



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2021 – 04:58 PM EDT

PDB ID : 7M2H  
Title : Structural Snapshots of Intermediates in the Gating of a K<sup>+</sup> Channel  
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Deposited on : 2021-03-16  
Resolution : 2.64 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 : 2.23.2  
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) : 2.23.2

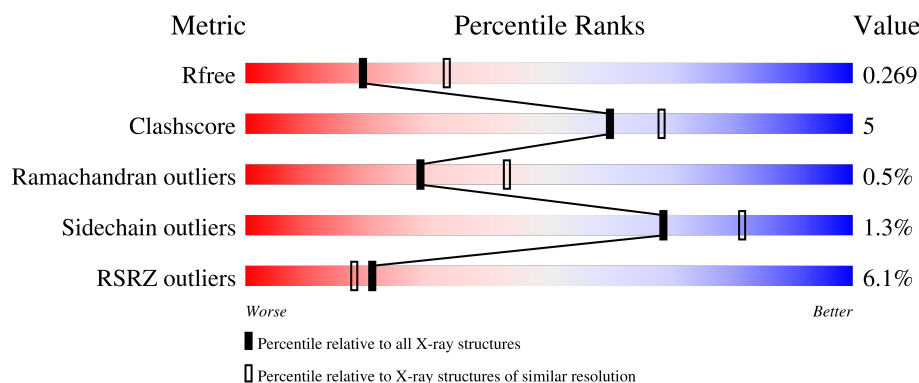
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	219	
1	D	219	
2	B	212	
2	E	212	
3	C	125	

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Mol	Chain	Length	Quality of chain
3	F	125	<div> <div>%</div> <div> </div> <div>77% 6% 18%</div> </div>

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
6	DGA	C	907	-	-	-	X
6	DGA	F	208	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8265 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 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1615	1024	270	315	6			
1	D	217	Total	C	N	O	S	0	0	0
			1580	1004	260	310	6			

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1642	1021	279	337	5			
2	E	209	Total	C	N	O	S	0	0	0
			1621	1009	275	332	5			

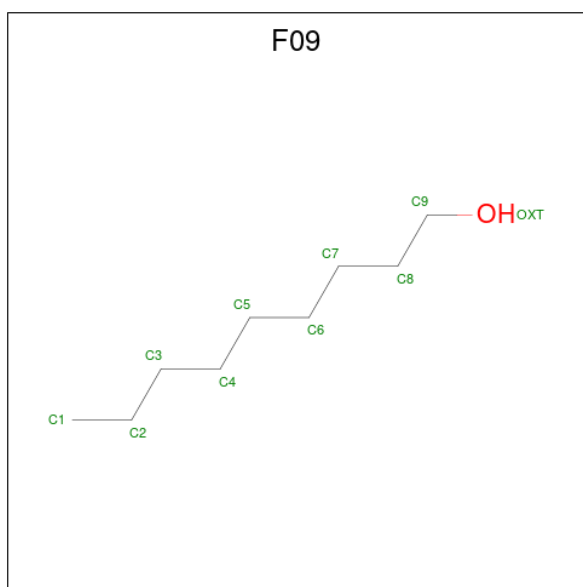
- Molecule 3 is a protein called pH-gated potassium channel KcsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	S	0	0	0
			776	513	131	131	1			
3	F	103	Total	C	N	O	S	0	0	0
			776	513	131	131	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP P0A334
C	2	ALA	-	expression tag	UNP P0A334
C	67	PHE	TRP	conflict	UNP P0A334
F	1	MET	-	initiating methionine	UNP P0A334
F	2	ALA	-	expression tag	UNP P0A334
F	67	PHE	TRP	conflict	UNP P0A334

- Molecule 4 is NONAN-1-OL (three-letter code: F09) (formula: C<sub>9</sub>H<sub>20</sub>O).

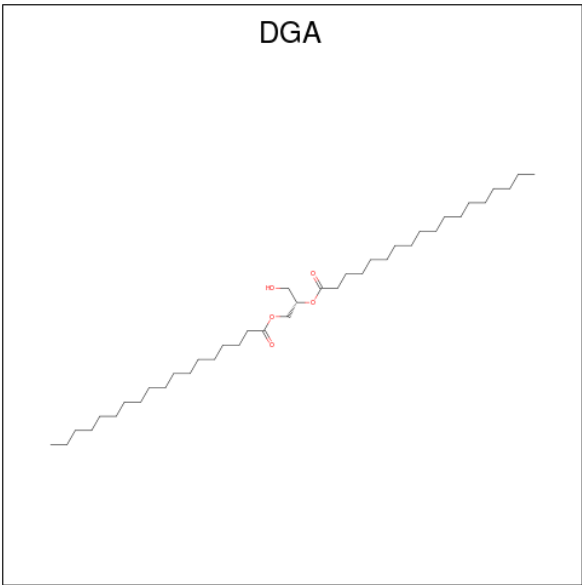


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	9	1		
4	D	1	Total	C	O	0	0
			10	9	1		

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

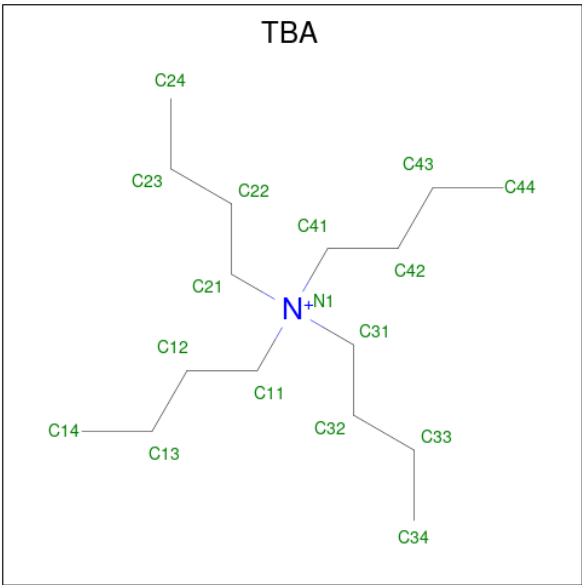
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	6	Total	K	0	0
			6	6		
5	F	6	Total	K	0	0
			6	6		

- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			31	26	5		
6	F	1	Total	C	O	0	0
			31	26	5		

- Molecule 7 is TETRABUTYLAMMONIUM ION (three-letter code: TBA) (formula: C<sub>16</sub>H<sub>36</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	N	0	0
			17	16	1		
7	F	1	Total	C	N	0	0
			17	16	1		

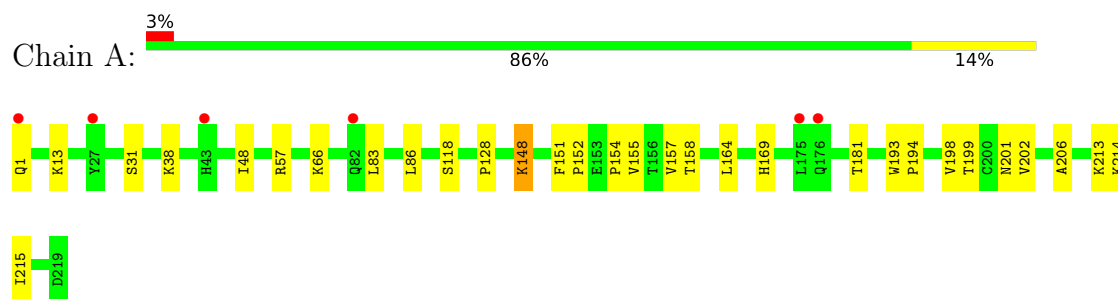
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	24	Total 24	O 24	0	0
8	B	28	Total 28	O 28	0	0
8	C	20	Total 20	O 20	0	0
8	D	6	Total 6	O 6	0	0
8	E	17	Total 17	O 17	0	0
8	F	32	Total 32	O 32	0	0

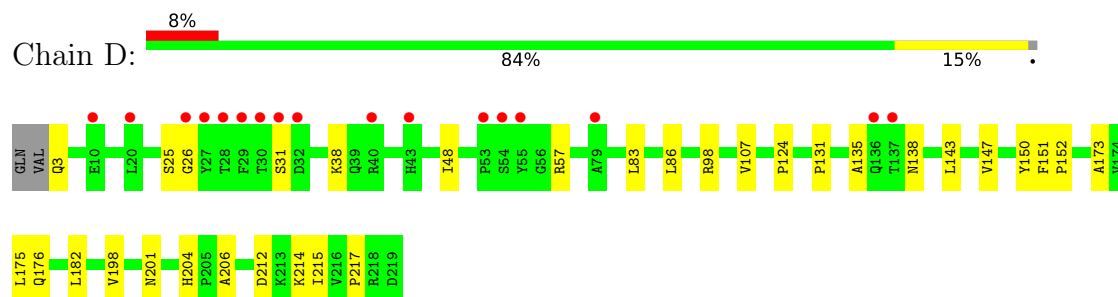
### 3 Residue-property plots [i](#)

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.

