3	C	801	KQD	O37-C36	-2.06	1.19	1.23
3	B	801	KQD	O65-C63	-2.04	1.19	1.23
3	A	601	KQD	O9-C7	-2.02	1.18	1.22
3	D	601	KQD	C15-C21	2.02	1.55	1.51
3	C	801	KQD	C1-C8	2.01	1.53	1.50
3	A	601	KQD	O65-C63	-2.01	1.19	1.23
3	D	601	KQD	C71-C72	2.00	1.53	1.50

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	KQD	C25-C26-C28	7.89	137.04	122.27
3	C	801	KQD	C42-C41-C43	7.85	136.97	122.27
3	B	801	KQD	C42-C41-C43	7.74	136.77	122.27
3	D	601	KQD	C42-C41-C43	7.55	136.41	122.27
3	A	601	KQD	C25-C26-C28	7.33	135.99	122.27
3	A	601	KQD	C42-C41-C43	7.32	135.97	122.27
3	B	801	KQD	C25-C26-C28	6.85	135.09	122.27
3	C	801	KQD	C25-C26-C28	6.61	134.65	122.27
3	A	601	KQD	C15-C21-N23	5.01	122.08	116.01
3	D	601	KQD	C15-C21-N23	4.99	122.05	116.01
3	D	601	KQD	C70-N66-C62	-4.77	114.96	123.25
3	C	801	KQD	C70-N66-C62	-4.19	115.96	123.25
3	C	801	KQD	C40-N38-C36	-4.09	116.13	123.25
3	B	801	KQD	C40-N38-C36	-3.78	116.67	123.25
3	A	601	KQD	C70-N66-C62	-3.77	116.68	123.25
3	B	801	KQD	C73-N67-C63	-3.48	117.19	123.25
3	D	601	KQD	O22-C21-N23	-3.21	117.21	122.96
3	D	601	KQD	C19-C63-N67	3.21	119.89	116.01
3	C	801	KQD	C29-C28-C26	-3.16	115.00	121.08
3	C	801	KQD	C1-C8-N12	-3.11	114.77	118.66
3	D	601	KQD	O9-C7-N11	-3.10	117.46	122.35
3	B	801	KQD	C29-C28-C26	-3.08	115.17	121.08
3	A	601	KQD	O9-C7-N11	-3.04	117.56	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	KQD	C40-N38-C36	-3.02	118.00	123.25
3	D	601	KQD	C40-N38-C36	-3.02	118.00	123.25
3	A	601	KQD	C19-C63-N67	2.99	119.64	116.01
3	C	801	KQD	C81-C76-C72	-2.96	115.41	121.08
3	A	601	KQD	C2-C1-C6	2.95	122.31	118.57
4	B	803	NAG	C2-N2-C7	2.92	126.81	122.90
3	A	601	KQD	O22-C21-N23	-2.88	117.80	122.96
3	D	601	KQD	O10-C8-N12	-2.70	118.09	122.35
3	A	601	KQD	O65-C63-N67	-2.68	118.16	122.96
3	D	601	KQD	C2-C1-C6	2.66	121.95	118.57
3	D	601	KQD	O65-C63-N67	-2.53	118.42	122.96
3	D	601	KQD	C81-C76-C77	2.48	121.38	118.30
3	D	601	KQD	C4-C7-N11	2.46	121.73	118.66
3	D	601	KQD	C81-C76-C72	-2.45	116.39	121.08
3	C	801	KQD	C73-N67-C63	-2.44	119.01	123.25
3	B	801	KQD	C87-C82-C74	-2.44	116.41	121.08
3	A	601	KQD	C4-C7-N11	2.42	121.68	118.66
3	D	601	KQD	C3-C4-C5	2.37	121.58	118.57
3	C	801	KQD	C4-C7-N11	-2.36	115.72	118.66
3	A	601	KQD	C3-C4-C5	2.30	121.49	118.57
3	A	601	KQD	C81-C76-C77	2.21	121.05	118.30
3	A	601	KQD	C17-C18-C19	2.21	108.13	104.11
3	A	601	KQD	O10-C8-N12	-2.21	118.88	122.35
3	C	801	KQD	C2-C1-C6	2.21	121.37	118.57
3	A	601	KQD	C5-C6-C1	-2.18	118.47	120.80
4	B	802	NAG	C1-O5-C5	2.16	115.08	112.19
3	B	801	KQD	C2-C1-C6	2.16	121.31	118.57
3	A	601	KQD	C81-C76-C72	-2.13	116.98	121.08
3	C	801	KQD	C81-C76-C77	2.13	120.94	118.30
3	D	601	KQD	C75-C74-C82	2.04	126.10	122.27
3	C	801	KQD	C33-C28-C26	2.01	124.93	121.08

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	NAG	C1-C2-N2-C7
4	D	603	NAG	C3-C2-N2-C7
3	A	601	KQD	C15-C21-N23-C24
3	A	601	KQD	C19-C63-N67-C73
3	D	601	KQD	C15-C21-N23-C24
3	D	601	KQD	C19-C63-N67-C73

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Mol	Chain	Res	Type	Atoms
4	A	604	NAG	O5-C5-C6-O6
4	B	802	NAG	O5-C5-C6-O6
4	A	605	NAG	C4-C5-C6-O6
4	B	802	NAG	C4-C5-C6-O6
4	B	803	NAG	C4-C5-C6-O6
4	A	606	NAG	C8-C7-N2-C2
4	A	606	NAG	O7-C7-N2-C2
4	A	607	NAG	C8-C7-N2-C2
4	A	607	NAG	O7-C7-N2-C2
4	B	803	NAG	C8-C7-N2-C2
4	B	803	NAG	O7-C7-N2-C2
3	A	601	KQD	O22-C21-N23-C24
3	D	601	KQD	O22-C21-N23-C24
3	A	601	KQD	O65-C63-N67-C73
3	D	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
4	C	802	NAG	C3-C2-N2-C7
3	C	801	KQD	C15-C14-C36-O37
3	B	801	KQD	C75-C74-C82-C87
3	C	801	KQD	C15-C14-C36-N38
3	C	801	KQD	C19-C18-C62-N66
3	C	801	KQD	C17-C18-C62-O64
3	B	801	KQD	C15-C14-C36-O37
3	B	801	KQD	C18-C19-C63-O65
3	C	801	KQD	C19-C18-C62-O64
3	C	801	KQD	C18-C19-C63-O65
3	B	801	KQD	C15-C14-C36-N38
3	B	801	KQD	C18-C19-C63-N67
4	C	802	NAG	C4-C5-C6-O6
3	C	801	KQD	C71-C72-C76-C81
3	B	801	KQD	C13-C14-C36-O37
3	C	801	KQD	C13-C14-C36-O37
3	C	801	KQD	C13-C14-C36-N38
3	C	801	KQD	C17-C18-C62-N66
4	B	803	NAG	C1-C2-N2-C7
4	C	802	NAG	O5-C5-C6-O6
3	B	801	KQD	C42-C41-C43-C48
3	B	801	KQD	C75-C74-C82-C83
3	C	801	KQD	C42-C41-C43-C48
3	C	801	KQD	C18-C19-C63-N67

