



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 9, 2021 – 02:32 PM EST

PDB ID : 7M2V
Title : Crystallographic Structure of the Rhombohedral Crystal Form of STMV
Grown from Chloride
Authors : McPherson, A.
Deposited on : 2021-03-17
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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	:	2.24
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)	:	2.24

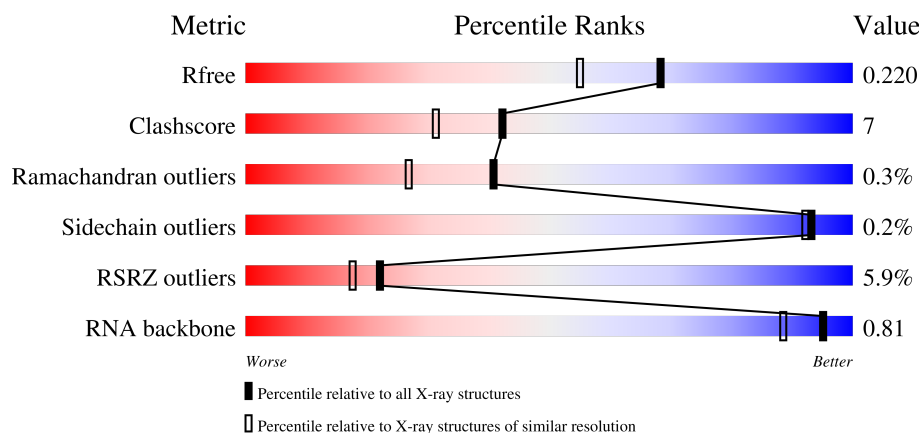
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)
RNA backbone	3102	1060 (2.40-1.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	159	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>8%</div> </div> </div>
1	B	159	<div> <div></div> <div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>
1	C	159	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>9%</div> </div> </div>
1	D	159	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	E	159	
1	FX	159	
1	G	159	
1	GG	159	
1	H	159	
1	HH	159	
1	I	159	
1	II	159	
1	J	159	
1	JJ	159	
1	K	159	
1	KK	159	
1	L	159	
1	M	159	
1	NN	159	
1	O	159	
2	QQ	12	
2	T	12	
2	e	12	
2	h	12	
2	i	12	
2	m	12	
2	n	12	
2	ww	12	
2	xx	12	

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Mol	Chain	Length	Quality of chain
2	yy	12	
3	P	12	
3	S	12	
3	TT	12	
3	U	12	
3	V	12	
3	X	12	
3	Y	12	
3	ff	12	
3	k	12	
3	zz	12	

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
4	CL	B	201	-	-	X	-
4	CL	H	201	-	-	X	-
4	CL	II	201	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 43122 atoms, of which 9956 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 Coat protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	146	Total	C	H	N	O	S	0	11	0
			2255	717	1115	201	216	6			
1	B	143	Total	C	H	N	O	S	0	12	0
			2205	703	1090	197	208	7			
1	C	144	Total	C	H	N	O	S	0	21	0
			2242	710	1113	202	211	6			
1	E	144	Total	C	H	N	O	S	0	18	0
			2218	708	1092	202	210	6			
1	J	150	Total	C	H	N	O	S	0	12	0
			2276	733	1104	210	223	6			
1	M	144	Total	C	H	N	O	S	0	10	0
			2259	714	1122	203	214	6			
1	HH	145	Total	C	H	N	O	S	0	14	0
			2262	715	1125	200	215	7			
1	II	143	Total	C	H	N	O	S	0	13	0
			2196	703	1080	197	210	6			
1	JJ	144	Total	C	H	N	O	S	0	17	0
			2236	705	1115	199	211	6			
1	FX	144	Total	C	N	O	S		0	14	0
			1189	757	206	217	9				
1	D	144	Total	C	N	O	S		0	14	0
			1186	754	206	217	9				
1	KK	144	Total	C	N	O	S		0	13	0
			1184	750	209	217	8				
1	G	144	Total	C	N	O	S		0	11	0
			1170	740	205	217	8				
1	H	144	Total	C	N	O	S		0	14	0
			1189	757	206	217	9				
1	GG	144	Total	C	N	O	S		0	15	0
			1205	767	212	217	9				
1	I	144	Total	C	N	O	S		0	15	0
			1205	767	212	217	9				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	144	Total	C	N	O	S	0	15	0
			1205	767	212	217	9			
1	O	144	Total	C	N	O	S	0	15	0
			1205	767	212	217	9			
1	K	144	Total	C	N	O	S	0	15	0
			1205	767	212	217	9			
1	NN	144	Total	C	N	O	S	0	15	0
			1205	767	212	217	9			

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QQ	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
2	h	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
2	ww	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
2	T	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
2	m	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
2	i	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
2	e	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
2	n	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
2	xx	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			
2	yy	10	Total	C	N	O	P	0	10	0
			201	90	20	81	10			

- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			
3	V	10	Total	C	N	O	P	0	10	0
			221	100	50	61	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	k	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
3	U	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
3	X	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
3	TT	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
3	P	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
3	Y	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
3	ff	10	Total 221	C 100	N 50	O 61	P 10	0	10	0
3	zz	10	Total 221	C 100	N 50	O 61	P 10	0	10	0

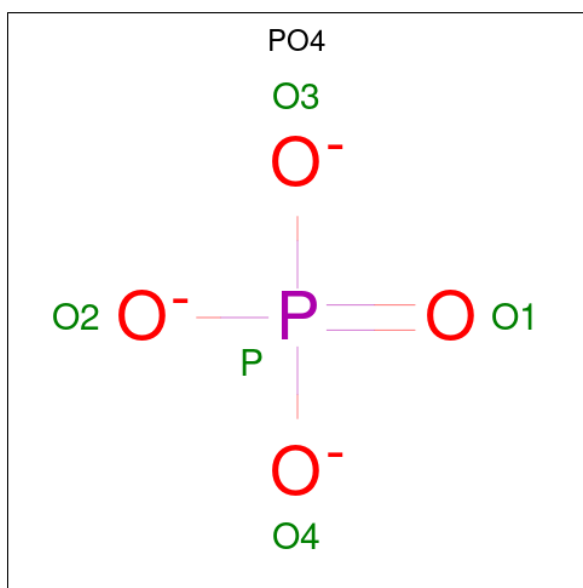
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	B	2	Total 2	Cl 2	0	0
4	II	1	Total 1	Cl 1	0	0
4	FX	1	Total 1	Cl 1	0	0
4	G	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0
4	GG	2	Total 2	Cl 2	0	0
4	K	2	Total 2	Cl 2	0	0
4	NN	2	Total 2	Cl 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0
5	II	1	Total Mg 1 1	0	0
5	FX	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0
5	O	1	Total Mg 1 1	0	0
5	K	1	Total Mg 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O P 5 4 1	0	0
6	FX	1	Total O P 5 4 1	0	0
6	GG	1	Total O P 5 4 1	0	0
6	K	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	195	Total O 195 195	0	0
7	B	313	Total O 313 313	0	0
7	C	195	Total O 195 195	0	0
7	E	194	Total O 194 194	0	0
7	J	194	Total O 194 194	0	0
7	M	273	Total O 273 273	0	0
7	HH	262	Total O 262 262	0	0
7	II	230	Total O 230 230	0	0
7	JJ	262	Total O 262 262	0	0
7	QQ	76	Total O 76 76	0	0
7	FX	184	Total O 184 184	0	0
7	S	40	Total O 40 40	0	0
7	h	43	Total O 43 43	0	0
7	D	212	Total O 212 212	0	0
7	KK	224	Total O 224 224	0	0
7	G	219	Total O 219 219	0	0
7	V	46	Total O 46 46	0	0
7	ww	51	Total O 51 51	0	0
7	k	46	Total O 46 46	0	0
7	H	321	Total O 321 321	0	0
7	T	47	Total O 47 47	0	0

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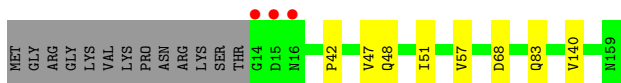
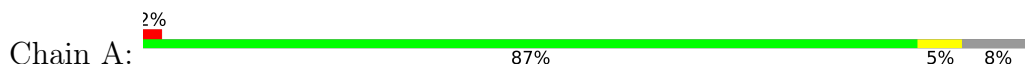
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	GG	212	Total 212	O 212	0	0
7	U	48	Total 48	O 48	0	0
7	I	167	Total 167	O 167	0	0
7	X	51	Total 51	O 51	0	0
7	m	54	Total 54	O 54	0	0
7	L	233	Total 233	O 233	0	0
7	TT	55	Total 55	O 55	0	0
7	i	68	Total 68	O 68	0	0
7	O	208	Total 208	O 208	0	0
7	P	38	Total 38	O 38	0	0
7	e	42	Total 42	O 42	0	0
7	K	277	Total 277	O 277	0	0
7	Y	51	Total 51	O 51	0	0
7	n	56	Total 56	O 56	0	0
7	ff	47	Total 47	O 47	0	0
7	xx	38	Total 38	O 38	0	0
7	NN	195	Total 195	O 195	0	0
7	yy	56	Total 56	O 56	0	0
7	zz	41	Total 41	O 41	0	0

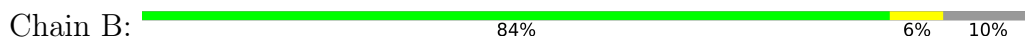
3 Residue-property plots [i](#)

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.

