Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 06:56 AM EDT

PDB ID	:	7M3T
Title	:	Crystallographic structure of a cubic crystal of STMV (80.7 degree rotation about 111) grown from chloride
Authors	:	McPherson, A.
Deposited on	:	2021-03-19
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

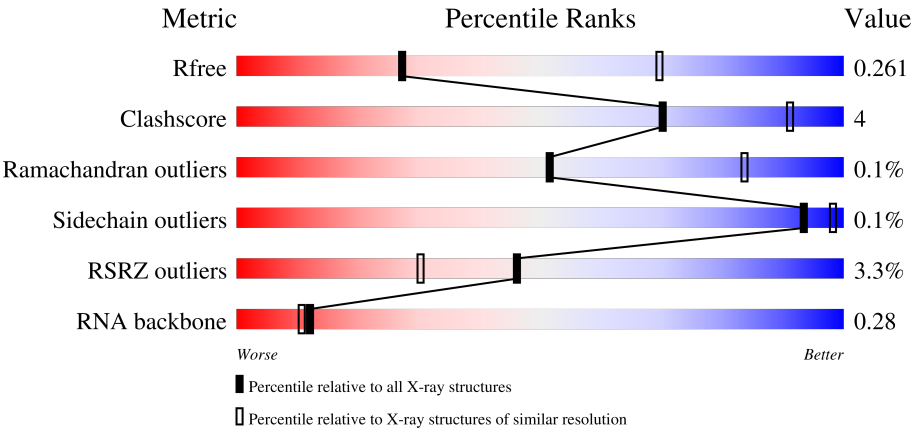
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	159	84% 7% 9%
1	B	159	84% 6% 10%
1	C	159	82% 8% 11%
1	D	159	81% 10% 9%

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Mol	Chain	Length	Quality of chain
1	E	159	81% 10% 9%
1	F	159	81% 10% 9%
1	GG	159	80% 11% 9%
1	H	159	84% 8% 9%
1	HH	159	83% 8% 9%
1	I	159	87% 9%
1	II	159	80% 10% 10%
1	J	159	82% 8% 9%
1	JJ	159	84% 7% 9%
1	K	159	85% 7% 8%
1	KK	159	80% 11% 9%
1	L	159	89% 10%
1	M	159	87% 9%
1	O	159	85% 9% 6%
2	G	159	83% 8% 9%
3	N	159	83% 8% 9%
4	P	10	30% 30% 30% 10% 30%
4	S	10	10% 40% 10% 50%
4	T	10	10% 20% 30% 50%
4	TT	10	50% 10% 40% 20% 30%
4	UU	10	40% 50% 10% 40%
4	V	10	50% 40% 20% 20% 20%
4	X	10	80% 30% 40% 20% 10%
4	Y	10	40% 60% 10% 30%
4	a	10	50% 40% 20% 40%

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Mol	Chain	Length	Quality of chain
5	WW	12	42% 25% 33% 8% 33%
5	e	12	83% 17% 75% 8%
6	h	12	33% 42% 25% 33%
7	i	11	9% 18% 27% 55%
7	ll	11	36% 36% 9% 55%
8	kk	10	30% 40% 30% 30%
8	m	10	40% 40% 50% 10%
9	n	8	38% 50% 50%
9	qq	8	38% 12% 38% 50%
10	bb	12	100% 42% 58%

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
11	PO4	H	503	-	-	-	X
12	CL	HH	201	-	-	X	-
12	CL	KK	202	-	-	-	X
12	CL	N	201	-	-	-	X
13	MG	G	201	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 26451 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 Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	6	0
			1118	703	199	210	6			
1	B	143	Total	C	N	O	S	0	10	0
			1115	703	197	208	7			
1	C	142	Total	C	N	O	S	0	13	0
			1104	696	196	206	6			
1	D	144	Total	C	N	O	S	0	12	0
			1118	703	199	210	6			
1	E	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	F	144	Total	C	N	O	S	0	6	0
			1121	705	199	211	6			
1	H	145	Total	C	N	O	S	0	8	0
			1126	707	200	213	6			
1	I	144	Total	C	N	O	S	0	8	0
			1118	703	199	210	6			
1	J	144	Total	C	N	O	S	0	8	0
			1118	703	199	210	6			
1	K	146	Total	C	N	O	S	0	6	0
			1150	723	206	215	6			
1	L	157	Total	C	N	O	S	0	0	0
			1215	761	221	227	6			
1	M	144	Total	C	N	O	S	0	0	0
			1118	703	199	210	6			
1	O	150	Total	C	N	O	S	0	17	0
			1168	732	209	220	7			
1	GG	144	Total	C	N	O	S	0	11	0
			1118	703	199	210	6			
1	HH	144	Total	C	N	O	S	0	7	0
			1118	703	199	210	6			
1	II	143	Total	C	N	O	S	0	8	0
			1110	699	197	208	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	JJ	144	Total	C	N	O	S	0	13	0
			1118	703	199	210	6			
1	KK	144	Total	C	N	O	S	0	8	0
			1118	703	199	210	6			

- Molecule 2 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	144	Total	C	N	O	S	0	7	0
			1117	702	199	210	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	128	SER	THR	conflict	UNP P17574

- Molecule 3 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	144	Total	C	N	O	S	0	1	0
			1125	709	199	210	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	137	VAL	ALA	conflict	UNP P17574

- Molecule 4 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	7	Total	C	N	O	P	0	7	0
			154	70	35	42	7			
4	S	5	Total	C	N	O	P	0	5	0
			110	50	25	30	5			
4	T	5	Total	C	N	O	P	0	5	0
			110	50	25	30	5			
4	V	8	Total	C	N	O	P	0	6	0
			176	80	40	48	8			
4	X	9	Total	C	N	O	P	0	8	0
			198	90	45	54	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Y	7	Total	C	N	O	P	0	6	0
			154	70	35	42	7			
4	a	6	Total	C	N	O	P	0	6	0
			132	60	30	36	6			
4	TT	7	Total	C	N	O	P	0	6	0
			154	70	35	42	7			
4	UU	6	Total	C	N	O	P	0	5	0
			132	60	30	36	6			

- Molecule 5 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
5	e	11	Total	C	N	O	P	0	10	0
			220	99	22	88	11			
5	WW	8	Total	C	N	O	P	0	2	0
			160	72	16	64	8			

- Molecule 6 is a RNA chain called RNA (5'-R(P*UP*AP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	h	8	Total	C	N	O	P	0	7	0
			162	73	19	62	8			

- Molecule 7 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	i	5	Total	C	N	O	P	0	5	0
			100	45	10	40	5			
7	ll	5	Total	C	N	O	P	0	5	0
			100	45	10	40	5			

- Molecule 8 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	m	9	Total	C	N	O	P	0	9	0
			180	81	18	72	9			
8	kk	7	Total	C	N	O	P	0	6	0
			140	63	14	56	7			

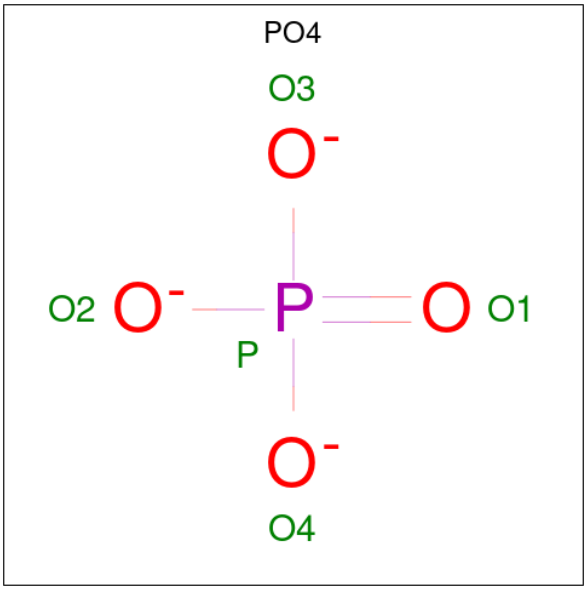
- Molecule 9 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	n	4	Total	C	N	O	P	0	4	0
			80	36	8	32	4			
9	qq	4	Total	C	N	O	P	0	2	0
			80	36	8	32	4			

- Molecule 10 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	bb	12	Total	C	N	O	P	0	8	0
			264	120	60	72	12			

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	P	0	0
			5	4	1		
11	H	1	Total	O	P	0	0
			5	4	1		
11	H	1	Total	O	P	0	0
			5	4	1		
11	L	1	Total	O	P	0	0
			5	4	1		
11	S	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	GG	1	Total O P 5 4 1	0	0
11	ll	1	Total O P 5 4 1	0	0

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total Cl 1 1	0	0
12	D	1	Total Cl 1 1	0	0
12	G	1	Total Cl 1 1	0	0
12	M	1	Total Cl 1 1	0	0
12	N	1	Total Cl 1 1	0	0
12	T	1	Total Cl 1 1	0	0
12	HH	1	Total Cl 1 1	0	0
12	JJ	1	Total Cl 1 1	0	0
12	KK	2	Total Cl 2 2	0	0
12	bb	3	Total Cl 3 3	0	0
12	qq	1	Total Cl 1 1	0	0
12	U	1	Total Cl 1 1	0	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	G	1	Total Mg 1 1	0	0
13	H	1	Total Mg 1 1	0	0
13	L	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	II	1	Total Mg 1 1	0	0
13	JJ	2	Total Mg 2 2	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	28	Total O 28 28	0	0
14	B	41	Total O 41 41	0	0
14	C	33	Total O 33 33	0	0
14	D	48	Total O 48 48	0	0
14	E	32	Total O 32 32	0	0
14	F	32	Total O 32 32	0	0
14	G	44	Total O 44 44	0	0
14	H	38	Total O 38 38	0	0
14	I	17	Total O 17 17	0	0
14	J	39	Total O 39 39	0	0
14	K	51	Total O 51 51	0	0
14	L	28	Total O 28 28	0	0
14	M	30	Total O 30 30	0	0
14	N	20	Total O 20 20	0	0
14	O	62	Total O 62 62	0	0
14	P	14	Total O 14 14	0	0
14	S	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	T	9	Total O 9 9	0	0
14	V	25	Total O 25 25	0	0
14	X	13	Total O 13 13	0	0
14	Y	18	Total O 18 18	0	0
14	a	6	Total O 6 6	0	0
14	e	30	Total O 30 30	0	0
14	h	21	Total O 21 21	0	0
14	i	3	Total O 3 3	0	0
14	m	15	Total O 15 15	0	0
14	n	9	Total O 9 9	0	0
14	GG	36	Total O 36 36	0	0
14	HH	57	Total O 57 57	0	0
14	II	65	Total O 65 65	0	0
14	JJ	30	Total O 30 30	0	0
14	KK	56	Total O 56 56	0	0
14	TT	3	Total O 3 3	0	0
14	UU	6	Total O 6 6	0	0
14	WW	14	Total O 14 14	0	0
14	bb	37	Total O 37 37	0	0
14	kk	30	Total O 30 30	0	0
14	ll	5	Total O 5 5	0	0

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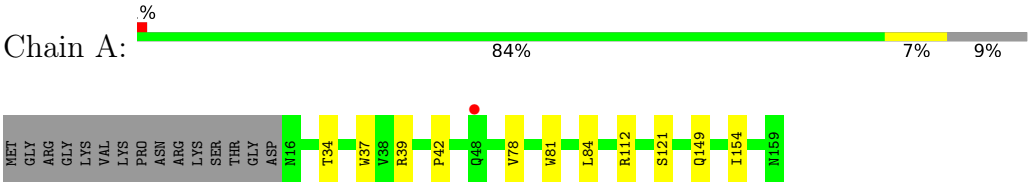
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	qq	6	Total	O	0	0
			6	6		

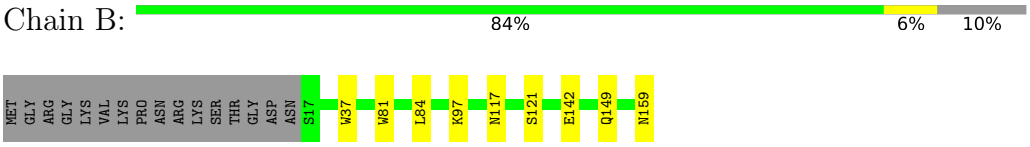
3 Residue-property plots (i)

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.

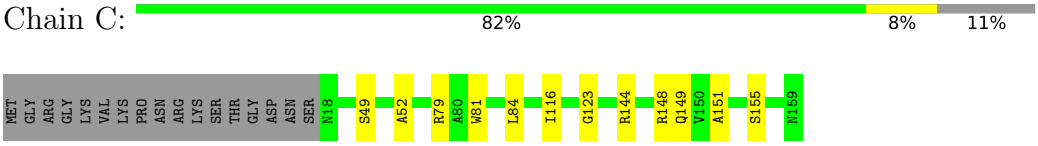
• Molecule 1: Coat protein



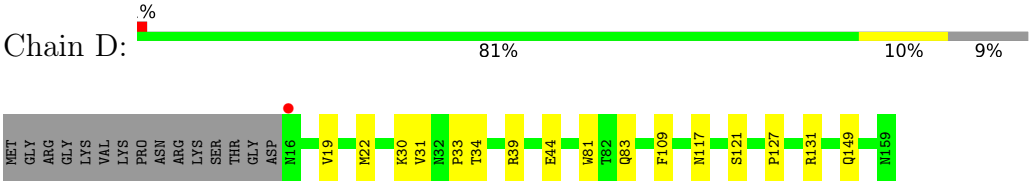
• Molecule 1: Coat protein



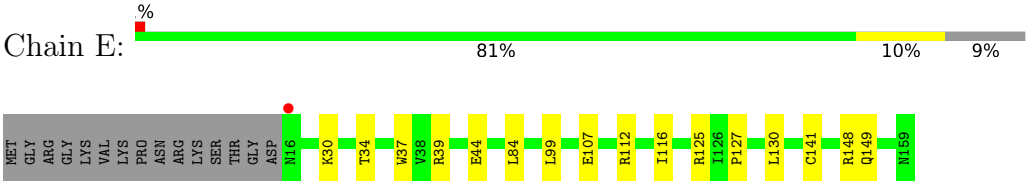
• Molecule 1: Coat protein



• Molecule 1: Coat protein

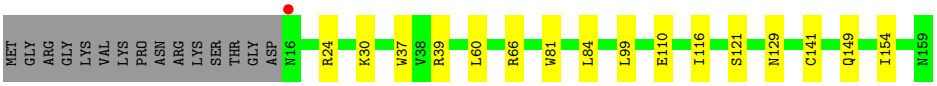


• Molecule 1: Coat protein



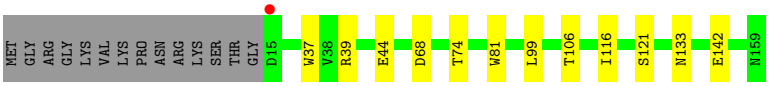
• Molecule 1: Coat protein

Chain F:



