wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2020 – 12:22 PM BST

PDB ID	:	5YPS
Title	:	The structural basis of histone chaperoneVps75
Authors	:	Chen, Y.; Zhang, Y.; Dou, Y.; Wang, M.; Xu, S.; Jiang, H.; Limper, A.; Su, D.
Deposited on	:	2017-11-03
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

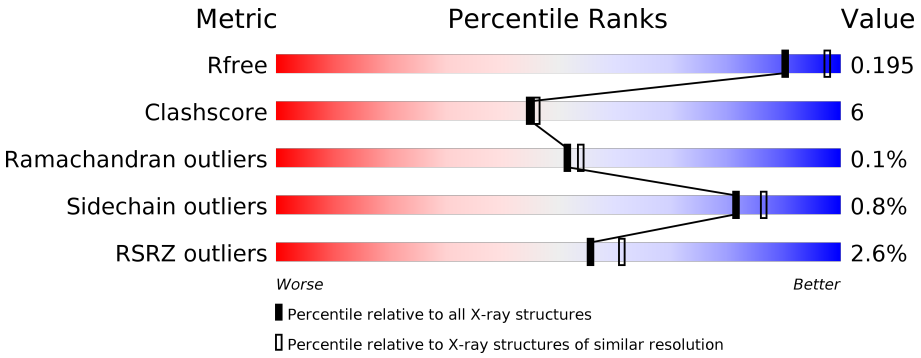
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	250	70% 10% • 19%
1	B	250	3% 73% 7% 20%
1	C	250	3% 71% 8% • 20%
1	D	250	2% 67% 13% 20%
1	E	250	3% 74% 7% 19%
1	F	250	72% 8% 20%

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
3	1PE	C	303	-	-	X	-
3	1PE	C	304	-	-	X	-
3	1PE	E	305	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10574 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 Vacuolar protein sorting-associated protein 75.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	Se	0	3	0
			1650	1061	261	324	4			
1	B	200	Total	C	N	O	Se	0	2	0
			1624	1049	256	316	3			
1	C	201	Total	C	N	O	Se	0	2	0
			1643	1060	258	322	3			
1	D	200	Total	C	N	O	Se	0	1	0
			1651	1062	259	327	3			
1	E	202	Total	C	N	O	Se	0	2	0
			1676	1077	264	331	4			
1	F	201	Total	C	N	O	Se	0	1	0
			1652	1063	260	326	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP A0A0W4ZF97
A	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
A	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
A	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97
B	1	MSE	-	initiating methionine	UNP A0A0W4ZF97
B	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
B	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
B	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97
C	1	MSE	-	initiating methionine	UNP A0A0W4ZF97
C	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
C	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
C	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97
D	1	MSE	-	initiating methionine	UNP A0A0W4ZF97
D	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
D	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
D	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97
E	1	MSE	-	initiating methionine	UNP A0A0W4ZF97

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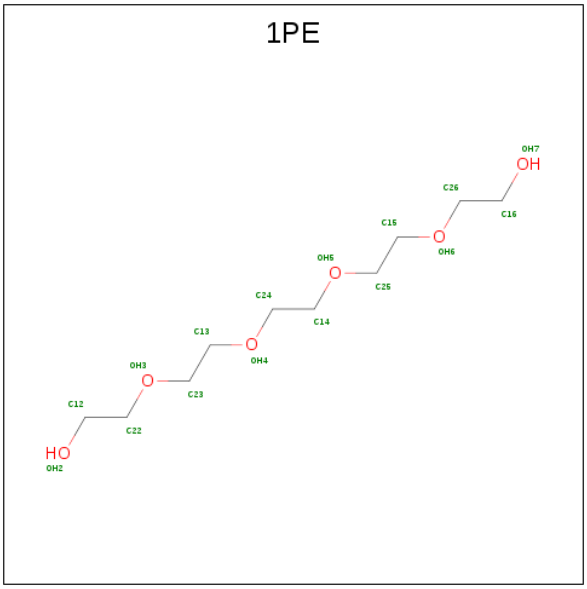
Chain	Residue	Modelled	Actual	Comment	Reference
E	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
E	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
E	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97
F	1	MSE	-	initiating methionine	UNP A0A0W4ZF97
F	56	MSE	ASN	engineered mutation	UNP A0A0W4ZF97
F	127	MSE	GLU	engineered mutation	UNP A0A0W4ZF97
F	194	GLU	GLY	engineered mutation	UNP A0A0W4ZF97

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

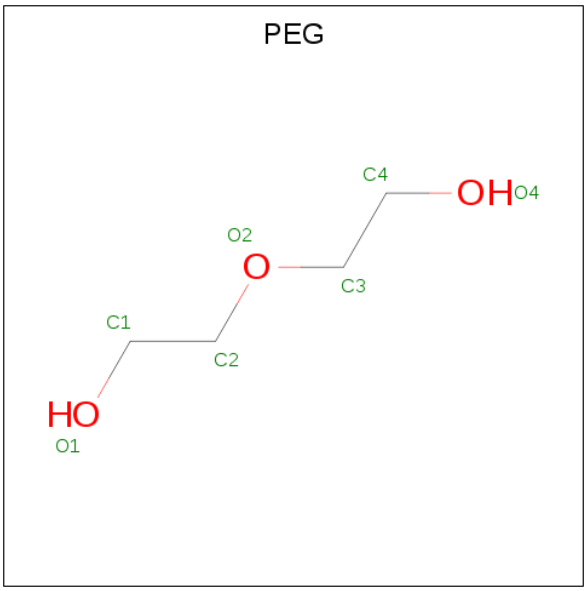
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Ca 2 2	0	0
2	E	2	Total Ca 2 2	0	0
2	B	3	Total Ca 3 3	0	0
2	C	1	Total Ca 1 1	0	0
2	A	2	Total Ca 2 2	0	0
2	F	2	Total Ca 2 2	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



