



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 08:33 PM JST

PDB ID : 7BRL  
Title : Atrial Natriuretic Peptide Receptor complexed with Deletion mutant of rat Atrial Natriuretic Peptide[4-17,23]  
Authors : Ogawa, H.  
Deposited on : 2020-03-29  
Resolution : 3.20 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>.

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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 : 2.36  
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) : 2.36

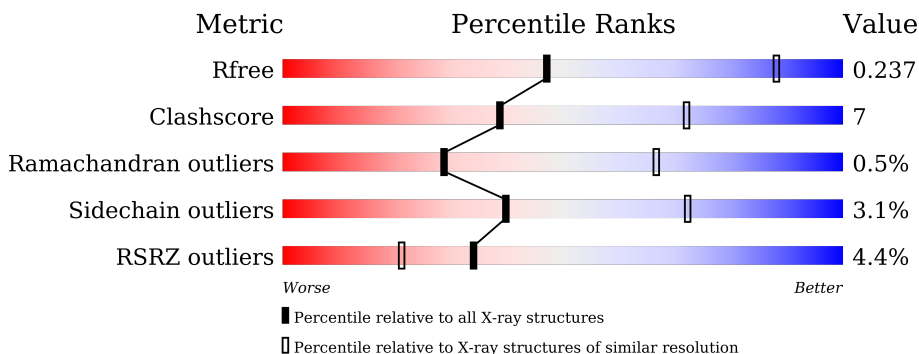
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	435	 3% 76% 21%
1	B	435	 4% 79% 18%
2	L	15	 33% 80% 13% 7%
3	C	3	 67% 33%
3	E	3	 33% 67%
4	D	4	 50% 50%

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Mol	Chain	Length	Quality of chain
4	F	4	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7166 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 Atrial natriuretic peptide receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	426	3383	2167	590	615	11	0	3	0
1	B	426	3383	2167	590	615	11	0	3	0

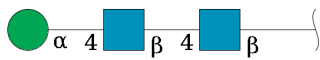
- Molecule 2 is a protein called Natriuretic peptides A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	15	220	128	48	40	4	0	15	0

There are 13 discrepancies between the modelled and reference sequences:

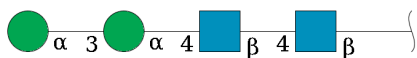
Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	SER	deletion	UNP P01161
L	?	-	LEU	deletion	UNP P01161
L	?	-	ARG	deletion	UNP P01161
L	?	-	GLN	deletion	UNP P01161
L	?	-	SER	deletion	UNP P01161
L	?	-	GLY	deletion	UNP P01161
L	?	-	LEU	deletion	UNP P01161
L	?	-	GLY	deletion	UNP P01161
L	?	-	ASN	deletion	UNP P01161
L	?	-	SER	deletion	UNP P01161
L	?	-	PHE	deletion	UNP P01161
L	?	-	ARG	deletion	UNP P01161
L	?	-	TYR	deletion	UNP P01161

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

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
4	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

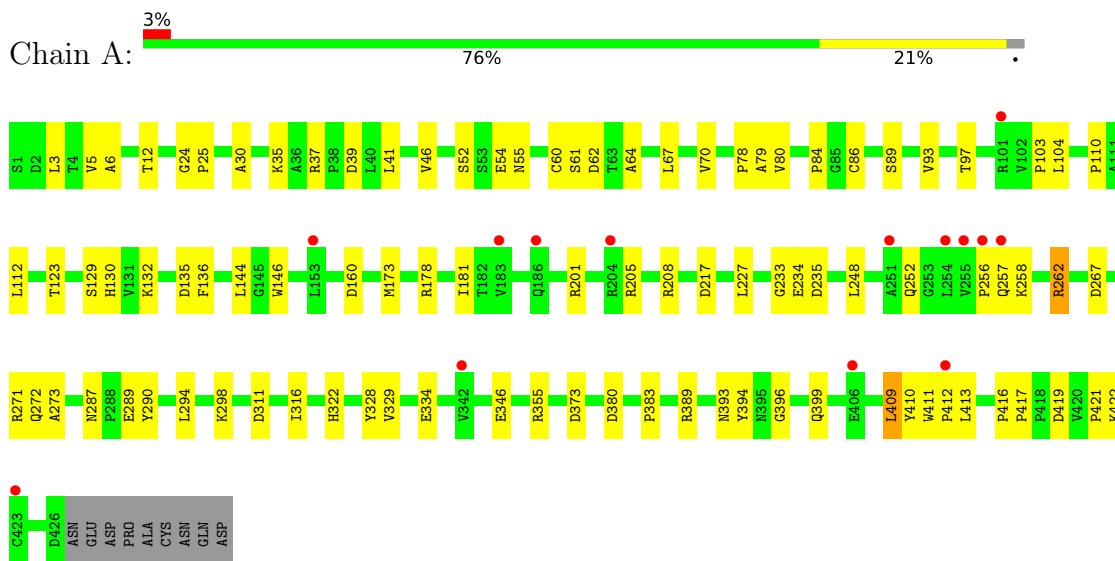
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

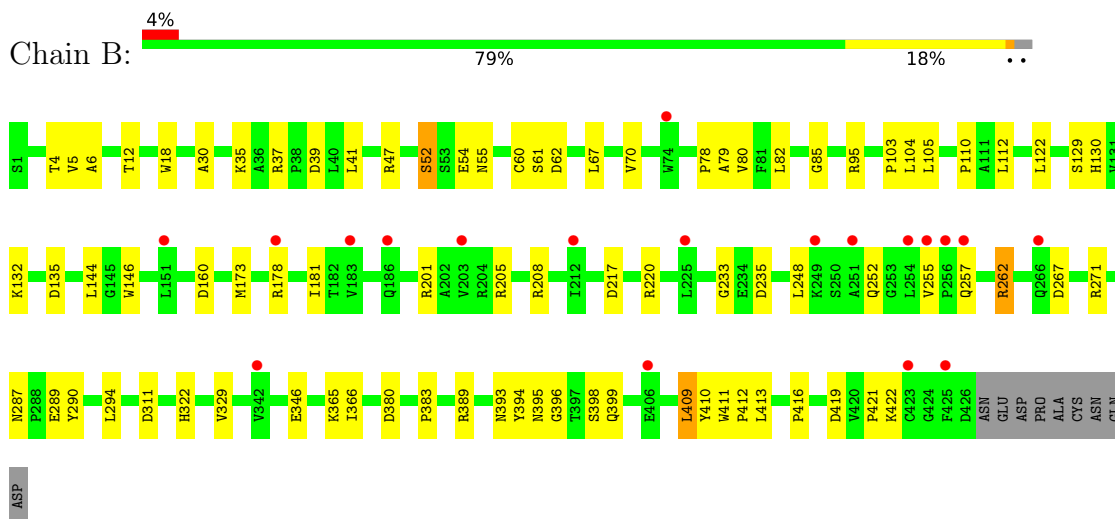
### 3 Residue-property plots

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.

