



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:14 AM BST

PDB ID : 6FKN  
Title : Drosophila Plexin A in complex with Semaphorin 1b  
Authors : Rozbesky, D.; Harlos, K.; Jones, E.Y.  
Deposited on : 2018-01-24  
Resolution : 4.80 Å(reported)

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

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

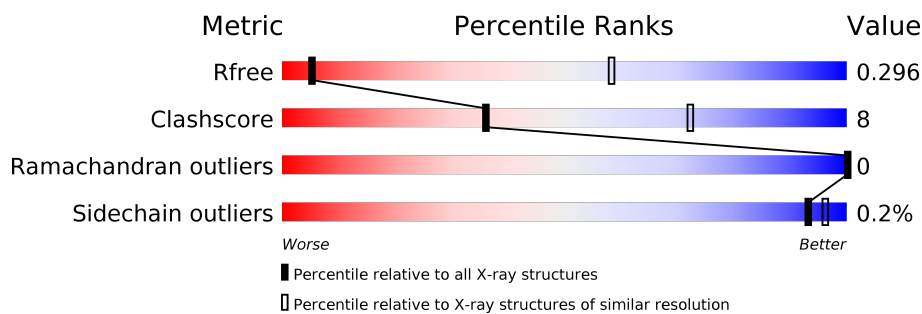
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1096 (5.80-3.80)
Clashscore	141614	1170 (5.80-3.80)
Ramachandran outliers	138981	1105 (5.80-3.80)
Sidechain outliers	138945	1085 (5.80-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	715	
1	C	715	
2	B	578	
2	D	578	
3	E	4	
4	F	3	
5	G	5	

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Mol	Chain	Length	Quality of chain
5	H	5	

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
3	NAG	E	1	X	-	-	-
5	NAG	G	2	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15600 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 Plexin A, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			3923	2466	654	777	26			
1	C	512	Total	C	N	O	S	0	0	0
			3931	2470	656	779	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLU	-	expression tag	UNP Q9V491
A	26	THR	-	expression tag	UNP Q9V491
A	27	GLY	-	expression tag	UNP Q9V491
A	731	GLY	-	expression tag	UNP Q9V491
A	732	THR	-	expression tag	UNP Q9V491
A	733	LYS	-	expression tag	UNP Q9V491
A	734	HIS	-	expression tag	UNP Q9V491
A	735	HIS	-	expression tag	UNP Q9V491
A	736	HIS	-	expression tag	UNP Q9V491
A	737	HIS	-	expression tag	UNP Q9V491
A	738	HIS	-	expression tag	UNP Q9V491
A	739	HIS	-	expression tag	UNP Q9V491
C	25	GLU	-	expression tag	UNP Q9V491
C	26	THR	-	expression tag	UNP Q9V491
C	27	GLY	-	expression tag	UNP Q9V491
C	731	GLY	-	expression tag	UNP Q9V491
C	732	THR	-	expression tag	UNP Q9V491
C	733	LYS	-	expression tag	UNP Q9V491
C	734	HIS	-	expression tag	UNP Q9V491
C	735	HIS	-	expression tag	UNP Q9V491
C	736	HIS	-	expression tag	UNP Q9V491
C	737	HIS	-	expression tag	UNP Q9V491
C	738	HIS	-	expression tag	UNP Q9V491
C	739	HIS	-	expression tag	UNP Q9V491

- Molecule 2 is a protein called MIP07328p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	478	Total	C	N	O	S	0	0	0
			3743	2376	646	702	19			
2	D	473	Total	C	N	O	S	0	0	0
			3708	2355	639	695	19			

There are 24 discrepancies between the modelled and reference sequences:

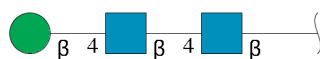
Chain	Residue	Modelled	Actual	Comment	Reference
B	34	GLU	-	expression tag	UNP Q7KK54
B	35	THR	-	expression tag	UNP Q7KK54
B	36	GLY	-	expression tag	UNP Q7KK54
B	603	GLY	-	expression tag	UNP Q7KK54
B	604	THR	-	expression tag	UNP Q7KK54
B	605	LYS	-	expression tag	UNP Q7KK54
B	606	HIS	-	expression tag	UNP Q7KK54
B	607	HIS	-	expression tag	UNP Q7KK54
B	608	HIS	-	expression tag	UNP Q7KK54
B	609	HIS	-	expression tag	UNP Q7KK54
B	610	HIS	-	expression tag	UNP Q7KK54
B	611	HIS	-	expression tag	UNP Q7KK54
D	34	GLU	-	expression tag	UNP Q7KK54
D	35	THR	-	expression tag	UNP Q7KK54
D	36	GLY	-	expression tag	UNP Q7KK54
D	603	GLY	-	expression tag	UNP Q7KK54
D	604	THR	-	expression tag	UNP Q7KK54
D	605	LYS	-	expression tag	UNP Q7KK54
D	606	HIS	-	expression tag	UNP Q7KK54
D	607	HIS	-	expression tag	UNP Q7KK54
D	608	HIS	-	expression tag	UNP Q7KK54
D	609	HIS	-	expression tag	UNP Q7KK54
D	610	HIS	-	expression tag	UNP Q7KK54
D	611	HIS	-	expression tag	UNP Q7KK54

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



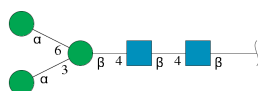
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 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
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 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>).