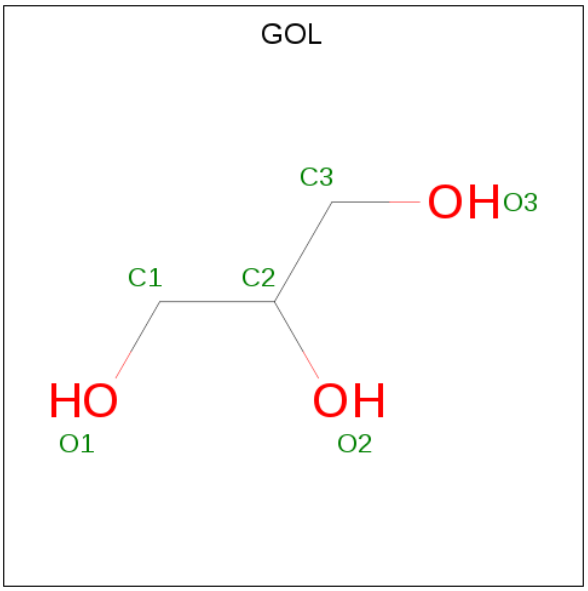
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 16 10 6	0	0
3	B	1	Total C O 16 10 6	0	0
3	B	1	Total C O 16 10 6	0	0
3	B	1	Total C O 16 10 6	0	0
3	C	1	Total C O 16 10 6	0	0
3	C	1	Total C O 16 10 6	0	0
3	C	1	Total C O 16 10 6	0	0
3	D	1	Total C O 16 10 6	0	0
3	D	1	Total C O 16 10 6	0	0
3	D	1	Total C O 16 10 6	0	0
3	E	1	Total C O 16 10 6	0	0
3	E	1	Total C O 16 10 6	0	0
3	E	1	Total C O 16 10 6	0	0
3	E	1	Total C O 16 10 6	0	0
3	F	1	Total C O 16 10 6	0	0
3	F	1	Total C O 16 10 6	0	0
3	F	1	Total C O 16 10 6	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



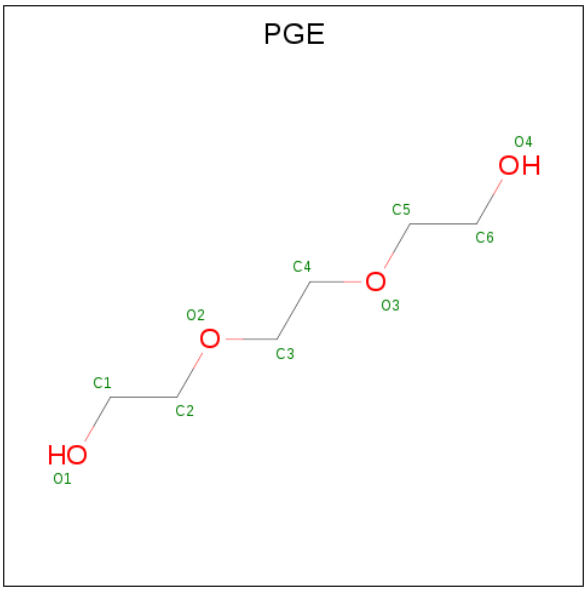
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 10 6 4	0	0

- Molecule 7 is water.

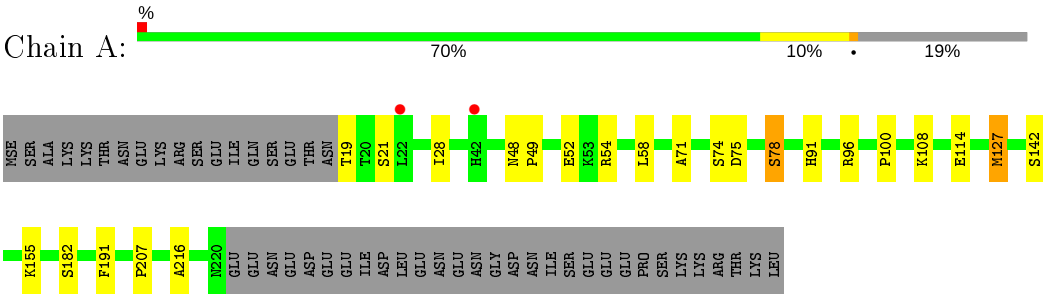
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	33	Total O 33 33	0	0
7	B	37	Total O 37 37	0	0
7	C	41	Total O 41 41	0	0
7	D	30	Total O 30 30	0	0
7	E	61	Total O 61 61	0	0
7	F	30	Total O 30 30	0	0

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.

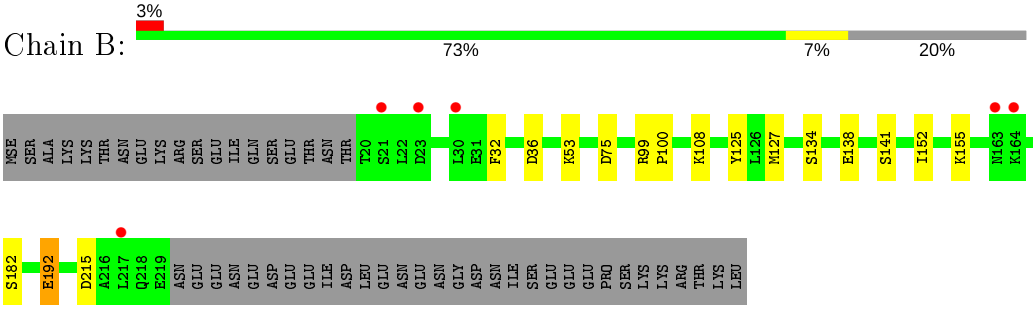
- Molecule 1: Vacuolar protein sorting-associated protein 75

Chain A:



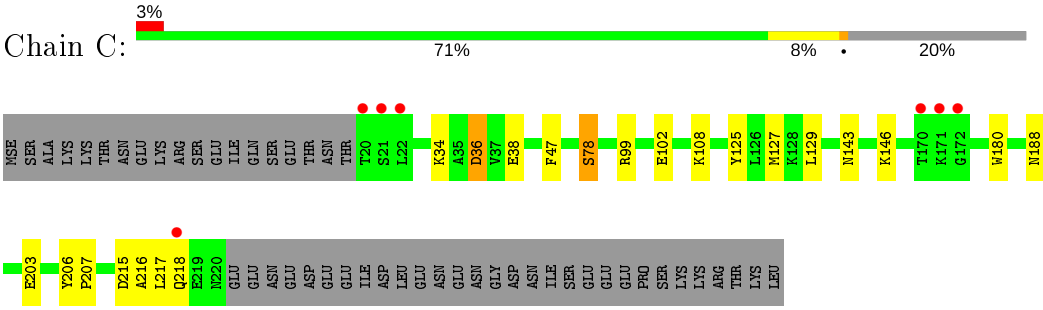
- Molecule 1: Vacuolar protein sorting-associated protein 75

