



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:52 AM BST

PDB ID : 2Z7X  
Title : Crystal structure of the TLR1-TLR2 heterodimer induced by binding of a tri-acylated lipopeptide  
Authors : Lee, J.O.; Jin, M.S.; Kim, S.E.; Heo, J.Y.  
Deposited on : 2007-08-29  
Resolution : 2.10 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

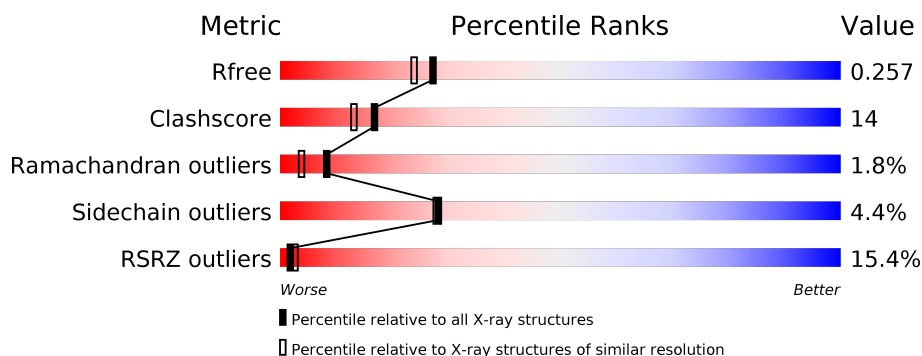
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



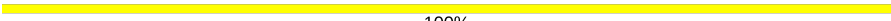
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	549	<div> <div>28%</div> <div>59%</div> <div>37%</div> <div>.</div> </div>
2	B	520	<div> <div>2%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
3	C	5	<div> <div>20%</div> <div>80%</div> <div>20%</div> </div>
4	D	3	<div> <div>33%</div> <div>67%</div> </div>
5	E	3	<div> <div>33%</div> <div>67%</div> </div>
6	F	3	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	D	3	-	-	-	X
5	MAN	E	3	-	-	-	X
8	NAG	A	901	X	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9088 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Toll-like receptor 2, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4366	2766	735	844	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	507	SER	-	linker	UNP O60603
A	508	ARG	-	linker	UNP O60603

- Molecule 2 is a protein called Toll-like receptor 1, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	520	Total	C	N	O	S	0	0	0
			4172	2671	697	784	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	476	ALA	-	linker	UNP Q15399
B	477	SER	-	linker	UNP Q15399

- Molecule 3 is a protein called Pam3CSK4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			43	27	9	7			

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



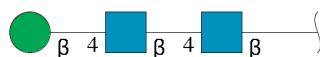
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



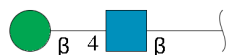
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

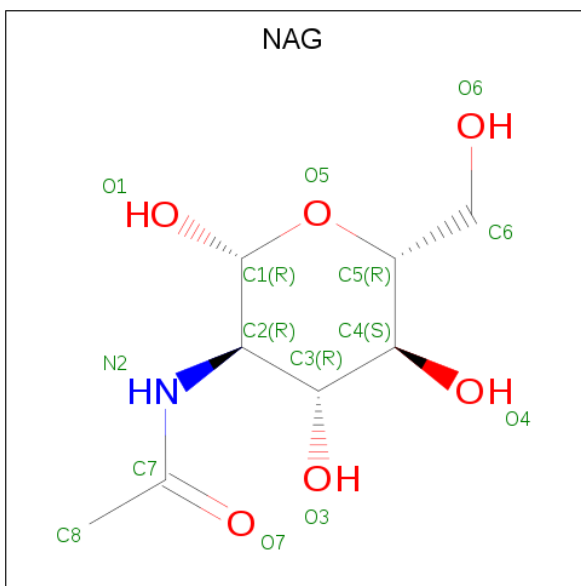
- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	2	Total	C	N	O	0	0	0
			25	14	1	10			

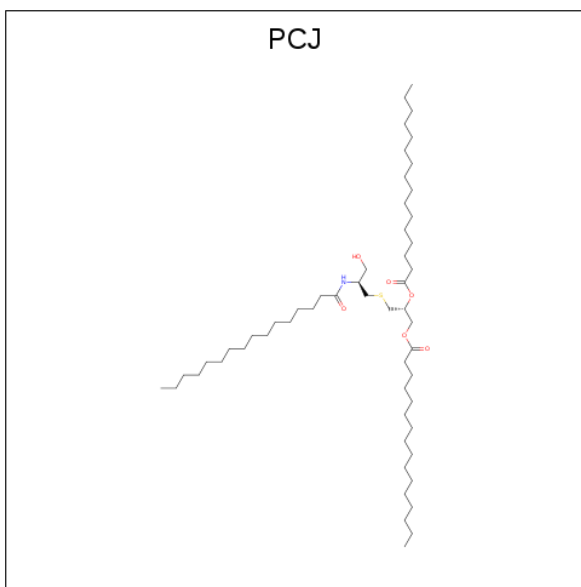
- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 9 is (2R)-3-{[(2S)-3-HYDROXY-2-(PALMITOYLAMINO)PROPYL]THIO}PROPANE-1,2-DIYL DIHEXADECANOATE (three-letter code: PCJ) (formula: C<sub>54</sub>H<sub>105</sub>NO<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	N	O	S	0	0
			62	54	1	6	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	70	Total	O	0	0
			70	70		
10	B	175	Total	O	0	0
			175	175		
10	C	2	Total	O	0	0
			2	2		

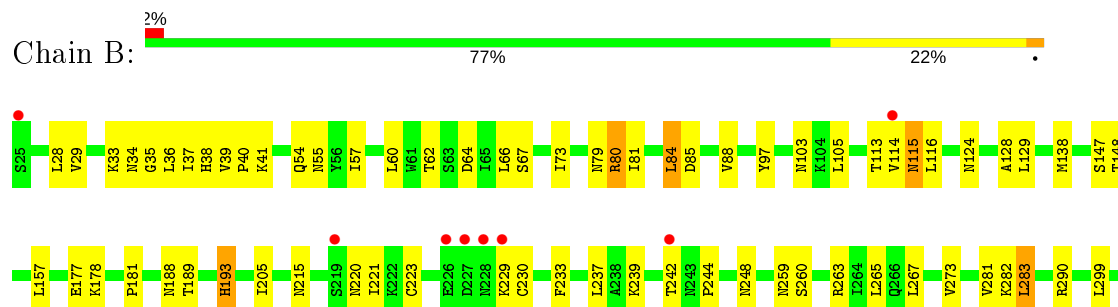
### 3 Residue-property plots

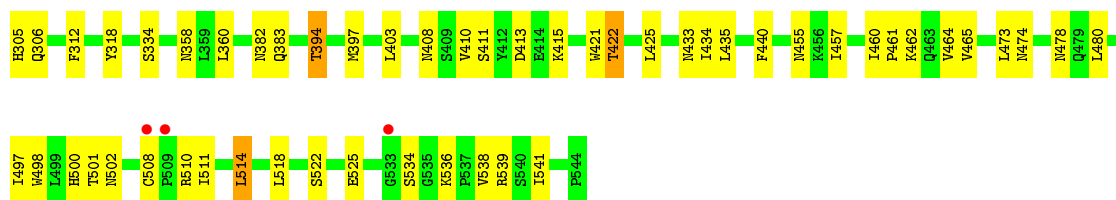
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

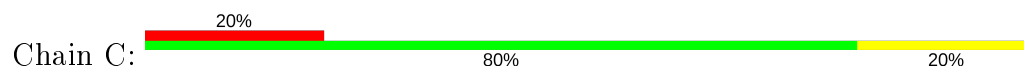


- Molecule 2: Toll-like receptor 1, Variable lymphocyte receptor B





- Molecule 3: Pam3CSK4



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



- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.30 Å   120.14 Å   74.12 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	45.85 – 2.10 45.85 – 2.08	Depositor EDS
% Data completeness (in resolution range)	94.5 (45.85-2.10) 93.0 (45.85-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.08 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.244   ,   0.270 0.234   ,   0.257	Depositor DCC
$R_{free}$ test set	5025 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: PCJ, BMA, NAG, NDG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.32	0/4442	0.60	2/6014 (0.0%)
2	B	0.38	0/4257	0.63	0/5766
3	C	0.38	0/42	0.50	0/49
All	All	0.35	0/8741	0.61	2/11829 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	PHE	N-CA-C	-5.74	95.51	111.00
1	A	351	VAL	N-CA-C	-5.03	97.41	111.00

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	4366	0	4418	155	0
2	B	4172	0	4221	91	0
3	C	43	0	56	0	0
4	D	39	0	33	4	0
5	E	39	0	34	0	0
6	F	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	25	0	22	2	0
8	A	42	0	39	1	0
8	B	14	0	13	0	0
9	C	62	0	102	4	0
10	A	70	0	0	3	0
10	B	175	0	0	3	0
10	C	2	0	0	0	0
All	All	9088	0	8972	251	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 14.

