Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 09:11 PM EDT

PDB ID	:	7V0I
Title	:	Crystal structure of a CelR catalytic domain active site mutant with bound cellohexaose substrate
Authors	:	Bingman, C.A.; Kuch, N.; Kutsche, M.E.; Parker, A.; Smith, R.W.; Fox, B.G.
Deposited on	:	2022-05-10
Resolution	:	1.90 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*
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:

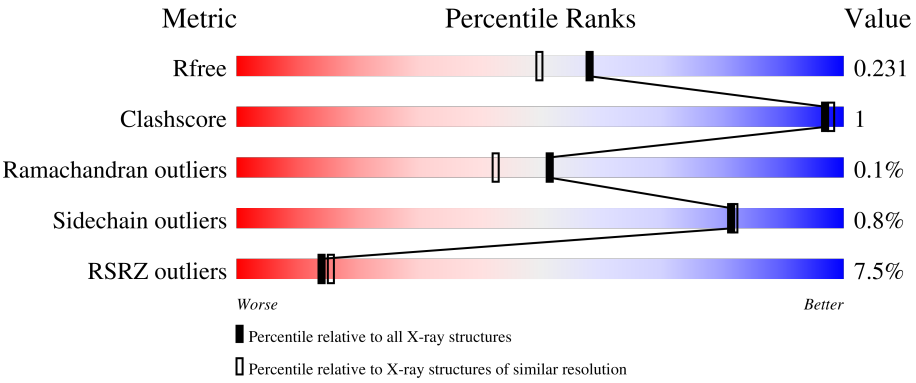
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 >=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 <=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	471	7% 94%
1	B	471	5% 94%
1	C	471	10% 91% 5%
2	D	6	83% 17%
2	E	6	83% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	6	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21883 atoms, of which 10237 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 Glucanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	451	Total	C	H	N	O	S	0	0	0
			6951	2307	3357	595	674	18			
1	B	451	Total	C	H	N	O	S	0	0	0
			6949	2307	3355	595	674	18			
1	C	451	Total	C	H	N	O	S	0	0	0
			6948	2307	3354	595	674	18			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP A3DCY5
A	439	GLN	GLU	conflict	UNP A3DCY5
A	473	ASN	-	expression tag	UNP A3DCY5
A	474	LEU	-	expression tag	UNP A3DCY5
A	475	TYR	-	expression tag	UNP A3DCY5
A	476	PHE	-	expression tag	UNP A3DCY5
A	477	GLN	-	expression tag	UNP A3DCY5
A	478	SER	-	expression tag	UNP A3DCY5
A	479	GLY	-	expression tag	UNP A3DCY5
A	480	SER	-	expression tag	UNP A3DCY5
A	481	HIS	-	expression tag	UNP A3DCY5
A	482	HIS	-	expression tag	UNP A3DCY5
A	483	HIS	-	expression tag	UNP A3DCY5
A	484	HIS	-	expression tag	UNP A3DCY5
A	485	HIS	-	expression tag	UNP A3DCY5
A	486	HIS	-	expression tag	UNP A3DCY5
A	487	HIS	-	expression tag	UNP A3DCY5
A	488	HIS	-	expression tag	UNP A3DCY5
B	18	MET	-	initiating methionine	UNP A3DCY5
B	439	GLN	GLU	conflict	UNP A3DCY5
B	473	ASN	-	expression tag	UNP A3DCY5
B	474	LEU	-	expression tag	UNP A3DCY5
B	475	TYR	-	expression tag	UNP A3DCY5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	476	PHE	-	expression tag	UNP A3DCY5
B	477	GLN	-	expression tag	UNP A3DCY5
B	478	SER	-	expression tag	UNP A3DCY5
B	479	GLY	-	expression tag	UNP A3DCY5
B	480	SER	-	expression tag	UNP A3DCY5
B	481	HIS	-	expression tag	UNP A3DCY5
B	482	HIS	-	expression tag	UNP A3DCY5
B	483	HIS	-	expression tag	UNP A3DCY5
B	484	HIS	-	expression tag	UNP A3DCY5
B	485	HIS	-	expression tag	UNP A3DCY5
B	486	HIS	-	expression tag	UNP A3DCY5
B	487	HIS	-	expression tag	UNP A3DCY5
B	488	HIS	-	expression tag	UNP A3DCY5
C	18	MET	-	initiating methionine	UNP A3DCY5
C	439	GLN	GLU	conflict	UNP A3DCY5
C	473	ASN	-	expression tag	UNP A3DCY5
C	474	LEU	-	expression tag	UNP A3DCY5
C	475	TYR	-	expression tag	UNP A3DCY5
C	476	PHE	-	expression tag	UNP A3DCY5
C	477	GLN	-	expression tag	UNP A3DCY5
C	478	SER	-	expression tag	UNP A3DCY5
C	479	GLY	-	expression tag	UNP A3DCY5
C	480	SER	-	expression tag	UNP A3DCY5
C	481	HIS	-	expression tag	UNP A3DCY5
C	482	HIS	-	expression tag	UNP A3DCY5
C	483	HIS	-	expression tag	UNP A3DCY5
C	484	HIS	-	expression tag	UNP A3DCY5
C	485	HIS	-	expression tag	UNP A3DCY5
C	486	HIS	-	expression tag	UNP A3DCY5
C	487	HIS	-	expression tag	UNP A3DCY5
C	488	HIS	-	expression tag	UNP A3DCY5

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	F	6	Total C H O 124 36 57 31	0	0	0
2	D	6	Total C H O 124 36 57 31	0	0	0
2	E	6	Total C H O 124 36 57 31	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

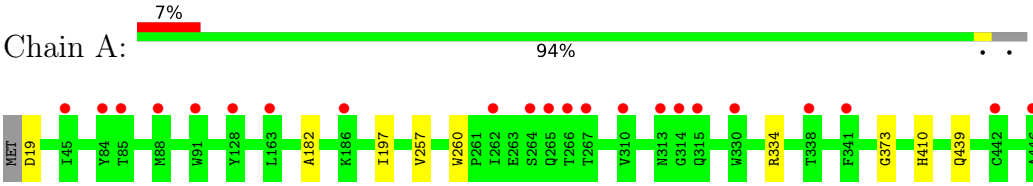
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	222	Total O 222 222	0	0
4	B	221	Total O 222 222	0	1
4	C	215	Total O 216 216	0	1

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.