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Mol	Chain	Res	Type	Atoms
3	B	801	KQD	C20-C19-C63-O65
3	B	801	KQD	C13-C14-C36-N38
3	B	801	KQD	C42-C41-C43-C44
3	C	801	KQD	C42-C41-C43-C44
3	C	801	KQD	C71-C72-C76-C77
3	B	801	KQD	C20-C19-C63-N67
3	B	801	KQD	C14-C15-C21-N23
3	A	601	KQD	C41-C40-N38-C36
3	B	801	KQD	C41-C40-N38-C36
3	C	801	KQD	C41-C40-N38-C36
3	D	601	KQD	C41-C40-N38-C36
3	B	801	KQD	C14-C15-C21-O22
3	C	801	KQD	C14-C15-C21-O22
3	C	801	KQD	C14-C15-C21-N23
3	B	801	KQD	C16-C15-C21-O22
3	C	801	KQD	C16-C15-C21-O22
3	C	801	KQD	C20-C19-C63-O65
3	B	801	KQD	C16-C15-C21-N23
3	C	801	KQD	C20-C19-C63-N67
4	B	803	NAG	C3-C2-N2-C7
3	C	801	KQD	C16-C15-C21-N23
3	B	801	KQD	C19-C18-C62-O64
3	B	801	KQD	C17-C18-C62-O64
3	B	801	KQD	C19-C18-C62-N66

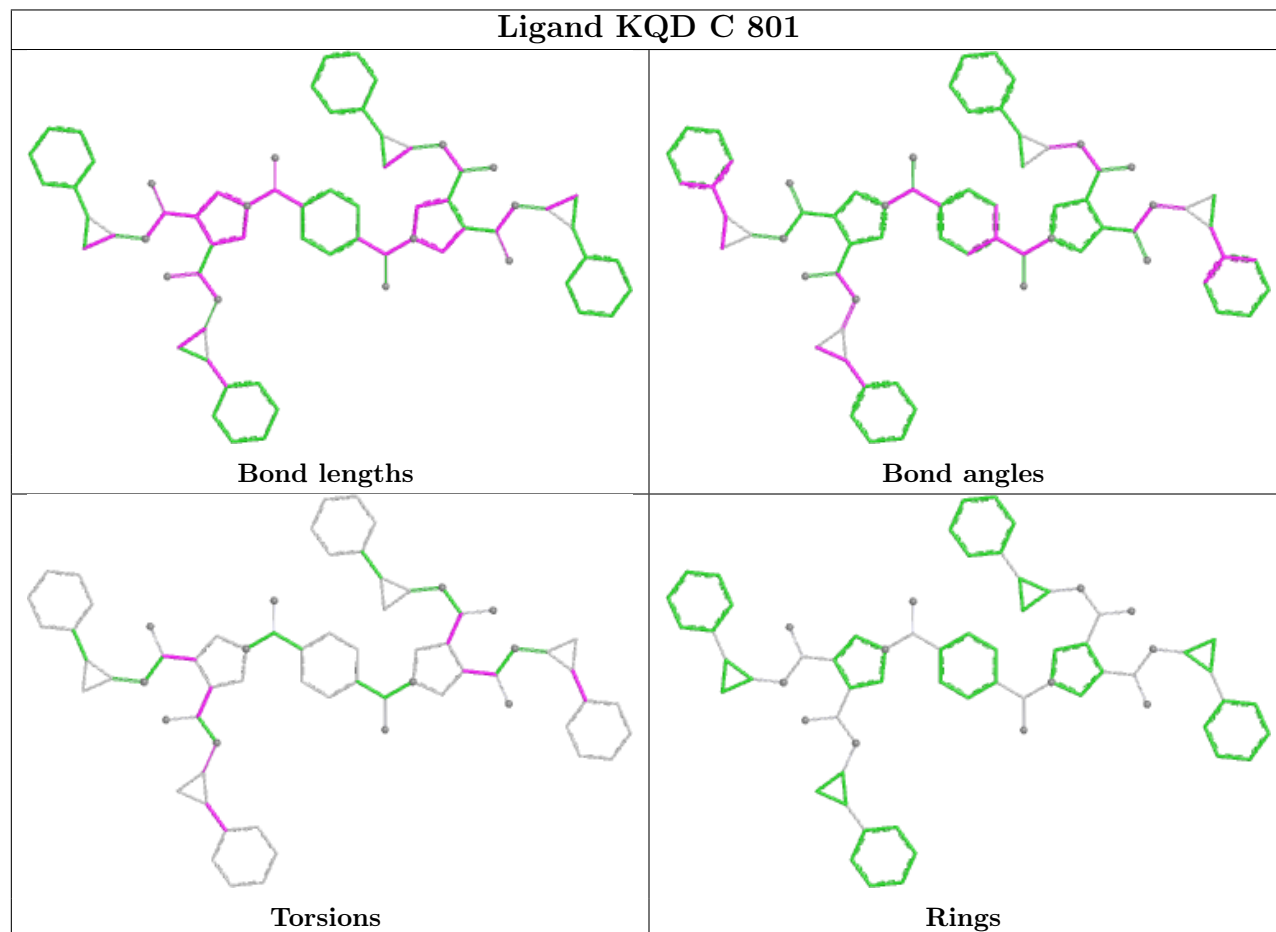
There are no ring outliers.