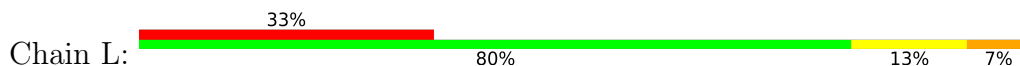
- Molecule 1: Atrial natriuretic peptide receptor 1



- Molecule 1: Atrial natriuretic peptide receptor 1



- Molecule 2: Natriuretic peptides A





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



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



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



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



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.27Å 100.27Å 270.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.52 – 3.20 33.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (33.52-3.20) 97.7 (33.52-3.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 3.18Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.198 , 0.237 0.198 , 0.237	Depositor DCC
$R_{free}$ test set	761 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.6	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 88.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: CL, 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	0.38	0/3475	0.53	0/4734
1	B	0.39	0/3475	0.52	0/4734
2	L	0.38	0/220	0.73	0/284
All	All	0.39	0/7170	0.53	0/9752

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	3383	0	3325	57	0
1	B	3383	0	3325	50	0
2	L	220	0	210	5	0
3	C	39	0	34	0	0
3	E	39	0	34	0	0
4	D	50	0	43	0	0
4	F	50	0	43	0	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
All	All	7166	0	7014	106	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 7.

All (106) 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:217:ASP:OD1	1:B:262:ARG:NH1	2.13	0.81
1:A:217:ASP:OD1	1:A:262:ARG:NH1	2.21	0.74
1:A:178:ARG:HH22	1:A:399:GLN:HE22	1.34	0.73
1:B:178:ARG:HH22	1:B:399:GLN:HE22	1.39	0.69
1:B:30:ALA:HB2	1:B:322:HIS:CD2	2.33	0.64
1:A:160:ASP:O	2:L:14[B]:ARG:NH2	2.32	0.63
1:A:84:PRO:HB3	5:A:508:CL:CL	2.38	0.61
1:A:30:ALA:HB2	1:A:322:HIS:CD2	2.36	0.60
1:B:419:ASP:N	1:B:419:ASP:OD1	2.32	0.60
1:B:4:THR:OG1	1:B:47:ARG:NH2	2.34	0.59
1:B:262:ARG:N	1:B:267:ASP:OD1	2.33	0.59
1:B:95[B]:ARG:NH2	2:L:13[B]:ASP:OD1	2.36	0.58
1:B:112:LEU:HD22	1:B:173:MET:HG3	1.85	0.58
1:A:419:ASP:OD1	1:A:419:ASP:N	2.33	0.58
1:A:62:ASP:OD2	2:L:11[A]:ARG:NH1	2.36	0.57
1:B:160:ASP:O	2:L:14[A]:ARG:NH2	2.39	0.55
1:A:41:LEU:HG	1:A:329:VAL:HG13	1.90	0.53
1:B:55:ASN:HB3	1:B:61:SER:HB2	1.90	0.53
1:A:52:SER:OG	1:A:54:GLU:HG2	2.09	0.53
1:A:12:THR:HB	1:A:54:GLU:OE2	2.08	0.52
1:A:54:GLU:HA	1:A:60:CYS:HA	1.91	0.52
1:A:144:LEU:HD23	1:A:146:TRP:CH2	2.45	0.52
1:A:233:GLY:HA3	1:A:412:PRO:HG2	1.92	0.52
1:B:248:LEU:HD22	1:B:257:GLN:HG3	1.92	0.52
1:A:409:LEU:HD13	1:A:411:TRP:HE1	1.75	0.52
1:B:233:GLY:HA3	1:B:412:PRO:HG2	1.92	0.52
1:A:112:LEU:HD22	1:A:173:MET:HG3	1.91	0.51
1:B:129:SER:HB2	1:B:132:LYS:HG2	1.91	0.51
1:B:62:ASP:OD2	2:L:11[B]:ARG:NH1	2.43	0.51
1:A:79:ALA:O	1:A:103:PRO:HD2	2.11	0.50
1:A:290:TYR:CE2	1:A:294:LEU:HD11	2.46	0.50
1:B:289:GLU:OE2	1:B:289:GLU:N	2.43	0.50
1:A:334:GLU:OE1	1:A:355:ARG:NH2	2.44	0.49
1:B:135:ASP:HB3	1:B:394:TYR:OH	2.12	0.49
1:B:144:LEU:HD21	1:B:411:TRP:HZ2	1.76	0.49
1:A:55:ASN:HB3	1:A:61:SER:HB2	1.93	0.49
1:A:70:VAL:HG11	1:B:70:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASN:HD22	1:A:289:GLU:HB2	1.78	0.49
1:B:54:GLU:HA	1:B:60:CYS:HA	1.95	0.49
1:B:346:GLU:OE2	1:B:346:GLU:N	2.45	0.49
1:B:52:SER:OG	1:B:54:GLU:HG2	2.13	0.49
1:B:409:LEU:HD13	1:B:411:TRP:HE1	1.78	0.49
1:A:3:LEU:HB3	1:A:46:VAL:HG22	1.96	0.48
1:B:144:LEU:HD23	1:B:146:TRP:CH2	2.48	0.48
1:A:262:ARG:N	1:A:267:ASP:OD1	2.34	0.48
1:B:287:ASN:HD22	1:B:289:GLU:HB2	1.79	0.48
1:A:201:ARG:HE	1:A:205:ARG:NH1	2.12	0.48
1:A:144:LEU:HD21	1:A:411:TRP:HZ2	1.78	0.48
1:B:12:THR:HB	1:B:54:GLU:OE2	2.13	0.48
1:B:144:LEU:HG	1:B:416:PRO:HG3	1.95	0.47
1:B:41:LEU:HG	1:B:329:VAL:HG13	1.97	0.47
1:A:256:PRO:HG2	1:A:258:LYS:HE3	1.96	0.47
1:B:110:PRO:HB2	1:B:130:HIS:CE1	2.50	0.46
1:A:86:CYS:HB2	1:A:89:SER:HB2	1.96	0.46
1:A:394:TYR:CE2	1:A:396:GLY:HA2	2.51	0.46
1:B:290:TYR:CE2	1:B:294:LEU:HD11	2.50	0.46
1:A:135:ASP:HB3	1:A:394:TYR:OH	2.16	0.46
1:B:103:PRO:HA	1:B:122:LEU:HB3	1.97	0.46
1:A:144:LEU:HG	1:A:416:PRO:HG3	1.98	0.46
1:A:208:ARG:HH21	1:A:421:PRO:HG3	1.81	0.45
1:B:79:ALA:O	1:B:103:PRO:HD2	2.16	0.45
1:A:289:GLU:OE2	1:A:289:GLU:N	2.44	0.45
1:A:346:GLU:N	1:A:346:GLU:OE2	2.49	0.45
1:B:394:TYR:CE2	1:B:396:GLY:HA2	2.52	0.45
1:A:5:VAL:HG22	1:A:80:VAL:CG1	2.47	0.45
1:B:365:LYS:HE2	1:B:366:ILE:O	2.16	0.45
1:A:144:LEU:HD23	1:A:146:TRP:CZ3	2.53	0.44
1:A:248:LEU:HD22	1:A:257:GLN:HG3	1.98	0.44
1:B:37:ARG:HB3	1:B:39:ASP:OD1	2.16	0.44
1:A:178:ARG:HH22	1:A:399:GLN:NE2	2.10	0.44
1:A:129:SER:HB2	1:A:132:LYS:HG2	1.98	0.44
1:B:144:LEU:HD23	1:B:146:TRP:CZ3	2.53	0.44
1:B:201:ARG:HE	1:B:205:ARG:NH1	2.16	0.43
1:B:18:TRP:CG	1:B:85:GLY:HA3	2.53	0.43
1:B:380:ASP:OD2	1:B:410:TYR:N	2.52	0.43
1:A:208:ARG:HB3	1:A:235:ASP:O	2.18	0.43
1:B:82:LEU:HD12	1:B:105:LEU:HB2	2.00	0.43
1:B:178:ARG:HH22	1:B:399:GLN:NE2	2.09	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:VAL:HG22	1:B:80:VAL:CG1	2.49	0.43
1:B:82:LEU:HD12	1:B:82:LEU:HA	1.91	0.42
1:A:37:ARG:HB3	1:A:39:ASP:OD1	2.18	0.42
1:A:61:SER:HB3	1:A:64:ALA:H	1.84	0.42
1:A:93:VAL:O	1:A:97:THR:HG23	2.19	0.42
1:B:144:LEU:HD21	1:B:411:TRP:CZ2	2.54	0.42
1:B:208:ARG:HB3	1:B:235:ASP:O	2.20	0.42
1:A:227:LEU:HD22	1:A:273:ALA:HB2	2.00	0.42
1:A:136:PHE:HD1	1:A:394:TYR:CB	2.33	0.42
1:A:6:ALA:HB2	1:A:78:PRO:HG3	2.02	0.42
1:A:132:LYS:HE3	1:A:373:ASP:HA	2.02	0.42
1:A:234:GLU:O	1:A:417:PRO:HB3	2.20	0.42
1:B:220:ARG:HD2	1:B:262:ARG:NH2	2.36	0.41
1:B:262:ARG:H	1:B:267:ASP:CG	2.19	0.41
1:A:144:LEU:HD21	1:A:411:TRP:CZ2	2.55	0.41
1:A:383:PRO:HG3	1:A:410:TYR:CD1	2.56	0.41
1:B:383:PRO:HG3	1:B:410:TYR:CD1	2.56	0.41
1:B:395:ASN:HB3	1:B:398:SER:OG	2.20	0.41
1:A:294:LEU:O	1:A:298:LYS:HG3	2.21	0.41
1:A:110:PRO:HB2	1:A:130:HIS:CE1	2.56	0.41
1:A:24:GLY:N	1:A:25:PRO:HD2	2.35	0.41
1:A:104:LEU:HD23	1:A:123:THR:HG23	2.03	0.41
1:A:380:ASP:OD2	1:A:410:TYR:N	2.54	0.41
1:B:252:GLN:NE2	1:B:311:ASP:HB3	2.36	0.40
1:A:252:GLN:NE2	1:A:311:ASP:HB3	2.36	0.40
1:B:6:ALA:HB2	1:B:78:PRO:HG3	2.03	0.40
1:A:316:ILE:HG21	1:A:316:ILE:HD13	1.81	0.40
1:A:3:LEU:HD21	1:A:328:TYR:HE2	1.86	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	427/435 (98%)	406 (95%)	20 (5%)	1 (0%)	47	79
1	B	427/435 (98%)	407 (95%)	18 (4%)	2 (0%)	29	67
2	L	26/15 (173%)	20 (77%)	4 (15%)	2 (8%)	1	6
All	All	880/885 (99%)	833 (95%)	42 (5%)	5 (1%)	29	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	LYS
1	B	422	LYS
2	L	14[A]	ARG
2	L	14[B]	ARG
1	B	421	PRO

