



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 09:43 PM EDT

PDB ID : 2GYS  
Title : 2.7 Å structure of the extracellular domains of the human beta common receptor involved in IL-3, IL-5, and GM-CSF signalling  
Authors : Carr, P.D.; Conlan, F.; Ford, S.; Ollis, D.L.; Young, I.G.  
Deposited on : 2006-05-09  
Resolution : 2.70 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.

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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

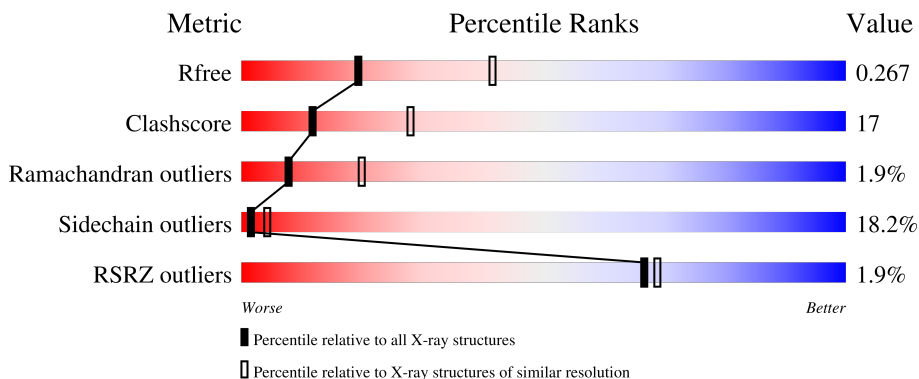
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	419	
1	B	419	
2	C	4	
2	E	4	
3	D	3	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	3	 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
2	NAG	C	1	X	-	-	-
2	FUC	E	4	-	-	-	X
3	NAG	F	1	X	-	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6454 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.

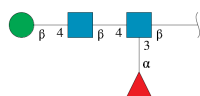
- Molecule 1 is a protein called Cytokine receptor common beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	3098	1953	551	578	16	0	0	0
1	B	406	3182	1995	575	595	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

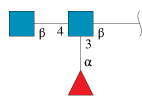
Chain	Residue	Modelled	Actual	Comment	Reference
A	328	GLN	ASN	engineered mutation	GB 47678387
B	328	GLN	ASN	engineered mutation	GB 47678387

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	4	49	28	2	19	0	0	0
2	E	4	49	28	2	19	0	0	0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.

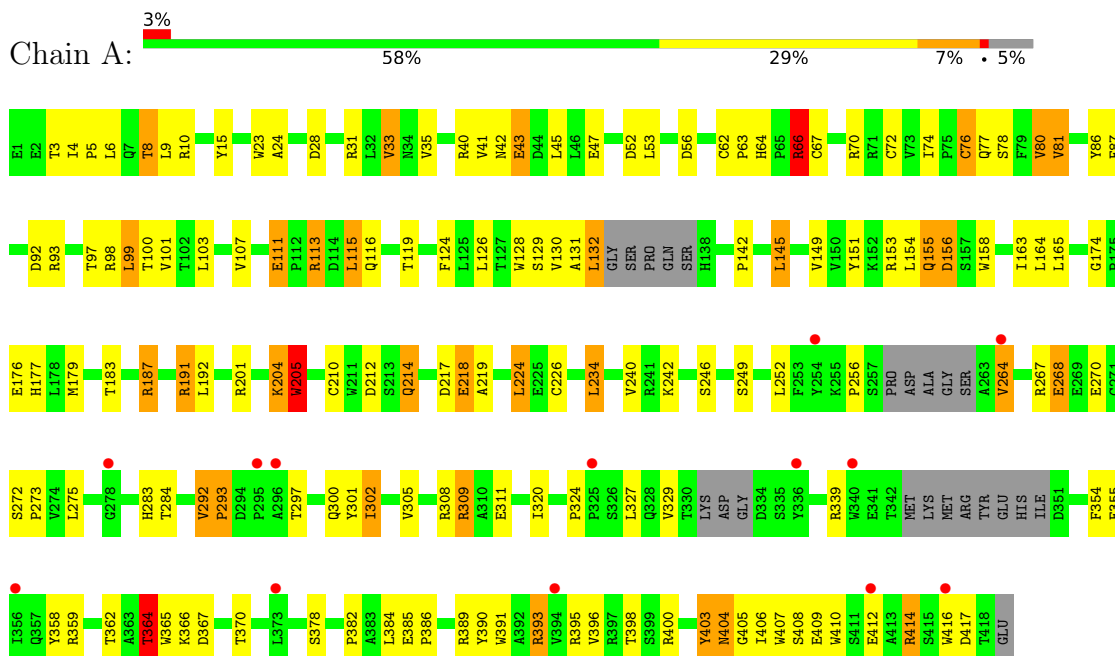


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	3	38	22	2	14	0	0	0
3	F	3	38	22	2	14	0	0	0

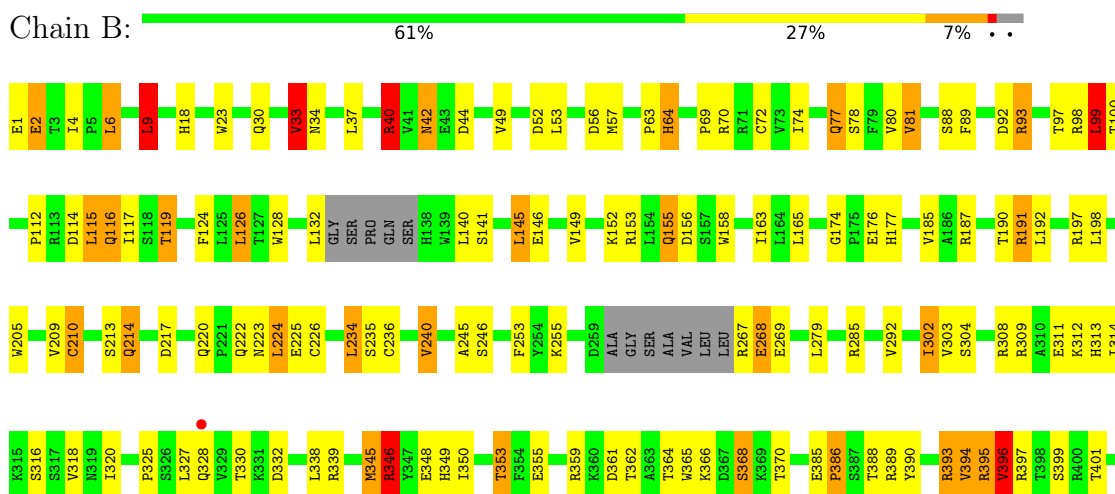
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cytokine receptor common beta chain



- Molecule 1: Cytokine receptor common beta chain





## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.91Å 184.91Å 101.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 46.23 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.4 (50.00-2.70) 91.4 (46.23-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.212 , 0.269 0.209 , 0.267	Depositor DCC
$R_{free}$ test set	1392 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtrriage
Anisotropy	0.310	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, FUC

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	0.97	5/3185 (0.2%)	1.02	9/4364 (0.2%)
1	B	0.95	3/3273 (0.1%)	1.02	10/4481 (0.2%)
All	All	0.96	8/6458 (0.1%)	1.02	19/8845 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	CYS	CB-SG	-7.39	1.69	1.82
1	A	80	VAL	CB-CG2	7.13	1.67	1.52
1	A	62	CYS	CB-SG	7.10	1.94	1.82
1	A	210	CYS	CB-SG	-6.57	1.71	1.82
1	A	205	TRP	CG-CD1	6.33	1.45	1.36
1	A	264	VAL	C-O	6.30	1.35	1.23
1	B	409	GLU	CG-CD	5.77	1.60	1.51
1	B	312	LYS	CE-NZ	5.58	1.62	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	VAL	CB-CA-C	-8.22	95.78	111.40

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	VAL	CB-CA-C	-7.58	96.99	111.40
1	A	10	ARG	CG-CD-NE	-6.64	97.85	111.80
1	A	66	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	40	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	308	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	396	VAL	CB-CA-C	-5.91	100.18	111.40
1	A	6	LEU	CB-CG-CD2	-5.84	101.07	111.00
1	B	33	VAL	CB-CA-C	-5.80	100.37	111.40
1	A	67	CYS	CA-CB-SG	-5.66	103.82	114.00
1	A	66	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	156	ASP	CB-CG-OD1	5.59	123.34	118.30
1	B	401	THR	C-N-CA	-5.43	110.89	122.30
1	A	164	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	80	VAL	CG1-CB-CG2	5.23	119.26	110.90
1	B	9	LEU	CA-CB-CG	5.12	127.07	115.30
1	B	99	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	346	ARG	CG-CD-NE	-5.08	101.13	111.80
1	B	126	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	76	CYS	Peptide
1	B	18	HIS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3098	0	2866	110	0
1	B	3182	0	2953	116	0
2	C	49	0	43	3	0
2	E	49	0	43	1	0
3	D	38	0	34	1	0
3	F	38	0	34	3	0
All	All	6454	0	5973	216	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 17.