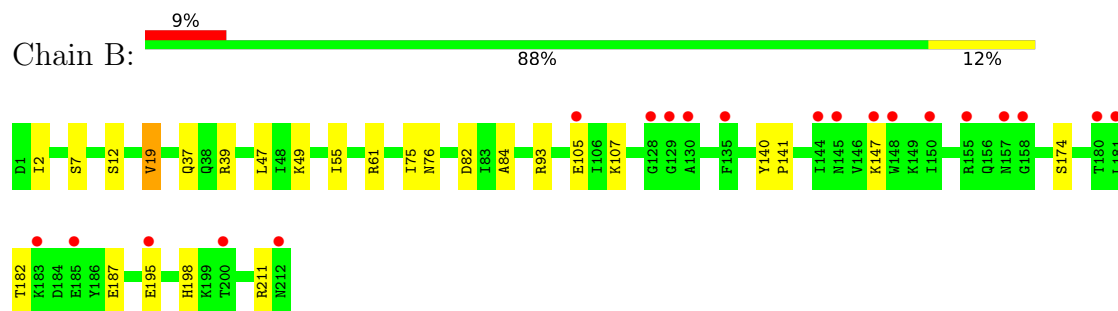
- Molecule 1: Fab heavy chain



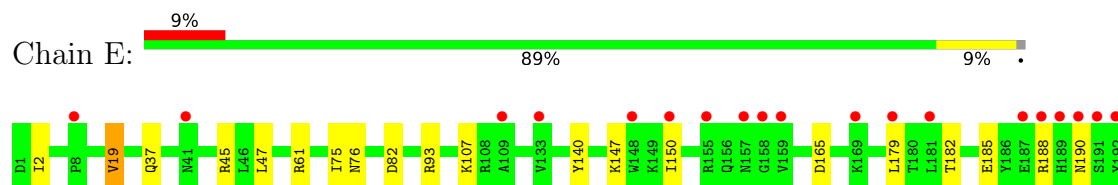
- Molecule 1: Fab heavy chain



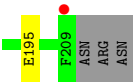
- Molecule 2: Fab light chain



- Molecule 2: Fab light chain



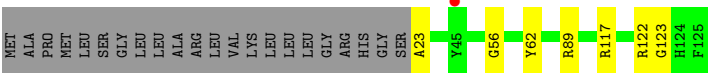
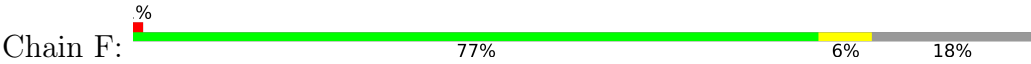




• Molecule 3: pH-gated potassium channel KcsA



• Molecule 3: pH-gated potassium channel KcsA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.32Å 154.32Å 74.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.64 48.80 – 2.64	Depositor EDS
% Data completeness (in resolution range)	92.1 (48.80-2.64) 91.4 (48.80-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.237 , 0.268 0.238 , 0.269	Depositor DCC
$R_{free}$ test set	1999 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DGA, F09, K, TBA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/1659	0.45	0/2275
1	D	0.25	0/1623	0.45	0/2227
2	B	0.39	0/1679	0.42	0/2278
2	E	0.24	0/1658	0.42	0/2251
3	C	0.23	0/796	0.40	0/1092
3	F	0.23	0/796	0.36	0/1092
All	All	0.31	0/8211	0.42	0/11215

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	1615	0	1549	21	0
1	D	1580	0	1502	20	0
2	B	1642	0	1565	16	0
2	E	1621	0	1551	12	0
3	C	776	0	791	7	0
3	F	776	0	791	5	0
4	A	10	0	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	10	0	20	1	0
5	C	6	0	0	0	0
5	F	6	0	0	0	0
6	C	31	0	44	0	0
6	F	31	0	44	2	0
7	C	17	0	36	1	0
7	F	17	0	36	1	0
8	A	24	0	0	0	0
8	B	28	0	0	3	0
8	C	20	0	0	2	0
8	D	6	0	0	1	0
8	E	17	0	0	0	0
8	F	32	0	0	1	0
All	All	8265	0	7949	74	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 5.

All (74) 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:A:1:GLN:HE22	1:D:217:PRO:HB3	1.37	0.89
1:A:1:GLN:HB2	1:D:131:PRO:HB2	1.68	0.75
2:B:198:HIS:NE2	8:B:301:HOH:O	2.18	0.75
2:B:141:PRO:O	8:B:301:HOH:O	2.09	0.71
1:D:83:LEU:HB3	1:D:86:LEU:HD21	1.75	0.66
2:B:2:ILE:HD11	2:B:93:ARG:HD2	1.77	0.66
1:A:157:VAL:HG22	1:A:202:VAL:HG22	1.78	0.66
1:D:38:LYS:HB2	1:D:48:ILE:HD11	1.79	0.65
1:A:199:THR:HG22	1:A:214:LYS:HA	1.76	0.65
1:A:38:LYS:HB2	1:A:48:ILE:HD11	1.78	0.65
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.80	0.63
3:C:120:GLU:O	3:C:122:ARG:N	2.31	0.61
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.81	0.61
1:D:173:ALA:HB2	1:D:182:LEU:HD23	1.84	0.59
1:A:83:LEU:HB3	1:A:86:LEU:HD21	1.85	0.59
1:D:214:LYS:NZ	1:D:215:ILE:O	2.32	0.58
2:B:147:LYS:HB3	2:B:195:GLU:HB2	1.87	0.56
2:B:61:ARG:NH1	2:B:82:ASP:OD1	2.40	0.54
1:A:158:THR:OG1	1:A:201:ASN:HB2	2.08	0.53
3:C:25:HIS:ND1	8:C:1001:HOH:O	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ASN:ND2	1:D:212:ASP:OD1	2.31	0.52
2:E:37:GLN:OE1	2:E:45:ARG:NH2	2.43	0.50
2:E:182:THR:OG1	2:E:185:GLU:OE1	2.27	0.50
2:E:61:ARG:NH1	2:E:82:ASP:OD1	2.46	0.49
1:A:152:PRO:HD2	1:A:206:ALA:CB	2.42	0.49
2:B:19:VAL:HG12	2:B:75:ILE:HB	1.93	0.49
2:E:185:GLU:HA	2:E:188:ARG:HG2	1.95	0.48
2:E:2:ILE:HD11	2:E:93:ARG:HD2	1.96	0.48
3:F:89:ARG:HH11	6:F:208:DGA:HA32	1.79	0.48
1:A:198:VAL:HG23	1:A:215:ILE:HB	1.96	0.47
1:A:1:GLN:H3	1:D:135:ALA:HB3	1.79	0.47
3:C:108:ALA:O	3:C:112:THR:HG23	2.14	0.47
1:D:175:LEU:HG	1:D:176:GLN:N	2.29	0.47
1:A:57:ARG:HH21	4:A:301:F09:H81	1.79	0.47
1:D:31:SER:HB2	3:F:62:TYR:CE1	2.50	0.47
1:A:151:PHE:HA	1:A:152:PRO:HA	1.68	0.46
1:A:66:LYS:HE2	1:A:66:LYS:HB3	1.82	0.46
1:D:143:LEU:HD12	1:D:198:VAL:HG11	1.98	0.46
2:E:93:ARG:NH1	3:F:56:GLY:O	2.49	0.45
2:E:61:ARG:HG3	2:E:76:ASN:O	2.17	0.45
1:A:128:PRO:HG3	1:A:213:LYS:HD2	1.98	0.45
1:D:26:GLY:O	8:D:401:HOH:O	2.21	0.45
2:B:39:ARG:HG2	2:B:84:ALA:HB2	2.00	0.44
2:E:19:VAL:HG12	2:E:75:ILE:HB	1.99	0.44
7:C:908:TBA:H322	7:C:908:TBA:H412	1.74	0.44
2:B:61:ARG:HG3	2:B:76:ASN:O	2.17	0.44
1:A:148:LYS:HB3	1:A:181:THR:HG23	1.99	0.44
3:F:89:ARG:HH11	6:F:208:DGA:CA3	2.31	0.44
1:A:1:GLN:N	1:D:135:ALA:HB3	2.32	0.43
2:B:49:LYS:HE3	8:B:303:HOH:O	2.17	0.43
2:B:93:ARG:NH1	3:C:56:GLY:O	2.51	0.43
2:E:147:LYS:HB3	2:E:195:GLU:HB2	2.00	0.43
2:B:107:LYS:HA	2:B:140:TYR:OH	2.19	0.42
1:D:3:GLN:HB3	1:D:25:SER:O	2.19	0.42
7:F:201:TBA:H322	7:F:201:TBA:H412	1.61	0.42
3:F:23:ALA:N	8:F:302:HOH:O	2.51	0.42
1:A:13:LYS:NZ	1:A:118:SER:O	2.51	0.42
1:D:124:PRO:HB3	1:D:150:TYR:HB3	2.01	0.42
1:D:98:ARG:HB3	1:D:107:VAL:HG13	2.02	0.42
1:D:204:HIS:CE1	1:D:206:ALA:HB3	2.54	0.42
2:B:12:SER:OG	2:B:105:GLU:OE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:PHE:HA	1:D:152:PRO:HA	1.84	0.41
2:E:150:ILE:HD11	2:E:179:LEU:HD21	2.02	0.41
1:A:148:LYS:HA	1:A:181:THR:HA	2.02	0.41
1:A:193:TRP:CD1	1:A:194:PRO:HA	2.55	0.41
3:C:80:ASP:OD1	3:C:80:ASP:N	2.54	0.41
3:C:23:ALA:N	8:C:1004:HOH:O	2.54	0.41
1:D:57:ARG:CZ	4:D:301:F09:H82	2.51	0.41
2:E:107:LYS:HA	2:E:140:TYR:OH	2.21	0.41
1:A:31:SER:HB2	3:C:62:TYR:CE1	2.56	0.40
2:B:49:LYS:HG2	2:B:55:ILE:HD11	2.03	0.40
1:A:169:HIS:CE1	2:B:174:SER:HG	2.39	0.40
2:B:187:GLU:OE2	2:B:211:ARG:NH2	2.54	0.40
1:D:147:VAL:HB	1:D:182:LEU:HD12	2.03	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	217/219 (99%)	206 (95%)	10 (5%)	1 (0%)	29	43
1	D	215/219 (98%)	203 (94%)	11 (5%)	1 (0%)	29	43
2	B	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
2	E	207/212 (98%)	198 (96%)	9 (4%)	0	100	100
3	C	101/125 (81%)	97 (96%)	3 (3%)	1 (1%)	15	22
3	F	101/125 (81%)	99 (98%)	0	2 (2%)	7	10
All	All	1051/1112 (94%)	1002 (95%)	44 (4%)	5 (0%)	29	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	122	ARG
1	D	138	ASN
3	F	122	ARG
3	F	123	GLY
1	A	154	PRO