### 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	356/361 (99%)	346 (97%)	10 (3%)	43	74
1	B	356/361 (99%)	344 (97%)	12 (3%)	37	70
2	L	22/11 (200%)	22 (100%)	0	100	100
All	All	734/733 (100%)	712 (97%)	22 (3%)	40	73

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	67	LEU
1	A	181	ILE
1	A	262	ARG
1	A	271	ARG
1	A	272	GLN
1	A	389	ARG
1	A	393	ASN

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Mol	Chain	Res	Type
1	A	409	LEU
1	A	413	LEU
1	B	35	LYS
1	B	52	SER
1	B	67	LEU
1	B	104	LEU
1	B	181	ILE
1	B	255	VAL
1	B	262	ARG
1	B	271	ARG
1	B	389	ARG
1	B	393	ASN
1	B	409	LEU
1	B	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	252	GLN
1	A	266	GLN
1	A	322	HIS
1	A	358	GLN
1	A	399	GLN
1	B	246	GLN
1	B	252	GLN
1	B	266	GLN
1	B	272	GLN
1	B	322	HIS
1	B	358	GLN
1	B	399	GLN

### 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
3	NAG	C	1	1,3	14,14,15	0.52	0	17,19,21	0.54	0
3	NAG	C	2	3	14,14,15	0.47	0	17,19,21	0.50	0
3	MAN	C	3	3	11,11,12	1.02	1 (9%)	15,15,17	1.52	2 (13%)
4	NAG	D	1	1,4	14,14,15	0.56	0	17,19,21	0.58	0
4	NAG	D	2	4	14,14,15	0.31	0	17,19,21	0.43	0
4	MAN	D	3	4	11,11,12	1.08	1 (9%)	15,15,17	1.82	2 (13%)
4	MAN	D	4	4	11,11,12	0.80	0	15,15,17	1.09	1 (6%)
3	NAG	E	1	1,3	14,14,15	0.61	0	17,19,21	0.52	0
3	NAG	E	2	3	14,14,15	0.60	1 (7%)	17,19,21	0.49	0
3	MAN	E	3	3	11,11,12	1.00	1 (9%)	15,15,17	1.54	2 (13%)
4	NAG	F	1	1,4	14,14,15	0.62	0	17,19,21	0.58	0
4	NAG	F	2	4	14,14,15	0.31	0	17,19,21	0.47	0
4	MAN	F	3	4	11,11,12	1.14	1 (9%)	15,15,17	1.80	2 (13%)
4	MAN	F	4	4	11,11,12	0.88	0	15,15,17	1.05	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	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	0/2/19/22	1/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	MAN	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	MAN	C2-C3	2.45	1.56	1.52
3	C	3	MAN	O5-C5	2.33	1.48	1.43
4	D	3	MAN	C2-C3	2.29	1.55	1.52
3	E	3	MAN	O5-C5	2.28	1.48	1.43
3	E	2	NAG	O5-C1	-2.09	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	MAN	C1-O5-C5	5.20	119.23	112.19
4	D	3	MAN	C1-O5-C5	5.09	119.08	112.19
3	E	3	MAN	C1-O5-C5	4.63	118.47	112.19
3	C	3	MAN	C1-O5-C5	4.60	118.43	112.19
4	D	3	MAN	O5-C1-C2	3.81	116.65	110.77
4	F	3	MAN	O5-C1-C2	3.72	116.52	110.77
4	D	4	MAN	C1-O5-C5	2.73	115.89	112.19
4	F	4	MAN	C1-O5-C5	2.61	115.73	112.19
3	C	3	MAN	O5-C1-C2	2.42	114.50	110.77
3	E	3	MAN	O5-C1-C2	2.35	114.40	110.77