All (216) 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:191:ARG:HG2	1:B:191:ARG:HH11	1.08	1.16
1:B:214:GLN:H	1:B:214:GLN:NE2	1.61	0.98
1:B:348:GLU:HG2	1:B:350:ILE:HD12	1.48	0.94
1:B:155:GLN:HE21	1:B:155:GLN:H	0.94	0.92
1:B:174:GLY:H	1:B:177:HIS:HD2	1.12	0.91
1:A:309:ARG:CZ	1:B:40:ARG:HH22	1.85	0.90
1:A:309:ARG:HG3	1:A:309:ARG:HH11	1.38	0.87
1:B:9:LEU:HD23	1:B:23:TRP:HB3	1.57	0.87
1:B:155:GLN:H	1:B:155:GLN:NE2	1.73	0.86
1:A:393:ARG:HG3	1:A:410:TRP:CE3	2.12	0.85
1:B:155:GLN:HE21	1:B:155:GLN:N	1.76	0.84
1:A:40:ARG:NH1	1:B:311:GLU:OE2	2.11	0.83
1:B:174:GLY:H	1:B:177:HIS:CD2	1.95	0.83
1:B:404:ASN:HD22	1:B:405:GLY:N	1.76	0.82
1:B:404:ASN:ND2	1:B:405:GLY:H	1.77	0.82
3:F:2:FUC:H5	3:F:3:NAG:H61	1.63	0.81
1:B:191:ARG:HG2	1:B:191:ARG:NH1	1.84	0.80
1:A:8:THR:HG21	1:A:24:ALA:H	1.47	0.79
1:B:404:ASN:HD22	1:B:405:GLY:H	1.27	0.78
1:B:415:SER:O	1:B:416:TRP:HB3	1.85	0.77
1:A:354:PHE:CD1	1:A:396:VAL:CG1	2.69	0.75
1:B:395:ARG:HG2	1:B:410:TRP:CZ3	2.22	0.75
1:B:214:GLN:H	1:B:214:GLN:HE21	1.33	0.74
2:C:2:NAG:O5	2:C:4:FUC:H4	1.87	0.74
1:B:395:ARG:HG2	1:B:410:TRP:CE3	2.24	0.73
2:E:2:NAG:H82	2:E:4:FUC:H5	1.72	0.72
1:A:115:LEU:HD22	1:A:126:LEU:HD11	1.71	0.71
1:A:309:ARG:HH11	1:A:309:ARG:CG	2.04	0.71
1:B:325:PRO:HG3	1:B:396:VAL:HG22	1.69	0.71
1:A:354:PHE:CE1	1:A:396:VAL:HG11	2.26	0.70
1:A:8:THR:HG23	1:A:23:TRP:HA	1.71	0.70
1:A:272:SER:HB2	1:A:273:PRO:HA	1.76	0.68
1:B:115:LEU:CD2	1:B:126:LEU:HD11	2.23	0.67
1:B:345:MET:O	1:B:346:ARG:C	2.30	0.67
1:A:64:HIS:HD2	1:A:66:ARG:H	1.43	0.67
1:A:92:ASP:OD1	1:A:93:ARG:HG2	1.93	0.67
1:B:191:ARG:HH11	1:B:191:ARG:CG	1.98	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ARG:HG3	1:A:410:TRP:CD2	2.30	0.67
1:A:246:SER:HB2	1:B:4:ILE:HD12	1.76	0.66
1:A:364:THR:OG1	1:A:365:TRP:N	2.28	0.66
1:A:113:ARG:HD3	1:A:129:SER:O	1.95	0.66
1:A:309:ARG:CZ	1:B:40:ARG:NH2	2.56	0.66
1:B:225:GLU:O	1:B:236:CYS:HA	1.95	0.65
1:B:348:GLU:CG	1:B:350:ILE:HD12	2.24	0.65
1:B:395:ARG:CG	1:B:410:TRP:CZ3	2.80	0.65
1:A:111:GLU:HG3	1:A:204:LYS:HG3	1.78	0.65
1:A:393:ARG:CG	1:A:410:TRP:CE3	2.80	0.65
1:B:209:VAL:HG22	1:B:210:CYS:N	2.12	0.65
1:B:325:PRO:HG3	1:B:396:VAL:CG2	2.27	0.65
1:A:412:GLU:OE1	1:A:414:ARG:NH2	2.30	0.64
1:A:80:VAL:HG22	1:A:81:VAL:H	1.63	0.63
1:B:92:ASP:OD1	1:B:93:ARG:HG2	1.98	0.63
1:B:348:GLU:HG2	1:B:350:ILE:CD1	2.27	0.63
1:B:397:ARG:HG2	1:B:407:TRP:CZ3	2.34	0.63
1:B:361:ASP:HB2	1:B:389:ARG:HB3	1.81	0.63
1:A:64:HIS:CD2	1:A:66:ARG:H	2.17	0.62
1:A:8:THR:HG21	1:A:24:ALA:N	2.15	0.62
1:B:152:LYS:HD3	1:B:158:TRP:CE3	2.35	0.62
1:A:155:GLN:H	1:A:155:GLN:HE21	1.48	0.61
1:A:309:ARG:HG3	1:A:309:ARG:NH1	2.05	0.61
1:A:320:ILE:O	1:A:405:GLY:HA3	1.99	0.61
1:B:115:LEU:HD22	1:B:126:LEU:HD11	1.83	0.61
1:B:209:VAL:HG22	1:B:210:CYS:H	1.66	0.61
1:A:224:LEU:HD13	1:B:99:LEU:HB2	1.83	0.61
1:A:4:ILE:O	1:A:8:THR:HB	2.03	0.59
1:A:365:TRP:C	1:A:367:ASP:H	2.05	0.59
1:A:42:ASN:O	1:A:43:GLU:C	2.40	0.59
1:B:213:SER:HB2	1:B:214:GLN:NE2	2.17	0.59
1:B:267:ARG:O	1:B:268:GLU:HB3	2.02	0.58
1:B:285:ARG:HG3	1:B:285:ARG:HH11	1.67	0.58
1:B:404:ASN:ND2	1:B:405:GLY:N	2.45	0.58
1:A:355:GLU:HG3	1:A:407:TRP:CH2	2.39	0.58
1:B:158:TRP:CH2	1:B:187:ARG:HG2	2.39	0.58
1:B:353:THR:HG23	1:B:399:SER:HB3	1.86	0.57
1:B:255:LYS:HB3	1:B:268:GLU:HA	1.85	0.57
1:A:77:GLN:H	1:A:77:GLN:CD	2.07	0.57
1:A:115:LEU:HD23	1:A:128:TRP:HB3	1.87	0.57
1:A:217:ASP:O	1:A:219:ALA:N	2.37	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:NH1	1:B:40:ARG:HH22	2.02	0.57
1:A:5:PRO:O	1:A:8:THR:HG22	2.04	0.56
1:A:187:ARG:HD2	1:A:205:TRP:CD1	2.39	0.56
1:A:354:PHE:CE1	1:A:396:VAL:CG1	2.87	0.56
1:A:99:LEU:HB2	1:B:224:LEU:HD13	1.87	0.56
1:B:214:GLN:H	1:B:214:GLN:CD	2.09	0.56
1:B:165:LEU:HD21	1:B:191:ARG:NH2	2.21	0.55
1:B:393:ARG:HD3	1:B:410:TRP:CE3	2.41	0.55
1:A:142:PRO:O	1:A:145:LEU:HB2	2.07	0.54
1:B:285:ARG:HG3	1:B:285:ARG:NH1	2.22	0.54
1:B:330:THR:HG21	1:B:339:ARG:HH11	1.73	0.54
1:B:37:LEU:HD23	1:B:49:VAL:HG11	1.88	0.54
1:A:187:ARG:CD	1:A:205:TRP:CG	2.91	0.54
1:B:6:LEU:HD13	1:B:89:PHE:CE1	2.42	0.54
1:A:309:ARG:NH1	1:B:40:ARG:NH2	2.55	0.54
1:B:327:LEU:HD12	1:B:414:ARG:HB2	1.89	0.54
1:B:253:PHE:HA	1:B:269:GLU:O	2.08	0.54
1:A:302:ILE:CD1	1:B:98:ARG:HB2	2.38	0.53
1:A:365:TRP:CH2	1:A:393:ARG:HD2	2.43	0.53
1:B:365:TRP:CH2	1:B:393:ARG:HG2	2.44	0.53
1:B:240:VAL:CG2	1:B:245:ALA:HB2	2.39	0.53
1:A:187:ARG:HD2	1:A:205:TRP:CG	2.44	0.52
1:B:23:TRP:CZ2	1:B:70:ARG:HG3	2.44	0.52
1:B:217:ASP:HB3	1:B:220:GLN:HG2	1.91	0.52
1:B:240:VAL:HG21	1:B:245:ALA:HB2	1.91	0.52
1:A:404:ASN:HD22	1:A:405:GLY:H	1.55	0.52
1:B:42:ASN:HD22	1:B:44:ASP:H	1.57	0.52
1:B:132:LEU:HD22	1:B:140:LEU:HD23	1.92	0.52
1:A:8:THR:CG2	1:A:24:ALA:H	2.20	0.52
1:A:389:ARG:HA	1:A:417:ASP:HA	1.92	0.51
1:A:395:ARG:HG2	1:A:410:TRP:CZ3	2.45	0.51
1:B:30:GLN:HA	1:B:33:VAL:O	2.10	0.50
1:B:77:GLN:H	1:B:77:GLN:NE2	2.09	0.50