Chain B:



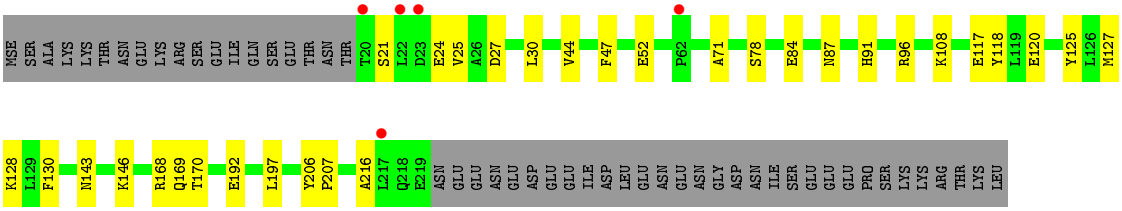
- Molecule 1: Vacuolar protein sorting-associated protein 75

Chain C:

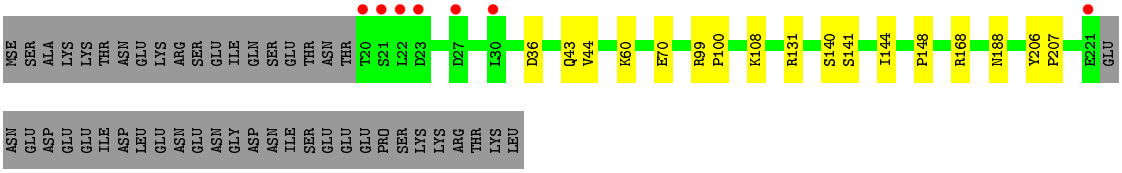


- Molecule 1: Vacuolar protein sorting-associated protein 75

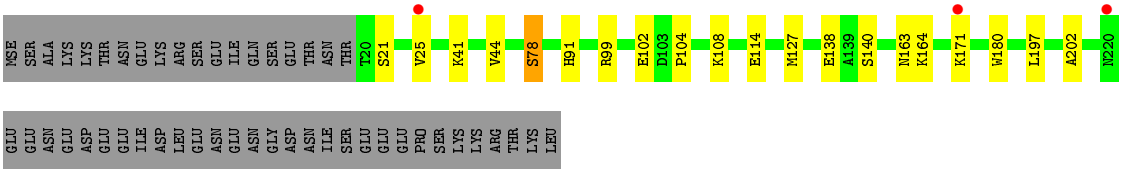
Chain D:



• Molecule 1: Vacuolar protein sorting-associated protein 75



• Molecule 1: Vacuolar protein sorting-associated protein 75



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.67Å 76.40Å 130.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.10 48.26 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.26-2.10) 99.6 (48.26-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.93 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.186 , 0.236 0.193 , 0.195	Depositor DCC
R_{free} test set	4185 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10574	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: PEG, GOL, CA, PGE, 1PE

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	0.40	0/1687	0.51	0/2291
1	B	0.46	1/1661 (0.1%)	0.53	0/2255
1	C	0.47	1/1680 (0.1%)	0.53	0/2278
1	D	0.47	0/1688	0.53	0/2288
1	E	0.48	0/1713	0.57	0/2320
1	F	0.46	0/1689	0.53	0/2290
All	All	0.46	2/10118 (0.0%)	0.53	0/13722

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	192	GLU	CB-CG	6.01	1.63	1.52
1	B	192	GLU	CB-CG	5.17	1.61	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1650	0	1555	21	0
1	B	1624	0	1543	20	0
1	C	1643	0	1563	28	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1651	0	1584	24	0
1	E	1676	0	1611	19	1
1	F	1652	0	1582	16	1
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	48	0	66	6	0
3	B	48	0	66	8	0
3	C	48	0	66	19	0
3	D	48	0	66	7	0
3	E	64	0	88	14	0
3	F	48	0	66	7	0
4	A	7	0	10	1	0
4	B	7	0	10	0	0
4	D	7	0	10	1	0
4	E	7	0	10	1	0
4	F	14	0	20	1	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	18	0	24	2	0
5	E	18	0	24	2	0
5	F	18	0	24	1	1
6	C	10	0	14	2	0
7	A	33	0	0	0	0
7	B	37	0	0	1	0
7	C	41	0	0	1	0
7	D	30	0	0	1	0
7	E	61	0	0	2	0
7	F	30	0	0	3	0
All	All	10574	0	10034	132	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 6.

The worst 5 of 132 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:B:192:GLU:OE2	7:B:401:HOH:O	1.95	0.85
1:C:192:GLU:OE2	7:C:401:HOH:O	1.96	0.83
1:C:99:ARG:HE	3:C:303:1PE:H142	1.41	0.83
1:B:99:ARG:HE	3:B:305:1PE:H232	1.46	0.80
1:C:108:LYS:HE2	3:C:304:1PE:H251	1.68	0.76

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:E:70:GLU:OE2	5:F:309:GOL:O2[2_565]	2.14	0.06
1:C:102:GLU:OE2	1:F:171:LYS:NZ[4_455]	2.16	0.04

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	203/250 (81%)	197 (97%)	6 (3%)	0	100	100
1	B	200/250 (80%)	191 (96%)	9 (4%)	0	100	100
1	C	201/250 (80%)	195 (97%)	5 (2%)	1 (0%)	29	26
1	D	199/250 (80%)	192 (96%)	7 (4%)	0	100	100
1	E	202/250 (81%)	197 (98%)	5 (2%)	0	100	100
1	F	200/250 (80%)	192 (96%)	8 (4%)	0	100	100
All	All	1205/1500 (80%)	1164 (97%)	40 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	217	LEU

