

# Full wwPDB X-ray Structure Validation Report (i)

#### Jul 20, 2023 – 02:09 AM EDT

PDB ID : 8CU1

Title: Structure of a K+ selective NaK mutant (NaK2K, Laue diffraction) in the

presence of an electric field of 0.8MV/cm along the crystallographic z axis,

500ns, with eightfold extrapolation of structure factor differences

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Deposited on : 2022-05-16

Resolution : 2.01 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.34

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.34

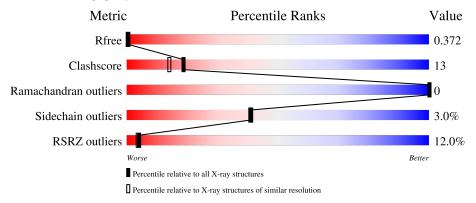


# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.01 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	96	79%	18%	
1	В	96	77%	22%	
2	D	2	100%		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	D	2	-	-	X	-
3	MPD	A	203	-	-	-	X
3	MPD	В	201	-	-	-	X
3	MPD	В	205	-	-	-	X
3	MPD	В	206	-	-	-	X
3	MPD	В	207[A]	-	-	-	X
3	MPD	В	207[B]	-	-	-	X



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4306 atoms, of which 2211 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 Potassium channel protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	95	Total	_	Н		0	0	25	0
			1882	627	956	137	162			
1	R	96	Total	С	Η	N	O	0	26	
1	ע	<i>9</i> 0	1927	635	981	143	168			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	-	expression tag	UNP B7HBV5
A	66	TYR	ASP	conflict	UNP B7HBV5
A	68	ASP	ASN	conflict	UNP B7HBV5
A	111	LEU	-	expression tag	UNP B7HBV5
A	112	VAL	-	expression tag	UNP B7HBV5
A	113	PRO	-	expression tag	UNP B7HBV5
A	114	ARG	-	expression tag	UNP B7HBV5
В	19	ALA	-	expression tag	UNP B7HBV5
В	66	TYR	ASP	conflict	UNP B7HBV5
В	68	ASP	ASN	conflict	UNP B7HBV5
В	111	LEU	-	expression tag	UNP B7HBV5
В	112	VAL	-	expression tag	UNP B7HBV5
В	113	PRO	-	expression tag	UNP B7HBV5
В	114	ARG	-	expression tag	UNP B7HBV5

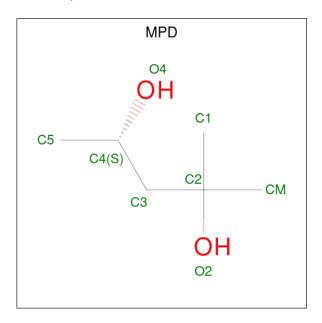
• Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	D	2	Total 45	C 12	H 22	O 11	0	0	0



• Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf				
3	Λ	1	Total C H	О	0	0				
3	A	1	22   6   14	2	U	0				
9	3 A	1	Total C H	О	0	0				
3		1	22   6   14	2	0	0				
3	A	1	Total C H	О	0	0				
0	Λ	1	22   6   14	2	0	0				
3	A	1	Total C H	О	0	0				
	Λ	1	22 6 14	2	0	U				
3	A	1	Total C H	O	0	0				
	11	1	22 6 14	2	O	U				
3	A	1	Total C H	Ο	0	0				
	11	1	22 6 14	2	O	Ŭ				
3	В	В	В 1	1	Total C H	Ο	0	0		
							ъ		1	22 6 14
3	В	1	Total C H	O	0	0				
		1	22 6 14	2	Ŭ	Ŭ				
3	В	1	Total C H	Ο	0	0				
		1	22 6 14	2	Ü	0				
3	В	1	Total C H	Ο	0	0				
		1	22 6 14	2	Ü	0				
3	В	1	Total C H	O	0	0				
		1	22 6 14	2	Ŭ					
3	В	1	Total C H	O	0	0				
		1	22 6 14	2						

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Mol	Chain	Residues	A	Atoms			ZeroOcc	AltConf	
3	В	1	Total	С	Н	О	0	1	
)	Ъ	1	44	12	28	4	0	1 0 0 0 0 0	
3	В	1	Total	С	Η	О	0	0	
0	D	1	22	6	14	2	0	U	
3	В	1	Total	С	Н	O	0	0	
9	D	D 1	22	6	14	2	U	U	
3	В	1	Total	С	Н	O	0	0	
9	D	1	22	6	14	2	0	U	
3	В	1	Total	С	Н	О	0	0	
3	ע	1	22	6	14	2			

• Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total K 7 7	0	0
4	В	6	Total K 6 6	0	0

• Molecule 5 is water.