1:B:63:PRO:O	1:B:64:HIS:HB2	2.11	0.50
1:A:214:GLN:H	1:A:214:GLN:NE2	2.10	0.50
1:B:226:CYS:HA	1:B:235:SER:O	2.10	0.50
1:A:103:LEU:O	1:A:107:VAL:HG12	2.12	0.49
1:A:3:THR:HB	1:B:246:SER:O	2.13	0.49
1:A:403:TYR:CD1	1:A:403:TYR:N	2.81	0.49
1:A:183:THR:OG1	1:A:212:ASP:OD1	2.29	0.49
1:A:256:PRO:HB3	1:A:301:TYR:CZ	2.48	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ASN:ND2	1:A:405:GLY:H	2.11	0.49
1:B:23:TRP:CE2	1:B:70:ARG:HG3	2.49	0.48
1:A:174:GLY:H	1:A:177:HIS:CD2	2.31	0.48
1:A:292:VAL:HA	1:A:293:PRO:HD3	1.74	0.48
1:B:77:GLN:H	1:B:77:GLN:HE21	1.60	0.48
1:A:153:ARG:HD3	1:A:179:MET:HE3	1.96	0.48
1:B:146:GLU:OE2	1:B:191:ARG:NH1	2.47	0.47
1:B:115:LEU:HD21	1:B:126:LEU:HD11	1.94	0.47
1:A:359:ARG:HD2	1:A:365:TRP:CH2	2.50	0.47
1:A:384:LEU:HB3	1:A:390:TYR:HE2	1.78	0.47
1:B:119:THR:HB	1:B:124:PHE:CE1	2.49	0.47
1:B:115:LEU:HD22	1:B:126:LEU:CD1	2.44	0.47
3:F:1:NAG:O7	3:F:2:FUC:O2	2.30	0.47
1:A:158:TRP:CH2	1:A:187:ARG:HG2	2.50	0.47
1:B:320:ILE:O	1:B:405:GLY:HA3	2.14	0.47
1:A:242:LYS:HE3	1:A:283:HIS:O	2.14	0.47
1:B:115:LEU:CD2	1:B:126:LEU:CD1	2.93	0.47
1:A:41:VAL:HG11	1:A:45:LEU:HD23	1.97	0.47
1:A:113:ARG:CZ	1:A:131:ALA:HB2	2.45	0.47
1:B:112:PRO:HB3	1:B:128:TRP:CD1	2.50	0.47
1:A:155:GLN:H	1:A:155:GLN:NE2	2.11	0.46
1:A:174:GLY:H	1:A:177:HIS:HD2	1.64	0.46
1:B:145:LEU:HG	1:B:190:THR:CG2	2.46	0.46
1:B:187:ARG:HD2	1:B:205:TRP:CD2	2.51	0.46
1:A:358:TYR:HA	1:A:391:TRP:O	2.16	0.46
1:A:155:GLN:HE21	1:A:155:GLN:N	2.12	0.46
1:A:267:ARG:HG2	1:A:268:GLU:N	2.30	0.46
1:B:6:LEU:HD13	1:B:89:PHE:HE1	1.79	0.46
1:B:395:ARG:HG3	1:B:410:TRP:CZ3	2.50	0.46
1:A:165:LEU:HD21	1:A:191:ARG:HH21	1.80	0.46
1:B:1:GLU:O	1:B:2:GLU:CB	2.63	0.46
1:A:217:ASP:O	1:A:218:GLU:C	2.54	0.46
1:A:324:PRO:HG3	1:A:409:GLU:HB2	1.97	0.46
1:B:359:ARG:HD2	1:B:365:TRP:CE2	2.51	0.46
3:F:1:NAG:H61	3:F:3:NAG:O7	2.16	0.46
1:B:1:GLU:O	1:B:2:GLU:HB3	2.17	0.45
1:B:152:LYS:HG3	1:B:153:ARG:O	2.17	0.45
1:A:77:GLN:OE1	1:A:77:GLN:N	2.23	0.45
1:A:187:ARG:HD3	1:A:205:TRP:CG	2.51	0.45
1:B:209:VAL:CG2	1:B:210:CYS:N	2.80	0.45
1:A:119:THR:HG22	1:A:124:PHE:CD2	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:HG3	1:B:302:ILE:CD1	2.46	0.44
1:A:359:ARG:HD3	1:A:391:TRP:HB2	1.99	0.44
1:B:292:VAL:O	1:B:292:VAL:CG2	2.65	0.44
1:A:87:PHE:CD2	1:B:314:ILE:HD12	2.53	0.44
1:A:87:PHE:O	1:B:311:GLU:HA	2.18	0.44
1:B:98:ARG:HE	1:B:98:ARG:HB3	1.63	0.44
1:A:64:HIS:HD2	1:A:66:ARG:N	2.13	0.44
1:A:365:TRP:C	1:A:367:ASP:N	2.71	0.44
1:B:327:LEU:HD22	1:B:339:ARG:O	2.18	0.44
1:B:355:GLU:OE1	1:B:395:ARG:NH1	2.51	0.44
1:B:57:MET:HG2	1:B:69:PRO:HB3	1.99	0.43
1:A:365:TRP:O	1:A:367:ASP:N	2.51	0.43
1:B:279:LEU:HD22	1:B:285:ARG:HD3	2.00	0.43
1:A:115:LEU:HD22	1:A:126:LEU:CD1	2.43	0.43
1:B:349:HIS:O	1:B:350:ILE:HG13	2.19	0.43
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.77	0.43
1:A:302:ILE:HD11	1:B:98:ARG:HB2	2.01	0.43
1:A:153:ARG:HB2	1:A:156:ASP:OD2	2.19	0.43
1:A:31:ARG:O	2:C:1:NAG:H83	2.19	0.42
1:A:385:GLU:HA	1:A:386:PRO:HD3	1.80	0.42
1:A:226:CYS:HB3	1:A:234:LEU:HD22	2.00	0.42
1:A:113:ARG:NH2	1:A:131:ALA:HB2	2.34	0.42
1:B:116:GLN:HG3	1:B:117:ILE:N	2.33	0.42
1:B:412:GLU:OE1	1:B:414:ARG:NH1	2.53	0.42
1:A:98:ARG:NH1	1:B:302:ILE:HD11	2.35	0.42
1:A:311:GLU:OE2	1:B:40:ARG:NH1	2.52	0.42
1:B:174:GLY:N	1:B:177:HIS:HD2	1.96	0.42
1:B:365:TRP:O	1:B:368:SER:HB2	2.20	0.42
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.57	0.42
1:A:252:LEU:HD12	1:A:305:VAL:HG22	2.01	0.42
1:B:385:GLU:HA	1:B:386:PRO:HD2	1.69	0.42
1:B:388:THR:HB	1:B:390:TYR:CE1	2.55	0.42
1:A:8:THR:HG23	1:A:23:TRP:CA	2.46	0.42
1:A:86:TYR:HD1	1:B:313:HIS:ND1	2.18	0.42
3:D:2:FUC:H3	3:D:3:NAG:H62	2.02	0.42
1:A:107:VAL:HG22	1:A:192:LEU:HD21	2.02	0.42
1:B:325:PRO:HD3	1:B:396:VAL:HG23	2.02	0.41
1:B:365:TRP:O	1:B:366:LYS:C	2.58	0.41
1:A:80:VAL:HG22	1:A:81:VAL:HG22	2.02	0.41
1:B:153:ARG:HB3	1:B:155:GLN:NE2	2.36	0.41
1:A:354:PHE:CD1	1:A:396:VAL:HG12	2.50	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:CD	1:A:205:TRP:CD1	3.03	0.41
1:A:242:LYS:HG2	1:A:284:THR:HG23	2.03	0.41
1:A:400:ARG:NH1	1:A:403:TYR:OH	2.54	0.41
1:B:395:ARG:HD3	1:B:407:TRP:CE3	2.56	0.41
1:A:270:GLU:OE2	1:A:308:ARG:HD2	2.21	0.41
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.71	0.41
1:A:52:ASP:OD1	1:A:52:ASP:N	2.52	0.40
1:A:151:TYR:OH	1:A:177:HIS:HB3	2.20	0.40
1:A:390:TYR:HB2	1:A:416:TRP:CZ2	2.56	0.40
1:B:30:GLN:HG2	1:B:34:ASN:OD1	2.21	0.40
1:A:116:GLN:O	1:A:126:LEU:HA	2.21	0.40
1:B:370:THR:HG23	1:B:370:THR:O	2.22	0.40
1:A:23:TRP:CZ2	1:A:70:ARG:HG3	2.56	0.40
1:B:153:ARG:HB2	1:B:156:ASP:OD2	2.21	0.40
2:C:4:FUC:H2	2:C:4:FUC:H63	2.04	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	387/419 (92%)	356 (92%)	23 (6%)	8 (2%)	7	18
1	B	400/419 (96%)	363 (91%)	30 (8%)	7 (2%)	8	21
All	All	787/838 (94%)	719 (91%)	53 (7%)	15 (2%)	8	20

