



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2021 – 04:04 PM EST

PDB ID : 6VHQ  
Title : Crystal structure of Bacillus subtilis levansucrase (D86A/E342A) in complex with oligosaccharides  
Authors : Diaz-Vilchis, A.; Raga-Carbajal, E.; Rojas-Trejo, S.; Olvera, C.; Rudino-Pinera, E.  
Deposited on : 2020-01-10  
Resolution : 2.05 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 : 2.16  
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) : 2.16

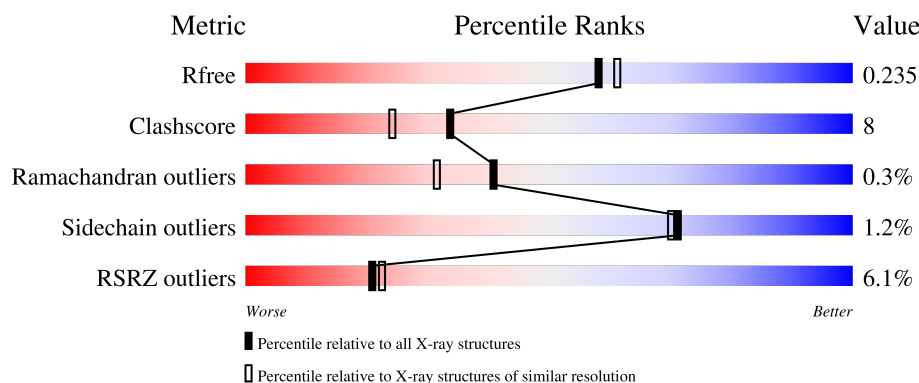
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


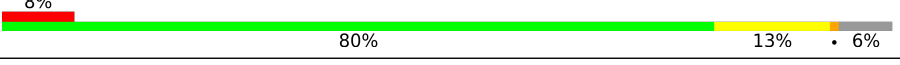
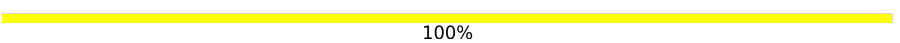

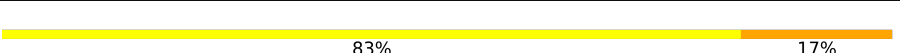
The reported resolution of this entry is 2.05 Å.

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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	466	 4% 80% 13% • 6%
1	B	466	 8% 80% 13% • 6%
2	C	6	 100%
2	D	6	 83% 17%
2	E	6	 83% 17%

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Mol	Chain	Length	Quality of chain
3	F	2	

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	FRU	E	2	-	-	-	X
3	FRU	F	1	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7871 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 Glycoside hydrolase family 68 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	6	0
			3528	2222	588	707	11			
1	B	440	Total	C	N	O	S	0	11	0
			3569	2248	598	712	11			

There are 48 discrepancies between the modelled and reference sequences:

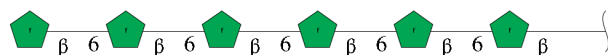
Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ALA	ASP	engineered mutation	UNP A0PFL2
A	342	ALA	GLU	engineered mutation	UNP A0PFL2
A	474	THR	-	expression tag	UNP A0PFL2
A	475	ASP	-	expression tag	UNP A0PFL2
A	476	PRO	-	expression tag	UNP A0PFL2
A	477	ASN	-	expression tag	UNP A0PFL2
A	478	SER	-	expression tag	UNP A0PFL2
A	479	SER	-	expression tag	UNP A0PFL2
A	480	SER	-	expression tag	UNP A0PFL2
A	481	VAL	-	expression tag	UNP A0PFL2
A	482	ASP	-	expression tag	UNP A0PFL2
A	483	LYS	-	expression tag	UNP A0PFL2
A	484	LEU	-	expression tag	UNP A0PFL2
A	485	ALA	-	expression tag	UNP A0PFL2
A	486	ALA	-	expression tag	UNP A0PFL2
A	487	ALA	-	expression tag	UNP A0PFL2
A	488	LEU	-	expression tag	UNP A0PFL2
A	489	GLU	-	expression tag	UNP A0PFL2
A	490	HIS	-	expression tag	UNP A0PFL2
A	491	HIS	-	expression tag	UNP A0PFL2
A	492	HIS	-	expression tag	UNP A0PFL2
A	493	HIS	-	expression tag	UNP A0PFL2
A	494	HIS	-	expression tag	UNP A0PFL2
A	495	HIS	-	expression tag	UNP A0PFL2
B	86	ALA	ASP	engineered mutation	UNP A0PFL2

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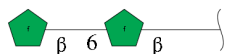
Chain	Residue	Modelled	Actual	Comment	Reference
B	342	ALA	GLU	engineered mutation	UNP A0PFL2
B	474	THR	-	expression tag	UNP A0PFL2
B	475	ASP	-	expression tag	UNP A0PFL2
B	476	PRO	-	expression tag	UNP A0PFL2
B	477	ASN	-	expression tag	UNP A0PFL2
B	478	SER	-	expression tag	UNP A0PFL2
B	479	SER	-	expression tag	UNP A0PFL2
B	480	SER	-	expression tag	UNP A0PFL2
B	481	VAL	-	expression tag	UNP A0PFL2
B	482	ASP	-	expression tag	UNP A0PFL2
B	483	LYS	-	expression tag	UNP A0PFL2
B	484	LEU	-	expression tag	UNP A0PFL2
B	485	ALA	-	expression tag	UNP A0PFL2
B	486	ALA	-	expression tag	UNP A0PFL2
B	487	ALA	-	expression tag	UNP A0PFL2
B	488	LEU	-	expression tag	UNP A0PFL2
B	489	GLU	-	expression tag	UNP A0PFL2
B	490	HIS	-	expression tag	UNP A0PFL2
B	491	HIS	-	expression tag	UNP A0PFL2
B	492	HIS	-	expression tag	UNP A0PFL2
B	493	HIS	-	expression tag	UNP A0PFL2
B	494	HIS	-	expression tag	UNP A0PFL2
B	495	HIS	-	expression tag	UNP A0PFL2

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	6	Total	C	O	0	0	0
			67	36	31			
2	D	6	Total	C	O	0	0	0
			67	36	31			
2	E	6	Total	C	O	0	0	0
			67	36	31			

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Br	0	0
			3	3		
5	A	6	Total	Br	0	0
			6	6		

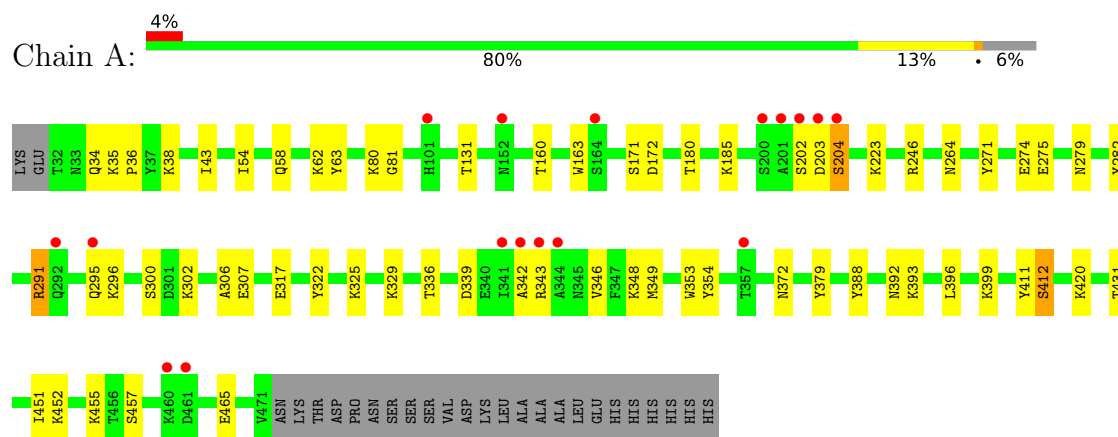
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	290	Total	O	0	0
			290	290		
6	B	250	Total	O	0	0
			250	250		

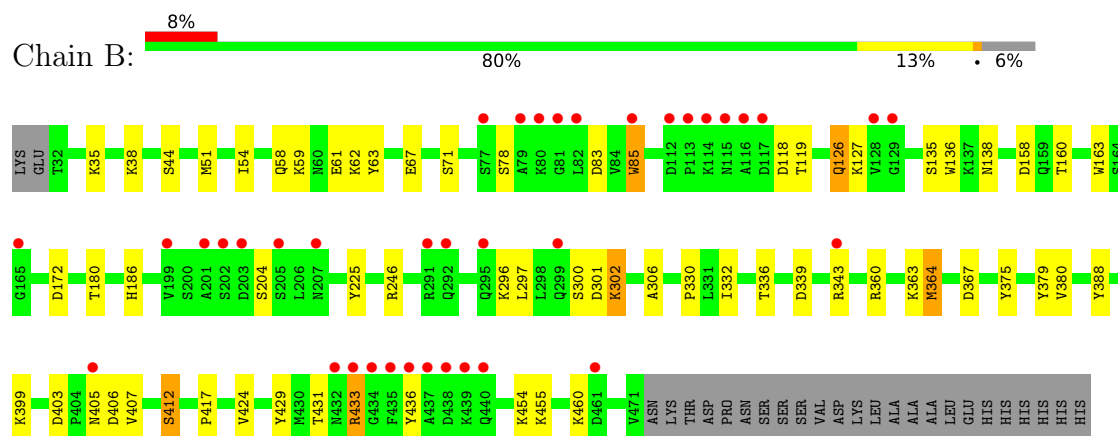
### 3 Residue-property plots

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.

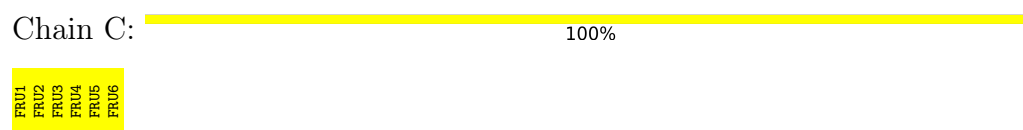
- Molecule 1: Glycoside hydrolase family 68 protein




- Molecule 1: Glycoside hydrolase family 68 protein



- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose




- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain D:  83% 17%


FRU1  
FRU2  
FRU3  
FRU4  
FRU5  
FRU6

- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain E:  83% 17%

FRU1  
FRU2  
FRU3  
FRU4  
FRU5  
FRU6

- Molecule 3: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain F:  50% 50%

FRU1  
FRU2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.31Å 78.67Å 78.73Å 90.00° 93.94° 90.00°	Depositor
Resolution (Å)	35.20 – 2.05 35.20 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.20-2.05) 99.2 (35.20-2.05)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.167 , 0.235 0.167 , 0.235	Depositor DCC
$R_{free}$ test set	2606 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 71.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BR, FRU

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	0.74	1/3605 (0.0%)	0.80	2/4872 (0.0%)
1	B	0.78	2/3649 (0.1%)	0.81	3/4932 (0.1%)
All	All	0.76	3/7254 (0.0%)	0.80	5/9804 (0.1%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85[A]	TRP	CB-CG	-7.39	1.36	1.50
1	B	85[B]	TRP	CB-CG	-7.39	1.36	1.50
1	A	271	TYR	CE2-CZ	6.13	1.46	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	ARG	NE-CZ-NH1	-9.98	115.31	120.30
1	B	364	MET	CG-SD-CE	9.26	115.02	100.20
1	A	291	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	246	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	246	ARG	NE-CZ-NH1	5.21	122.91	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	375	TYR	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	3528	0	3387	48	0
1	B	3569	0	3417	76	0
2	C	67	0	57	0	0
2	D	67	0	57	1	0
2	E	67	0	58	1	0
3	F	22	0	18	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	6	0	0	0	0
5	B	3	0	0	2	0
6	A	290	0	0	9	0
6	B	250	0	0	13	0
All	All	7871	0	6994	122	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 8.