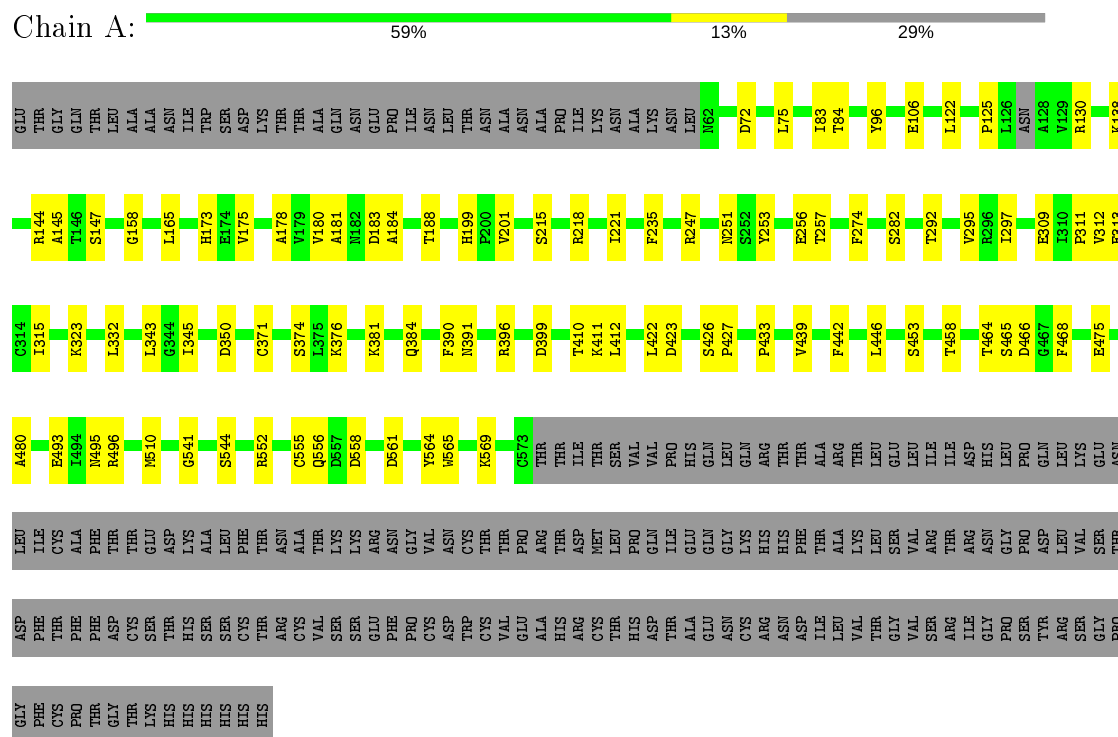


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

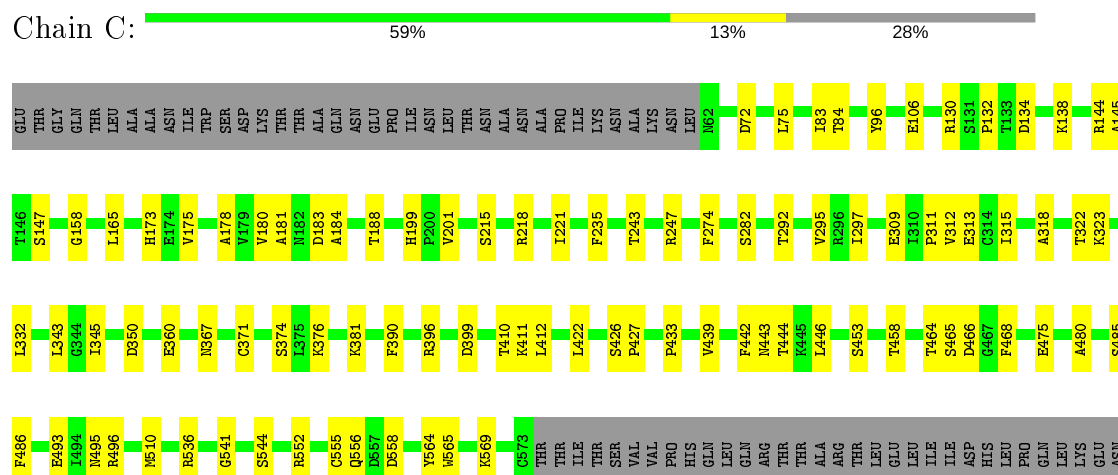
### 3 Residue-property plots

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. 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. 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: Plexin A, isoform A



#### • Molecule 1: Plexin A, isoform A









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

Chain F:



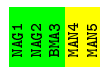
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.63 Å 153.63 Å 425.37 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	133.05 – 4.80 133.05 – 4.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (133.05-4.80) 89.0 (133.05-4.80)	Depositor EDS
$R_{merge}$	0.34	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 4.88 Å)	Xtriage
Refinement program	PHENIX (1.13rc2_2986: ???)	Depositor
R, $R_{free}$	0.285 , 0.297 0.285 , 0.296	Depositor DCC
$R_{free}$ test set	819 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	185.7	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 204.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	15600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	271.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% 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: BMA, NAG, 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	0/4001	0.52	0/5436
1	C	0.32	0/4010	0.52	0/5450
2	B	0.31	0/3830	0.51	0/5200
2	D	0.31	0/3793	0.51	0/5150
All	All	0.32	0/15634	0.52	0/21236

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	3923	0	3825	67	7
1	C	3931	0	3832	81	5
2	B	3743	0	3658	84	24
2	D	3708	0	3630	51	32
3	E	50	0	43	10	0
4	F	39	0	34	0	0
5	G	61	0	52	15	0
5	H	61	0	52	0	0
6	A	42	0	39	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	42	0	39	2	0
All	All	15600	0	15204	245	37

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 8.