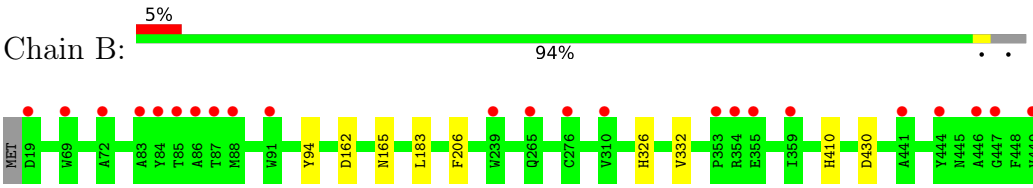
• Molecule 1: Glucanase

Chain A:



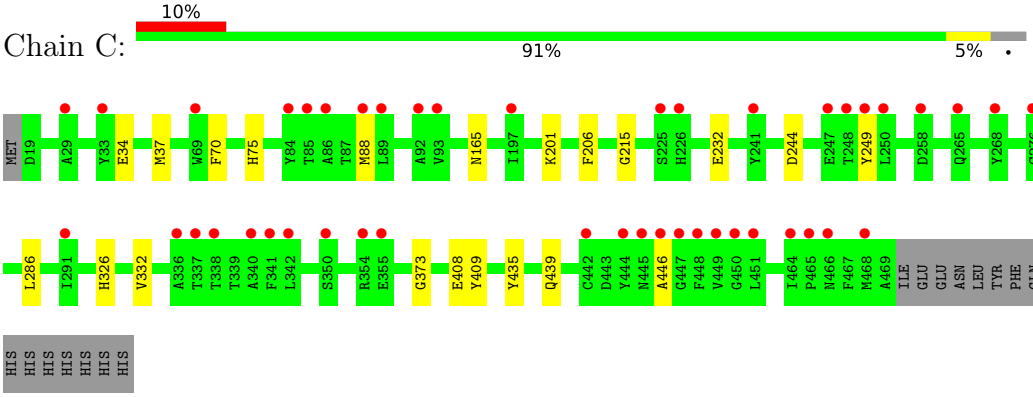
• Molecule 1: Glucanase

Chain B:



• Molecule 1: Glucanase

Chain C:



• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F:

• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain D:

• Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	93.30Å 162.42Å 210.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.87 – 1.90 39.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.87-1.90) 99.8 (39.87-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.185 , 0.232 0.185 , 0.231	Depositor DCC
R_{free} test set	3037 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.044 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.046 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21883	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BGC

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	0.28	0/3711	0.49	0/5059
1	B	0.28	0/3711	0.48	0/5059
1	C	0.28	0/3711	0.49	0/5059
All	All	0.28	0/11133	0.49	0/15177

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

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	3594	3357	3354	3	0
1	B	3594	3355	3354	3	0
1	C	3594	3354	3354	12	0
2	D	67	57	57	1	0
2	E	67	57	57	0	0
2	F	67	57	57	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	222	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	222	0	0	0	0
4	C	216	0	0	1	0
All	All	11646	10237	10233	19	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 1.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:BGC:H6C1	2:F:3:BGC:H2	1.92	0.51
1:C:326:HIS:CD2	1:C:332:VAL:HG21	2.47	0.49
1:C:408:GLU:HG2	1:C:409:TYR:CD2	2.47	0.49
1:C:435:TYR:O	1:C:439:GLN:HB2	2.14	0.47
1:C:286:LEU:O	1:C:286:LEU:HD23	2.15	0.47
1:A:257:VAL:HG22	1:A:260:TRP:CZ2	2.50	0.47
1:B:326:HIS:CD2	1:B:332:VAL:HG21	2.51	0.45
1:C:88:MET:HB2	1:C:446:ALA:HB1	2.00	0.43
1:A:439:GLN:NE2	2:D:3:BGC:O5	2.52	0.43
1:C:439:GLN:HG2	2:F:3:BGC:H6C2	1.99	0.43
1:C:232:GLU:OE2	4:C:601:HOH:O	2.21	0.42
1:C:165:ASN:HB3	1:C:215:GLY:HA3	2.02	0.41
1:B:94:TYR:CD1	1:B:183:LEU:HD21	2.56	0.41
1:B:162:ASP:OD1	1:B:165:ASN:N	2.53	0.41
1:C:34:GLU:O	1:C:37:MET:HE2	2.21	0.41
1:C:201:LYS:HD3	1:C:249:TYR:CE1	2.57	0.40
1:A:182:ALA:CB	1:A:197:ILE:HG13	2.51	0.40
1:C:70:PHE:CD1	1:C:75:HIS:HA	2.57	0.40
1:C:278:ASP:OD2	2:F:6:BGC:O2	2.17	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	449/471 (95%)	433 (96%)	15 (3%)	1 (0%)	47 38
1	B	449/471 (95%)	433 (96%)	16 (4%)	0	100 100
1	C	449/471 (95%)	431 (96%)	17 (4%)	1 (0%)	47 38
All	All	1347/1413 (95%)	1297 (96%)	48 (4%)	2 (0%)	51 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	GLY
1	C	373	GLY