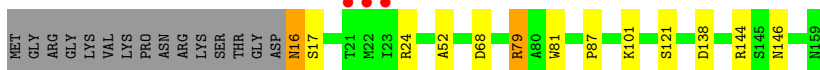
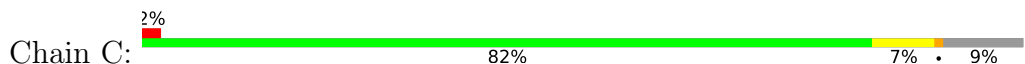
- Molecule 1: Coat protein



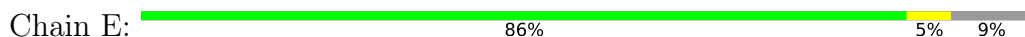
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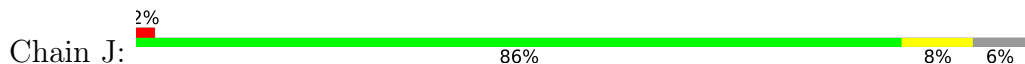
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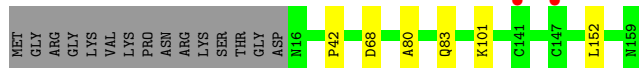
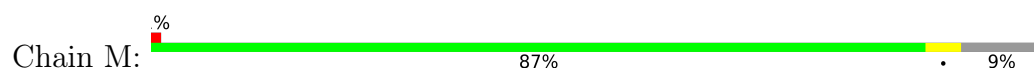
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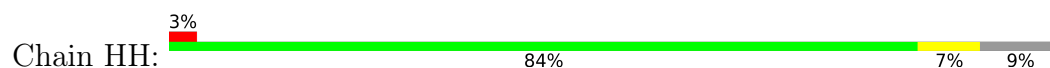
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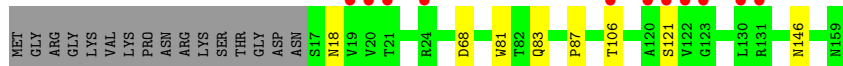
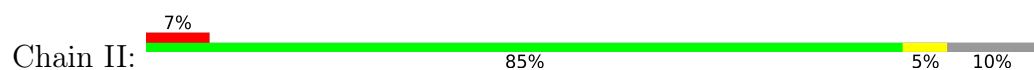
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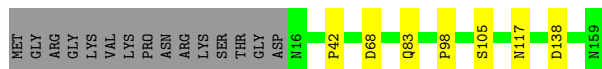
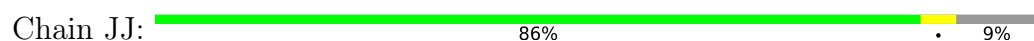
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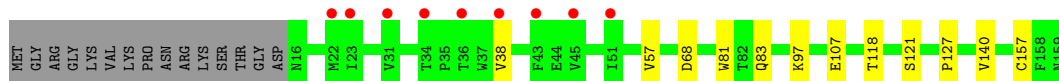
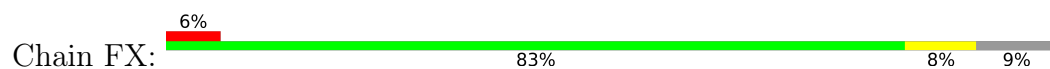
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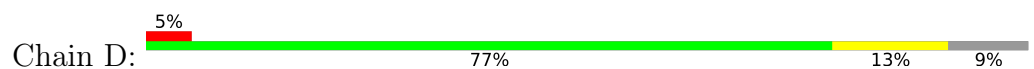
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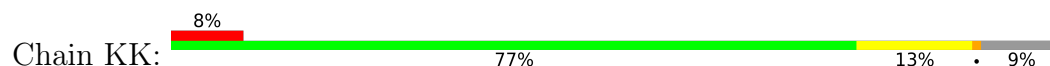
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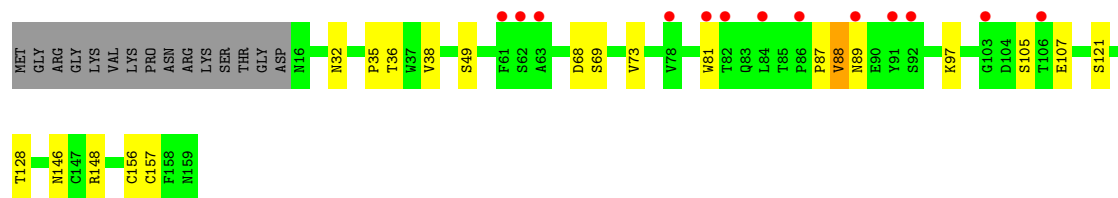


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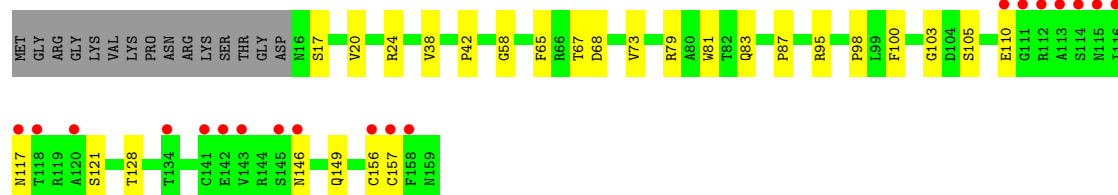
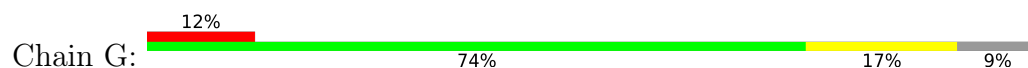


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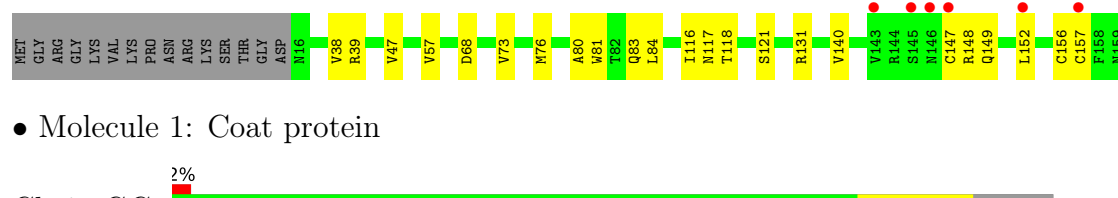
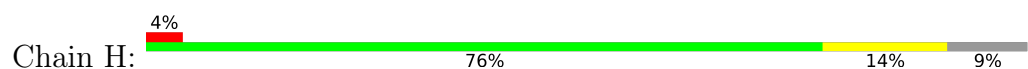




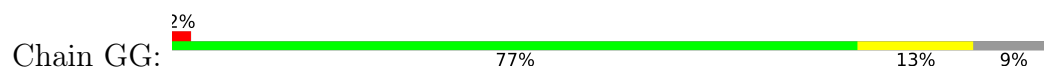
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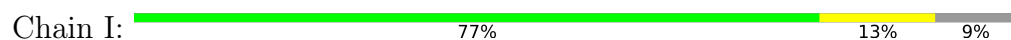
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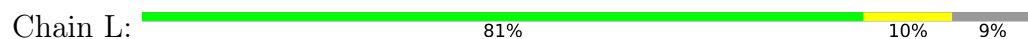
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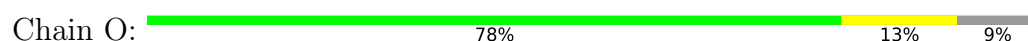
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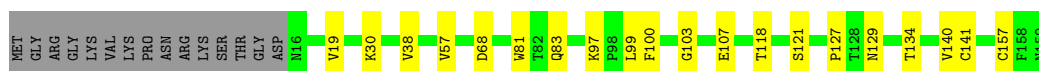


- Molecule 1: Coat protein

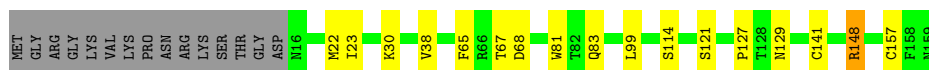
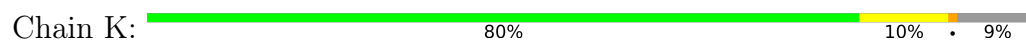


- Molecule 1: Coat protein





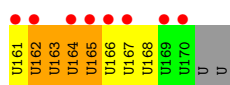
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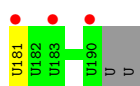
- Molecule 1: Coat protein



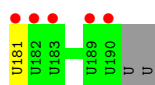
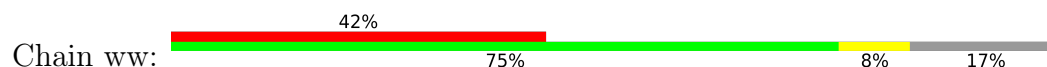
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



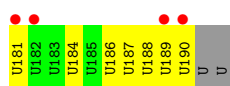
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



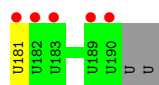
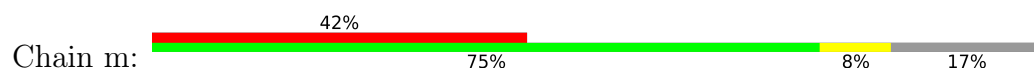
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



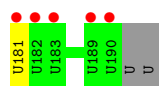
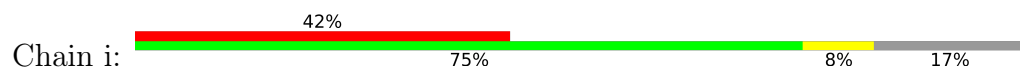
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



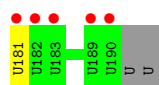
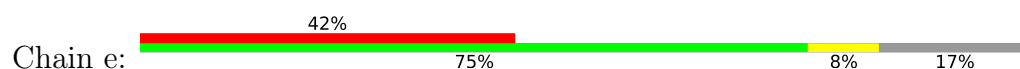
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



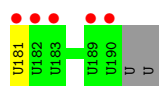
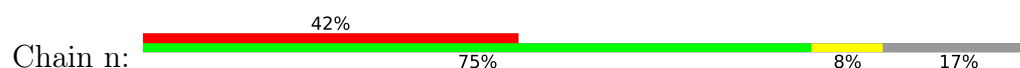
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



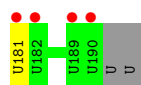
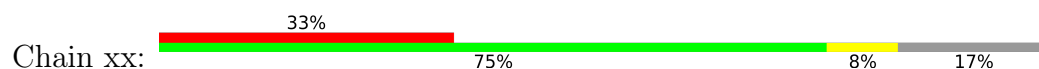
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



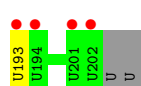
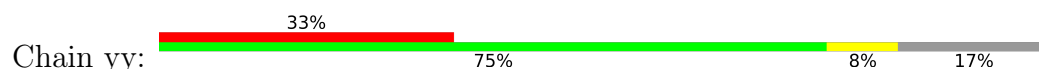
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



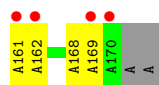
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



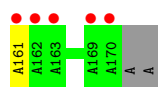
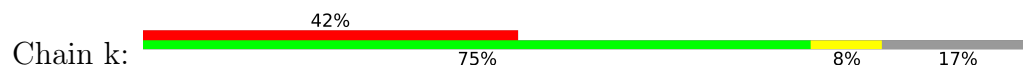
- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