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

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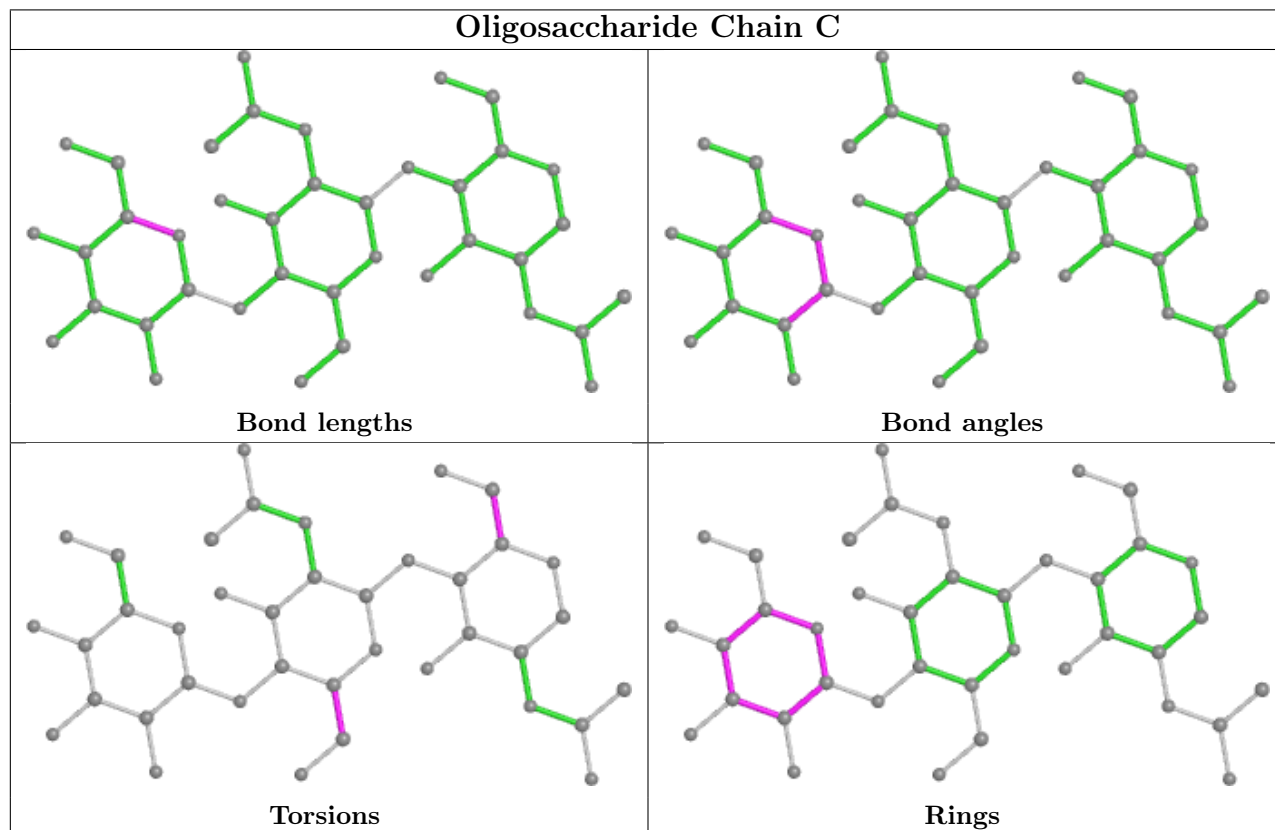
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6