All (122) 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:85[A]:TRP:CD1	1:B:433:ARG:HD3	1.62	1.35
5:B:502:BR:BR	6:B:831:HOH:O	2.19	1.12
1:B:85[A]:TRP:NE1	1:B:433:ARG:CD	2.13	1.11
1:B:85[A]:TRP:CE2	1:B:433:ARG:HD2	1.92	1.05
1:B:85[A]:TRP:CE2	1:B:433:ARG:CD	2.44	1.01
1:B:85[A]:TRP:CG	1:B:433:ARG:HD3	1.95	1.01
1:B:85[A]:TRP:CD1	1:B:433:ARG:CD	2.44	0.99
1:B:85[A]:TRP:NE1	1:B:433:ARG:HD3	1.75	0.95
1:B:85[B]:TRP:CZ2	1:B:433:ARG:NH2	2.45	0.84
1:B:403:ASP:HB2	6:B:609:HOH:O	1.79	0.81
1:B:296:LYS:HE2	1:B:367:ASP:OD2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85[A]:TRP:CE2	1:B:433:ARG:HD3	2.13	0.79
1:B:85[A]:TRP:NE1	1:B:433:ARG:CG	2.47	0.76
1:A:35:LYS:HD3	1:A:36:PRO:HD2	1.66	0.75
1:B:85[B]:TRP:CD2	1:B:433:ARG:HD3	2.22	0.75
1:B:85[A]:TRP:CD2	1:B:433:ARG:HD3	2.23	0.73
1:A:300:SER:OG	1:A:302:LYS:HG2	1.89	0.72
1:B:78:SER:HB2	1:B:138:ASN:HB2	1.71	0.72
1:A:80:LYS:HD2	1:A:81:GLY:N	2.10	0.66
1:B:85[A]:TRP:CD1	1:B:433:ARG:HG2	2.31	0.65
1:B:300:SER:OG	1:B:302:LYS:HG2	1.97	0.65
1:A:185:LYS:HA	1:A:185:LYS:HE2	1.78	0.65
1:B:85[A]:TRP:CD1	1:B:433:ARG:CG	2.80	0.64
1:B:158:ASP:OD2	1:B:186[B]:HIS:NE2	2.28	0.64
1:B:61:GLU:OE2	1:B:460:LYS:HE2	1.99	0.63
1:B:380:VAL:HG11	1:B:454:LYS:HD2	1.81	0.63
1:B:403:ASP:HB3	6:B:733:HOH:O	1.99	0.63
1:A:317:GLU:OE1	1:A:325:LYS:NZ	2.30	0.63
1:A:80:LYS:HA	6:A:822:HOH:O	1.99	0.62
1:B:406:ASP:N	6:B:609:HOH:O	2.32	0.61
1:B:360:ARG:NH1	1:B:363:LYS:HD2	2.16	0.60
1:B:51[A]:MET:HE1	1:B:364:MET:HE1	1.84	0.59
1:B:85[A]:TRP:CZ2	1:B:433:ARG:HD2	2.38	0.58
1:A:452:LYS:NZ	6:A:609:HOH:O	2.32	0.58
1:B:38:LYS:HE2	6:B:826:HOH:O	2.03	0.58
1:B:163:TRP:HB2	1:B:180:THR:HB	1.85	0.58
1:B:85[A]:TRP:NE1	1:B:433:ARG:HD2	1.99	0.58
1:A:296:LYS:HB3	1:A:296:LYS:HZ2	1.70	0.57
1:A:349[A]:MET:HE1	1:A:451:ILE:HB	1.85	0.57
1:A:62:LYS:HG3	1:A:457[A]:SER:HB2	1.88	0.56
1:A:452:LYS:NZ	1:B:59:LYS:HE3	2.20	0.56
1:A:131:THR:HB	1:A:465:GLU:HG3	1.88	0.56
1:A:343:ARG:HD3	1:A:412:SER:OG	2.07	0.54
1:A:223:LYS:HE2	6:A:870:HOH:O	2.06	0.54
1:A:393:LYS:NZ	1:B:67:GLU:HG3	2.23	0.54
1:B:85[B]:TRP:CE2	1:B:433:ARG:NH2	2.76	0.54
1:B:301:ASP:OD1	1:B:301:ASP:N	2.41	0.53
1:B:62:LYS:HE2	1:B:63:TYR:CZ	2.44	0.53
1:B:58:GLN:HG3	1:B:399:LYS:HE2	1.89	0.53
1:B:51[A]:MET:CE	1:B:364:MET:HE1	2.39	0.53
5:B:504:BR:BR	6:B:841:HOH:O	2.74	0.53
1:A:393:LYS:HZ1	1:B:67:GLU:HG3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85[A]:TRP:CD2	1:B:433:ARG:CD	2.89	0.51
1:A:317:GLU:CD	1:A:325:LYS:HZ1	2.14	0.51
1:B:160:THR:HA	3:F:1:FRU:H61	1.93	0.50
1:B:85[A]:TRP:NE1	1:B:433:ARG:HG2	2.23	0.50
1:B:71[B]:SER:OG	6:B:602:HOH:O	2.19	0.49
1:A:202:SER:C	1:A:204:SER:H	2.15	0.49
1:A:317:GLU:CD	1:A:325:LYS:NZ	2.67	0.49
1:A:163:TRP:HB2	1:A:180:THR:HB	1.94	0.49
1:A:296:LYS:HB3	1:A:296:LYS:NZ	2.27	0.48
1:B:455:LYS:CD	1:B:455:LYS:N	2.76	0.48
1:B:455:LYS:HD3	1:B:455:LYS:N	2.28	0.48
1:A:62:LYS:HE3	1:A:63:TYR:CE1	2.48	0.47
1:B:454:LYS:C	1:B:455:LYS:HD2	2.35	0.47
1:B:83:ASP:HB3	1:B:85[A]:TRP:CZ2	2.49	0.47
1:B:83:ASP:HB3	1:B:85[A]:TRP:CE2	2.49	0.47
1:B:85[B]:TRP:CG	1:B:433:ARG:HD3	2.44	0.46
1:A:172:ASP:N	1:A:172:ASP:OD1	2.46	0.46
1:A:34:GLN:NE2	1:A:275:GLU:OE2	2.36	0.46
1:B:58:GLN:NE2	6:B:616:HOH:O	2.43	0.46
1:B:405:ASN:HB2	6:B:609:HOH:O	2.16	0.46
1:B:380:VAL:CG1	1:B:454:LYS:HD2	2.45	0.46
1:B:85[B]:TRP:CZ2	1:B:119:THR:HG23	2.50	0.45
1:A:379:TYR:HB3	1:A:388:TYR:HB3	1.97	0.45
1:B:78:SER:HB2	1:B:138:ASN:CB	2.42	0.45
1:A:38:LYS:NZ	6:A:615:HOH:O	2.39	0.45
1:B:78:SER:OG	1:B:136:TRP:O	2.19	0.45
1:A:279:ASN:HB3	1:A:282:TYR:CD2	2.52	0.44
1:B:225:TYR:CE1	1:B:330:PRO:HG3	2.53	0.44
1:A:342:ALA:HB2	6:A:689:HOH:O	2.17	0.44
1:A:54:ILE:HG12	1:A:396:LEU:HB2	2.00	0.44
1:B:85[B]:TRP:HB2	1:B:429:TYR:CE2	2.52	0.44
1:A:452:LYS:HZ2	1:B:59:LYS:HE3	1.82	0.44
1:A:346:VAL:HA	1:A:354:TYR:O	2.18	0.44
1:B:62:LYS:HE2	1:B:63:TYR:CE1	2.53	0.44
1:B:379:TYR:HB3	1:B:388:TYR:HB3	2.00	0.44
1:A:322:TYR:OH	6:A:601:HOH:O	2.16	0.43
1:A:348:LYS:HE3	1:A:353:TRP:NE1	2.33	0.43
1:B:172:ASP:N	1:B:172:ASP:OD1	2.42	0.43
1:A:372:ASN:ND2	6:A:629:HOH:O	2.50	0.43
1:B:85[A]:TRP:HE1	1:B:433:ARG:CG	2.28	0.43
1:A:392:ASN:O	1:A:393:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:VAL:HG12	1:B:436:TYR:HE2	1.83	0.43
1:B:51[A]:MET:CE	1:B:364:MET:CE	2.96	0.43
1:A:306:ALA:O	1:A:336:THR:HA	2.17	0.43
1:A:411:TYR:CG	1:A:412:SER:N	2.87	0.43
6:B:623:HOH:O	2:E:5:FRU:H5	2.18	0.42
1:B:127:LYS:NZ	6:B:631:HOH:O	2.51	0.42
1:B:126:GLN:NE2	1:B:135:SER:OG	2.52	0.42
1:B:343[B]:ARG:NE	1:B:412:SER:OG	2.52	0.42
1:A:58:GLN:NE2	6:A:639:HOH:O	2.52	0.42
1:A:455:LYS:HD3	6:A:611:HOH:O	2.19	0.42
1:B:306:ALA:O	1:B:336:THR:HA	2.19	0.42
1:B:417:PRO:HA	1:B:424:VAL:HG12	2.02	0.42
1:A:274:GLU:HA	1:A:307:GLU:HG2	2.02	0.42
1:B:297:LEU:HD12	1:B:297:LEU:HA	1.80	0.42
1:B:35:LYS:HD2	1:B:35:LYS:HA	1.76	0.41
1:A:291:ARG:O	1:A:295:GLN:HG2	2.21	0.41
1:B:158:ASP:CG	1:B:186[B]:HIS:HE2	2.20	0.41
1:A:452:LYS:HZ1	1:B:59:LYS:HE3	1.85	0.41
1:A:264:ASN:ND2	1:A:339:ASP:OD1	2.53	0.41
1:A:202:SER:O	1:A:203:ASP:HB2	2.20	0.41
1:B:85[B]:TRP:CH2	1:B:433:ARG:NH2	2.87	0.41
1:B:433:ARG:NH1	6:B:623:HOH:O	2.48	0.41
1:A:160:THR:HA	2:D:4:FRU:H61	2.03	0.41
1:A:80:LYS:HD2	1:A:80:LYS:C	2.40	0.41
1:A:43:ILE:HG22	1:A:329:LYS:HD2	2.03	0.40
1:A:202:SER:O	1:A:204:SER:N	2.42	0.40
1:B:118:ASP:OD1	6:B:603:HOH:O	2.21	0.40
1:B:44:SER:O	1:B:332:ILE:HG13	2.20	0.40
1:B:51[A]:MET:HE3	1:B:54:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/466 (95%)	424 (96%)	19 (4%)	1 (0%)	47	39
1	B	448/466 (96%)	433 (97%)	13 (3%)	2 (0%)	34	24
All	All	892/932 (96%)	857 (96%)	32 (4%)	3 (0%)	41	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	SER
1	A	431	THR
1	B	431	THR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/406 (96%)	384 (99%)	5 (1%)	69	67
1	B	393/406 (97%)	389 (99%)	4 (1%)	76	75
All	All	782/812 (96%)	773 (99%)	9 (1%)	71	70

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	SER
1	A	204	SER
1	A	399	LYS
1	A	412	SER
1	A	420	LYS
1	B	126	GLN
1	B	302	LYS
1	B	339	ASP
1	B	412	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	152	ASN
1	B	405	ASN

### 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 ⓘ

20 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	FRU	C	1	2	11,12,12	4.57	7 (63%)	10,18,18	1.80	2 (20%)
2	FRU	C	2	2	11,11,12	4.42	8 (72%)	15,15,18	1.17	2 (13%)
2	FRU	C	3	2	11,11,12	4.28	8 (72%)	15,15,18	2.53	8 (53%)
2	FRU	C	4	2	11,11,12	4.45	8 (72%)	15,15,18	1.25	2 (13%)
2	FRU	C	5	2	11,11,12	4.29	8 (72%)	15,15,18	1.84	4 (26%)
2	FRU	C	6	2	11,11,12	4.12	8 (72%)	15,15,18	1.32	2 (13%)
2	FRU	D	1	2	11,12,12	4.64	7 (63%)	10,18,18	4.92	1 (10%)
2	FRU	D	2	2	11,11,12	4.51	8 (72%)	15,15,18	1.31	1 (6%)
2	FRU	D	3	2	11,11,12	4.51	8 (72%)	15,15,18	1.16	1 (6%)
2	FRU	D	4	2	11,11,12	4.09	8 (72%)	15,15,18	2.20	5 (33%)
2	FRU	D	5	2	11,11,12	4.32	8 (72%)	15,15,18	1.70	2 (13%)
2	FRU	D	6	2	11,11,12	4.50	8 (72%)	15,15,18	0.95	1 (6%)
2	FRU	E	1	2	11,12,12	4.47	7 (63%)	10,18,18	3.62	2 (20%)
2	FRU	E	2	2	11,11,12	4.50	8 (72%)	15,15,18	1.48	3 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FRU	E	3	2	11,11,12	4.52	8 (72%)	15,15,18	1.74	4 (26%)
2	FRU	E	4	2	11,11,12	4.50	8 (72%)	15,15,18	2.72	3 (20%)
2	FRU	E	5	2	11,11,12	4.74	7 (63%)	15,15,18	1.48	3 (20%)
2	FRU	E	6	2	11,11,12	4.26	8 (72%)	15,15,18	1.82	6 (40%)
3	FRU	F	1	3	11,12,12	4.36	7 (63%)	10,18,18	1.10	1 (10%)
3	FRU	F	2	3	10,10,12	5.18	8 (80%)	12,14,18	1.89	2 (16%)

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	FRU	C	1	2	-	3/5/24/24	0/1/1/1
2	FRU	C	2	2	-	1/4/20/24	0/1/1/1
2	FRU	C	3	2	-	1/4/20/24	0/1/1/1
2	FRU	C	4	2	-	1/4/20/24	0/1/1/1
2	FRU	C	5	2	-	2/4/20/24	0/1/1/1
2	FRU	C	6	2	-	0/4/20/24	0/1/1/1
2	FRU	D	1	2	-	3/5/24/24	0/1/1/1
2	FRU	D	2	2	-	2/4/20/24	0/1/1/1
2	FRU	D	3	2	-	2/4/20/24	0/1/1/1
2	FRU	D	4	2	-	0/4/20/24	0/1/1/1
2	FRU	D	5	2	-	2/4/20/24	0/1/1/1
2	FRU	D	6	2	-	0/4/20/24	0/1/1/1
2	FRU	E	1	2	-	3/5/24/24	0/1/1/1
2	FRU	E	2	2	-	2/4/20/24	0/1/1/1
2	FRU	E	3	2	-	4/4/20/24	0/1/1/1
2	FRU	E	4	2	-	4/4/20/24	0/1/1/1
2	FRU	E	5	2	-	3/4/20/24	0/1/1/1
2	FRU	E	6	2	-	0/4/20/24	0/1/1/1
3	FRU	F	1	3	-	0/5/24/24	0/1/1/1
3	FRU	F	2	3	-	2/2/18/24	0/1/1/1