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	364/383 (95%)	361 (99%)	3 (1%)	81 82
1	B	364/383 (95%)	361 (99%)	3 (1%)	81 82
1	C	364/383 (95%)	361 (99%)	3 (1%)	81 82
All	All	1092/1149 (95%)	1083 (99%)	9 (1%)	81 82

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

Mol	Chain	Res	Type
1	A	19	ASP
1	A	334	ARG
1	A	410	HIS
1	B	206	PHE
1	B	410	HIS
1	B	430	ASP
1	C	206	PHE
1	C	244	ASP
1	C	281	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

18 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	BGC	D	1	2	12,12,12	0.11	0	17,17,17	0.47	0
2	BGC	D	2	2	11,11,12	0.26	0	15,15,17	0.62	0
2	BGC	D	3	2	11,11,12	0.25	0	15,15,17	1.89	3 (20%)
2	BGC	D	4	2	11,11,12	0.20	0	15,15,17	0.59	0
2	BGC	D	5	2	11,11,12	0.23	0	15,15,17	0.47	0
2	BGC	D	6	2	11,11,12	0.21	0	15,15,17	0.39	0
2	BGC	E	1	2	12,12,12	0.11	0	17,17,17	0.34	0
2	BGC	E	2	2	11,11,12	0.37	0	15,15,17	0.66	0
2	BGC	E	3	2	11,11,12	0.25	0	15,15,17	1.97	3 (20%)
2	BGC	E	4	2	11,11,12	0.27	0	15,15,17	0.52	0
2	BGC	E	5	2	11,11,12	0.22	0	15,15,17	0.47	0
2	BGC	E	6	2	11,11,12	0.24	0	15,15,17	0.52	0
2	BGC	F	1	2	12,12,12	0.12	0	17,17,17	0.52	0
2	BGC	F	2	2	11,11,12	0.32	0	15,15,17	0.81	1 (6%)
2	BGC	F	3	2	11,11,12	0.28	0	15,15,17	2.04	4 (26%)
2	BGC	F	4	2	11,11,12	0.21	0	15,15,17	0.52	0
2	BGC	F	5	2	11,11,12	0.20	0	15,15,17	0.49	0
2	BGC	F	6	2	11,11,12	0.24	0	15,15,17	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	BGC	D	2	2	-	2/2/19/22	0/1/1/1
2	BGC	D	3	2	-	2/2/19/22	0/1/1/1
2	BGC	D	4	2	-	2/2/19/22	0/1/1/1
2	BGC	D	5	2	-	0/2/19/22	0/1/1/1
2	BGC	D	6	2	-	2/2/19/22	0/1/1/1
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	E	5	2	-	0/2/19/22	0/1/1/1
2	BGC	E	6	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	BGC	F	2	2	-	2/2/19/22	0/1/1/1
2	BGC	F	3	2	-	0/2/19/22	0/1/1/1
2	BGC	F	4	2	-	0/2/19/22	0/1/1/1
2	BGC	F	5	2	-	0/2/19/22	0/1/1/1
2	BGC	F	6	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	3	BGC	C1-C2-C3	5.41	116.31	109.67
2	E	3	BGC	C1-O5-C5	4.96	118.91	112.19
2	D	3	BGC	C1-C2-C3	4.71	115.46	109.67
2	D	3	BGC	C1-O5-C5	4.26	117.96	112.19
2	E	3	BGC	C1-C2-C3	4.21	114.84	109.67
2	F	3	BGC	C1-O5-C5	4.19	117.87	112.19
2	F	3	BGC	O5-C1-C2	2.83	115.15	110.77
2	E	3	BGC	O5-C1-C2	2.68	114.90	110.77
2	D	3	BGC	O5-C1-C2	2.61	114.80	110.77
2	F	2	BGC	C1-O5-C5	2.31	115.32	112.19
2	F	3	BGC	C3-C4-C5	-2.07	106.54	110.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

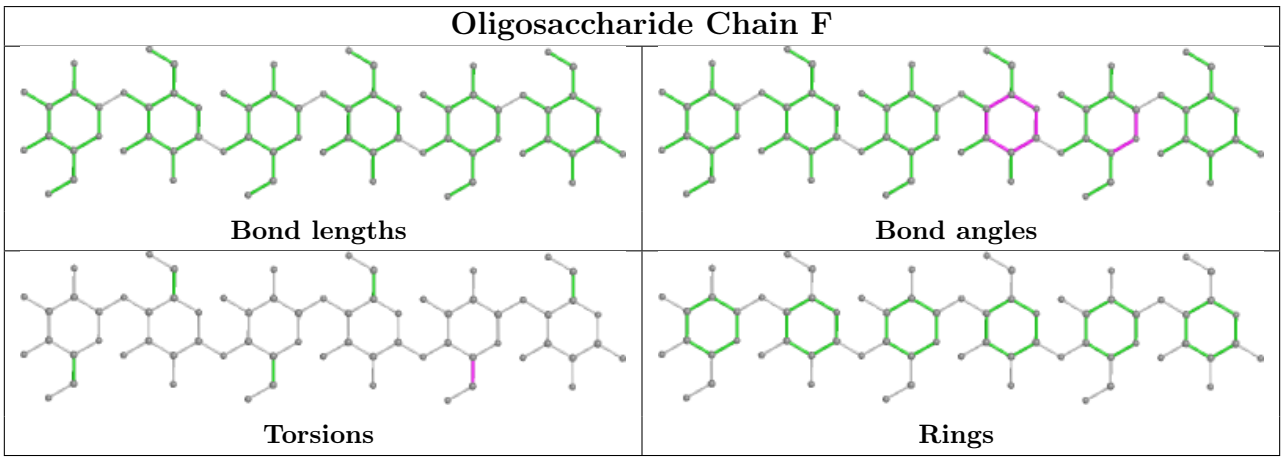
Mol	Chain	Res	Type	Atoms
2	F	2	BGC	O5-C5-C6-O6
2	D	2	BGC	O5-C5-C6-O6
2	D	2	BGC	C4-C5-C6-O6
2	F	2	BGC	C4-C5-C6-O6
2	D	4	BGC	O5-C5-C6-O6
2	D	3	BGC	C4-C5-C6-O6
2	D	3	BGC	O5-C5-C6-O6
2	D	6	BGC	C4-C5-C6-O6
2	D	6	BGC	O5-C5-C6-O6
2	D	4	BGC	C4-C5-C6-O6