All (251) 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:A:511:LEU:H	1:A:533:ASN:HD22	1.01	0.95
2:B:229:LYS:HD2	2:B:263:ARG:HE	1.32	0.94
1:A:456:PRO:HG2	1:A:459:LEU:HD13	1.59	0.84
1:A:372:MET:H	1:A:397:ASN:HD22	1.25	0.84
2:B:81:ILE:H	2:B:103:ASN:HD22	1.27	0.81
1:A:170:PHE:HA	1:A:173:LEU:HD21	1.62	0.81
1:A:469:LEU:H	1:A:487:ASN:HD22	1.28	0.79
1:A:56:SER:HA	1:A:80:ALA:HB3	1.65	0.79
2:B:457:ILE:H	2:B:478:ASN:HD22	1.29	0.79
2:B:410:VAL:H	2:B:433:ASN:HD22	1.34	0.76
1:A:30:CYS:HA	1:A:36:CYS:HA	1.67	0.76
1:A:239:PHE:H	1:A:268:GLN:HE21	1.34	0.75
2:B:435:LEU:H	2:B:455:ASN:HD22	1.33	0.74
2:B:55:ASN:HB2	2:B:79:ASN:HD21	1.53	0.73
1:A:123:LEU:HD13	1:A:126:LEU:HD22	1.69	0.72
1:A:511:LEU:H	1:A:533:ASN:ND2	1.84	0.72
1:A:183:ALA:HB1	1:A:186:LEU:HB2	1.72	0.71
2:B:229:LYS:HD2	2:B:263:ARG:NE	2.04	0.71
2:B:54:GLN:HE22	4:D:2:NDG:H8C3	1.55	0.71
1:A:121:LYS:HB3	1:A:122:PRO:HD3	1.73	0.69
1:A:346:SER:H	1:A:370:ASN:HD21	1.38	0.69
2:B:103:ASN:HB2	2:B:124:ASN:HD21	1.57	0.69
2:B:410:VAL:H	2:B:433:ASN:ND2	1.89	0.69
1:A:571:SER:O	1:A:572:ILE:HG23	1.93	0.69
1:A:64:ILE:HB	1:A:86:ASN:HB3	1.74	0.69
1:A:166:GLN:HA	1:A:190:GLU:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:LEU:N	1:A:533:ASN:HD22	1.84	0.68
1:A:38:GLY:H	1:A:58:ASP:HB3	1.57	0.68
1:A:487:ASN:HB2	1:A:509:ASN:HD21	1.58	0.68
1:A:218:VAL:HG12	1:A:244:THR:HB	1.77	0.67
1:A:112:LEU:H	1:A:134:ASN:HD22	1.42	0.66
1:A:489:LEU:H	1:A:509:ASN:HD22	1.43	0.66
1:A:158:ASN:HD22	1:A:160:ASP:HB2	1.59	0.66
1:A:59:LEU:HD12	1:A:64:ILE:HD11	1.78	0.66
1:A:112:LEU:HD22	1:A:115:LEU:HD23	1.78	0.65
1:A:239:PHE:H	1:A:268:GLN:NE2	1.95	0.65
2:B:408:ASN:HB2	2:B:433:ASN:HD21	1.61	0.65
7:G:1:NAG:H62	7:G:2:BMA:O5	1.96	0.64
2:B:115:ASN:ND2	2:B:138:MET:HA	2.13	0.63
1:A:110:ASN:HB2	1:A:134:ASN:HD21	1.64	0.63
2:B:54:GLN:HE22	4:D:2:NDG:C8	2.12	0.63
1:A:310:GLU:HG3	1:A:311:THR:HG23	1.80	0.62
2:B:62:THR:HA	2:B:88:VAL:HG13	1.80	0.62
1:A:68:SER:HA	1:A:92:GLU:HB2	1.80	0.62
1:A:158:ASN:ND2	1:A:160:ASP:HB2	2.13	0.62
1:A:43:LEU:HD12	1:A:43:LEU:H	1.62	0.62
1:A:489:LEU:HB2	1:A:509:ASN:HD22	1.64	0.62
2:B:397:MET:O	2:B:422:THR:HG21	2.01	0.61
2:B:281:VAL:HG12	2:B:283:LEU:HD13	1.82	0.61
2:B:360:LEU:H	2:B:382:ASN:HD22	1.48	0.61
1:A:489:LEU:HB2	1:A:509:ASN:ND2	2.15	0.61
2:B:239:LYS:O	2:B:242:THR:HG22	2.00	0.60
1:A:270:MET:HB3	1:A:304:ILE:HD12	1.83	0.60
2:B:57:ILE:H	2:B:79:ASN:HD22	1.49	0.60
9:C:1:PCJ:H321	9:C:1:PCJ:H113	1.82	0.60
1:A:395:ARG:O	1:A:421:SER:O	2.20	0.60
2:B:455:ASN:HB2	2:B:478:ASN:HD21	1.66	0.60
1:A:113:SER:HB3	1:A:135:PRO:HB2	1.84	0.60
2:B:433:ASN:HB2	2:B:455:ASN:HD21	1.67	0.60
1:A:73:GLN:HA	1:A:98:SER:HB2	1.82	0.59
2:B:460:ILE:HG23	2:B:464:VAL:HG21	1.83	0.59
1:A:522:LEU:H	1:A:522:LEU:HD22	1.68	0.58
1:A:569:VAL:HA	1:A:572:ILE:HD11	1.85	0.58
1:A:78:LEU:HD23	1:A:99:LEU:HD22	1.84	0.58
1:A:234:LEU:HB3	1:A:261:ILE:HD12	1.86	0.57
1:A:52:GLU:OE1	1:A:76:VAL:HG12	2.04	0.57
2:B:36:LEU:HD13	2:B:40:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:HA	1:A:172:GLY:HA3	1.86	0.57
1:A:346:SER:H	1:A:370:ASN:ND2	2.02	0.57
1:A:446:THR:CG2	1:A:448:ILE:HG23	2.35	0.56
2:B:242:THR:O	2:B:244:PRO:HD3	2.04	0.56
7:G:1:NAG:H4	7:G:2:BMA:O2	2.04	0.56
1:A:425:PHE:O	1:A:446:THR:O	2.23	0.56
1:A:378:LYS:HA	1:A:408:THR:HG23	1.87	0.56
1:A:537:CYS:HA	1:A:542:ILE:HG21	1.87	0.56
2:B:36:LEU:H	2:B:55:ASN:ND2	2.02	0.56
1:A:35:ILE:HG23	1:A:56:SER:HB2	1.87	0.56
1:A:481:GLU:HG2	1:A:503:VAL:HB	1.88	0.56
2:B:358:ASN:HB2	2:B:382:ASN:HD21	1.70	0.56
1:A:79:GLN:HA	1:A:102:LEU:HA	1.88	0.55
1:A:82:VAL:HA	1:A:106:ASP:HB3	1.89	0.55
1:A:85:SER:HA	1:A:109:TYR:O	2.07	0.55
1:A:335:THR:HB	1:A:359:LEU:HD23	1.89	0.55
2:B:80:ARG:HG2	2:B:80:ARG:HH11	1.72	0.55
2:B:230:CYS:HA	10:B:858:HOH:O	2.06	0.54
1:A:356:SER:HB3	1:A:385:ALA:HB1	1.89	0.54
1:A:506:ILE:HD12	1:A:511:LEU:HD11	1.88	0.54
1:A:540:PRO:O	1:A:541:ARG:HG3	2.07	0.54
2:B:282:LYS:HG2	10:B:817:HOH:O	2.06	0.54
2:B:538:VAL:HA	2:B:541:ILE:HD13	1.88	0.54
2:B:66:LEU:HD12	2:B:67:SER:N	2.23	0.54
2:B:273:VAL:HG23	2:B:299:LEU:HD21	1.90	0.54
1:A:535:TRP:CD1	1:A:560:ALA:HB1	2.42	0.53
2:B:193:HIS:HD2	10:B:889:HOH:O	1.91	0.53
2:B:522:SER:HA	2:B:539:ARG:HH21	1.72	0.53
1:A:212:LEU:HD22	1:A:215:GLU:OE1	2.09	0.53
1:A:469:LEU:H	1:A:487:ASN:ND2	2.02	0.53
1:A:36:CYS:HB2	1:A:57:LEU:HD23	1.89	0.53
1:A:506:ILE:O	1:A:506:ILE:HG23	2.08	0.53
1:A:129:LEU:HG	1:A:131:LEU:HD21	1.91	0.53
1:A:369:GLU:HA	1:A:396:GLN:O	2.10	0.52
2:B:147:SER:O	2:B:148:THR:HG23	2.08	0.52
1:A:121:LYS:H	1:A:122:PRO:CD	2.23	0.52
2:B:113:THR:HG23	2:B:114:VAL:O	2.10	0.52
1:A:573:ILE:N	1:A:573:ILE:HD12	2.24	0.52
1:A:377:LEU:HG	1:A:408:THR:HG21	1.91	0.51
1:A:138:THR:HG22	1:A:139:LEU:H	1.75	0.51
1:A:556:GLU:OE1	1:A:559:SER:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:SER:O	1:A:150:LYS:HD3	2.11	0.51
1:A:65:THR:HG23	1:A:89:ASN:OD1	2.10	0.51
2:B:34:ASN:H	2:B:55:ASN:HD21	1.59	0.51
1:A:467:ASN:HB2	1:A:487:ASN:HD21	1.75	0.51
1:A:370:ASN:HB2	1:A:397:ASN:HD21	1.76	0.50
1:A:137:LYS:HA	1:A:162:PHE:HA	1.94	0.50
1:A:167:ARG:C	1:A:169:ASP:H	2.15	0.50
1:A:446:THR:HG22	1:A:448:ILE:HG23	1.93	0.50
1:A:443:LEU:O	1:A:446:THR:HB	2.11	0.50
1:A:510:GLN:NE2	1:A:534:PRO:HG2	2.27	0.50
2:B:215:ASN:HD22	2:B:248:ASN:HB2	1.75	0.50
1:A:548:TRP:HE3	1:A:549:LEU:HD12	1.76	0.50
2:B:435:LEU:H	2:B:455:ASN:ND2	2.05	0.49
1:A:50:LEU:H	1:A:50:LEU:HD12	1.78	0.49
2:B:394:THR:CG2	2:B:422:THR:H	2.25	0.49
2:B:57:ILE:H	2:B:79:ASN:ND2	2.09	0.49
2:B:229:LYS:HB2	2:B:260:SER:OG	2.12	0.49
1:A:96:PHE:CE1	1:A:119:TRP:HB3	2.48	0.49
2:B:312:PHE:O	9:C:1:PCJ:H651	2.13	0.49
1:A:139:LEU:HB2	1:A:169:ASP:OD1	2.13	0.48