### 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	174/185 (94%)	171 (98%)	3 (2%)	60	76
1	D	168/185 (91%)	168 (100%)	0	100	100
2	B	188/190 (99%)	185 (98%)	3 (2%)	62	78
2	E	187/190 (98%)	184 (98%)	3 (2%)	62	78
3	C	74/92 (80%)	73 (99%)	1 (1%)	67	80
3	F	74/92 (80%)	73 (99%)	1 (1%)	67	80
All	All	865/934 (93%)	854 (99%)	11 (1%)	69	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LYS
1	A	155	VAL
1	A	164	LEU
2	B	7	SER
2	B	19	VAL
2	B	182	THR
3	C	35	LEU
2	E	19	VAL
2	E	165	ASP
2	E	190	ASN
3	F	117	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	169	HIS
2	E	27	GLN
2	E	190	ASN
3	F	119	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	DGA	F	208	-	30,30,43	1.35	3 (10%)	32,32,45	1.24	2 (6%)
7	TBA	C	908	-	16,16,16	0.93	0	18,18,18	0.64	0
6	DGA	C	907	-	30,30,43	1.37	3 (10%)	32,32,45	1.23	2 (6%)
4	F09	D	301	-	9,9,9	0.30	0	8,8,8	0.79	0
4	F09	A	301	-	9,9,9	0.31	0	8,8,8	0.81	0
7	TBA	F	201	-	16,16,16	0.91	0	18,18,18	0.64	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
6	DGA	F	208	-	-	13/32/32/45	-
7	TBA	C	908	-	-	2/20/20/20	-
6	DGA	C	907	-	-	11/32/32/45	-
4	F09	D	301	-	-	1/7/7/7	-
4	F09	A	301	-	-	1/7/7/7	-
7	TBA	F	201	-	-	1/20/20/20	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	208	DGA	OG1-CA1	3.64	1.44	1.33
6	C	907	DGA	OG1-CA1	3.54	1.43	1.33
6	C	907	DGA	OG2-CB1	2.90	1.42	1.34
6	F	208	DGA	OG2-CB1	2.87	1.42	1.34
6	F	208	DGA	OG2-CG2	-2.71	1.39	1.46
6	C	907	DGA	OG2-CG2	-2.60	1.40	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	907	DGA	OG2-CB1-CB2	4.04	120.20	111.50
6	F	208	DGA	OG2-CB1-CB2	3.94	120.00	111.50
6	F	208	DGA	OG1-CA1-CA2	2.45	119.59	111.91
6	C	907	DGA	OG1-CA1-CA2	2.39	119.42	111.91

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	907	DGA	OB1-CB1-OG2-CG2
6	C	907	DGA	CG1-CG2-CG3-OXT
6	C	907	DGA	OG2-CG2-CG3-OXT
6	F	208	DGA	CA2-CA1-OG1-CG1
6	F	208	DGA	OA1-CA1-OG1-CG1
6	F	208	DGA	OB1-CB1-OG2-CG2
6	C	907	DGA	CB2-CB1-OG2-CG2
6	F	208	DGA	CB2-CB1-OG2-CG2
6	C	907	DGA	CB3-CB4-CB5-CB6
6	C	907	DGA	CA1-CA2-CA3-CA4