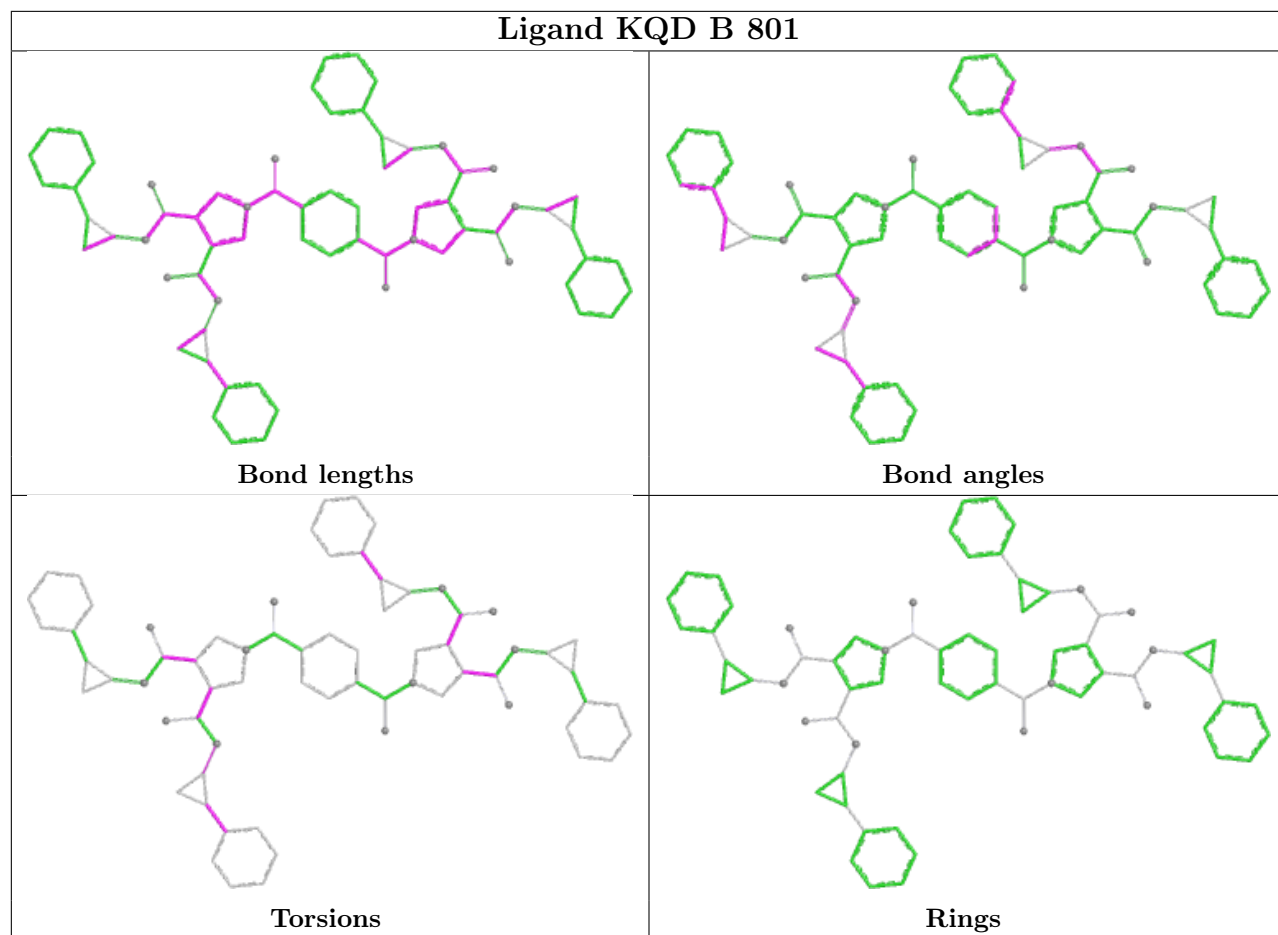
6 monomers are involved in 7 short contacts:

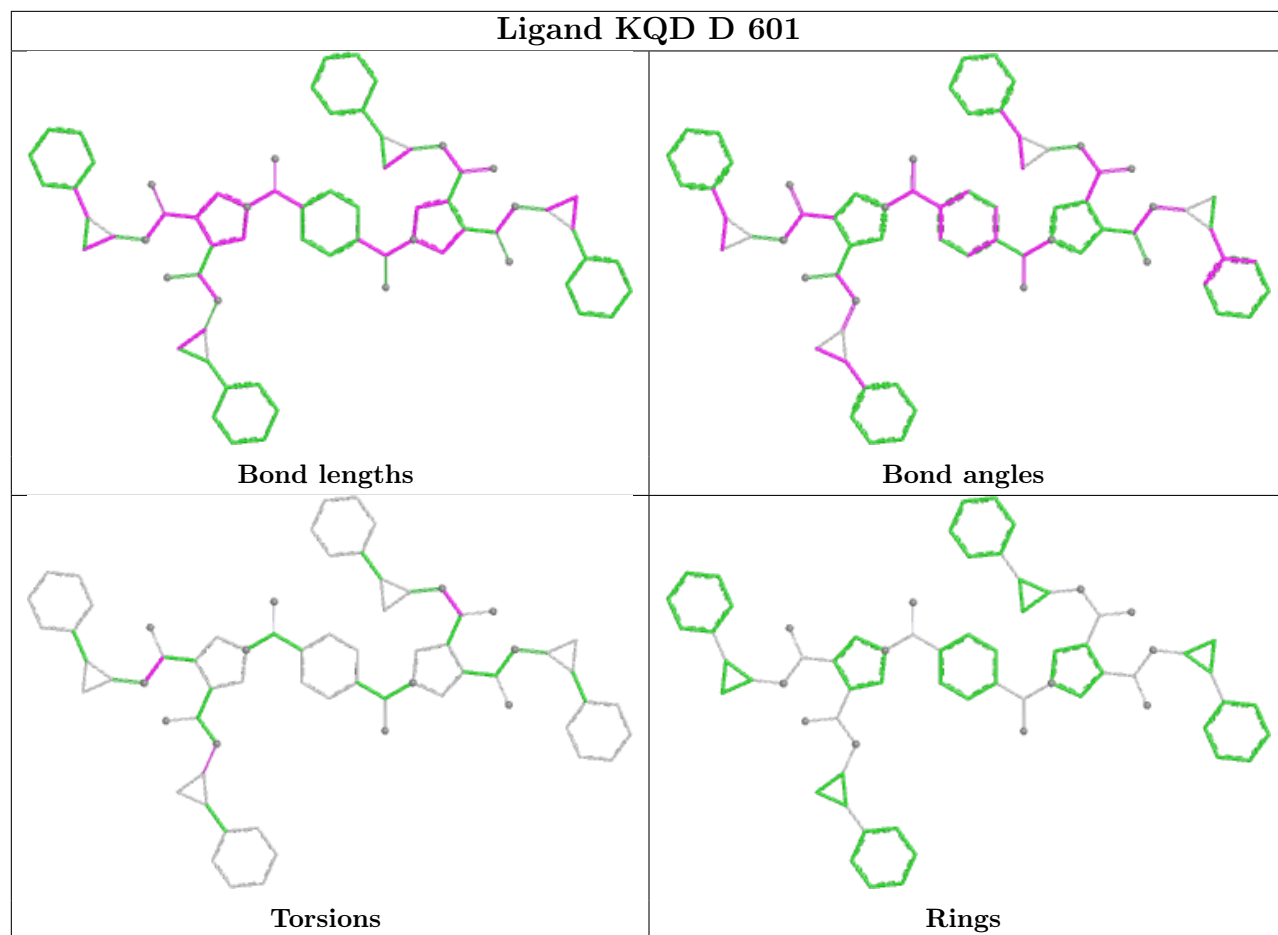
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	NAG	2	0
4	D	603	NAG	1	0
3	D	601	KQD	1	0
4	C	802	NAG	1	0
4	A	605	NAG	1	0
3	A	601	KQD	1	0