All (245) 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)
2:B:294:GLY:N	3:E:2:NAG:C7	1.96	1.28
2:B:386:ILE:HG23	2:B:390:PHE:CZ	1.69	1.25
2:D:293:PRO:CA	5:G:2:NAG:H82	1.67	1.24
2:B:386:ILE:HG22	2:B:390:PHE:CE2	1.81	1.16
2:B:349:GLU:OE2	1:C:486:PHE:CB	1.96	1.12
2:B:386:ILE:CG2	2:B:390:PHE:CZ	2.32	1.12
2:B:294:GLY:N	3:E:2:NAG:C8	2.15	1.09
2:D:293:PRO:HA	5:G:2:NAG:H82	1.15	1.09
2:D:293:PRO:C	5:G:2:NAG:C8	2.25	1.05
2:D:293:PRO:HA	5:G:2:NAG:C8	1.88	1.03
2:D:400:ALA:HB3	5:G:1:NAG:H82	1.37	1.02
2:D:400:ALA:HB3	5:G:1:NAG:C8	1.90	1.01
2:B:386:ILE:CG2	2:B:390:PHE:CE2	2.42	1.01
6:A:803:NAG:O4	1:C:132:PRO:HG2	1.59	1.00
2:B:349:GLU:OE2	1:C:486:PHE:HA	1.64	0.98
2:D:293:PRO:CA	5:G:2:NAG:C8	2.42	0.98
1:A:256:GLU:O	1:C:360:GLU:OE1	1.84	0.96
2:B:252:MET:HB2	1:C:443:ASN:OD1	1.67	0.95
2:B:349:GLU:OE2	1:C:486:PHE:CA	2.16	0.94
2:B:252:MET:CB	1:C:443:ASN:OD1	2.17	0.92
2:B:294:GLY:O	3:E:2:NAG:O3	1.91	0.87
2:B:252:MET:CG	1:C:443:ASN:OD1	2.23	0.87
2:B:352:SER:HB2	1:C:444:THR:HG21	1.57	0.86
2:B:349:GLU:OE2	1:C:486:PHE:HB3	1.75	0.85
2:D:400:ALA:CB	5:G:1:NAG:H82	2.06	0.84
6:A:803:NAG:O3	1:C:132:PRO:O	1.97	0.82
2:B:386:ILE:HG23	2:B:390:PHE:HZ	1.41	0.80
2:D:297:PRO:HG3	5:G:2:NAG:O7	1.82	0.79
1:C:311:PRO:HG2	1:C:433:PRO:HB3	1.66	0.77
1:A:257:THR:HA	1:C:360:GLU:CD	2.04	0.77
2:B:294:GLY:N	3:E:2:NAG:O7	2.17	0.77
1:A:311:PRO:HG2	1:A:433:PRO:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:GLY:N	3:E:2:NAG:H83	1.99	0.76
2:B:352:SER:HB2	1:C:444:THR:CG2	2.20	0.71
2:B:349:GLU:OE2	1:C:486:PHE:HB2	1.88	0.70
2:B:252:MET:HG3	1:C:443:ASN:OD1	1.92	0.67
1:A:199:HIS:O	1:A:201:VAL:N	2.25	0.67
1:A:464:THR:HG22	1:A:466:ASP:H	1.59	0.67
1:C:464:THR:HG22	1:C:466:ASP:H	1.59	0.66
2:B:252:MET:HB2	1:C:443:ASN:CG	2.16	0.66
2:B:209:LEU:HD13	2:B:211:TYR:HB2	1.76	0.66
2:D:209:LEU:HD13	2:D:211:TYR:HB2	1.76	0.65
2:D:293:PRO:C	5:G:2:NAG:H83	2.15	0.64
1:C:243:THR:O	2:D:219:GLN:NE2	2.28	0.64
2:D:238:GLY:HA2	2:D:267:LYS:HE2	1.80	0.63
1:C:199:HIS:O	1:C:201:VAL:N	2.25	0.62
1:A:411:LYS:HB2	2:B:107:LEU:HD12	1.81	0.62
2:D:534:THR:HG22	2:D:536:GLU:H	1.64	0.62
2:D:400:ALA:HB3	5:G:1:NAG:H81	1.81	0.62
2:B:534:THR:HG22	2:B:536:GLU:H	1.64	0.62
6:A:803:NAG:O4	1:C:132:PRO:CG	2.43	0.62
2:D:400:ALA:CB	5:G:1:NAG:C8	2.72	0.62
1:A:138:LYS:HB2	1:A:180:VAL:HG11	1.82	0.61
1:A:122:LEU:HD22	2:B:274:TYR:CZ	2.34	0.61
2:B:238:GLY:HA2	2:B:267:LYS:HE2	1.81	0.61
2:B:394:HIS:CE1	1:C:466:ASP:OD1	2.53	0.61
2:D:293:PRO:CB	5:G:2:NAG:H82	2.31	0.61
2:B:553:LEU:HD21	2:B:566:LEU:HB3	1.82	0.61
2:B:299:TYR:OH	3:E:1:NAG:O3	2.14	0.61
2:D:553:LEU:HD21	2:D:566:LEU:HB3	1.82	0.61
1:C:138:LYS:HB2	1:C:180:VAL:HG11	1.82	0.60
2:B:349:GLU:OE1	1:C:485:SER:O	2.20	0.59
6:A:803:NAG:H81	1:C:134:ASP:CG	2.22	0.59
1:C:315:ILE:HD12	1:C:323:LYS:HG2	1.85	0.59
2:D:129:GLU:HG3	2:D:146:THR:HG22	1.83	0.59
2:B:129:GLU:HG3	2:B:146:THR:HG22	1.83	0.59
2:B:349:GLU:CD	1:C:486:PHE:HA	2.21	0.59
1:C:72:ASP:OD1	1:C:96:TYR:OH	2.21	0.58
1:A:315:ILE:HD12	1:A:323:LYS:HG2	1.85	0.58
1:A:253:TYR:CE2	2:B:222:LEU:HD13	2.38	0.58
1:A:253:TYR:HE2	2:B:222:LEU:HD13	1.67	0.58
2:D:293:PRO:C	5:G:2:NAG:H81	2.19	0.58
1:A:72:ASP:OD1	1:A:96:TYR:OH	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ASP:HB3	2:B:76:LYS:HB2	1.85	0.57
1:A:125:PRO:HB3	2:B:386:ILE:HD11	1.86	0.57
1:C:345:ILE:HG22	1:C:376:LYS:HD3	1.86	0.57
2:B:252:MET:CE	1:C:367:ASN:OD1	2.52	0.57
2:D:521:LEU:HB3	2:D:563:ALA:HB1	1.86	0.57
2:D:59:ASP:HB3	2:D:76:LYS:HB2	1.85	0.57
1:A:215:SER:HB3	1:A:218:ARG:HG2	1.86	0.56
1:C:215:SER:HB3	1:C:218:ARG:HG2	1.86	0.56
2:B:412:LYS:HD2	2:B:419:LEU:HD11	1.87	0.56
1:C:464:THR:HB	1:C:468:PHE:H	1.69	0.56
1:A:464:THR:HB	1:A:468:PHE:H	1.69	0.56
1:A:544:SER:N	1:A:564:TYR:O	2.39	0.56
2:D:412:LYS:HD2	2:D:419:LEU:HD11	1.86	0.56
1:A:345:ILE:HG22	1:A:376:LYS:HD3	1.86	0.56
2:B:521:LEU:HB3	2:B:563:ALA:HB1	1.86	0.55
1:A:410:THR:HG22	1:A:412:LEU:H	1.70	0.55
1:C:544:SER:N	1:C:564:TYR:O	2.39	0.55
1:C:410:THR:HG22	1:C:412:LEU:H	1.70	0.55
1:C:495:ASN:OD1	1:C:496:ARG:N	2.40	0.54
1:A:343:LEU:HD13	1:A:374:SER:HB3	1.89	0.54
2:B:386:ILE:O	2:B:390:PHE:CG	2.60	0.54
1:A:282:SER:HB3	1:A:399:ASP:OD2	2.07	0.54
2:D:377:VAL:HG11	2:D:383:LEU:HD21	1.89	0.54
1:C:274:PHE:HB2	1:C:295:VAL:HB	1.90	0.54
1:C:426:SER:HB2	1:C:427:PRO:HD3	1.90	0.53
1:A:122:LEU:HD22	2:B:274:TYR:CE1	2.43	0.53
1:A:495:ASN:OD1	1:A:496:ARG:N	2.40	0.53
2:B:377:VAL:HG11	2:B:383:LEU:HD21	1.89	0.53
2:B:252:MET:HE3	1:C:367:ASN:OD1	2.08	0.53
1:C:343:LEU:HD13	1:C:374:SER:HB3	1.89	0.53
1:A:251:ASN:ND2	2:B:220:TYR:O	2.41	0.53
1:C:282:SER:HB3	1:C:399:ASP:OD2	2.08	0.53
2:B:252:MET:HA	1:C:443:ASN:HD21	1.75	0.52
1:A:426:SER:HB2	1:A:427:PRO:HD3	1.90	0.52
2:B:250:GLU:OE1	2:B:261:ARG:NH1	2.40	0.52
1:A:274:PHE:HB2	1:A:295:VAL:HB	1.90	0.52
2:B:212:ARG:HG2	2:B:213:GLU:H	1.75	0.52
2:D:212:ARG:HG2	2:D:213:GLU:H	1.75	0.52
1:C:453:SER:OG	1:C:458:THR:HG22	2.10	0.52
2:D:250:GLU:OE1	2:D:261:ARG:NH1	2.40	0.52
1:C:396:ARG:HD2	1:C:427:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:HG13	1:A:188:THR:HG21	1.91	0.51
1:C:180:VAL:HG13	1:C:188:THR:HG21	1.91	0.51
1:A:453:SER:OG	1:A:458:THR:HG22	2.10	0.51
2:B:453:ASN:HB3	2:B:466:LEU:HD11	1.91	0.51
1:A:422:LEU:O	1:A:426:SER:OG	2.28	0.51
1:A:396:ARG:HD2	1:A:427:PRO:HD2	1.91	0.51
1:A:399:ASP:N	1:A:399:ASP:OD1	2.43	0.51
2:D:453:ASN:HB3	2:D:466:LEU:HD11	1.91	0.51
2:B:299:TYR:OH	3:E:1:NAG:C3	2.60	0.49
1:A:130:ARG:O	6:A:803:NAG:H82	2.12	0.49
1:A:183:ASP:OD1	1:A:184:ALA:N	2.45	0.49
1:A:423:ASP:HB2	2:B:108:LYS:HE3	1.94	0.49
1:C:475:GLU:OE2	1:C:569:LYS:NZ	2.38	0.49
1:A:75:LEU:HD13	1:A:510:MET:HE2	1.94	0.49
1:C:183:ASP:OD1	1:C:184:ALA:N	2.45	0.49
1:C:130:ARG:O	6:C:803:NAG:H82	2.13	0.49
2:B:144:HIS:HB2	2:B:170:ARG:HB3	1.95	0.49
1:A:83:ILE:HG13	1:A:84:THR:HG23	1.96	0.48
1:A:122:LEU:CD2	2:B:274:TYR:CZ	2.96	0.48
1:C:175:VAL:HG21	1:C:235:PHE:HD2	1.79	0.48
1:C:541:GLY:HA3	1:C:565:TRP:CE2	2.49	0.48
1:C:75:LEU:HD13	1:C:510:MET:HE2	1.95	0.48
2:D:476:VAL:HG11	2:D:497:VAL:HG21	1.96	0.48
2:B:299:TYR:HH	3:E:1:NAG:HO3	1.57	0.48
2:D:144:HIS:HB2	2:D:170:ARG:HB3	1.95	0.48
1:A:541:GLY:HA3	1:A:565:TRP:CE2	2.49	0.48
1:C:83:ILE:HG13	1:C:84:THR:HG23	1.96	0.48
2:B:476:VAL:HG11	2:B:497:VAL:HG21	1.96	0.47
1:C:422:LEU:O	1:C:426:SER:OG	2.28	0.47
2:D:293:PRO:HB3	5:G:1:NAG:O6	2.14	0.47
1:A:181:ALA:HA	1:A:218:ARG:HH22	1.78	0.47
1:A:475:GLU:OE2	1:A:569:LYS:NZ	2.39	0.47
1:A:442:PHE:CD1	1:A:446:LEU:HD11	2.50	0.47
2:B:386:ILE:HG22	2:B:390:PHE:HE2	1.65	0.47
1:C:181:ALA:HA	1:C:218:ARG:HH22	1.78	0.47
1:C:552:ARG:HG2	1:C:565:TRP:CE2	2.50	0.47
1:C:442:PHE:CD1	1:C:446:LEU:HD11	2.50	0.47
2:D:199:THR:OG1	2:D:200:VAL:N	2.48	0.47
1:A:257:THR:HA	1:C:360:GLU:OE1	2.14	0.46
1:A:552:ARG:HG2	1:A:565:TRP:CE2	2.50	0.46
1:C:399:ASP:N	1:C:399:ASP:OD1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:ASP:OD1	2:B:532:LEU:N	2.48	0.46
2:D:136:ASN:HB3	2:D:139:LYS:O	2.15	0.46
1:A:122:LEU:HD23	2:B:274:TYR:OH	2.13	0.46
1:A:175:VAL:HG21	1:A:235:PHE:HD2	1.79	0.46
2:B:219:GLN:HG2	2:B:220:TYR:CD2	2.51	0.46
1:C:552:ARG:HG2	1:C:565:TRP:CD2	2.51	0.46
2:D:219:GLN:HG2	2:D:220:TYR:CD2	2.51	0.46
2:B:199:THR:OG1	2:B:200:VAL:N	2.48	0.46
1:A:158:GLY:HA3	1:A:180:VAL:O	2.16	0.46
1:A:552:ARG:HG2	1:A:565:TRP:CD2	2.51	0.46
1:A:390:PHE:CD2	1:A:412:LEU:HD12	2.50	0.45
1:C:158:GLY:HA3	1:C:180:VAL:O	2.16	0.45
2:D:351:LYS:HD2	2:D:396:LEU:HD23	1.98	0.45
2:D:531:ASP:OD1	2:D:532:LEU:N	2.48	0.45
1:C:536:ARG:NH2	3:E:4:MAN:O2	2.50	0.45
1:C:411:LYS:HB2	2:D:107:LEU:HD12	1.99	0.45
1:C:390:PHE:CD2	1:C:412:LEU:HD12	2.50	0.45
2:B:351:LYS:HD2	2:B:396:LEU:HD23	1.98	0.45
1:C:247:ARG:HG3	1:C:247:ARG:HH11	1.82	0.45
1:A:292:THR:HG22	1:A:312:VAL:HB	1.97	0.45
1:A:295:VAL:HG22	1:A:309:GLU:HG2	1.98	0.45
2:B:136:ASN:HB3	2:B:139:LYS:O	2.16	0.45
1:C:292:THR:HG22	1:C:312:VAL:HB	1.98	0.45
1:A:122:LEU:CD2	2:B:274:TYR:CE1	3.00	0.45
2:B:119:LEU:HA	2:B:119:LEU:HD23	1.74	0.45
1:C:295:VAL:HG22	1:C:309:GLU:HG2	1.98	0.45
1:A:253:TYR:HE2	2:B:222:LEU:CD1	2.29	0.45
1:C:175:VAL:HG21	1:C:235:PHE:CD2	2.51	0.45
1:C:313:GLU:HB3	1:C:315:ILE:HD11	1.99	0.45
1:A:175:VAL:HG21	1:A:235:PHE:CD2	2.52	0.45
1:A:247:ARG:HH11	1:A:247:ARG:HG3	1.82	0.45
2:D:555:SER:OG	2:D:558:SER:OG	2.34	0.44
1:A:313:GLU:HB3	1:A:315:ILE:HD11	1.99	0.44
2:B:221:ASP:OD1	2:B:223:LYS:HG2	2.18	0.44
2:D:221:ASP:OD1	2:D:223:LYS:HG2	2.18	0.44
6:A:803:NAG:H81	1:C:134:ASP:OD2	2.18	0.44
1:A:178:ALA:HB1	1:A:221:ILE:HD11	2.00	0.43
2:B:135:THR:HB	2:B:180:TYR:O	2.19	0.43
1:C:465:SER:HA	1:C:493:GLU:HG3	2.00	0.43
2:D:121:VAL:HB	2:D:133:CYS:HB2	2.00	0.43
1:C:178:ALA:HB1	1:C:221:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:LEU:HD23	2:D:119:LEU:HA	1.74	0.43
2:B:121:VAL:HB	2:B:133:CYS:HB2	2.00	0.43
1:A:332:LEU:HD11	1:A:350:ASP:HB3	2.00	0.43
1:C:556:GLN:HG3	1:C:558:ASP:H	1.83	0.43
1:A:439:VAL:HB	1:A:480:ALA:HB3	2.01	0.43
2:B:323:THR:HB	2:B:418:ARG:NH1	2.34	0.43
1:C:332:LEU:HD11	1:C:350:ASP:HB3	2.00	0.43
2:D:323:THR:HB	2:D:418:ARG:NH1	2.34	0.43
1:A:381:LYS:HD2	1:A:381:LYS:HA	1.91	0.43
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.83	0.42
1:A:465:SER:HA	1:A:493:GLU:HG3	2.00	0.42
1:C:318:ALA:O	1:C:322:THR:OG1	2.30	0.42
2:B:310:VAL:HG13	2:B:426:PRO:HB3	2.02	0.42
1:C:165:LEU:HD23	1:C:165:LEU:HA	1.83	0.42
2:B:118:TYR:O	2:B:135:THR:HG23	2.20	0.42
2:D:104:LEU:O	2:D:108:LYS:HG3	2.20	0.42
2:B:485:GLU:O	2:B:486:LEU:HD23	2.20	0.42
1:A:412:LEU:HA	1:A:412:LEU:HD23	1.74	0.42
2:B:386:ILE:O	2:B:390:PHE:CD2	2.72	0.42
1:C:439:VAL:HB	1:C:480:ALA:HB3	2.01	0.42
2:D:485:GLU:O	2:D:486:LEU:HD23	2.20	0.42
1:A:556:GLN:HG3	1:A:558:ASP:H	1.83	0.41
2:B:502:SER:O	2:B:503:LEU:HD23	2.20	0.41
2:B:104:LEU:O	2:B:108:LYS:HG3	2.20	0.41
1:C:381:LYS:HD2	1:C:381:LYS:HA	1.91	0.41
2:B:252:MET:CA	1:C:443:ASN:HD21	2.33	0.41
2:D:135:THR:HB	2:D:180:TYR:O	2.19	0.41
2:D:321:VAL:HG23	2:D:422:ILE:HB	2.01	0.41
1:A:251:ASN:ND2	2:B:220:TYR:HB3	2.35	0.41
2:B:177:LEU:HD22	2:B:195:LEU:HD23	2.03	0.41
2:B:299:TYR:OH	3:E:1:NAG:H3	2.20	0.41
2:D:78:VAL:HG21	2:D:80:TYR:CZ	2.56	0.41
2:D:409:LEU:HB3	2:D:453:ASN:OD1	2.21	0.41
2:D:502:SER:O	2:D:503:LEU:HD23	2.20	0.41
1:A:561:ASP:OD1	1:A:561:ASP:N	2.52	0.41
2:B:312:SER:OG	2:B:437:ASP:OD2	2.34	0.41
2:B:78:VAL:HG21	2:B:80:TYR:CZ	2.56	0.41
2:B:252:MET:HE1	1:C:367:ASN:OD1	2.18	0.41
2:D:118:TYR:O	2:D:135:THR:HG23	2.20	0.41
2:B:196:TYR:CE2	2:B:212:ARG:HD3	2.56	0.41
1:C:106:GLU:OE2	6:C:801:NAG:O7	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:HIS:CE1	1:C:175:VAL:HG12	2.56	0.41
2:D:177:LEU:HD22	2:D:195:LEU:HD23	2.03	0.41
1:A:173:HIS:CE1	1:A:175:VAL:HG12	2.56	0.40
1:A:106:GLU:OE2	6:A:801:NAG:O7	2.39	0.40
2:D:310:VAL:HG13	2:D:426:PRO:HB3	2.01	0.40
1:A:555:CYS:SG	1:A:565:TRP:HD1	2.44	0.40
2:B:321:VAL:HG23	2:B:422:ILE:HB	2.01	0.40
1:C:555:CYS:SG	1:C:565:TRP:HD1	2.44	0.40