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	176/228 (77%)	173 (98%)	3 (2%)	60	67
1	B	173/228 (76%)	173 (100%)	0	100	100
1	C	176/228 (77%)	173 (98%)	3 (2%)	60	67
1	D	181/228 (79%)	180 (99%)	1 (1%)	86	90
1	E	184/228 (81%)	183 (100%)	1 (0%)	88	92
1	F	180/228 (79%)	179 (99%)	1 (1%)	86	90
All	All	1070/1368 (78%)	1061 (99%)	9 (1%)	81	86

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	78	SER
1	F	78	SER
1	D	78	SER
1	A	127[B]	MSE
1	C	215	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	E	43	GLN
1	E	48	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 51 ligands modelled in this entry, 12 are monoatomic - leaving 39 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	$\#\|Z\| > 2$
3	1PE	A	303	-	15,15,15	0.74	0	14,14,14	0.36	0
3	1PE	C	303	-	15,15,15	0.78	0	14,14,14	0.31	0
4	PEG	B	307	-	6,6,6	0.55	0	5,5,5	0.30	0
3	1PE	F	304	-	15,15,15	0.75	0	14,14,14	0.30	0
4	PEG	A	306	-	6,6,6	0.58	0	5,5,5	0.29	0
4	PEG	E	307	-	6,6,6	0.56	0	5,5,5	0.23	0
5	GOL	A	307	-	5,5,5	0.39	0	5,5,5	0.21	0
3	1PE	F	303	-	15,15,15	0.77	0	14,14,14	0.25	0
3	1PE	E	306	-	15,15,15	0.73	0	14,14,14	0.31	0
5	GOL	D	308	-	5,5,5	0.36	0	5,5,5	0.26	0
5	GOL	F	308	-	5,5,5	0.31	0	5,5,5	0.98	0
4	PEG	D	306	-	6,6,6	0.54	0	5,5,5	0.29	0
3	1PE	B	305	-	15,15,15	0.81	0	14,14,14	0.25	0
5	GOL	B	308	-	5,5,5	0.34	0	5,5,5	0.27	0
3	1PE	E	304	-	15,15,15	0.73	0	14,14,14	0.38	0
3	1PE	B	304	-	15,15,15	0.74	0	14,14,14	0.41	0
5	GOL	E	308	-	5,5,5	0.35	0	5,5,5	0.33	0
3	1PE	E	305	-	15,15,15	0.76	0	14,14,14	0.27	0
3	1PE	C	302	-	15,15,15	0.78	0	14,14,14	0.29	0
3	1PE	B	306	-	15,15,15	0.75	0	14,14,14	0.27	0
5	GOL	D	307	-	5,5,5	0.34	0	5,5,5	0.42	0
3	1PE	F	305	-	15,15,15	0.74	0	14,14,14	0.38	0
6	PGE	C	306	-	9,9,9	0.31	0	8,8,8	0.43	0
5	GOL	E	309	-	5,5,5	0.33	0	5,5,5	0.31	0
3	1PE	C	304	-	15,15,15	0.76	0	14,14,14	0.27	0
4	PEG	F	306	-	6,6,6	0.54	0	5,5,5	0.30	0
3	1PE	A	304	-	15,15,15	0.78	0	14,14,14	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	D	309	-	5,5,5	0.35	0	5,5,5	0.35	0
5	GOL	F	309	-	5,5,5	0.45	0	5,5,5	0.22	0
3	1PE	D	303	-	15,15,15	0.69	0	14,14,14	0.39	0
5	GOL	F	310	-	5,5,5	0.39	0	5,5,5	0.26	0
5	GOL	A	308	-	5,5,5	0.35	0	5,5,5	0.39	0
5	GOL	E	310	-	5,5,5	0.37	0	5,5,5	0.34	0
3	1PE	D	305	-	15,15,15	0.75	0	14,14,14	0.41	0
4	PEG	F	307	-	6,6,6	0.52	0	5,5,5	0.50	0
3	1PE	E	303	-	15,15,15	0.74	0	14,14,14	0.38	0
3	1PE	D	304	-	15,15,15	0.74	0	14,14,14	0.38	0
5	GOL	C	305	-	5,5,5	0.45	0	5,5,5	0.18	0
3	1PE	A	305	-	15,15,15	0.76	0	14,14,14	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	303	-	-	8/13/13/13	-
3	1PE	C	303	-	-	9/13/13/13	-
4	PEG	B	307	-	-	2/4/4/4	-
3	1PE	F	304	-	-	9/13/13/13	-
4	PEG	A	306	-	-	1/4/4/4	-
4	PEG	E	307	-	-	1/4/4/4	-
5	GOL	A	307	-	-	2/4/4/4	-
3	1PE	F	303	-	-	10/13/13/13	-
3	1PE	E	306	-	-	3/13/13/13	-
5	GOL	D	308	-	-	2/4/4/4	-
5	GOL	F	308	-	-	4/4/4/4	-
4	PEG	D	306	-	-	3/4/4/4	-
3	1PE	B	305	-	-	7/13/13/13	-
5	GOL	B	308	-	-	1/4/4/4	-
3	1PE	E	304	-	-	8/13/13/13	-
3	1PE	B	304	-	-	10/13/13/13	-
5	GOL	E	308	-	-	2/4/4/4	-
3	1PE	E	305	-	-	9/13/13/13	-
3	1PE	C	302	-	-	4/13/13/13	-
3	1PE	B	306	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	307	-	-	4/4/4/4	-
3	1PE	F	305	-	-	6/13/13/13	-
6	PGE	C	306	-	-	2/7/7/7	-
5	GOL	E	309	-	-	0/4/4/4	-
3	1PE	C	304	-	-	10/13/13/13	-
4	PEG	F	306	-	-	2/4/4/4	-
3	1PE	A	304	-	-	8/13/13/13	-
5	GOL	D	309	-	-	0/4/4/4	-
5	GOL	F	309	-	-	2/4/4/4	-
3	1PE	D	303	-	-	6/13/13/13	-
5	GOL	F	310	-	-	2/4/4/4	-
5	GOL	A	308	-	-	4/4/4/4	-
5	GOL	E	310	-	-	2/4/4/4	-
3	1PE	D	305	-	-	7/13/13/13	-
4	PEG	F	307	-	-	1/4/4/4	-
3	1PE	E	303	-	-	5/13/13/13	-
3	1PE	D	304	-	-	4/13/13/13	-
5	GOL	C	305	-	-	2/4/4/4	-
3	1PE	A	305	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 178 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	308	GOL	C1-C2-C3-O3
5	C	305	GOL	C1-C2-C3-O3
5	D	307	GOL	O1-C1-C2-C3
5	D	307	GOL	C1-C2-C3-O3
5	F	309	GOL	O1-C1-C2-O2

There are no ring outliers.