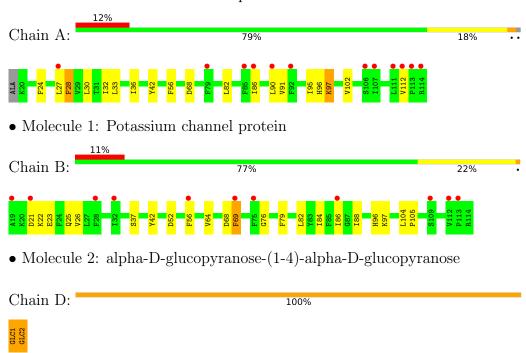
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O 23 23	0	0
5	В	20	Total O 20 20	0	0



# 3 Residue-property plots (i)

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

• Molecule 1: Potassium channel protein





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants	68.82Å 68.82Å 90.36Å	Donositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	21.42 - 2.01	Depositor
Resolution (A)	27.59 - 2.01	EDS
% Data completeness	67.2 (21.42-2.01)	Depositor
(in resolution range)	$67.2\ (27.59-2.01)$	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.60 \; (at \; 2.01 \text{Å})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
$R, R_{free}$	0.334 , 0.371	Depositor
Tt, Ttfree	0.333 , $0.372$	DCC
$R_{free}$ test set	533 reflections $(5.25%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.43, 73.0	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.087 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	4306	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.21% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MPD, GLC, K

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		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.38	0/949	0.49	0/1293	
1	В	0.45	0/978	0.53	0/1323	
All	All	0.42	0/1927	0.51	0/2616	

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	926	956	944	22	0
1	В	946	981	962	23	0
2	D	23	22	19	9	0
3	A	48	84	84	6	0
3	В	96	168	168	6	0
4	A	7	0	0	0	0
4	В	6	0	0	0	0
5	A	23	0	0	0	0
5	В	20	0	0	2	0
All	All	2095	2211	2177	56	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 13.