2:B:440:PHE:CD2	2:B:464:VAL:HG22	2.49	0.48
1:A:306:PRO:HG3	1:A:334:LEU:HA	1.96	0.48
1:A:218:VAL:HG13	1:A:242:LEU:HD22	1.95	0.48
1:A:198:GLN:HG2	1:A:199:ASN:OD1	2.13	0.48
2:B:480:LEU:H	2:B:502:ASN:HD22	1.62	0.48
2:B:500:HIS:HD2	2:B:501:THR:OG1	1.97	0.47
1:A:87:GLY:HA2	1:A:111:TYR:CD1	2.50	0.47
1:A:345:ASN:HA	1:A:369:GLU:O	2.15	0.47
1:A:234:LEU:HD22	1:A:259:VAL:HG11	1.96	0.47
1:A:512:LYS:HA	1:A:534:PRO:O	2.15	0.47
2:B:273:VAL:HG23	2:B:299:LEU:CD2	2.44	0.47
2:B:129:LEU:HA	2:B:148:THR:CG2	2.44	0.47
2:B:33:LYS:HE3	4:D:1:NAG:C6	2.45	0.47
1:A:298:SER:HB3	1:A:303:VAL:HG12	1.97	0.46
1:A:118:SER:O	1:A:122:PRO:HD3	2.14	0.46
2:B:129:LEU:HA	2:B:148:THR:HG23	1.98	0.46
1:A:158:ASN:OD1	1:A:162:PHE:HB2	2.16	0.46
2:B:462:LYS:O	2:B:465:VAL:HG22	2.16	0.46
1:A:161:THR:O	1:A:163:THR:HG23	2.16	0.46
2:B:518:LEU:HG	2:B:525:GLU:OE2	2.16	0.46
2:B:115:ASN:HD21	2:B:138:MET:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:ASN:HA	2:B:498:TRP:HB2	1.98	0.45
2:B:413:ASP:OD1	2:B:415:LYS:HG2	2.16	0.45
2:B:534:SER:OG	2:B:536:LYS:HG3	2.14	0.45
1:A:125:SER:HA	1:A:150:LYS:HD3	1.97	0.45
1:A:132:LEU:HD11	1:A:155:ARG:HB3	1.99	0.45
1:A:182:ASP:HA	1:A:206:HIS:HB2	1.97	0.45
1:A:469:LEU:N	1:A:487:ASN:HD22	2.04	0.45
1:A:173:LEU:N	1:A:173:LEU:HD23	2.31	0.45
1:A:328:LEU:HA	10:A:930:HOH:O	2.17	0.45
1:A:385:ALA:O	1:A:386:TRP:C	2.55	0.45
1:A:475:ASN:HA	1:A:497:LEU:HB3	1.99	0.45
2:B:28:LEU:HD22	2:B:29:VAL:N	2.30	0.45
2:B:37:ILE:HG13	2:B:38:HIS:CD2	2.52	0.45
1:A:398:HIS:ND1	2:B:383:GLN:NE2	2.64	0.44
2:B:305:HIS:CD2	2:B:334:SER:HB2	2.52	0.44
1:A:383:GLU:O	1:A:384:ASP:HB2	2.17	0.44
2:B:221:ILE:HD13	2:B:233:PHE:CZ	2.52	0.44
2:B:514:LEU:O	2:B:518:LEU:HB2	2.17	0.44
2:B:115:ASN:HA	2:B:115:ASN:HD22	1.58	0.44
2:B:541:ILE:HD12	2:B:541:ILE:N	2.33	0.44
1:A:28:LEU:HD13	1:A:36:CYS:HB3	2.00	0.44
2:B:181:PRO:HG3	2:B:205:ILE:HD12	2.00	0.44
8:A:911:NAG:C7	10:A:968:HOH:O	2.66	0.44
1:A:138:THR:HG22	1:A:139:LEU:N	2.32	0.44
1:A:460:GLU:HG3	1:A:480:LYS:HG2	2.00	0.44
2:B:114:VAL:HG12	2:B:115:ASN:H	1.83	0.44
2:B:358:ASN:HB2	2:B:382:ASN:ND2	2.33	0.44
1:A:176:LEU:HD11	1:A:200:VAL:HG22	1.99	0.43
2:B:394:THR:HG21	2:B:421:TRP:HE3	1.83	0.43
1:A:52:GLU:C	1:A:54:VAL:H	2.22	0.43
1:A:67:ILE:HB	1:A:91:ILE:HG12	2.00	0.43
2:B:411:SER:HB3	2:B:434:ILE:HG13	1.99	0.43
1:A:115:LEU:HA	1:A:119:TRP:HZ3	1.84	0.43
1:A:132:LEU:HA	1:A:157:GLY:O	2.19	0.43
1:A:542:ILE:HD12	1:A:546:SER:OG	2.18	0.43
2:B:79:ASN:HB2	2:B:103:ASN:HD21	1.83	0.43
1:A:142:THR:O	1:A:143:SER:C	2.56	0.43
1:A:43:LEU:HD12	1:A:43:LEU:N	2.30	0.43
2:B:457:ILE:H	2:B:478:ASN:ND2	2.06	0.43
2:B:177:GLU:O	2:B:178:LYS:C	2.57	0.43
2:B:290:ARG:HD2	2:B:318:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:NAG:H61	4:D:2:NDG:H8C3	1.99	0.43
1:A:176:LEU:CD1	1:A:200:VAL:HG22	2.49	0.42
1:A:535:TRP:NE1	1:A:560:ALA:HB1	2.35	0.42
2:B:480:LEU:H	2:B:502:ASN:ND2	2.16	0.42
1:A:560:ALA:O	1:A:561:LYS:HD2	2.20	0.42
2:B:73:ILE:HG23	2:B:97:TYR:CD2	2.54	0.42
1:A:484:ILE:HG12	1:A:484:ILE:O	2.19	0.42
1:A:61:ASN:HA	1:A:85:SER:O	2.19	0.42
2:B:128:ALA:C	2:B:148:THR:HG22	2.40	0.42
1:A:402:LEU:HD12	1:A:428:MET:HB3	2.02	0.42
1:A:519:PHE:HB2	1:A:544:TYR:OH	2.20	0.42
2:B:39:VAL:HG11	2:B:64:ASP:HB3	2.02	0.42
1:A:505:LYS:HA	1:A:529:TRP:HB2	2.01	0.42
1:A:41:GLY:HA2	1:A:62:ASN:OD1	2.20	0.42
1:A:195:LYS:HB2	1:A:219:ASP:HB3	2.02	0.42
2:B:229:LYS:HE2	2:B:259:ASN:HB2	2.02	0.42
2:B:511:ILE:O	2:B:511:ILE:HG13	2.20	0.42
1:A:134:ASN:HA	1:A:135:PRO:HD3	1.89	0.41
1:A:348:VAL:H	1:A:370:ASN:ND2	2.18	0.41
2:B:394:THR:O	2:B:422:THR:HG23	2.19	0.41
1:A:82:VAL:O	1:A:82:VAL:HG13	2.20	0.41
1:A:446:THR:HG22	1:A:448:ILE:HG12	2.02	0.41
1:A:451:VAL:HG21	1:A:472:PHE:CD1	2.55	0.41
1:A:74:ARG:O	1:A:74:ARG:HG3	2.20	0.41
2:B:84:LEU:HD22	2:B:85:ASP:N	2.35	0.41
1:A:131:LEU:HD22	1:A:131:LEU:N	2.34	0.41
2:B:105:LEU:H	2:B:124:ASN:HD22	1.69	0.41
2:B:28:LEU:HD22	2:B:29:VAL:H	1.85	0.41
1:A:158:ASN:HD21	1:A:161:THR:H	1.68	0.41
1:A:290:ASN:HB2	10:A:932:HOH:O	2.19	0.41
1:A:78:LEU:HD23	1:A:99:LEU:CD2	2.50	0.41
2:B:73:ILE:HG12	2:B:97:TYR:HB3	2.03	0.41
1:A:139:LEU:HD21	1:A:156:VAL:HG21	2.02	0.41
1:A:506:ILE:HG22	1:A:529:TRP:O	2.21	0.41
1:A:141:GLU:HB3	1:A:168:LYS:HD2	2.03	0.41
1:A:418:ILE:HD12	1:A:438:MET:SD	2.61	0.41
1:A:515:PRO:HB2	1:A:518:ILE:HB	2.02	0.41
1:A:538:SER:O	1:A:542:ILE:HG12	2.20	0.41
1:A:565:SER:C	1:A:567:LYS:H	2.24	0.41
1:A:58:ASP:HA	1:A:82:VAL:CG1	2.50	0.41
2:B:360:LEU:H	2:B:382:ASN:ND2	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:GLY:N	2:B:55:ASN:ND2	2.69	0.41
2:B:440:PHE:CD1	2:B:461:PRO:HD2	2.56	0.41
2:B:508:CYS:C	2:B:510:ARG:H	2.23	0.41
1:A:282:LEU:CD1	9:C:1:PCJ:H312	2.51	0.41
1:A:224:VAL:HG12	1:A:225:GLU:N	2.36	0.41
9:C:1:PCJ:H652	9:C:1:PCJ:HA	1.84	0.41
1:A:121:LYS:HA	1:A:147:HIS:HD2	1.86	0.41
1:A:50:LEU:N	1:A:50:LEU:HD12	2.36	0.41
2:B:113:THR:OG1	2:B:114:VAL:N	2.52	0.41
1:A:112:LEU:H	1:A:134:ASN:ND2	2.15	0.40
1:A:573:ILE:HG22	1:A:574:CYS:N	2.36	0.40
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.87	0.40
1:A:234:LEU:HD22	1:A:259:VAL:CG1	2.51	0.40
2:B:473:LEU:O	2:B:497:ILE:HA	2.21	0.40
1:A:159:MET:H	1:A:159:MET:HG3	1.65	0.40
2:B:237:LEU:HB3	2:B:267:LEU:HD22	2.03	0.40
1:A:103:GLU:HA	1:A:126:LEU:HA	2.02	0.40
1:A:145:PHE:HB3	1:A:148:LEU:HD11	2.02	0.40
1:A:230:ARG:HG2	1:A:257:ARG:HB3	2.03	0.40
1:A:84:THR:HG23	1:A:108:SER:HB2	2.02	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	547/549 (100%)	458 (84%)	72 (13%)	17 (3%)	4	1
2	B	518/520 (100%)	480 (93%)	36 (7%)	2 (0%)	34	32
3	C	3/5 (60%)	3 (100%)	0	0	100	100
All	All	1068/1074 (99%)	941 (88%)	108 (10%)	19 (2%)	8	4