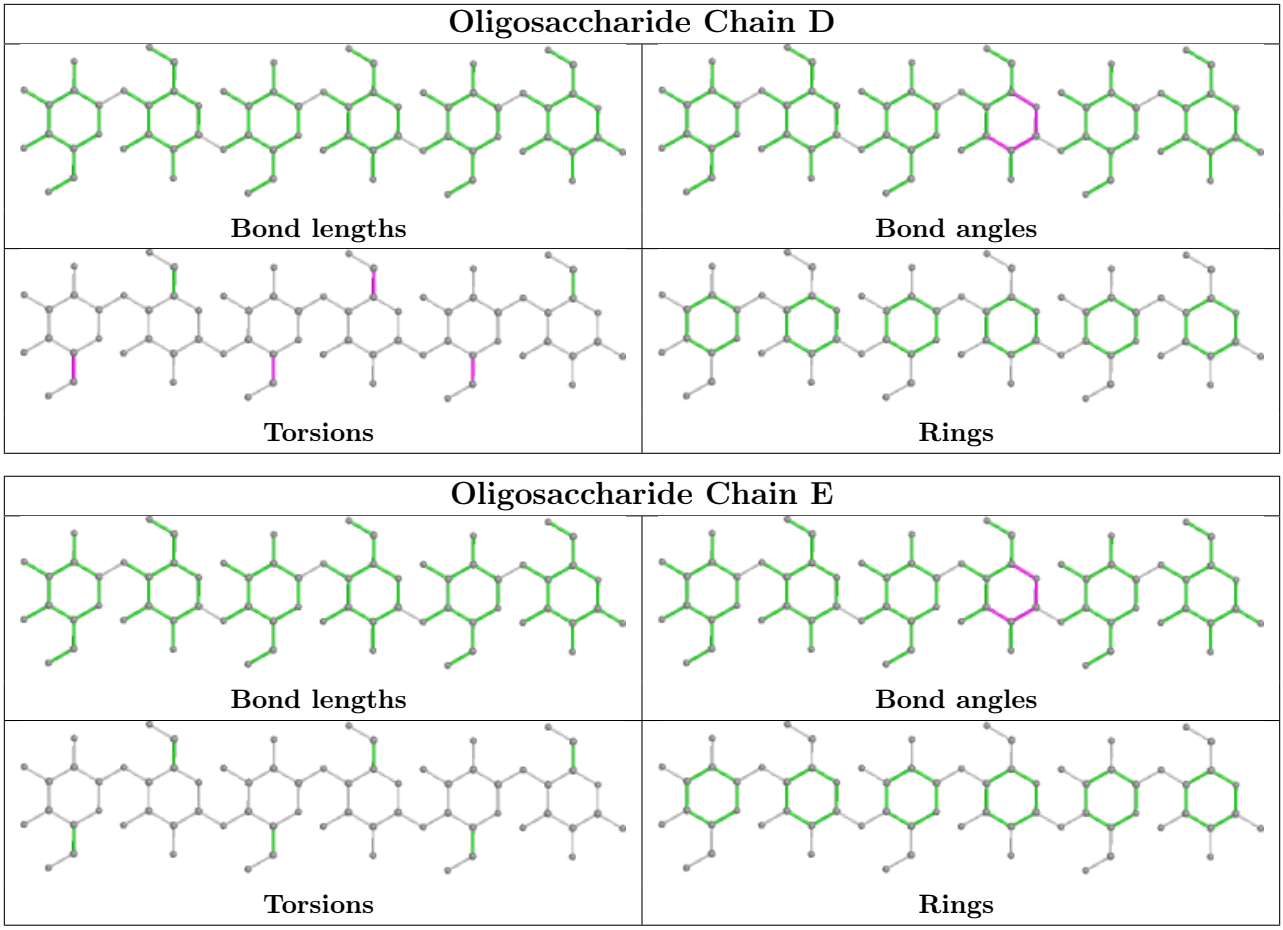
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	6	BGC	1	0
2	F	3	BGC	2	0
2	D	3	BGC	1	0
2	F	2	BGC	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)