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	FRU	C4-C3	-11.10	1.22	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	FRU	C4-C3	-10.50	1.24	1.53
2	E	3	FRU	C4-C3	-10.36	1.25	1.53
2	E	2	FRU	C4-C3	-10.25	1.25	1.53
2	C	5	FRU	C4-C3	-10.25	1.25	1.53
2	E	4	FRU	C4-C3	-10.17	1.25	1.53
2	D	5	FRU	C4-C3	-10.12	1.25	1.53
2	D	2	FRU	C4-C3	-10.11	1.25	1.53
2	C	2	FRU	C4-C3	-10.04	1.25	1.53
2	D	6	FRU	C4-C3	-9.89	1.26	1.53
2	C	3	FRU	C4-C3	-9.60	1.27	1.53
3	F	2	FRU	C4-C5	9.48	1.66	1.52
2	C	4	FRU	C4-C3	-9.48	1.27	1.53
2	D	3	FRU	C4-C3	-9.42	1.27	1.53
2	D	4	FRU	C4-C3	-9.15	1.28	1.53
2	E	6	FRU	C4-C3	-8.93	1.28	1.53
2	C	6	FRU	C4-C3	-8.55	1.29	1.53
2	E	5	FRU	O5-C5	-7.71	1.27	1.45
2	C	1	FRU	C1-C2	-7.61	1.39	1.52
3	F	1	FRU	C1-C2	-7.42	1.40	1.52
2	E	1	FRU	C1-C2	-7.26	1.40	1.52
2	D	1	FRU	C1-C2	-7.26	1.40	1.52
2	C	1	FRU	C4-C3	-6.76	1.24	1.52
3	F	1	FRU	C4-C3	-6.71	1.24	1.52
2	D	1	FRU	C4-C3	-6.70	1.24	1.52
2	E	1	FRU	C4-C3	-6.37	1.26	1.52
2	D	1	FRU	O5-C5	-6.22	1.30	1.43
2	D	3	FRU	C4-C5	6.19	1.68	1.53
2	D	1	FRU	O5-C2	6.16	1.52	1.43
2	C	4	FRU	C4-C5	6.15	1.68	1.53
2	E	6	FRU	O5-C5	-6.07	1.31	1.45
2	D	6	FRU	C4-C5	6.03	1.68	1.53
2	C	5	FRU	O5-C5	-6.01	1.31	1.45
2	E	4	FRU	O5-C5	-5.94	1.31	1.45
2	E	3	FRU	O5-C5	-5.91	1.31	1.45
2	E	2	FRU	C4-C5	5.89	1.68	1.53
2	E	4	FRU	C4-C5	5.86	1.68	1.53
2	E	1	FRU	C4-C5	5.86	1.68	1.53
2	D	6	FRU	O5-C5	-5.82	1.32	1.45
2	C	1	FRU	C4-C5	5.82	1.67	1.53
2	C	1	FRU	O5-C2	5.80	1.52	1.43
2	D	1	FRU	C4-C5	5.79	1.67	1.53
2	C	6	FRU	C4-C5	5.79	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	FRU	O5-C5	-5.77	1.32	1.45
2	C	4	FRU	O5-C5	-5.76	1.32	1.45
2	D	2	FRU	C4-C5	5.75	1.67	1.53
2	E	3	FRU	C4-C5	5.66	1.67	1.53
2	E	1	FRU	O5-C5	-5.62	1.31	1.43
2	D	2	FRU	O5-C5	-5.61	1.32	1.45
3	F	1	FRU	C4-C5	5.60	1.67	1.53
2	E	6	FRU	C4-C5	5.60	1.67	1.53
2	C	3	FRU	C4-C5	5.59	1.67	1.53
2	C	1	FRU	O5-C5	-5.55	1.31	1.43
2	D	5	FRU	O5-C5	-5.50	1.32	1.45
3	F	1	FRU	O5-C5	-5.49	1.31	1.43
2	E	1	FRU	O5-C2	5.48	1.51	1.43
2	D	4	FRU	O5-C5	-5.45	1.32	1.45
2	C	2	FRU	O5-C5	-5.42	1.32	1.45
2	C	2	FRU	C4-C5	5.37	1.66	1.53
2	D	3	FRU	O5-C5	-5.29	1.33	1.45
2	C	3	FRU	O5-C5	-5.25	1.33	1.45
2	D	5	FRU	C4-C5	5.20	1.66	1.53
2	C	6	FRU	O5-C5	-5.19	1.33	1.45
2	E	5	FRU	C4-C5	4.88	1.65	1.53
2	E	1	FRU	O3-C3	4.83	1.52	1.42
3	F	1	FRU	O5-C2	4.78	1.50	1.43
2	C	5	FRU	C4-C5	4.70	1.65	1.53
2	D	4	FRU	C4-C5	4.60	1.64	1.53
2	D	1	FRU	O3-C3	4.58	1.51	1.42
2	C	1	FRU	O3-C3	4.26	1.51	1.42
2	D	3	FRU	C3-C2	4.14	1.63	1.53
3	F	2	FRU	O5-C5	-4.14	1.32	1.44
2	C	6	FRU	O5-C2	4.11	1.54	1.45
3	F	1	FRU	O3-C3	4.09	1.50	1.42
2	E	3	FRU	O3-C3	3.98	1.52	1.43
2	C	2	FRU	O3-C3	3.96	1.52	1.43
3	F	2	FRU	O3-C3	3.90	1.52	1.43
2	C	3	FRU	O5-C2	3.84	1.53	1.45
2	D	3	FRU	O3-C3	3.79	1.51	1.43
2	D	4	FRU	O3-C3	3.76	1.51	1.43
2	C	4	FRU	C3-C2	3.76	1.62	1.53
2	E	4	FRU	C1-C2	-3.76	1.39	1.51
2	D	5	FRU	O5-C2	3.71	1.53	1.45
2	D	6	FRU	O3-C3	3.70	1.51	1.43
2	D	3	FRU	O5-C2	3.62	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	FRU	O3-C3	3.60	1.51	1.43
2	D	6	FRU	C3-C2	3.56	1.62	1.53
2	C	4	FRU	C1-C2	-3.54	1.40	1.51
2	D	4	FRU	C3-C2	3.52	1.62	1.53
2	E	6	FRU	O5-C2	3.48	1.52	1.45
2	C	6	FRU	C3-C2	3.48	1.61	1.53
2	C	2	FRU	C1-C2	-3.47	1.40	1.51
2	D	2	FRU	C1-C2	-3.43	1.40	1.51
2	E	2	FRU	C1-C2	-3.42	1.40	1.51
2	D	2	FRU	O3-C3	3.42	1.51	1.43
2	D	2	FRU	O5-C2	3.42	1.52	1.45
2	E	3	FRU	C3-C2	3.41	1.61	1.53
2	E	2	FRU	O5-C2	3.40	1.52	1.45
2	C	2	FRU	C3-C2	3.40	1.61	1.53
2	C	4	FRU	O3-C3	3.37	1.50	1.43
2	E	6	FRU	C3-C2	3.37	1.61	1.53
2	D	6	FRU	O5-C2	3.36	1.52	1.45
2	D	3	FRU	O4-C4	3.36	1.50	1.43
2	D	2	FRU	C3-C2	3.35	1.61	1.53
2	E	5	FRU	C1-C2	-3.34	1.40	1.51
2	E	2	FRU	O3-C3	3.33	1.50	1.43
2	C	5	FRU	O3-C3	3.32	1.50	1.43
2	D	3	FRU	C1-C2	-3.31	1.40	1.51
2	C	6	FRU	O4-C4	3.31	1.50	1.43
2	E	6	FRU	O4-C4	3.31	1.50	1.43
2	D	5	FRU	C3-C2	3.19	1.61	1.53
3	F	2	FRU	C1-C2	-3.18	1.41	1.51
2	C	3	FRU	O3-C3	3.18	1.50	1.43
3	F	2	FRU	O5-C2	3.17	1.52	1.45
2	D	5	FRU	O3-C3	3.12	1.50	1.43
2	C	5	FRU	C3-C2	3.08	1.60	1.53
2	E	5	FRU	O3-C3	3.05	1.50	1.43
3	F	2	FRU	C3-C2	3.05	1.60	1.53
2	C	3	FRU	C3-C2	3.02	1.60	1.53
2	E	3	FRU	C1-C2	-3.01	1.41	1.51
2	E	6	FRU	C1-C2	-2.99	1.41	1.51
2	C	3	FRU	C1-C2	-2.98	1.41	1.51
2	C	4	FRU	O5-C2	2.97	1.51	1.45
2	C	2	FRU	O5-C2	2.97	1.51	1.45
2	D	2	FRU	O4-C4	2.95	1.49	1.43
2	D	6	FRU	C1-C2	-2.91	1.42	1.51
2	E	2	FRU	C3-C2	2.90	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	FRU	O5-C2	2.87	1.51	1.45
2	E	3	FRU	O5-C2	2.84	1.51	1.45
2	C	4	FRU	O4-C4	2.80	1.49	1.43
2	D	6	FRU	O4-C4	2.79	1.49	1.43
2	D	4	FRU	C1-C2	-2.75	1.42	1.51
2	E	4	FRU	O5-C2	2.75	1.51	1.45
2	E	4	FRU	C3-C2	2.71	1.59	1.53
2	C	1	FRU	O4-C4	2.66	1.49	1.43
2	E	6	FRU	O3-C3	2.65	1.49	1.43
2	C	6	FRU	O3-C3	2.65	1.49	1.43
2	E	5	FRU	C3-C2	2.61	1.59	1.53
2	C	2	FRU	O4-C4	2.60	1.49	1.43
3	F	2	FRU	O4-C4	2.55	1.49	1.43
2	C	5	FRU	O5-C2	2.54	1.50	1.45
2	C	3	FRU	O4-C4	2.53	1.48	1.43
2	C	6	FRU	C1-C2	-2.51	1.43	1.51
2	C	5	FRU	C1-C2	-2.51	1.43	1.51
2	E	5	FRU	O5-C2	2.48	1.50	1.45
2	E	4	FRU	O4-C4	2.48	1.48	1.43
3	F	1	FRU	O4-C4	2.40	1.48	1.43
2	D	1	FRU	O4-C4	2.38	1.48	1.43
2	D	5	FRU	O4-C4	2.37	1.48	1.43
2	E	1	FRU	O4-C4	2.37	1.48	1.43
2	D	4	FRU	O4-C4	2.35	1.48	1.43
2	C	5	FRU	O4-C4	2.23	1.48	1.43
2	E	2	FRU	O4-C4	2.22	1.48	1.43
2	D	5	FRU	C1-C2	-2.17	1.44	1.51
2	E	3	FRU	O4-C4	2.15	1.48	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	FRU	O6-C6-C5	15.07	162.99	111.29
2	E	1	FRU	O6-C6-C5	11.05	149.22	111.29
2	E	4	FRU	O6-C6-C5	9.27	143.10	111.29
2	C	3	FRU	O5-C2-C1	6.37	122.98	109.21
3	F	2	FRU	C6-C5-C4	-5.60	109.81	115.70
2	C	1	FRU	O6-C6-C5	-4.75	94.99	111.29
2	D	5	FRU	O6-C6-C5	-4.54	95.73	111.29
2	D	4	FRU	O5-C2-C3	-4.27	96.67	105.11
2	E	3	FRU	O6-C6-C5	3.87	124.57	111.29
2	E	5	FRU	O5-C5-C6	-3.75	101.11	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	FRU	O5-C2-C1	3.69	117.18	109.21
2	D	4	FRU	O4-C4-C5	-3.67	100.44	111.05
2	D	2	FRU	O6-C6-C5	-3.65	98.77	111.29
2	E	6	FRU	O3-C3-C2	-3.38	101.29	111.05
2	D	4	FRU	O5-C2-C1	3.16	116.05	109.21
2	C	3	FRU	O5-C2-C3	-3.15	98.88	105.11
2	D	4	FRU	O6-C6-C5	-3.15	100.50	111.29
2	D	5	FRU	C6-C5-C4	-3.13	107.53	115.09
2	E	2	FRU	C1-C2-C3	-3.11	107.60	115.09
2	C	3	FRU	O5-C5-C6	3.09	115.90	109.21
2	E	3	FRU	C3-C4-C5	3.01	108.49	102.64
2	C	5	FRU	C6-C5-C4	-3.00	107.86	115.09
2	E	6	FRU	O5-C2-C1	2.90	115.48	109.21
2	E	5	FRU	C6-C5-C4	-2.86	108.18	115.09
2	C	3	FRU	C6-C5-C4	-2.81	108.32	115.09
2	D	4	FRU	C6-C5-C4	-2.79	108.35	115.09
2	C	4	FRU	C6-C5-C4	-2.72	108.52	115.09
2	C	4	FRU	O6-C6-C5	2.71	120.57	111.29
2	E	6	FRU	O5-C2-C3	-2.69	99.80	105.11
2	E	3	FRU	C1-C2-C3	-2.66	108.67	115.09
2	E	6	FRU	C6-C5-C4	-2.55	108.93	115.09
2	C	5	FRU	O5-C2-C3	-2.43	100.30	105.11
2	C	3	FRU	O3-C3-C2	-2.41	104.08	111.05
2	E	4	FRU	C1-C2-C3	-2.40	109.31	115.09
2	E	2	FRU	C3-C4-C5	2.37	107.25	102.64
2	C	5	FRU	O3-C3-C2	-2.37	104.20	111.05
2	E	5	FRU	O6-C6-C5	-2.36	103.19	111.29
2	D	6	FRU	C3-C4-C5	2.35	107.20	102.64
2	C	1	FRU	C6-C5-C4	-2.34	109.45	115.09
2	C	3	FRU	C4-C3-C2	-2.33	98.11	102.64
3	F	1	FRU	O1-C1-C2	-2.29	106.99	111.86
2	C	3	FRU	O4-C4-C5	-2.25	104.55	111.05
2	C	6	FRU	O5-C2-C1	2.25	114.07	109.21
3	F	2	FRU	O5-C2-C1	2.24	114.06	109.21
2	E	6	FRU	O4-C4-C3	2.21	118.96	111.82
2	C	2	FRU	C1-C2-C3	-2.19	109.80	115.09
2	C	3	FRU	C1-C2-C3	-2.19	109.80	115.09
2	D	3	FRU	C6-C5-C4	-2.16	109.89	115.09
2	E	2	FRU	C6-C5-C4	-2.15	109.90	115.09
2	E	3	FRU	C4-C3-C2	2.13	106.78	102.64
2	E	1	FRU	C5-C4-C3	2.13	108.74	101.91
2	E	6	FRU	O1-C1-C2	2.06	118.35	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	FRU	O1-C1-C2	-2.05	104.27	111.29
2	C	6	FRU	O4-C4-C3	2.01	118.34	111.82
2	C	2	FRU	C6-C5-C4	-2.00	110.25	115.09