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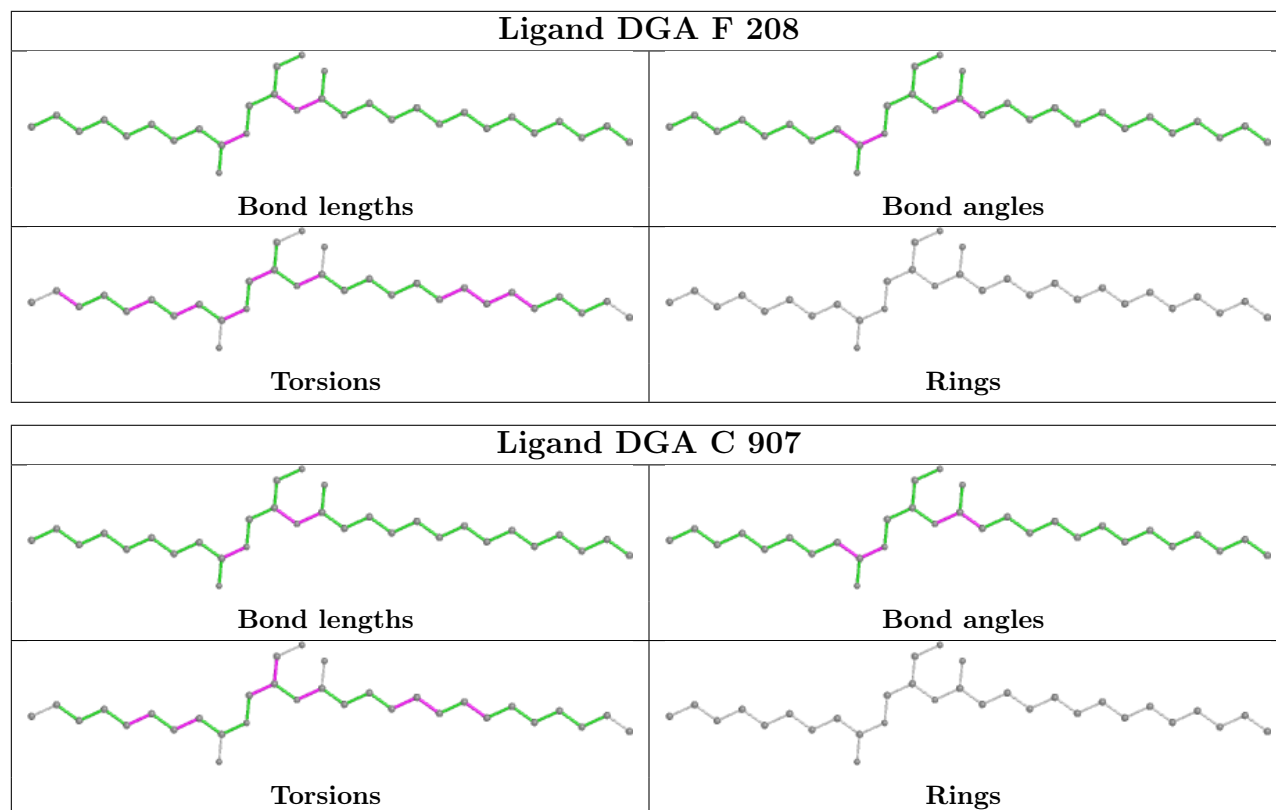
Mol	Chain	Res	Type	Atoms
6	F	208	DGA	CA1-CA2-CA3-CA4
7	C	908	TBA	N1-C11-C12-C13
7	C	908	TBA	N1-C31-C32-C33
7	F	201	TBA	N1-C31-C32-C33
6	F	208	DGA	CB7-CB8-CB9-CAB
6	C	907	DGA	CB6-CB7-CB8-CB9
6	F	208	DGA	CA3-CA4-CA5-CA6
4	D	301	F09	C6-C7-C8-C9
6	C	907	DGA	CB4-CB5-CB6-CB7
6	F	208	DGA	CB5-CB6-CB7-CB8
6	F	208	DGA	CA6-CA7-CA8-CA9
6	C	907	DGA	OG1-CG1-CG2-CG3
6	C	907	DGA	OG1-CG1-CG2-OG2
6	F	208	DGA	OG1-CG1-CG2-OG2
6	F	208	DGA	CB6-CB7-CB8-CB9
6	C	907	DGA	CA3-CA4-CA5-CA6
6	F	208	DGA	CBB-CAB-CB9-CB8
6	F	208	DGA	OG1-CG1-CG2-CG3
4	A	301	F09	C1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	208	DGA	2	0
7	C	908	TBA	1	0
4	D	301	F09	1	0
4	A	301	F09	1	0
7	F	201	TBA	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	219/219 (100%)	0.20	6 (2%) 54 50	18, 44, 70, 85	0
1	D	217/219 (99%)	0.43	17 (7%) 13 10	20, 42, 60, 81	0
2	B	212/212 (100%)	0.55	20 (9%) 8 6	12, 43, 77, 90	0
2	E	209/212 (98%)	0.54	20 (9%) 8 6	17, 41, 70, 87	0
3	C	103/125 (82%)	0.15	1 (0%) 82 81	11, 19, 29, 35	0
3	F	103/125 (82%)	0.22	1 (0%) 82 81	15, 21, 32, 40	0
All	All	1063/1112 (95%)	0.38	65 (6%) 21 18	11, 37, 68, 90	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	187	GLU	6.1
2	E	191	SER	5.0
1	A	27	TYR	4.8
2	E	190	ASN	4.7
1	D	30	THR	4.5
2	B	181	LEU	4.5
2	E	189	HIS	4.2
2	E	109	ALA	3.8
1	D	137	THR	3.8
2	E	188	ARG	3.7
1	D	53	PRO	3.7
2	B	155	ARG	3.7
2	B	195	GLU	3.6
2	E	192	TYR	3.6
2	B	147	LYS	3.5
1	A	1	GLN	3.5
2	E	181	LEU	3.5
1	D	43	HIS	3.3
2	E	41	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	128	GLY	3.3
2	B	183	LYS	3.3
2	E	179	LEU	3.3
1	A	43	HIS	3.2
2	B	158	GLY	3.2
2	E	148	TRP	3.1
2	B	129	GLY	3.0
2	E	157	ASN	3.0
2	E	8	PRO	2.9
1	D	27	TYR	2.9
1	D	10	GLU	2.9
1	D	26	GLY	2.8
2	B	144	ILE	2.8
1	D	55	TYR	2.8
2	E	209	PHE	2.8
2	B	200	THR	2.8
2	B	145	ASN	2.8
1	D	136	GLN	2.7
1	D	79	ALA	2.7
2	E	155	ARG	2.7
2	B	180	THR	2.7
1	A	175	LEU	2.7
2	B	135	PHE	2.6
2	E	133	VAL	2.6
1	D	31	SER	2.6
3	F	45	TYR	2.5
2	E	158	GLY	2.4
2	B	130	ALA	2.4
1	A	82	GLN	2.4
2	B	157	ASN	2.4
3	C	79	GLY	2.4
2	B	148	TRP	2.4
2	E	150	ILE	2.3
1	D	20	LEU	2.3
2	B	105	GLU	2.2
2	B	212	ASN	2.2
1	D	28	THR	2.2
2	E	159	VAL	2.2
2	B	150	ILE	2.2
2	E	169	LYS	2.1
1	A	176	GLN	2.1
1	D	54	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	40	ARG	2.1
1	D	32	ASP	2.1
1	D	29	PHE	2.0
2	B	185	GLU	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 ⓘ

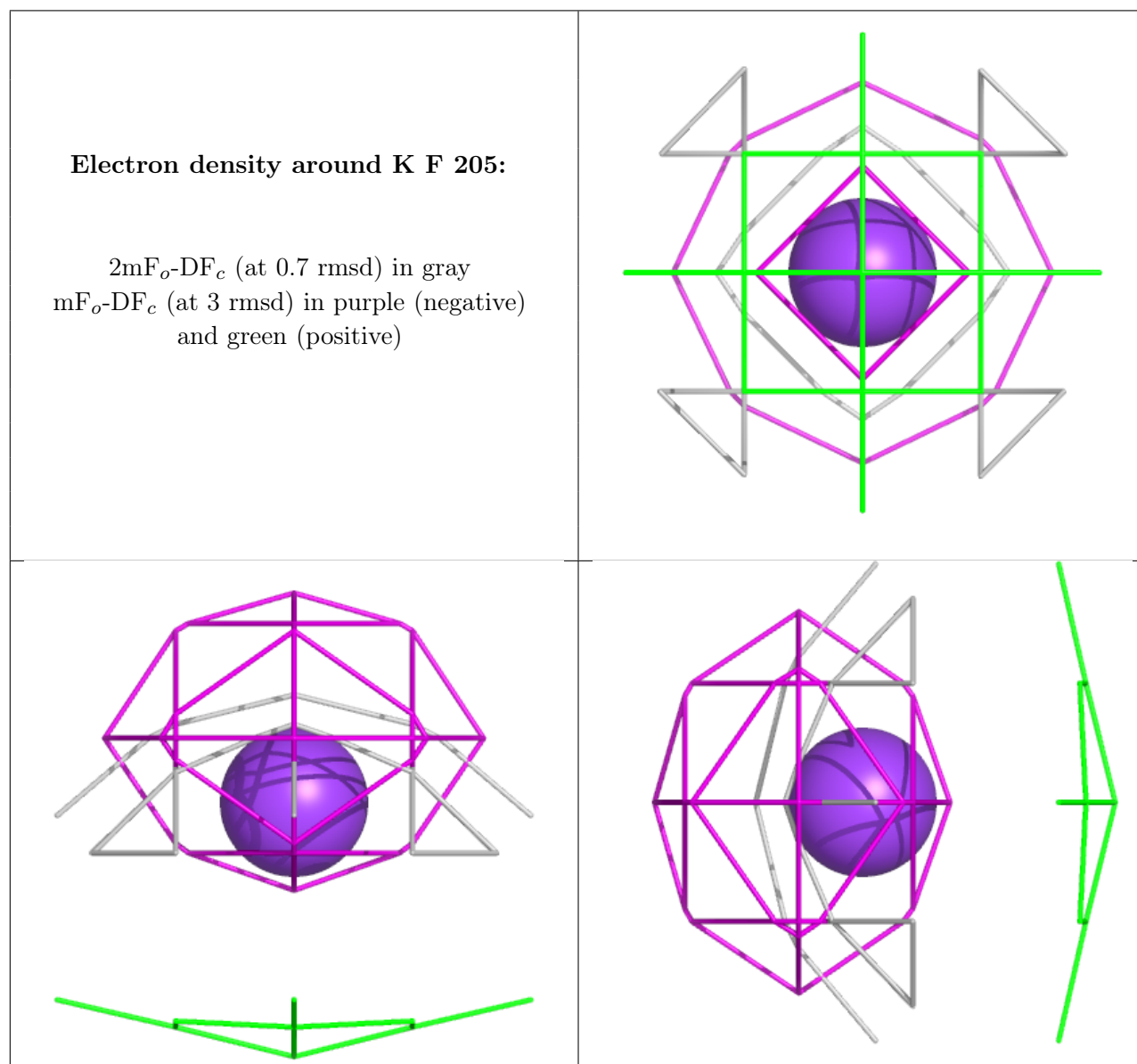
There are no monosaccharides in this entry.