All (37) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:VAL:O	2:D:414:ASN:OD1[8_665]	1.13	1.07
2:D:549:THR:CG2	2:D:551:THR:CB[10_555]	1.13	1.07
2:B:414:ASN:CB	2:D:327:ASN:CB[8_665]	1.32	0.88
2:B:327:ASN:CB	2:D:414:ASN:CB[8_665]	1.36	0.84
1:A:391:ASN:ND2	2:D:514:ILE:CD1[8_665]	1.39	0.81
1:A:145:ALA:O	1:C:147:SER:OG[6_554]	1.43	0.77
2:B:414:ASN:CA	2:D:327:ASN:CB[8_665]	1.45	0.75
2:D:549:THR:CG2	2:D:551:THR:OG1[10_555]	1.55	0.65
2:B:414:ASN:OD1	2:D:326:VAL:O[8_665]	1.55	0.65
2:D:549:THR:CB	2:D:551:THR:OG1[10_555]	1.57	0.63
2:D:549:THR:CB	2:D:551:THR:CB[10_555]	1.59	0.61
2:B:57:SER:OG	2:D:57:SER:OG[8_665]	1.65	0.55
2:B:326:VAL:C	2:D:414:ASN:OD1[8_665]	1.65	0.55
1:A:144:ARG:CD	1:C:144:ARG:CD[6_554]	1.68	0.52
2:D:549:THR:OG1	2:D:551:THR:OG1[10_555]	1.70	0.50
2:B:414:ASN:CG	2:D:327:ASN:CB[8_665]	1.74	0.46
1:A:145:ALA:O	1:C:147:SER:CB[6_554]	1.80	0.40
1:A:147:SER:OG	1:C:145:ALA:O[6_554]	1.80	0.40
2:B:327:ASN:CB	2:D:414:ASN:CA[8_665]	1.82	0.38
2:B:414:ASN:OD1	2:D:327:ASN:CB[8_665]	1.83	0.37
2:B:327:ASN:CB	2:D:414:ASN:CG[8_665]	1.84	0.36
2:B:414:ASN:CB	2:D:327:ASN:CG[8_665]	1.85	0.35
2:D:549:THR:CB	2:D:551:THR:CG2[10_555]	1.86	0.34
2:B:414:ASN:OD1	2:D:327:ASN:CA[8_665]	1.91	0.29
1:A:384:GLN:OE1	2:D:569:HIS:O[8_665]	1.92	0.28
2:B:327:ASN:CA	2:D:414:ASN:OD1[8_665]	1.93	0.27
2:B:414:ASN:CB	2:D:327:ASN:ND2[8_665]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ASN:N	2:D:414:ASN:OD1[8_665]	1.94	0.26
2:B:326:VAL:O	2:D:414:ASN:CG[8_665]	1.95	0.25
2:B:327:ASN:OD1	2:D:329:ILE:CG2[8_665]	1.96	0.24
1:A:145:ALA:C	1:C:147:SER:OG[6_554]	1.98	0.22
2:B:327:ASN:CB	2:D:414:ASN:OD1[8_665]	2.01	0.19
2:B:414:ASN:OD1	2:D:327:ASN:C[8_665]	2.01	0.19
2:B:330:PRO:CG	2:D:327:ASN:N[8_665]	2.11	0.09
2:B:330:PRO:CD	2:D:328:ALA:N[8_665]	2.13	0.07
2:B:414:ASN:OD1	2:D:326:VAL:C[8_665]	2.16	0.04
2:B:327:ASN:N	2:D:330:PRO:CG[8_665]	2.19	0.01