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	143	SER
1	A	241	GLU
1	A	572	ILE
1	A	85	SER
1	A	395	ARG
1	A	494	ASP
1	A	40	SER
1	A	71	ASP
2	B	220	ASN
1	A	121	LYS
1	A	145	PHE
1	A	541	ARG
1	A	550	ASN
2	B	306	GLN
1	A	32	ARG
1	A	168	LYS
1	A	49	GLY
1	A	100	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	518/518 (100%)	492 (95%)	26 (5%)	24	23
2	B	494/494 (100%)	476 (96%)	18 (4%)	35	36
3	C	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	1017/1017 (100%)	972 (96%)	45 (4%)	28	28

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	55	LYS

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Mol	Chain	Res	Type
1	A	148	LEU
1	A	159	MET
1	A	173	LEU
1	A	176	LEU
1	A	205	LEU
1	A	207	MET
1	A	227	LEU
1	A	229	LEU
1	A	234	LEU
1	A	242	LEU
1	A	254	PHE
1	A	270	MET
1	A	282	LEU
1	A	324	LEU
1	A	325	PHE
1	A	371	LEU
1	A	402	LEU
1	A	446	THR
1	A	459	LEU
1	A	470	ASN
1	A	490	MET
1	A	506	ILE
1	A	522	LEU
1	A	523	THR
2	B	41	LYS
2	B	60	LEU
2	B	80	ARG
2	B	84	LEU
2	B	115	ASN
2	B	116	LEU
2	B	157	LEU
2	B	188	ASN
2	B	189	THR
2	B	193	HIS
2	B	223	CYS
2	B	265	LEU
2	B	283	LEU
2	B	394	THR
2	B	403	LEU
2	B	422	THR
2	B	425	LEU
2	B	514	LEU

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Mol	Chain	Res	Type
3	C	3	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	62	ASN
1	A	73	GLN
1	A	86	ASN
1	A	134	ASN
1	A	147	HIS
1	A	158	ASN
1	A	202	HIS
1	A	258	ASN
1	A	268	GLN
1	A	290	ASN
1	A	370	ASN
1	A	397	ASN
1	A	417	ASN
1	A	423	ASN
1	A	470	ASN
1	A	475	ASN
1	A	478	GLN
1	A	487	ASN
1	A	509	ASN
1	A	510	GLN
1	A	526	GLN
1	A	531	HIS
1	A	533	ASN
1	A	557	GLN
2	B	38	HIS
2	B	54	GLN
2	B	55	ASN
2	B	79	ASN
2	B	82	GLN
2	B	92	ASN
2	B	103	ASN
2	B	115	ASN
2	B	118	HIS
2	B	124	ASN
2	B	188	ASN
2	B	193	HIS

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Mol	Chain	Res	Type
2	B	199	ASN
2	B	215	ASN
2	B	243	ASN
2	B	358	ASN
2	B	367	ASN
2	B	382	ASN
2	B	383	GLN
2	B	402	GLN
2	B	408	ASN
2	B	433	ASN
2	B	455	ASN
2	B	471	GLN
2	B	478	ASN
2	B	479	GLN
2	B	500	HIS
2	B	502	ASN
2	B	526	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 ⓘ

11 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	$\# Z  > 2$
4	NAG	D	1	2,4	14,14,15	0.77	0	17,19,21	0.71	0
4	NDG	D	2	4	14,14,15	0.90	0	17,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	D	3	4	11,11,12	0.77	0	15,15,17	0.82	0
5	NAG	E	1	2,5	14,14,15	0.60	0	17,19,21	1.00	1 (5%)
5	NAG	E	2	5	14,14,15	0.69	0	17,19,21	0.73	1 (5%)
5	MAN	E	3	5	11,11,12	0.71	0	15,15,17	0.71	0
6	NAG	F	1	2,6	14,14,15	0.61	0	17,19,21	0.74	0
6	NAG	F	2	6	14,14,15	0.63	0	17,19,21	0.61	0
6	BMA	F	3	6	11,11,12	0.52	0	15,15,17	0.27	0
7	NAG	G	1	7	14,14,15	0.74	0	17,19,21	0.88	0
7	BMA	G	2	7	11,11,12	0.67	0	15,15,17	0.34	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	1	2,4	-	3/6/23/26	0/1/1/1
4	NDG	D	2	4	-	2/6/23/26	0/1/1/1
4	MAN	D	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	MAN	E	3	5	-	2/2/19/22	0/1/1/1
6	NAG	F	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
7	NAG	G	1	7	-	2/6/23/26	0/1/1/1
7	BMA	G	2	7	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C2-N2-C7	-2.62	119.17	122.90
5	E	2	NAG	C2-N2-C7	-2.04	120.00	122.90

There are no chirality outliers.

All (21) torsion outliers are listed below:

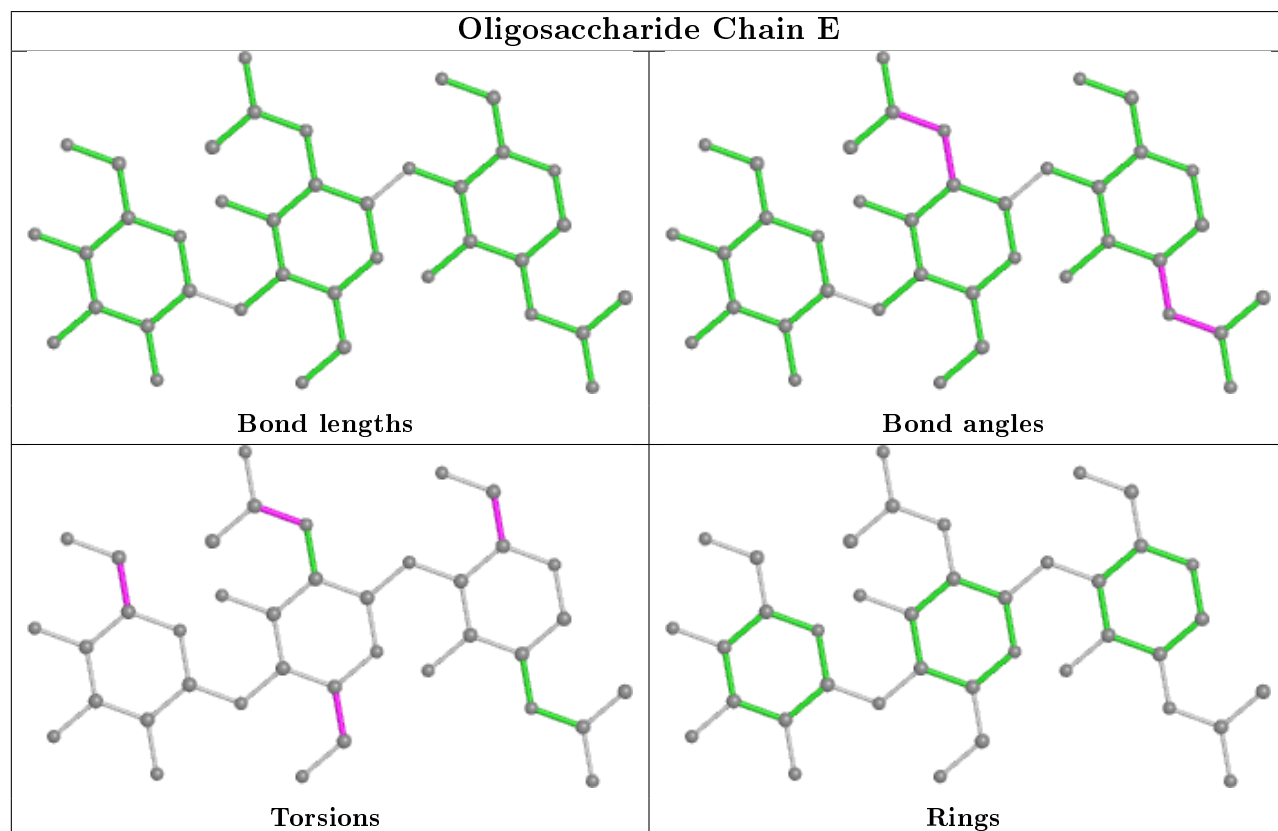
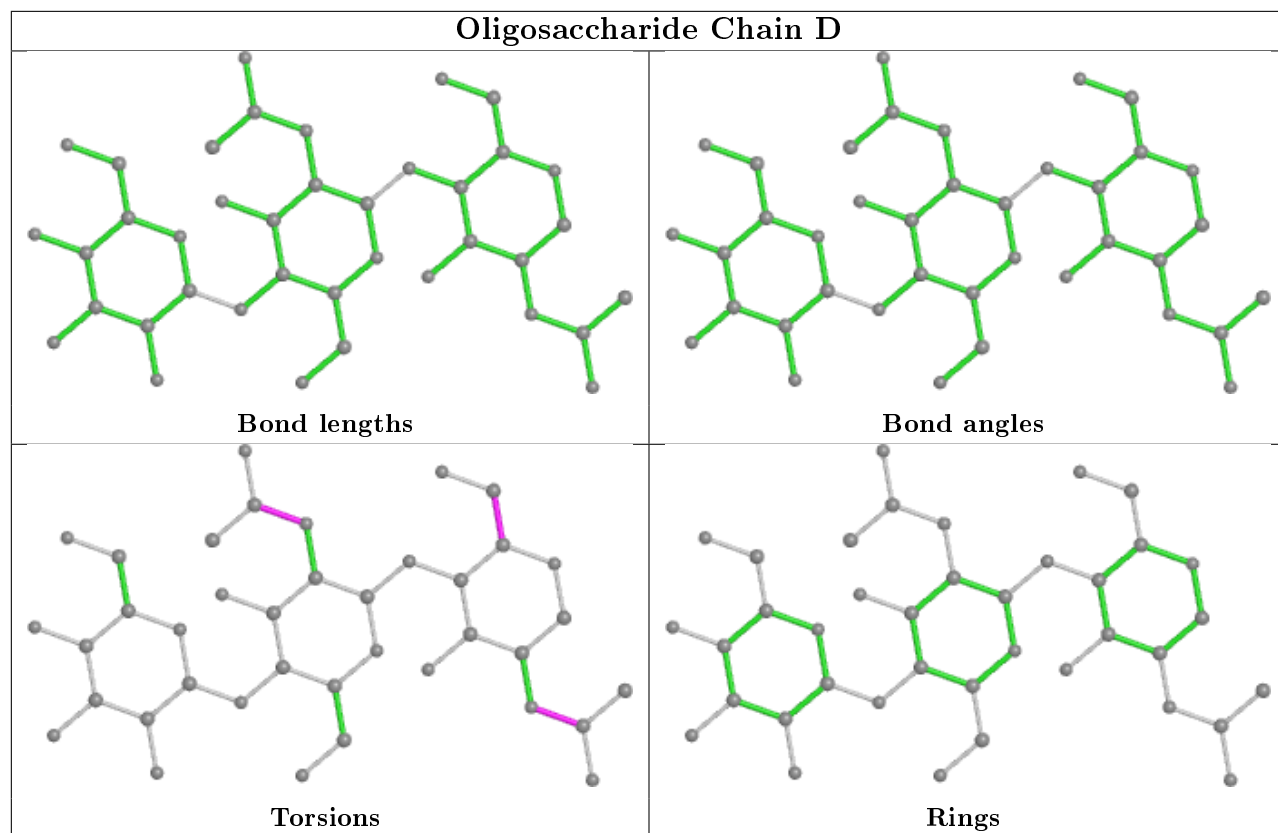
Mol	Chain	Res	Type	Atoms
7	G	1	NAG	C8-C7-N2-C2
7	G	1	NAG	O7-C7-N2-C2
4	D	2	NDG	C8-C7-N2-C2
4	D	2	NDG	O7-C7-N2-C2
5	E	3	MAN	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
5	E	3	MAN	C4-C5-C6-O6
6	F	3	BMA	C4-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
7	G	2	BMA	C4-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O7-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
7	G	2	BMA	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