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	FRU	O1-C1-C2-C3
2	E	1	FRU	O1-C1-C2-O2
2	E	1	FRU	O1-C1-C2-O5
2	D	1	FRU	O1-C1-C2-C3
2	C	1	FRU	O1-C1-C2-C3
2	C	1	FRU	O1-C1-C2-O2
2	D	3	FRU	O1-C1-C2-O5
3	F	2	FRU	O1-C1-C2-O5
2	D	3	FRU	O1-C1-C2-C3
2	D	2	FRU	O1-C1-C2-O5
2	D	2	FRU	O1-C1-C2-C3
2	E	3	FRU	O1-C1-C2-C3
2	E	4	FRU	C4-C5-C6-O6
2	E	4	FRU	O1-C1-C2-O5
3	F	2	FRU	O1-C1-C2-C3
2	C	5	FRU	O1-C1-C2-O5
2	E	3	FRU	O1-C1-C2-O5
2	E	4	FRU	O1-C1-C2-C3
2	E	4	FRU	O5-C5-C6-O6
2	D	1	FRU	O1-C1-C2-O5
2	C	1	FRU	O1-C1-C2-O5
2	C	5	FRU	O1-C1-C2-C3
2	E	5	FRU	C4-C5-C6-O6
2	C	4	FRU	O1-C1-C2-O5
2	E	2	FRU	O1-C1-C2-C3
2	D	1	FRU	O1-C1-C2-O2
2	E	5	FRU	O1-C1-C2-O5
2	E	5	FRU	O5-C5-C6-O6
2	E	3	FRU	O5-C5-C6-O6
2	C	3	FRU	O1-C1-C2-O5
2	D	5	FRU	O1-C1-C2-C3
2	E	2	FRU	O1-C1-C2-O5
2	D	5	FRU	O1-C1-C2-O5
2	C	2	FRU	O1-C1-C2-O5

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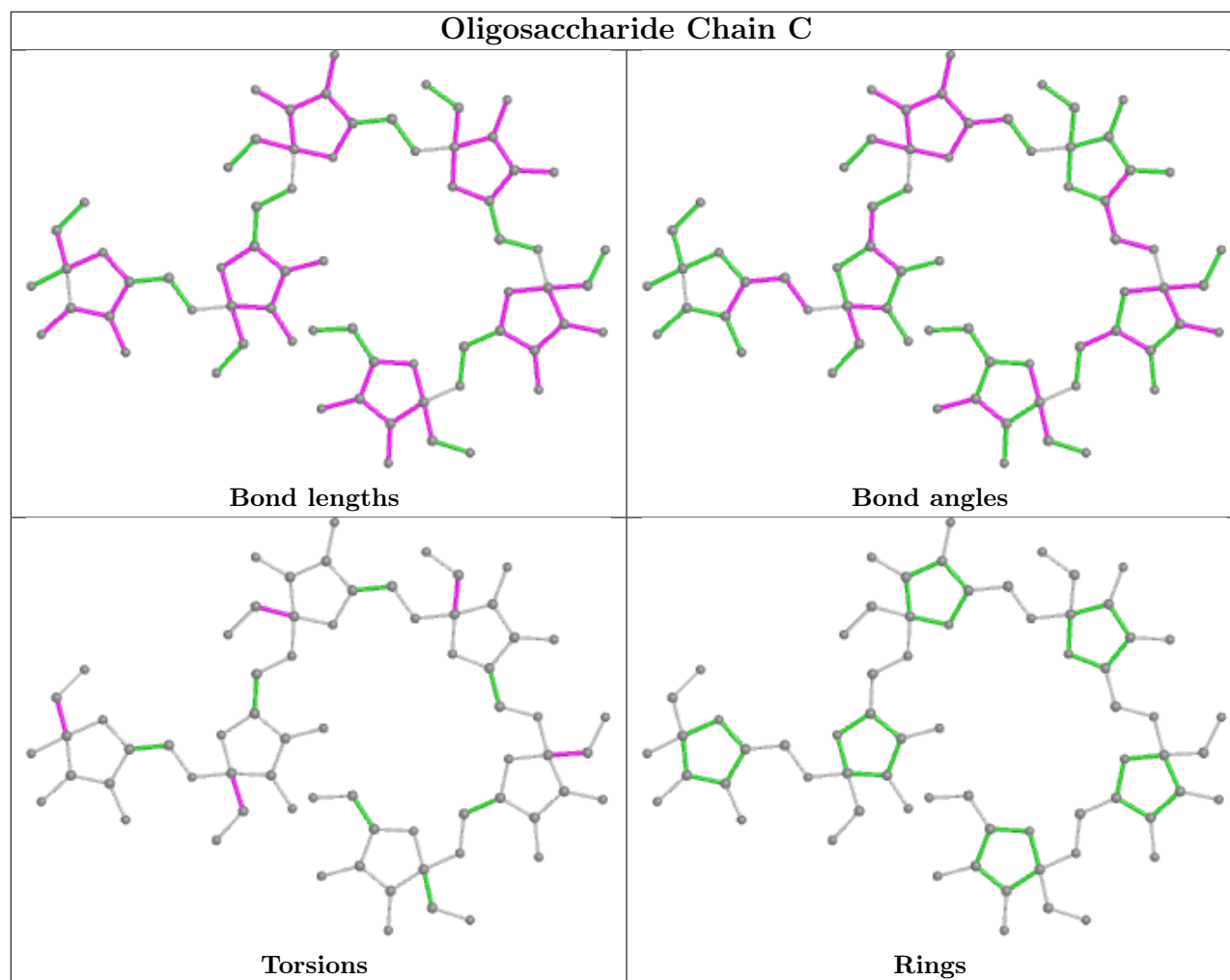
Mol	Chain	Res	Type	Atoms
2	E	3	FRU	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

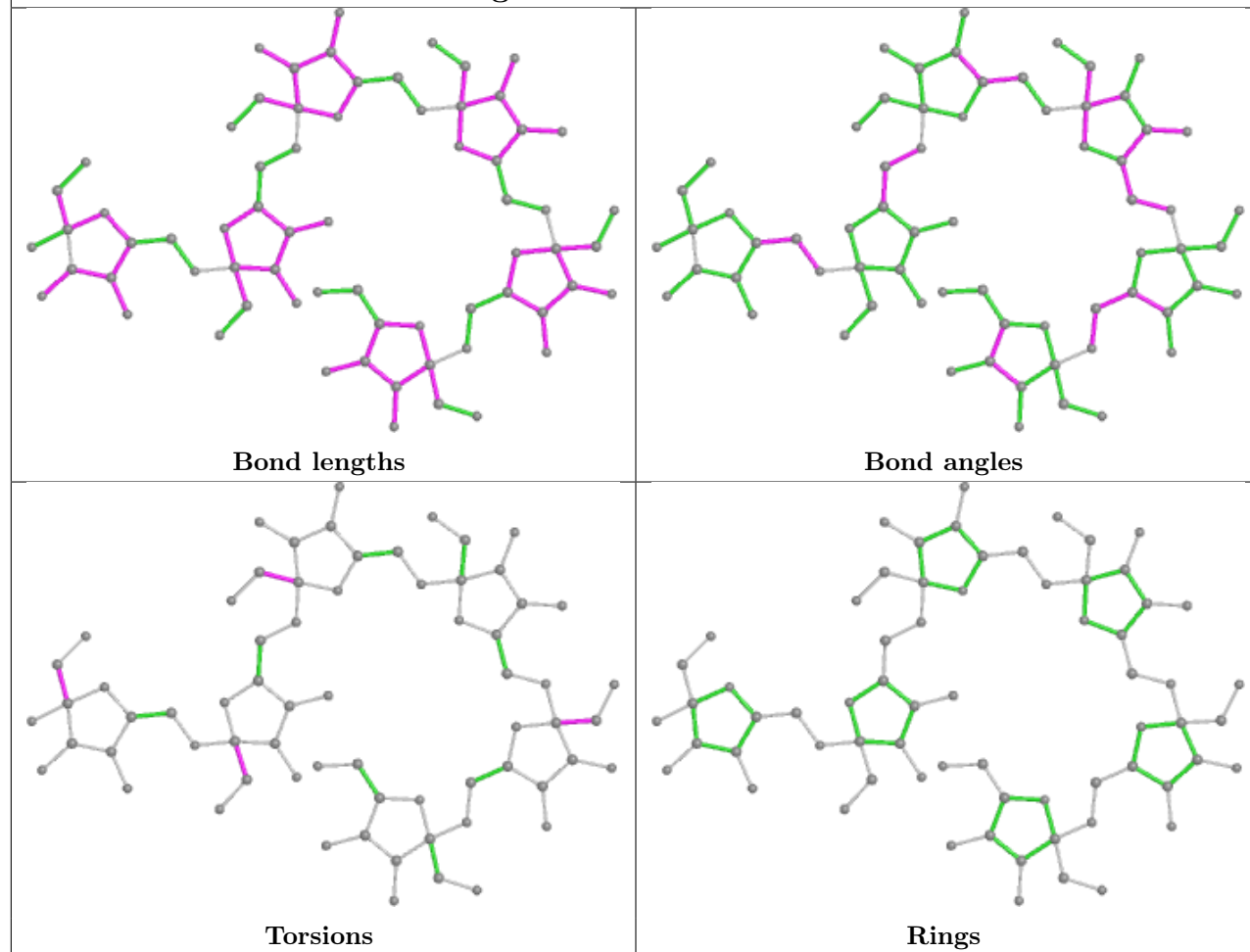
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	5	FRU	1	0
3	F	1	FRU	1	0
2	D	4	FRU	1	0