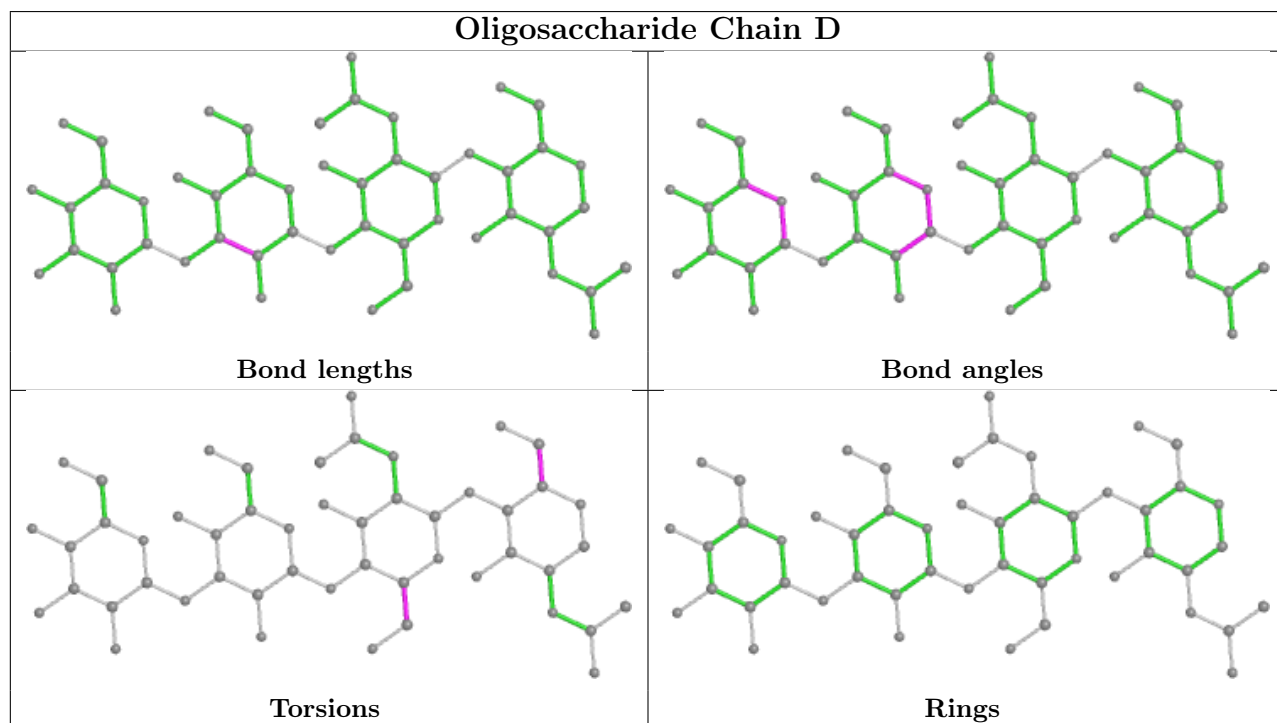
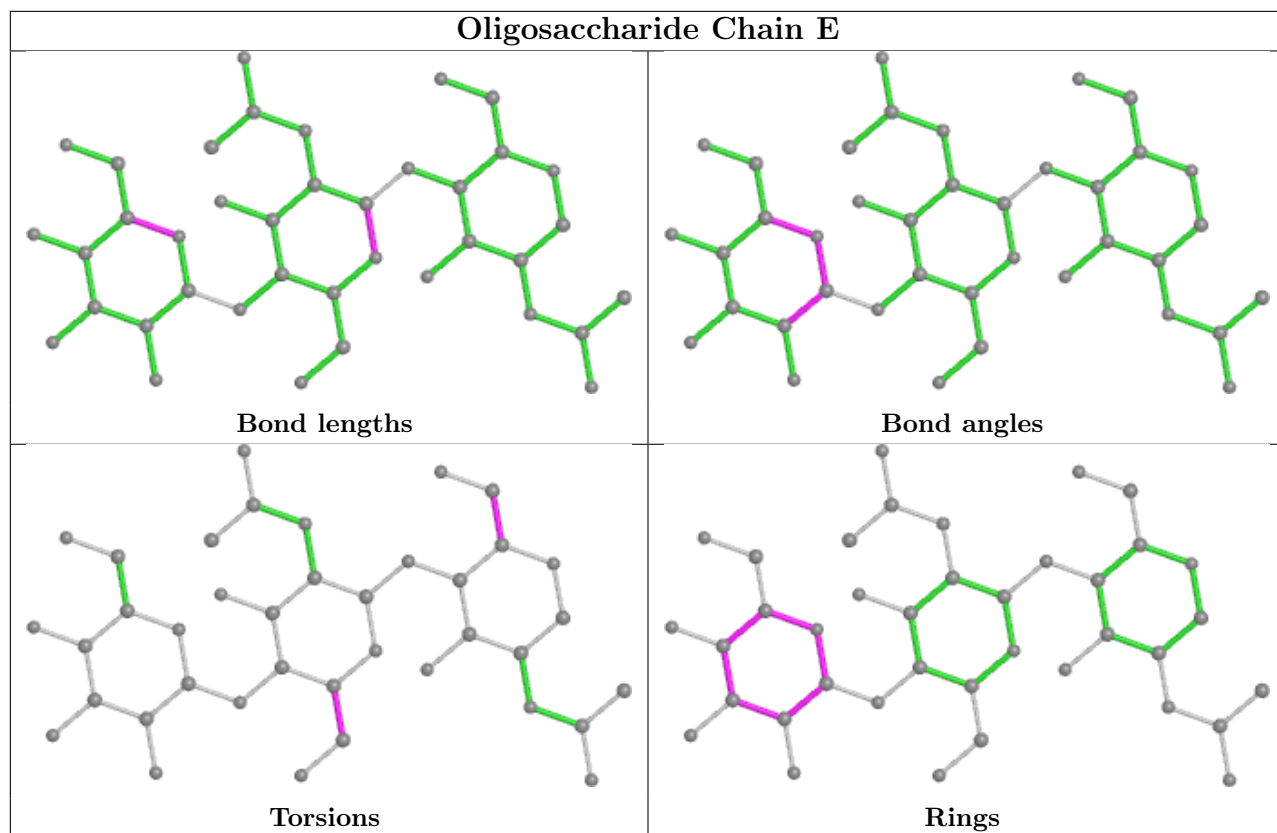
All (2) ring outliers are listed below:

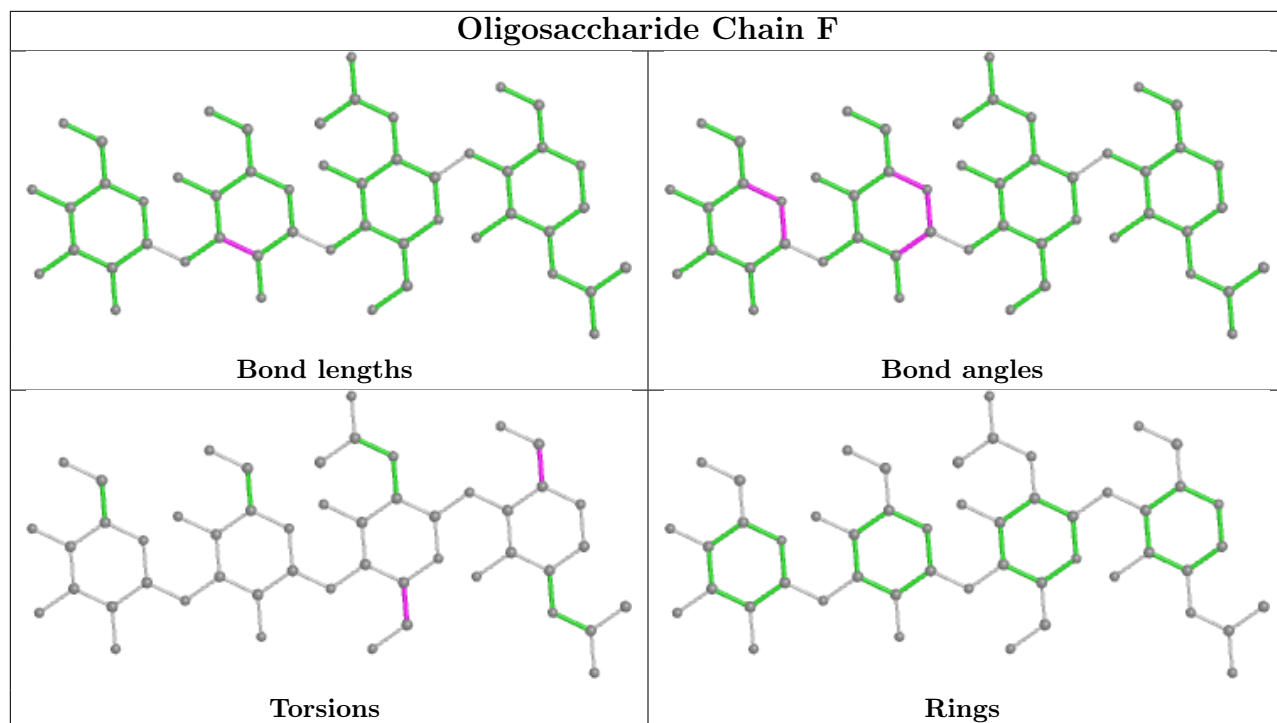
Mol	Chain	Res	Type	Atoms
3	E	3	MAN	C1-C2-C3-C4-C5-O5
3	C	3	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	426/435 (97%)	0.47	14 (3%) 46 30	61, 108, 183, 267	0
1	B	426/435 (97%)	0.48	19 (4%) 33 21	61, 108, 177, 265	0
2	L	15/15 (100%)	2.16	5 (33%) 0 0	89, 111, 187, 202	0
All	All	867/885 (97%)	0.50	38 (4%) 34 21	61, 108, 183, 267	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	17[A]	ALA	8.6
1	B	256	PRO	7.7
1	A	256	PRO	7.4
1	B	254	LEU	6.2
1	B	255	VAL	5.5
1	A	254	LEU	4.6
2	L	16[A]	GLY	4.5
1	A	255	VAL	4.3
1	A	186	GLN	3.8
1	B	406	GLU	3.4
2	L	6[A]	SER	3.3
1	B	342	VAL	3.3
1	A	406	GLU	2.9
1	B	423	CYS	2.7
1	B	212	ILE	2.6
2	L	15[A]	ILE	2.5
1	B	183	VAL	2.5
1	B	186	GLN	2.5
1	B	251	ALA	2.5
1	B	425	PHE	2.5
1	B	74[A]	TRP	2.4
1	A	342	VAL	2.3
1	A	183	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLN	2.3
1	B	249	LYS	2.2
1	B	178	ARG	2.2
1	A	204	ARG	2.2
1	B	257	GLN	2.2
1	A	101	ARG	2.2
1	A	251	ALA	2.2
1	B	203	VAL	2.1
1	A	153	LEU	2.1
1	A	412	PRO	2.1
2	L	12[A]	ILE	2.0
1	B	225	LEU	2.0
1	B	151	LEU	2.0
1	A	423	CYS	2.0
1	B	266	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