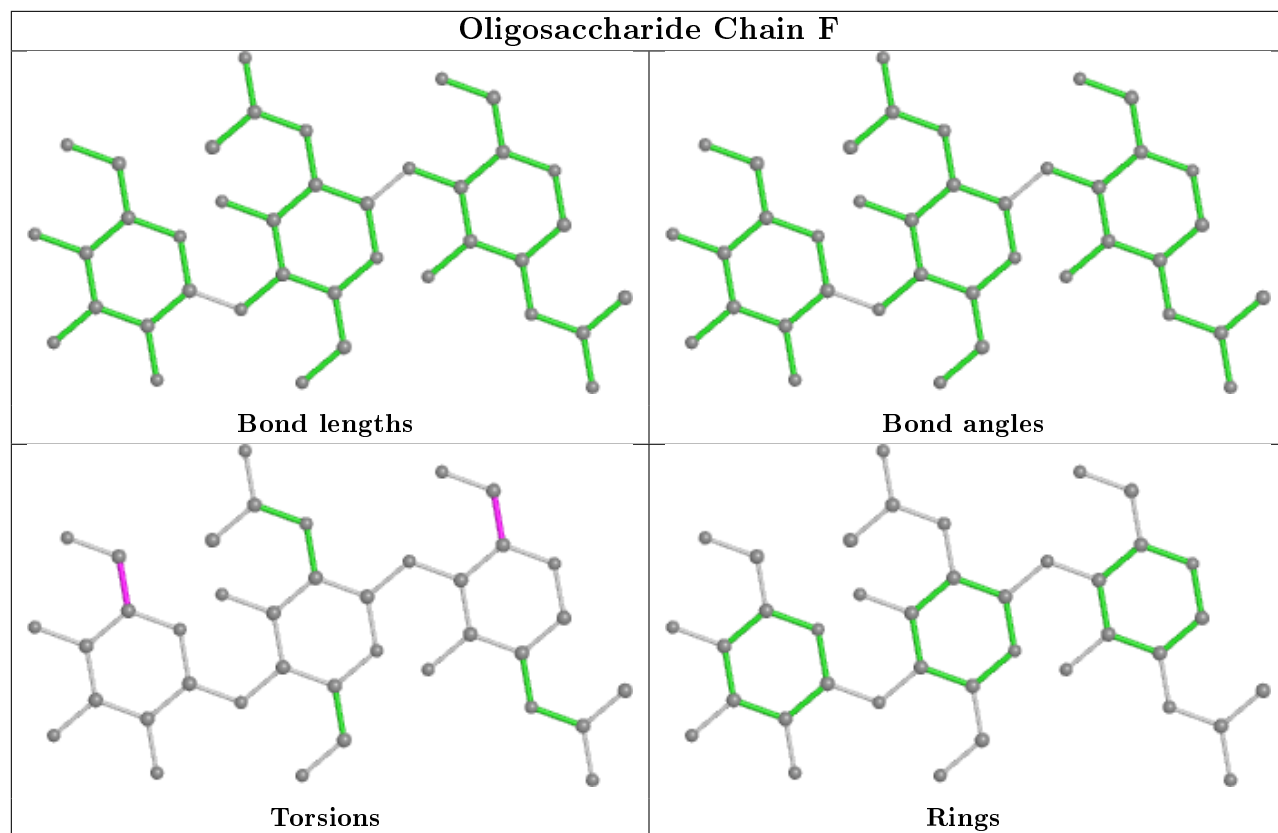
There are no ring outliers.

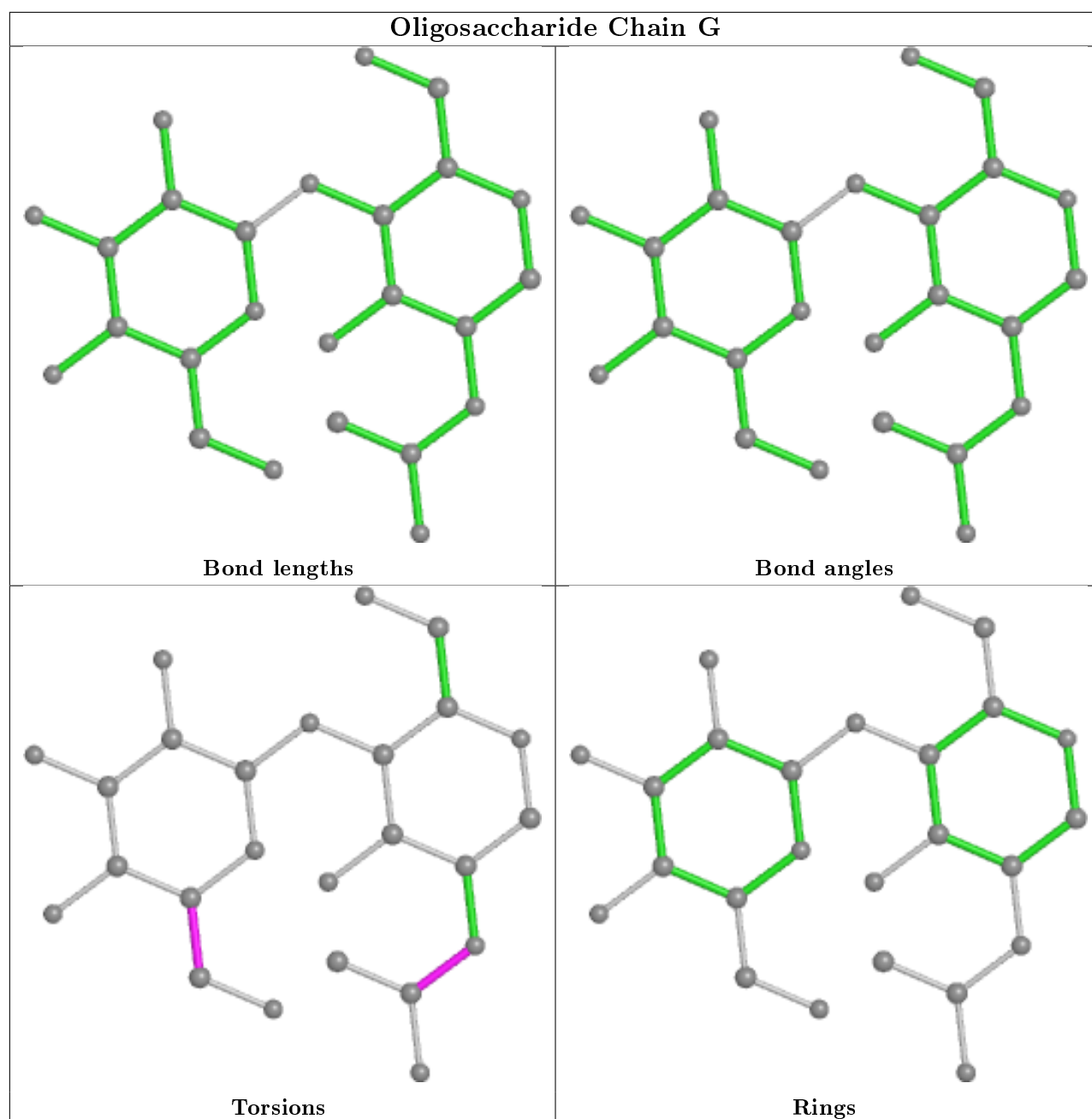
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	2	BMA	2	0
7	G	1	NAG	2	0
4	D	1	NAG	2	0
4	D	2	NDG	3	0