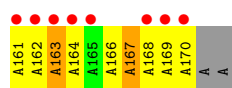
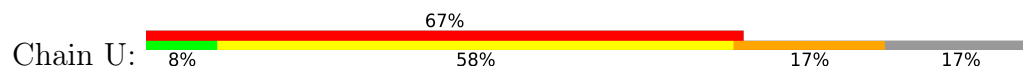
- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



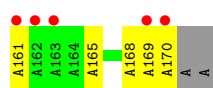
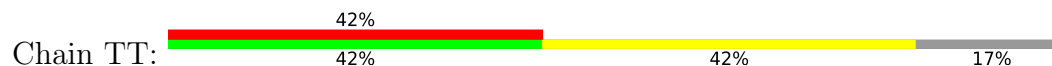
- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

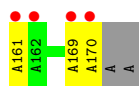


- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

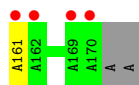
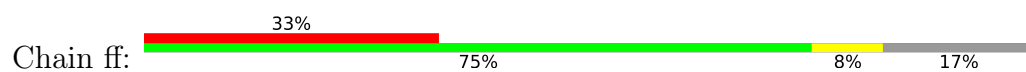


- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

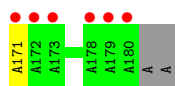
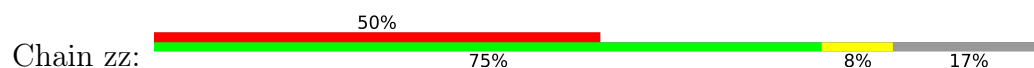




- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	165.63Å 165.63Å 433.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.80 55.25 – 1.80	Depositor EDS
% Data completeness (in resolution range)	84.0 (50.00-1.80) 84.1 (55.25-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.205 , 0.217 0.209 , 0.220	Depositor DCC
R_{free} test set	17134 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , -3.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.479 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	43122	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PO4, CL, MG

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	0.42	0/1173	0.63	0/1598
1	B	0.41	0/1154	0.61	0/1571
1	C	0.42	0/1159	0.62	0/1578
1	D	0.41	0/1249	0.61	0/1698
1	E	0.43	0/1165	0.61	0/1586
1	FX	0.44	0/1253	0.61	0/1702
1	G	0.41	0/1224	0.60	0/1665
1	GG	0.39	0/1275	0.62	0/1730
1	H	0.40	0/1253	0.61	0/1702
1	HH	0.39	0/1177	0.62	0/1603
1	I	0.40	0/1275	0.62	0/1730
1	II	0.43	0/1164	0.61	0/1585
1	J	0.40	0/1196	0.62	0/1627
1	JJ	0.39	0/1148	0.62	0/1564
1	K	0.42	0/1275	0.61	0/1730
1	KK	0.40	0/1244	0.60	0/1690
1	L	0.42	0/1275	0.61	0/1730
1	M	0.40	0/1179	0.62	0/1605
1	NN	0.39	0/1275	0.61	0/1730
1	O	0.41	0/1275	0.63	0/1730
2	QQ	0.74	1/220 (0.5%)	0.77	0/336
2	T	0.74	1/220 (0.5%)	0.77	0/336
2	e	0.74	1/220 (0.5%)	0.72	0/336
2	h	0.75	1/220 (0.5%)	0.74	0/336
2	i	0.74	1/220 (0.5%)	0.75	0/336
2	m	0.74	1/220 (0.5%)	0.74	0/336
2	n	0.73	1/220 (0.5%)	0.72	0/336
2	ww	0.74	1/220 (0.5%)	0.75	0/336
2	xx	0.74	1/220 (0.5%)	0.71	0/336
2	yy	0.74	1/220 (0.5%)	0.77	0/336
3	P	0.73	1/250 (0.4%)	0.68	0/386
3	S	0.71	1/250 (0.4%)	0.68	0/386

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	TT	0.70	1/250 (0.4%)	0.70	0/386
3	U	0.73	1/250 (0.4%)	0.86	0/386
3	V	0.71	1/250 (0.4%)	0.63	0/386
3	X	0.72	1/250 (0.4%)	0.66	0/386
3	Y	0.73	1/250 (0.4%)	0.64	0/386
3	ff	0.71	1/250 (0.4%)	0.68	0/386
3	k	0.69	1/250 (0.4%)	0.67	0/386
3	zz	0.71	1/250 (0.4%)	0.69	0/386
All	All	0.47	20/29088 (0.1%)	0.63	0/40374

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	161[A]	A	OP3-P	-10.74	1.48	1.61
2	e	181[A]	U	OP3-P	-10.66	1.48	1.61
3	X	161[A]	A	OP3-P	-10.65	1.48	1.61
3	U	161[A]	A	OP3-P	-10.63	1.48	1.61
2	T	181[A]	U	OP3-P	-10.63	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	79	ARG	Sidechain

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	1140	1115	1120	5	0
1	B	1115	1090	1093	6	0
1	C	1129	1113	1070	10	0
1	D	1186	0	1230	17	0
1	E	1126	1092	1070	7	0
1	FX	1189	0	1228	10	0
1	G	1170	0	1197	18	1
1	GG	1205	0	1254	16	0
1	H	1189	0	1228	20	1
1	HH	1137	1125	1087	9	0
1	I	1205	0	1254	17	0
1	II	1116	1080	1073	5	0
1	J	1172	1104	1130	9	0
1	JJ	1121	1115	1084	5	0
1	K	1205	0	1254	15	0
1	KK	1184	0	1223	26	1
1	L	1205	0	1254	10	1
1	M	1137	1122	1111	4	0
1	NN	1205	0	1254	7	0
1	O	1205	0	1254	16	0
2	QQ	201	0	71	20	2
2	T	201	0	101	6	2
2	e	201	0	101	0	0
2	h	201	0	101	0	0
2	i	201	0	101	0	0
2	m	201	0	101	0	0
2	n	201	0	101	0	0
2	ww	201	0	101	0	0
2	xx	201	0	101	0	0
2	yy	201	0	101	0	0
3	P	221	0	111	6	0
3	S	221	0	111	2	0
3	TT	221	0	111	4	0
3	U	221	0	111	10	0
3	V	221	0	111	5	0
3	X	221	0	111	6	1
3	Y	221	0	111	1	0
3	ff	221	0	111	0	0
3	k	221	0	111	0	0
3	zz	221	0	111	0	0
4	A	1	0	0	0	0
4	B	2	0	0	2	0
4	FX	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1	0	0	0	0
4	GG	2	0	0	1	0
4	H	1	0	0	3	0
4	II	1	0	0	2	0
4	K	2	0	0	1	0
4	NN	2	0	0	1	0
5	A	1	0	0	0	0
5	FX	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	II	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	O	1	0	0	0	0
6	C	5	0	0	1	0
6	FX	5	0	0	1	0
6	GG	5	0	0	1	0
6	K	5	0	0	0	0
7	A	195	0	0	1	3
7	B	313	0	0	2	3
7	C	195	0	0	4	4
7	D	212	0	0	2	1
7	E	194	0	0	3	0
7	FX	184	0	0	3	3
7	G	219	0	0	5	2
7	GG	212	0	0	5	3
7	H	321	0	0	0	1
7	HH	262	0	0	1	0
7	I	167	0	0	2	1
7	II	230	0	0	2	2
7	J	194	0	0	4	2
7	JJ	262	0	0	2	3
7	K	277	0	0	4	1
7	KK	224	0	0	5	2
7	L	233	0	0	2	2
7	M	273	0	0	2	2
7	NN	195	0	0	2	2
7	O	208	0	0	3	0
7	P	38	0	0	1	1
7	QQ	76	0	0	9	2
7	S	40	0	0	1	0
7	T	47	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	TT	55	0	0	0	1
7	U	48	0	0	1	1
7	V	46	0	0	1	0
7	X	51	0	0	2	0
7	Y	51	0	0	0	0
7	e	42	0	0	0	0
7	ff	47	0	0	0	0
7	h	43	0	0	0	1
7	i	68	0	0	0	0
7	k	46	0	0	0	1
7	m	54	0	0	0	1
7	n	56	0	0	0	0
7	ww	51	0	0	0	0
7	xx	38	0	0	0	1
7	yy	56	0	0	0	0
7	zz	41	0	0	0	0
All	All	33166	9956	25558	271	28

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 271 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:H:148:ARG:NH2	4:H:201:CL:CL	2.31	1.00
2:QQ:166[A]:U:H4'	1:KK:35:PRO:HB2	1.44	0.99
1:HH:15:ASP:HB2	1:G:128:THR:HB	1.43	0.98
1:O:68:ASP:OD1	7:O:301:HOH:O	1.85	0.94
1:D:68:ASP:OD1	7:D:201:HOH:O	1.84	0.94

The worst 5 of 28 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:KK:295:HOH:O	7:NN:307:HOH:O[9_554]	1.78	0.42
1:L:68:ASP:OD1	7:B:390:HOH:O[3_555]	1.86	0.34
1:H:68:ASP:OD1	7:JJ:357:HOH:O[3_555]	1.91	0.29
2:QQ:166[A]:U:OP1	7:G:1501:HOH:O[2_555]	1.93	0.27
7:QQ:215:HOH:O	7:GG:412:HOH:O[2_555]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	147/159 (92%)	141 (96%)	5 (3%)	1 (1%)	22	10
1	B	143/159 (90%)	137 (96%)	6 (4%)	0	100	100
1	C	144/159 (91%)	137 (95%)	7 (5%)	0	100	100
1	D	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	12
1	E	144/159 (91%)	139 (96%)	4 (3%)	1 (1%)	22	10
1	FX	156/159 (98%)	150 (96%)	6 (4%)	0	100	100
1	G	153/159 (96%)	147 (96%)	5 (3%)	1 (1%)	22	10
1	GG	158/159 (99%)	153 (97%)	5 (3%)	0	100	100
1	H	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
1	HH	147/159 (92%)	140 (95%)	7 (5%)	0	100	100
1	I	158/159 (99%)	151 (96%)	6 (4%)	1 (1%)	25	12
1	II	145/159 (91%)	139 (96%)	6 (4%)	0	100	100
1	J	149/159 (94%)	139 (93%)	9 (6%)	1 (1%)	22	10
1	JJ	143/159 (90%)	138 (96%)	4 (3%)	1 (1%)	22	10
1	K	158/159 (99%)	152 (96%)	6 (4%)	0	100	100
1	KK	155/159 (98%)	148 (96%)	7 (4%)	0	100	100
1	L	158/159 (99%)	154 (98%)	4 (2%)	0	100	100
1	M	146/159 (92%)	141 (97%)	4 (3%)	1 (1%)	22	10
1	NN	158/159 (99%)	152 (96%)	6 (4%)	0	100	100
1	O	158/159 (99%)	153 (97%)	5 (3%)	0	100	100
All	All	3032/3180 (95%)	2913 (96%)	111 (4%)	8 (0%)	41	27