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	VAL
1	B	2	GLU
1	B	386	PRO

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	218	GLU
1	A	366	LYS
1	B	64	HIS
1	B	332	ASP
1	B	346	ARG
1	A	364	THR
1	B	268	GLU
1	A	63	PRO
1	A	382	PRO
1	A	78	SER
1	A	293	PRO
1	B	81	VAL

### 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	327/379 (86%)	266 (81%)	61 (19%)	1	4
1	B	339/379 (89%)	279 (82%)	60 (18%)	2	4
All	All	666/758 (88%)	545 (82%)	121 (18%)	1	4

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	9	LEU
1	A	15	TYR
1	A	28	ASP
1	A	33	VAL
1	A	35	VAL
1	A	43	GLU
1	A	47	GLU
1	A	53	LEU
1	A	56	ASP
1	A	66	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	72	CYS
1	A	74	ILE
1	A	76	CYS
1	A	81	VAL
1	A	97	THR
1	A	99	LEU
1	A	100	THR
1	A	101	VAL
1	A	111	GLU
1	A	113	ARG
1	A	115	LEU
1	A	130	VAL
1	A	132	LEU
1	A	145	LEU
1	A	149	VAL
1	A	154	LEU
1	A	155	GLN
1	A	163	ILE
1	A	176	GLU
1	A	187	ARG
1	A	191	ARG
1	A	201	ARG
1	A	204	LYS
1	A	205	TRP
1	A	214	GLN
1	A	224	LEU
1	A	234	LEU
1	A	240	VAL
1	A	249	SER
1	A	268	GLU
1	A	275	LEU
1	A	292	VAL
1	A	297	THR
1	A	300	GLN
1	A	302	ILE
1	A	309	ARG
1	A	327	LEU
1	A	329	VAL
1	A	339	ARG
1	A	362	THR
1	A	364	THR
1	A	370	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	378	SER
1	A	393	ARG
1	A	398	THR
1	A	403	TYR
1	A	404	ASN
1	A	406	ILE
1	A	408	SER
1	A	414	ARG
1	B	6	LEU
1	B	9	LEU
1	B	33	VAL
1	B	40	ARG
1	B	42	ASN
1	B	52	ASP
1	B	53	LEU
1	B	56	ASP
1	B	72	CYS
1	B	74	ILE
1	B	77	GLN
1	B	78	SER
1	B	80	VAL
1	B	81	VAL
1	B	88	SER
1	B	93	ARG
1	B	97	THR
1	B	99	LEU
1	B	100	THR
1	B	114	ASP
1	B	115	LEU
1	B	116	GLN
1	B	119	THR
1	B	141	SER
1	B	145	LEU
1	B	149	VAL
1	B	155	GLN
1	B	163	ILE
1	B	176	GLU
1	B	185	VAL
1	B	191	ARG
1	B	192	LEU
1	B	197	ARG
1	B	198	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	214	GLN
1	B	222	GLN
1	B	223	ASN
1	B	224	LEU
1	B	234	LEU
1	B	240	VAL
1	B	302	ILE
1	B	303	VAL
1	B	304	SER
1	B	309	ARG
1	B	316	SER
1	B	318	VAL
1	B	328	GLN
1	B	338	LEU
1	B	345	MET
1	B	353	THR
1	B	362	THR
1	B	364	THR
1	B	368	SER
1	B	393	ARG
1	B	394	VAL
1	B	395	ARG
1	B	396	VAL
1	B	404	ASN
1	B	414	ARG
1	B	418	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	30	GLN
1	A	64	HIS
1	A	105	GLN
1	A	155	GLN
1	A	177	HIS
1	A	214	GLN
1	A	283	HIS
1	A	287	HIS
1	A	289	GLN
1	A	319	ASN
1	A	374	GLN
1	A	404	ASN

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	B	18	HIS
1	B	42	ASN
1	B	64	HIS
1	B	77	GLN
1	B	155	GLN
1	B	177	HIS
1	B	214	GLN
1	B	223	ASN
1	B	287	HIS
1	B	289	GLN
1	B	319	ASN
1	B	328	GLN
1	B	404	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