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







## 5.6 Ligand geometry [i](#)

5 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
9	PCJ	C	1	3	60,61,61	0.75	1 (1%)	59,65,65	1.05	4 (6%)
8	NAG	B	811	2	14,14,15	0.57	0	17,19,21	0.67	1 (5%)
8	NAG	A	921	1	14,14,15	0.56	0	17,19,21	0.62	0
8	NAG	A	911	1	14,14,15	0.63	0	17,19,21	0.57	0
8	NAG	A	901	1	14,14,15	0.59	0	17,19,21	0.61	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
9	PCJ	C	1	3	-	17/66/66/66	-
8	NAG	B	811	2	-	2/6/23/26	0/1/1/1
8	NAG	A	921	1	-	0/6/23/26	0/1/1/1
8	NAG	A	911	1	-	4/6/23/26	0/1/1/1
8	NAG	A	901	1	1/1/5/7	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1	PCJ	O-C	-4.68	1.22	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1	PCJ	O2-C46-C45	3.58	119.22	111.50
9	C	1	PCJ	O-C-CA	3.32	120.54	111.95
9	C	1	PCJ	C2-O2-C46	-2.80	110.91	117.79
9	C	1	PCJ	O3-C26-C25	2.57	119.97	111.91
8	B	811	NAG	C2-N2-C7	-2.15	119.84	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	901	NAG	C1

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1	PCJ	O-C-CA-CB
9	C	1	PCJ	O-C-CA-N
8	B	811	NAG	C8-C7-N2-C2
8	B	811	NAG	O7-C7-N2-C2
8	A	911	NAG	C8-C7-N2-C2
8	A	911	NAG	O7-C7-N2-C2
8	A	901	NAG	C8-C7-N2-C2
8	A	901	NAG	O7-C7-N2-C2
9	C	1	PCJ	C65-C66-N-CA
9	C	1	PCJ	O67-C66-N-CA
8	A	911	NAG	O5-C5-C6-O6
8	A	911	NAG	C4-C5-C6-O6
9	C	1	PCJ	C23-C24-C25-C26
9	C	1	PCJ	C22-C23-C24-C25
9	C	1	PCJ	C39-C40-C41-C42
9	C	1	PCJ	C19-C20-C21-C22
8	A	901	NAG	O5-C5-C6-O6
9	C	1	PCJ	C38-C39-C40-C41
9	C	1	PCJ	C25-C26-O3-C3
9	C	1	PCJ	O2-C2-C3-O3
9	C	1	PCJ	C60-C61-C62-C63
9	C	1	PCJ	O28-C26-O3-C3
9	C	1	PCJ	C18-C19-C20-C21
9	C	1	PCJ	C1-C2-C3-O3
9	C	1	PCJ	C24-C25-C26-O3
9	C	1	PCJ	C24-C25-C26-O28

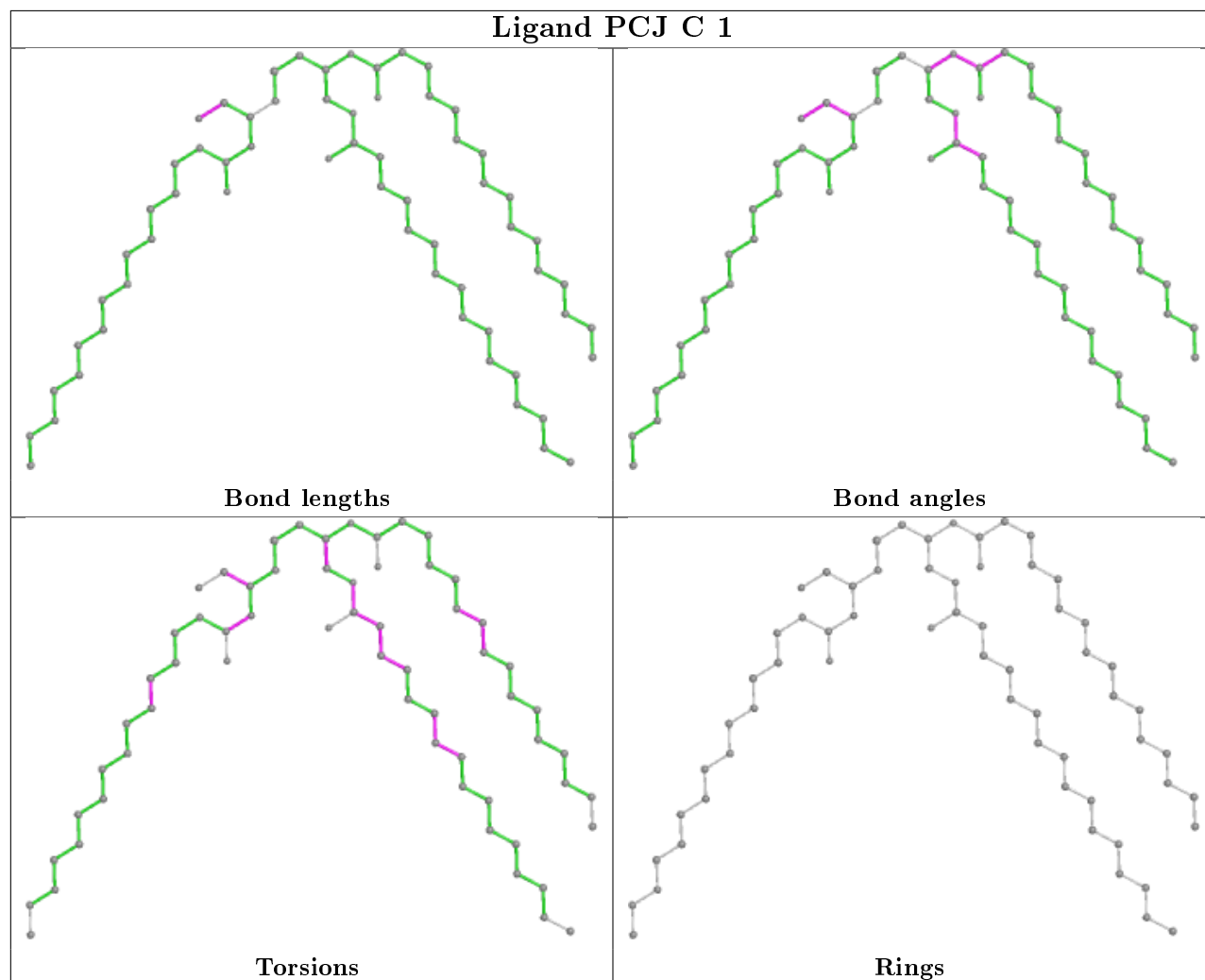
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1	PCJ	4	0
8	A	911	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 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	549/549 (100%)	1.54	153 (27%) 0 0	22, 59, 130, 137	0
2	B	520/520 (100%)	0.15	11 (2%) 63 68	20, 35, 60, 83	0
3	C	5/5 (100%)	1.26	1 (20%) 1 1	41, 57, 74, 83	0
All	All	1074/1074 (100%)	0.87	165 (15%) 2 2	20, 43, 125, 137	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	LEU	11.3
1	A	244	THR	11.3
1	A	67	ILE	10.9
1	A	35	ILE	10.7
1	A	46	ILE	10.3
1	A	99	LEU	10.2
1	A	48	SER	9.5
1	A	83	LEU	9.4
1	A	247	THR	9.2
1	A	573	ILE	9.1
1	A	59	LEU	8.9
1	A	57	LEU	8.7
1	A	96	PHE	8.5
1	A	76	VAL	8.2
1	A	31	ASP	8.0
1	A	33	ASN	7.9
1	A	39	SER	7.9
1	A	40	SER	7.9
1	A	38	GLY	7.9
1	A	50	LEU	7.9
1	A	572	ILE	7.8
1	A	53	ALA	7.7
1	A	47	PRO	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	66	TYR	7.7
1	A	43	LEU	7.6
1	A	27	SER	7.6
1	A	32	ARG	7.4
1	A	36	CYS	7.3
1	A	242	LEU	7.0
1	A	105	LEU	7.0
1	A	141	GLU	6.8
1	A	107	LEU	6.7
1	A	51	THR	6.6
1	A	245	GLY	6.6
1	A	78	LEU	6.5
1	A	74	ARG	6.4
1	A	574	CYS	6.1
1	A	29	SER	6.1
1	A	30	CYS	6.1
1	A	115	LEU	6.1
1	A	55	LYS	5.9
1	A	243	SER	5.9
1	A	68	SER	5.9
2	B	228	ASN	5.7
1	A	117	SER	5.7
1	A	175	PHE	5.6
1	A	72	LEU	5.6
1	A	90	THR	5.6
1	A	61	ASN	5.5
1	A	81	LEU	5.5
1	A	102	LEU	5.5
1	A	302	ARG	5.3
1	A	112	LEU	5.2
1	A	164	LYS	5.2
2	B	227	ASP	5.2
1	A	86	ASN	5.0
1	A	120	PHE	5.0
1	A	575	PRO	5.0
1	A	63	ARG	5.0
1	A	56	SER	4.9
1	A	91	ILE	4.9
1	A	129	LEU	4.8
1	A	145	PHE	4.8
1	A	49	GLY	4.6
1	A	140	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	77	ASN	4.5
1	A	88	ILE	4.5
1	A	151	LEU	4.4
1	A	564	GLY	4.3
1	A	170	PHE	4.3
1	A	37	LYS	4.3
2	B	25	SER	4.3
1	A	114	ASN	4.2
1	A	103	GLU	4.2
1	A	159	MET	4.2
1	A	143	SER	4.2
1	A	75	CYS	4.2
1	A	300	ASN	4.2
1	A	44	ASN	4.1
1	A	126	LEU	4.1
1	A	135	PRO	4.1
1	A	111	TYR	4.1
1	A	123	LEU	4.1
1	A	148	LEU	4.1
1	A	87	GLY	4.0
1	A	176	LEU	4.0
1	A	551	LYS	4.0
1	A	58	ASP	4.0
1	A	248	ASN	4.0
1	A	144	LEU	3.9
1	A	137	LYS	3.9
1	A	34	GLY	3.8
3	C	6	LYS	3.8
1	A	198	GLN	3.8
1	A	519	PHE	3.7
1	A	301	ASP	3.6
1	A	62	ASN	3.6
2	B	508	CYS	3.6
1	A	570	ARG	3.5
1	A	73	GLN	3.5
1	A	160	ASP	3.5
1	A	547	ARG	3.5
1	A	121	LYS	3.4
2	B	533	GLY	3.4
1	A	246	GLU	3.4
1	A	569	VAL	3.3
1	A	65	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	82	VAL	3.2
1	A	84	THR	3.2
1	A	54	VAL	3.1
1	A	42	SER	3.1
1	A	539	CYS	3.1
1	A	558	GLY	3.1
1	A	571	SER	3.1
2	B	226	GLU	3.1
1	A	89	ASN	3.0
1	A	168	LYS	3.0
1	A	104	HIS	3.0
1	A	94	ASP	3.0
1	A	41	GLY	2.9
1	A	541	ARG	2.9
1	A	70	SER	2.8
1	A	125	SER	2.8
1	A	147	HIS	2.8
1	A	109	TYR	2.7
1	A	92	GLU	2.7
1	A	79	GLN	2.7
1	A	298	SER	2.6
1	A	542	ILE	2.6
1	A	173	LEU	2.6
1	A	52	GLU	2.6
1	A	150	LYS	2.6
1	A	119	TRP	2.6
1	A	128	PHE	2.6
1	A	261	ILE	2.5
2	B	219	SER	2.5
2	B	114	VAL	2.5
1	A	45	SER	2.4
1	A	136	TYR	2.4
1	A	152	GLN	2.4
1	A	156	VAL	2.4
2	B	229	LYS	2.4
1	A	71	ASP	2.4
1	A	211	ILE	2.4
1	A	139	LEU	2.3
1	A	490	MET	2.3
1	A	153	ILE	2.3
1	A	187	GLN	2.3
1	A	510	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	540	PRO	2.3
1	A	535	TRP	2.2
2	B	509	PRO	2.2
2	B	242	THR	2.2
1	A	93	GLU	2.2
1	A	543	ASP	2.2
1	A	118	SER	2.2
1	A	172	GLY	2.2
1	A	69	ASN	2.2
1	A	549	LEU	2.1
1	A	60	SER	2.1
1	A	516	ASP	2.1
1	A	64	ILE	2.1
1	A	544	TYR	2.1
1	A	167	ARG	2.0
1	A	520	ASP	2.0