### 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	507/715 (71%)	485 (96%)	22 (4%)	0	100	100
1	C	510/715 (71%)	487 (96%)	23 (4%)	0	100	100
2	B	470/578 (81%)	449 (96%)	21 (4%)	0	100	100
2	D	463/578 (80%)	443 (96%)	20 (4%)	0	100	100
All	All	1950/2586 (75%)	1864 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

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	451/633 (71%)	449 (100%)	2 (0%)	91	94
1	C	452/633 (71%)	450 (100%)	2 (0%)	91	94
2	B	416/502 (83%)	416 (100%)	0	100	100
2	D	413/502 (82%)	413 (100%)	0	100	100
All	All	1732/2270 (76%)	1728 (100%)	4 (0%)	93	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	ILE
1	A	371	CYS
1	C	297	ILE
1	C	371	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
2	B	394	HIS
1	C	278	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 ⓘ

17 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	$\# Z  > 2$
3	NAG	E	1	3,2	14,14,15	0.36	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	0.49	0
3	BMA	E	3	3	11,11,12	0.38	0	15,15,17	1.23	3 (20%)
3	MAN	E	4	3	11,11,12	0.27	0	15,15,17	1.13	1 (6%)
4	NAG	F	1	2,4	14,14,15	0.31	0	17,19,21	0.50	0
4	NAG	F	2	4	14,14,15	0.36	0	17,19,21	0.51	0
4	BMA	F	3	4	11,11,12	0.83	0	15,15,17	0.75	0
5	NAG	G	1	2,5	14,14,15	0.36	0	17,19,21	0.48	0
5	NAG	G	2	5	14,14,15	0.29	0	17,19,21	0.49	0
5	BMA	G	3	5	11,11,12	0.38	0	15,15,17	2.32	4 (26%)
5	MAN	G	4	5	11,11,12	1.01	1 (9%)	15,15,17	1.05	2 (13%)
5	MAN	G	5	5	11,11,12	0.26	0	15,15,17	0.73	0
5	NAG	H	1	2,5	14,14,15	0.30	0	17,19,21	0.51	0
5	NAG	H	2	5	14,14,15	0.36	0	17,19,21	0.49	0
5	BMA	H	3	5	11,11,12	0.83	0	15,15,17	0.77	0
5	MAN	H	4	5	11,11,12	0.97	1 (9%)	15,15,17	1.22	2 (13%)
5	MAN	H	5	5	11,11,12	0.82	0	15,15,17	1.08	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	1/2/19/22	0/1/1/1
4	NAG	F	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
5	NAG	H	1	2,5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	4	MAN	C1-C2	2.54	1.58	1.52
5	G	4	MAN	O5-C5	2.00	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	C1-C2-C3	-6.90	101.19	109.67
5	H	4	MAN	C1-O5-C5	3.44	116.85	112.19
3	E	4	MAN	O5-C1-C2	-3.07	106.03	110.77
5	H	5	MAN	C1-O5-C5	3.07	116.35	112.19
5	G	3	BMA	O3-C3-C4	2.99	117.26	110.35
5	G	3	BMA	O3-C3-C2	2.82	115.40	109.99
5	G	4	MAN	C1-O5-C5	2.54	115.63	112.19
5	G	3	BMA	C2-C3-C4	-2.34	106.84	110.89
3	E	3	BMA	C1-O5-C5	2.34	115.36	112.19
3	E	3	BMA	O3-C3-C4	2.32	115.72	110.35
5	H	4	MAN	O2-C2-C3	-2.18	105.76	110.14
3	E	3	BMA	O5-C1-C2	-2.08	107.56	110.77
5	G	4	MAN	O2-C2-C3	-2.08	105.98	110.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	1	NAG	C1

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7
5	H	1	NAG	C1-C2-N2-C7
5	H	3	BMA	C4-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
5	G	5	MAN	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6

There are no ring outliers.

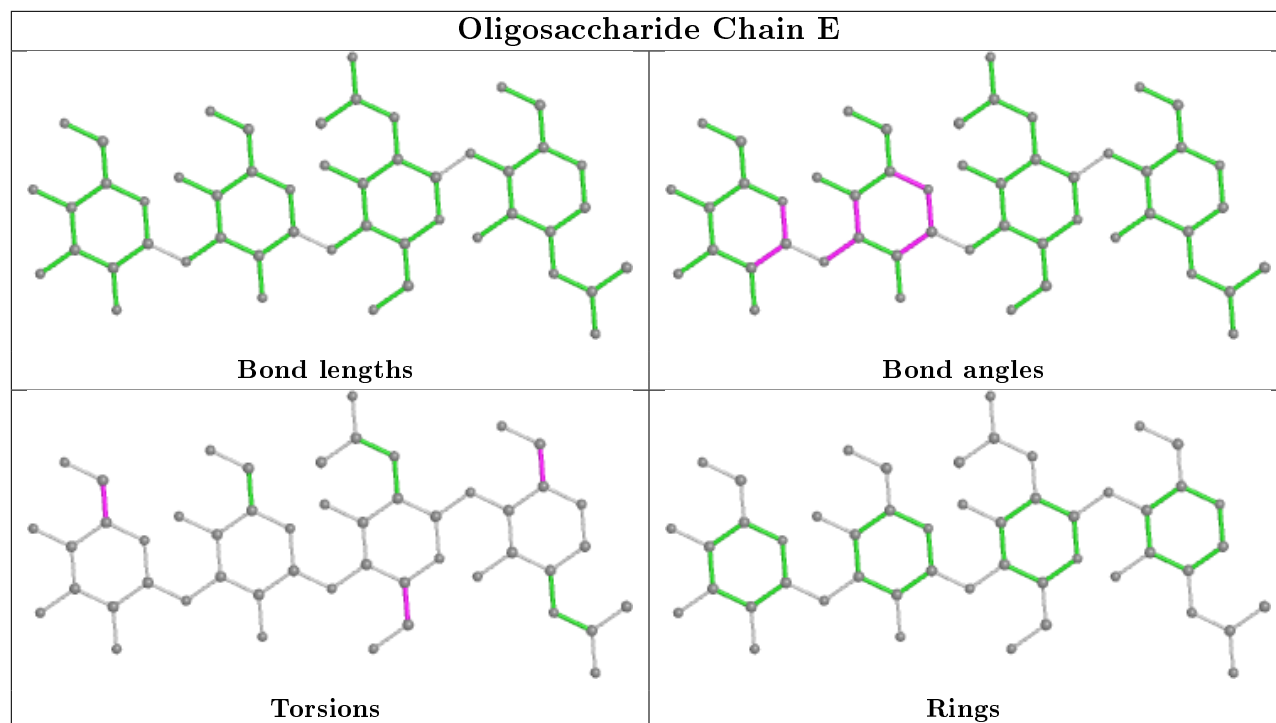
5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	5	0
5	G	1	NAG	6	0
3	E	1	NAG	4	0
5	G	2	NAG	9	0
3	E	4	MAN	1	0