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

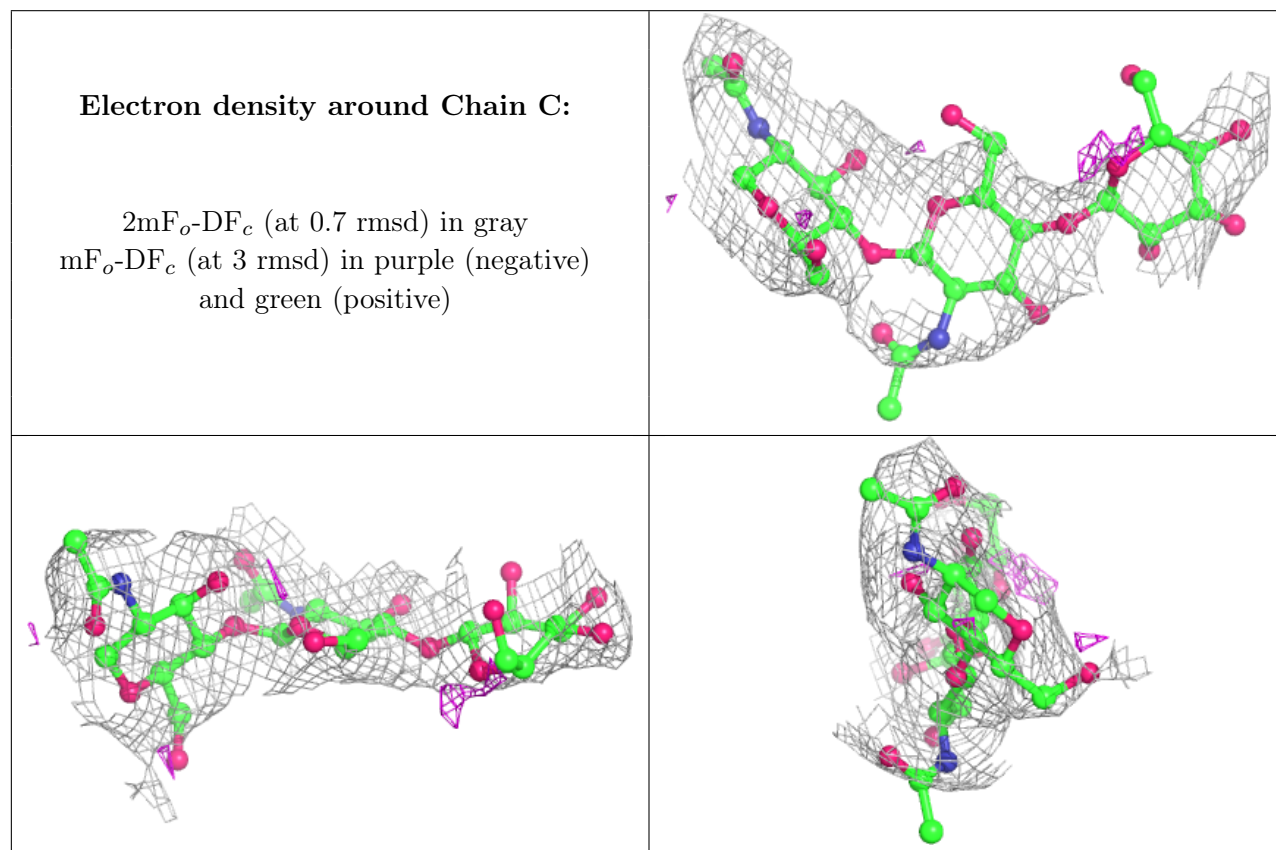
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	C	3	11/12	0.49	0.34	178,188,198,204	0
4	MAN	F	3	11/12	0.56	0.19	203,209,213,217	0
4	MAN	D	3	11/12	0.57	0.18	216,222,228,234	0
3	MAN	E	3	11/12	0.69	0.25	164,172,188,193	0
4	MAN	D	4	11/12	0.80	0.17	226,230,235,236	0
4	MAN	F	4	11/12	0.83	0.14	203,208,214,216	0
3	NAG	E	2	14/15	0.84	0.30	121,142,150,163	0
4	NAG	D	1	14/15	0.90	0.17	107,114,136,142	0
4	NAG	F	2	14/15	0.91	0.15	151,162,175,192	0
3	NAG	C	2	14/15	0.91	0.28	123,147,161,176	0
4	NAG	F	1	14/15	0.91	0.17	104,113,130,135	0
4	NAG	D	2	14/15	0.93	0.16	160,173,186,203	0
3	NAG	C	1	14/15	0.94	0.20	59,81,99,105	0

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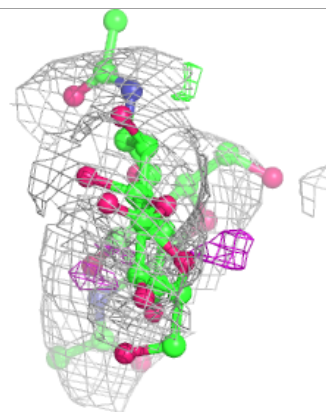
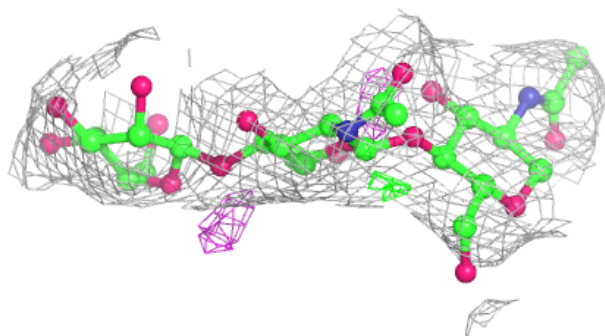
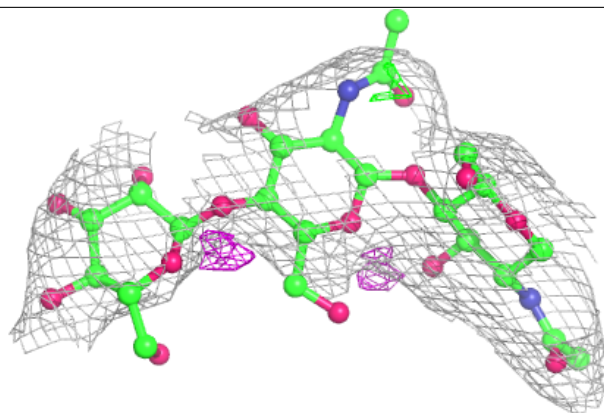
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	1	14/15	0.94	0.22	57,77,95,102	0

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.