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

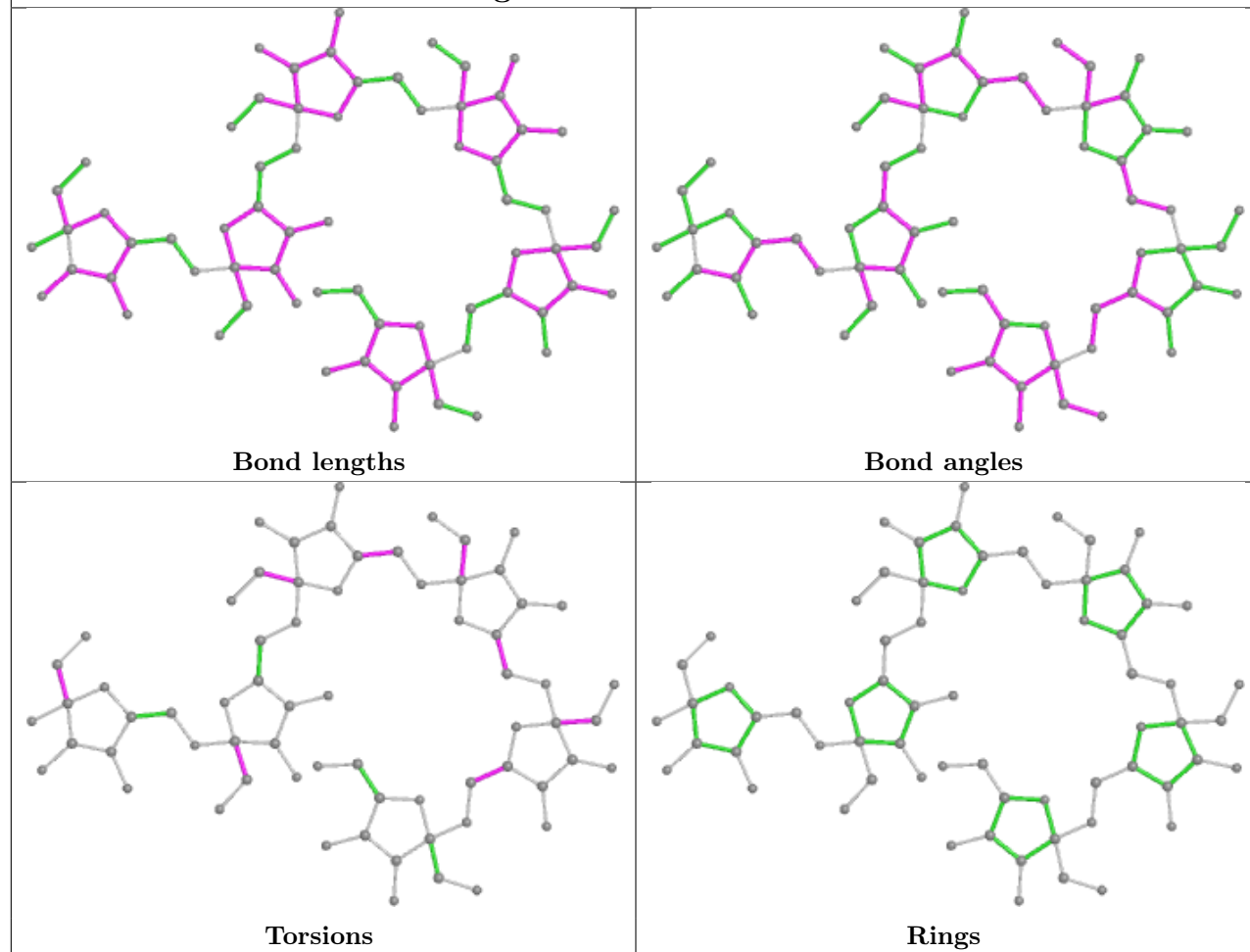


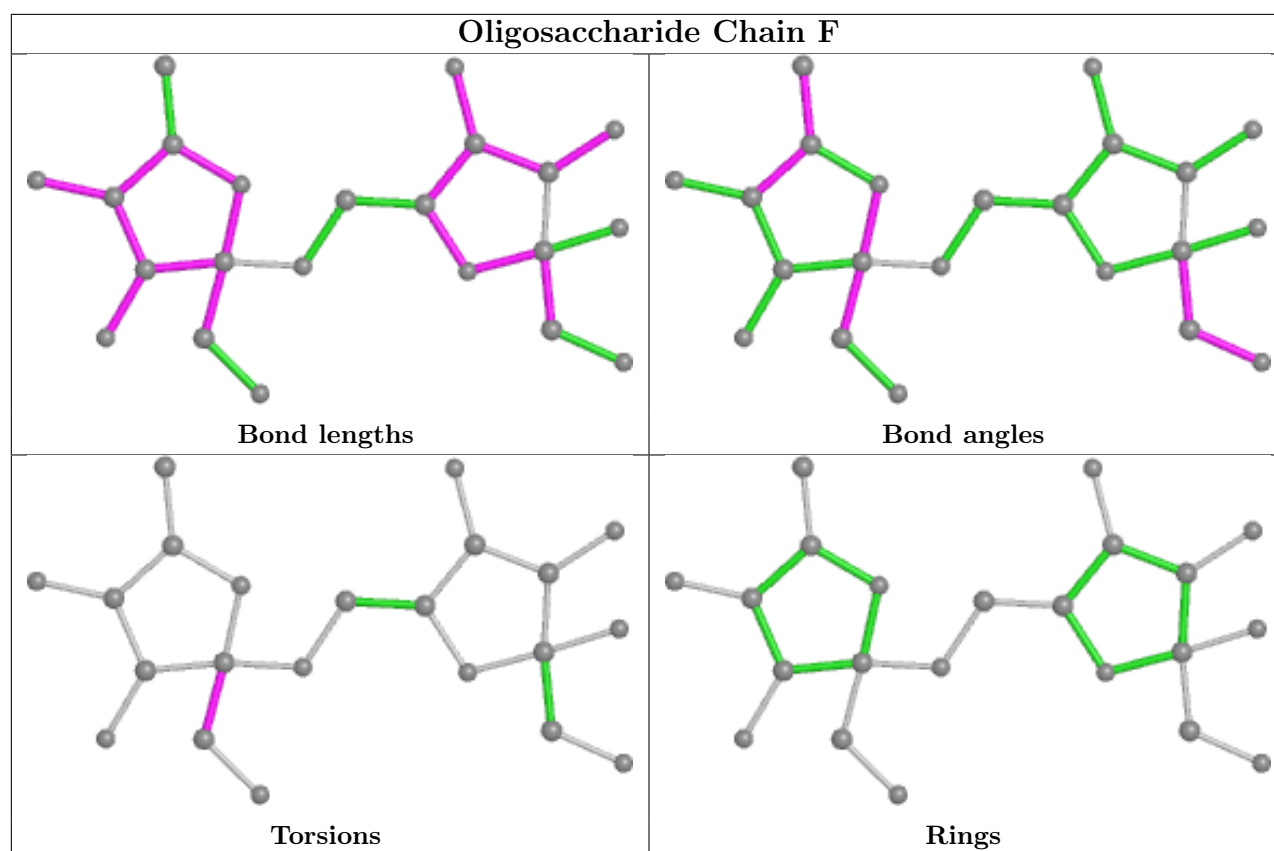


## Oligosaccharide Chain D



## Oligosaccharide Chain E





## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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	440/466 (94%)	0.01	17 (3%) 39 42	13, 24, 45, 78	0
1	B	440/466 (94%)	0.21	37 (8%) 11 11	10, 25, 55, 86	0
All	All	880/932 (94%)	0.11	54 (6%) 21 22	10, 24, 49, 86	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	ASP	6.3
1	A	202	SER	5.6
1	B	116	ALA	5.6
1	B	436	TYR	5.3
1	B	434	GLY	5.1
1	B	295	GLN	4.2
1	B	201	ALA	4.0
1	B	205	SER	3.9
1	B	438	ASP	3.9
1	B	113	PRO	3.8
1	A	201	ALA	3.8
1	B	81	GLY	3.7
1	B	440	GLN	3.7
1	B	115	ASN	3.7
1	A	203	ASP	3.6
1	B	435	PHE	3.5
1	B	437	ALA	3.4
1	B	292	GLN	3.4
1	B	299	GLN	3.3
1	A	152	ASN	3.3
1	B	433	ARG	3.2
1	B	128	VAL	3.2
1	A	342	ALA	3.1
1	B	129	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	291	ARG	3.0
1	B	79	ALA	3.0
1	B	112	ASP	2.9
1	B	461	ASP	2.9
1	B	80	LYS	2.9
1	A	344	ALA	2.8
1	B	432	ASN	2.6
1	B	439	LYS	2.5
1	A	164[A]	SER	2.5
1	B	82	LEU	2.4
1	A	341	ILE	2.4
1	B	405	ASN	2.4
1	A	460	LYS	2.3
1	A	343	ARG	2.3
1	A	295	GLN	2.3
1	B	85[A]	TRP	2.3
1	B	202[A]	SER	2.3
1	A	292	GLN	2.3
1	A	204	SER	2.2
1	A	461	ASP	2.2
1	B	207	ASN	2.2
1	B	199	VAL	2.1
1	B	343[A]	ARG	2.1
1	B	117	ASP	2.1
1	A	200	SER	2.1
1	B	77	SER	2.1
1	A	357	THR	2.1
1	A	101[A]	HIS	2.1
1	B	114	LYS	2.0
1	B	165	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

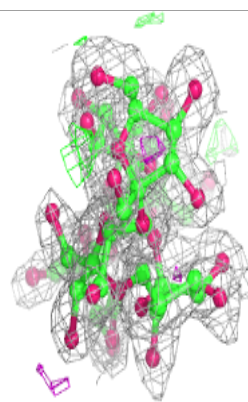
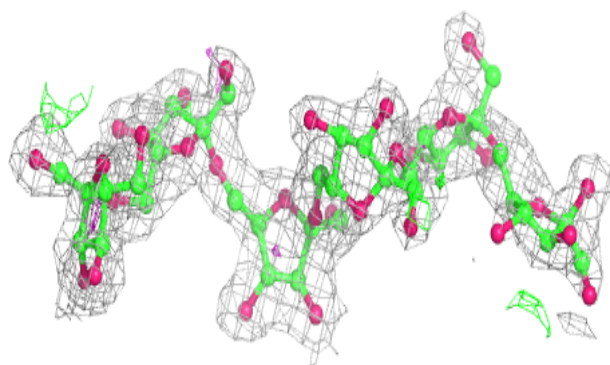
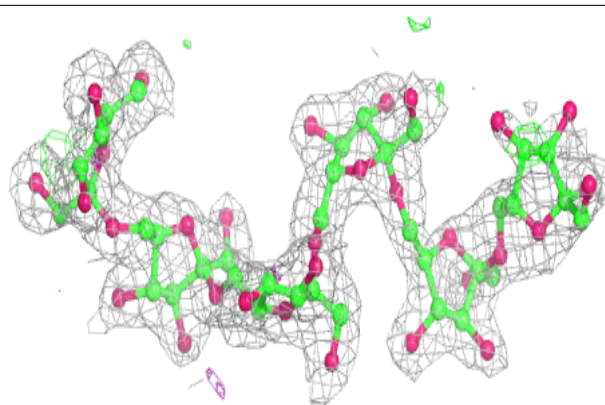
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FRU	E	2	11/12	0.34	0.44	65,70,81,87	1
3	FRU	F	1	12/12	0.47	0.56	40,51,59,68	12
2	FRU	E	1	12/12	0.57	0.35	68,78,93,93	0
3	FRU	F	2	10/12	0.58	0.38	29,51,55,58	10
2	FRU	E	3	11/12	0.67	0.23	52,55,65,70	11
2	FRU	D	1	12/12	0.73	0.29	38,48,59,61	0
2	FRU	E	6	11/12	0.74	0.34	16,27,40,41	11
2	FRU	D	6	11/12	0.79	0.24	35,50,57,61	0
2	FRU	E	4	11/12	0.82	0.22	28,44,48,48	11
2	FRU	C	1	12/12	0.82	0.27	54,62,66,68	0
2	FRU	C	2	11/12	0.83	0.27	38,50,65,65	0
2	FRU	D	5	11/12	0.85	0.15	27,33,46,49	0
2	FRU	D	4	11/12	0.86	0.22	25,31,36,39	0
2	FRU	E	5	11/12	0.86	0.22	30,39,53,58	11
2	FRU	D	2	11/12	0.89	0.27	44,46,53,58	0
2	FRU	C	6	11/12	0.89	0.21	15,23,32,37	0
2	FRU	C	3	11/12	0.90	0.12	28,37,44,44	0
2	FRU	D	3	11/12	0.91	0.14	35,42,52,59	0
2	FRU	C	5	11/12	0.93	0.13	25,30,42,45	0
2	FRU	C	4	11/12	0.94	0.10	23,28,33,34	0

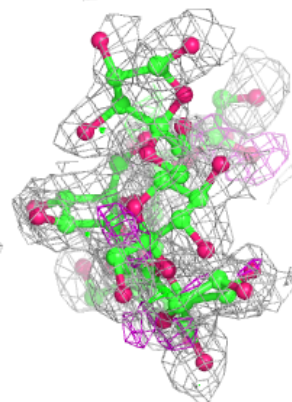
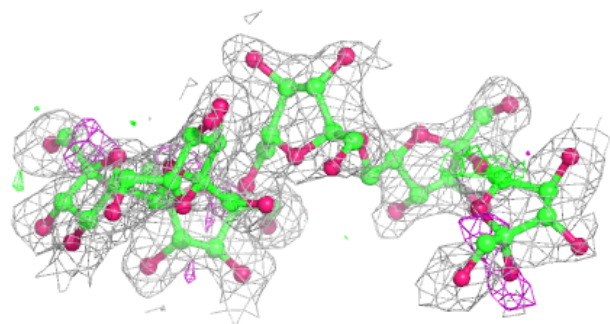
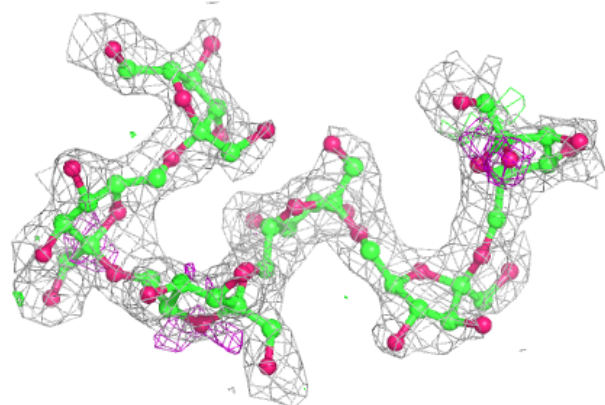
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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)