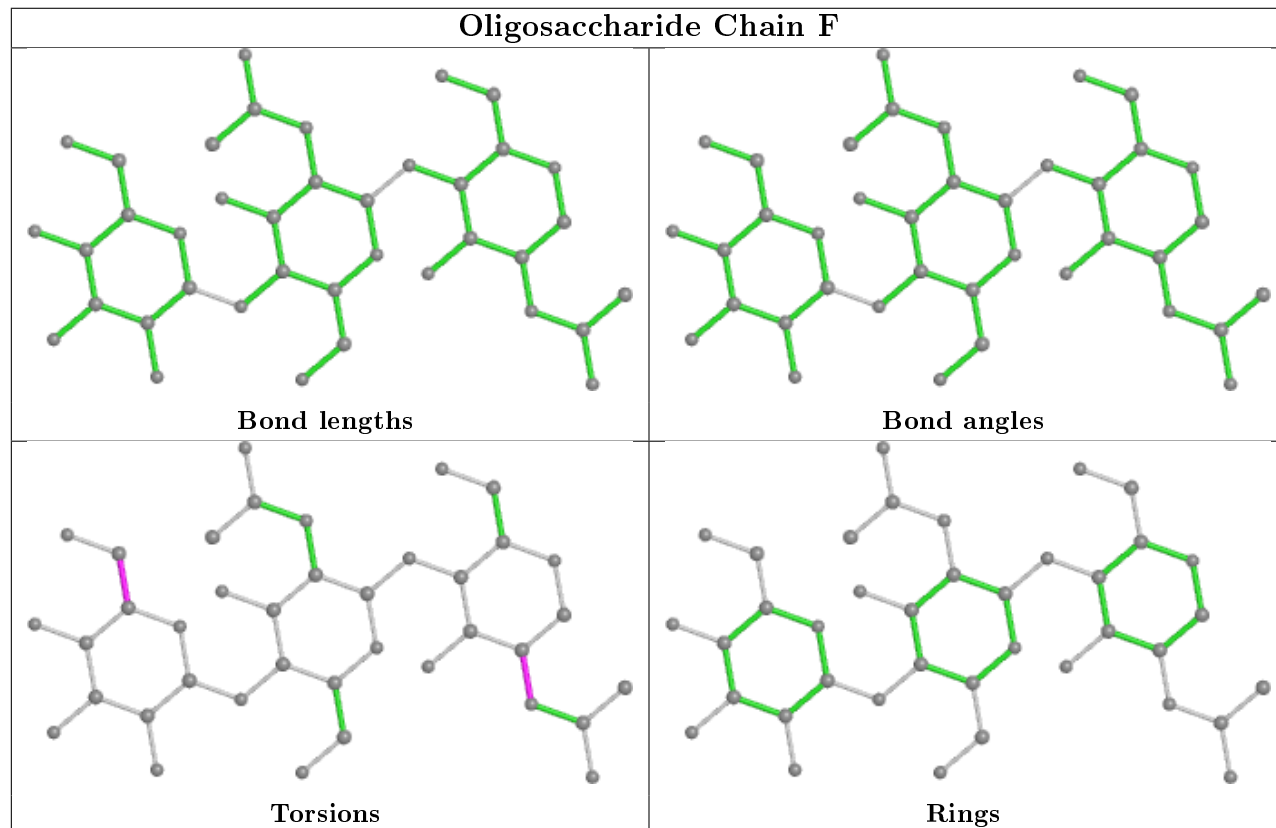
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