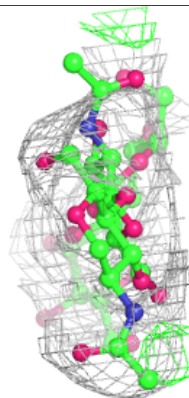
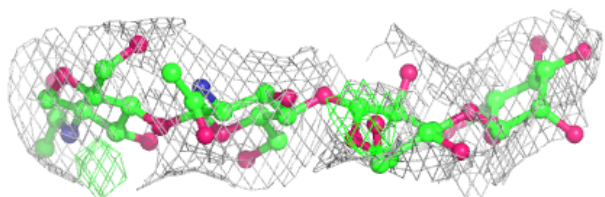
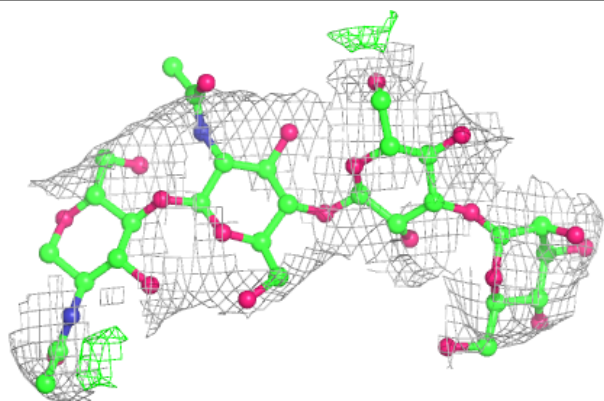


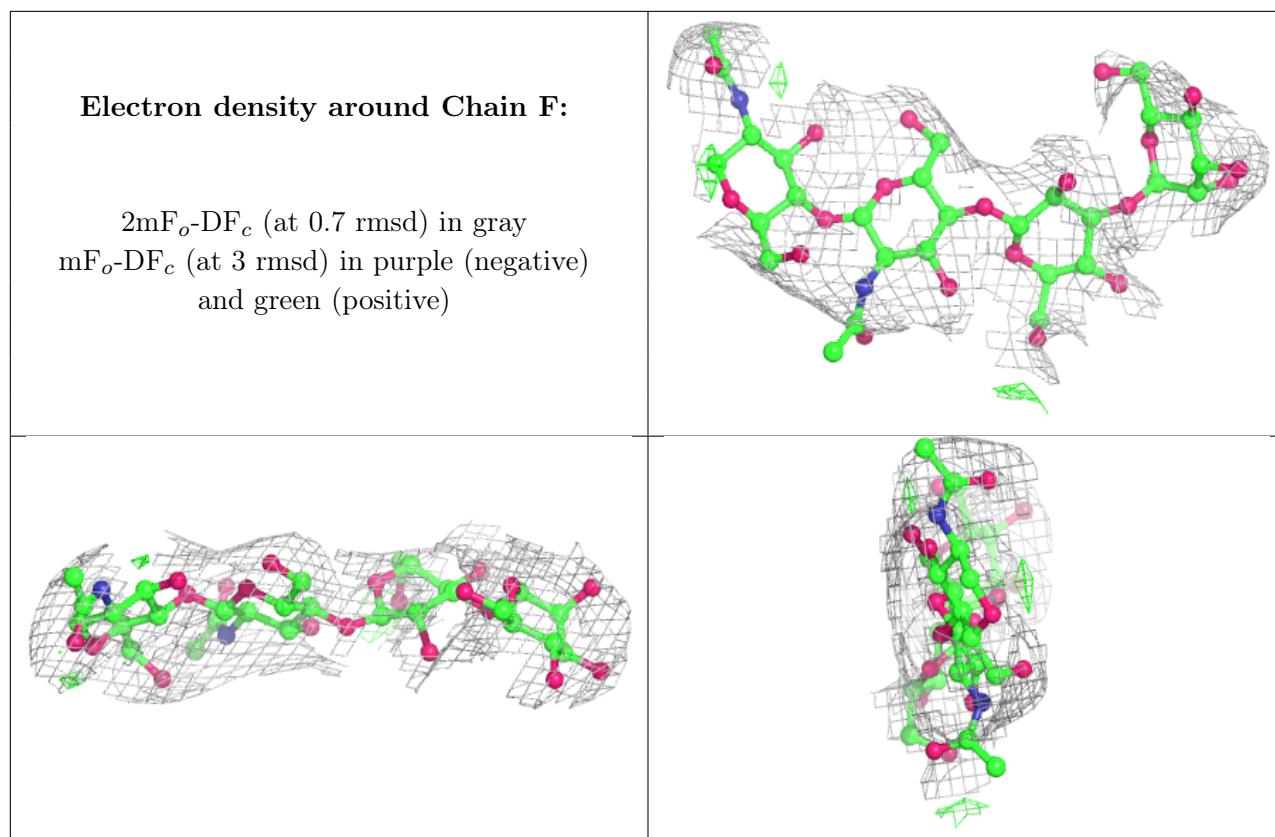
**Electron density around Chain E:**

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

**Electron density around Chain 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](#)

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.