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

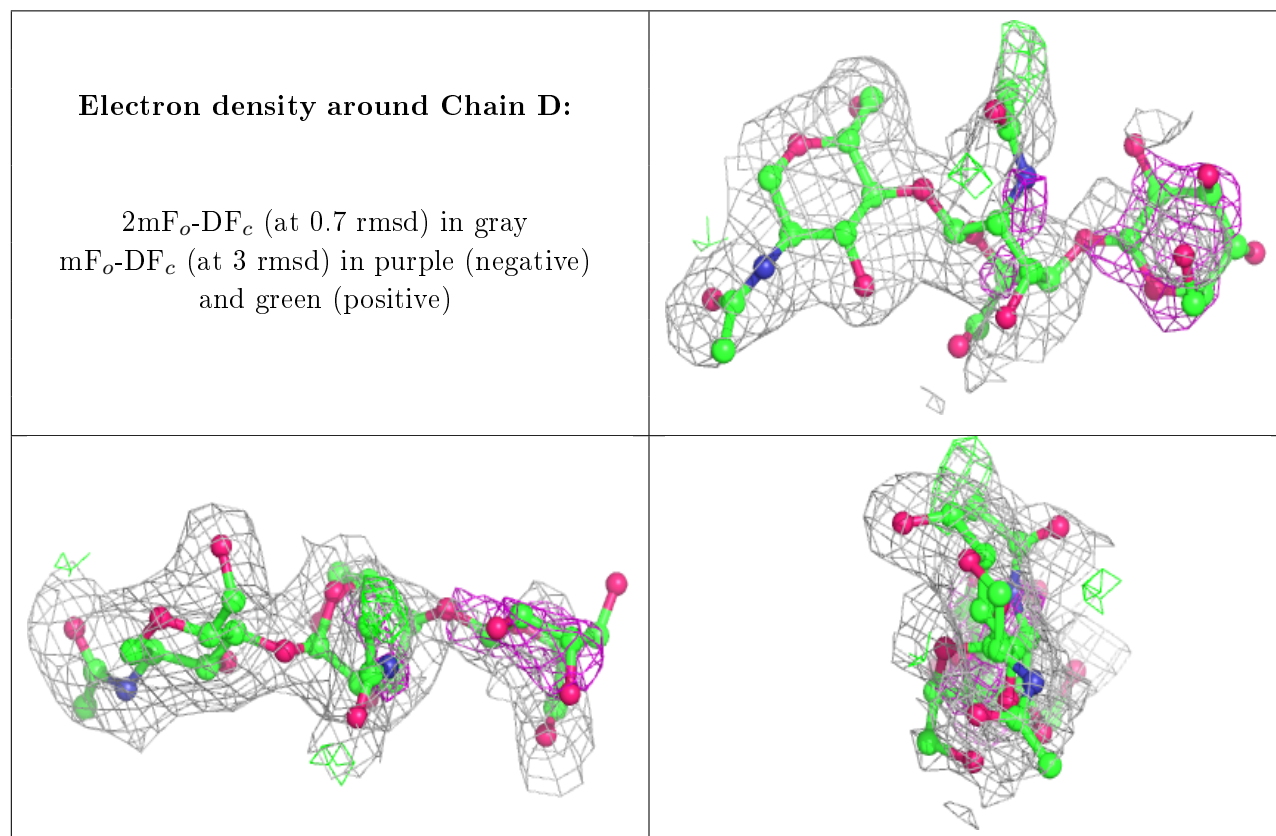
There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 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.

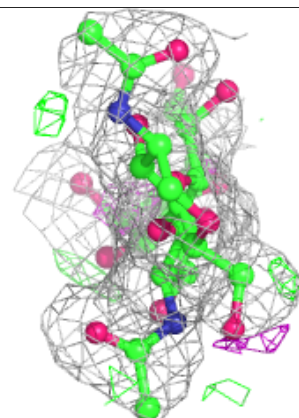
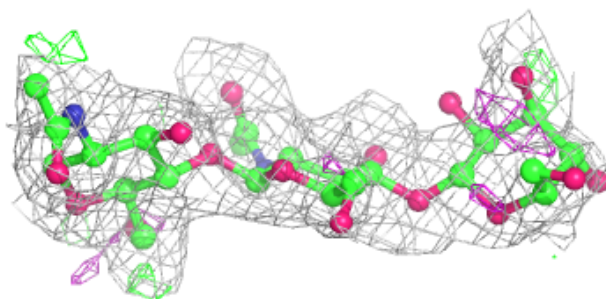
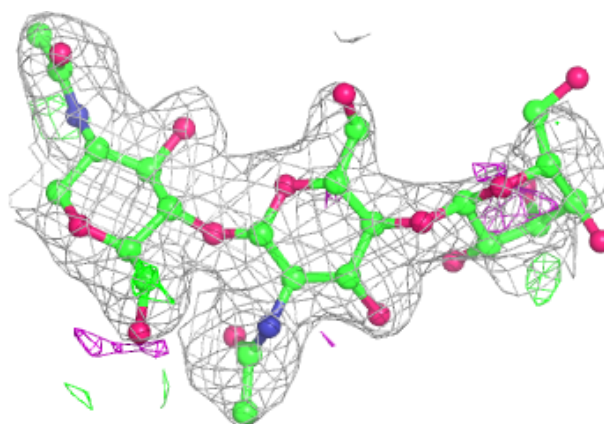
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MAN	D	3	11/12	0.36	0.70	98,100,102,102	0
7	NAG	G	1	14/15	0.44	0.28	90,93,96,96	0
7	BMA	G	2	11/12	0.47	0.31	96,98,99,99	0
4	NDG	D	2	14/15	0.61	0.29	80,85,89,94	0
5	MAN	E	3	11/12	0.72	0.46	81,84,86,88	0
6	BMA	F	3	11/12	0.78	0.18	68,72,74,77	0
5	NAG	E	2	14/15	0.84	0.19	55,65,71,75	0
5	NAG	E	1	14/15	0.91	0.11	41,46,52,56	0
4	NAG	D	1	14/15	0.93	0.09	53,58,62,72	0
6	NAG	F	2	14/15	0.93	0.10	35,48,54,62	0
6	NAG	F	1	14/15	0.95	0.10	24,30,33,40	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.