All (56) 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:D:1:GLC:O3	2:D:2:GLC:O2	1.54	1.26
1:A:27:LEU:CD2	1:A:97:LYS:NZ	2.20	1.04
1:B:96:HIS:NE2	2:D:2:GLC:O4	2.00	0.93
1:A:27:LEU:HD21	1:A:97:LYS:NZ	1.85	0.89
1:B:96:HIS:CE1	2:D:2:GLC:O4	2.24	0.89
1:A:27:LEU:HD22	1:A:97:LYS:NZ	1.86	0.88
1:A:27:LEU:CD2	1:A:97:LYS:HZ3	1.91	0.82
1:A:27:LEU:HD21	1:A:97:LYS:HZ1	1.47	0.78
3:A:201:MPD:O4	3:A:201:MPD:O2	2.01	0.77
1:B:96:HIS:CE1	2:D:2:GLC:HO4	1.99	0.77
1:B:68:ASP:OD1	5:B:301:HOH:O	2.03	0.76
1:B:76:GLY:O	5:B:302:HOH:O	2.04	0.76
1:A:27:LEU:HD22	1:A:97:LYS:HZ3	1.48	0.75
3:A:204:MPD:H53	3:A:204:MPD:H12	1.67	0.75
1:B:96:HIS:CD2	2:D:2:GLC:O4	2.41	0.73
1:B:52:ASP:HB3	1:B:69[A]:PHE:CE2	2.27	0.69
1:B:79:PHE:HE1	3:B:202:MPD:H53	1.61	0.66
1:B:79:PHE:CE1	3:B:202:MPD:H53	2.32	0.65
2:D:2:GLC:H62	2:D:2:GLC:O3	1.97	0.63
1:A:24[B]:PHE:CZ	1:A:102:VAL:HG21	2.36	0.61
3:B:207[B]:MPD:O4	3:B:207[B]:MPD:O2	2.16	0.56
1:A:82:LEU:O	1:A:86[B]:ILE:HG22	2.06	0.55
1:B:96:HIS:CD2	2:D:2:GLC:HO4	2.18	0.55
1:A:42:TYR:CZ	1:A:56:PHE:HE2	2.25	0.55
1:B:52:ASP:HB3	1:B:69[A]:PHE:HE2	1.70	0.54
1:A:33[A]:LEU:HD23	1:A:33[A]:LEU:O	2.08	0.54
1:A:97:LYS:HZ2	1:A:97:LYS:HB2	1.74	0.53
1:B:86[B]:ILE:HD13	3:B:202:MPD:H12	1.91	0.52
1:B:104:LEU:HB3	1:B:105:PRO:HD3	1.92	0.51
1:A:27:LEU:HD22	1:A:97:LYS:HZ2	1.72	0.50
1:B:21[A]:ASP:O	1:B:25:GLN:HG3	2.11	0.50
1:B:42[B]:TYR:CZ	1:B:56:PHE:HE2	2.30	0.49
1:B:42[A]:TYR:CZ	1:B:56:PHE:HE2	2.31	0.48
1:A:112[B]:VAL:O	1:A:112[B]:VAL:HG23	2.13	0.48
3:A:204:MPD:H12	3:A:204:MPD:C5	2.38	0.48
1:A:28[A]:PHE:CE1	1:A:32[A]:ILE:HD11	2.49	0.47
1:A:32[A]:ILE:O	1:A:36:ILE:HG13	2.15	0.47
1:B:82:LEU:O	1:B:86[B]:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:GLC:O4	2:D:1:GLC:O6	2.28	0.46
1:B:21[B]:ASP:O	1:B:25:GLN:HG3	2.15	0.46
1:A:91[B]:VAL:O	1:A:95:ILE:HG13	2.17	0.45
1:B:37[A]:SER:OG	3:B:202:MPD:HM1	2.18	0.44
1:B:84:ILE:O	1:B:88:ILE:HG13	2.17	0.43
1:A:82:LEU:HD21	3:A:201:MPD:H4	2.01	0.42
1:A:68:ASP:OD1	1:A:68:ASP:N	2.52	0.42
1:B:56:PHE:CE1	1:B:69[A]:PHE:O	2.71	0.42
1:A:32[B]:ILE:O	1:A:36:ILE:HG13	2.19	0.42
3:A:205:MPD:O4	3:A:205:MPD:O2	2.23	0.42
1:A:27:LEU:CD2	1:A:97:LYS:HZ2	2.23	0.42
1:A:30:LEU:HB3	1:A:90[A]:LEU:HD11	2.01	0.42
1:A:90[A]:LEU:C	1:A:90[A]:LEU:HD23	2.39	0.42
3:B:202:MPD:O2	3:B:202:MPD:O4	2.37	0.42
3:A:206:MPD:H12	3:A:206:MPD:O4	2.20	0.41
1:B:23[B]:GLU:OE1	1:B:97[B]:LYS:NZ	2.51	0.41
1:B:22[B]:LYS:O	1:B:26:VAL:HG23	2.21	0.41
2:D:2:GLC:C2	2:D:2:GLC:C6	2.93	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	tliers   Percentiles	
1	A	117/96 (122%)	117 (100%)	0	0	100	100
1	В	117/96 (122%)	116 (99%)	1 (1%)	0	100	100
All	All	$234/192\ (122\%)$	233 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.



#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Rotameric Outliers		
1	A	103/85 (121%)	99 (96%)	4 (4%)	32	30
1	В	108/85 (127%)	105 (97%)	3 (3%)	43	44
All	All	211/170 (124%)	204 (97%)	7 (3%)	41	37

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	$\mathbf{Type}$	
1	A	28[A]	PHE	
1	A	28[B]	PHE	
1	A	96	HIS	
1	A	97	LYS	
1	В	64[A]	VAL	
1	В	69[A]	PHE	
1	В	69[B]	PHE	

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

#### 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)

2 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		
WIOI					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	D	1	2	12,12,12	0.56	0	17,17,17	1.36	2 (11%)
2	GLC	D	2	2	11,11,12	0.66	0	15,15,17	2.45	5 (33%)

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	GLC	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	D	2	GLC	C1-C2-C3	7.45	118.82	109.67
2	D	1	GLC	C3-C4-C5	-3.04	104.81	110.24
2	D	2	GLC	O5-C1-C2	2.94	115.31	110.77
2	D	2	GLC	O2-C2-C3	-2.86	104.41	110.14
2	D	1	GLC	O5-C5-C4	-2.51	105.14	109.69
2	D	2	GLC	C1-O5-C5	2.49	115.57	112.19
2	D	2	GLC	O5-C5-C6	2.12	110.52	107.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	GLC	O5-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6