## 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.

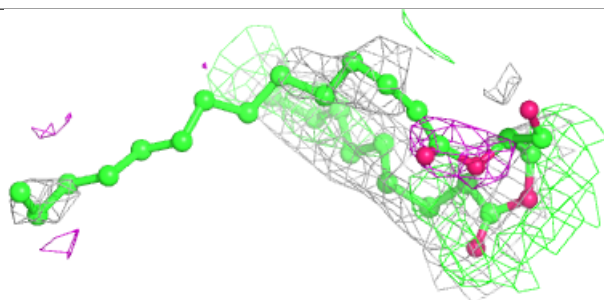
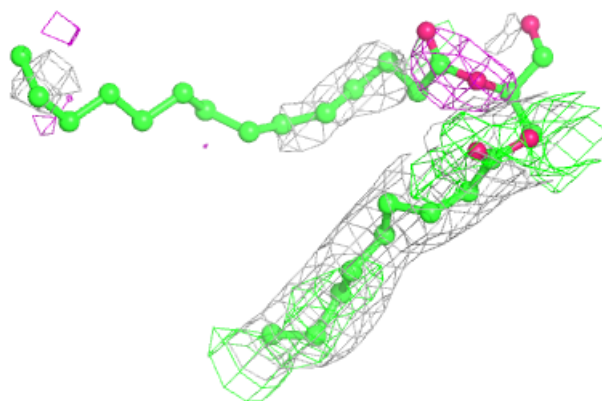
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	K	F	205	1/1	0.09	0.32	30,30,30,30	1
6	DGA	F	208	31/44	0.30	0.66	66,68,72,75	0
6	DGA	C	907	31/44	0.46	0.72	66,68,72,75	0
5	K	C	901	1/1	0.49	0.36	30,30,30,30	1
4	F09	D	301	10/10	0.76	0.28	20,20,20,20	0
5	K	F	204	1/1	0.79	0.27	30,30,30,30	1
4	F09	A	301	10/10	0.85	0.17	20,20,20,20	0
5	K	F	203	1/1	0.86	0.39	30,30,30,30	1
5	K	C	902	1/1	0.92	0.36	30,30,30,30	1
5	K	C	904	1/1	0.93	0.28	30,30,30,30	1
5	K	F	207	1/1	0.94	0.33	30,30,30,30	1
5	K	C	905	1/1	0.94	0.32	30,30,30,30	1
5	K	F	206	1/1	0.94	0.33	30,30,30,30	1
7	TBA	C	908	17/17	0.94	0.31	20,20,20,20	17
5	K	C	906	1/1	0.95	0.35	30,30,30,30	1
7	TBA	F	201	17/17	0.97	0.21	20,20,20,20	17
5	K	F	202	1/1	0.98	0.27	30,30,30,30	1
5	K	C	903	1/1	0.98	0.34	30,30,30,30	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.

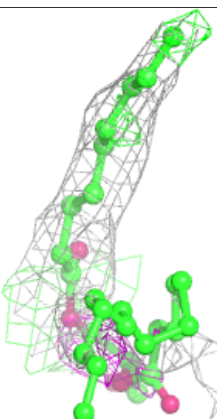
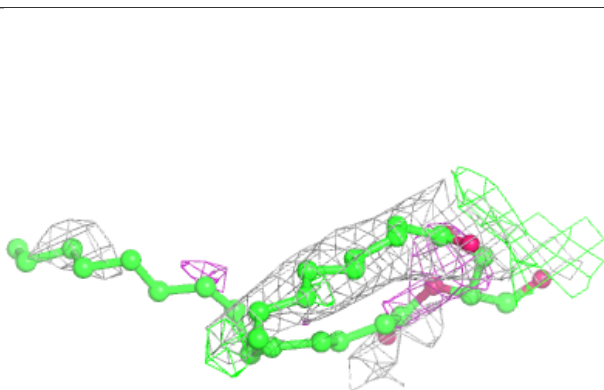
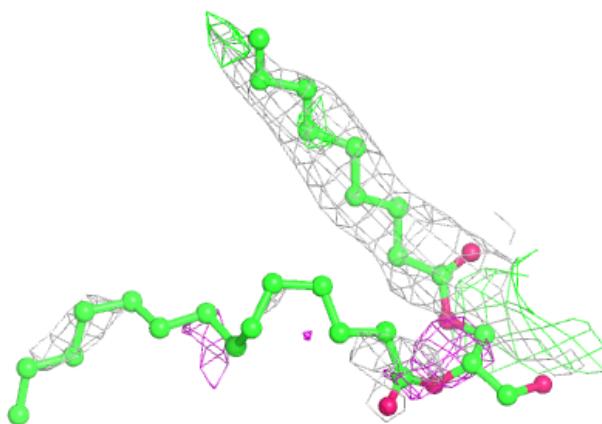


**Electron density around DGA F 208:**

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

**Electron density around DGA C 907:**

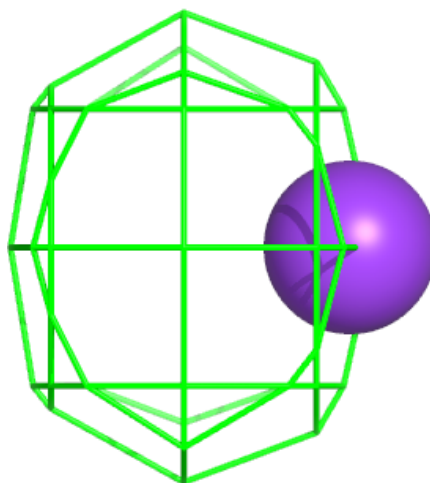
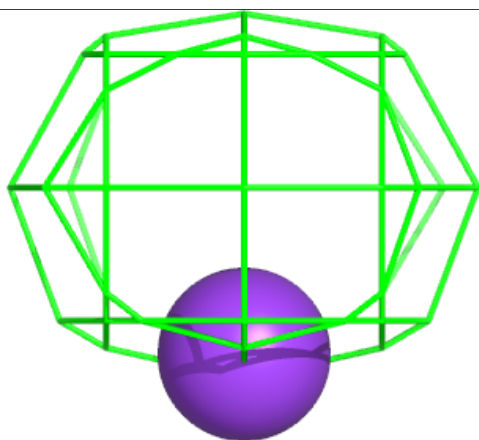
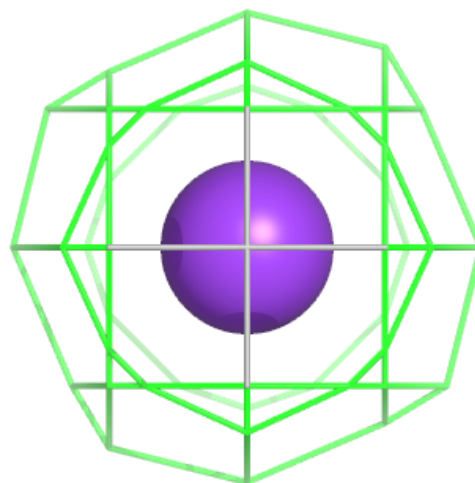
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





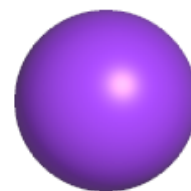
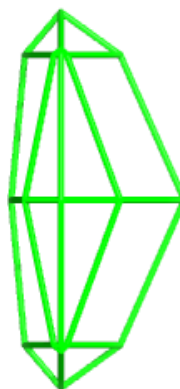
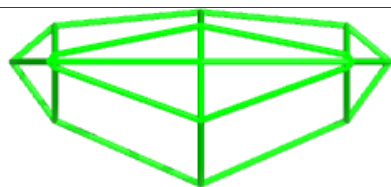
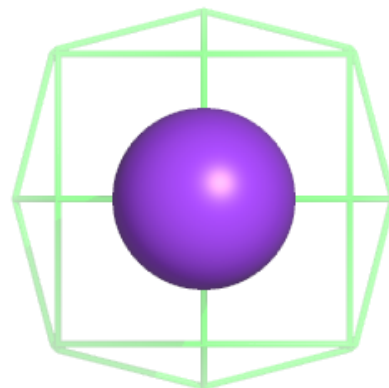
**Electron density around K C 901:**