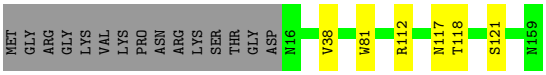
• Molecule 1: Coat protein

Chain H:



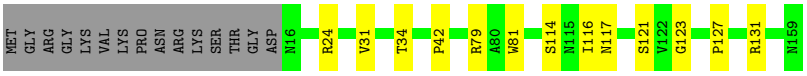
• Molecule 1: Coat protein

Chain I:



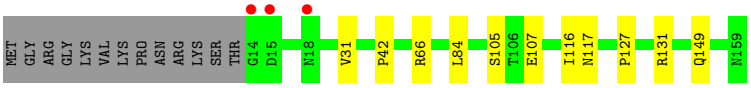
• Molecule 1: Coat protein

Chain J:



• Molecule 1: Coat protein

Chain K:

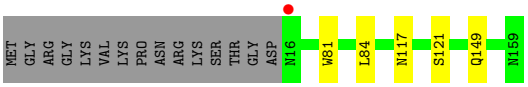


• Molecule 1: Coat protein

Chain L:

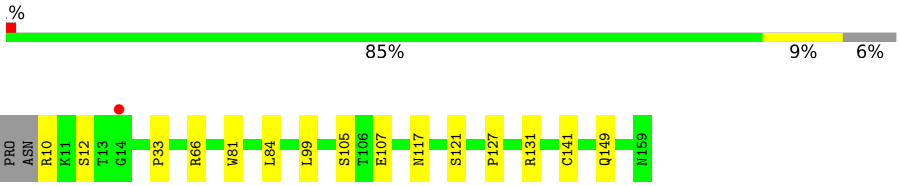
• Molecule 1: Coat protein

Chain M:



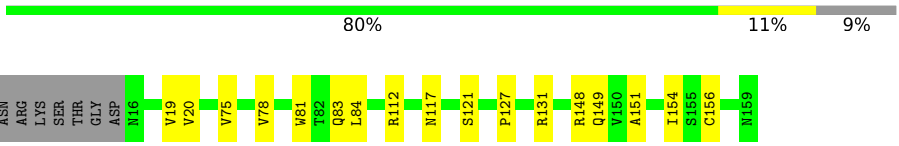
• Molecule 1: Coat protein

Chain O:



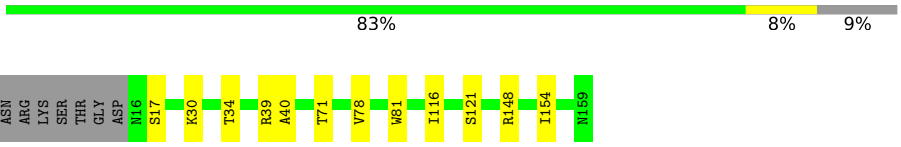
• Molecule 1: Coat protein

Chain GG:



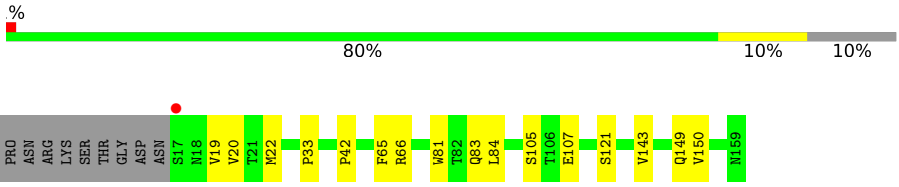
• Molecule 1: Coat protein

Chain HH:



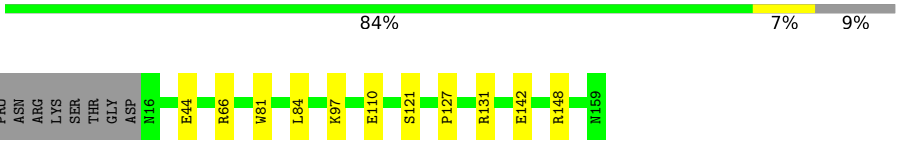
• Molecule 1: Coat protein

Chain II:



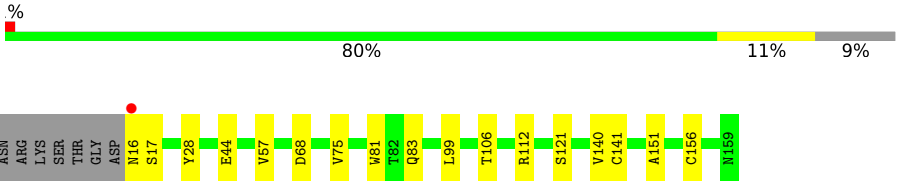
• Molecule 1: Coat protein

Chain JJ:



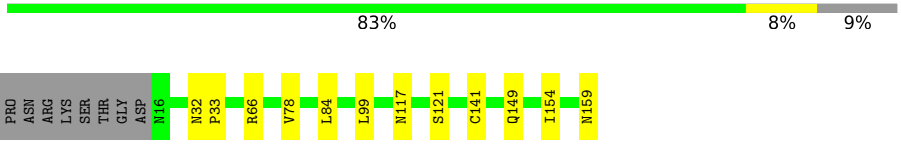
• Molecule 1: Coat protein

Chain KK:



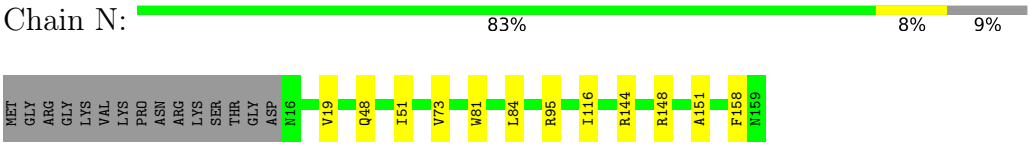
• Molecule 2: Coat protein

Chain G:



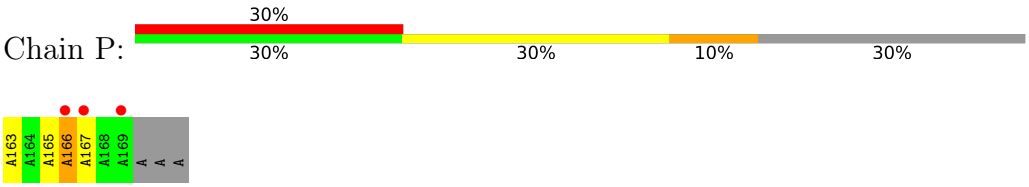
• Molecule 3: Coat protein

Chain N:



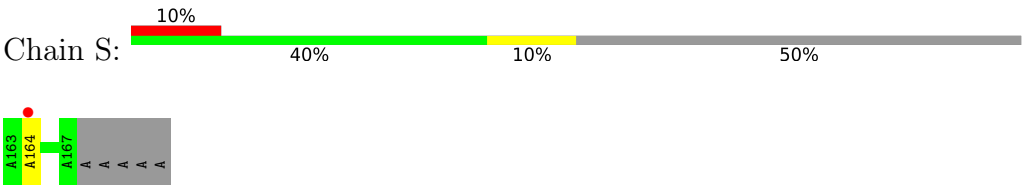
• Molecule 4: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain P:



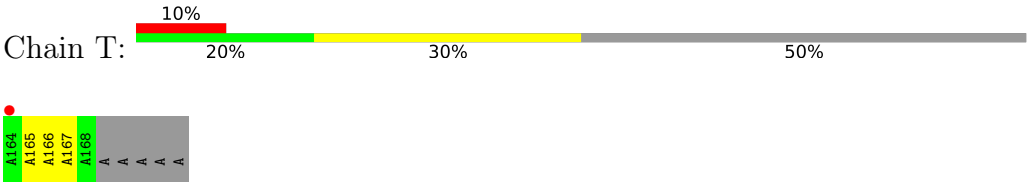
• Molecule 4: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain S:



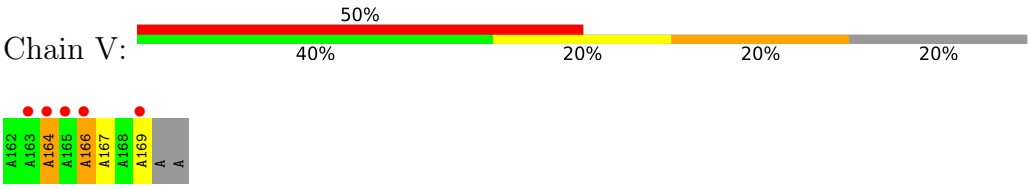
• Molecule 4: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain T:



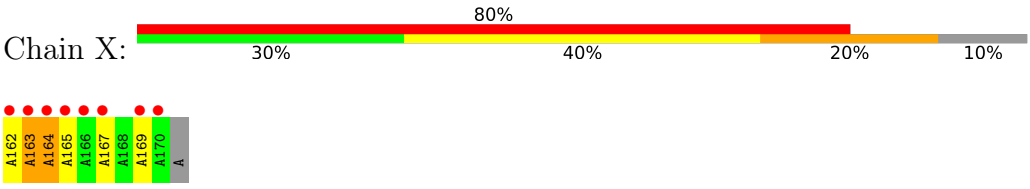
• Molecule 4: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain V:



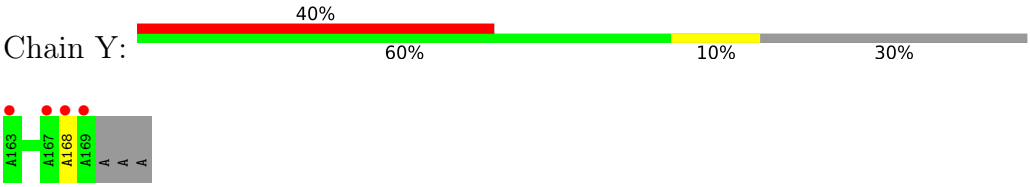
• Molecule 4: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain X:



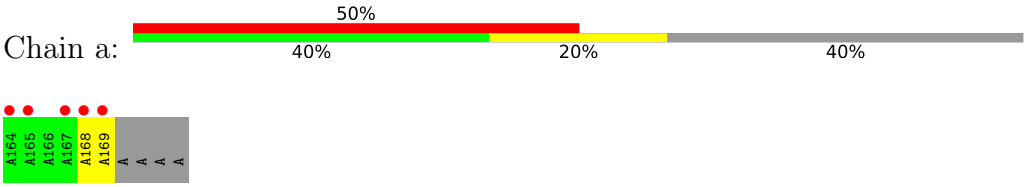
• Molecule 4: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain Y:



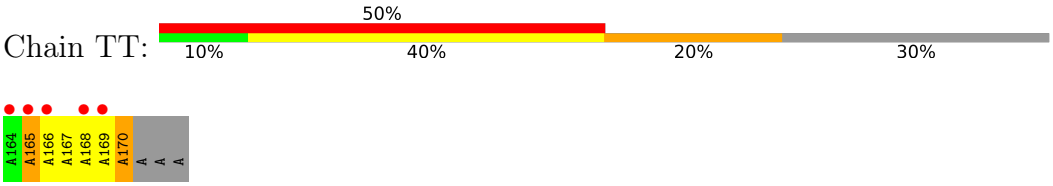
• Molecule 4: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain a:



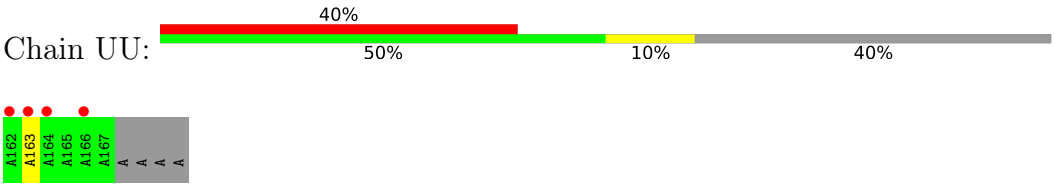
• Molecule 4: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain TT:



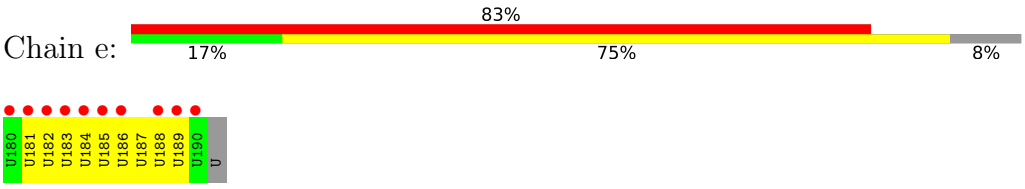
• Molecule 4: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain UU:



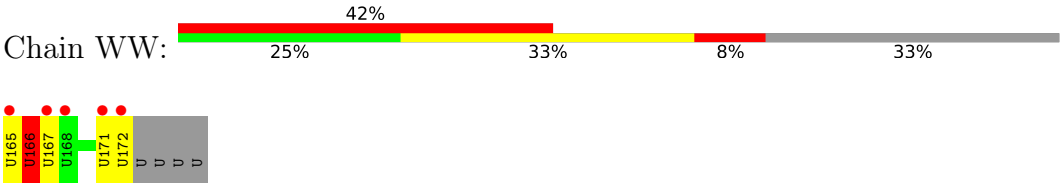
• Molecule 5: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain e:



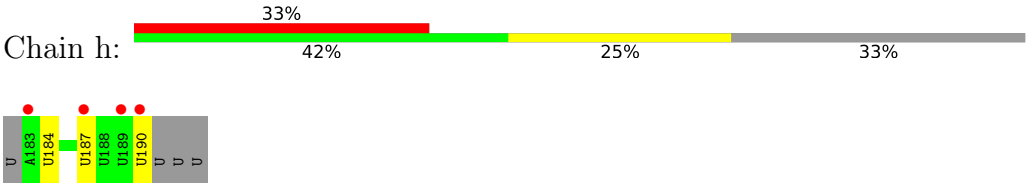
• Molecule 5: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain WW:



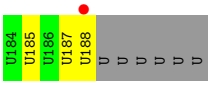
• Molecule 6: RNA (5'-R(P*UP*AP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain h:



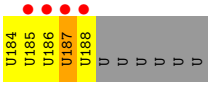
• Molecule 7: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain i:



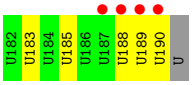
• Molecule 7: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain ll:



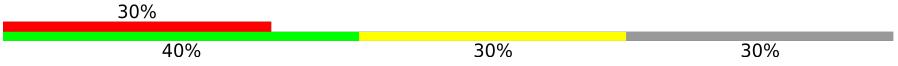
• Molecule 8: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

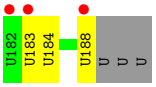
Chain m:



• Molecule 8: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

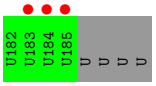
Chain kk:





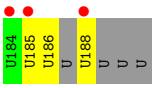
• Molecule 9: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain n:



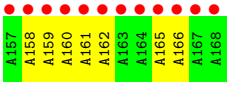
• Molecule 9: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain qq:



• Molecule 10: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain bb:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α, β, γ	234.05Å 234.05Å 234.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.81 – 3.20 46.81 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.81-3.20) 98.7 (46.81-3.20)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	4.54 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.215 , 0.254 0.222 , 0.261	Depositor DCC
R_{free} test set	3531 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 1.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	26451	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, CL

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	0.27	0/1142	0.53	0/1556
1	B	0.28	0/1142	0.54	0/1555
1	C	0.28	0/1128	0.54	0/1537
1	D	0.29	0/1142	0.53	0/1556
1	E	0.29	0/1142	0.53	0/1556
1	F	0.28	0/1148	0.53	0/1564
1	GG	0.28	0/1142	0.53	0/1556
1	H	0.28	0/1150	0.53	0/1567
1	HH	0.29	0/1142	0.53	0/1556
1	I	0.28	0/1142	0.53	0/1556
1	II	0.28	0/1134	0.54	0/1545
1	J	0.28	0/1142	0.53	0/1556
1	JJ	0.30	0/1142	0.54	0/1556
1	K	0.27	0/1181	0.53	0/1608
1	KK	0.31	0/1142	0.54	0/1556
1	L	0.27	0/1240	0.53	0/1685
1	M	0.26	0/1142	0.53	0/1556
1	O	0.27	0/1195	0.53	0/1625
2	G	0.29	0/1141	0.53	0/1554
3	N	0.29	0/1152	0.52	0/1569
4	P	0.37	0/174	0.90	0/269
4	S	0.20	0/124	0.72	0/191
4	T	0.30	0/124	0.83	0/191
4	TT	0.35	0/174	0.98	0/269
4	UU	0.15	0/149	0.64	0/230
4	V	0.25	0/199	0.74	0/308
4	X	0.28	0/223	0.75	0/343
4	Y	0.14	0/173	0.64	0/265
4	a	0.27	0/149	0.77	0/230
5	WW	0.29	0/175	1.25	3/268 (1.1%)
5	e	0.30	0/241	1.08	1/370 (0.3%)
6	h	0.18	0/178	0.72	0/273

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
7	i	0.24	0/109	0.88	0/166
7	ll	0.30	0/109	1.16	1/166 (0.6%)
8	kk	0.22	0/153	0.82	0/234
8	m	0.30	0/197	0.97	0/302
9	n	0.24	0/87	0.94	0/132
9	qq	0.33	0/86	1.41	3/128 (2.3%)
10	bb	0.28	0/299	0.87	0/464
All	All	0.28	0/26154	0.60	8/36168 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	WW	166[A]	U	C2-N1-C1'	7.80	127.06	117.70
5	e	181[A]	U	OP1-P-OP2	-7.33	108.61	119.60
5	WW	166[A]	U	N3-C2-O2	-6.38	117.74	122.20
5	WW	166[A]	U	N1-C2-O2	6.03	127.02	122.80
9	qq	188	U	C2-N1-C1'	6.01	124.91	117.70
9	qq	188	U	N1-C2-O2	5.94	126.96	122.80
7	ll	184[A]	U	C2-N1-C1'	5.32	124.09	117.70
9	qq	188	U	N3-C2-O2	-5.26	118.52	122.20

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	1118	0	1110	8	0
1	B	1115	0	1112	5	0
1	C	1104	0	1094	6	2
1	D	1118	0	1103	14	0
1	E	1118	0	1105	12	0
1	F	1121	0	1113	11	0
1	GG	1118	0	1103	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1126	0	1110	9	0
1	HH	1118	0	1109	10	0
1	I	1118	0	1106	6	0
1	II	1110	0	1105	11	0
1	J	1118	0	1108	10	0
1	JJ	1118	0	1105	8	0
1	K	1150	0	1149	10	0
1	KK	1118	0	1106	11	0
1	L	1215	0	1216	9	0
1	M	1118	0	1112	3	0
1	O	1168	0	1155	9	0
2	G	1117	0	1106	9	0
3	N	1125	0	1125	7	0
4	P	154	0	78	5	0
4	S	110	0	56	0	0
4	T	110	0	56	1	0
4	TT	154	0	78	3	0
4	UU	132	0	67	0	0
4	V	176	0	89	3	0
4	X	198	0	101	4	0
4	Y	154	0	79	0	0
4	a	132	0	67	0	0
5	WW	160	0	75	1	0
5	e	220	0	111	0	0
6	h	162	0	82	0	0
7	i	100	0	51	0	0
7	ll	100	0	51	0	1
8	kk	140	0	71	0	0
8	m	180	0	91	0	0
9	n	80	0	41	0	0
9	qq	80	0	42	0	0
10	bb	264	0	133	0	0
11	A	5	0	0	0	0
11	GG	5	0	0	0	0
11	H	10	0	0	1	0
11	L	5	0	0	0	0
11	S	5	0	0	0	0
11	ll	5	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
12	G	1	0	0	0	0
12	HH	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	JJ	1	0	0	0	0
12	KK	2	0	0	0	0
12	M	1	0	0	0	0
12	N	1	0	0	0	0
12	T	1	0	0	0	0
12	U	1	0	0	0	0
12	bb	3	0	0	0	0
12	qq	1	0	0	0	0
13	G	1	0	0	0	0
13	H	1	0	0	0	0
13	II	1	0	0	0	0
13	JJ	2	0	0	0	0
13	L	1	0	0	0	0
14	A	28	0	0	0	0
14	B	41	0	0	0	0
14	C	33	0	0	0	0
14	D	48	0	0	0	0
14	E	32	0	0	0	0
14	F	32	0	0	2	0
14	G	44	0	0	1	0
14	GG	36	0	0	0	0
14	H	38	0	0	0	0
14	HH	57	0	0	0	0
14	I	17	0	0	0	0
14	II	65	0	0	1	0
14	J	39	0	0	0	0
14	JJ	30	0	0	0	0
14	K	51	0	0	0	0
14	KK	56	0	0	1	0
14	L	28	0	0	0	0
14	M	30	0	0	0	0
14	N	20	0	0	0	0
14	O	62	0	0	1	0
14	P	14	0	0	1	0
14	S	7	0	0	0	0
14	T	9	0	0	0	0
14	TT	3	0	0	1	0
14	UU	6	0	0	0	0
14	V	25	0	0	0	0
14	WW	14	0	0	0	0
14	X	13	0	0	2	0
14	Y	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	a	6	0	0	0	0
14	bb	37	0	0	0	0
14	e	30	0	0	0	0
14	h	21	0	0	0	0
14	i	3	0	0	0	0
14	kk	30	0	0	0	0
14	ll	5	0	0	0	0
14	m	15	0	0	0	0
14	n	9	0	0	0	0
14	qq	6	0	0	0	0
All	All	26451	0	23771	152	2

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 4.

All (152) 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:HH:71:THR:OG1	12:HH:201:CL:CL	2.39	0.76
1:KK:28:TYR:O	14:KK:301:HOH:O	2.09	0.70
1:II:143:VAL:HG11	1:II:150:VAL:HG11	1.73	0.69
1:I:38:VAL:HB	4:X:163[A]:A:C2	2.32	0.64
1:H:68:ASP:N	11:H:503:PO4:O4	2.31	0.63
1:J:24:ARG:NH2	4:P:167[A]:A:OP2	2.33	0.61
1:L:12:SER:OG	1:L:16:ASN:O	2.19	0.61
4:TT:170[A]:A:N6	14:TT:201:HOH:O	2.34	0.60
1:KK:57:VAL:HG22	1:KK:140:VAL:HG13	1.84	0.60
4:X:162[A]:A:N6	14:X:201:HOH:O	2.35	0.59
1:O:10:ARG:O	14:O:201:HOH:O	2.17	0.58
1:II:83:GLN:NE2	14:II:303:HOH:O	2.36	0.57
3:N:48:GLN:HG3	3:N:51:ILE:HB	1.84	0.57
1:K:84:LEU:HG	1:K:149:GLN:HB3	1.87	0.57
3:N:84:LEU:HD12	3:N:148:ARG:HB3	1.87	0.57
1:L:11:LYS:HE2	1:L:21:THR:HB	1.87	0.56
1:II:105[A]:SER:OG	1:II:107:GLU:OE1	2.22	0.56
1:D:22:MET:H	4:V:164[A]:A:H5'	1.70	0.56
4:T:165[A]:A:H4'	1:HH:17:SER:HA	1.87	0.55
1:L:48:GLN:HB2	1:L:51:ILE:HG22	1.89	0.55
4:V:166[A]:A:H2'	4:V:167[A]:A:O4'	2.05	0.55
2:G:159:ASN:OXT	14:G:301:HOH:O	2.18	0.55
3:N:81:TRP:O	3:N:151:ALA:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HG	1:B:149[A]:GLN:HB2	1.90	0.53
1:E:84:LEU:HG	1:E:149[A]:GLN:HB2	1.90	0.53
1:GG:84:LEU:HD12	1:GG:148:ARG:HB2	1.90	0.53
1:D:81:TRP:CD1	1:D:121:SER:HB3	2.44	0.53
1:M:84:LEU:HG	1:M:149:GLN:HB2	1.91	0.52
1:C:79:ARG:HG3	1:C:123:GLY:HA3	1.90	0.52
1:I:117:ASN:HB3	1:J:116:ILE:HG12	1.92	0.52
1:E:84:LEU:HD12	1:E:148:ARG:HB2	1.93	0.51
1:J:79:ARG:HG2	1:J:123:GLY:HA3	1.91	0.51
1:II:19:VAL:HG22	1:II:20:VAL:H	1.75	0.51
1:J:81:TRP:CD1	1:J:121:SER:HB3	2.45	0.51
1:A:39:ARG:NH2	1:O:33:PRO:O	2.44	0.51
1:A:121:SER:O	1:F:30:LYS:NZ	2.37	0.51
1:F:110:GLU:HB3	1:K:31:VAL:HG23	1.93	0.51
3:N:95:ARG:HB2	3:N:144:ARG:HB2	1.93	0.51
1:GG:78:VAL:HG13	1:GG:154:ILE:HG12	1.93	0.51
1:D:31:VAL:HG23	1:JJ:110:GLU:HB3	1.93	0.51
1:J:31:VAL:HB	1:K:42:PRO:HG3	1.94	0.50
1:I:38:VAL:HB	4:X:163[A]:A:H2	1.74	0.50
1:F:81:TRP:CD1	1:F:121:SER:HB3	2.47	0.49
1:GG:83:GLN:OE1	1:GG:151:ALA:HB2	2.13	0.49
1:E:125:ARG:NH1	14:F:201:HOH:O	2.45	0.49
1:B:159:ASN:HD22	3:N:19:VAL:HG12	1.77	0.49
1:KK:75:VAL:HA	1:KK:156:CYS:HB3	1.94	0.49
2:G:33:PRO:O	1:HH:39:ARG:NH2	2.46	0.48
1:II:84:LEU:HG	1:II:149[A]:GLN:HB2	1.95	0.48
1:E:127:PRO:HG2	1:E:130:LEU:HB2	1.96	0.48
1:H:106:THR:HG23	12:HH:201:CL:CL	2.49	0.48
4:P:163[A]:A:N7	14:P:201:HOH:O	2.35	0.48
1:D:39:ARG:NH2	1:II:33:PRO:O	2.46	0.48
1:D:109:PHE:CD1	1:II:22:MET:HB2	2.49	0.47
1:GG:83:GLN:HB3	1:GG:149:GLN:HB3	1.96	0.47
1:E:30:LYS:NZ	2:G:121:SER:O	2.38	0.47
1:M:117:ASN:HB3	3:N:116:ILE:HG12	1.96	0.47
1:O:84:LEU:HG	1:O:149:GLN:HB3	1.96	0.47
1:II:81:TRP:CD1	1:II:121:SER:HB3	2.50	0.47
1:JJ:81:TRP:CD1	1:JJ:121:SER:HB3	2.50	0.47
1:A:84:LEU:HG	1:A:149[A]:GLN:HB2	1.96	0.47
1:HH:78:VAL:HG13	1:HH:154:ILE:HG12	1.97	0.47
1:C:84:LEU:HD12	1:C:148:ARG:HB2	1.97	0.47
4:V:164[A]:A:H2	1:HH:39:ARG:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:GLU:OE2	1:I:112:ARG:NH2	2.39	0.47
1:GG:81:TRP:CD1	1:GG:121:SER:HB3	2.50	0.46
1:A:78:VAL:HG13	1:A:154:ILE:HG12	1.98	0.46
1:M:81:TRP:CD1	1:M:121:SER:HB3	2.50	0.46
1:O:81:TRP:CD1	1:O:121:SER:HB3	2.50	0.46
1:C:84:LEU:HG	1:C:149[A]:GLN:HB2	1.96	0.46
1:K:116:ILE:HG12	1:O:117:ASN:HB3	1.97	0.46
1:GG:75:VAL:HA	1:GG:156:CYS:HB3	1.98	0.46
1:F:84:LEU:HG	1:F:149:GLN:HB2	1.96	0.45
1:H:121:SER:O	1:HH:30:LYS:NZ	2.41	0.45
4:P:165[A]:A:H2'	4:P:165[A]:A:N3	2.32	0.45
1:H:81:TRP:CD1	1:H:121:SER:HB3	2.52	0.45
1:C:52:ALA:HB2	1:C:144:ARG:HE	1.80	0.45
1:O:127:PRO:O	1:O:131:ARG:HG3	2.17	0.45
1:GG:117:ASN:HB3	1:HH:116:ILE:HG12	1.98	0.45
1:K:66:ARG:NH2	1:L:106:THR:OG1	2.33	0.45
1:HH:81:TRP:CD1	1:HH:121:SER:HB3	2.52	0.45
1:JJ:44:GLU:OE2	1:KK:112:ARG:NH1	2.36	0.45
1:A:112:ARG:NH2	1:E:44:GLU:OE2	2.38	0.45
2:G:84:LEU:HG	2:G:149:GLN:HB2	1.98	0.45
1:H:37:TRP:CE2	1:H:39:ARG:HD3	2.52	0.45
1:GG:19:VAL:HG12	1:GG:20:VAL:H	1.82	0.44
1:HH:40:ALA:HA	1:HH:154:ILE:O	2.17	0.44
1:H:74:THR:OG1	1:H:133:ASN:OD1	2.31	0.44
1:D:127:PRO:O	1:D:131:ARG:HG3	2.17	0.44
1:JJ:97:LYS:HB3	1:JJ:142:GLU:HB2	1.98	0.44
2:G:117:ASN:HB3	1:H:116:ILE:HG12	1.98	0.44
1:JJ:127:PRO:O	1:JJ:131:ARG:HG3	2.18	0.44
1:B:97[A]:LYS:HB3	1:B:142:GLU:HB2	2.00	0.43
1:O:105[A]:SER:HB3	1:O:107:GLU:OE1	2.18	0.43
2:G:99:LEU:HG	2:G:141:CYS:HA	2.00	0.43
1:L:84:LEU:HD12	1:L:148:ARG:HB2	1.99	0.43
1:K:117:ASN:HB3	1:L:116:ILE:HG12	2.00	0.43
4:P:166[A]:A:H2'	4:P:167[A]:A:O4'	2.18	0.43
1:L:81:TRP:O	1:L:151:ALA:N	2.37	0.43
1:I:81:TRP:CD1	1:I:121:SER:HB3	2.54	0.43
1:D:30:LYS:NZ	1:JJ:121:SER:O	2.37	0.43
1:A:37:TRP:CE2	1:A:39:ARG:HD3	2.53	0.42
1:D:117:ASN:HB3	1:E:116:ILE:HG12	2.01	0.42
1:E:34:THR:HB	1:F:66:ARG:NH2	2.33	0.42
1:JJ:66:ARG:NH2	1:KK:106:THR:OG1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GG:127:PRO:O	1:GG:131:ARG:HG3	2.19	0.42
1:F:129:ASN:ND2	1:K:131:ARG:O	2.47	0.42
1:H:99:LEU:HD11	1:H:142:GLU:HG3	2.01	0.42
1:O:99:LEU:HG	1:O:141:CYS:HA	2.01	0.42
1:GG:112:ARG:NH2	1:KK:44:GLU:OE2	2.40	0.42
1:A:34:THR:HB	1:O:66:ARG:NH2	2.35	0.42
1:KK:99:LEU:HG	1:KK:141:CYS:HA	2.02	0.42
1:B:117:ASN:HB3	1:C:116:ILE:HG12	2.01	0.42
1:KK:83:GLN:OE1	1:KK:151:ALA:HB2	2.20	0.42
1:F:37:TRP:CE2	1:F:39:ARG:HD3	2.54	0.42
1:D:31:VAL:HB	1:II:42:PRO:HG3	2.01	0.42
1:L:37:TRP:CE2	1:L:39:ARG:HD3	2.55	0.42
1:D:83:GLN:HB3	1:D:149:GLN:HB3	2.01	0.42
1:GG:81:TRP:O	1:GG:151:ALA:N	2.47	0.42
1:J:34:THR:HB	1:K:66:ARG:NH2	2.34	0.41
1:K:127:PRO:O	1:K:131:ARG:HG3	2.19	0.41
4:X:164[A]:A:H5'	14:X:204:HOH:O	2.20	0.41
1:E:37:TRP:CE2	1:E:39:ARG:HD3	2.55	0.41
1:F:99:LEU:HG	1:F:141:CYS:HA	2.02	0.41
1:J:127:PRO:O	1:J:131:ARG:HG3	2.21	0.41
1:KK:81:TRP:CD1	1:KK:121:SER:HB3	2.55	0.41
4:TT:165:A:H2'	4:TT:165:A:N3	2.34	0.41
1:D:33:PRO:O	1:II:65:PHE:HA	2.20	0.41
1:J:79:ARG:NH1	1:J:81:TRP:HH2	2.18	0.41
1:E:99:LEU:HG	1:E:141:CYS:HA	2.03	0.41
1:F:24:ARG:NH2	14:F:203:HOH:O	2.53	0.41
1:JJ:84:LEU:HD12	1:JJ:148:ARG:HB2	2.03	0.41
3:N:73:VAL:HG23	3:N:158:PHE:HA	2.03	0.41
1:C:81:TRP:O	1:C:151:ALA:N	2.41	0.41
1:L:127:PRO:HB2	1:L:129:ASN:OD1	2.21	0.41
1:D:34:THR:HB	1:II:66:ARG:NH2	2.36	0.41
1:I:118:THR:HA	1:J:114:SER:O	2.21	0.41
1:KK:16:ASN:HB3	1:KK:17:SER:H	1.67	0.41
1:A:81:TRP:CD1	1:A:121:SER:HB3	2.56	0.40
1:F:60:LEU:HD21	1:F:154:ILE:HD12	2.03	0.40
1:F:116:ILE:HG12	1:J:117:ASN:HB3	2.03	0.40
2:G:78:VAL:HG13	2:G:154:ILE:HG12	2.03	0.40
1:B:81:TRP:CD1	1:B:121:SER:HB3	2.57	0.40
1:D:22:MET:HE1	2:G:32:ASN:HB2	2.04	0.40
1:K:105:SER:HB2	1:K:107:GLU:OE1	2.22	0.40
4:TT:168[A]:A:H2'	4:TT:169[A]:A:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:166[A]:A:H3'	4:P:167[A]:A:H8	1.87	0.40
1:D:44:GLU:OE2	1:E:112:ARG:NH2	2.44	0.40
2:G:66:ARG:NH2	1:HH:34:THR:HB	2.37	0.40