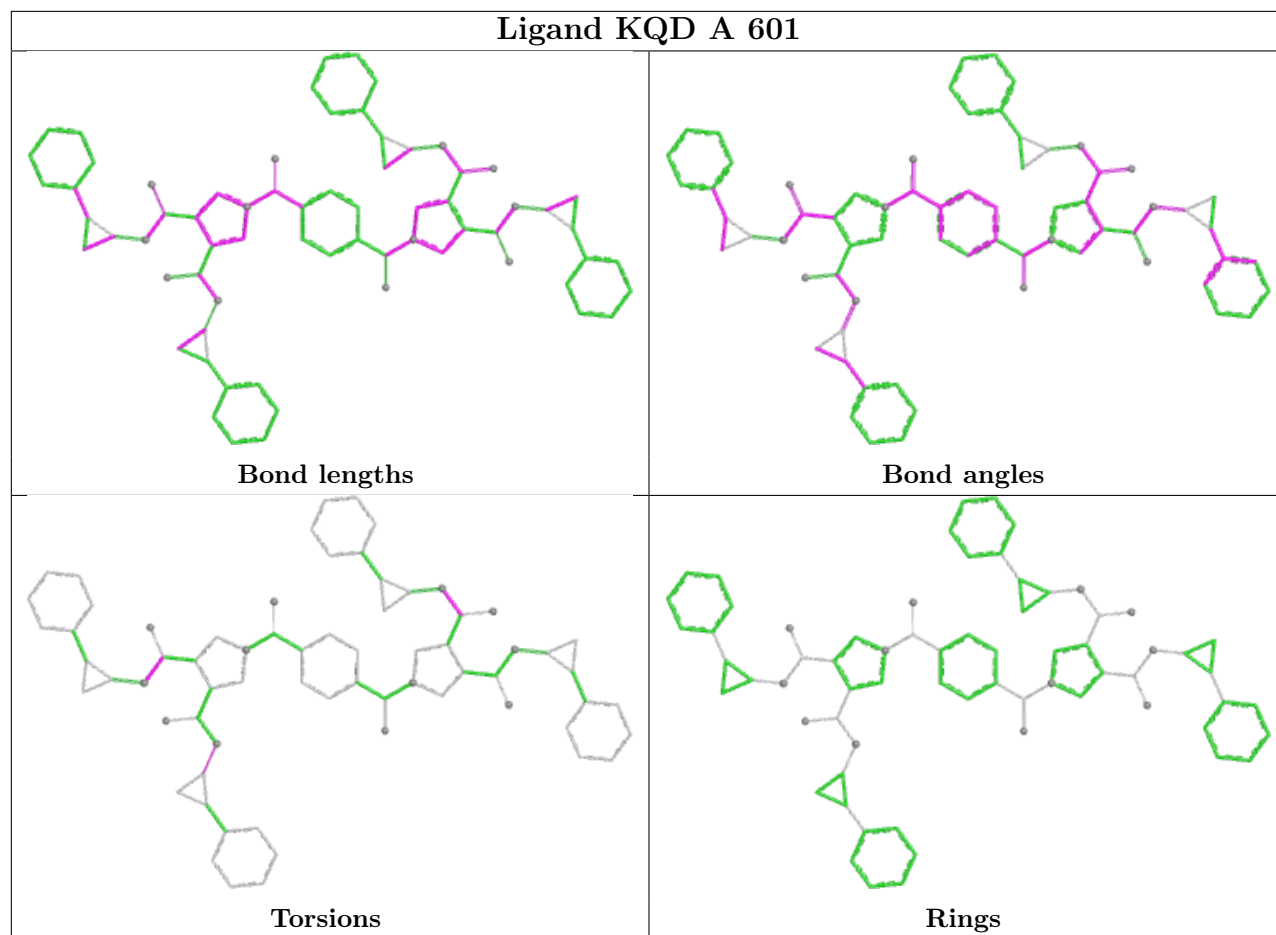
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	546/576 (94%)	0.69	44 (8%) 18 20	55, 82, 129, 214	0
1	B	545/576 (94%)	1.05	81 (14%) 5 6	53, 91, 165, 205	0
1	C	549/576 (95%)	1.09	83 (15%) 5 6	56, 95, 161, 230	0
1	D	546/576 (94%)	0.86	61 (11%) 10 12	42, 83, 145, 223	1 (0%)
All	All	2186/2304 (94%)	0.92	269 (12%) 8 10	42, 87, 156, 230	1 (0%)