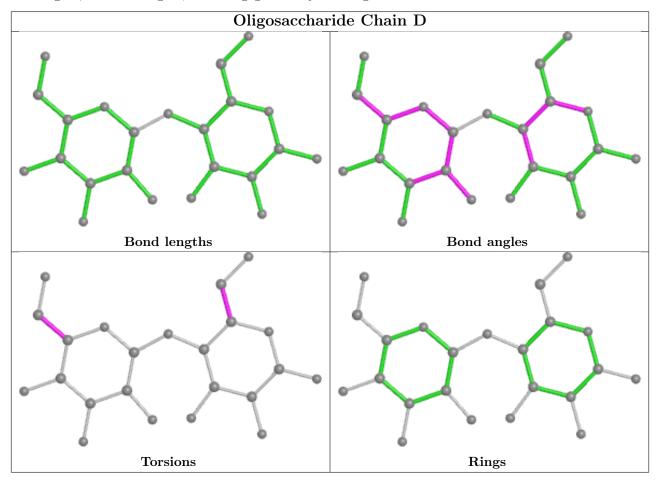
There are no ring outliers.

2 monomers are involved in 9 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	GLC	8	0
2	D	1	GLC	2	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 31 ligands modelled in this entry, 13 are monoatomic - leaving 18 for Mogul analysis.

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).

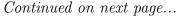
1	/[a]	Type	Chain	Res	Link	Bond lengths			Bond angles		
10.	Mol	туре				Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
	3	MPD	A	205	-	7,7,7	0.25	0	9,10,10	0.30	0



Mol	Type	Chain	Res	Link	В	ond leng	$_{ m gths}$	В	ond ang	gles
WIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MPD	В	203	-	7,7,7	0.28	0	9,10,10	0.23	0
3	MPD	В	205	-	7,7,7	0.25	0	9,10,10	0.22	0
3	MPD	В	201	-	7,7,7	0.28	0	9,10,10	0.14	0
3	MPD	В	207[B]	-	7,7,7	0.27	0	9,10,10	0.20	0
3	MPD	В	204	-	7,7,7	0.25	0	9,10,10	0.19	0
3	MPD	A	201	-	7,7,7	0.27	0	9,10,10	0.17	0
3	MPD	В	206	-	7,7,7	0.28	0	9,10,10	0.28	0
3	MPD	A	206	-	7,7,7	0.28	0	9,10,10	0.23	0
3	MPD	A	203	-	7,7,7	0.38	0	9,10,10	0.50	0
3	MPD	В	207[A]	-	7,7,7	0.25	0	9,10,10	0.26	0
3	MPD	В	208	-	7,7,7	0.23	0	9,10,10	0.38	0
3	MPD	В	209	-	7,7,7	0.27	0	9,10,10	0.30	0
3	MPD	A	202	-	7,7,7	0.28	0	9,10,10	0.47	0
3	MPD	В	202	-	7,7,7	0.26	0	9,10,10	0.31	0
3	MPD	В	210	-	7,7,7	0.30	0	9,10,10	0.29	0
3	MPD	В	211	-	7,7,7	0.28	0	9,10,10	0.16	0
3	MPD	A	204	-	7,7,7	0.45	0	9,10,10	1.24	2 (22%)

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	MPD	A	205	-	-	2/5/5/5	-
3	MPD	В	203	-	-	0/5/5/5	-
3	MPD	В	205	-	-	0/5/5/5	-
3	MPD	В	201	-	-	0/5/5/5	-
3	MPD	В	207[B]	-	-	2/5/5/5	-
3	MPD	В	204	-	-	0/5/5/5	-
3	MPD	A	201	-	-	3/5/5/5	-
3	MPD	В	206	-	-	1/5/5/5	-
3	MPD	A	206	-	-	2/5/5/5	-
3	MPD	A	203	-	-	2/5/5/5	-
3	MPD	В	207[A]	-	-	1/5/5/5	-
3	MPD	В	208	-	-	0/5/5/5	-
3	MPD	В	209	-	-	2/5/5/5	-
3	MPD	A	202	-	-	2/5/5/5	-
3	MPD	В	202	-	-	0/5/5/5	-
3	MPD	В	210	-	-	0/5/5/5	-
3	MPD	В	211	-	-	2/5/5/5	-





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Mo	l Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	A	204	-	-	1/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	204	MPD	C5-C4-C3	2.50	123.47	111.69
3	A	204	MPD	O4-C4-C3	-2.24	102.34	111.36

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	MPD	C2-C3-C4-O4
3	A	201	MPD	C2-C3-C4-C5
3	A	204	MPD	C2-C3-C4-C5
3	A	205	MPD	C2-C3-C4-O4
3	A	206	MPD	C2-C3-C4-O4
3	A	202	MPD	C2-C3-C4-C5
3	A	205	MPD	C2-C3-C4-C5
3	A	206	MPD	C2-C3-C4-C5
3	В	207[B]	MPD	C2-C3-C4-O4
3	A	203	MPD	C1-C2-C3-C4
3	A	201	MPD	O2-C2-C3-C4
3	A	203	MPD	O2-C2-C3-C4
3	В	207[A]	MPD	C2-C3-C4-C5
3	В	207[B]	MPD	C2-C3-C4-C5
3	В	209	MPD	C2-C3-C4-C5
3	В	211	MPD	C2-C3-C4-C5
3	A	202	MPD	C2-C3-C4-O4
3	В	206	MPD	C2-C3-C4-O4
3	В	209	MPD	C2-C3-C4-O4
3	В	211	MPD	C2-C3-C4-O4

There are no ring outliers.