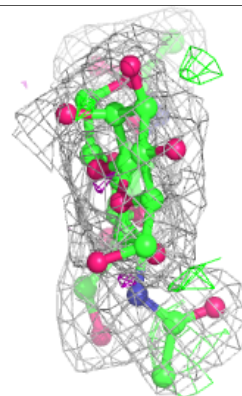
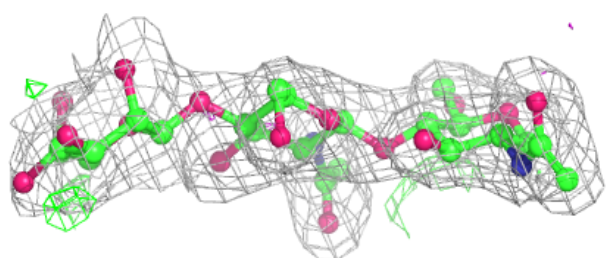
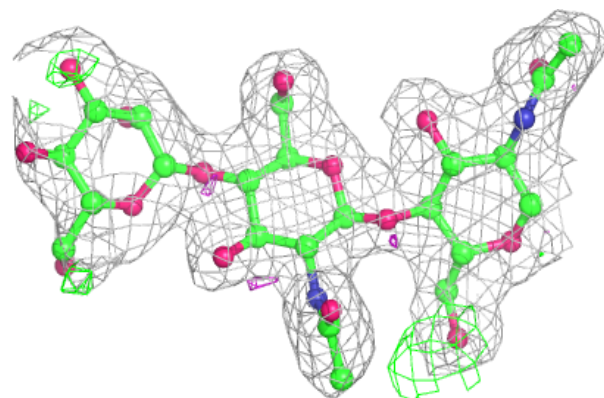


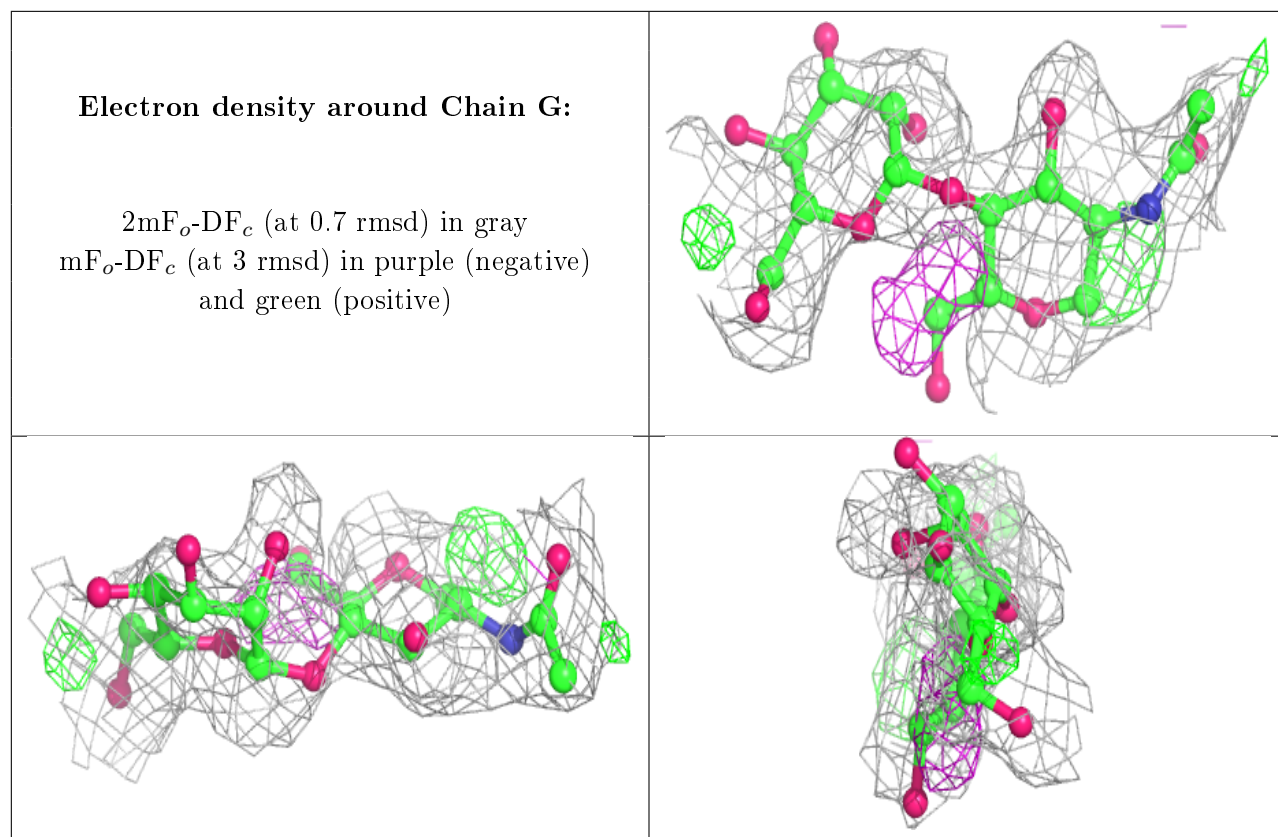
**Electron density around Chain E:**

$2mF_o-DF_c$  (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)



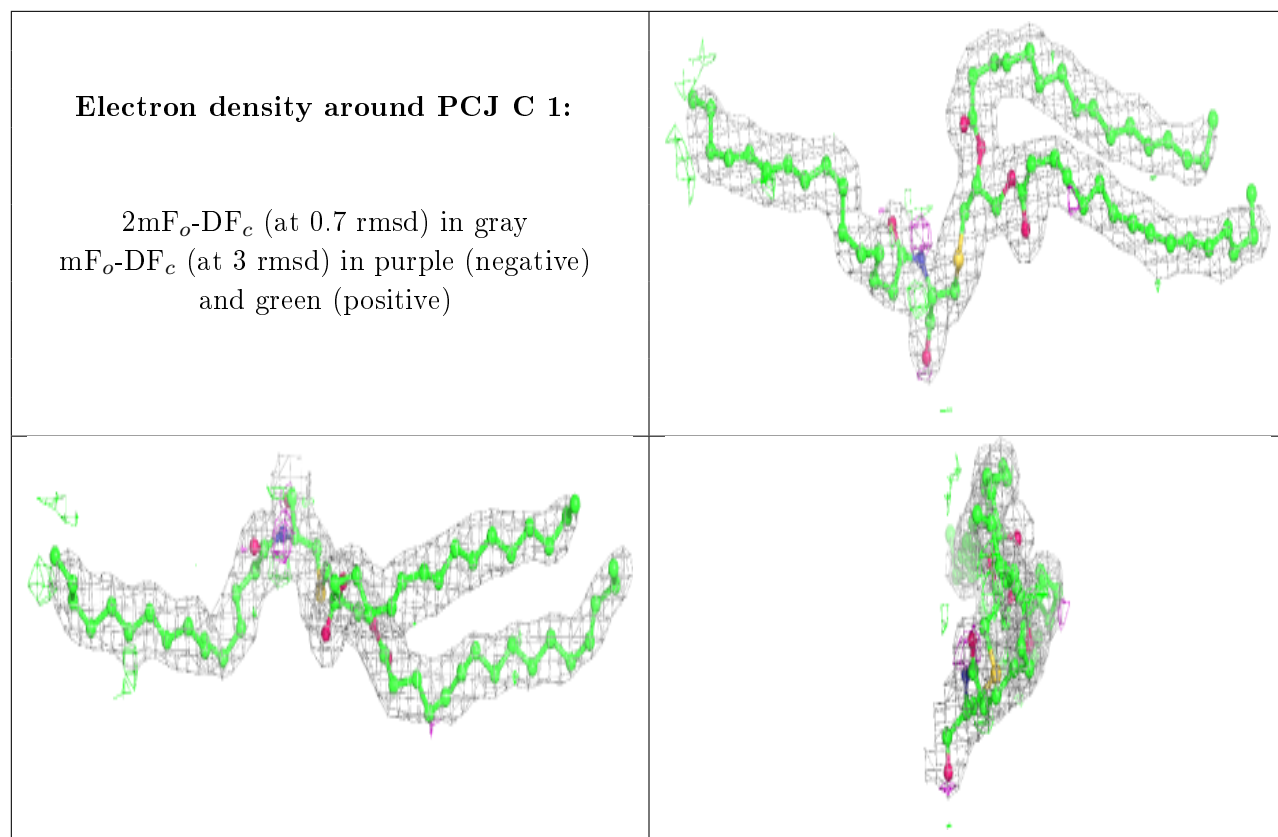


## 6.4 Ligands [i](#)

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
8	NAG	A	911	14/15	0.55	0.22	71,74,77,78	0
8	NAG	A	901	14/15	0.67	0.46	104,106,107,107	0
8	NAG	B	811	14/15	0.70	0.28	74,78,80,81	0
9	PCJ	C	1	62/62	0.93	0.20	28,37,53,56	0
8	NAG	A	921	14/15	0.94	0.08	31,34,37,37	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.