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	LEU	7.0
1	B	72	LEU	6.2
1	B	138	THR	6.0
1	B	64	ILE	5.7
1	B	88	ILE	5.6
1	A	67	ILE	5.5
1	C	138	THR	5.4
1	B	304	ILE	5.3
1	C	376	TYR	5.2
1	A	87	GLY	5.0
1	A	112	LEU	4.8
1	D	40	SER	4.8
1	B	99	LEU	4.8
1	A	88	ILE	4.8
1	C	406	GLY	4.8
1	D	66	TYR	4.7
1	C	297	ALA	4.7
1	C	67	ILE	4.6
1	D	90	THR	4.6
1	A	90	THR	4.6
1	B	90	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	303	VAL	4.5
1	A	376	TYR	4.4
1	C	575	PRO	4.4
1	C	529	TRP	4.2
1	D	522	LEU	4.0
1	A	244	THR	4.0
1	B	164	LYS	3.8
1	D	497	LEU	3.8
1	C	239	PHE	3.8
1	D	27	SER	3.8
1	C	211	ILE	3.8
1	D	479	LEU	3.8
1	D	251	ILE	3.8
1	B	490	MET	3.7
1	A	304	ILE	3.7
1	C	227	LEU	3.7
1	A	89	ASN	3.7
1	B	110	ASN	3.7
1	B	133	GLY	3.7
1	B	166	GLN	3.6
1	C	373	VAL	3.6
1	B	46	ILE	3.6
1	C	88	ILE	3.6
1	C	66	TYR	3.6
1	D	349	PHE	3.5
1	D	115	LEU	3.5
1	C	349	PHE	3.5
1	A	575	PRO	3.4
1	C	72	LEU	3.4
1	A	66	TYR	3.4
1	C	453	GLY	3.4
1	C	91	ILE	3.3
1	B	354	LEU	3.3
1	A	276	ILE	3.3
1	D	575	PRO	3.2
1	D	244	THR	3.2
1	C	212	LEU	3.2
1	C	223	SER	3.2
1	C	302	ARG	3.2
1	A	251	ILE	3.2
1	C	64	ILE	3.2
1	C	251	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	247	THR	3.2
1	D	53	ALA	3.1
1	B	139	LEU	3.1
1	C	534	PRO	3.1
1	D	490	MET	3.1
1	B	175	PHE	3.1
1	B	540	PRO	3.1
1	C	112	LEU	3.1
1	C	410	LEU	3.1
1	C	224	VAL	3.1
1	D	164	LYS	3.1
1	D	67	ILE	3.1
1	D	276	ILE	3.1
1	C	254	PHE	3.1
1	C	139	LEU	3.1
1	D	78	LEU	3.1
1	A	495	ALA	3.0
1	B	373	VAL	3.0
1	A	27	SER	3.0
1	A	349	PHE	3.0
1	A	303	VAL	3.0
1	C	187	GLN	3.0
1	D	222	SER	3.0
1	B	575	PRO	3.0
1	D	573	ILE	3.0
1	A	53	ALA	2.9
1	D	492	LEU	2.9
1	D	196	SER	2.9
1	B	381	ALA	2.9
1	C	50	LEU	2.9
1	C	81	LEU	2.9
1	C	530	LEU	2.9
1	A	574	CYS	2.9
1	B	67	ILE	2.9
1	B	197	ILE	2.9
1	D	294	ASN	2.9
1	C	175	PHE	2.9
1	C	93	GLU	2.9
1	C	243	SER	2.8
1	D	217	PHE	2.8
1	D	138	THR	2.8
1	B	66	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	126	LEU	2.8
1	D	297	ALA	2.8
1	B	136	TYR	2.8
1	B	45	SER	2.7
1	C	573	ILE	2.7
1	C	434	TRP	2.7
1	D	173	LEU	2.7
1	B	349	PHE	2.7
1	B	224	VAL	2.7
1	C	49	GLY	2.7
1	C	293	GLY	2.7
1	B	297	ALA	2.6
1	A	34	GLY	2.6
1	A	41	GLY	2.6
1	A	539	CYS	2.6
1	B	36	CYS	2.6
1	B	50	LEU	2.6
1	D	71	ASP	2.6
1	C	259	VAL	2.6
1	B	102	LEU	2.6
1	B	371	LEU	2.6
1	C	99	LEU	2.6
1	C	539	CYS	2.6
1	B	120	PHE	2.6
1	D	500	MET	2.6
1	B	295	PHE	2.6
1	C	36	CYS	2.5
1	B	134	ASN	2.5
1	D	159	MET	2.5
1	C	140	GLY	2.5
1	D	41	GLY	2.5
1	D	254	PHE	2.5
1	C	303	VAL	2.5
1	A	138	THR	2.5
1	A	249	SER	2.5
1	B	123	LEU	2.5
1	B	242	LEU	2.5
1	D	494	ASP	2.5
1	B	49	GLY	2.5
1	A	76	VAL	2.5
1	B	118	SER	2.5
1	B	141	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	98	SER	2.5
1	B	261	ILE	2.5
1	A	354	LEU	2.5
1	D	510	GLN	2.5
1	B	446	THR	2.4
1	C	166	GLN	2.4
1	C	407	GLU	2.4
1	A	35	ILE	2.4
1	B	514	VAL	2.4
1	B	198	GLN	2.4
1	A	171	ALA	2.4
1	B	564	GLY	2.4
1	C	27	SER	2.4
1	D	323	TYR	2.4
1	B	169	ASP	2.4
1	C	247	THR	2.4
1	C	435	PRO	2.3
1	B	560	ALA	2.3
1	B	163	THR	2.3
1	A	159	MET	2.3
1	C	30	CYS	2.3
1	C	574	CYS	2.3
1	D	412	LEU	2.3
1	D	476	LEU	2.3
1	B	89	ASN	2.3
1	A	553	SER	2.3
1	C	159	MET	2.3
1	A	321	ARG	2.3
1	B	91	ILE	2.3
1	A	514	VAL	2.3
1	A	412	LEU	2.3
1	C	57	LEU	2.3
1	B	119	TRP	2.3
1	D	152	GLN	2.3
1	D	211	ILE	2.3
1	B	80	ALA	2.3
1	D	238[A]	HIS	2.3
1	D	318	HIS	2.3
1	C	43	LEU	2.2
1	D	495	ALA	2.2
1	B	465	SER	2.2
1	C	535	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	347	LYS	2.2
1	B	35	ILE	2.2
1	C	214	LEU	2.2
1	C	354	LEU	2.2
1	A	301	ASP	2.2
1	D	199	ASN	2.2
1	C	47	PRO	2.2
1	C	75	CYS	2.2
1	D	30	CYS	2.2
1	D	521	ARG	2.2
1	C	141	GLU	2.2
1	B	573	ILE	2.2
1	D	54	VAL	2.2
1	A	169	ASP	2.2
1	B	521	ARG	2.2
1	C	32	ARG	2.2
1	B	161	THR	2.2
1	B	495	ALA	2.2
1	A	525	LEU	2.2
1	B	415	LEU	2.2
1	D	572	ILE	2.2
1	B	162	PHE	2.2
1	A	47	PRO	2.2
1	D	478	GLN	2.2
1	D	574	CYS	2.2
1	B	105	LEU	2.1
1	C	455	ILE	2.1
1	D	418	ILE	2.1
1	D	518	ILE	2.1
1	B	299	ASP	2.1
1	B	569	VAL	2.1
1	C	540	PRO	2.1
1	A	510	GLN	2.1
1	C	209	GLN	2.1
1	A	297	ALA	2.1
1	B	146	SER	2.1
1	C	45	SER	2.1
1	D	68	SER	2.1
1	A	299	ASP	2.1
1	C	526	GLN	2.1
1	B	142	THR	2.1
1	C	497	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	398	HIS	2.1
1	C	120	PHE	2.1
1	D	170	PHE	2.1
1	C	240	SER	2.1
1	C	537	CYS	2.1
1	D	42	SER	2.1
1	C	246	GLU	2.1
1	A	328	LEU	2.1
1	C	176	LEU	2.1
1	A	64	ILE	2.1
1	C	357	GLN	2.1
1	D	354	LEU	2.1
1	C	323	TYR	2.1
1	A	373	VAL	2.1
1	B	254	PHE	2.1
1	B	559	SER	2.0
1	D	116	SER	2.0
1	B	212	LEU	2.0
1	C	115	LEU	2.0
1	C	148	LEU	2.0
1	D	474	LEU	2.0
1	D	530	LEU	2.0
1	B	259	VAL	2.0
1	C	156	VAL	2.0
1	D	292	VAL	2.0
1	B	140	GLY	2.0
1	C	162	PHE	2.0
1	C	386	TRP	2.0
1	A	161	THR	2.0
1	D	171	ALA	2.0
1	B	537	CYS	2.0
1	B	144	LEU	2.0
1	B	186	LEU	2.0
1	B	522	LEU	2.0
1	C	199	ASN	2.0
1	C	324	LEU	2.0
1	B	251	ILE	2.0
1	B	572	ILE	2.0