6 monomers are involved in 12 short contacts:

$\mathbf{Mol}$	Chain	Res	Type	Clashes	Symm-Clashes
3	A	205	MPD	1	0
3	В	207[B]	MPD	1	0

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Mol	Chain	$\operatorname{Res}$	Type	Clashes	Symm-Clashes
3	A	201	MPD	2	0
3	A	206	MPD	1	0
3	В	202	MPD	5	0
3	A	204	MPD	2	0

# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

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

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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9	
1	A	95/96~(98%)	0.98	12 (12%)	3	3	7, 21, 46, 58	0
1	В	96/96 (100%)	0.77	11 (11%)	4	4	12, 21, 36, 50	0
All	All	191/192 (99%)	0.88	23 (12%)	4	3	7, 21, 41, 58	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113[A]	PRO	8.1
1	A	27	LEU	5.9
1	В	32	ILE	4.1
1	A	90[A]	LEU	4.0
1	В	86[A]	ILE	3.8
1	В	112	VAL	3.7
1	В	69[A]	PHE	3.6
1	В	21[A]	ASP	3.6
1	В	56	PHE	3.1
1	A	107	ILE	2.9
1	В	109[A]	SER	2.8
1	A	114	ARG	2.6
1	A	111[A]	LEU	2.6
1	В	113[A]	PRO	2.5
1	A	85	PHE	2.4
1	A	106	SER	2.4
1	A	79	PHE	2.3
1	В	75	PHE	2.3
1	A	92[A]	PHE	2.2
1	В	19	ALA	2.2
1	В	28	PHE	2.1
1	A	86[A]	ILE	2.1
1	A	112[A]	VAL	2.0



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

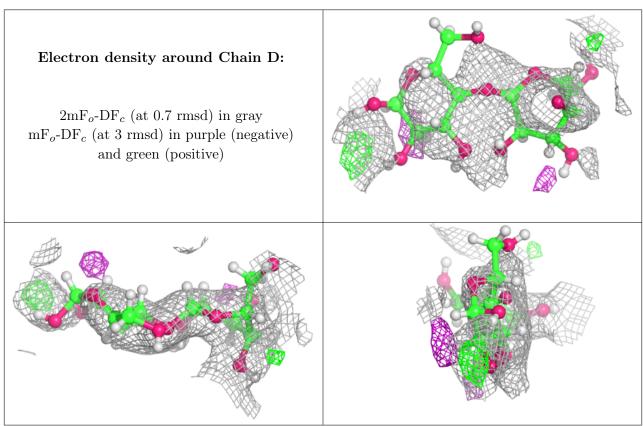
There are no non-standard protein/DNA/RNA residues in this entry.

## 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	GLC	D	1	12/12	0.66	0.29	68,94,127,133	0
2	GLC	D	2	11/12	0.75	0.31	46,67,84,137	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.