29 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	1PE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	303	1PE	7	0
3	F	304	1PE	3	0
4	A	306	PEG	1	0
4	E	307	PEG	1	0
3	F	303	1PE	1	0
3	E	306	1PE	1	0
5	D	308	GOL	1	0
5	F	308	GOL	1	0
4	D	306	PEG	1	0
3	B	305	1PE	2	0
3	E	304	1PE	2	0
3	B	304	1PE	5	0
3	E	305	1PE	8	0
3	C	302	1PE	4	0
3	B	306	1PE	1	0
5	D	307	GOL	2	0
3	F	305	1PE	3	0
6	C	306	PGE	2	0
5	E	309	GOL	1	0
3	C	304	1PE	8	0
3	A	304	1PE	3	0
5	F	309	GOL	0	1
3	D	303	1PE	2	0
5	E	310	GOL	1	0
3	D	305	1PE	2	0
4	F	307	PEG	1	0
3	E	303	1PE	3	0
3	D	304	1PE	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	200/250 (80%)	-0.04	2 (1%)	82	85	28, 44, 69, 105	0
1	B	198/250 (79%)	-0.01	7 (3%)	44	50	25, 44, 82, 114	0
1	C	199/250 (79%)	0.05	7 (3%)	44	50	25, 42, 84, 108	0
1	D	198/250 (79%)	0.11	5 (2%)	57	62	29, 46, 76, 110	0
1	E	200/250 (80%)	0.08	7 (3%)	44	50	23, 39, 79, 119	0
1	F	199/250 (79%)	0.10	3 (1%)	73	77	27, 46, 76, 108	0
All	All	1194/1500 (79%)	0.05	31 (2%)	56	61	23, 44, 77, 119	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	THR	5.8
1	E	20	THR	4.8
1	D	23	ASP	4.2
1	C	171	LYS	4.1
1	B	163	ASN	4.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (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
5	GOL	B	308	6/6	0.38	0.26	85,96,98,100	0
4	PEG	E	307	7/7	0.54	0.24	64,73,77,78	0
3	1PE	B	306	16/16	0.57	0.18	91,98,109,109	0
5	GOL	E	309	6/6	0.69	0.24	71,73,77,77	0
3	1PE	E	306	16/16	0.70	0.30	78,95,99,101	0
5	GOL	F	308	6/6	0.70	0.27	53,58,65,67	0
3	1PE	E	305	16/16	0.72	0.26	47,79,93,95	0
5	GOL	D	309	6/6	0.72	0.15	71,78,79,80	0
4	PEG	B	307	7/7	0.73	0.18	64,68,75,77	0
3	1PE	C	303	16/16	0.73	0.31	50,69,81,81	0
3	1PE	D	305	16/16	0.73	0.21	49,85,99,100	0
6	PGE	C	306	10/10	0.74	0.18	67,76,78,83	0
5	GOL	A	308	6/6	0.75	0.18	67,79,81,81	0
5	GOL	E	308	6/6	0.76	0.14	82,86,88,91	0
3	1PE	F	305	16/16	0.76	0.26	65,80,102,103	0
5	GOL	C	305	6/6	0.76	0.36	50,59,66,67	0
3	1PE	A	305	16/16	0.76	0.34	83,90,106,106	0
3	1PE	B	305	16/16	0.78	0.20	53,73,90,91	0
3	1PE	F	303	16/16	0.78	0.30	75,94,126,127	0
3	1PE	C	304	16/16	0.79	0.18	66,73,91,97	0
3	1PE	C	302	16/16	0.79	0.20	54,75,87,88	0
4	PEG	A	306	7/7	0.80	0.27	62,79,81,81	0
3	1PE	E	304	16/16	0.80	0.20	59,84,91,94	0
3	1PE	A	304	16/16	0.80	0.20	56,69,81,84	0
3	1PE	B	304	16/16	0.81	0.16	45,67,82,83	0
5	GOL	F	310	6/6	0.81	0.18	44,80,82,88	0
5	GOL	D	308	6/6	0.81	0.17	72,91,94,96	0
4	PEG	F	307	7/7	0.83	0.19	61,64,70,73	0
3	1PE	A	303	16/16	0.84	0.18	41,65,74,76	0
5	GOL	F	309	6/6	0.85	0.17	54,62,80,81	0
3	1PE	E	303	16/16	0.86	0.13	51,64,80,83	0
5	GOL	A	307	6/6	0.87	0.18	62,73,80,85	0
4	PEG	D	306	7/7	0.87	0.19	47,65,76,79	0
3	1PE	F	304	16/16	0.88	0.20	55,71,87,87	0
3	1PE	D	303	16/16	0.88	0.19	38,70,87,89	0
5	GOL	D	307	6/6	0.88	0.17	55,83,90,92	0
4	PEG	F	306	7/7	0.89	0.14	67,71,78,81	0