14 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	C	1	2,1	14,14,15	0.74	0	17,19,21	2.30	4 (23%)
2	NAG	C	2	2	14,14,15	0.80	1 (7%)	17,19,21	2.35	4 (23%)
2	BMA	C	3	2	11,11,12	0.90	0	15,15,17	1.72	3 (20%)
2	FUC	C	4	2	10,10,11	1.40	1 (10%)	14,14,16	2.09	8 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	D	1	3,1	14,14,15	0.73	0	17,19,21	2.33	7 (41%)
3	FUC	D	2	3	10,10,11	0.94	0	14,14,16	1.25	1 (7%)
3	NAG	D	3	3	14,14,15	1.03	1 (7%)	17,19,21	2.69	6 (35%)
2	NAG	E	1	2,1	14,14,15	0.59	0	17,19,21	2.10	6 (35%)
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.31	2 (11%)
2	BMA	E	3	2	11,11,12	1.22	2 (18%)	15,15,17	2.28	4 (26%)
2	FUC	E	4	2	10,10,11	1.18	1 (10%)	14,14,16	3.23	7 (50%)
3	NAG	F	1	3,1	14,14,15	1.43	2 (14%)	17,19,21	3.41	8 (47%)
3	FUC	F	2	3	10,10,11	1.17	2 (20%)	14,14,16	2.17	4 (28%)
3	NAG	F	3	3	14,14,15	0.91	1 (7%)	17,19,21	2.44	6 (35%)

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	C	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
3	NAG	D	3	3	-	4/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	FUC	E	4	2	-	-	0/1/1/1
3	NAG	F	1	3,1	1/1/5/7	3/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
3	NAG	F	3	3	-	3/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C1-C2	3.45	1.57	1.52
3	D	3	NAG	C1-C2	3.00	1.56	1.52
2	E	3	BMA	C2-C3	2.89	1.56	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	FUC	C2-C3	2.74	1.56	1.52
3	F	1	NAG	C3-C2	2.30	1.57	1.52
3	F	2	FUC	C1-C2	2.30	1.57	1.52
2	C	2	NAG	O5-C1	-2.26	1.40	1.43
2	E	4	FUC	C4-C5	2.22	1.57	1.52
2	E	3	BMA	C1-C2	2.14	1.57	1.52
3	F	3	NAG	C1-C2	2.10	1.55	1.52
3	F	2	FUC	C2-C3	2.09	1.55	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-O5-C5	8.32	123.47	112.19
3	F	1	NAG	C2-N2-C7	8.15	134.51	122.90
2	E	4	FUC	C1-C2-C3	-7.17	100.85	109.67
2	C	1	NAG	O5-C1-C2	-7.04	100.17	111.29
2	C	2	NAG	C2-N2-C7	-6.89	113.10	122.90
3	D	3	NAG	C1-O5-C5	6.69	121.25	112.19
2	E	3	BMA	C1-C2-C3	6.64	117.83	109.67
3	F	3	NAG	C4-C3-C2	6.20	120.10	111.02
2	E	1	NAG	O5-C5-C6	5.35	115.59	107.20
3	F	1	NAG	O3-C3-C2	4.87	119.55	109.47
3	F	2	FUC	O5-C1-C2	4.78	118.16	110.77
2	E	4	FUC	C1-O5-C5	4.72	123.48	112.78
3	D	3	NAG	O5-C1-C2	4.68	118.67	111.29
3	D	1	NAG	O5-C5-C6	4.53	114.30	107.20
2	C	2	NAG	C4-C3-C2	4.48	117.59	111.02
3	F	3	NAG	C1-O5-C5	4.43	118.19	112.19
2	C	3	BMA	C1-C2-C3	-4.29	104.39	109.67
3	D	1	NAG	O5-C5-C4	-4.25	100.50	110.83
3	D	3	NAG	C4-C3-C2	-4.06	105.07	111.02
2	E	4	FUC	O2-C2-C3	3.90	117.95	110.14
3	F	2	FUC	C1-O5-C5	3.81	121.42	112.78
2	E	4	FUC	O5-C5-C4	3.64	116.05	109.52
2	E	1	NAG	C2-N2-C7	3.63	128.07	122.90
2	E	4	FUC	O3-C3-C2	3.57	116.84	109.99
3	D	1	NAG	O5-C1-C2	3.56	116.91	111.29
3	F	3	NAG	C3-C4-C5	3.53	116.54	110.24
2	C	4	FUC	C3-C4-C5	3.29	114.90	109.77
3	F	2	FUC	C1-C2-C3	3.21	113.61	109.67
3	F	1	NAG	O5-C5-C6	3.11	112.08	107.20
2	E	4	FUC	O3-C3-C4	3.10	117.53	110.35

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C5-C6	3.07	112.02	107.20
3	D	1	NAG	O4-C4-C5	3.00	116.76	109.30
3	D	1	NAG	C3-C4-C5	-2.96	104.96	110.24
2	E	2	NAG	C4-C3-C2	2.96	115.35	111.02
3	F	3	NAG	C8-C7-N2	2.92	121.05	116.10
3	D	3	NAG	C3-C4-C5	-2.90	105.07	110.24
2	E	1	NAG	C1-O5-C5	2.79	115.97	112.19
3	D	1	NAG	C6-C5-C4	2.75	119.44	113.00
2	E	3	BMA	O5-C1-C2	2.73	114.98	110.77
2	E	4	FUC	C2-C3-C4	-2.72	106.19	110.89
2	C	1	NAG	O7-C7-C8	-2.69	117.05	122.06
2	E	3	BMA	C2-C3-C4	2.68	115.53	110.89
3	D	3	NAG	O5-C5-C6	2.66	111.37	107.20
3	D	2	FUC	C3-C4-C5	2.66	113.91	109.77
3	D	3	NAG	C2-N2-C7	2.63	126.64	122.90
2	C	4	FUC	O4-C4-C3	2.60	116.36	110.35
2	C	1	NAG	O5-C5-C4	-2.58	104.56	110.83
2	C	4	FUC	C1-O5-C5	2.57	118.60	112.78
2	E	2	NAG	C1-O5-C5	-2.54	108.74	112.19
3	F	1	NAG	O4-C4-C3	2.53	116.21	110.35
2	C	4	FUC	O2-C2-C3	2.53	115.20	110.14
2	C	2	NAG	C3-C4-C5	2.48	114.66	110.24
3	D	1	NAG	C2-N2-C7	2.47	126.42	122.90
2	C	3	BMA	O3-C3-C4	2.47	116.06	110.35
2	C	4	FUC	O5-C5-C6	2.46	112.62	107.33
3	F	3	NAG	O7-C7-C8	-2.44	117.53	122.06
2	C	3	BMA	C1-O5-C5	-2.42	108.91	112.19
3	F	1	NAG	O7-C7-N2	2.34	126.26	121.95
3	F	2	FUC	O2-C2-C1	2.33	113.92	109.15
2	E	1	NAG	O7-C7-C8	-2.32	117.75	122.06
2	C	4	FUC	O3-C3-C2	2.29	114.38	109.99
2	E	1	NAG	C1-C2-N2	2.26	114.35	110.49
2	C	4	FUC	C6-C5-C4	2.24	117.21	113.07
3	F	1	NAG	O5-C5-C4	2.19	116.16	110.83
3	F	3	NAG	C2-N2-C7	2.19	126.02	122.90
3	F	1	NAG	O7-C7-C8	-2.13	118.11	122.06
2	E	1	NAG	O7-C7-N2	2.08	125.78	121.95
2	E	3	BMA	O5-C5-C6	2.07	110.45	107.20
2	C	4	FUC	O4-C4-C5	2.04	114.18	109.67
2	C	2	NAG	O4-C4-C3	-2.01	105.71	110.35

All (2) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
2	C	1	NAG	C1
3	F	1	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C3-C2-N2-C7
3	F	3	NAG	C8-C7-N2-C2
3	F	3	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	3	NAG	O5-C5-C6-O6
3	D	3	NAG	C4-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	D	3	NAG	C8-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	D	3	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	F	3	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 8 short contacts:

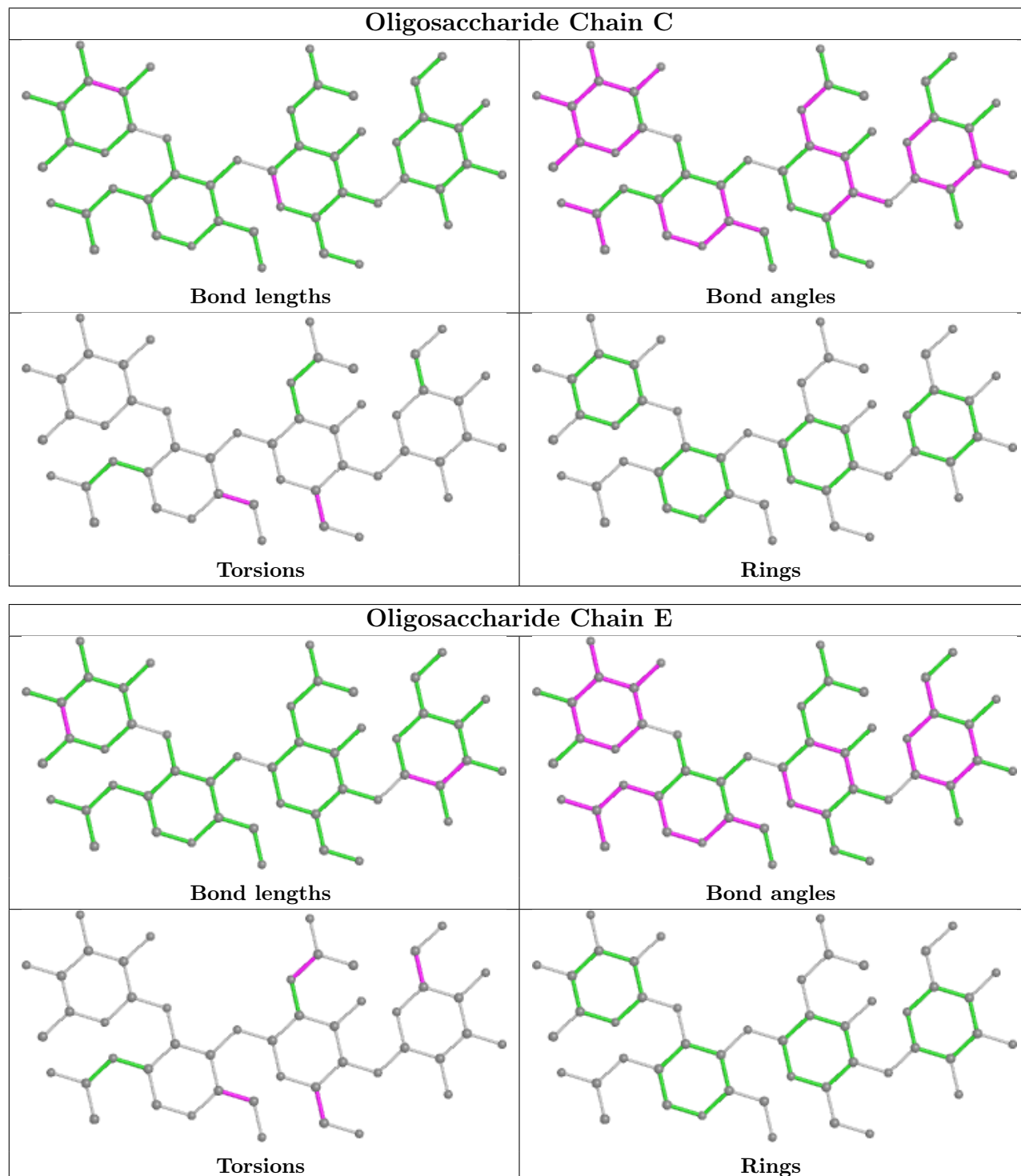
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	FUC	2	0
2	E	4	FUC	1	0
3	D	2	FUC	1	0
2	C	2	NAG	1	0
2	E	2	NAG	1	0
3	F	2	FUC	2	0
3	F	3	NAG	2	0
3	D	3	NAG	1	0