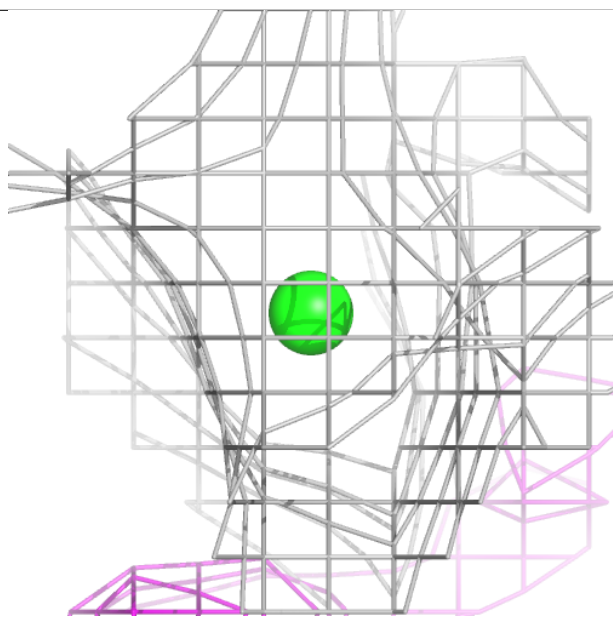
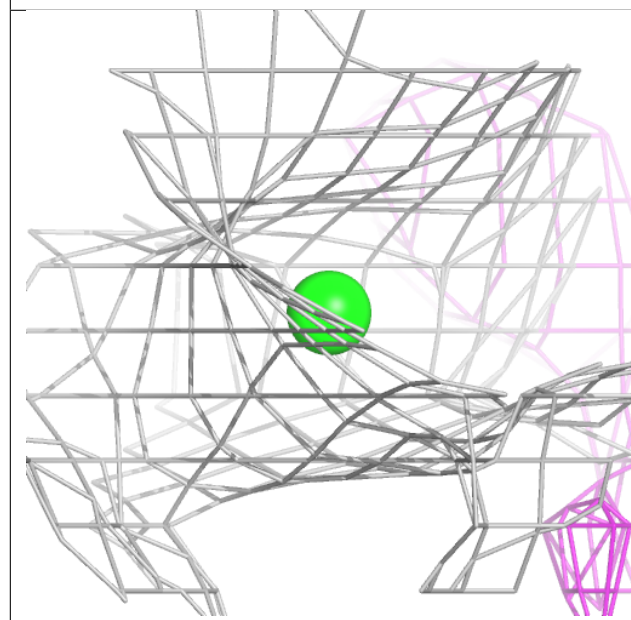
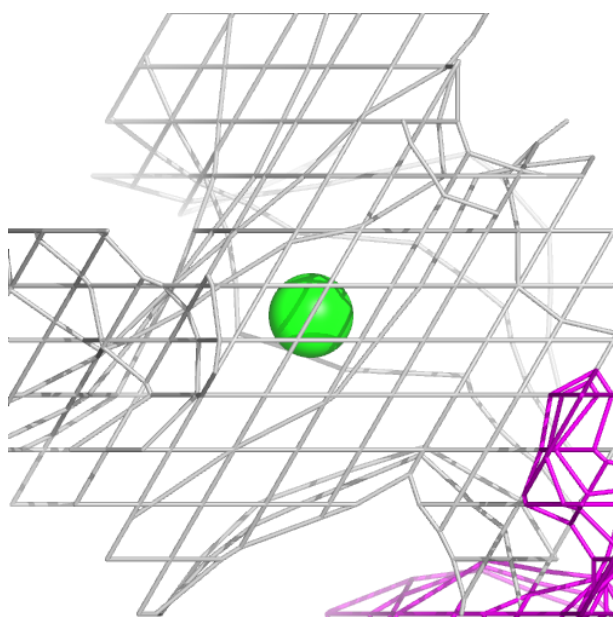
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	CL	A	508	1/1	0.96	0.30	90,90,90,90	0
5	CL	B	508	1/1	0.98	0.22	67,67,67,67	0

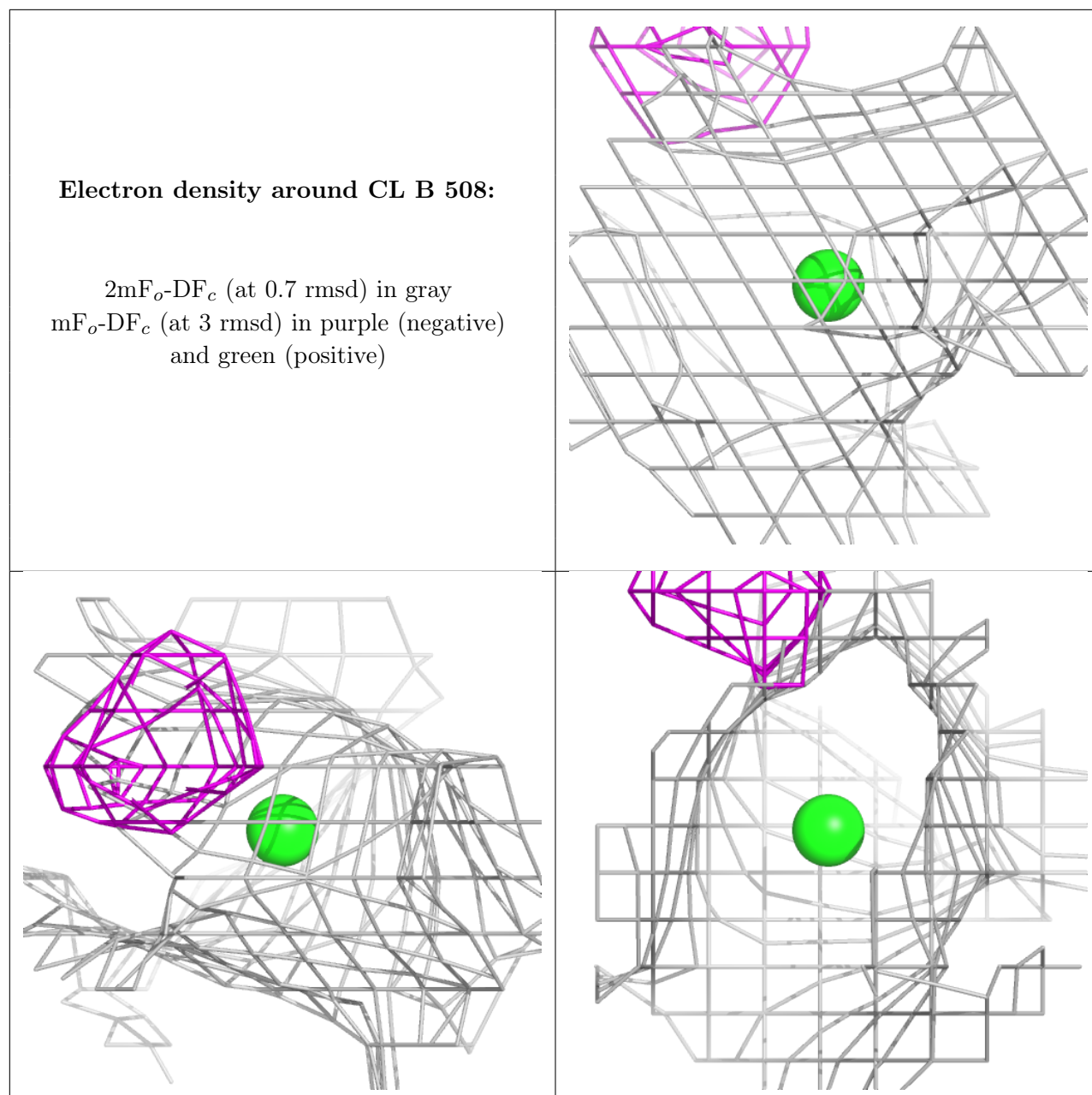
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around CL A 508:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.