All (2) 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)
1:C:49[A]:SER:OG	1:C:49[A]:SER:OG[2_675]	2.04	0.16
1:C:155[A]:SER:OG	7:ll:187[A]:U:O2'[12_665]	2.04	0.16

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	142/159 (89%)	136 (96%)	5 (4%)	1 (1%)	22	61
1	B	142/159 (89%)	134 (94%)	7 (5%)	1 (1%)	22	61
1	C	140/159 (88%)	132 (94%)	8 (6%)	0	100	100
1	D	142/159 (89%)	136 (96%)	6 (4%)	0	100	100
1	E	142/159 (89%)	131 (92%)	11 (8%)	0	100	100
1	F	143/159 (90%)	133 (93%)	10 (7%)	0	100	100
1	GG	142/159 (89%)	135 (95%)	7 (5%)	0	100	100
1	H	143/159 (90%)	132 (92%)	11 (8%)	0	100	100
1	HH	142/159 (89%)	133 (94%)	9 (6%)	0	100	100
1	I	142/159 (89%)	134 (94%)	8 (6%)	0	100	100
1	II	141/159 (89%)	129 (92%)	12 (8%)	0	100	100
1	J	142/159 (89%)	134 (94%)	7 (5%)	1 (1%)	22	61
1	JJ	142/159 (89%)	136 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	147/159 (92%)	137 (93%)	10 (7%)	0	100 100
1	KK	142/159 (89%)	133 (94%)	9 (6%)	0	100 100
1	L	155/159 (98%)	140 (90%)	15 (10%)	0	100 100
1	M	142/159 (89%)	135 (95%)	7 (5%)	0	100 100
1	O	149/159 (94%)	141 (95%)	7 (5%)	1 (1%)	22 61
2	G	142/159 (89%)	132 (93%)	10 (7%)	0	100 100
3	N	143/159 (90%)	136 (95%)	7 (5%)	0	100 100
All	All	2865/3180 (90%)	2689 (94%)	172 (6%)	4 (0%)	51 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	TRP
1	O	12	SER
1	A	42	PRO
1	J	42	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	128/140 (91%)	128 (100%)	0	100 100
1	B	128/140 (91%)	128 (100%)	0	100 100
1	C	126/140 (90%)	126 (100%)	0	100 100
1	D	128/140 (91%)	127 (99%)	1 (1%)	81 93
1	E	128/140 (91%)	128 (100%)	0	100 100
1	F	129/140 (92%)	129 (100%)	0	100 100
1	GG	128/140 (91%)	128 (100%)	0	100 100
1	H	129/140 (92%)	129 (100%)	0	100 100
1	HH	128/140 (91%)	127 (99%)	1 (1%)	81 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	128/140 (91%)	128 (100%)	0	100	100
1	II	127/140 (91%)	127 (100%)	0	100	100
1	J	128/140 (91%)	128 (100%)	0	100	100
1	JJ	128/140 (91%)	128 (100%)	0	100	100
1	K	132/140 (94%)	132 (100%)	0	100	100
1	KK	128/140 (91%)	128 (100%)	0	100	100
1	L	138/140 (99%)	138 (100%)	0	100	100
1	M	128/140 (91%)	128 (100%)	0	100	100
1	O	134/140 (96%)	134 (100%)	0	100	100
2	G	128/140 (91%)	128 (100%)	0	100	100
3	N	130/141 (92%)	130 (100%)	0	100	100
All	All	2581/2801 (92%)	2579 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	19	VAL
1	HH	148	ARG

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	bb	11/12 (91%)	7 (63%)	0
4	P	6/10 (60%)	1 (16%)	0
4	S	4/10 (40%)	1 (25%)	0
4	T	4/10 (40%)	2 (50%)	1 (25%)
4	TT	6/10 (60%)	4 (66%)	1 (16%)
4	UU	5/10 (50%)	1 (20%)	0
4	V	7/10 (70%)	3 (42%)	0
4	X	7/10 (70%)	5 (71%)	0
4	Y	5/10 (50%)	1 (20%)	0
4	a	5/10 (50%)	2 (40%)	0
5	WW	8/12 (66%)	4 (50%)	1 (12%)
5	e	10/12 (83%)	8 (80%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	h	7/12 (58%)	3 (42%)	0
7	i	4/11 (36%)	3 (75%)	0
7	ll	4/11 (36%)	4 (100%)	0
8	kk	6/10 (60%)	3 (50%)	0
8	m	8/10 (80%)	5 (62%)	0
9	n	3/8 (37%)	0	0
9	qq	2/8 (25%)	2 (100%)	0
All	All	112/196 (57%)	59 (52%)	3 (2%)

All (59) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	P	166[A]	A
4	S	164[A]	A
4	T	166[A]	A
4	T	167[A]	A
4	V	164[A]	A
4	V	166[A]	A
4	V	169[A]	A
4	X	163[A]	A
4	X	164[A]	A
4	X	165[A]	A
4	X	167[A]	A
4	X	169[A]	A
4	Y	168[A]	A
4	a	168[A]	A
4	a	169[A]	A
5	e	182[A]	U
5	e	183[A]	U
5	e	184[A]	U
5	e	185[A]	U
5	e	186[A]	U
5	e	187[A]	U
5	e	188[A]	U
5	e	189[A]	U
6	h	184[A]	U
6	h	187[A]	U
6	h	190[A]	U
7	i	185[A]	U
7	i	187[A]	U
7	i	188[A]	U
8	m	183[A]	U

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Mol	Chain	Res	Type
8	m	185[A]	U
8	m	188[A]	U
8	m	189[A]	U
8	m	190[A]	U
4	TT	165	A
4	TT	166[A]	A
4	TT	167[A]	A
4	TT	170[A]	A
4	UU	163[A]	A
5	WW	166[A]	U
5	WW	167[A]	U
5	WW	171	U
5	WW	172	U
10	bb	158	A
10	bb	159	A
10	bb	160	A
10	bb	161[A]	A
10	bb	162[A]	A
10	bb	165[A]	A
10	bb	166[A]	A
8	kk	183[A]	U
8	kk	184[A]	U
8	kk	188[A]	U
7	ll	185[A]	U
7	ll	186[A]	U
7	ll	187[A]	U
7	ll	188[A]	U
9	qq	185[A]	U
9	qq	186	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	T	166[A]	A
4	TT	166[A]	A
5	WW	165	U

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 28 ligands modelled in this entry, 21 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
11	PO4	H	501	-	4,4,4	1.02	0	6,6,6	0.47	0
11	PO4	L	901	-	4,4,4	1.05	0	6,6,6	0.48	0
11	PO4	ll	201	-	4,4,4	0.90	0	6,6,6	0.48	0
11	PO4	H	503	-	4,4,4	0.99	0	6,6,6	0.37	0
11	PO4	A	701	-	4,4,4	1.03	0	6,6,6	0.42	0
11	PO4	GG	401	-	4,4,4	1.07	0	6,6,6	0.47	0
11	PO4	S	201	-	4,4,4	0.94	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	503	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	X	1
4	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	169[A]:A	O3'	170:A	P	4.35
1	Y	168[A]:A	O3'	169:A	P	3.93

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	144/159 (90%)	-0.31	1 (0%) 87 81	15, 25, 46, 78	0
1	B	143/159 (89%)	-0.42	0 100 100	16, 24, 40, 53	0
1	C	142/159 (89%)	-0.44	0 100 100	15, 21, 34, 54	0
1	D	144/159 (90%)	-0.27	1 (0%) 87 81	13, 22, 35, 71	0
1	E	144/159 (90%)	-0.37	1 (0%) 87 81	13, 20, 34, 94	0
1	F	144/159 (90%)	-0.41	1 (0%) 87 81	17, 25, 38, 89	0
1	GG	144/159 (90%)	-0.40	0 100 100	13, 19, 35, 84	0
1	H	145/159 (91%)	-0.41	1 (0%) 87 81	13, 21, 39, 78	0
1	HH	144/159 (90%)	-0.44	0 100 100	14, 20, 33, 64	0
1	I	144/159 (90%)	-0.32	0 100 100	19, 26, 41, 67	0
1	II	143/159 (89%)	-0.33	1 (0%) 87 81	13, 21, 34, 69	0
1	J	144/159 (90%)	-0.32	0 100 100	22, 29, 43, 57	0
1	JJ	144/159 (90%)	-0.37	0 100 100	13, 18, 28, 61	0
1	K	146/159 (91%)	-0.15	3 (2%) 63 49	21, 31, 56, 110	0
1	KK	144/159 (90%)	-0.45	1 (0%) 87 81	11, 17, 29, 63	0
1	L	157/159 (98%)	-0.10	3 (1%) 66 53	25, 33, 75, 97	0
1	M	144/159 (90%)	-0.23	1 (0%) 87 81	25, 32, 49, 72	0
1	O	150/159 (94%)	-0.18	1 (0%) 87 81	17, 32, 53, 88	0
2	G	144/159 (90%)	-0.36	0 100 100	16, 23, 40, 81	0
3	N	144/159 (90%)	-0.23	0 100 100	20, 29, 49, 72	0
4	P	7/10 (70%)	1.78	3 (42%) 0 0	71, 78, 107, 109	0
4	S	5/10 (50%)	1.33	1 (20%) 1 1	75, 77, 86, 105	0
4	T	5/10 (50%)	1.89	1 (20%) 1 1	80, 101, 109, 109	0
4	TT	7/10 (70%)	2.36	5 (71%) 0 0	91, 98, 125, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
4	UU	6/10 (60%)	2.09	4 (66%)	0	67, 79, 97, 130	0
4	V	8/10 (80%)	2.77	5 (62%)	0	79, 88, 96, 127	0
4	X	9/10 (90%)	3.09	8 (88%)	0	94, 109, 141, 152	0
4	Y	7/10 (70%)	3.06	4 (57%)	0	81, 90, 117, 124	0
4	a	6/10 (60%)	3.39	5 (83%)	0	87, 96, 121, 138	0
5	WW	8/12 (66%)	2.24	5 (62%)	0	77, 105, 135, 139	0
5	e	11/12 (91%)	3.41	10 (90%)	0	103, 121, 132, 133	0
6	h	8/12 (66%)	1.92	4 (50%)	0	71, 81, 115, 166	0
7	i	5/11 (45%)	1.18	1 (20%)	1	63, 73, 100, 115	0
7	ll	5/11 (45%)	3.50	4 (80%)	0	78, 86, 95, 113	0
8	kk	7/10 (70%)	2.40	3 (42%)	0	75, 82, 103, 108	0
8	m	9/10 (90%)	2.11	4 (44%)	0	85, 98, 128, 133	0
9	n	4/8 (50%)	4.05	3 (75%)	0	92, 108, 110, 113	0
9	qq	4/8 (50%)	4.24	3 (75%)	0	110, 122, 124, 129	0
10	bb	12/12 (100%)	4.72	12 (100%)	0	79, 111, 131, 146	0
All	All	3031/3376 (89%)	-0.19	100 (3%)	46	11, 25, 73, 166	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	bb	160	A	9.5
9	qq	188	U	9.2
9	n	185[A]	U	7.7
10	bb	157	A	7.6
4	Y	169	A	7.1
5	e	190[A]	U	7.0
4	a	169[A]	A	6.3
10	bb	161[A]	A	6.3
10	bb	158	A	6.1
7	ll	188[A]	U	6.1
10	bb	159	A	5.8
8	kk	182	U	5.6
9	n	184[A]	U	5.6
5	e	189[A]	U	5.5
4	V	164[A]	A	5.2
8	m	189[A]	U	5.0
4	a	168[A]	A	5.0