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



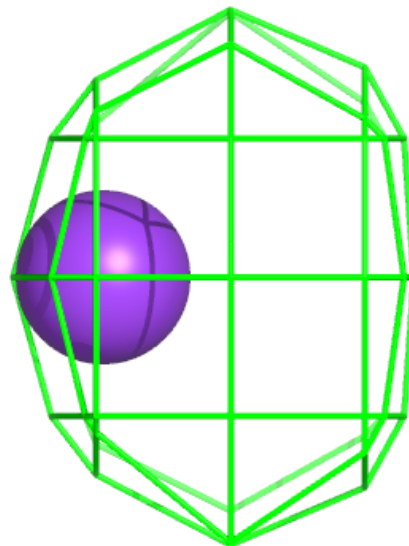
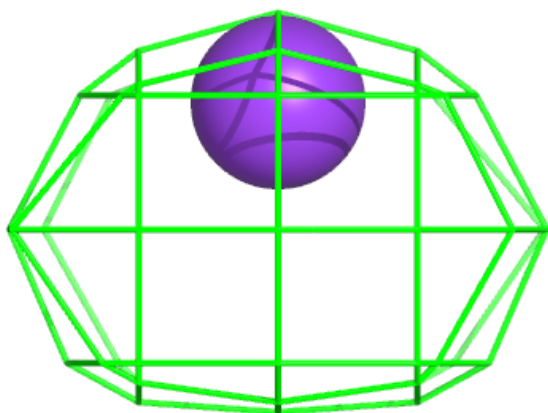
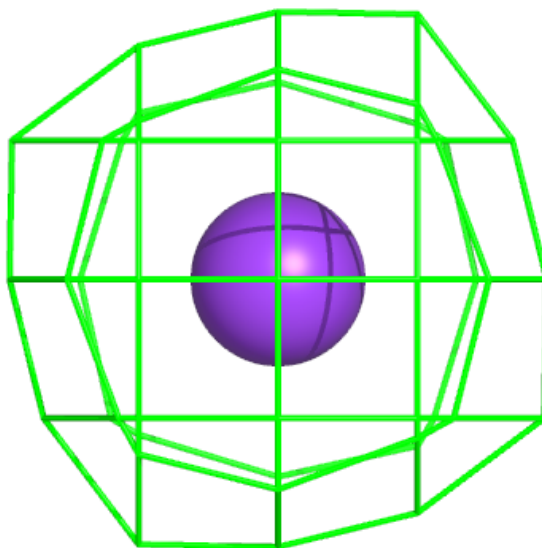
**Electron density around K F 204:**

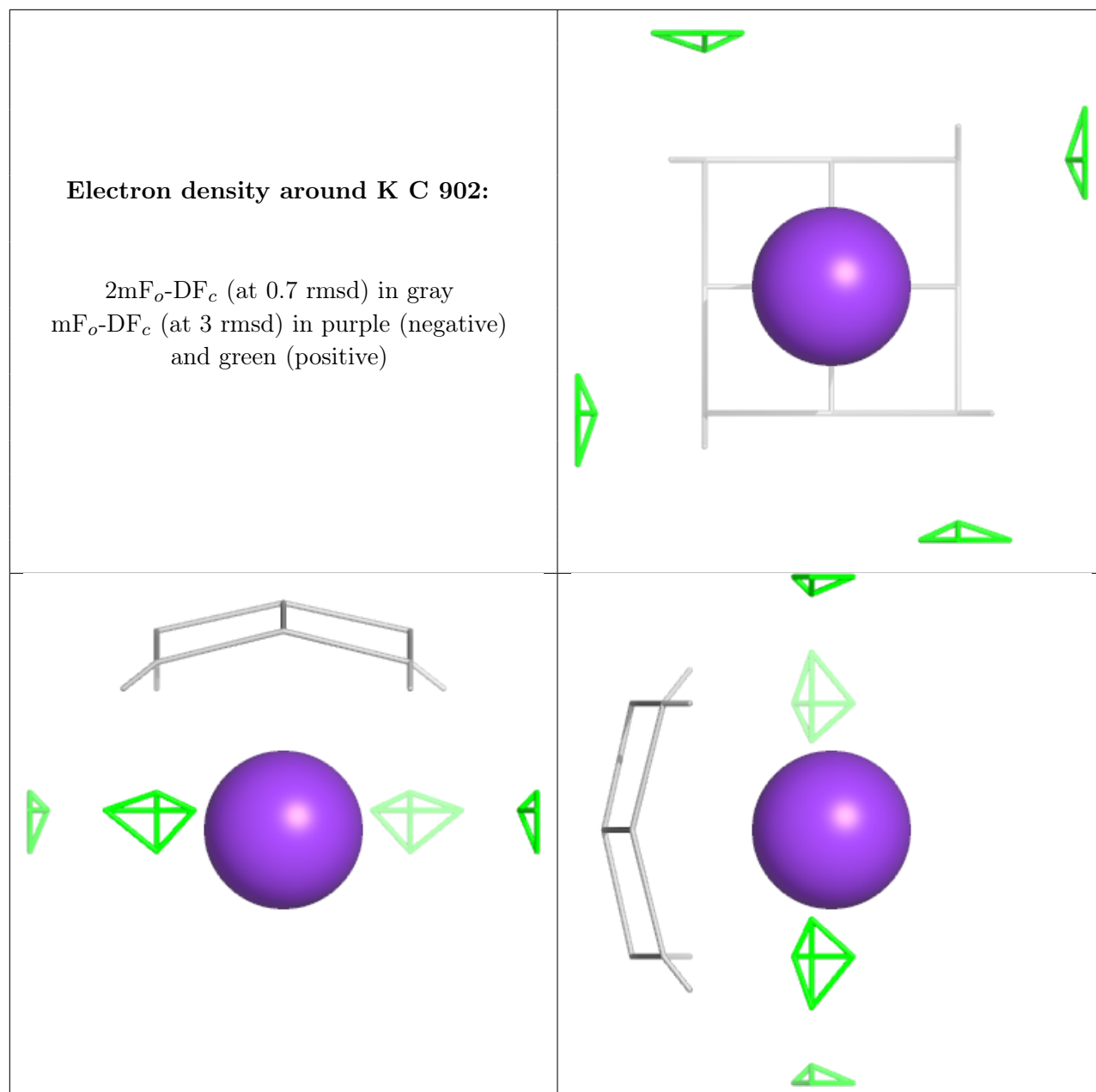
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around K F 203:**

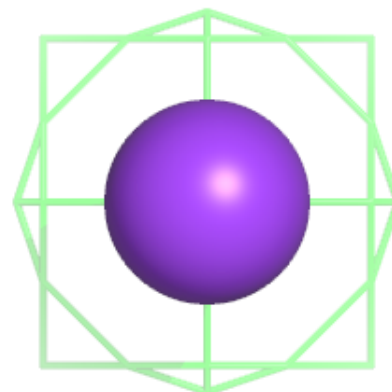
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