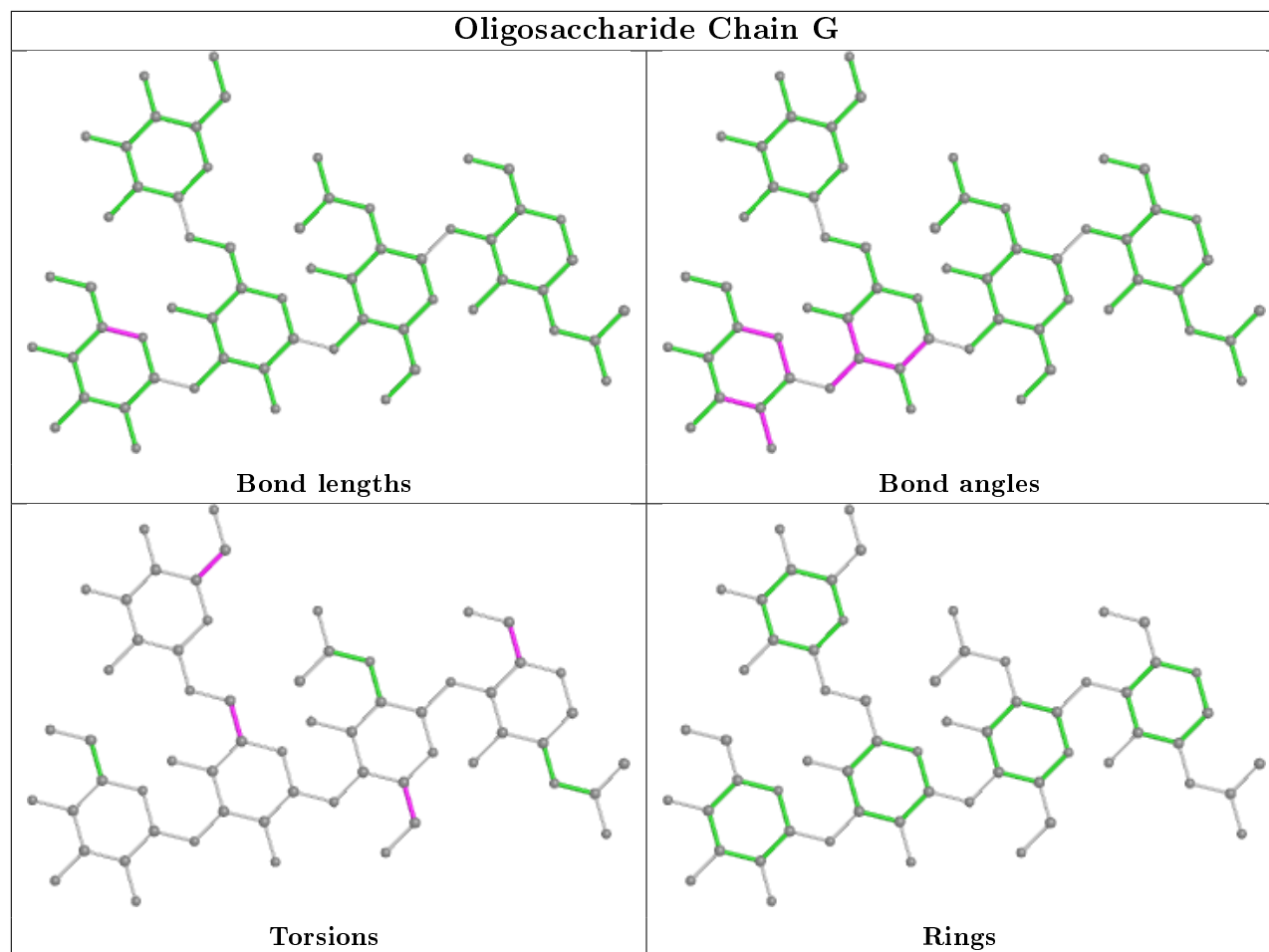


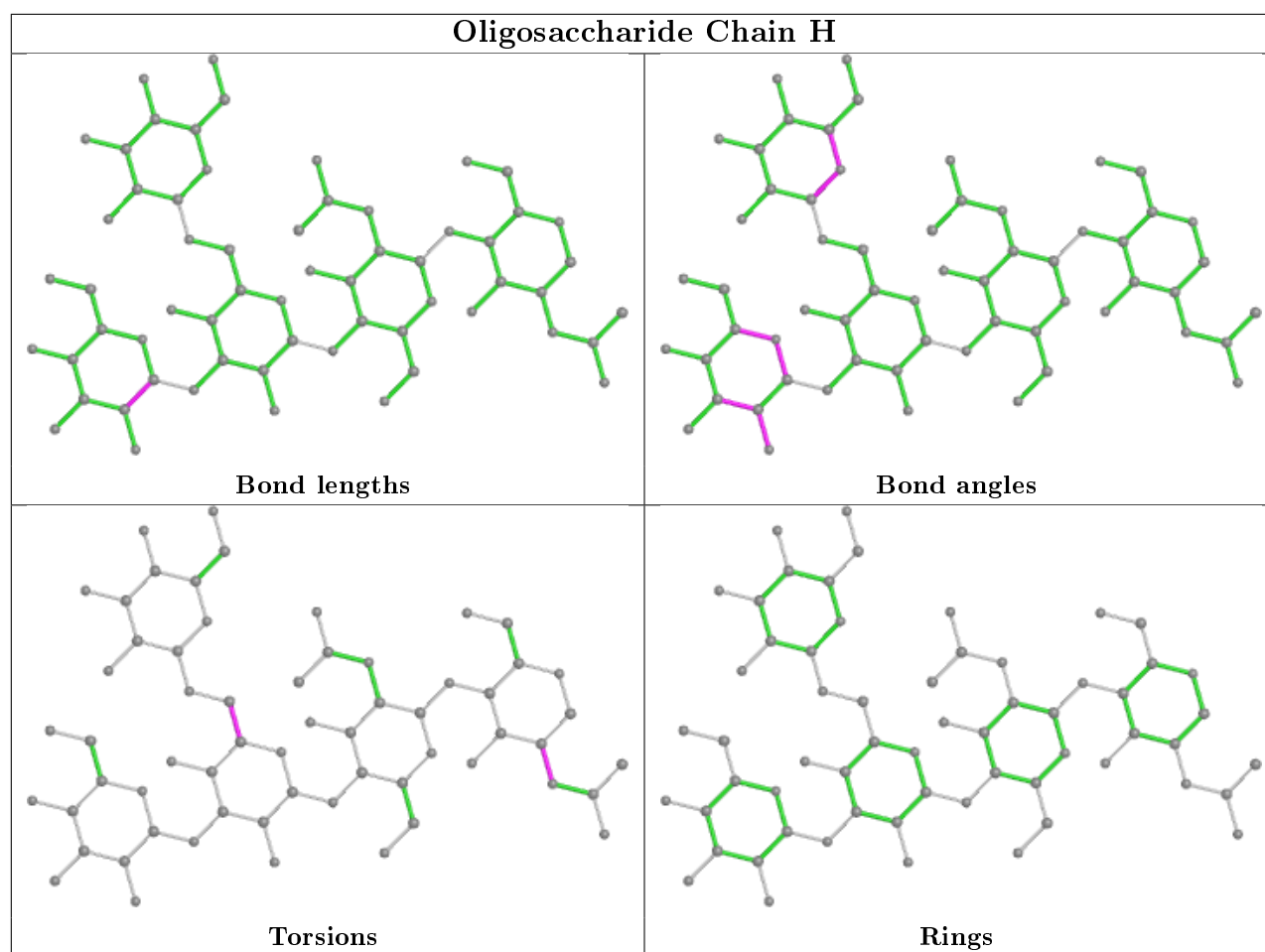
## Oligosaccharide Chain E



## Oligosaccharide Chain F







## 5.6 Ligand geometry [i](#)

6 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$
6	NAG	C	803	1	14,14,15	0.61	1 (7%)	17,19,21	0.44	0
6	NAG	A	803	1	14,14,15	0.64	1 (7%)	17,19,21	0.44	0
6	NAG	A	802	1	14,14,15	0.23	0	17,19,21	0.58	0
6	NAG	C	802	1	14,14,15	0.21	0	17,19,21	0.59	0
6	NAG	A	801	1	14,14,15	0.22	0	17,19,21	0.78	0
6	NAG	C	801	1	14,14,15	0.22	0	17,19,21	0.78	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
6	NAG	C	803	1	-	4/6/23/26	0/1/1/1
6	NAG	A	803	1	-	4/6/23/26	0/1/1/1
6	NAG	A	802	1	-	2/6/23/26	0/1/1/1
6	NAG	C	802	1	-	2/6/23/26	0/1/1/1
6	NAG	A	801	1	-	1/6/23/26	0/1/1/1
6	NAG	C	801	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	803	NAG	C1-C2	2.16	1.55	1.52
6	C	803	NAG	C1-C2	2.06	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	803	NAG	C1-C2-N2-C7
6	A	803	NAG	C1-C2-N2-C7
6	A	801	NAG	C3-C2-N2-C7
6	C	801	NAG	C3-C2-N2-C7
6	A	803	NAG	C4-C5-C6-O6
6	C	803	NAG	C4-C5-C6-O6
6	A	802	NAG	C4-C5-C6-O6
6	C	802	NAG	C4-C5-C6-O6
6	A	803	NAG	O5-C5-C6-O6
6	C	803	NAG	O5-C5-C6-O6
6	C	802	NAG	O5-C5-C6-O6
6	A	802	NAG	O5-C5-C6-O6
6	C	803	NAG	C3-C2-N2-C7
6	A	803	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	803	NAG	1	0
6	A	803	NAG	6	0
6	A	801	NAG	1	0
6	C	801	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

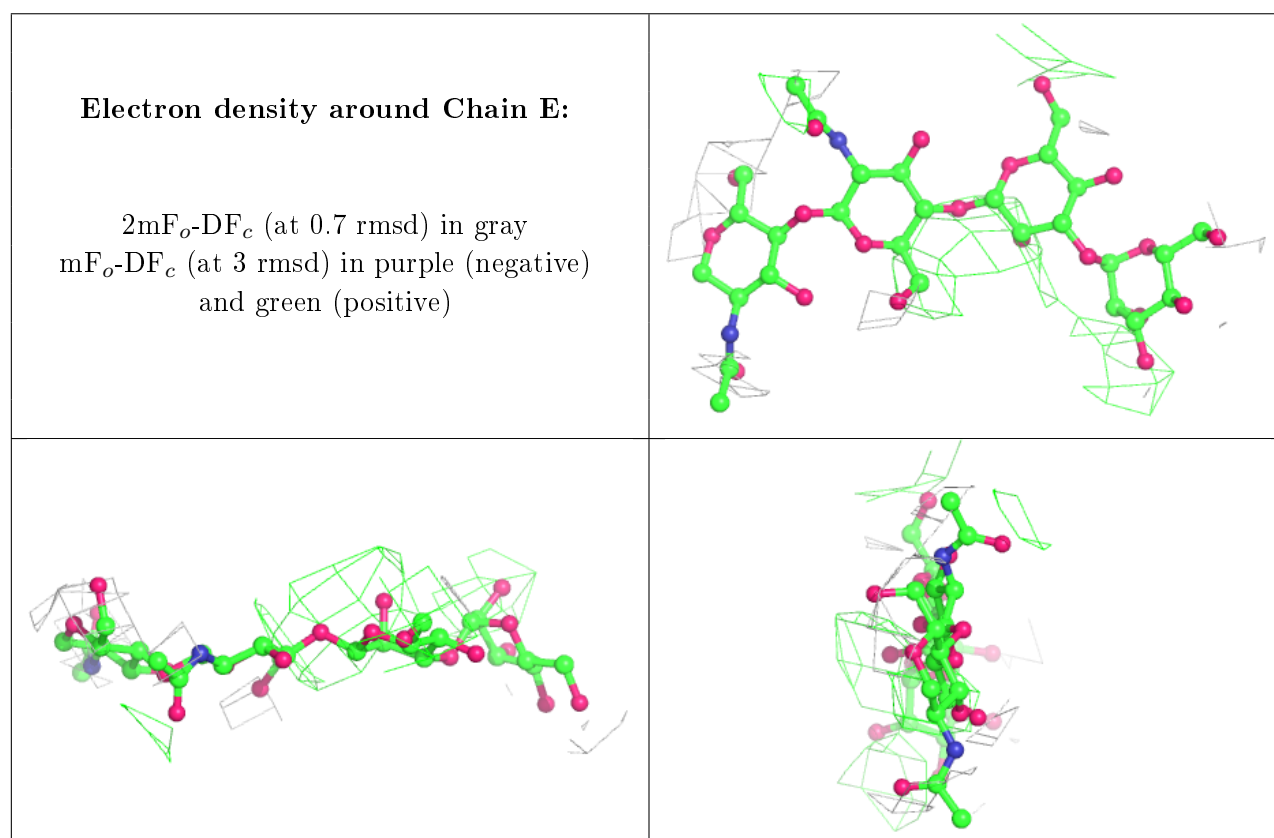
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