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Mol	Chain	Res	Type	RSRZ
4	X	162[A]	A	4.8
1	K	15	ASP	4.7
5	e	185[A]	U	4.4
6	h	183	A	4.3
4	X	164[A]	A	4.3
8	m	190[A]	U	4.3
4	X	165[A]	A	4.2
10	bb	162[A]	A	4.0
4	V	165[A]	A	4.0
1	L	15	ASP	3.9
7	ll	187[A]	U	3.9
10	bb	165[A]	A	3.9
4	TT	165	A	3.8
5	e	186[A]	U	3.8
4	Y	168[A]	A	3.8
9	qq	184[A]	U	3.7
5	WW	171	U	3.5
4	T	164[A]	A	3.5
8	kk	183[A]	U	3.5
1	K	14	GLY	3.4
1	II	17	SER	3.4
4	TT	168[A]	A	3.3
1	L	5	LYS	3.3
10	bb	163[A]	A	3.2
6	h	189[A]	U	3.2
4	P	167[A]	A	3.2
4	X	163[A]	A	3.2
4	Y	167[A]	A	3.1
5	e	188[A]	U	3.1
7	ll	186[A]	U	3.1
4	V	166[A]	A	3.1
4	a	167[A]	A	3.1
10	bb	167[A]	A	3.1
7	i	188[A]	U	3.0
4	V	169[A]	A	3.0
7	ll	185[A]	U	3.0
4	P	166[A]	A	3.0
4	a	165[A]	A	2.9
1	M	16	ASN	2.8
4	TT	164[A]	A	2.8
8	kk	188[A]	U	2.8
5	e	180	U	2.8

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Mol	Chain	Res	Type	RSRZ
9	qq	185[A]	U	2.8
4	X	170	A	2.8
4	UU	163[A]	A	2.7
5	e	183[A]	U	2.7
5	WW	167[A]	U	2.7
1	H	15	ASP	2.7
4	a	164[A]	A	2.7
4	X	169[A]	A	2.7
4	UU	162	A	2.6
5	e	184[A]	U	2.6
4	V	163	A	2.6
4	Y	163[A]	A	2.5
4	UU	164[A]	A	2.5
10	bb	168[A]	A	2.5
9	n	183[A]	U	2.5
10	bb	164[A]	A	2.5
5	e	182[A]	U	2.4
1	A	48	GLN	2.4
6	h	190[A]	U	2.4
6	h	187[A]	U	2.4
1	D	16	ASN	2.3
5	WW	165	U	2.3
8	m	188[A]	U	2.3
5	WW	172	U	2.3
4	X	166[A]	A	2.2
5	WW	168	U	2.2
4	UU	166[A]	A	2.2
5	e	181[A]	U	2.2
4	TT	169[A]	A	2.2
8	m	187[A]	U	2.2
1	F	16	ASN	2.2
4	X	167[A]	A	2.2
1	E	16	ASN	2.1
1	KK	16	ASN	2.1
1	O	14	GLY	2.1
4	S	164[A]	A	2.1
4	TT	166[A]	A	2.1
4	P	169[A]	A	2.0
10	bb	166[A]	A	2.0
1	K	18	ASN	2.0
1	L	6	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)

There are no monosaccharides in this entry.

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	B-factors(Å^2)	Q<0.9
12	CL	N	201	1/1	-0.20	0.92	102,102,102,102	0
12	CL	KK	202	1/1	0.54	0.46	68,68,68,68	1
12	CL	T	201	1/1	0.58	0.34	86,86,86,86	0
12	CL	JJ	203	1/1	0.71	0.20	104,104,104,104	1
13	MG	JJ	202	1/1	0.72	0.34	26,26,26,26	0
11	PO4	H	503	5/5	0.75	0.40	54,58,70,92	0
12	CL	bb	201	1/1	0.78	0.28	67,67,67,67	1
13	MG	G	201	1/1	0.79	0.81	44,44,44,44	0
11	PO4	S	201	5/5	0.82	0.35	75,76,94,104	0
11	PO4	ll	201	5/5	0.83	0.35	80,85,109,116	0
12	CL	bb	203	1/1	0.85	0.11	65,65,65,65	1
13	MG	JJ	201	1/1	0.86	0.65	20,20,20,20	0
12	CL	C	201	1/1	0.87	0.30	68,68,68,68	0
12	CL	D	201	1/1	0.88	0.50	71,71,71,71	1
12	CL	KK	201	1/1	0.88	0.77	34,34,34,34	1
12	CL	qq	201	1/1	0.90	0.17	71,71,71,71	0
12	CL	G	202	1/1	0.92	0.46	39,39,39,39	0
12	CL	HH	201	1/1	0.93	0.25	50,50,50,50	0
13	MG	L	902	1/1	0.94	0.13	31,31,31,31	0
12	CL	M	201	1/1	0.95	0.30	52,52,52,52	1
13	MG	H	502	1/1	0.96	0.48	28,28,28,28	0
12	CL	bb	202	1/1	0.96	0.08	73,73,73,73	1
11	PO4	H	501	5/5	0.97	0.21	24,24,27,43	0
13	MG	II	201	1/1	0.97	0.41	51,51,51,51	0
11	PO4	GG	401	5/5	0.98	0.14	14,15,19,21	0
11	PO4	A	701	5/5	0.98	0.17	18,21,25,29	0
11	PO4	L	901	5/5	0.99	0.15	24,24,33,38	0

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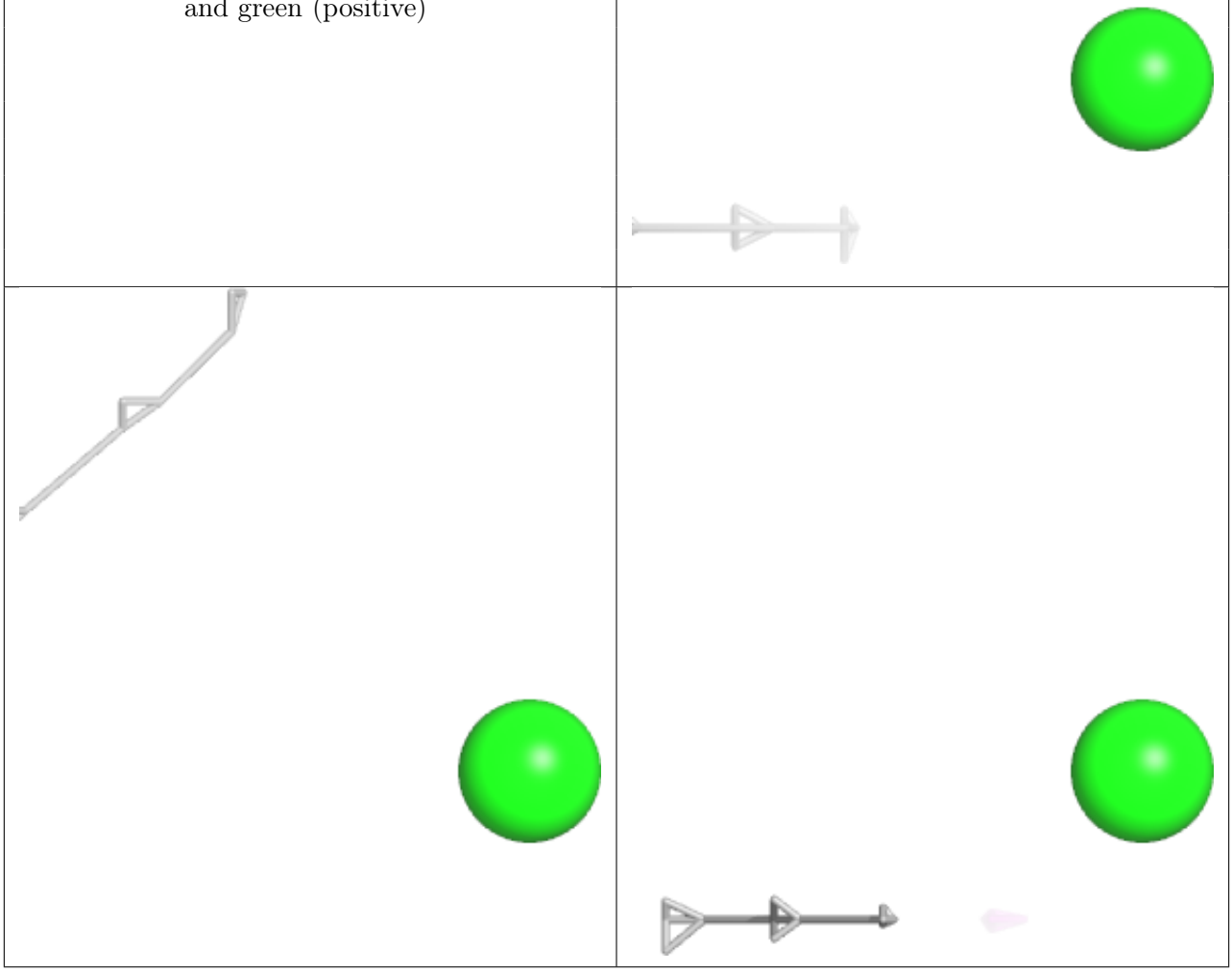
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CL	U	5	1/1	1.00	0.22	171,171,171,171	1

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.

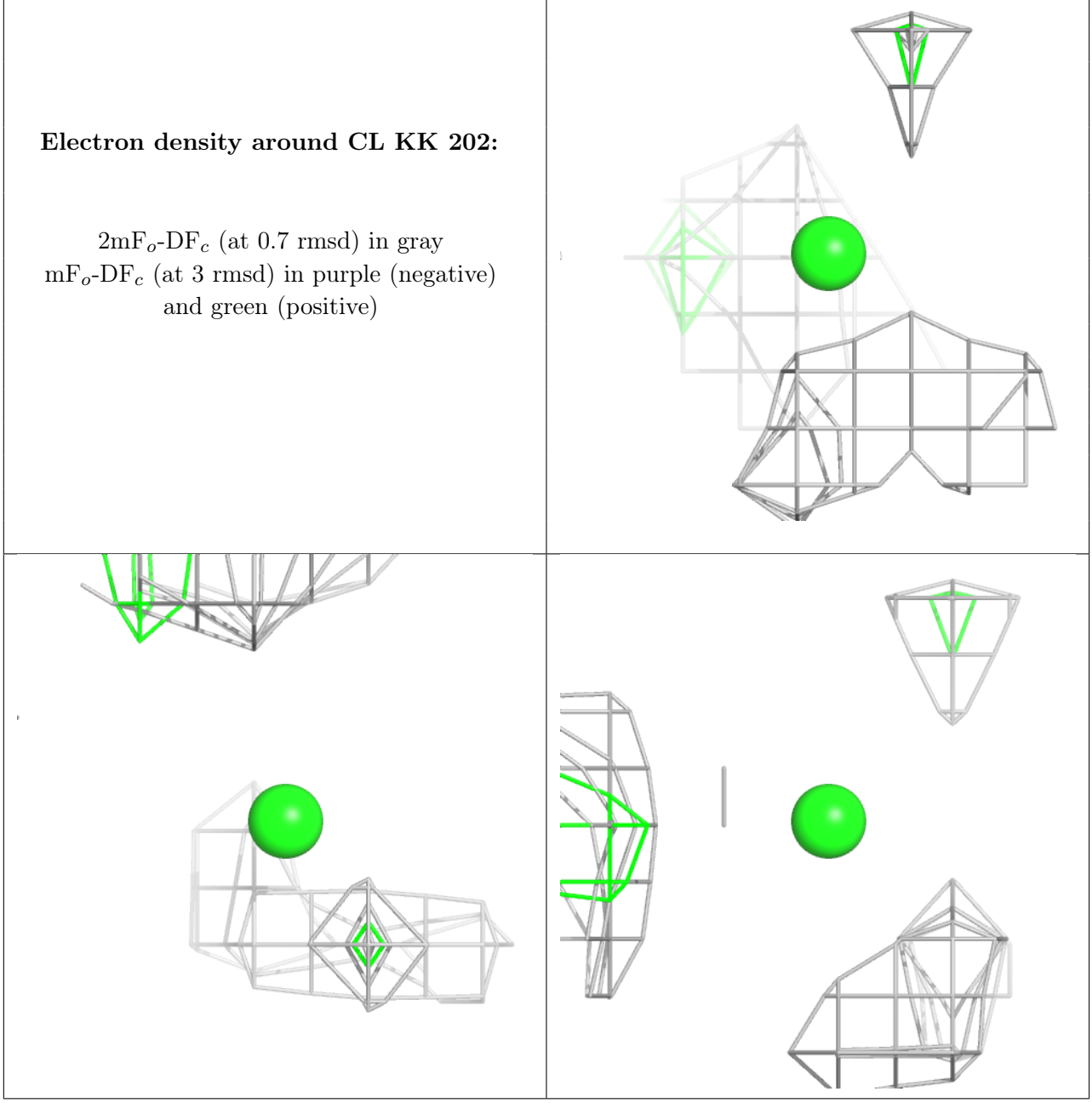
Electron density around CL N 201:

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



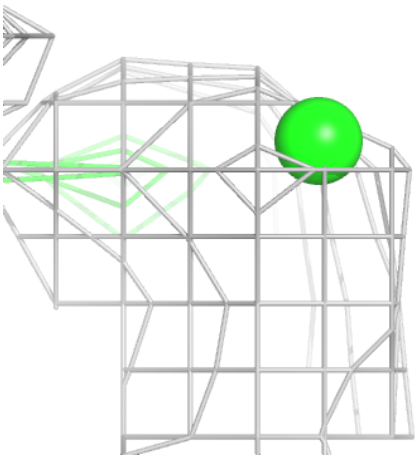
Electron density around CL KK 202:

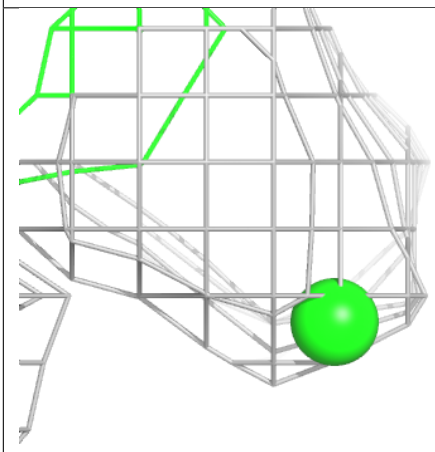
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

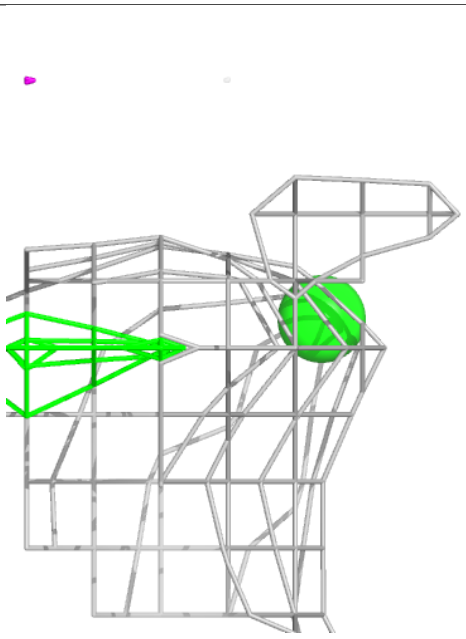


Electron density around CL T 201:

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

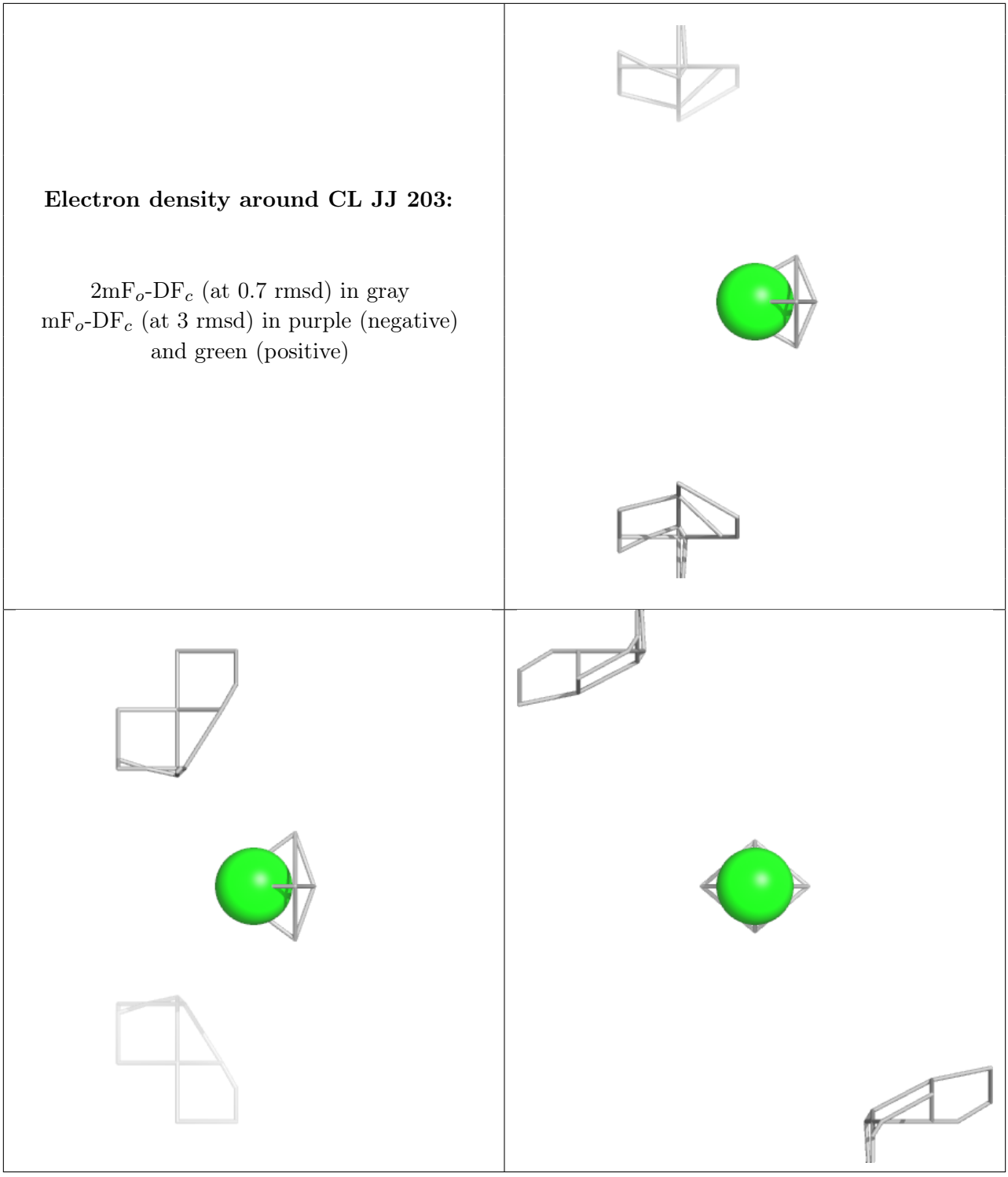






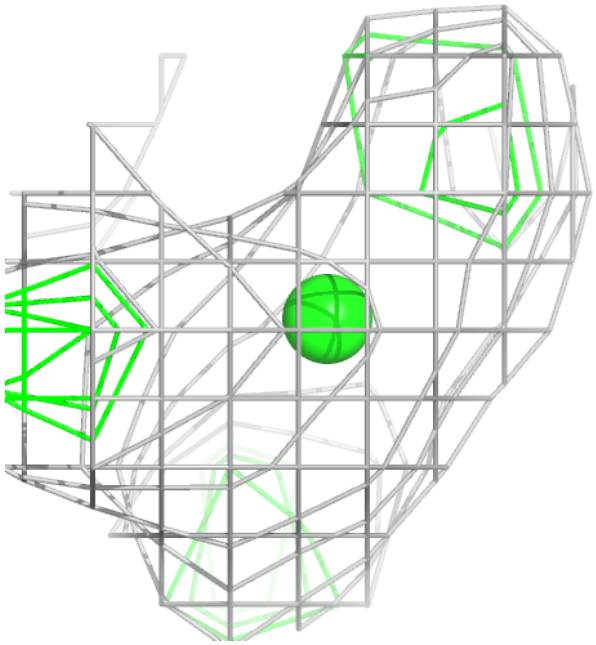
Electron density around CL JJ 203:

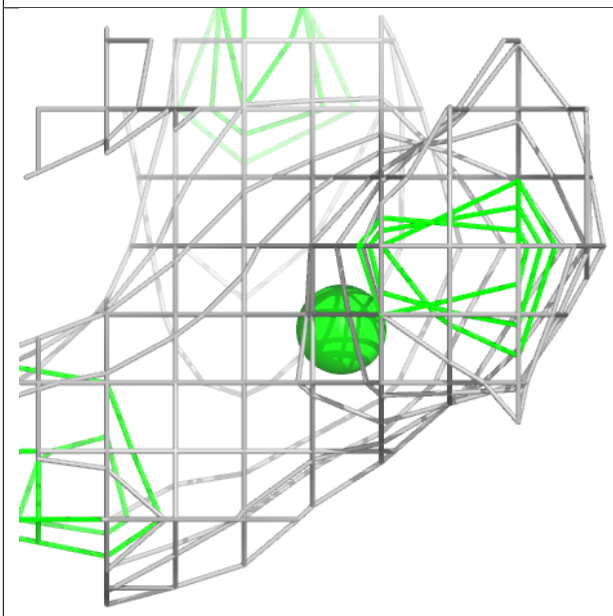
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

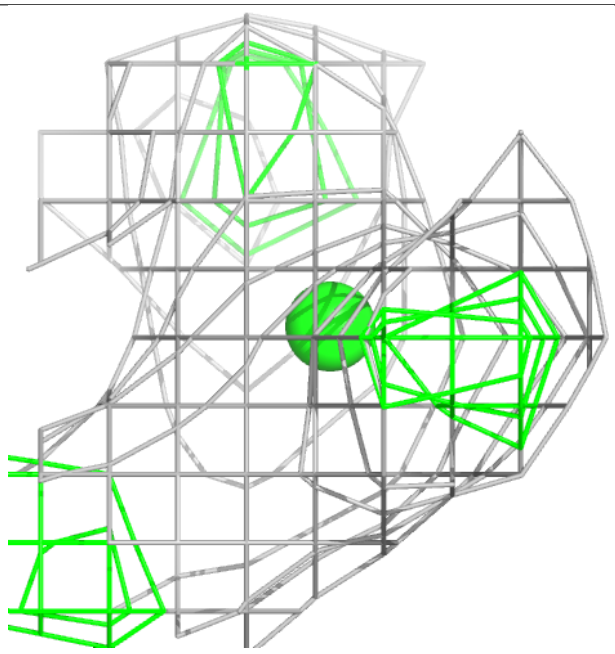


Electron density around CL bb 201:

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

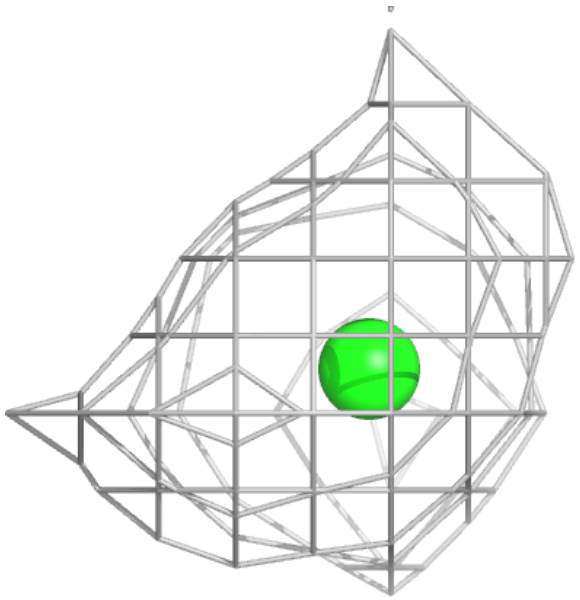


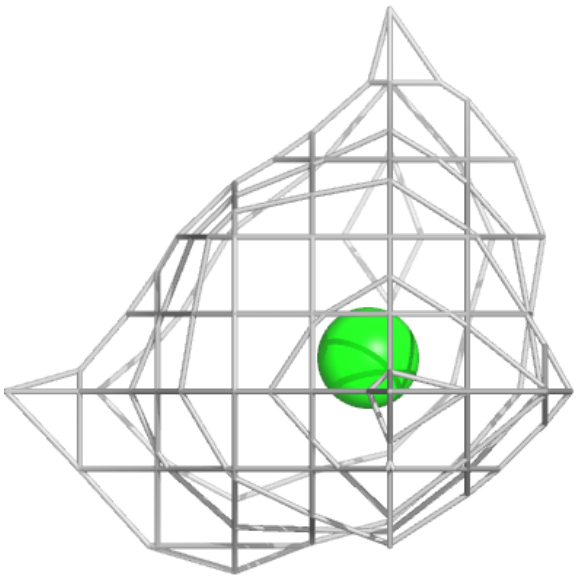


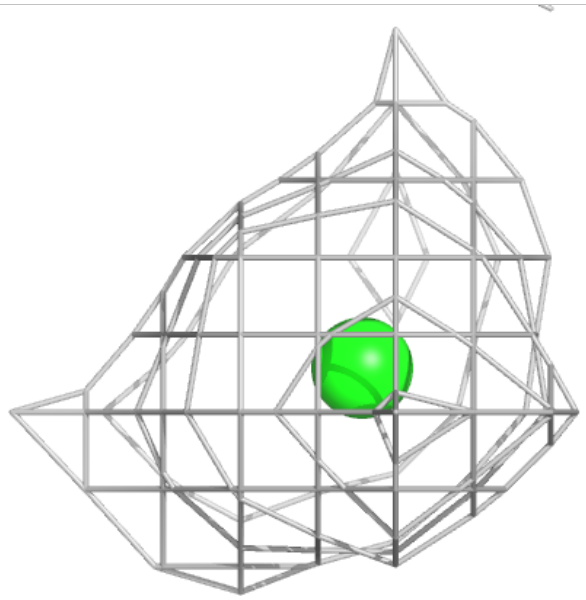


Electron density around CL bb 203:

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

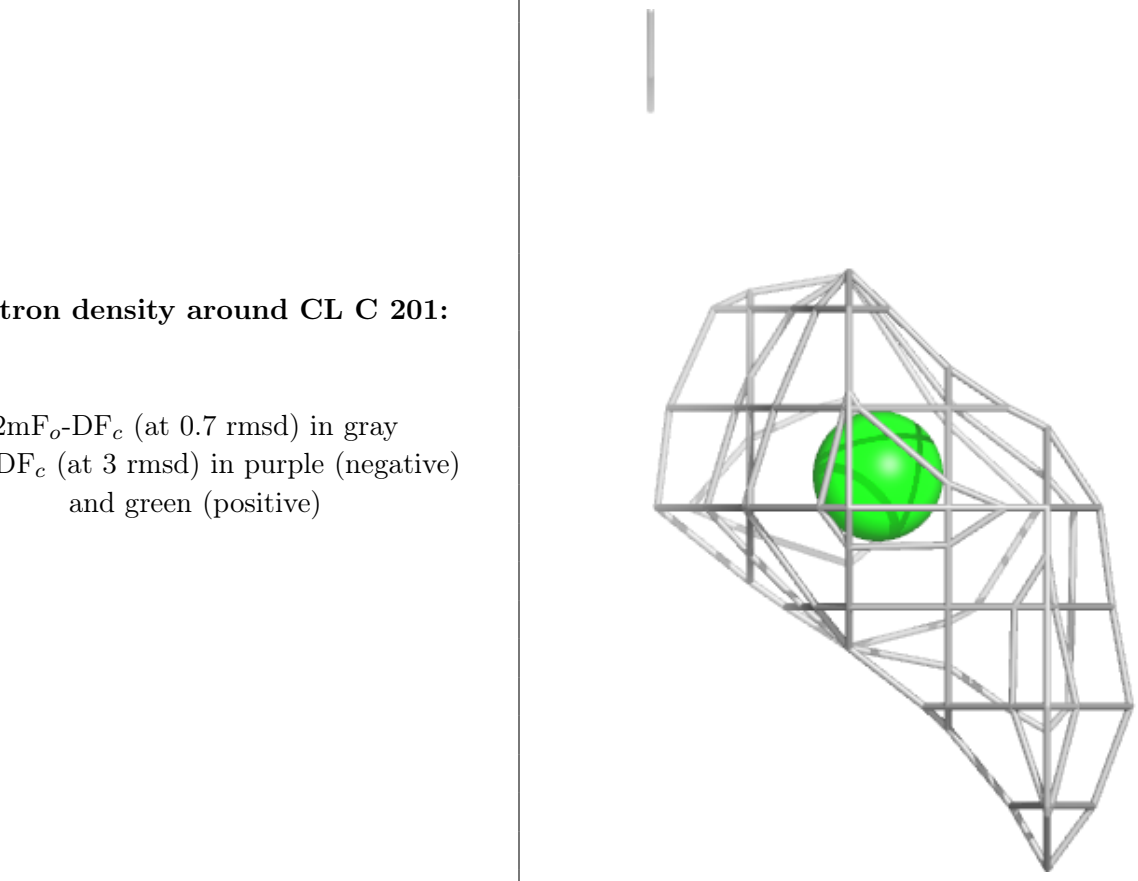


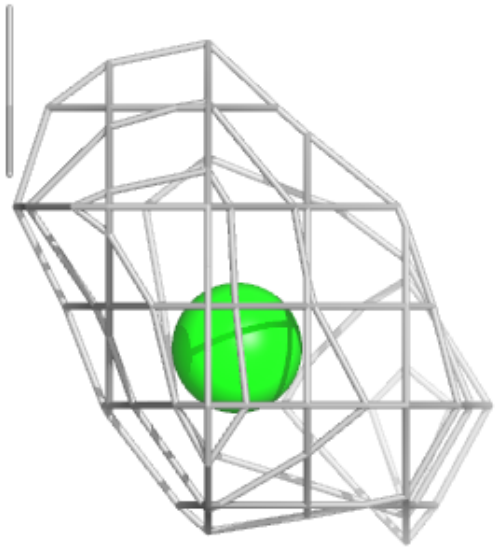


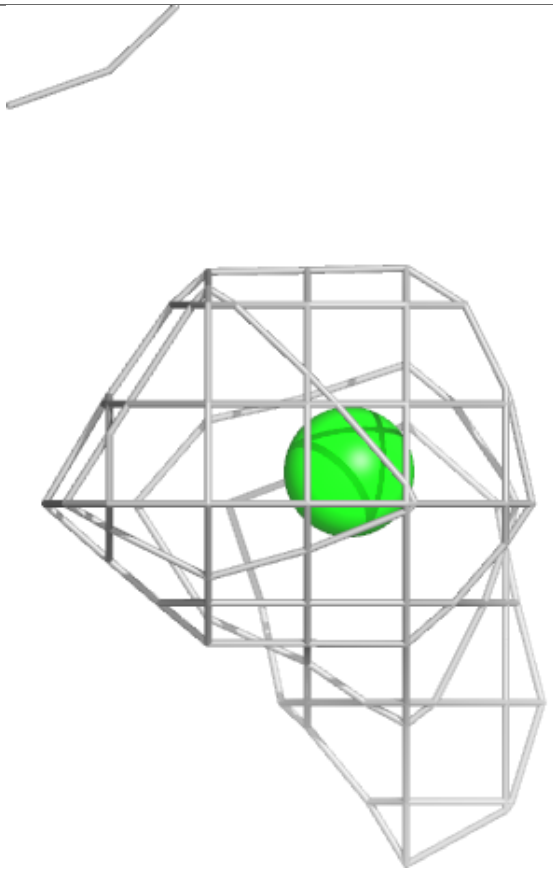


Electron density around CL C 201:

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

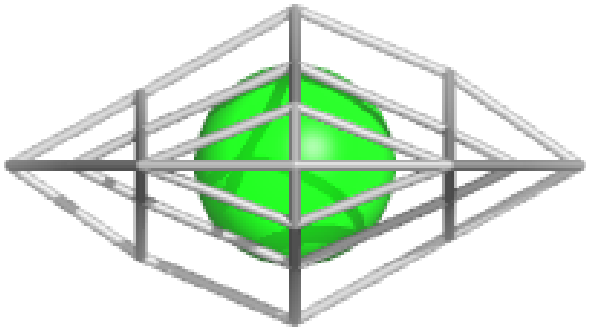


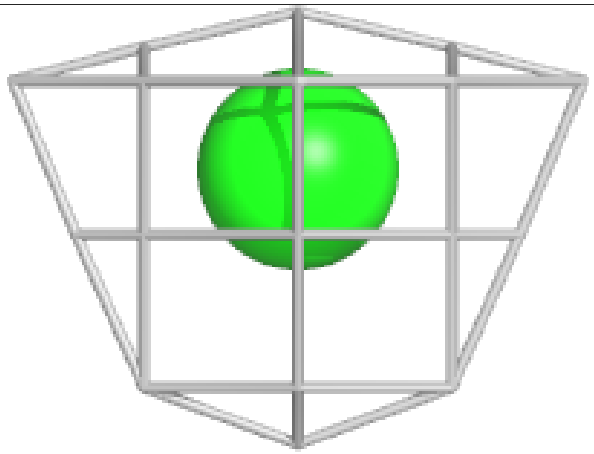


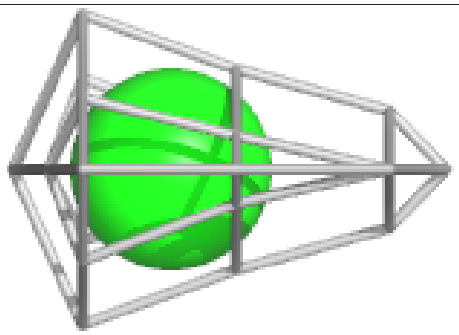


Electron density around CL D 201:

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

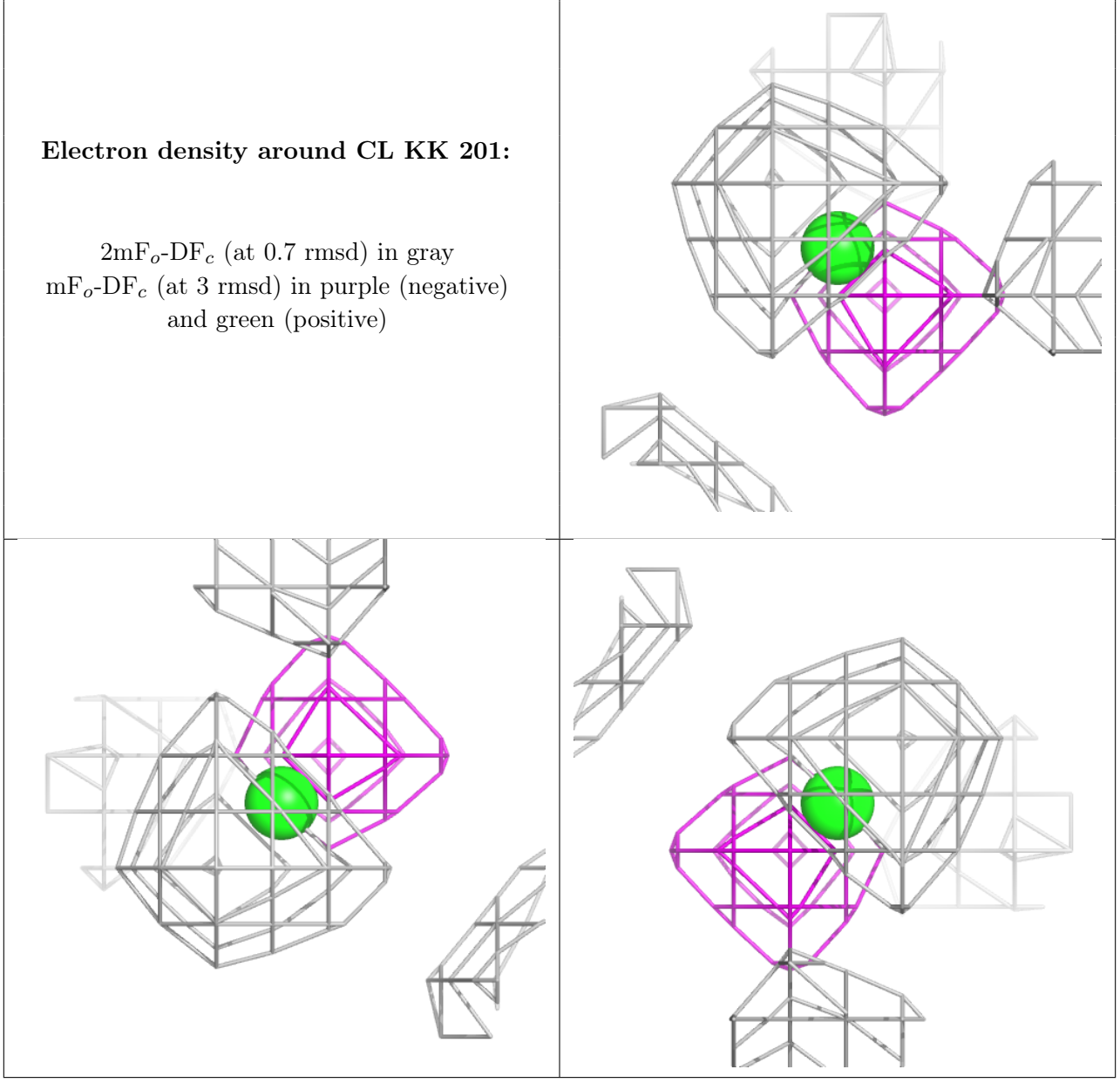






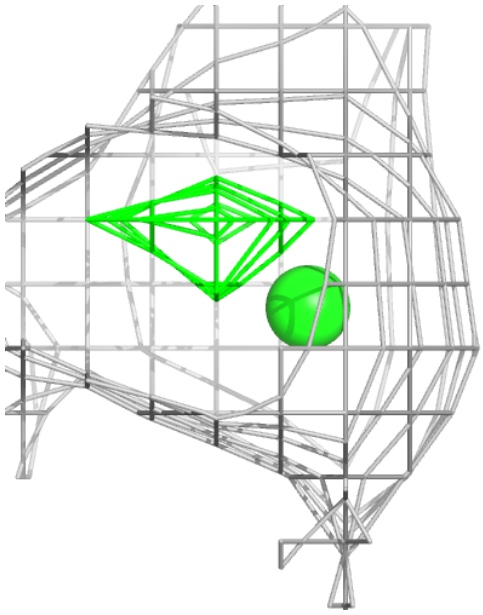
Electron density around CL KK 201:

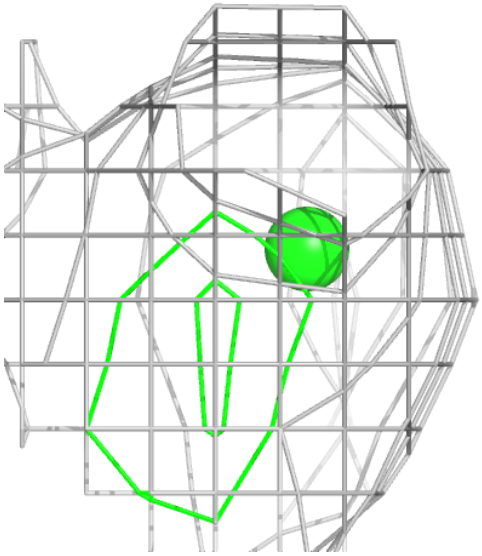
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

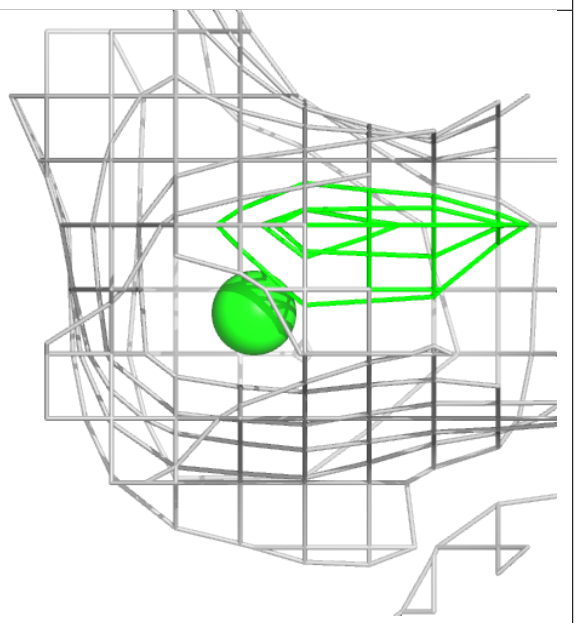


Electron density around CL qq 201:

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

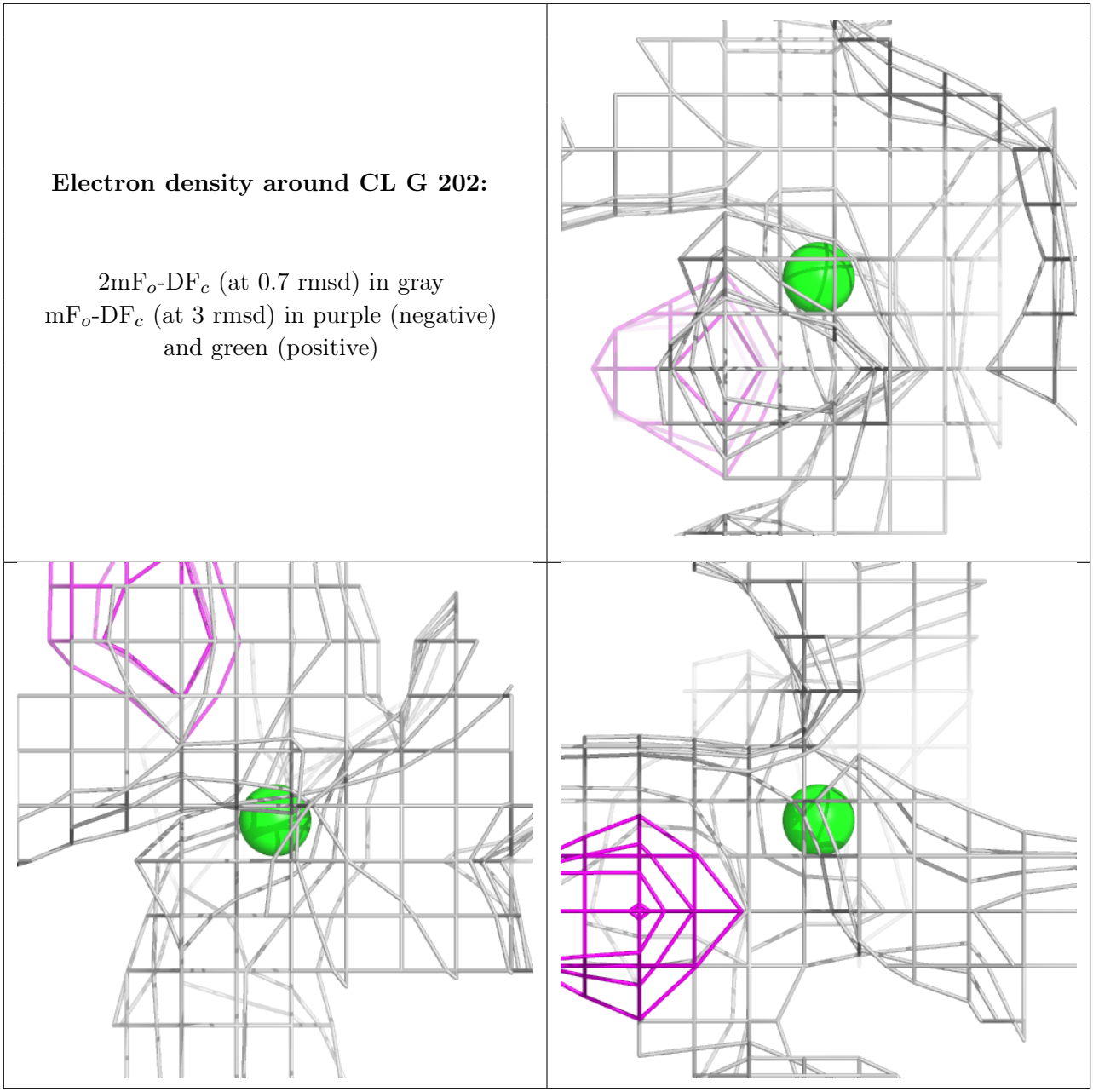






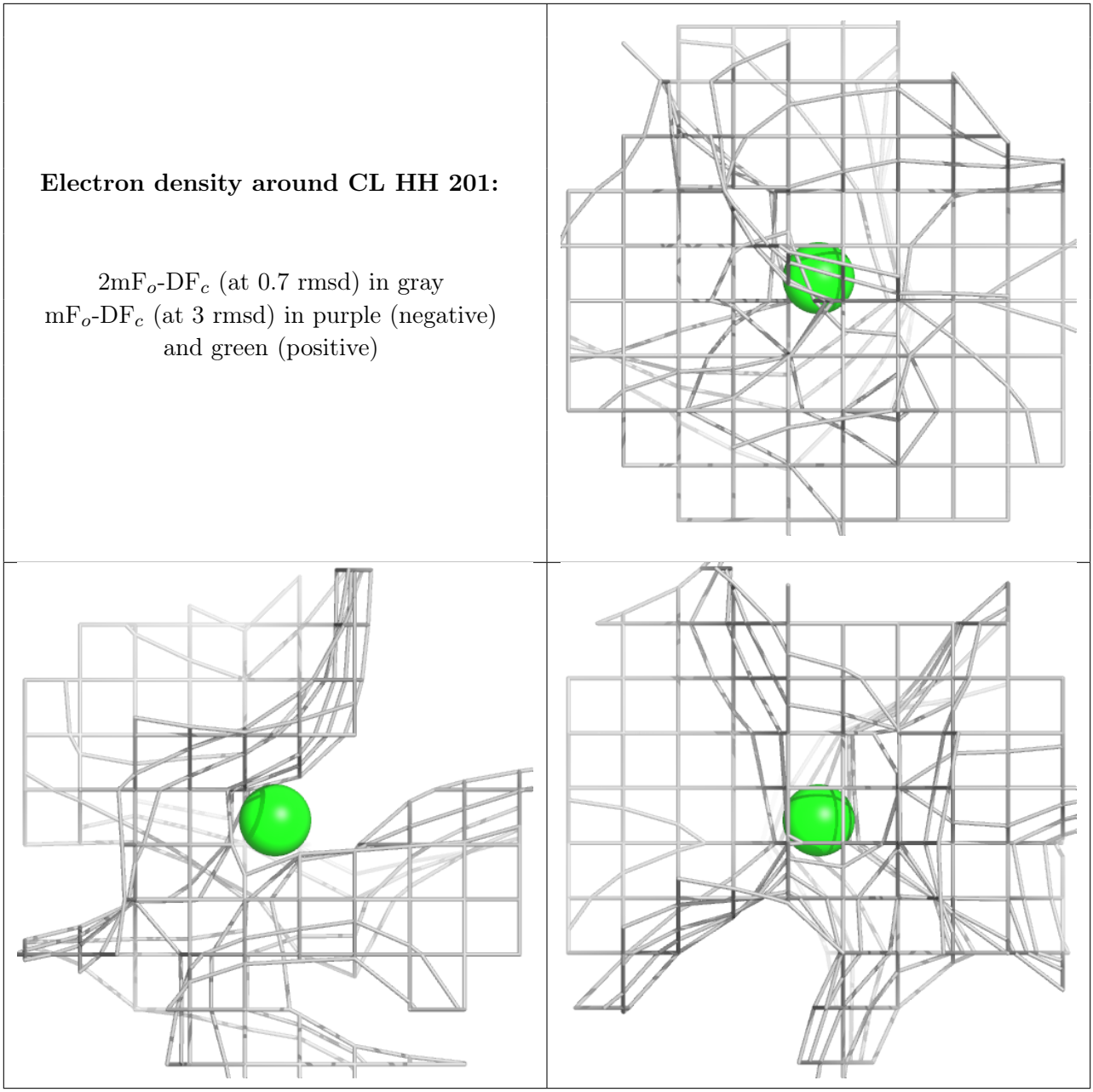
Electron density around CL G 202:

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



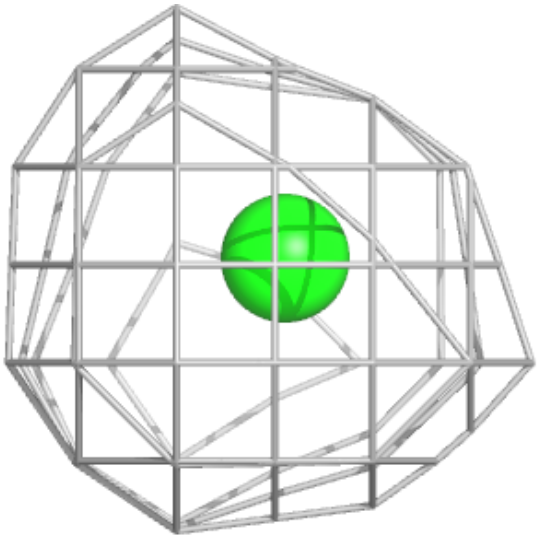
Electron density around CL HH 201:

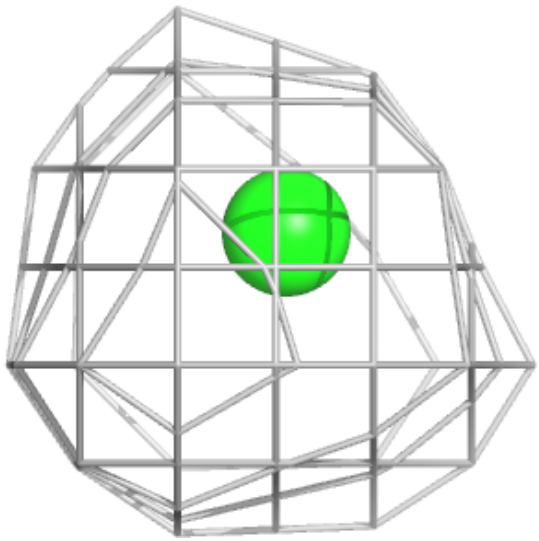
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

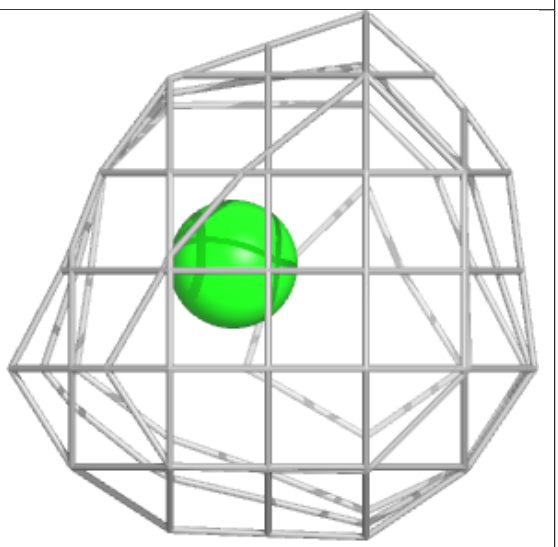


Electron density around CL M 201:

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

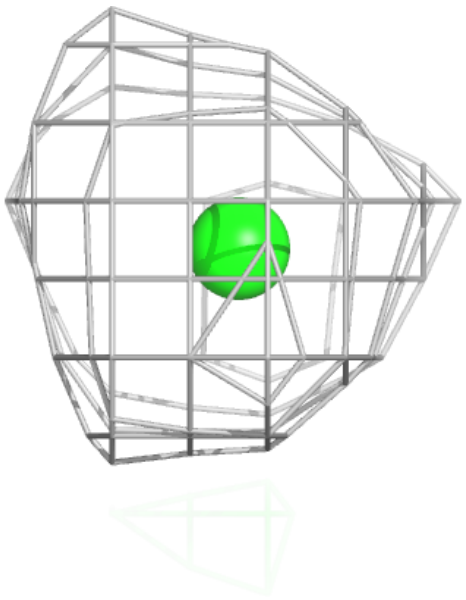


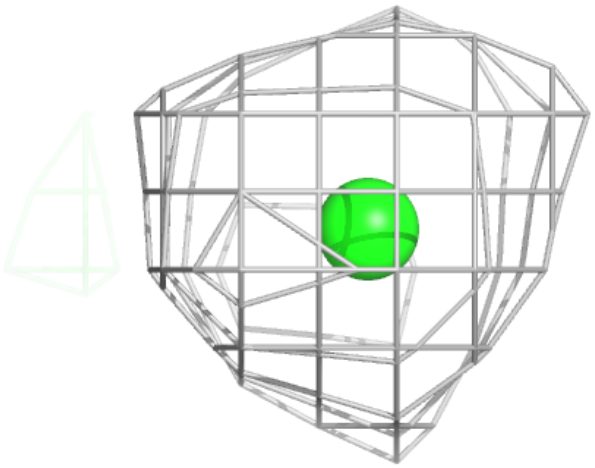


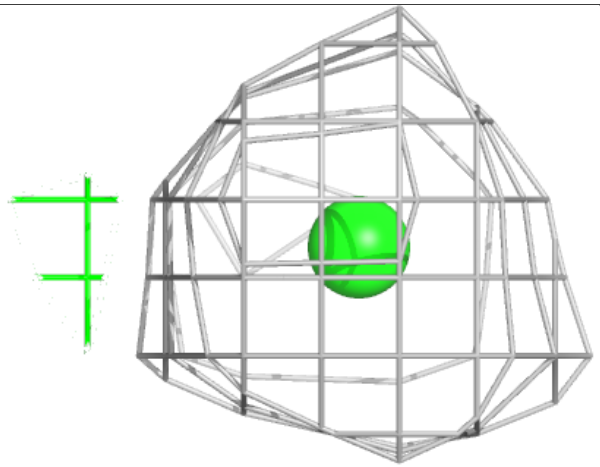


Electron density around CL bb 202:

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

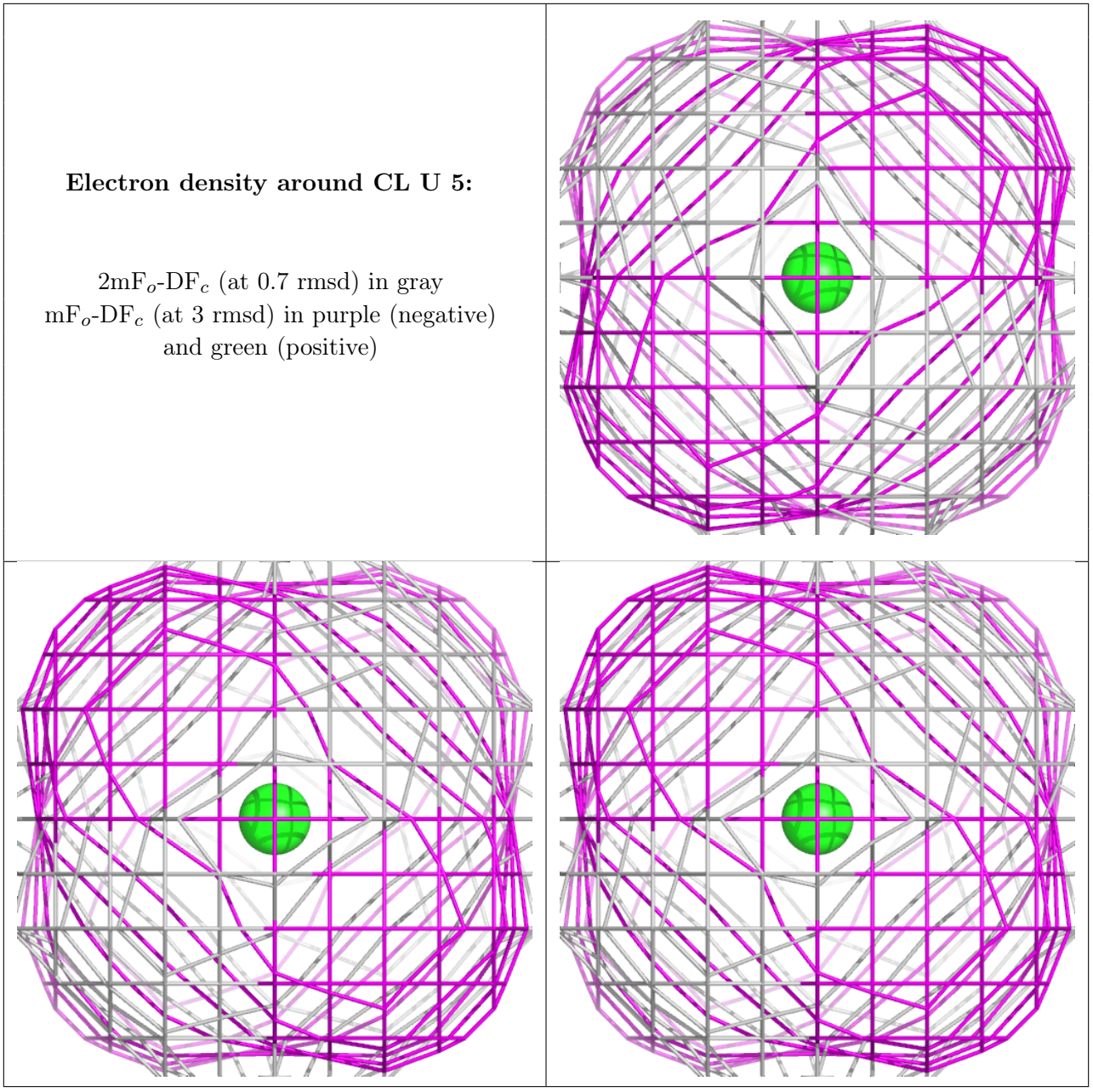






Electron density around CL U 5:

$2mF_o$-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.