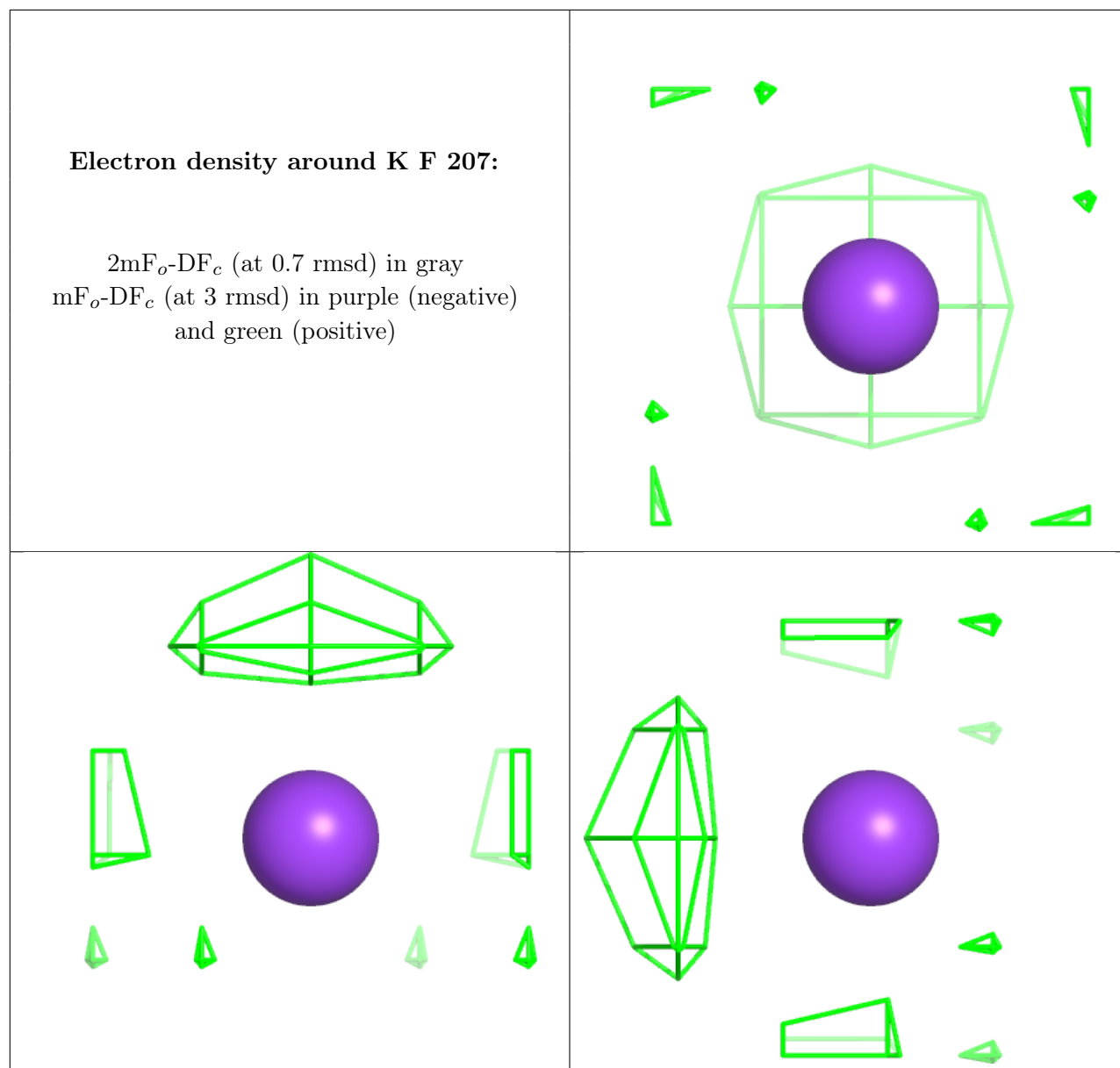




**Electron density around K C 904:**

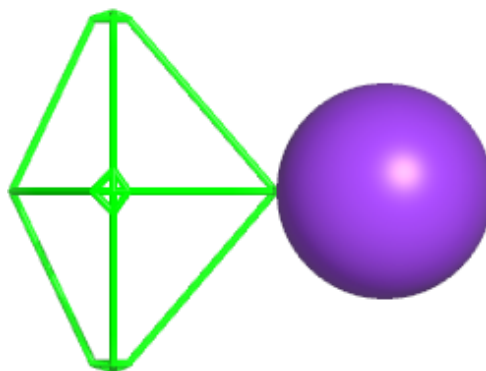
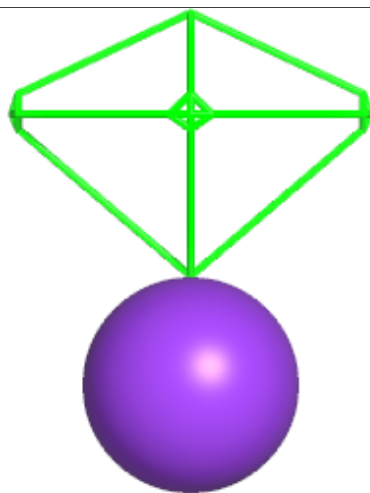
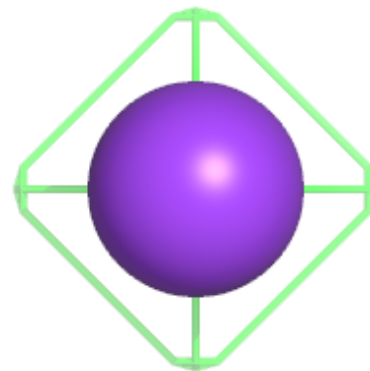
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





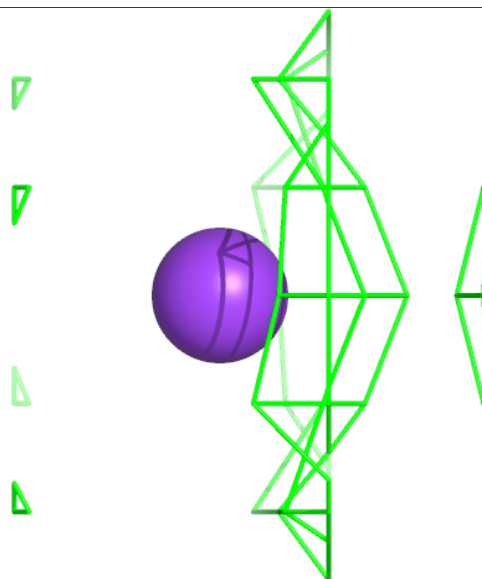
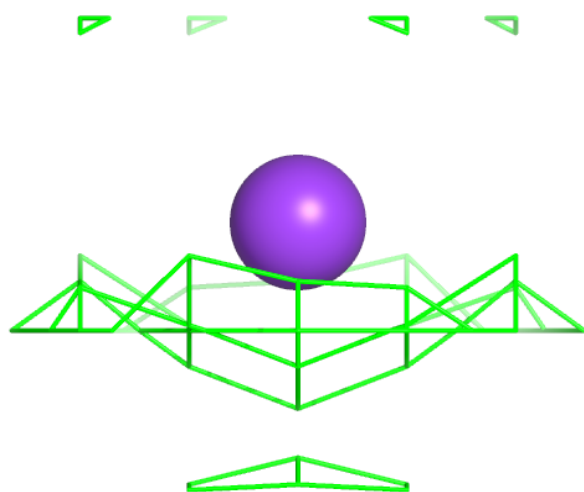
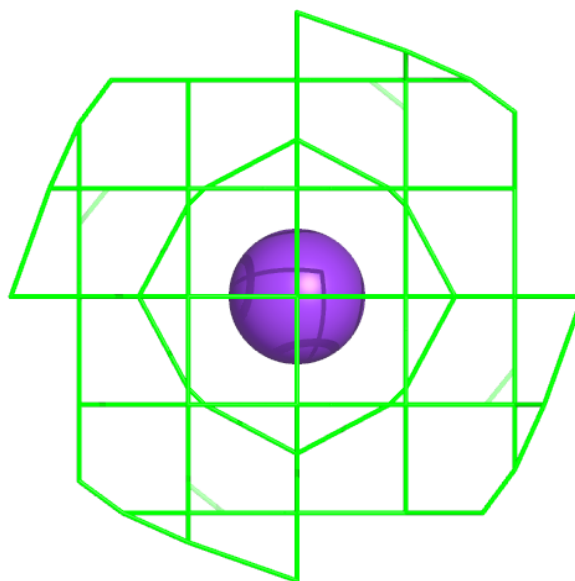
**Electron density around K C 905:**

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



**Electron density around K F 206:**

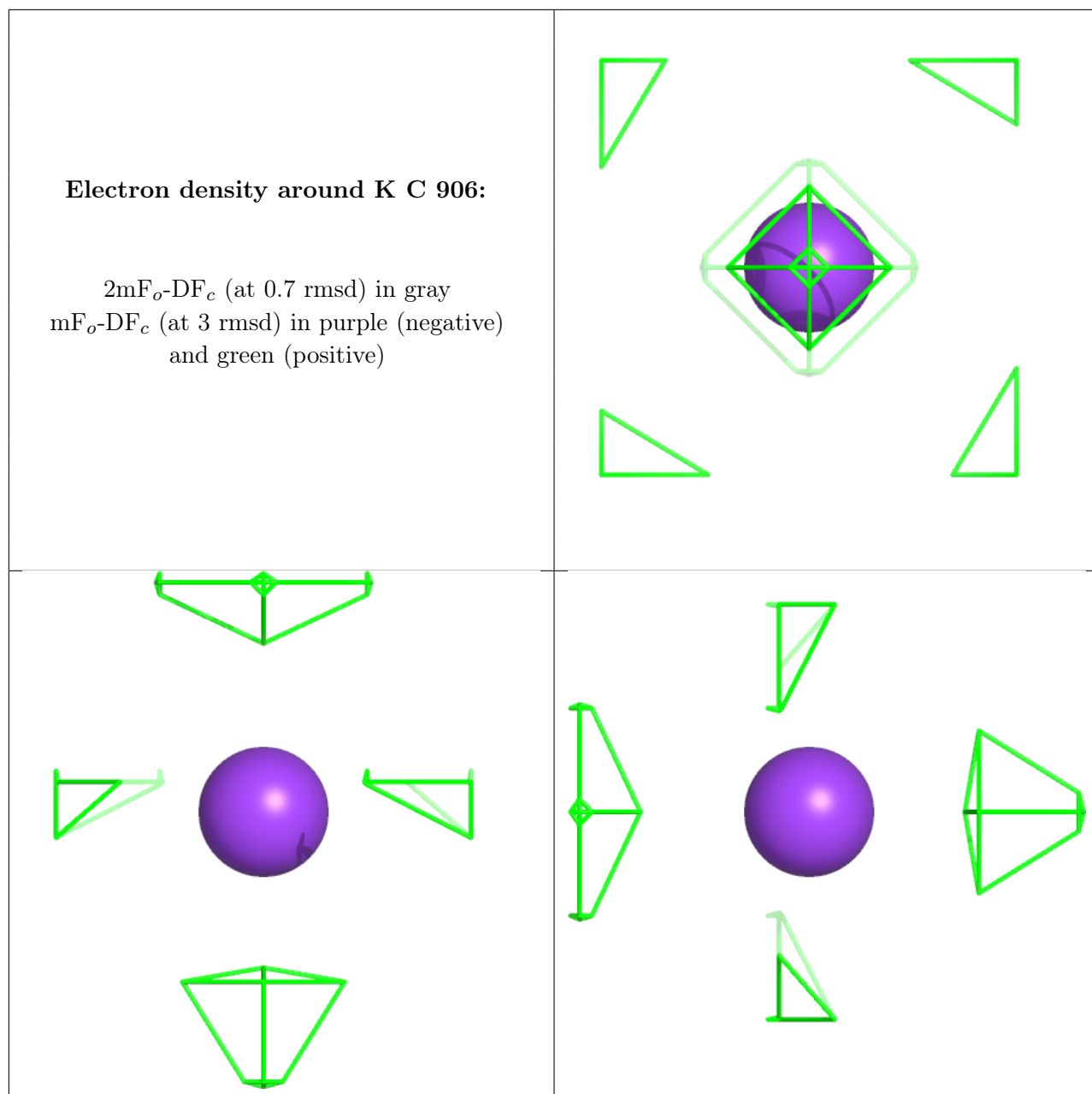
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