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

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

6.3 Carbohydrates

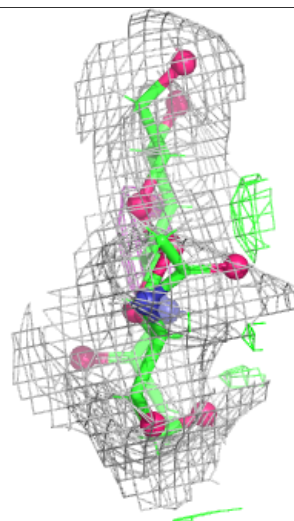
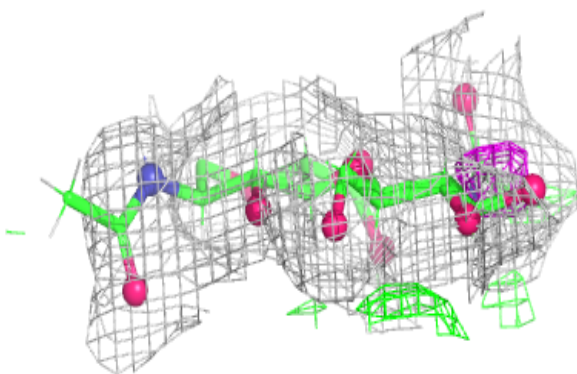
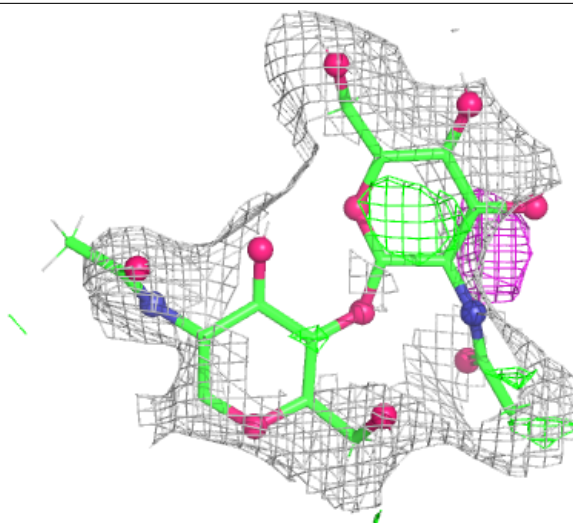
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.25	0.14	104,110,131,133	0
2	NAG	E	1	14/15	0.55	0.14	91,104,123,124	0
2	NAG	H	2	14/15	0.61	0.15	84,97,116,121	0
2	NAG	G	2	14/15	0.68	0.14	84,98,117,119	0
2	NAG	F	2	14/15	0.75	0.14	81,93,111,112	0
2	NAG	H	1	14/15	0.94	0.09	52,67,78,81	0
2	NAG	G	1	14/15	0.94	0.08	53,64,75,76	0
2	NAG	F	1	14/15	0.95	0.07	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.

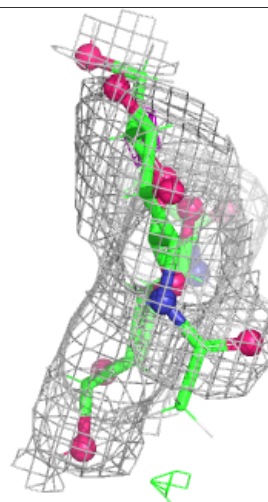
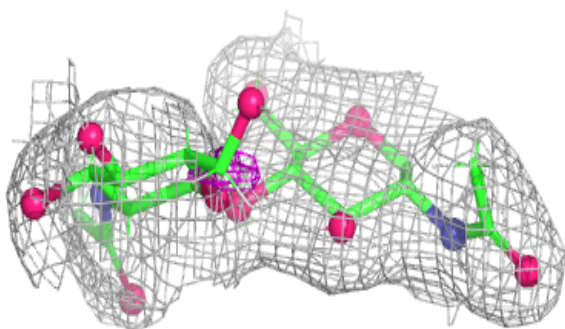
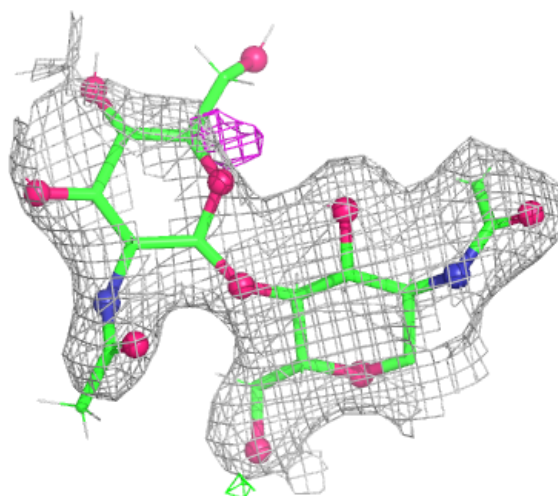
Electron density around Chain E:

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



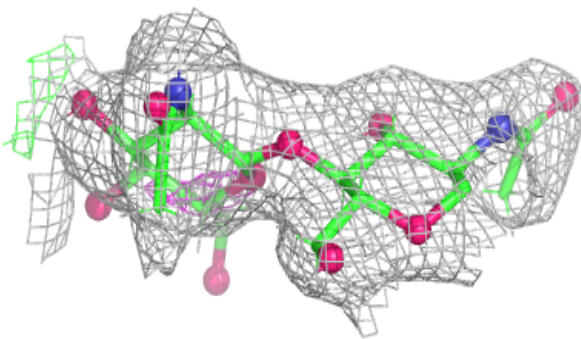
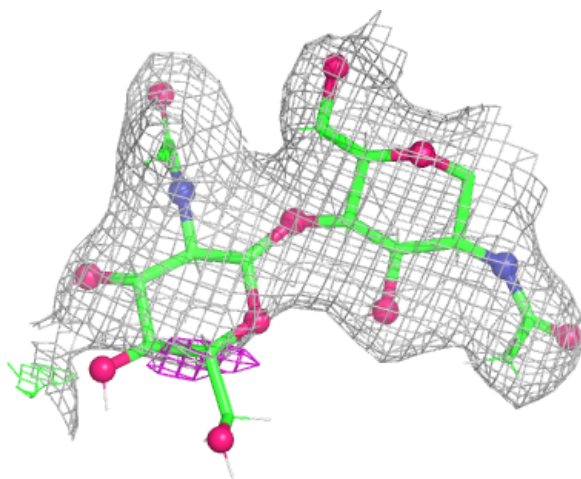
Electron density around Chain F:

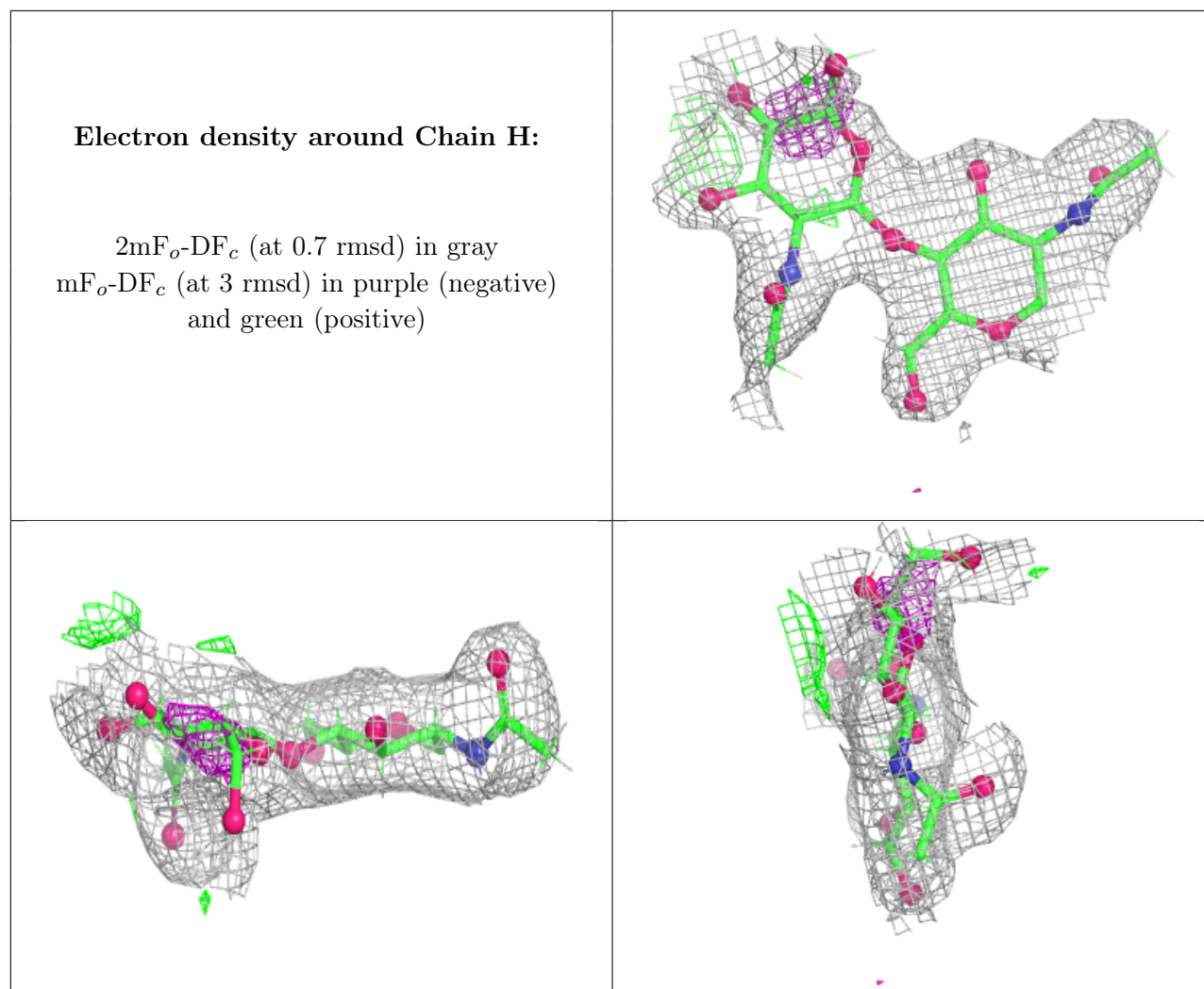
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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
4	NAG	B	802	14/15	0.37	0.17	78,92,110,111	0
4	NAG	C	802	14/15	0.55	0.14	83,94,113,114	0
4	NAG	B	803	14/15	0.59	0.14	99,116,139,139	0
4	NAG	A	605	14/15	0.60	0.13	75,92,110,110	0
4	NAG	D	602	14/15	0.64	0.12	83,94,112,113	0
4	NAG	A	604	14/15	0.67	0.13	79,94,112,112	0
4	NAG	A	607	14/15	0.69	0.16	87,97,117,118	0
4	NAG	D	603	14/15	0.69	0.11	99,115,138,138	0
3	KQD	B	801	68/68	0.91	0.11	59,71,83,91	0

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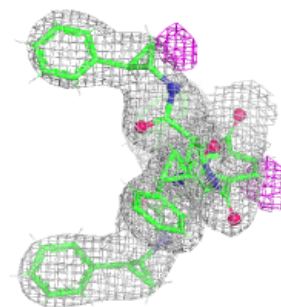
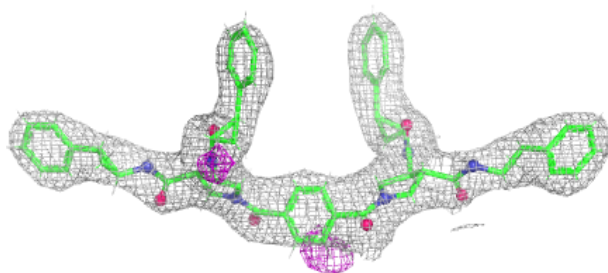
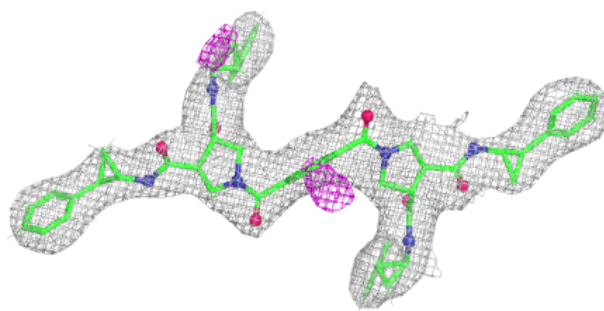
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	KQD	A	601	68/68	0.92	0.12	57,67,79,81	0
3	KQD	C	801	68/68	0.93	0.09	59,68,81,84	0
3	KQD	D	601	68/68	0.94	0.11	56,65,78,79	0
4	NAG	A	606	14/15	0.95	0.07	49,65,76,79	0

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.