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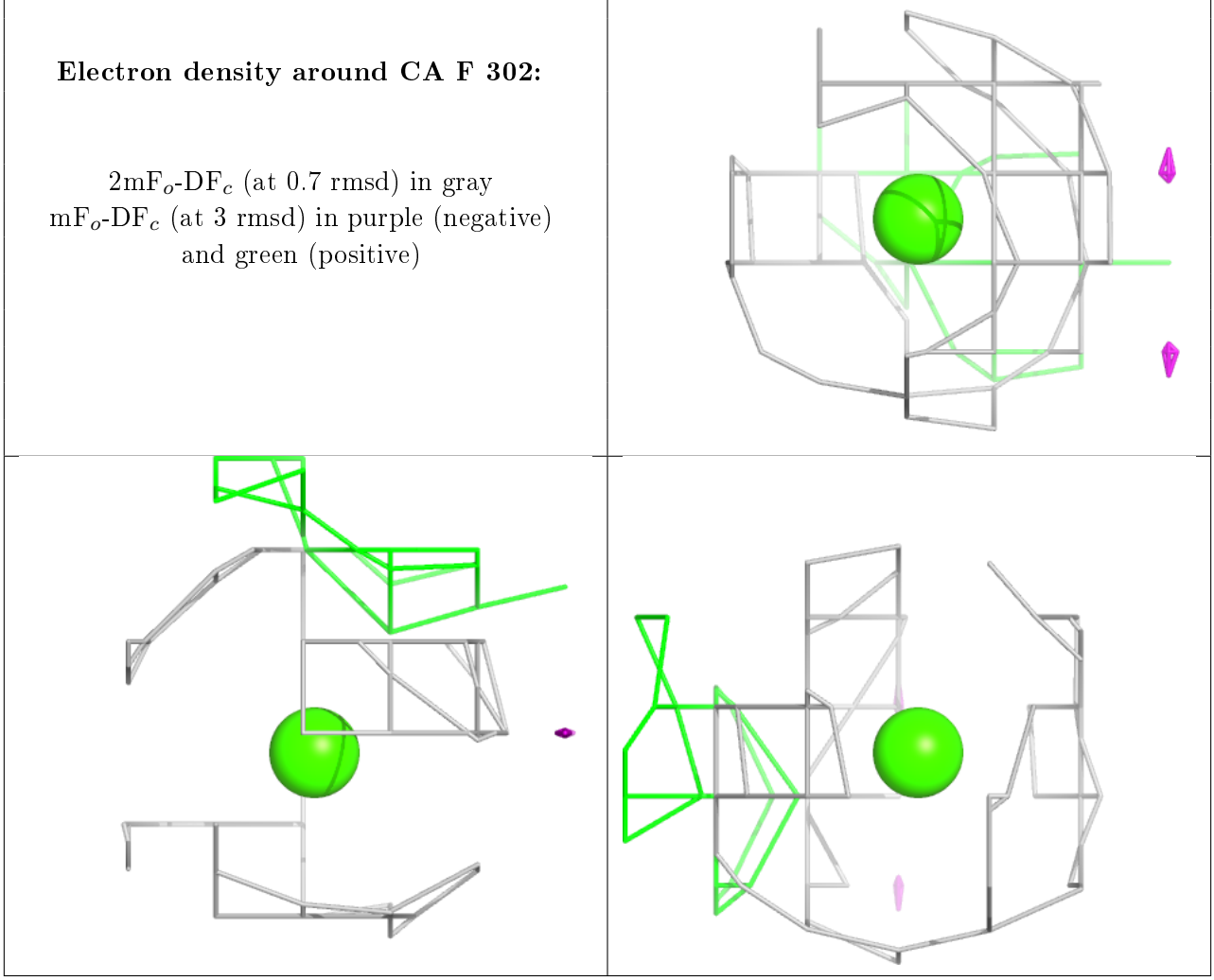
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	1PE	D	304	16/16	0.89	0.17	57,63,89,90	0
5	GOL	E	310	6/6	0.90	0.39	81,83,84,86	0
2	CA	F	302	1/1	0.96	0.18	32,32,32,32	0
2	CA	B	303	1/1	0.96	0.14	32,32,32,32	0
2	CA	A	302	1/1	0.97	0.18	30,30,30,30	0
2	CA	A	301	1/1	0.97	0.19	31,31,31,31	0
2	CA	D	301	1/1	0.97	0.17	30,30,30,30	0
2	CA	C	301	1/1	0.97	0.16	31,31,31,31	0
2	CA	E	302	1/1	0.98	0.18	28,28,28,28	0
2	CA	F	301	1/1	0.98	0.12	27,27,27,27	0
2	CA	B	302	1/1	0.99	0.15	30,30,30,30	0
2	CA	B	301	1/1	0.99	0.14	29,29,29,29	0
2	CA	D	302	1/1	0.99	0.17	32,32,32,32	0
2	CA	E	301	1/1	1.00	0.19	25,25,25,25	0

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

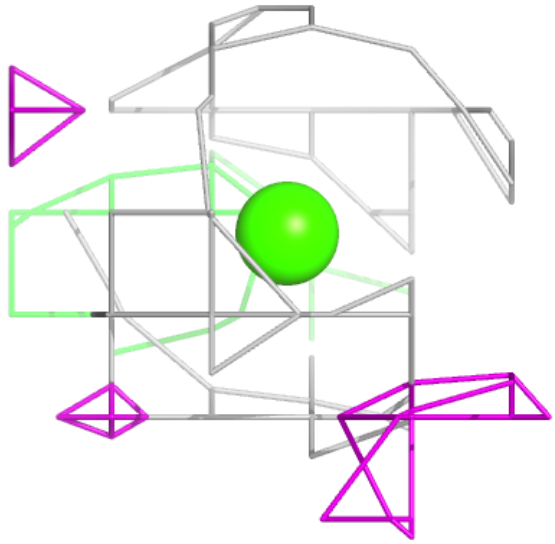
Electron density around CA F 302:

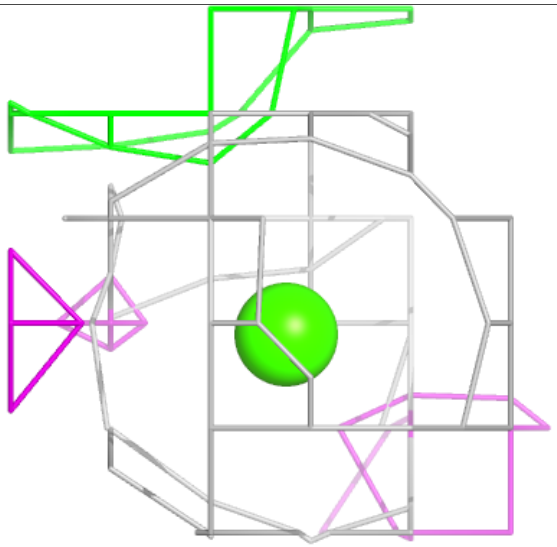
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