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	JJ	42	PRO

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Mol	Chain	Res	Type
1	D	42	PRO
1	G	42	PRO
1	E	42	PRO
1	I	42	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	132/140 (94%)	132 (100%)	0	100	100
1	B	129/140 (92%)	129 (100%)	0	100	100
1	C	130/140 (93%)	129 (99%)	1 (1%)	81	78
1	D	142/140 (101%)	142 (100%)	0	100	100
1	E	130/140 (93%)	130 (100%)	0	100	100
1	FX	142/140 (101%)	142 (100%)	0	100	100
1	G	139/140 (99%)	139 (100%)	0	100	100
1	GG	144/140 (103%)	144 (100%)	0	100	100
1	H	142/140 (101%)	142 (100%)	0	100	100
1	HH	133/140 (95%)	133 (100%)	0	100	100
1	I	144/140 (103%)	144 (100%)	0	100	100
1	II	131/140 (94%)	130 (99%)	1 (1%)	81	78
1	J	134/140 (96%)	133 (99%)	1 (1%)	84	81
1	JJ	129/140 (92%)	129 (100%)	0	100	100
1	K	144/140 (103%)	141 (98%)	3 (2%)	53	42
1	KK	141/140 (101%)	140 (99%)	1 (1%)	84	81
1	L	144/140 (103%)	144 (100%)	0	100	100
1	M	132/140 (94%)	132 (100%)	0	100	100
1	NN	144/140 (103%)	144 (100%)	0	100	100
1	O	144/140 (103%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2750/2800 (98%)	2743 (100%)	7 (0%)	93 91

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	KK	88	VAL
1	K	148[A]	ARG
1	K	148[C]	ARG
1	K	148[B]	ARG
1	II	106	THR

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	QQ	9/12 (75%)	5 (55%)	0
2	T	9/12 (75%)	0	0
2	e	9/12 (75%)	0	0
2	h	9/12 (75%)	0	0
2	i	9/12 (75%)	0	0
2	m	9/12 (75%)	0	0
2	n	9/12 (75%)	0	0
2	ww	9/12 (75%)	0	0
2	xx	9/12 (75%)	0	0
2	yy	9/12 (75%)	0	0
3	P	9/12 (75%)	0	0
3	S	9/12 (75%)	0	0
3	TT	9/12 (75%)	0	0
3	U	9/12 (75%)	4 (44%)	0
3	V	9/12 (75%)	0	0
3	X	9/12 (75%)	0	0
3	Y	9/12 (75%)	0	0
3	ff	9/12 (75%)	0	0
3	k	9/12 (75%)	0	0
3	zz	9/12 (75%)	0	0
All	All	180/240 (75%)	9 (5%)	0

5 of 9 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	QQ	162[A]	U
2	QQ	163[A]	U
2	QQ	164[A]	U
2	QQ	165[A]	U
2	QQ	168[A]	U

There are no RNA pucker outliers to report.

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 25 ligands modelled in this entry, 21 are monoatomic - leaving 4 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	PO4	K	201	-	4,4,4	2.02	3 (75%)	6,6,6	0.81	0
6	PO4	FX	201	-	4,4,4	1.84	3 (75%)	6,6,6	0.86	0
6	PO4	C	201	-	4,4,4	1.70	1 (25%)	6,6,6	0.62	0
6	PO4	GG	201	-	4,4,4	1.71	1 (25%)	6,6,6	1.11	0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	201	PO4	P-O3	-2.41	1.47	1.54
6	K	201	PO4	P-O2	-2.16	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	201	PO4	P-O2	-2.12	1.48	1.54
6	FX	201	PO4	P-O2	-2.08	1.48	1.54
6	K	201	PO4	P-O4	-2.08	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	FX	201	PO4	1	0
6	C	201	PO4	1	0
6	GG	201	PO4	1	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 ⓘ

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, 95th 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	146/159 (91%)	-0.57	3 (2%) 63 59	7, 11, 20, 62	0
1	B	143/159 (89%)	-0.66	0 100 100	8, 11, 15, 27	0
1	C	144/159 (90%)	-0.55	3 (2%) 63 59	8, 11, 17, 44	0
1	D	144/159 (90%)	-0.09	8 (5%) 24 19	8, 11, 16, 36	0
1	E	144/159 (90%)	-0.64	0 100 100	8, 11, 16, 37	0
1	FX	144/159 (90%)	-0.08	9 (6%) 20 15	7, 11, 16, 45	0
1	G	144/159 (90%)	0.23	19 (13%) 3 2	8, 11, 15, 41	0
1	GG	144/159 (90%)	-0.49	3 (2%) 63 59	7, 12, 16, 34	0
1	H	144/159 (90%)	-0.35	6 (4%) 36 30	8, 11, 16, 36	0
1	HH	145/159 (91%)	0.55	4 (2%) 53 47	8, 12, 17, 39	0
1	I	144/159 (90%)	-0.68	0 100 100	8, 11, 15, 44	0
1	II	143/159 (89%)	-0.05	11 (7%) 13 10	8, 12, 16, 39	0
1	J	150/159 (94%)	-0.50	3 (2%) 65 61	8, 11, 28, 116	0
1	JJ	144/159 (90%)	-0.71	0 100 100	8, 11, 16, 54	2 (1%)
1	K	144/159 (90%)	-0.65	0 100 100	7, 11, 16, 34	0
1	KK	144/159 (90%)	0.17	13 (9%) 9 7	8, 11, 17, 38	0
1	L	144/159 (90%)	-0.62	0 100 100	7, 11, 15, 35	0
1	M	144/159 (90%)	0.19	2 (1%) 75 72	8, 11, 15, 40	0
1	NN	144/159 (90%)	-0.63	0 100 100	8, 10, 16, 35	0
1	O	144/159 (90%)	-0.60	0 100 100	7, 10, 15, 45	0
2	QQ	10/12 (83%)	3.52	8 (80%) 0 0	41, 56, 76, 125	9 (90%)
2	T	10/12 (83%)	2.68	4 (40%) 0 0	32, 46, 59, 64	6 (60%)
2	e	10/12 (83%)	3.64	5 (50%) 0 0	31, 47, 58, 60	6 (60%)
2	h	10/12 (83%)	1.99	3 (30%) 0 0	36, 48, 86, 92	5 (50%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
2	i	10/12 (83%)	4.09	5 (50%)	0	0	30, 46, 66, 80	6 (60%)
2	m	10/12 (83%)	2.86	5 (50%)	0	0	31, 43, 53, 60	6 (60%)
2	n	10/12 (83%)	3.16	5 (50%)	0	0	30, 42, 61, 83	6 (60%)
2	ww	10/12 (83%)	3.35	5 (50%)	0	0	34, 40, 69, 83	6 (60%)
2	xx	10/12 (83%)	2.83	4 (40%)	0	0	31, 46, 99, 105	5 (50%)
2	yy	10/12 (83%)	3.38	4 (40%)	0	0	28, 43, 58, 70	6 (60%)
3	P	10/12 (83%)	4.79	5 (50%)	0	0	34, 44, 50, 58	6 (60%)
3	S	10/12 (83%)	1.41	4 (40%)	0	0	32, 39, 62, 62	6 (60%)
3	TT	10/12 (83%)	4.02	5 (50%)	0	0	30, 37, 68, 74	6 (60%)
3	U	10/12 (83%)	5.31	8 (80%)	0	0	45, 64, 102, 109	6 (60%)
3	V	10/12 (83%)	3.22	5 (50%)	0	0	34, 44, 61, 63	5 (50%)
3	X	10/12 (83%)	2.84	4 (40%)	0	0	34, 55, 93, 121	4 (40%)
3	Y	10/12 (83%)	3.55	4 (40%)	0	0	31, 44, 64, 71	5 (50%)
3	ff	10/12 (83%)	1.92	4 (40%)	0	0	32, 52, 73, 78	4 (40%)
3	k	10/12 (83%)	3.32	5 (50%)	0	0	34, 41, 57, 59	6 (60%)
3	zz	10/12 (83%)	4.50	6 (60%)	0	0	31, 46, 49, 57	6 (60%)
All	All	3087/3420 (90%)	-0.10	182 (5%)	22	17	7, 11, 40, 125	117 (3%)

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	161[A]	A	14.3
3	zz	171[A]	A	13.3
3	U	170[A]	A	13.0
3	zz	180[A]	A	12.6
2	T	181[A]	U	12.2

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](#)

There are no monosaccharides in this entry.