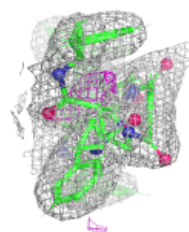
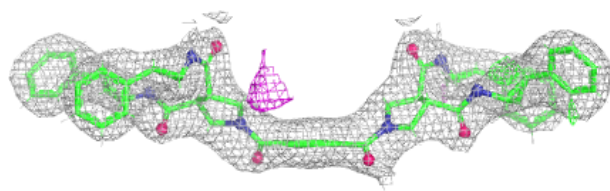
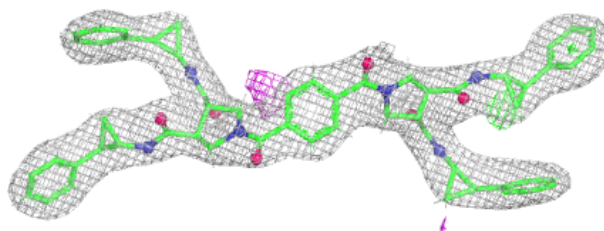
Electron density around KQD B 801:

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

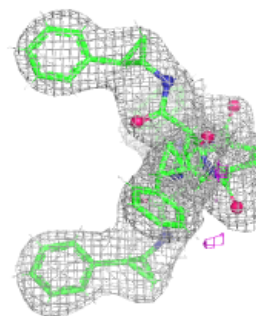
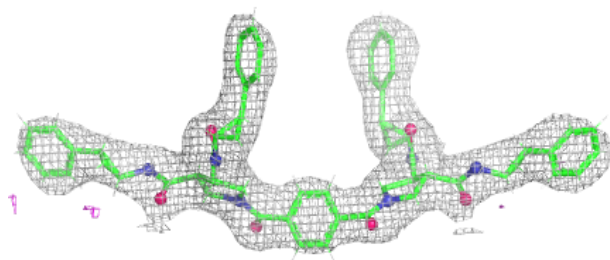
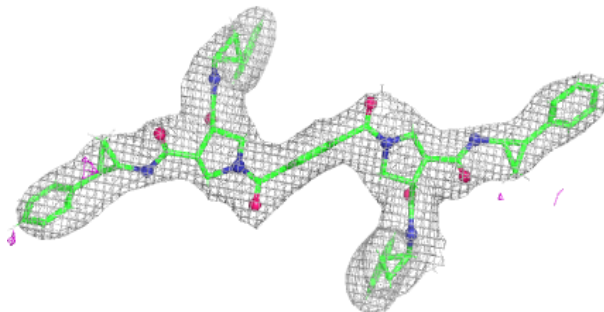


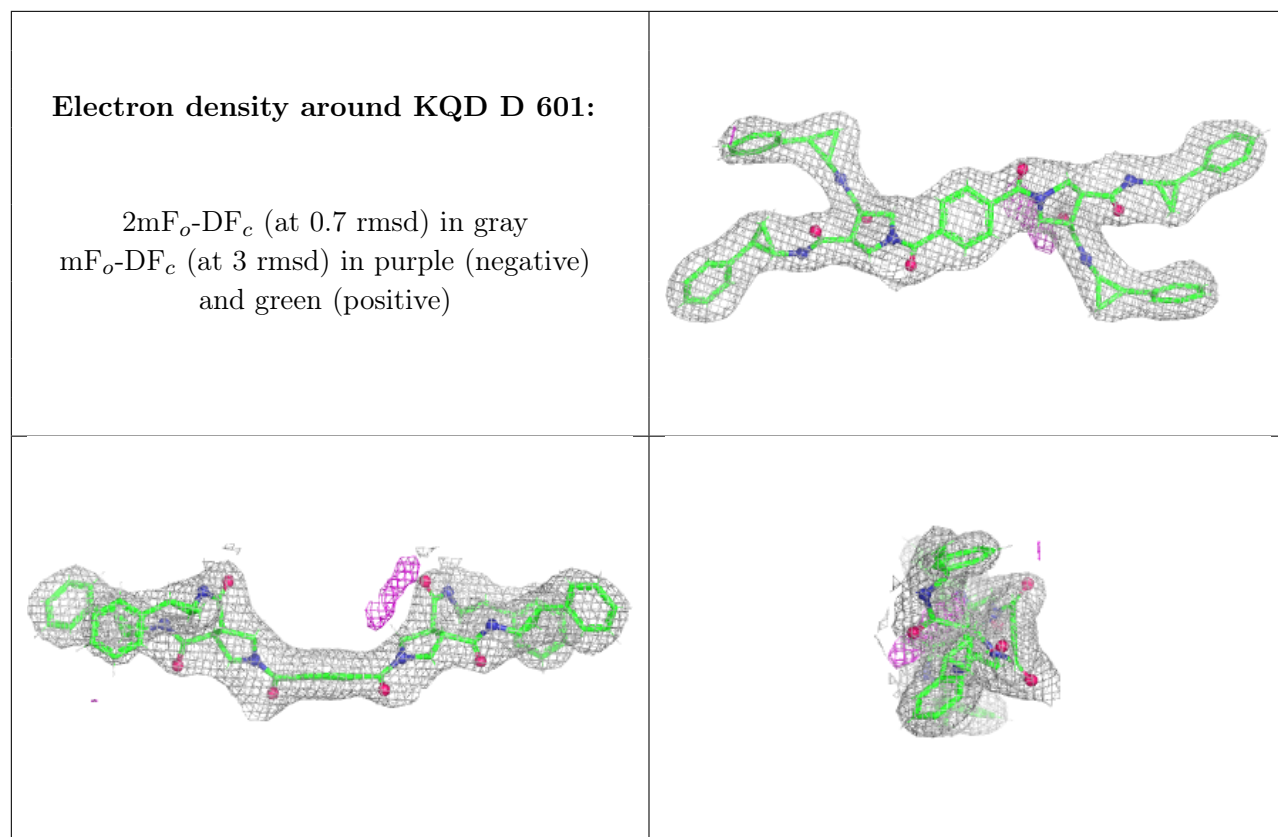
Electron density around KQD A 601:

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

**Electron density around KQD C 801:**

$2mF_o-DF_c$ (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.