# 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,

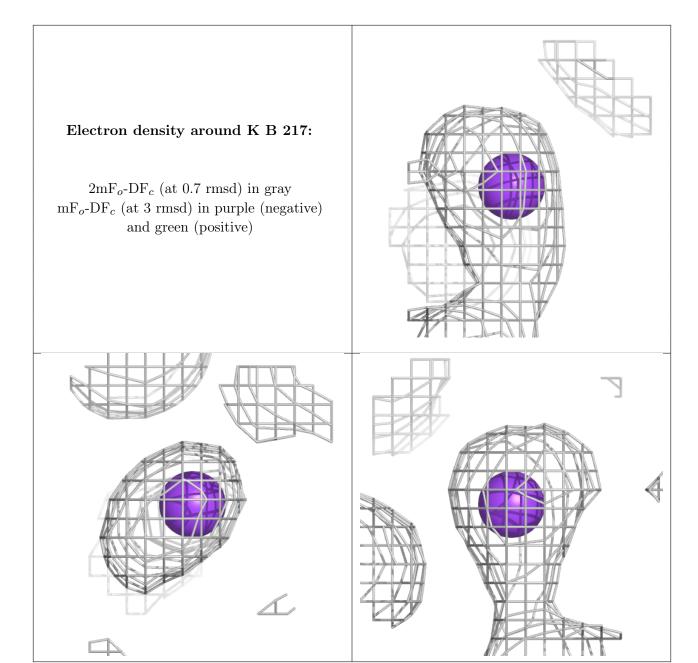


median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$oxed{ \mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2) }$	Q<0.9
3	MPD	В	203	8/8	-0.06	0.35	62,77,121,121	0
3	MPD	A	202	8/8	0.41	0.27	42,60,70,96	0
3	MPD	В	210	8/8	0.48	0.26	27,36,46,55	0
3	MPD	В	201	8/8	0.49	0.48	30,48,66,66	0
3	MPD	A	201	8/8	0.55	0.23	32,50,59,60	0
3	MPD	В	205	8/8	0.56	0.56	45,63,72,105	0
3	MPD	A	204	8/8	0.58	0.38	44,62,84,105	0
3	MPD	В	206	8/8	0.59	0.61	46,57,62,69	0
3	MPD	В	209	8/8	0.62	0.39	32,41,51,61	0
3	MPD	A	203	8/8	0.66	0.48	39,59,86,86	0
3	MPD	В	208	8/8	0.67	0.33	42,59,71,95	0
3	MPD	A	206	8/8	0.68	0.18	58,74,86,99	0
3	MPD	В	211	8/8	0.70	0.25	32,53,69,69	0
3	MPD	A	205	8/8	0.72	0.35	39,49,58,59	0
3	MPD	В	204	8/8	0.72	0.34	44,58,75,90	0
3	MPD	В	202	8/8	0.74	0.38	38,50,53,67	0
4	K	В	217	1/1	0.75	0.12	58,58,58,58	0
3	MPD	В	207[B]	8/8	0.78	0.53	72,88,101,148	22
3	MPD	В	207[A]	8/8	0.78	0.53	64,83,89,145	22
4	K	A	213	1/1	0.79	0.08	55,55,55,55	1
4	K	A	211	1/1	0.82	0.24	59,59,59,59	1
4	K	A	212	1/1	0.93	0.51	36,36,36,36	1
4	K	В	215	1/1	0.94	0.18	17,17,17,17	1
4	K	A	210	1/1	0.98	0.07	12,12,12,12	1
4	K	A	207	1/1	0.98	0.09	7,7,7,7	1
4	K	A	209	1/1	0.98	0.15	14,14,14,14	1
4	K	В	213	1/1	0.99	0.16	15,15,15,15	1
4	K	В	216	1/1	0.99	0.32	60,60,60,60	1
4	K	В	214	1/1	0.99	0.10	17,17,17,17	1
4	K	В	212	1/1	1.00	0.08	18,18,18,18	1
4	K	A	208	1/1	1.00	0.12	9,9,9,9	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.

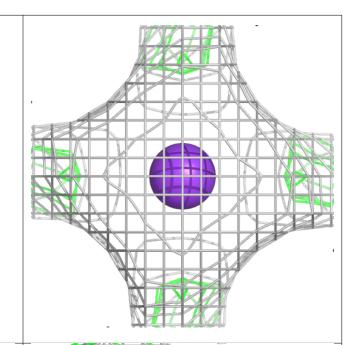


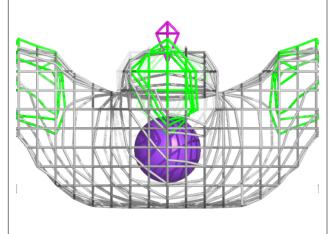


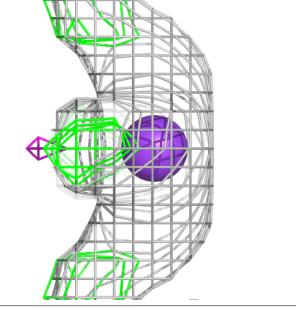


#### Electron density around K A 213:

 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)