6.4 Ligands

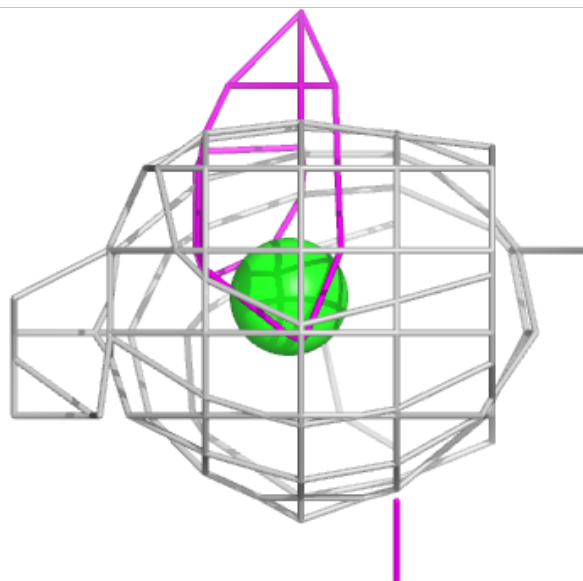
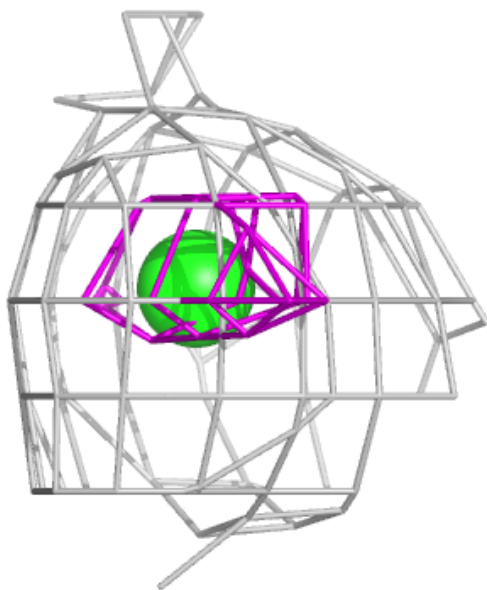
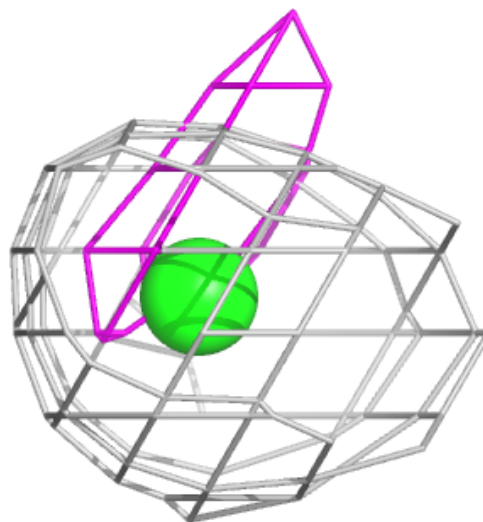
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	GG	202	1/1	0.89	0.09	32,32,32,32	0
5	MG	A	202	1/1	0.91	0.31	15,15,15,15	0
5	MG	J	201	1/1	0.94	0.11	17,17,17,17	0
4	CL	H	201	1/1	0.95	0.10	30,30,30,30	0
4	CL	K	202	1/1	0.95	0.12	27,27,27,27	0
5	MG	G	1402	1/1	0.95	0.10	15,15,15,15	0
5	MG	FX	203	1/1	0.96	0.21	14,14,14,14	0
4	CL	NN	201	1/1	0.97	0.06	21,21,21,21	0
5	MG	H	202	1/1	0.97	0.20	16,16,16,16	0
6	PO4	C	201	5/5	0.97	0.11	14,14,29,30	0
6	PO4	FX	201	5/5	0.97	0.13	15,18,25,27	0
6	PO4	GG	201	5/5	0.97	0.12	15,17,31,31	0
5	MG	O	201	1/1	0.98	0.12	11,11,11,11	0
5	MG	II	202	1/1	0.98	0.19	16,16,16,16	0
6	PO4	K	201	5/5	0.98	0.13	10,16,19,20	0
4	CL	G	1401	1/1	0.99	0.05	15,15,15,15	0
5	MG	K	203	1/1	0.99	0.04	12,12,12,12	0
4	CL	K	204	1/1	0.99	0.05	15,15,15,15	0
4	CL	II	201	1/1	0.99	0.12	43,43,43,43	0
4	CL	NN	202	1/1	0.99	0.07	28,28,28,28	0
4	CL	FX	202	1/1	0.99	0.05	28,28,28,28	0
4	CL	B	202	1/1	1.00	0.08	30,30,30,30	0
4	CL	A	201	1/1	1.00	0.02	17,17,17,17	0
4	CL	B	201	1/1	1.00	0.05	21,21,21,21	0
4	CL	GG	203	1/1	1.00	0.01	17,17,17,17	0

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

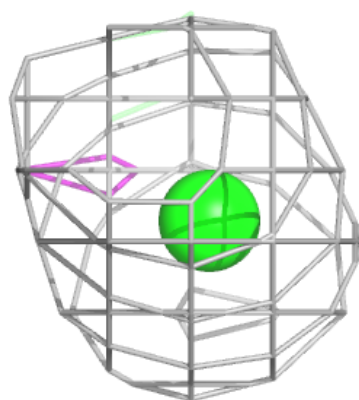
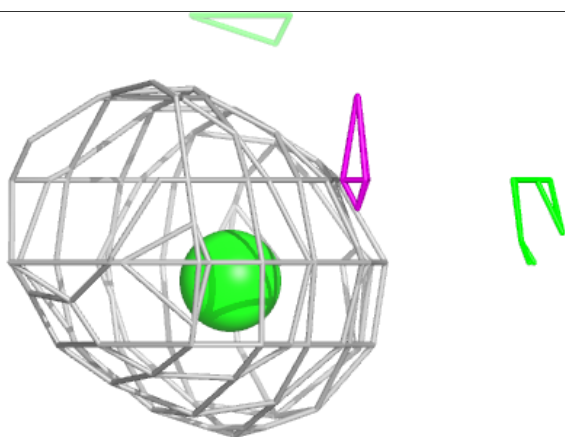
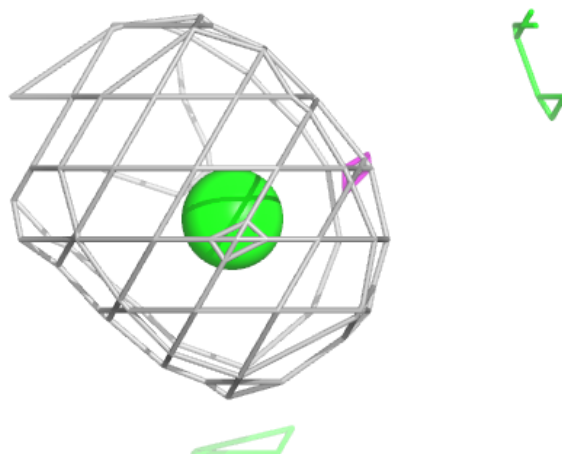
Electron density around CL GG 202:

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



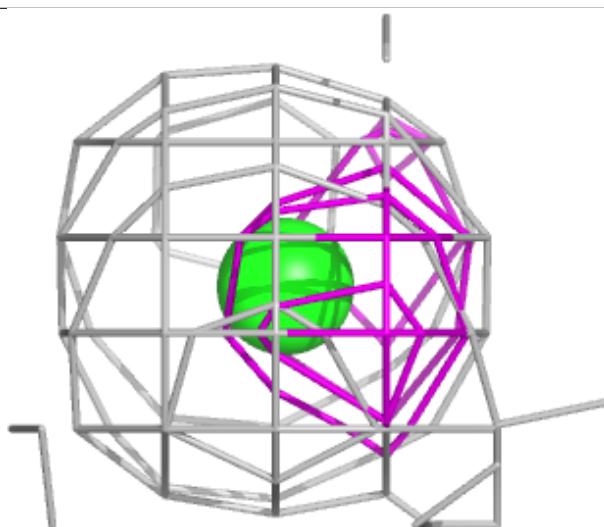
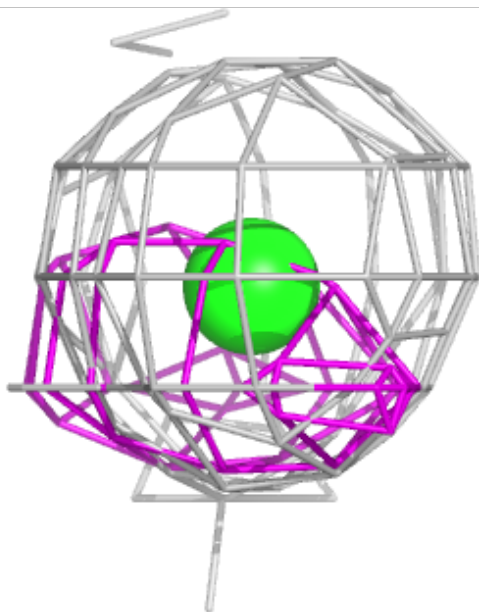
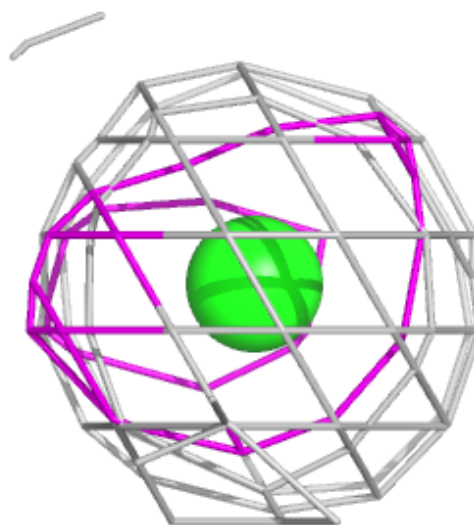
Electron density around CL H 201:

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



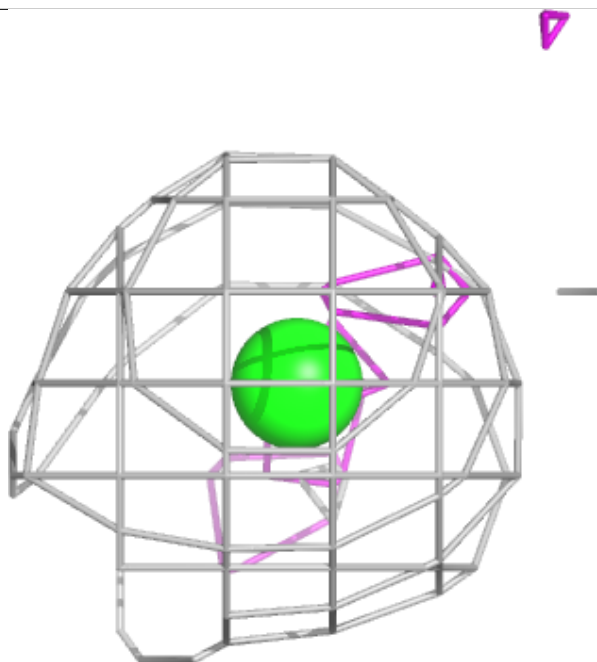
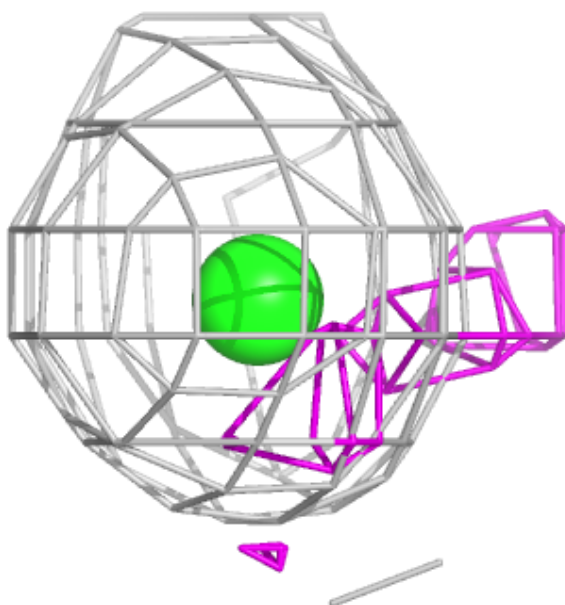
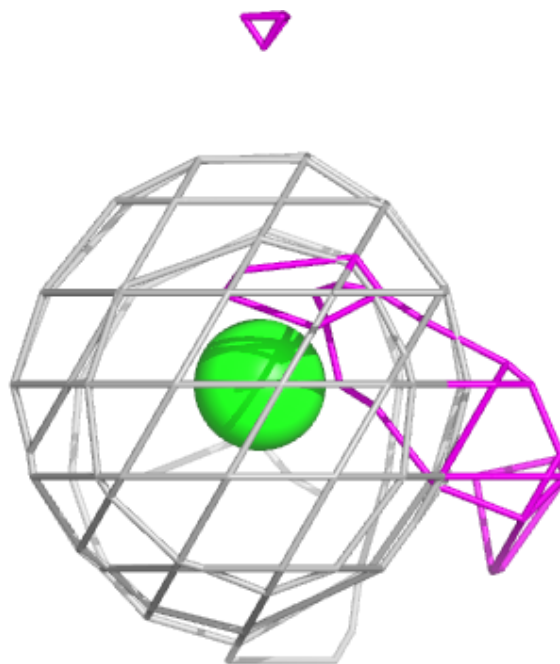
Electron density around CL K 202:

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and green (positive)



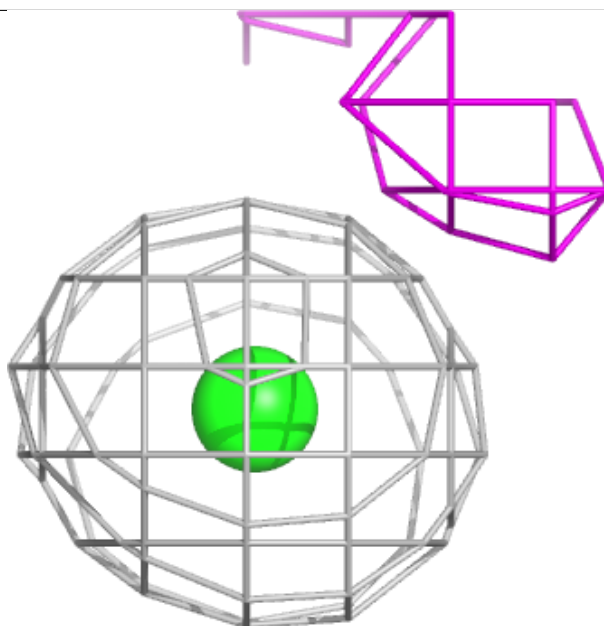
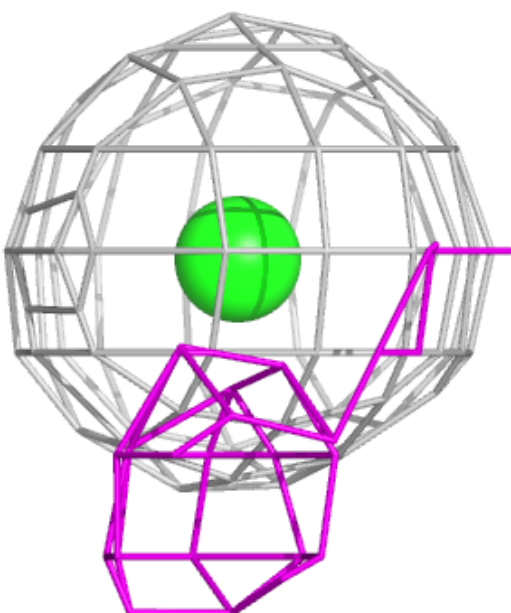
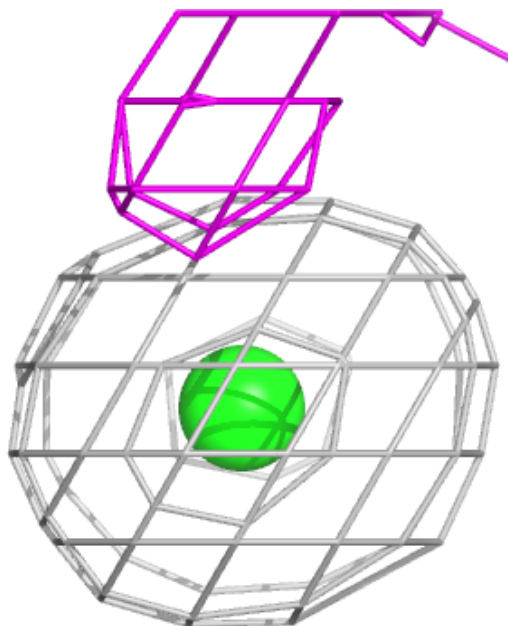
Electron density around CL NN 201:

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and green (positive)



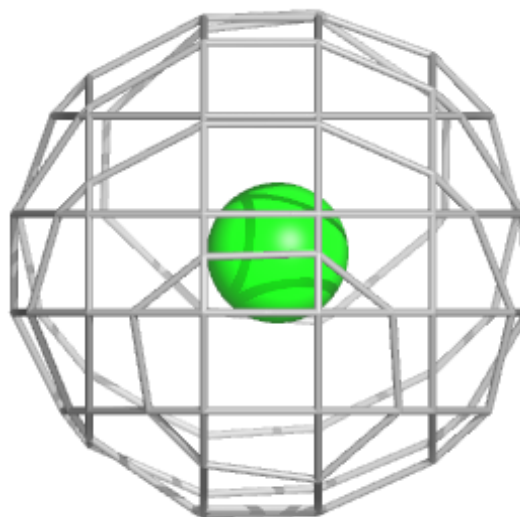
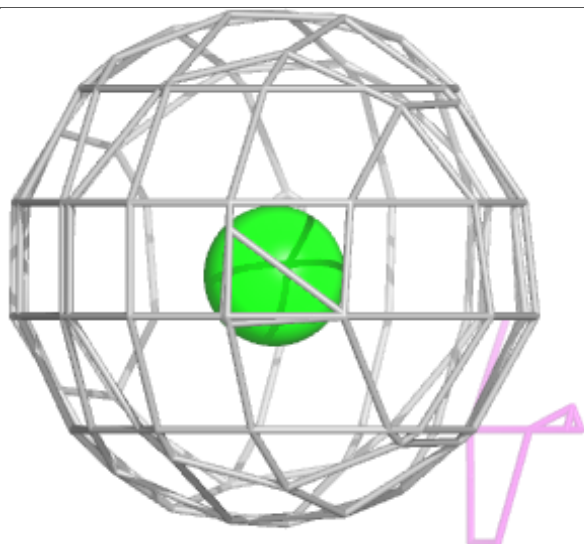
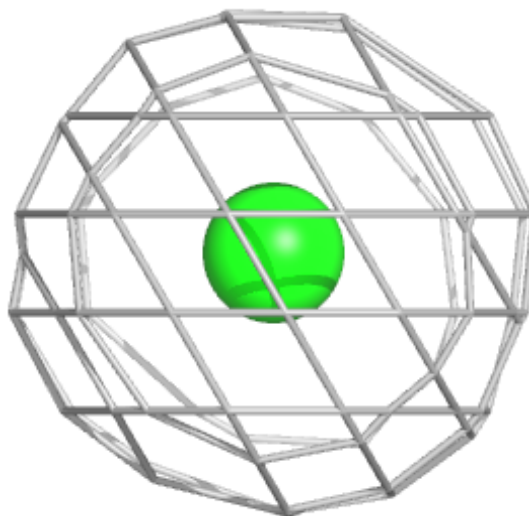
Electron density around CL G 1401:

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



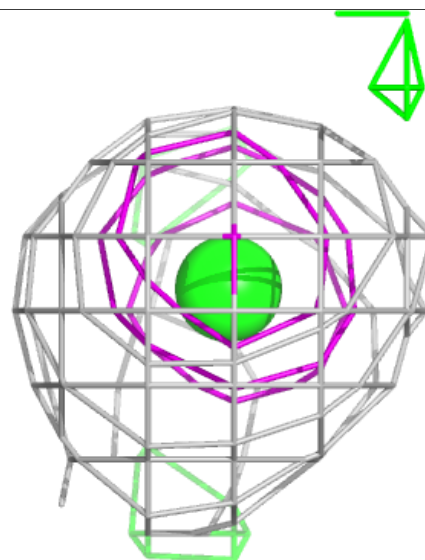
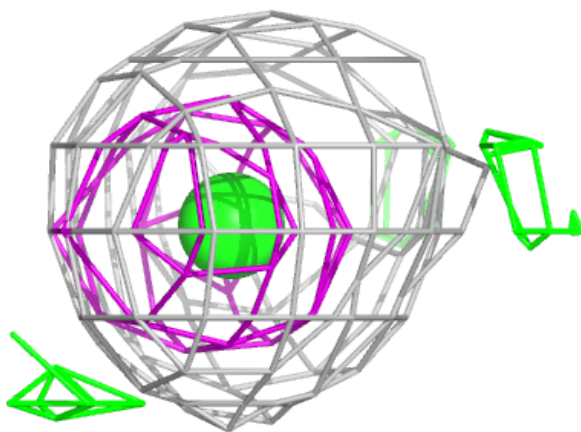
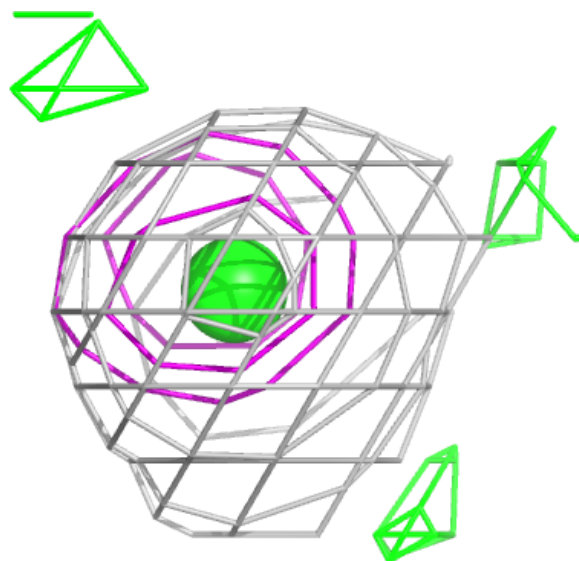
Electron density around CL K 204:

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and green (positive)



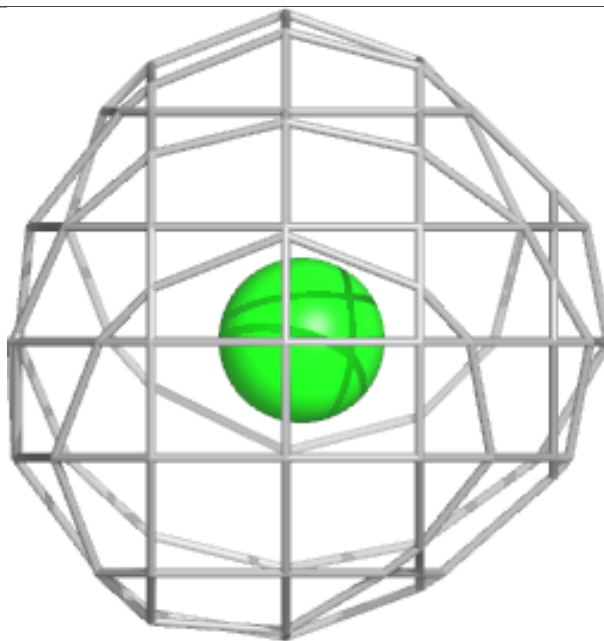
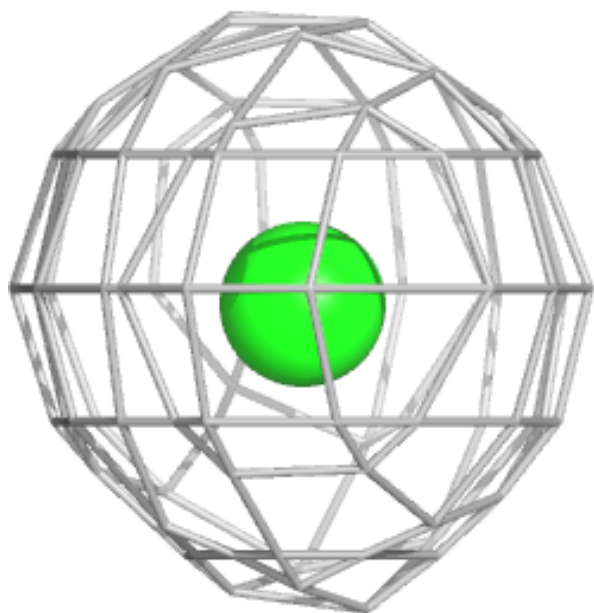
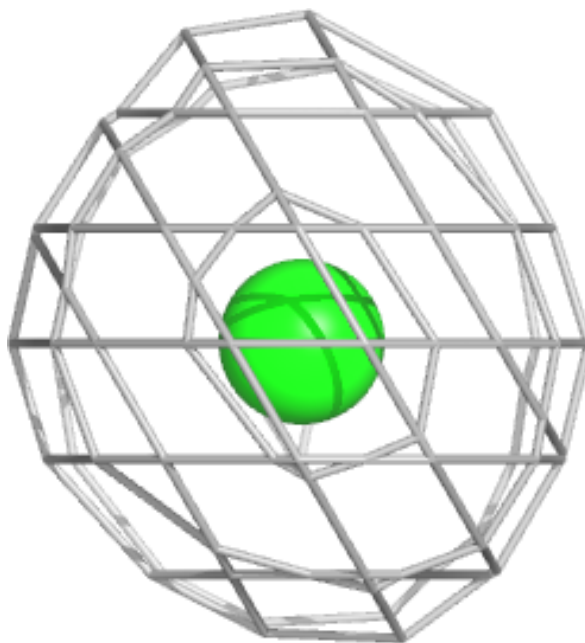
Electron density around CL II 201:

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



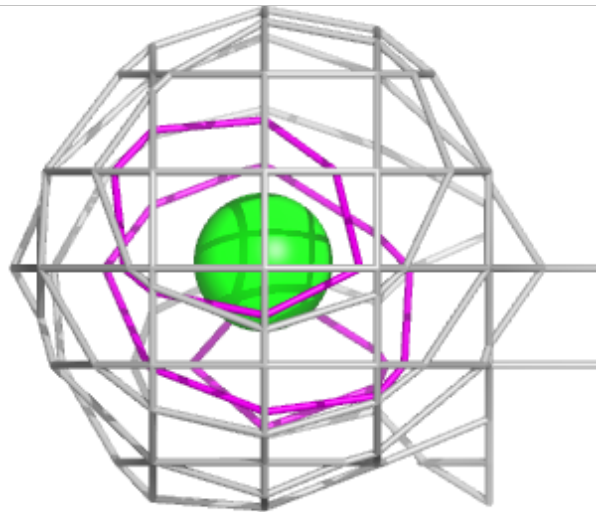
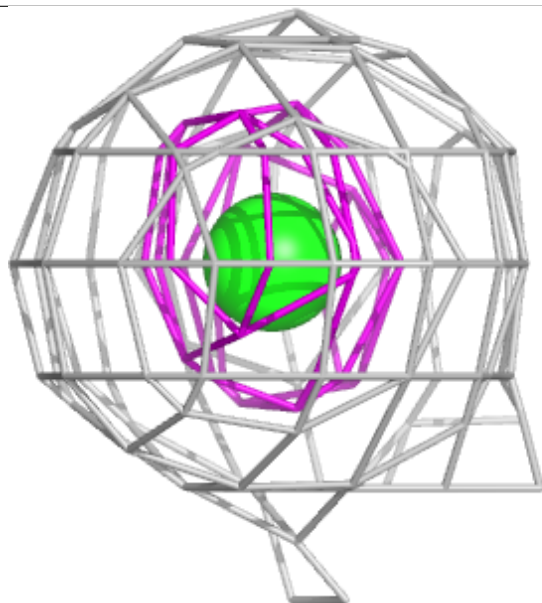
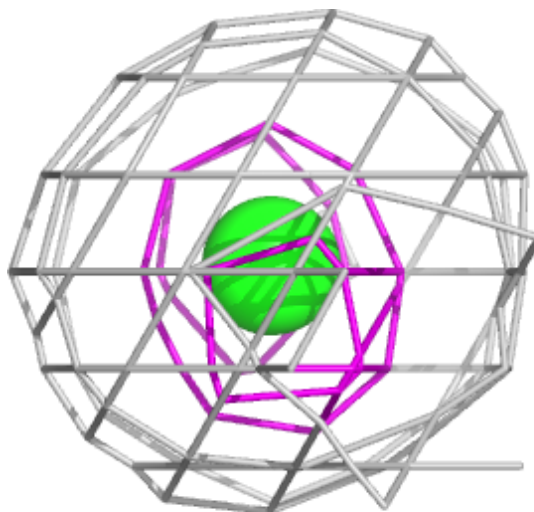
Electron density around CL NN 202:

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



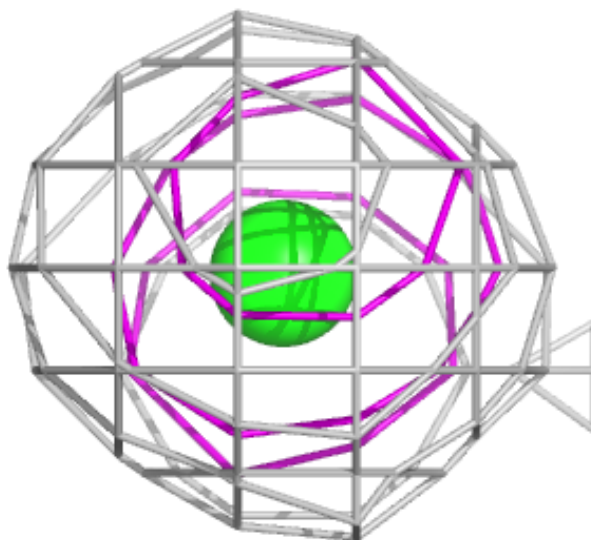
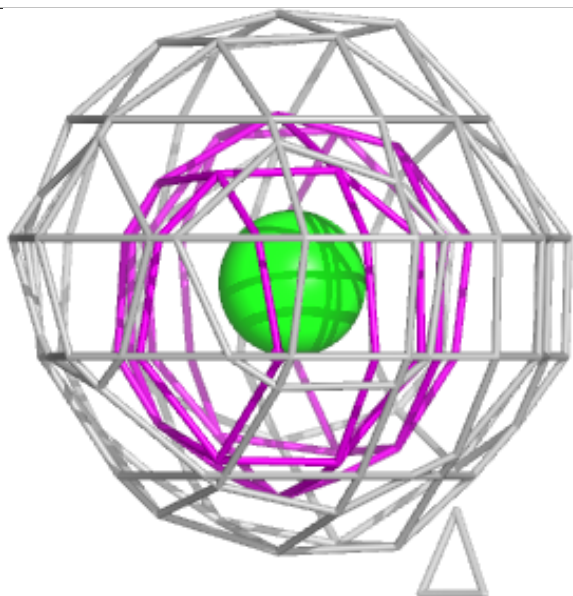
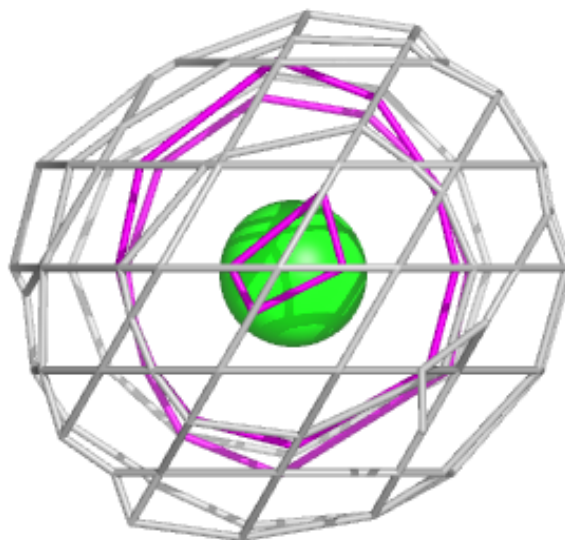
Electron density around CL FX 202:

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



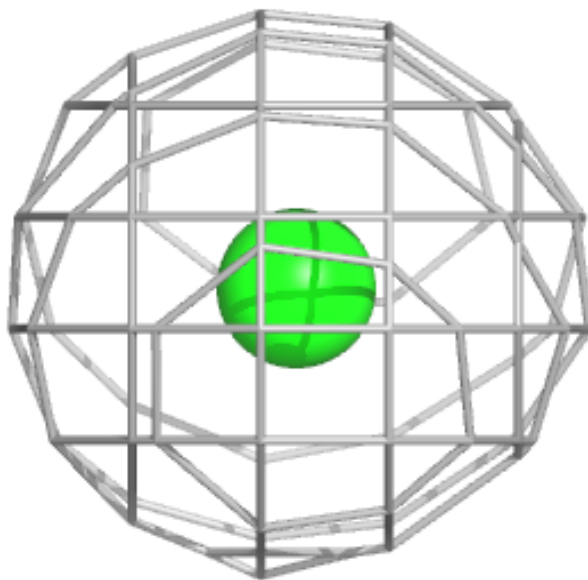
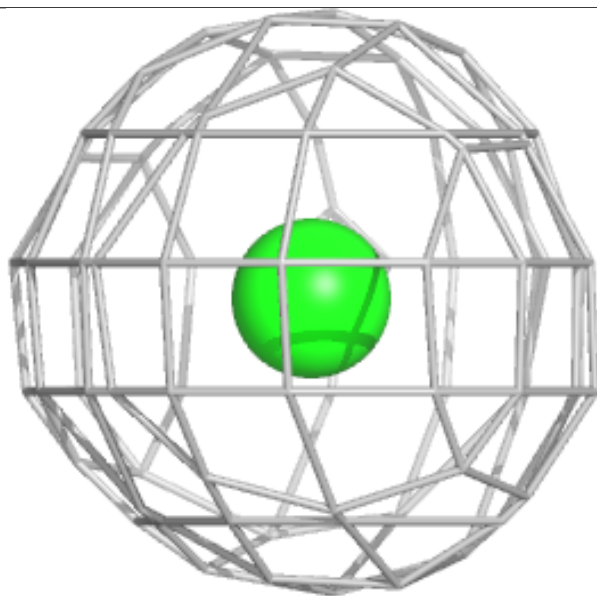
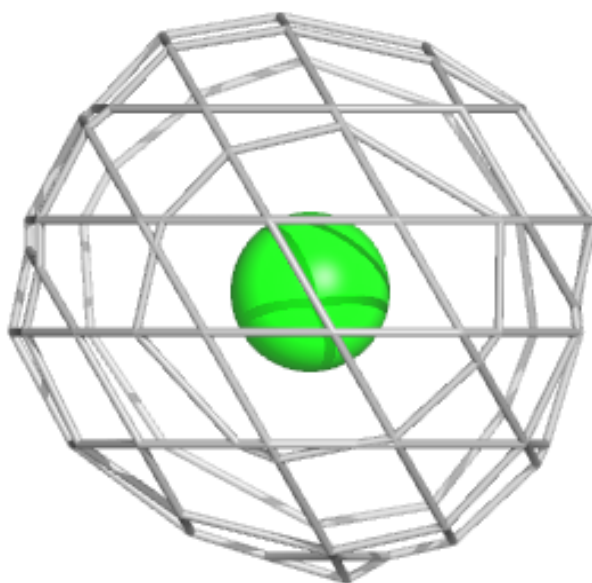
Electron density around CL B 202:

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



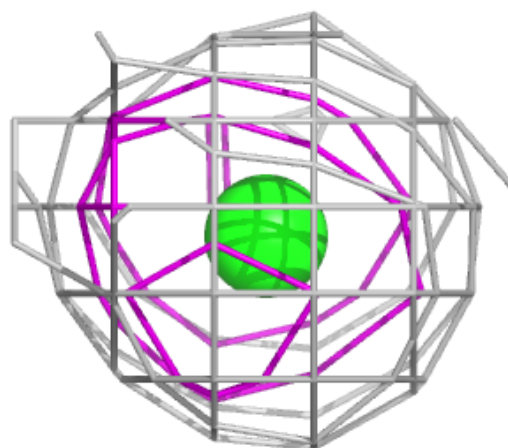
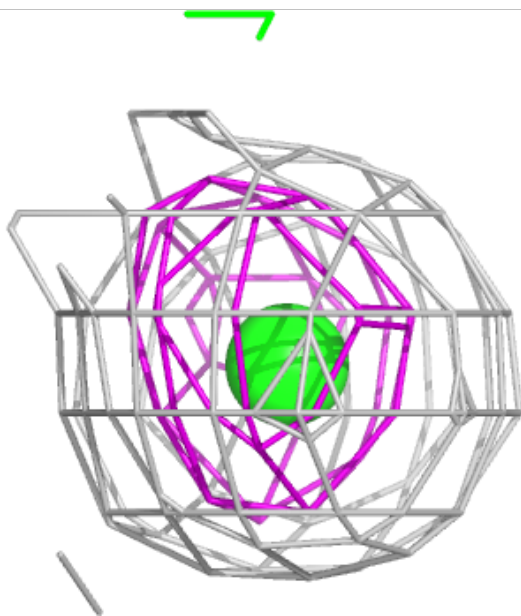
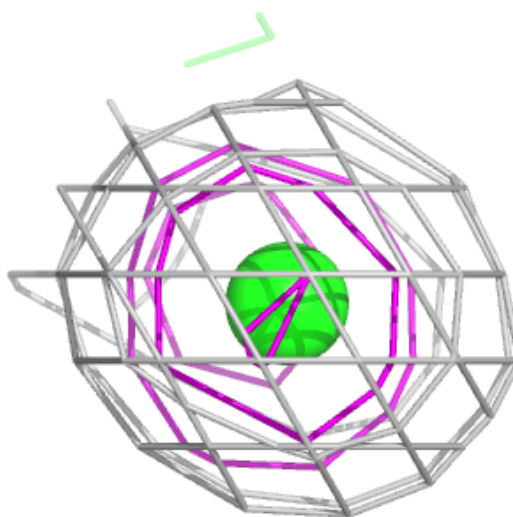
Electron density around CL A 201:

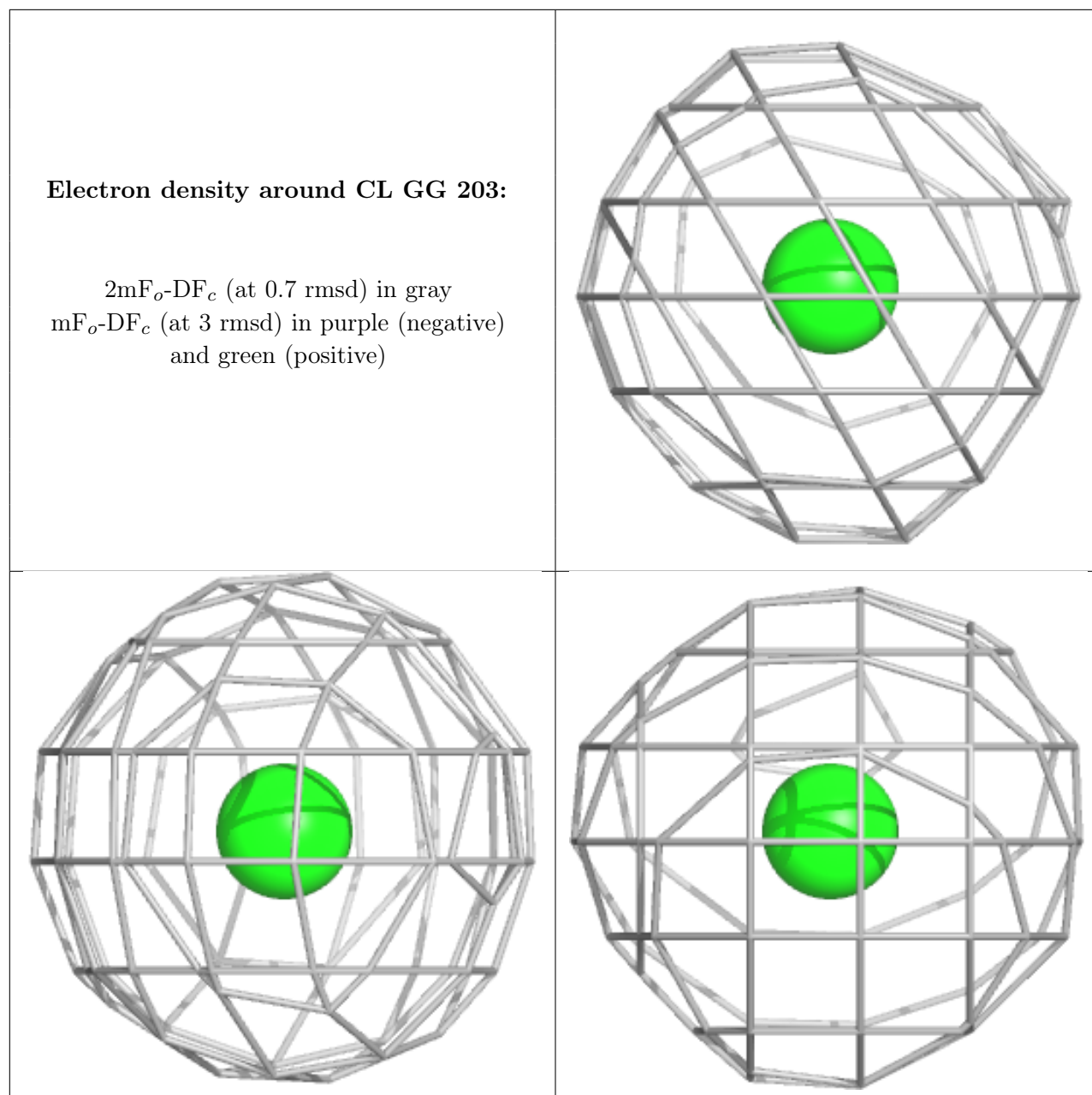
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL B 201:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.