Of 3 ligands modelled in this entry, 3 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^{th} 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^2)	Q<0.9
1	A	451/471 (95%)	0.27	31 (6%) 16 19	27, 42, 63, 90	0
1	B	451/471 (95%)	0.29	25 (5%) 25 28	25, 42, 63, 97	0
1	C	451/471 (95%)	0.46	45 (9%) 7 8	27, 45, 67, 85	0
All	All	1353/1413 (95%)	0.34	101 (7%) 14 15	25, 43, 64, 97	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	GLN	4.9
1	A	466	ASN	4.8
1	C	447	GLY	4.5
1	A	465	PRO	4.1
1	C	89	LEU	4.1
1	B	84	TYR	3.9
1	C	464	ILE	3.8
1	C	442	CYS	3.8
1	C	448	PHE	3.7
1	C	92	ALA	3.7
1	C	446	ALA	3.7
1	B	355	GLU	3.6
1	A	467	PHE	3.5
1	C	354	ARG	3.5
1	C	248	THR	3.5
1	B	354	ARG	3.5
1	A	469	ALA	3.4
1	C	241	TYR	3.3
1	B	310	VAL	3.3
1	C	341	PHE	3.3
1	C	265	GLN	3.3
1	A	267	THR	3.2
1	C	465	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	85	THR	3.2
1	A	84	TYR	3.1
1	C	338	THR	3.1
1	A	313	ASN	3.1
1	C	468	MET	3.1
1	C	249	TYR	3.1
1	A	468	MET	3.0
1	B	441	ALA	3.0
1	A	264	SER	3.0
1	B	465	PRO	3.0
1	A	163	LEU	3.0
1	C	451	LEU	3.0
1	B	91	TRP	3.0
1	C	84	TYR	2.9
1	A	314	GLY	2.9
1	B	85	THR	2.9
1	A	262	ILE	2.9
1	C	449	VAL	2.9
1	A	186	LYS	2.9
1	A	446	ALA	2.8
1	B	444	TYR	2.8
1	C	86	ALA	2.8
1	C	268	TYR	2.8
1	C	466	ASN	2.7
1	C	342	LEU	2.7
1	B	353	PRO	2.7
1	C	337	THR	2.7
1	C	250	LEU	2.6
1	A	464	ILE	2.6
1	C	336	ALA	2.6
1	C	450	GLY	2.6
1	C	445	ASN	2.5
1	C	29	ALA	2.5
1	C	444	TYR	2.5
1	A	330	TRP	2.5
1	C	226	HIS	2.4
1	C	340	ALA	2.4
1	C	88	MET	2.4
1	C	247	GLU	2.4
1	A	338	THR	2.4
1	A	315	GLN	2.4
1	C	225	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	197	ILE	2.3
1	B	88	MET	2.3
1	B	459	TYR	2.3
1	B	69	TRP	2.3
1	A	85	THR	2.3
1	A	88	MET	2.3
1	B	359	ILE	2.3
1	C	355	GLU	2.3
1	B	72	ALA	2.3
1	C	276	CYS	2.3
1	B	446	ALA	2.2
1	B	19	ASP	2.2
1	C	291	ILE	2.2
1	B	239	TRP	2.2
1	A	341	PHE	2.2
1	B	449	VAL	2.2
1	C	93	VAL	2.2
1	B	86	ALA	2.2
1	C	350	SER	2.1
1	A	128	TYR	2.1
1	A	463	PRO	2.1
1	B	83	ALA	2.1
1	C	69	TRP	2.1
1	B	265	GLN	2.1
1	C	33	TYR	2.1
1	A	266	THR	2.1
1	A	45	ILE	2.1
1	A	442	CYS	2.1
1	B	447	GLY	2.1
1	B	276	CYS	2.1
1	B	87	THR	2.0
1	A	310	VAL	2.0
1	A	447	GLY	2.0
1	A	450	GLY	2.0
1	C	258	ASP	2.0
1	A	91	TRP	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)

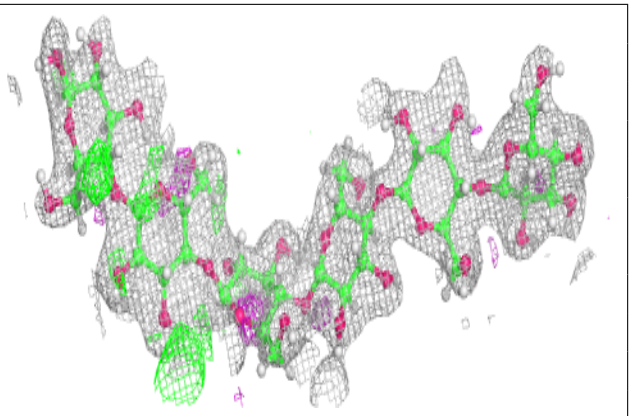
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

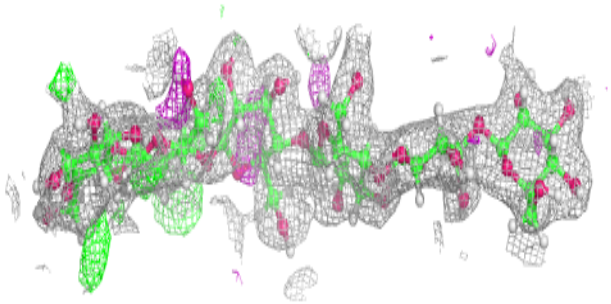
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	D	6	11/12	0.68	0.21	75,85,101,103	0
2	BGC	D	1	12/12	0.73	0.24	60,82,102,111	0
2	BGC	D	5	11/12	0.74	0.24	63,71,84,85	0
2	BGC	E	6	11/12	0.76	0.17	68,82,94,99	0
2	BGC	D	4	11/12	0.78	0.20	59,68,77,87	0
2	BGC	E	4	11/12	0.78	0.17	49,58,68,69	0
2	BGC	D	3	11/12	0.78	0.29	54,66,79,82	0
2	BGC	F	3	11/12	0.79	0.21	44,53,63,67	0
2	BGC	F	2	11/12	0.82	0.17	41,47,54,65	0
2	BGC	E	5	11/12	0.83	0.13	56,64,74,79	0
2	BGC	D	2	11/12	0.83	0.16	45,54,67,71	0
2	BGC	F	1	12/12	0.86	0.16	49,61,70,79	0
2	BGC	E	2	11/12	0.87	0.17	42,50,57,64	0
2	BGC	F	5	11/12	0.87	0.16	46,56,68,70	0
2	BGC	E	1	12/12	0.88	0.15	50,65,83,97	0
2	BGC	F	4	11/12	0.88	0.12	46,54,64,65	0
2	BGC	E	3	11/12	0.88	0.17	44,55,69,69	0
2	BGC	F	6	11/12	0.91	0.18	50,57,68,76	0

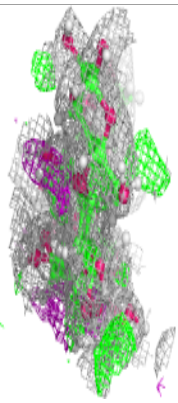
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain F:

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

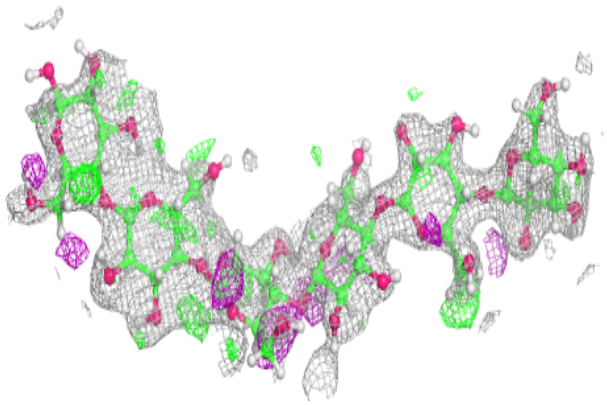


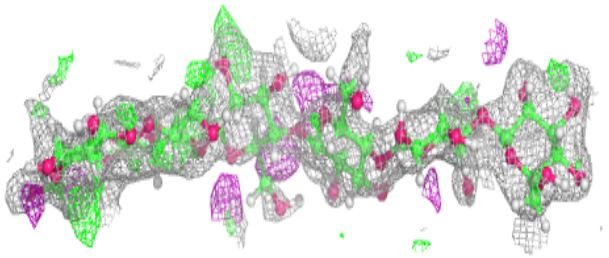


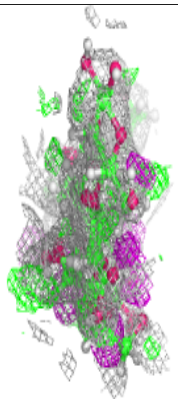


Electron density around Chain D:

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

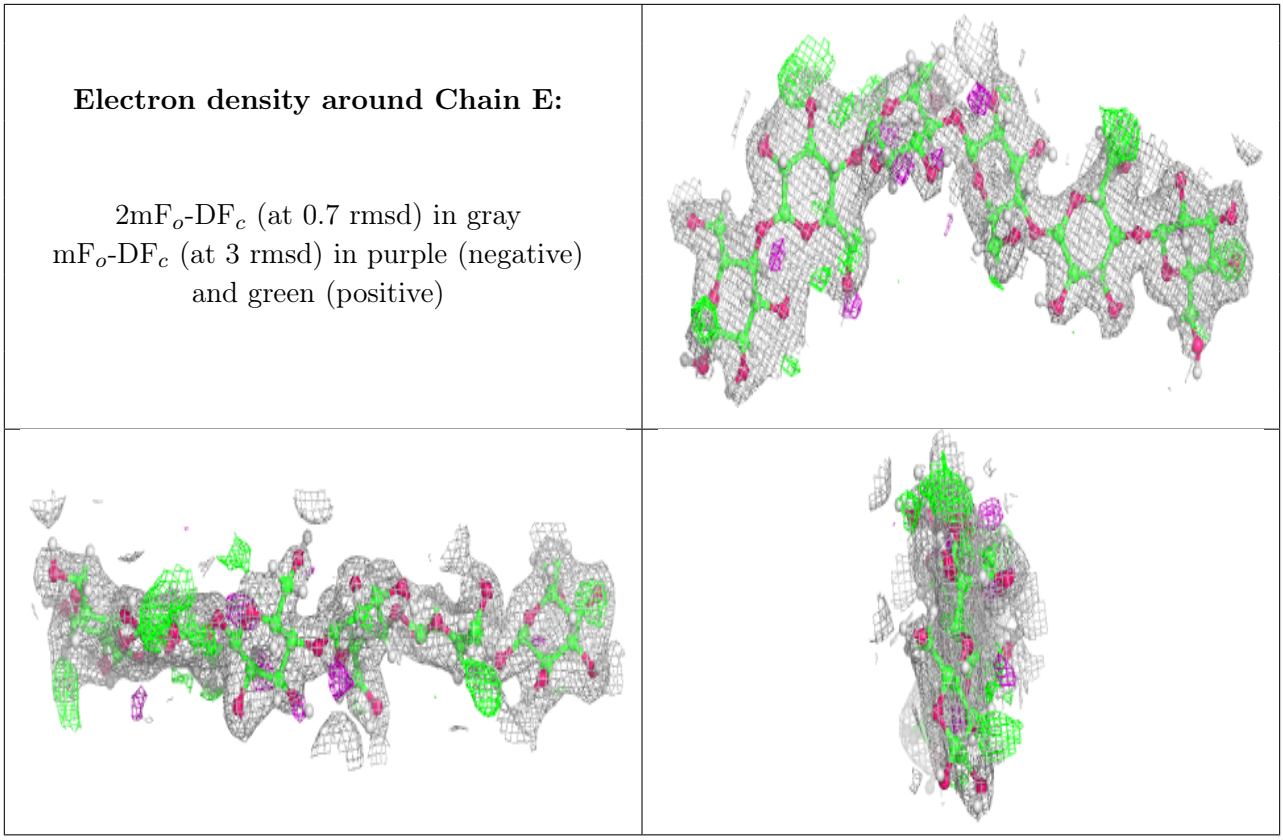






Electron density around Chain E:

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



6.4 Ligands

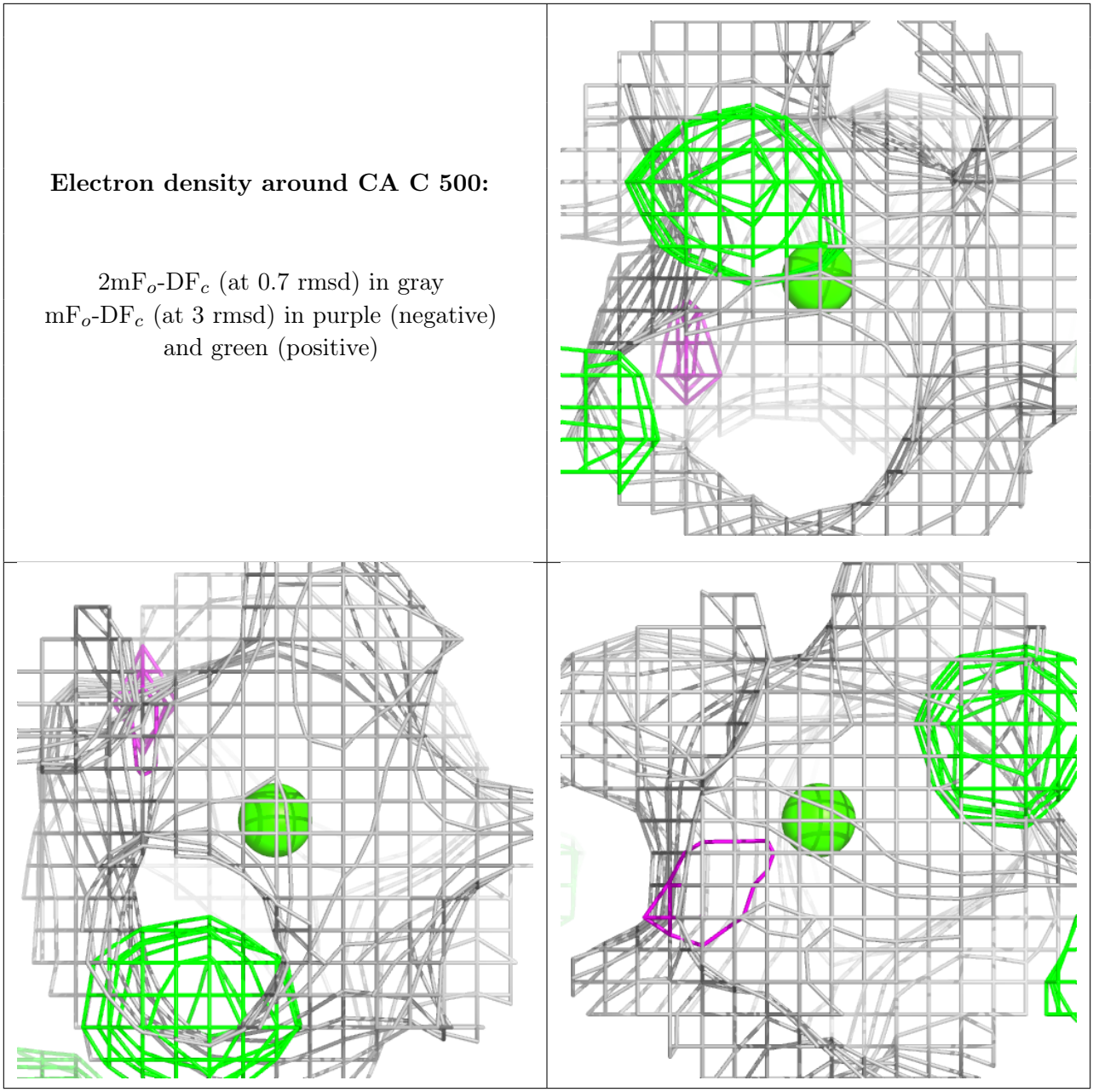
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	C	500	1/1	0.95	0.04	55,55,55,55	0
3	CA	A	500	1/1	0.96	0.06	56,56,56,56	0
3	CA	B	500	1/1	0.97	0.06	52,52,52,52	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.

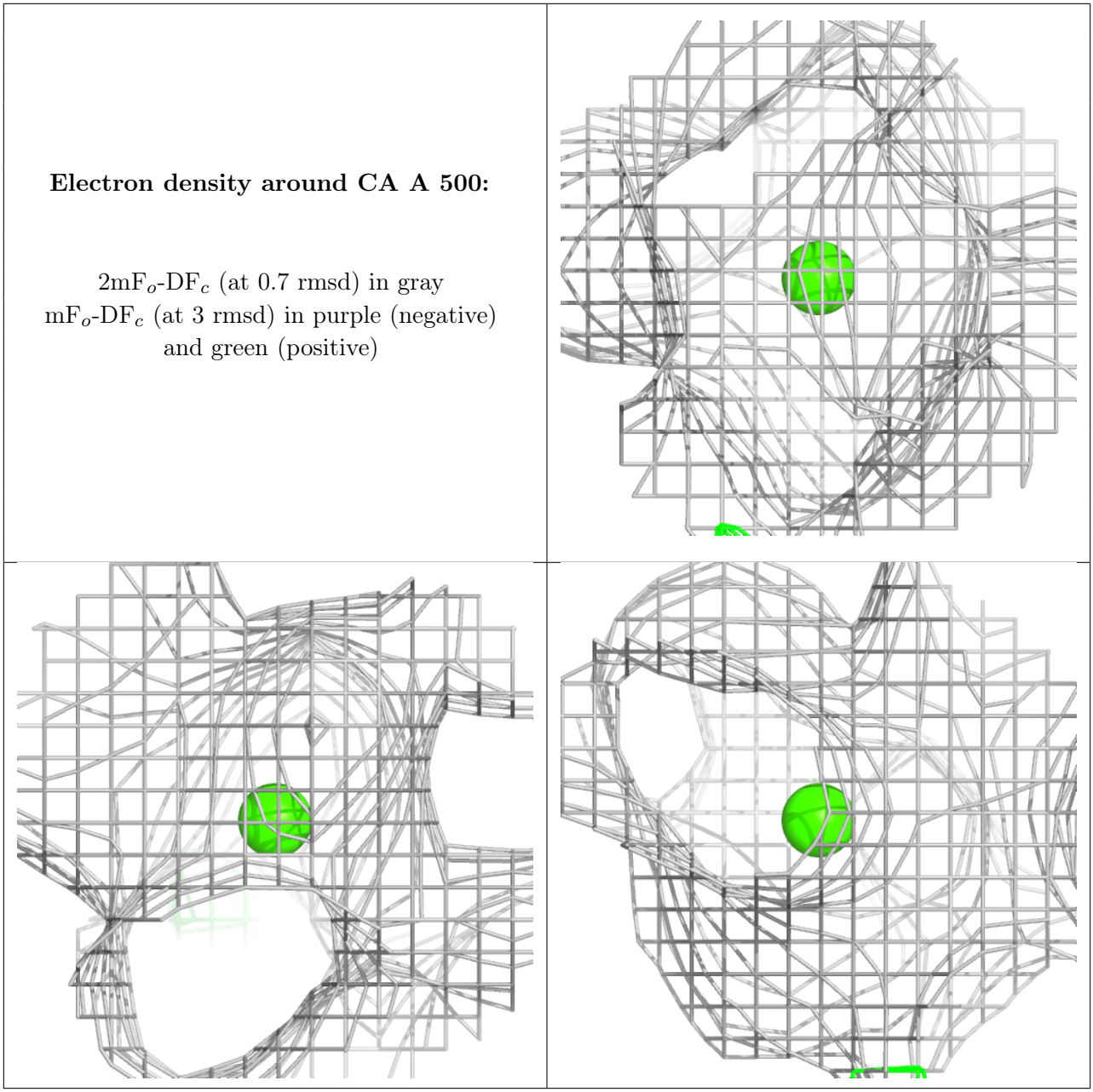
Electron density around CA C 500:

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



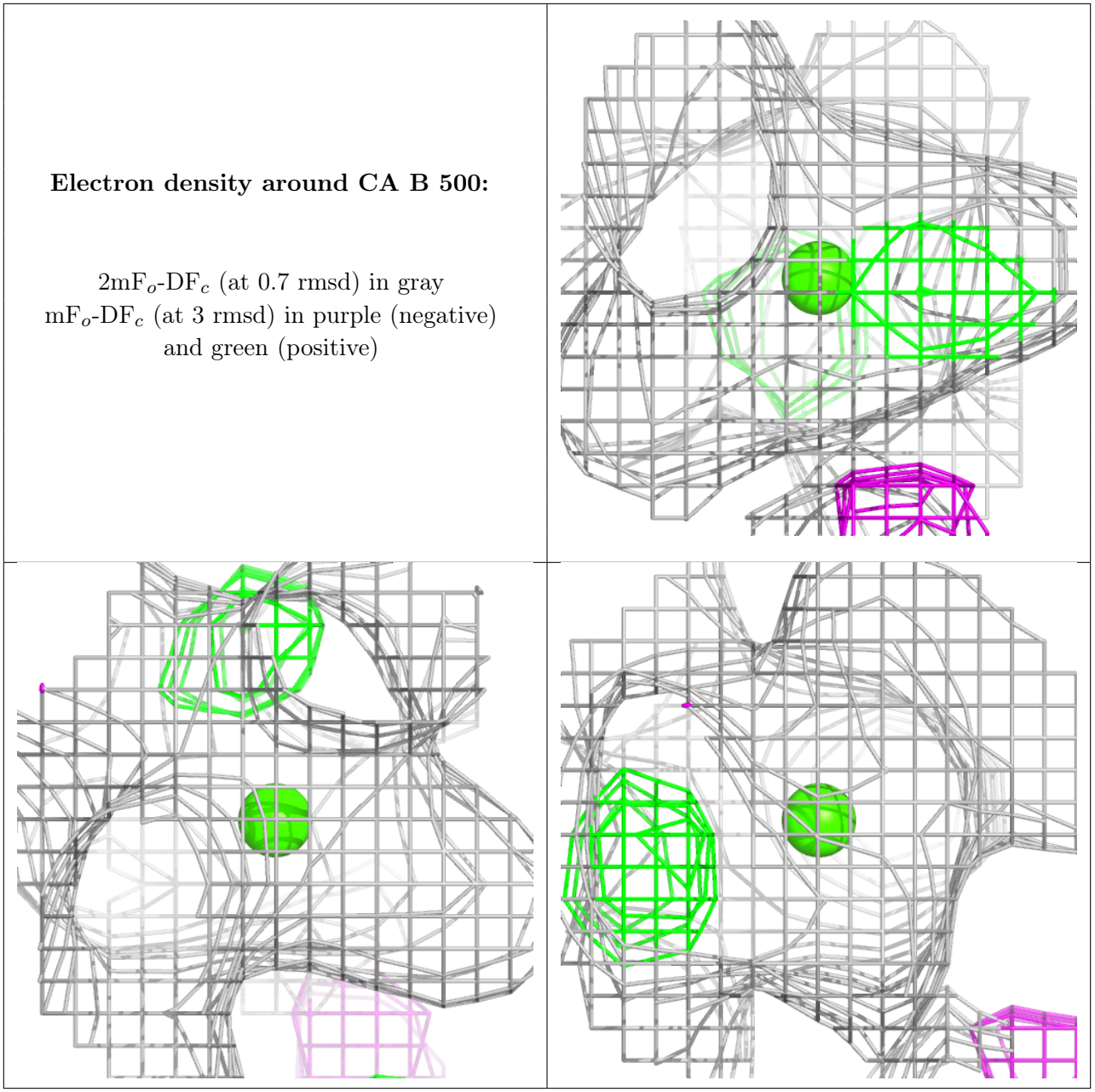
Electron density around CA A 500:

$2mF_o$-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 500:

$2mF_o$-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.