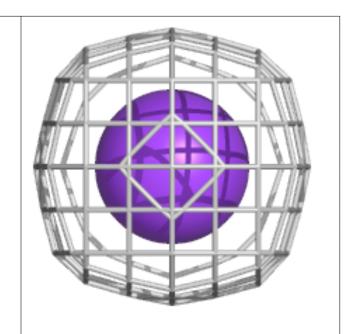


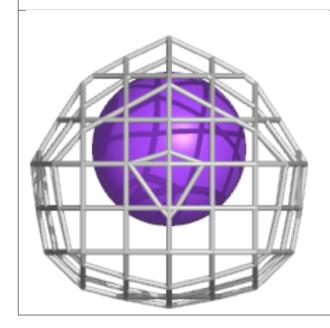


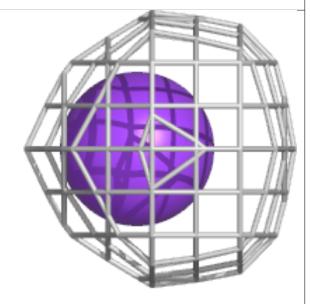


#### Electron density around K A 211:

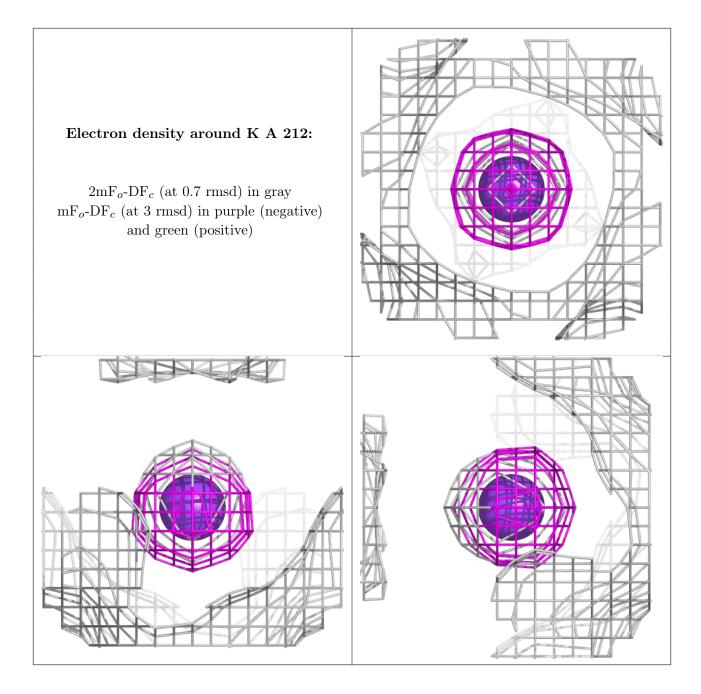
 $2 {
m mF}_o {
m -DF}_c$  (at 0.7 rmsd) in gray  ${
m mF}_o {
m -DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)