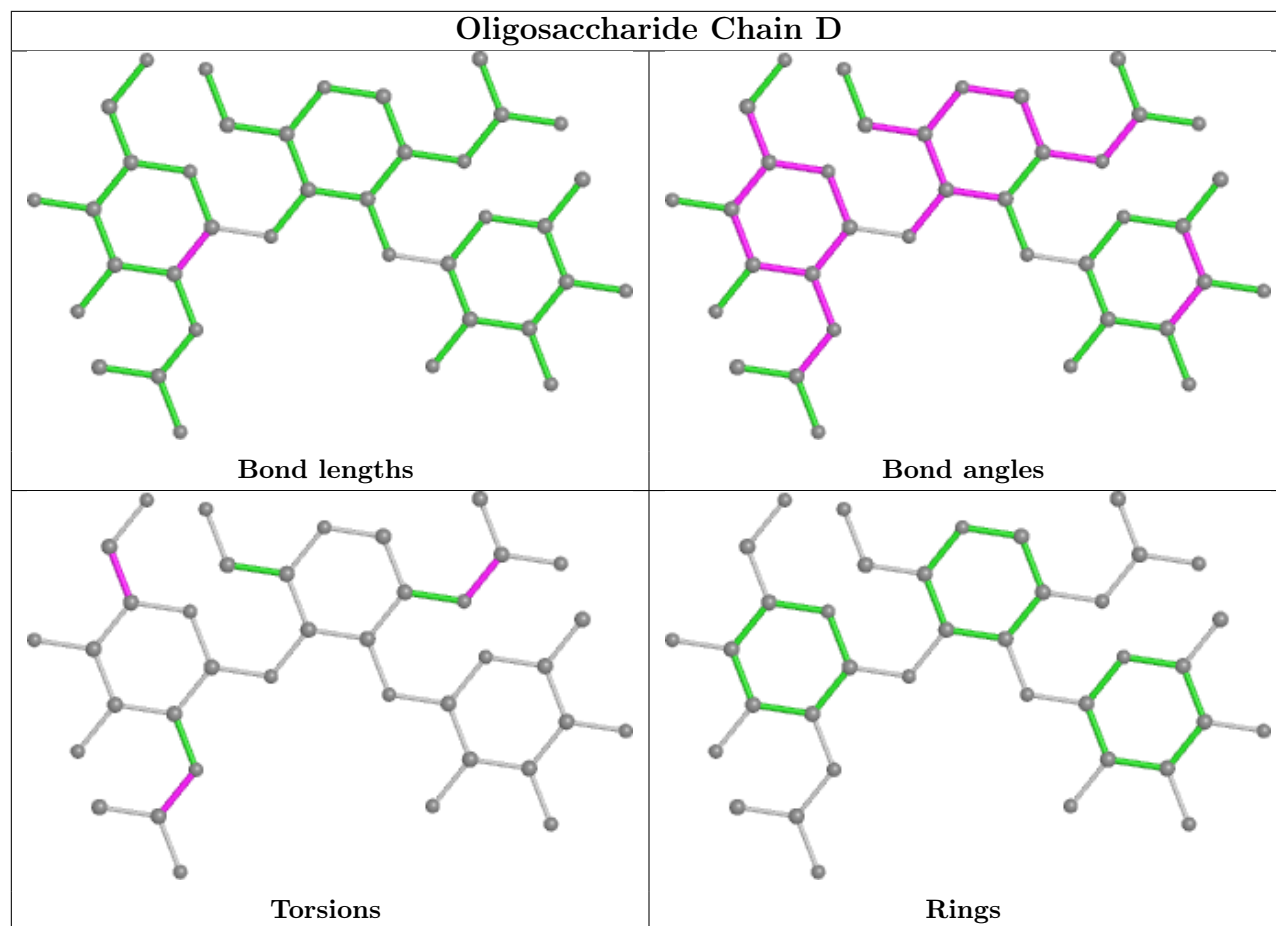
*Continued on next page...*

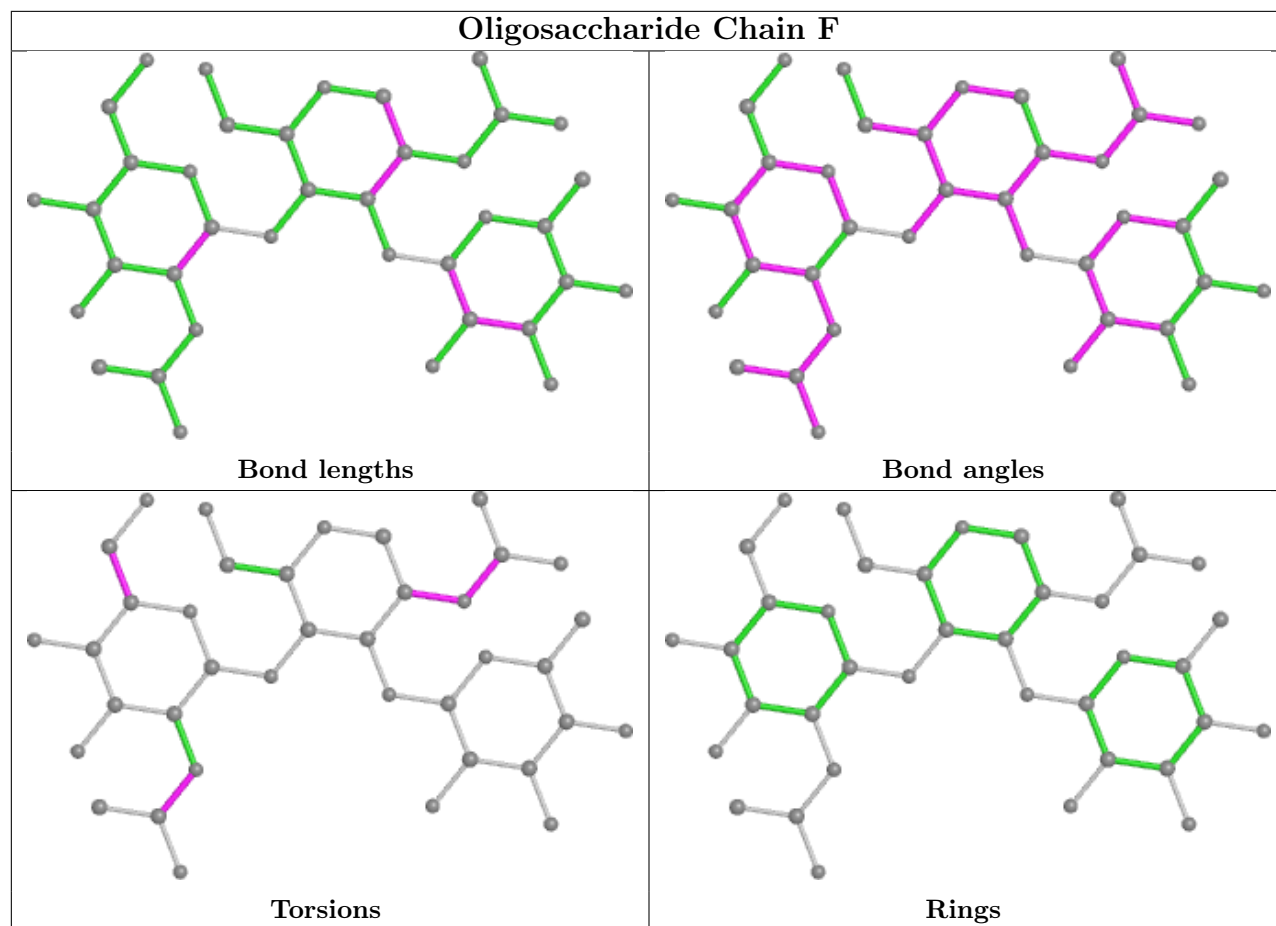
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	2	0
2	C	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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	397/419 (94%)	0.30	13 (3%) 46 46	36, 50, 60, 69	0
1	B	406/419 (96%)	0.17	2 (0%) 91 92	35, 49, 58, 61	0
All	All	803/838 (95%)	0.24	15 (1%) 66 69	35, 50, 58, 69	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	PRO	3.8
1	A	264	VAL	3.2
1	A	416	TRP	3.2
1	A	373	LEU	3.0
1	A	325	PRO	3.0
1	A	340	TRP	2.9
1	B	413	ALA	2.7
1	A	278	GLY	2.7
1	A	356	ILE	2.5
1	A	254	TYR	2.5
1	A	394	VAL	2.3
1	B	328	GLN	2.3
1	A	412	GLU	2.2
1	A	296	ALA	2.2
1	A	336	TYR	2.1

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

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

### 6.3 Carbohydrates i

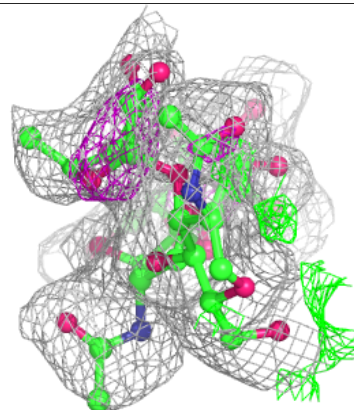
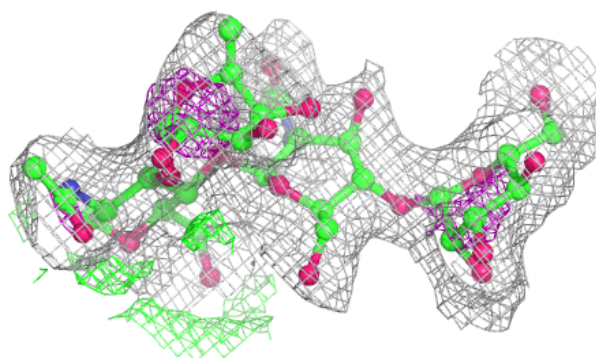
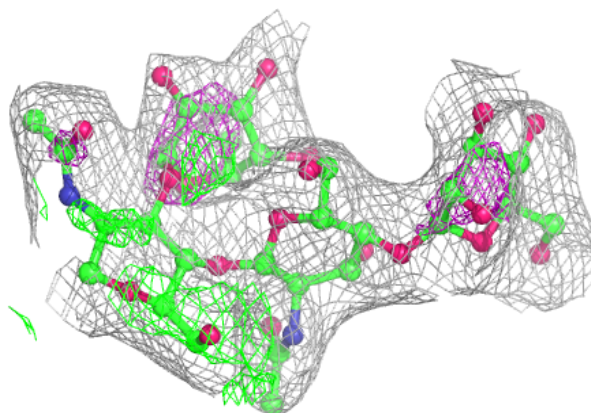
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	FUC	F	2	10/11	0.56	0.24	96,100,100,101	0
2	FUC	E	4	10/11	0.66	0.44	93,95,97,97	0
3	FUC	D	2	10/11	0.74	0.25	95,97,99,99	0
3	NAG	F	1	14/15	0.75	0.20	84,91,94,97	0
2	BMA	C	3	11/12	0.77	0.32	93,96,97,97	0
2	BMA	E	3	11/12	0.82	0.37	99,101,102,102	0
3	NAG	F	3	14/15	0.82	0.17	94,96,97,98	0
3	NAG	D	3	14/15	0.84	0.21	95,98,100,100	0
2	NAG	E	2	14/15	0.87	0.23	93,95,99,99	0
2	FUC	C	4	10/11	0.87	0.38	76,80,82,82	0
3	NAG	D	1	14/15	0.89	0.18	84,91,96,96	0
2	NAG	E	1	14/15	0.90	0.15	72,77,87,87	0
2	NAG	C	1	14/15	0.92	0.11	42,52,64,66	0
2	NAG	C	2	14/15	0.92	0.20	66,75,81,88	0