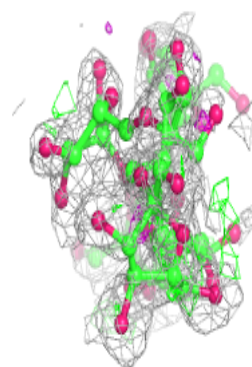
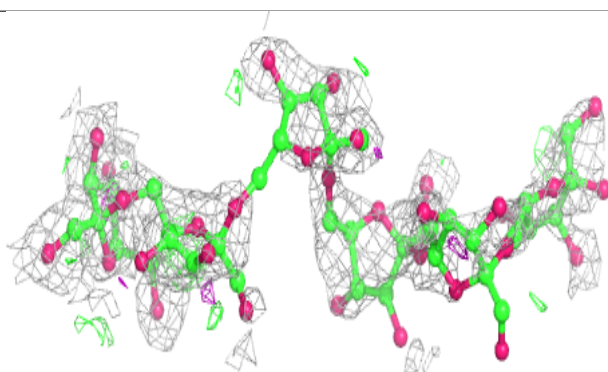
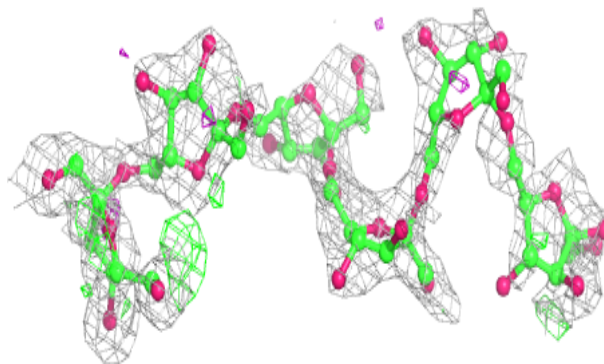
**Electron density around Chain D:**

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

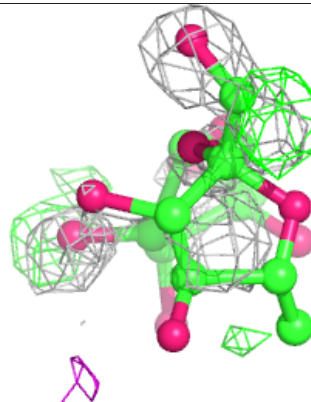
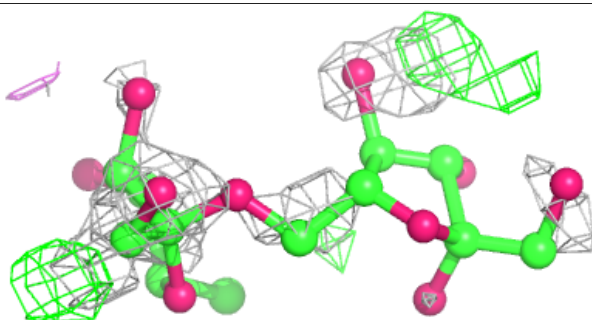
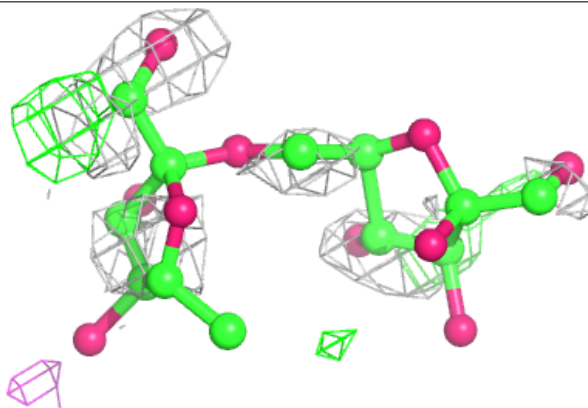


**Electron density around Chain E:**

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

**Electron density around Chain F:**

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





## 6.4 Ligands

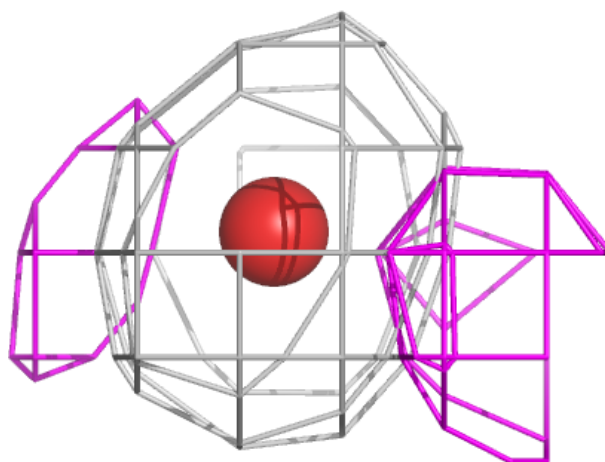
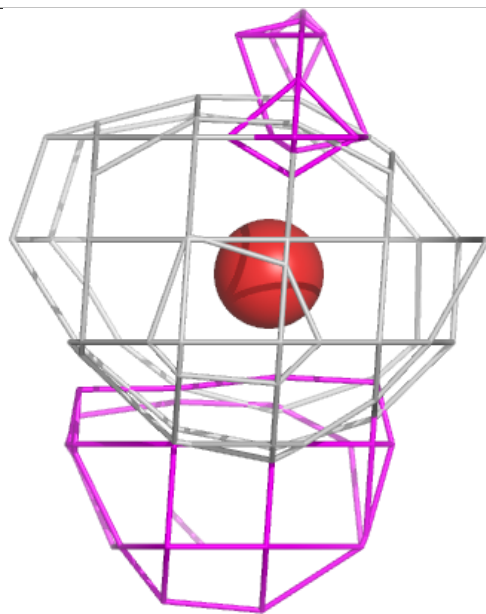
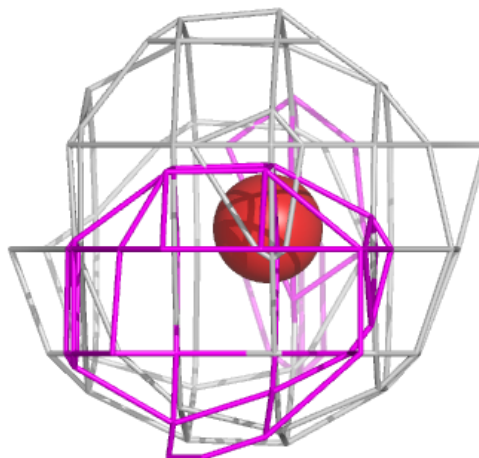
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	BR	A	507	1/1	0.95	0.18	79,79,79,79	0
5	BR	B	502	1/1	0.96	0.08	45,45,45,45	1
5	BR	B	503	1/1	0.98	0.04	38,38,38,38	1
5	BR	B	504	1/1	0.98	0.06	34,34,34,34	1
5	BR	A	506	1/1	0.99	0.06	38,38,38,38	1
5	BR	A	505	1/1	0.99	0.04	25,25,25,25	0
4	CA	A	501	1/1	0.99	0.06	14,14,14,14	0
5	BR	A	502	1/1	0.99	0.06	25,25,25,25	1
4	CA	B	501	1/1	1.00	0.09	15,15,15,15	0
5	BR	A	504	1/1	1.00	0.05	22,22,22,22	1
5	BR	A	503	1/1	1.00	0.04	24,24,24,24	1

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.

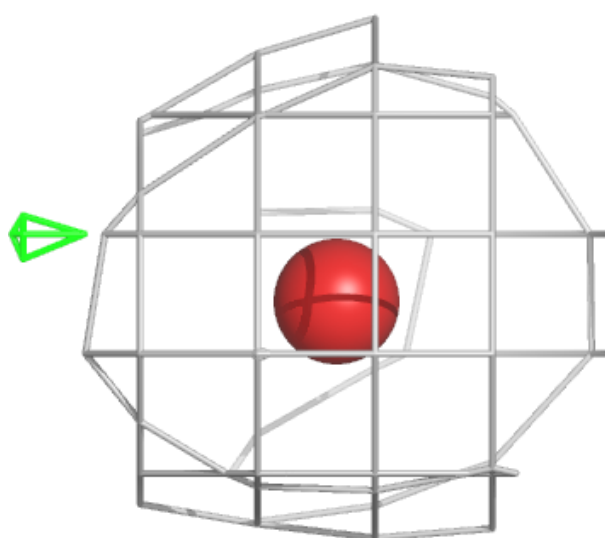
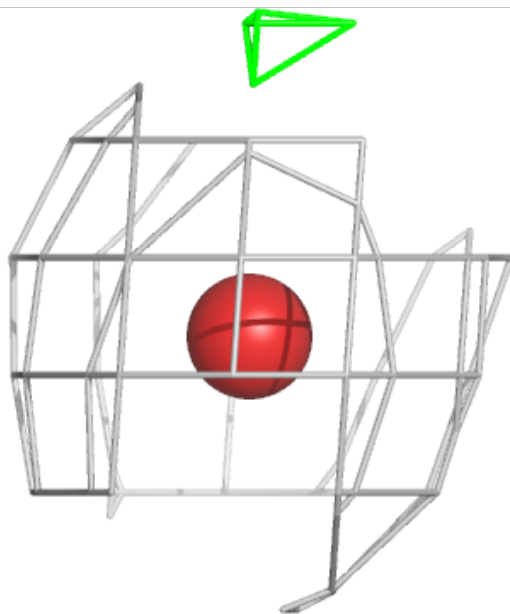
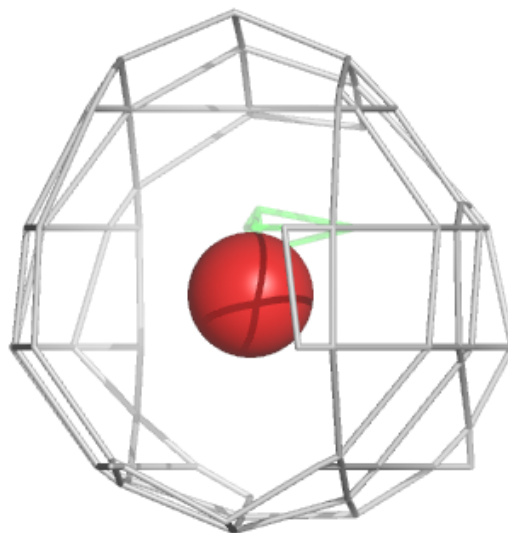
**Electron density around BR A 507:**

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



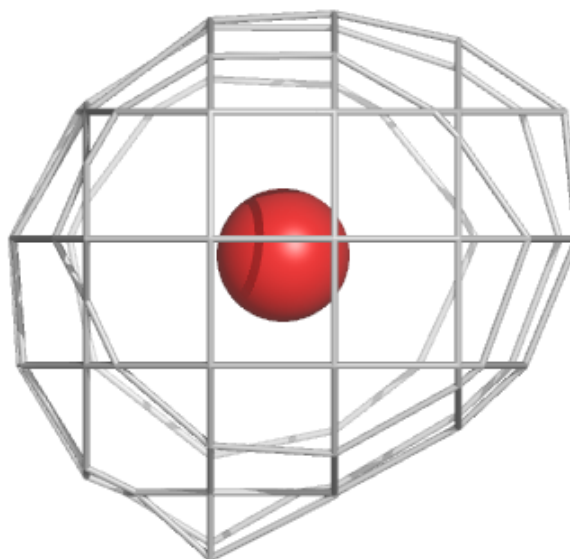
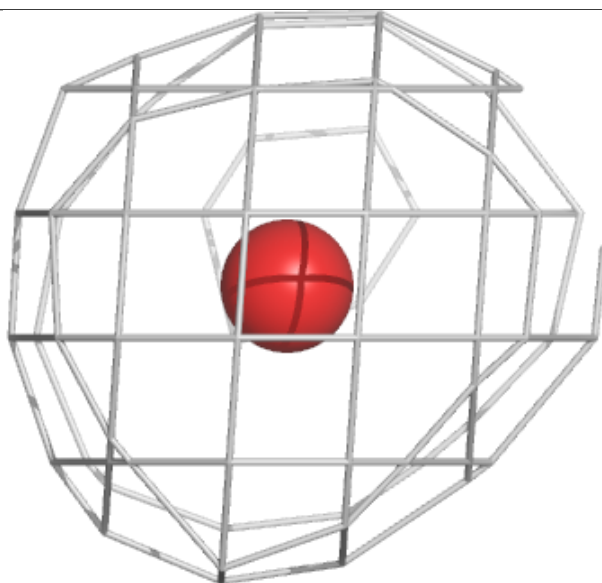
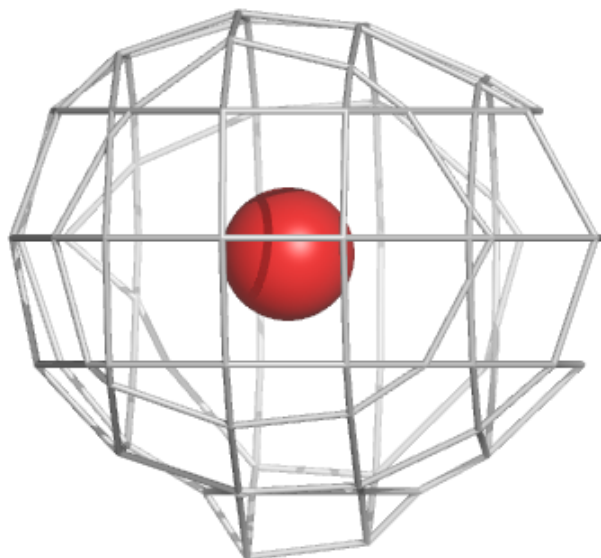
**Electron density around BR B 502:**