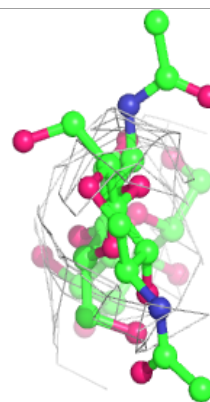
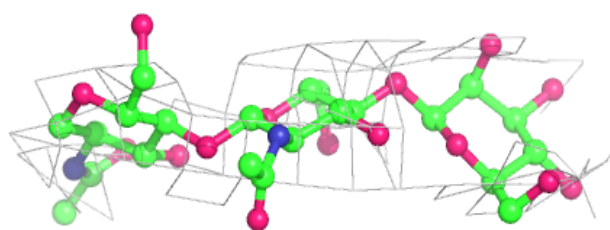
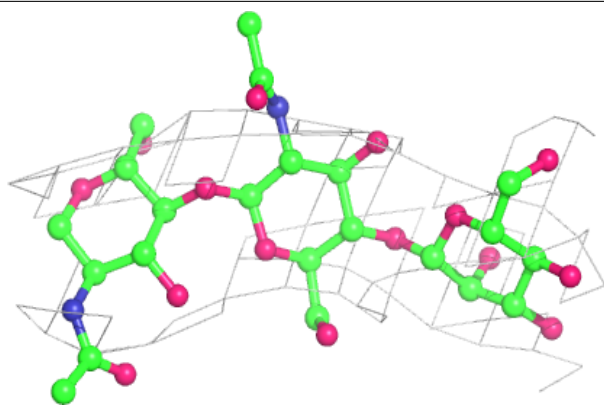
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

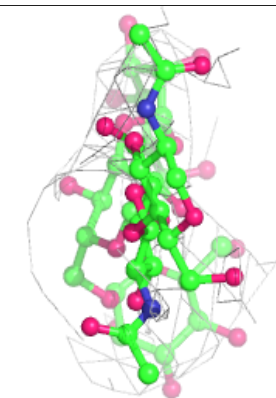
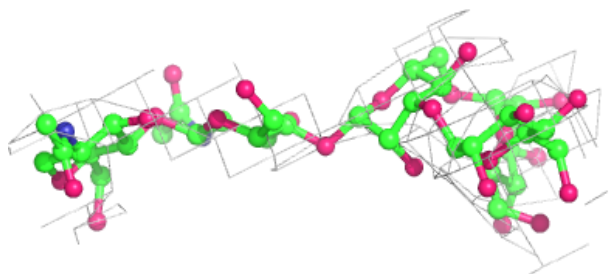
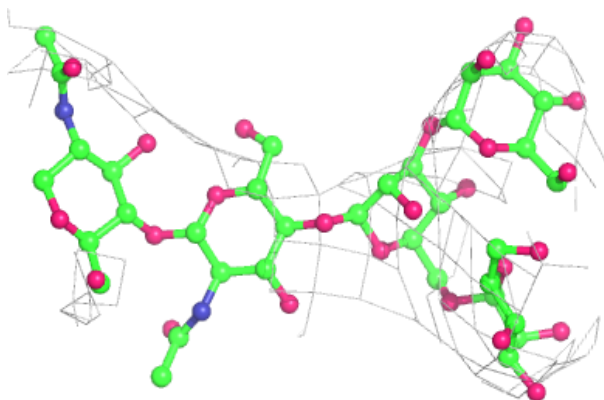


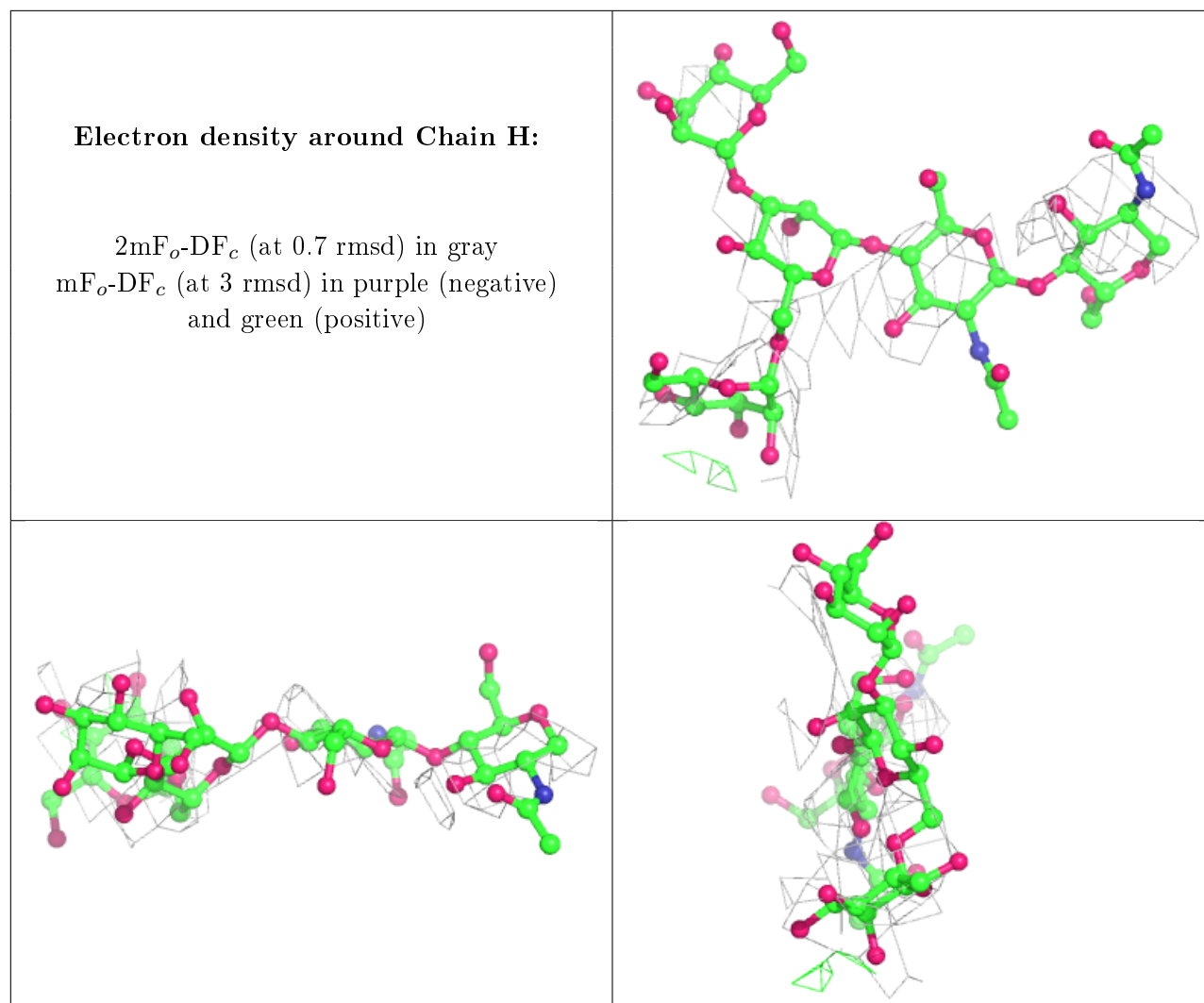
**Electron density around Chain F:**

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

**Electron density around Chain G:**

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





## 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.