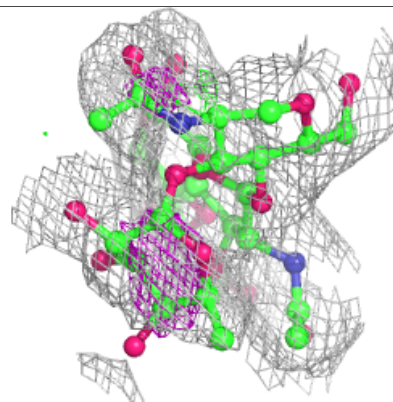
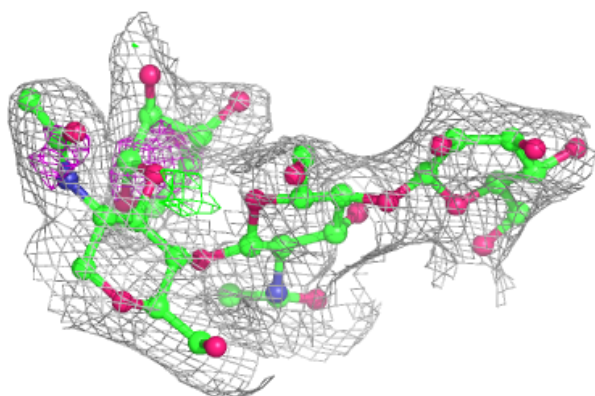
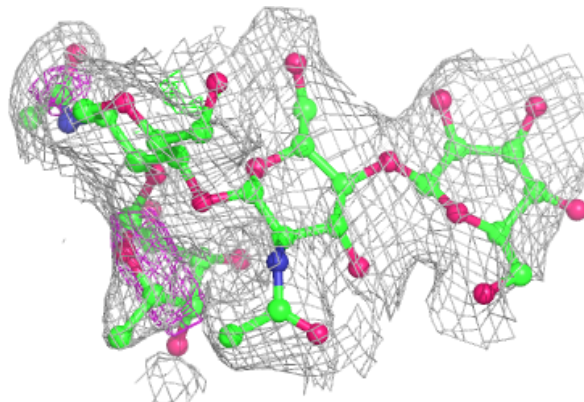
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

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

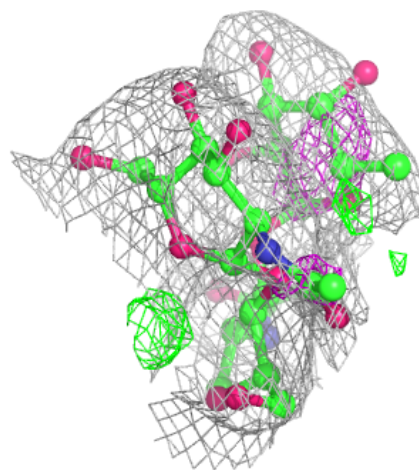
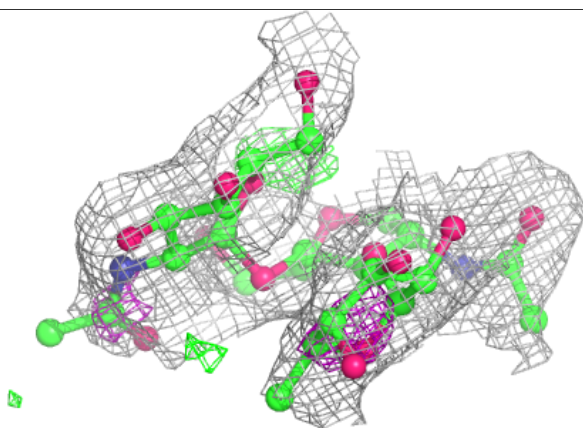
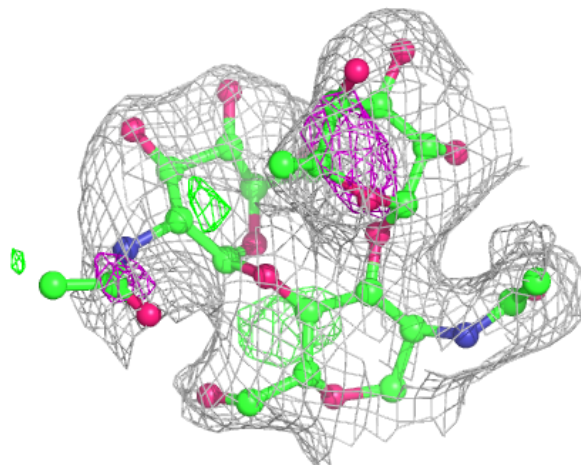
**Electron density around Chain E:**

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

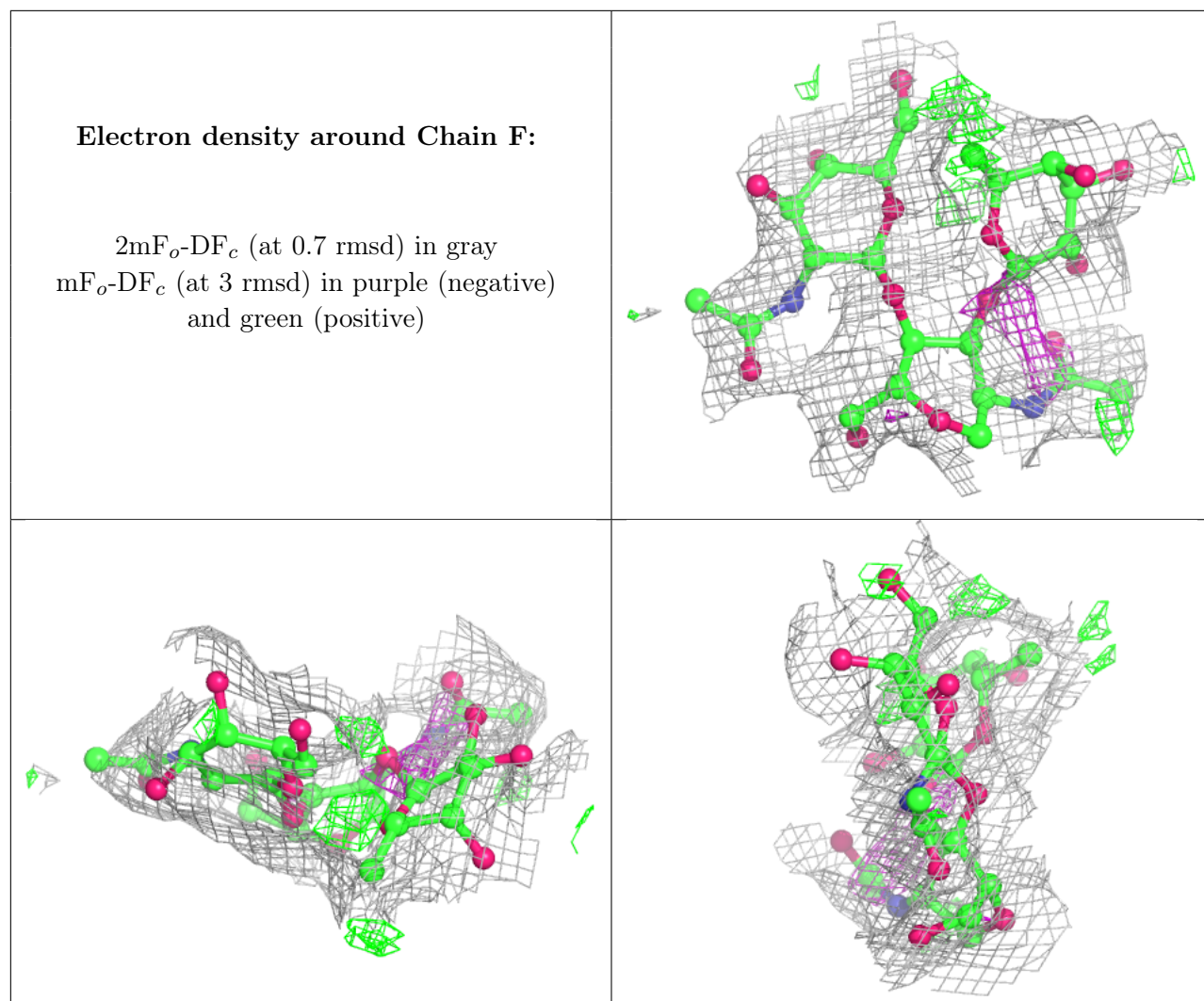


**Electron density around Chain D:**

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







## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.