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



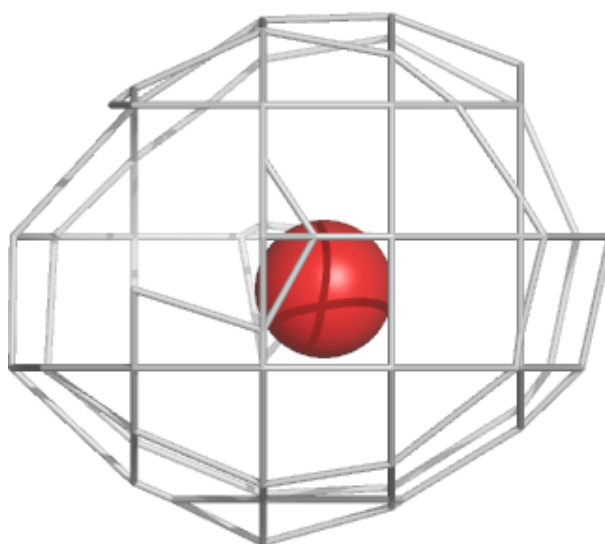
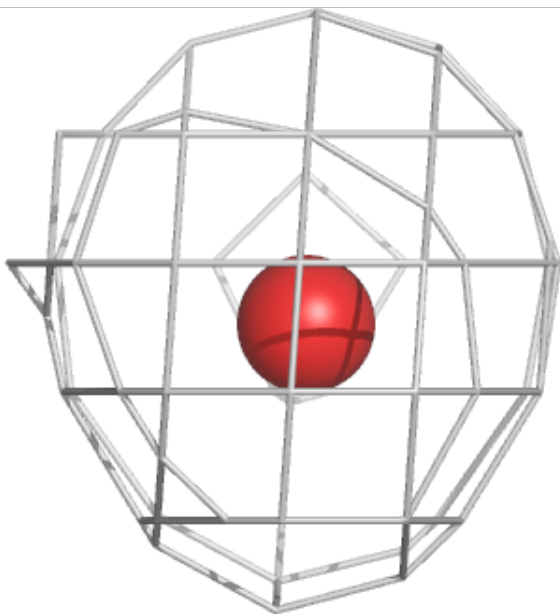
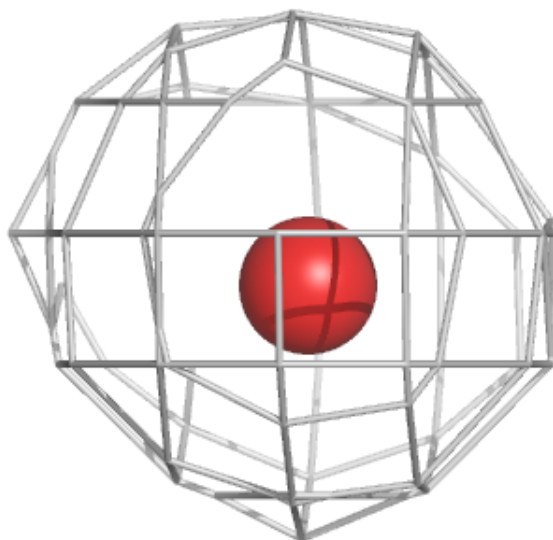
**Electron density around BR B 503:**

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



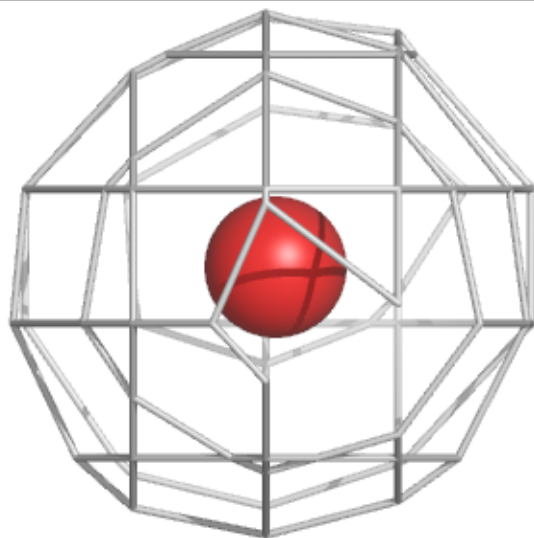
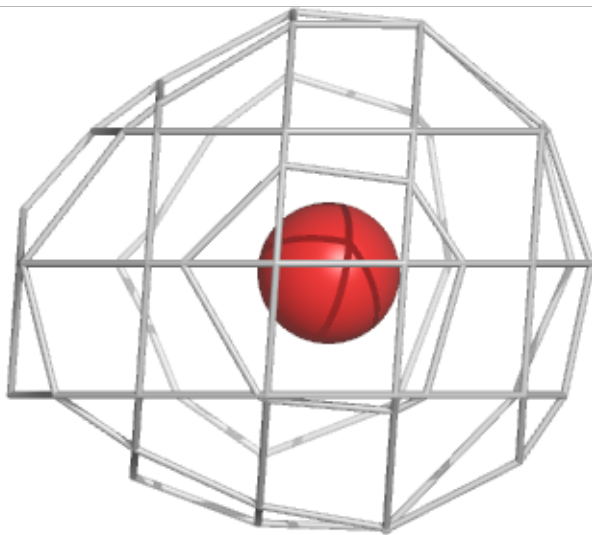
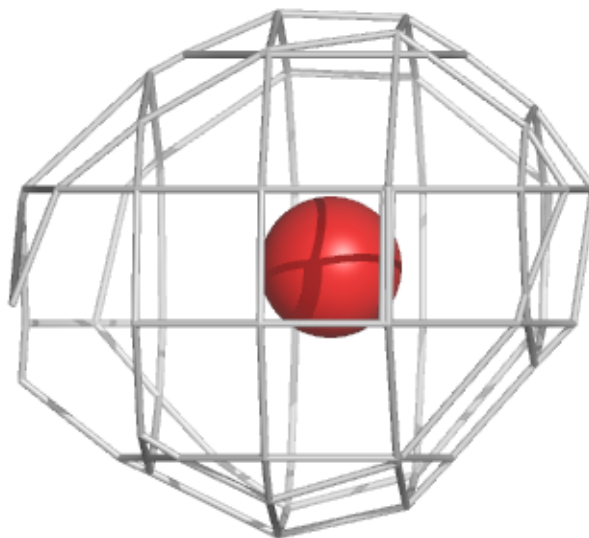
**Electron density around BR B 504:**

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



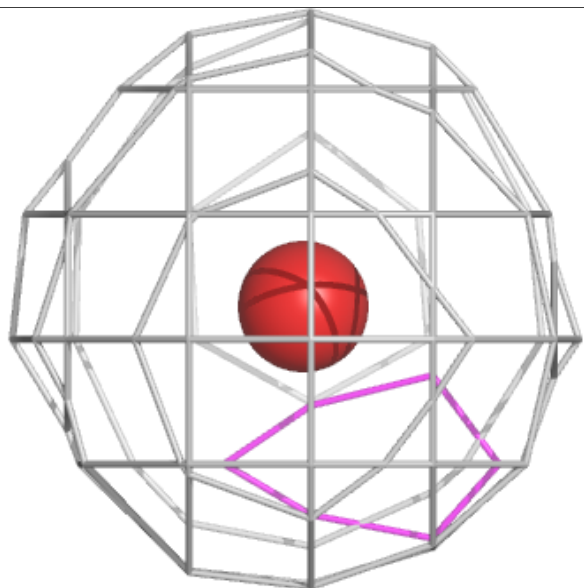
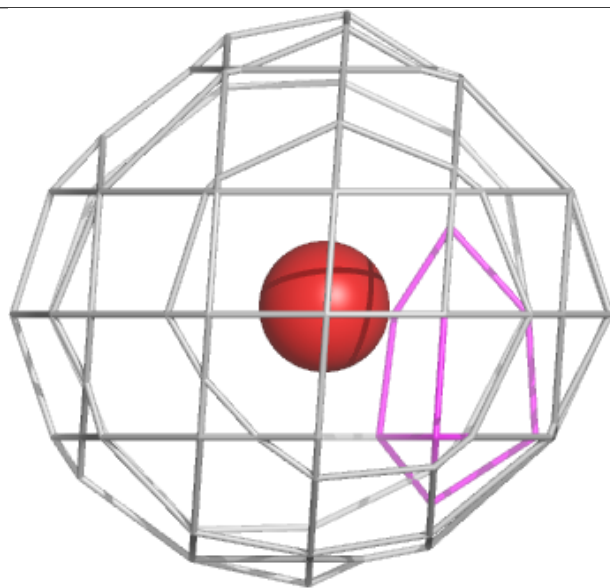
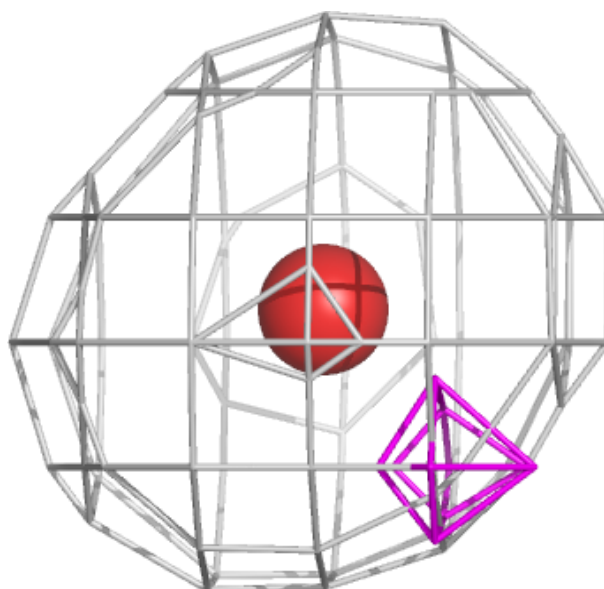
**Electron density around BR A 506:**

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



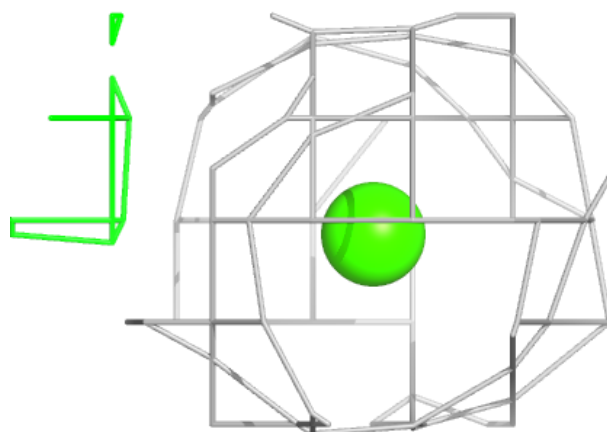
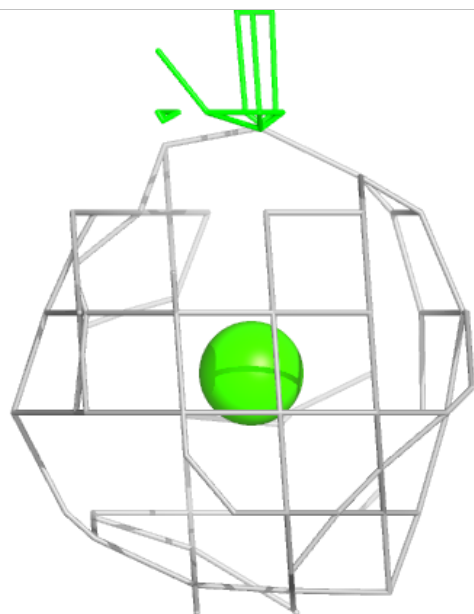
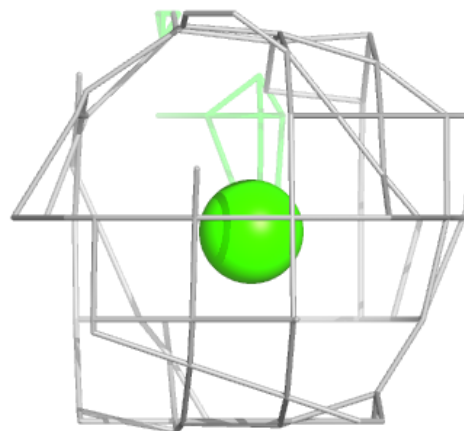
**Electron density around BR A 505:**