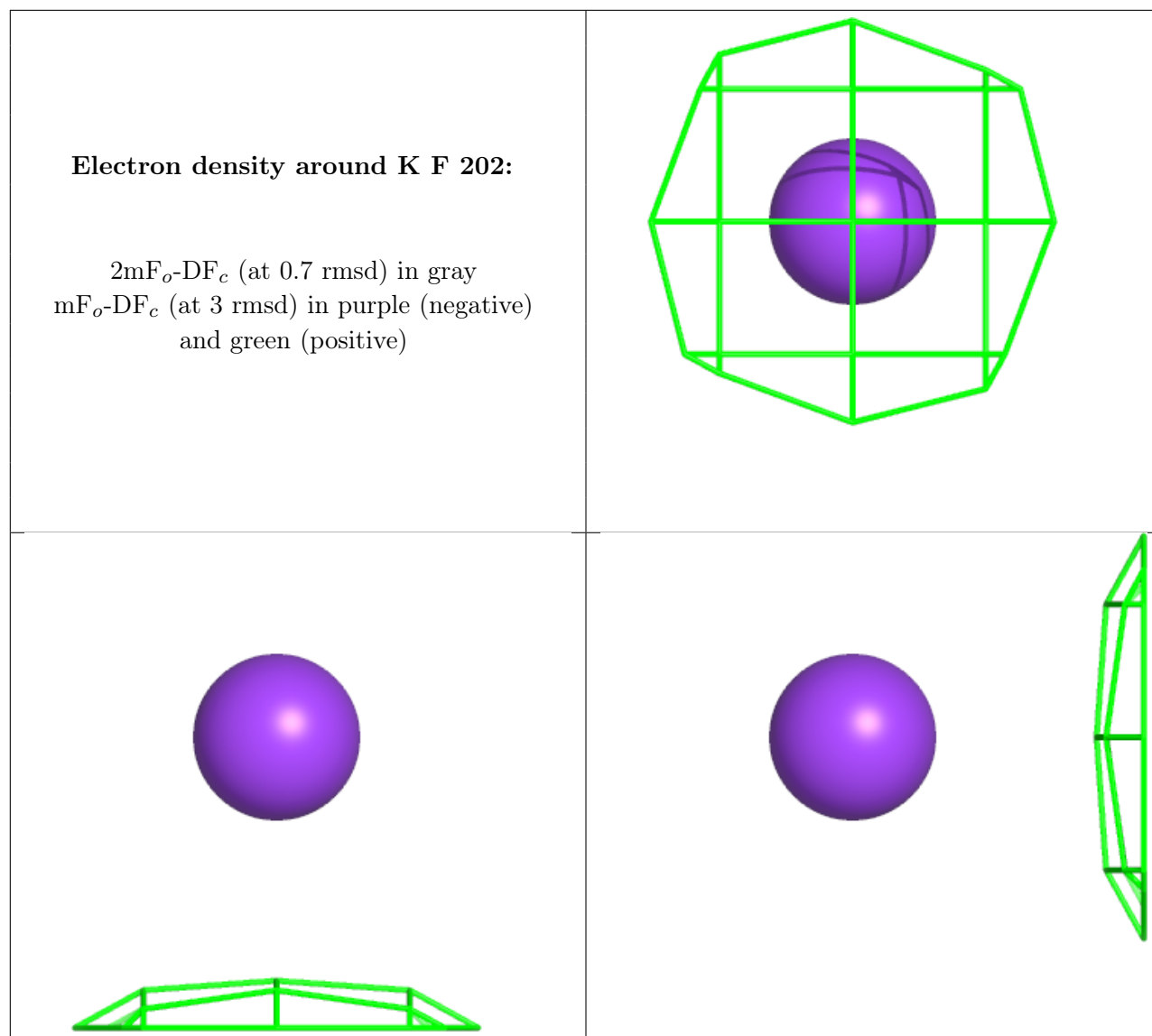


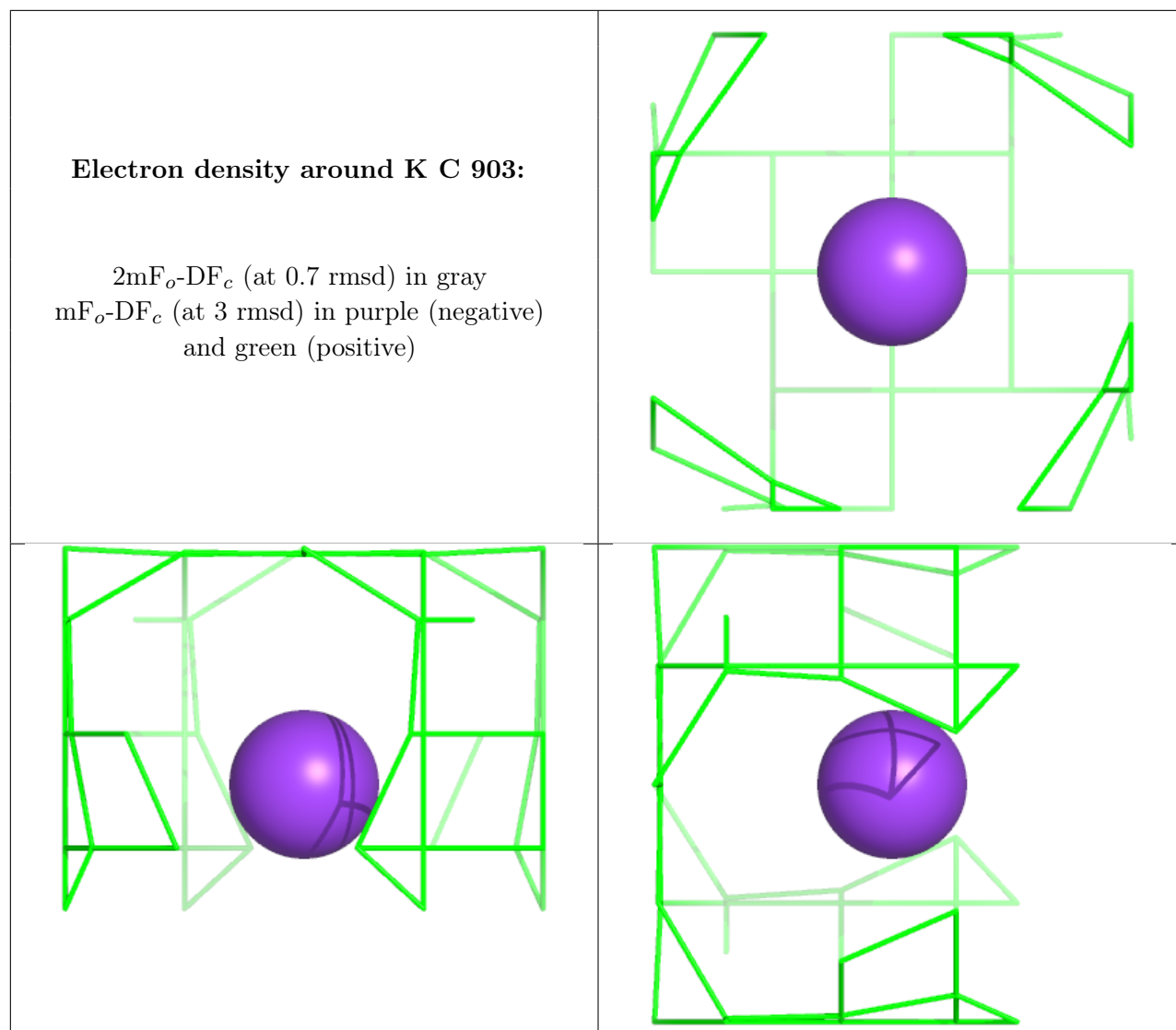


**Electron density around K C 906:**

$2mF_o-DF_c$  (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.