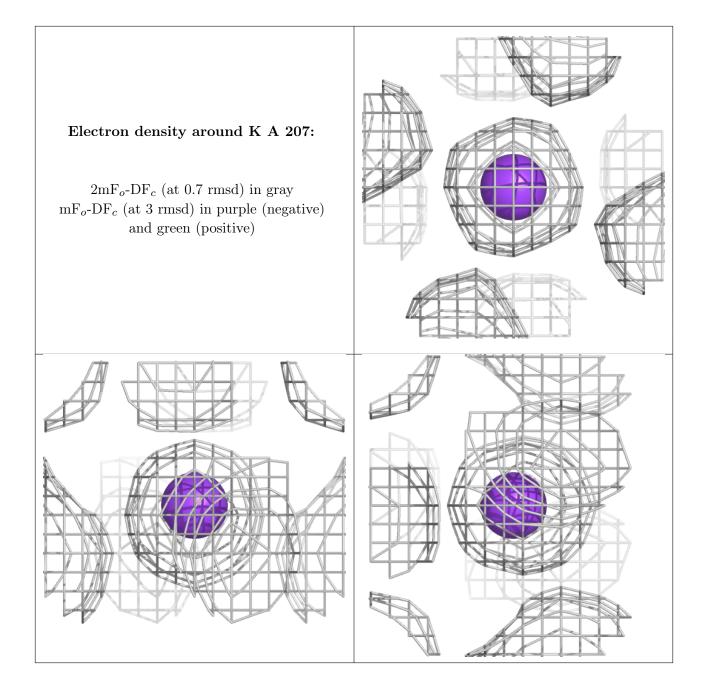


# Electron density around K B 215: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

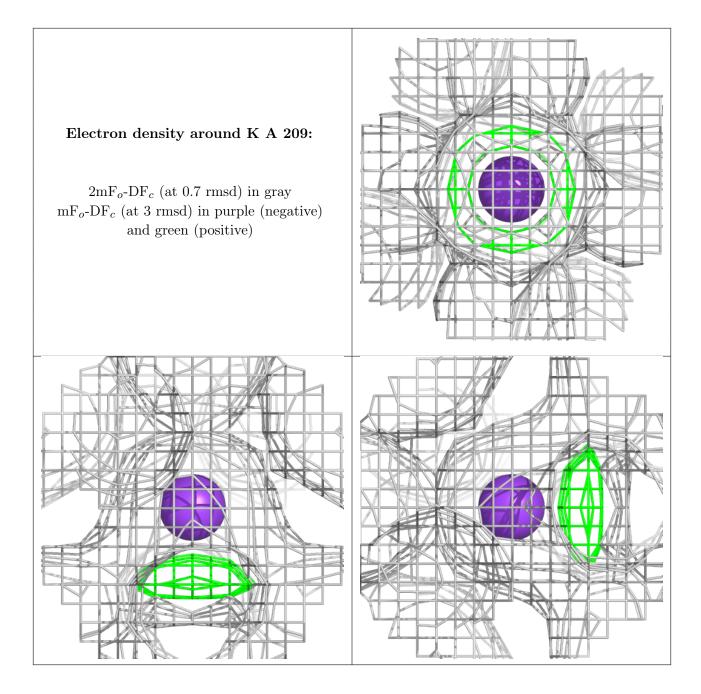


# 









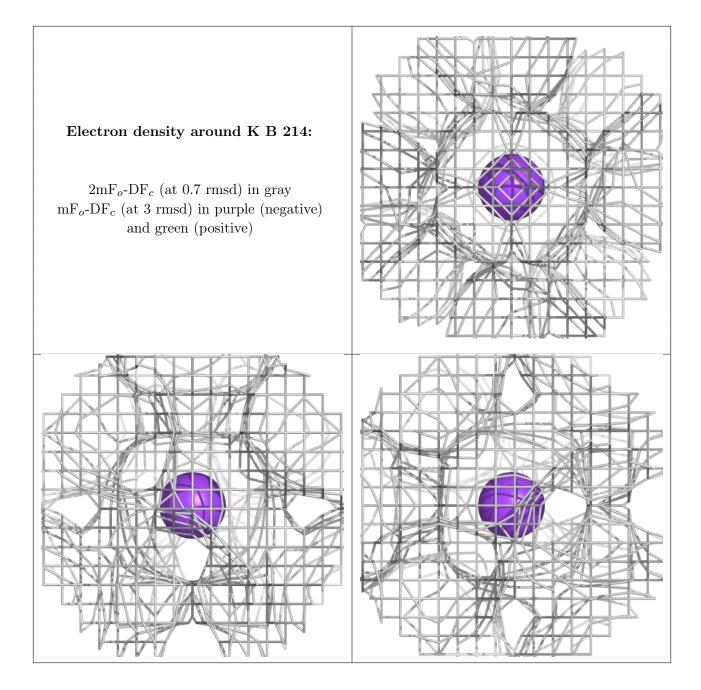


# Electron density around K B 213: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



# Electron density around K B 216: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

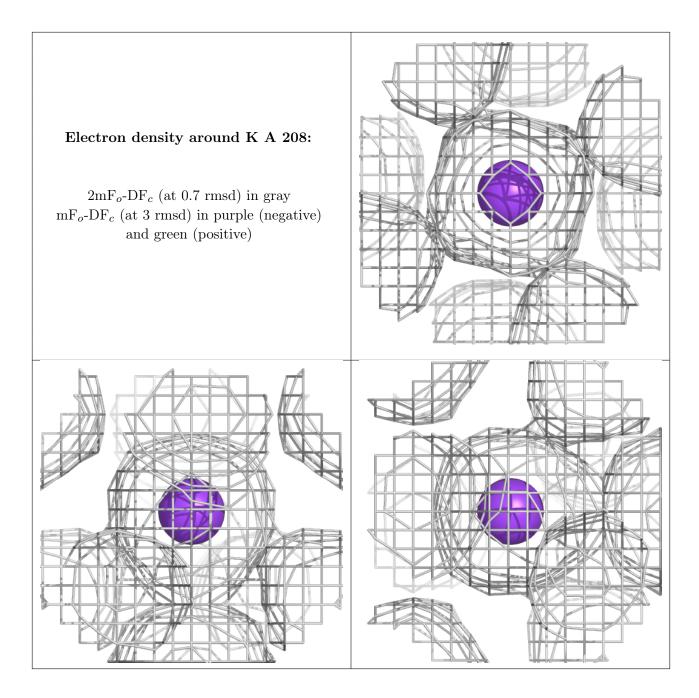






# Electron density around K B 212: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





# 6.5 Other polymers (i)

There are no such residues in this entry.