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



**Electron density around CA A 501:**

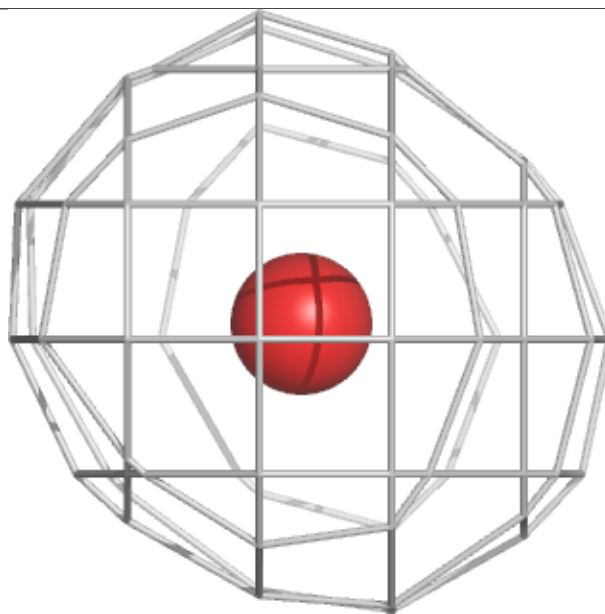
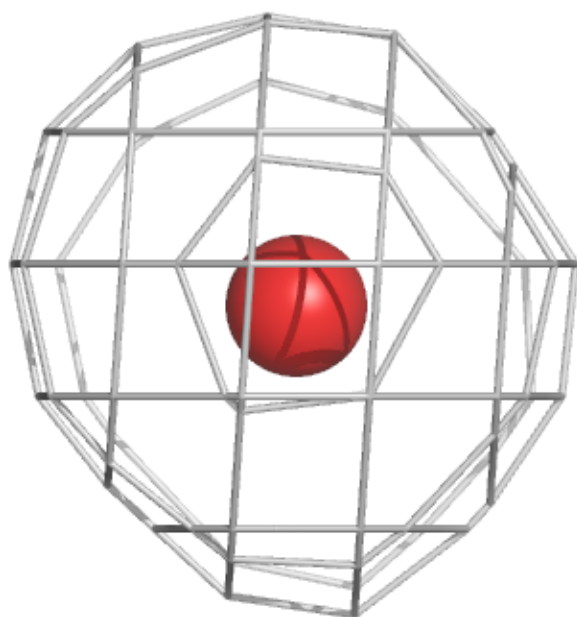
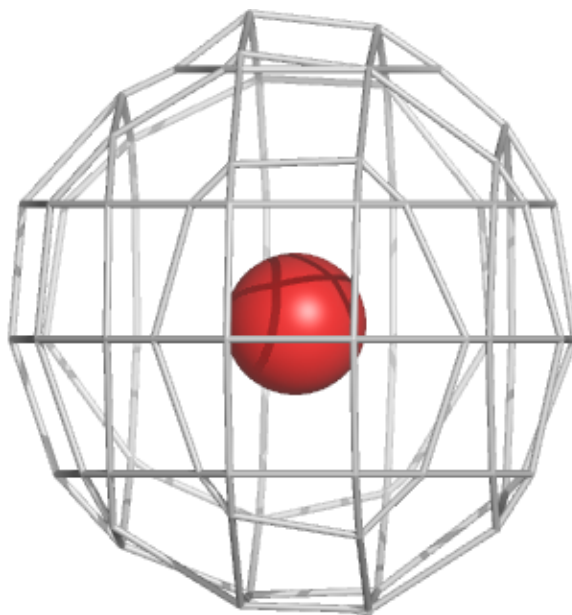
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





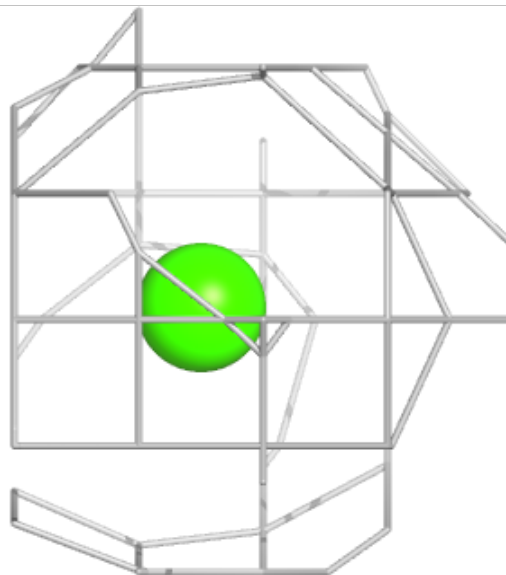
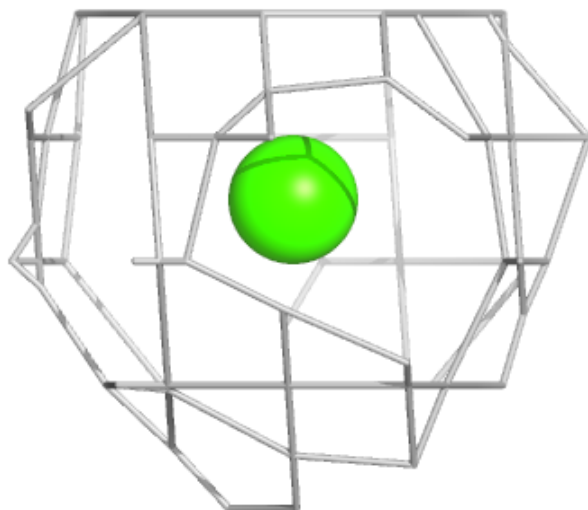
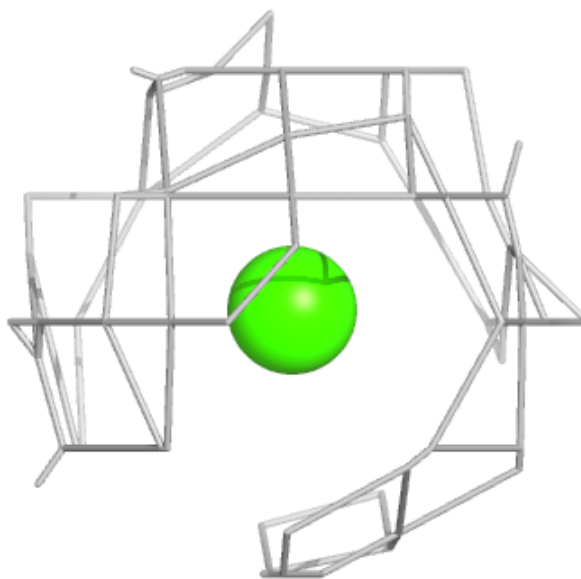
**Electron density around BR A 502:**

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



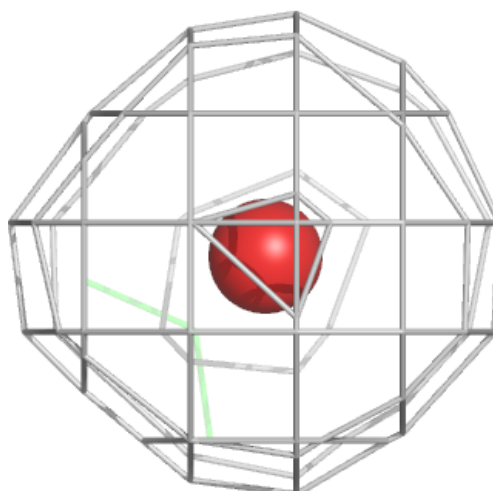
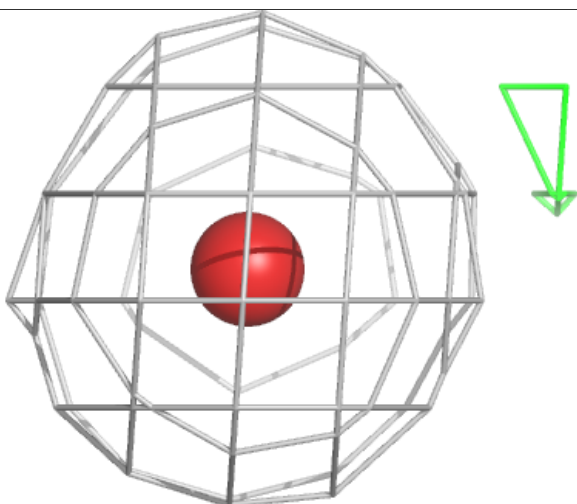
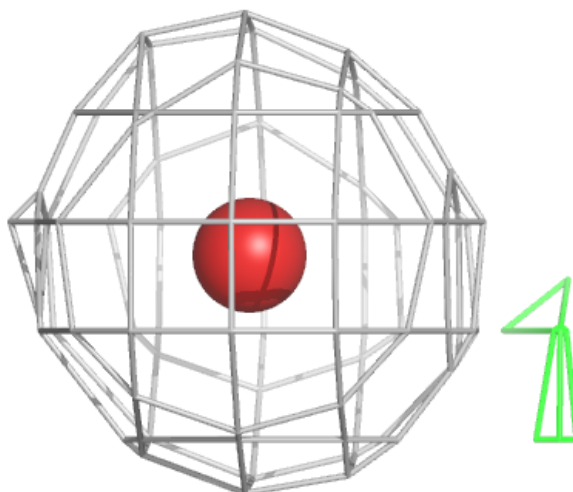
**Electron density around CA B 501:**

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



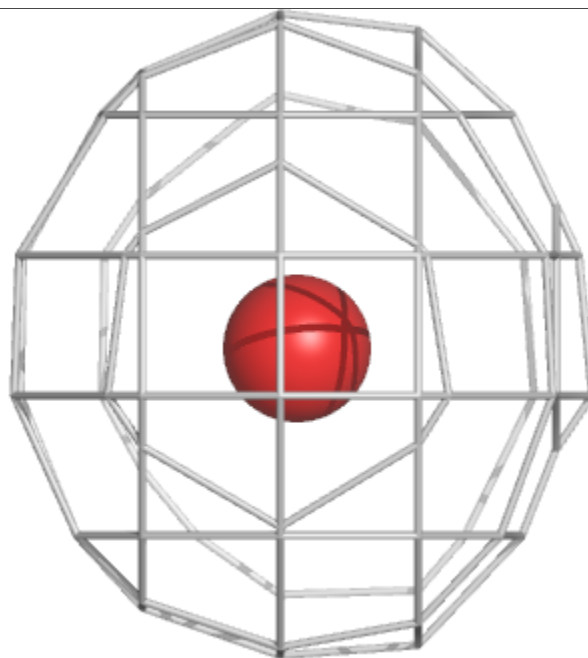
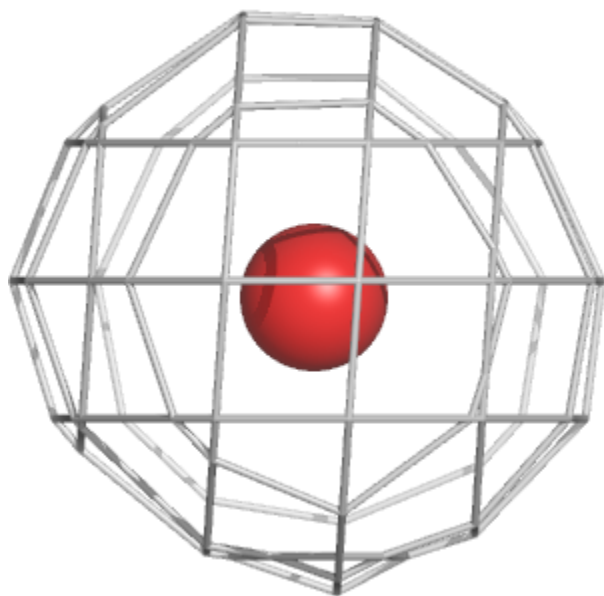
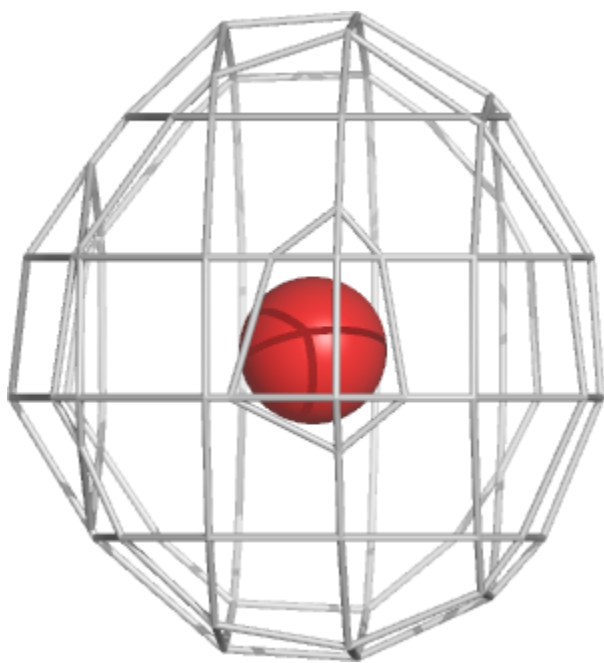
**Electron density around BR A 504:**

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



**Electron density around BR A 503:**

$2mF_o-DF_c$  (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.