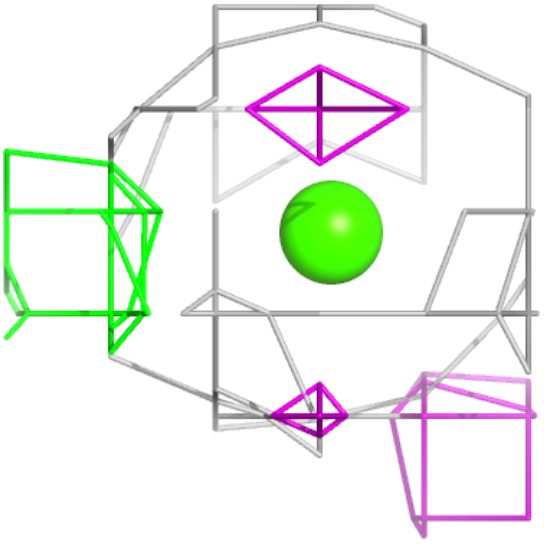


Electron density around CA B 303:

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

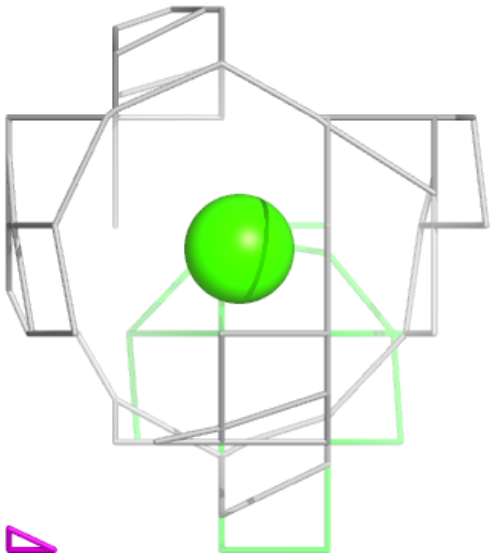


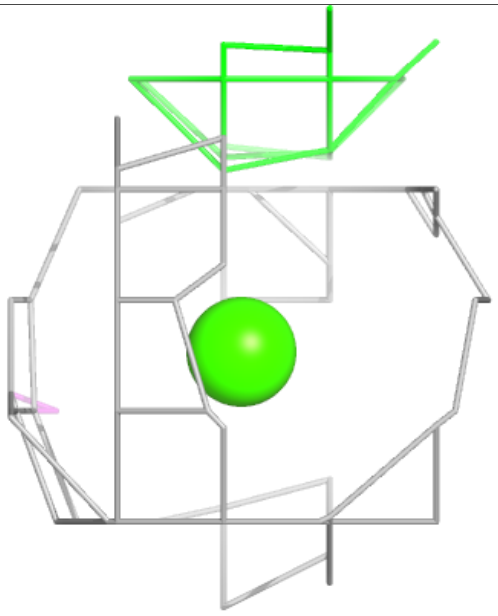


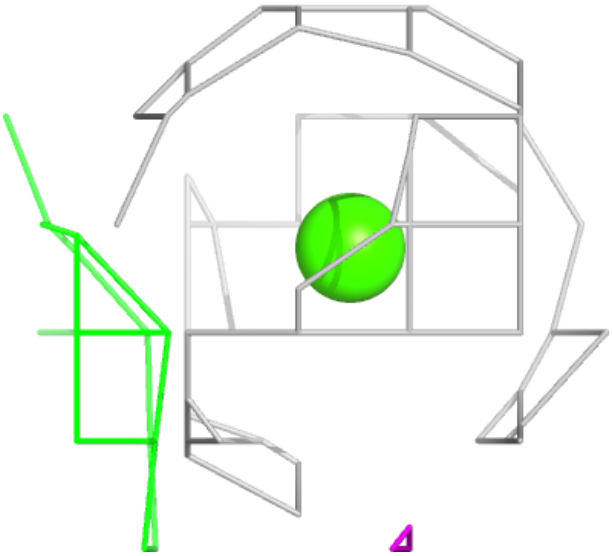


Electron density around CA A 302:

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

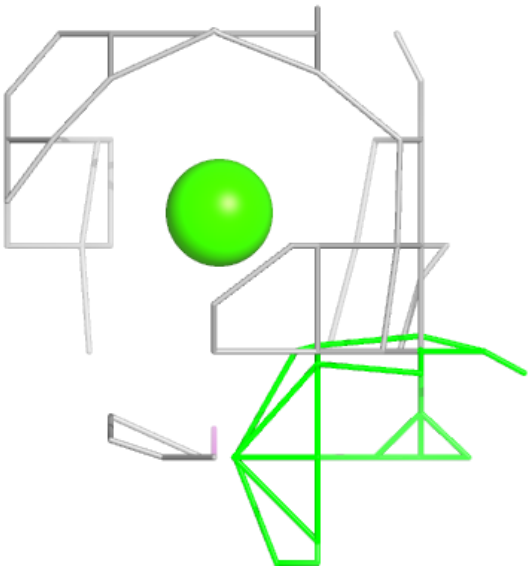


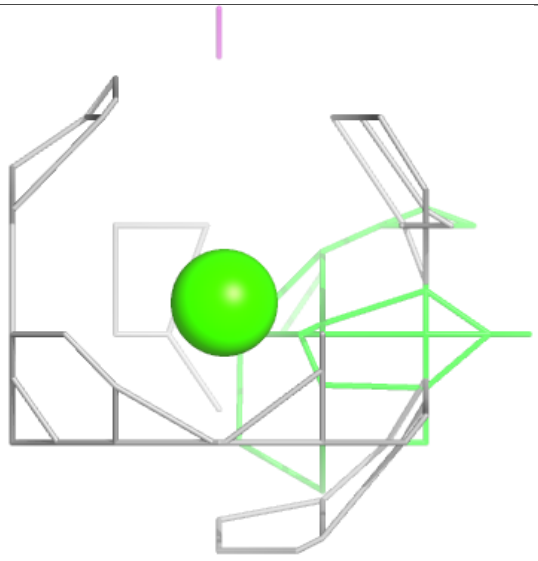


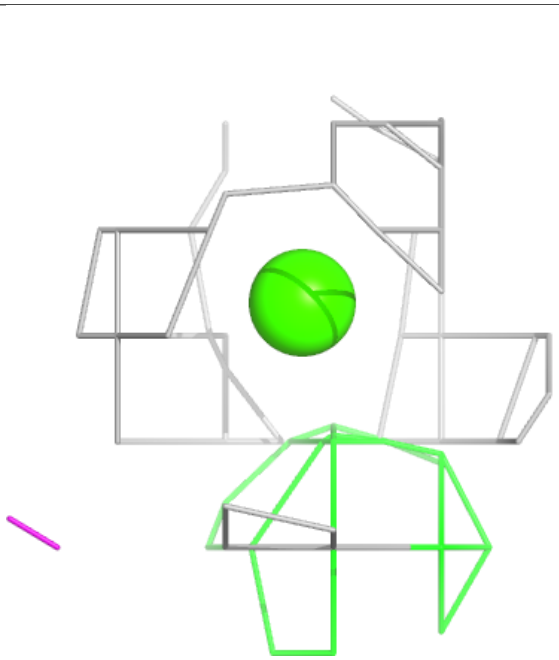


Electron density around CA A 301:

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

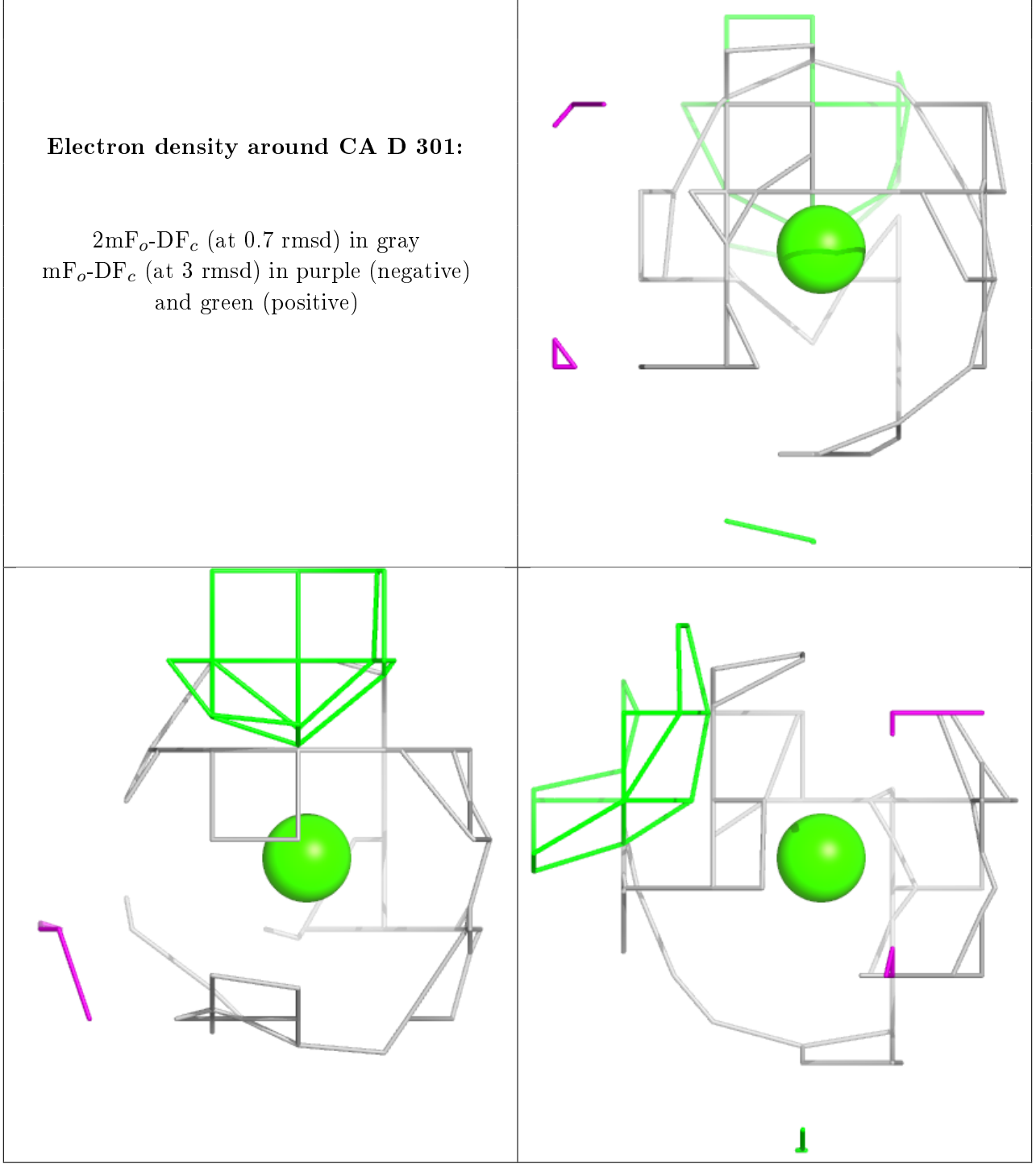






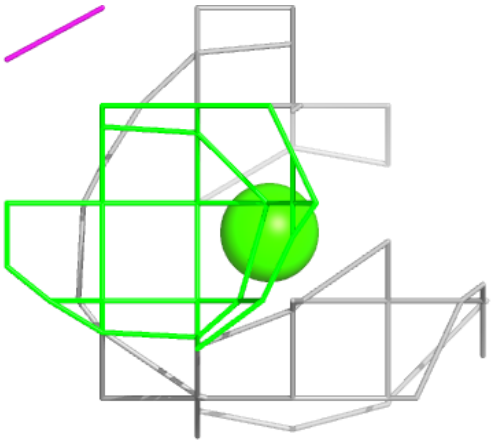
Electron density around CA D 301:

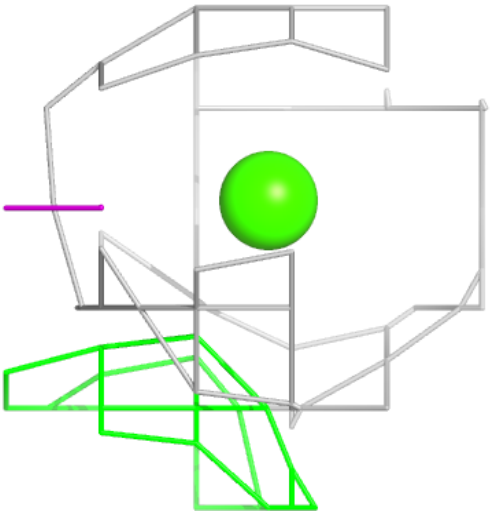
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

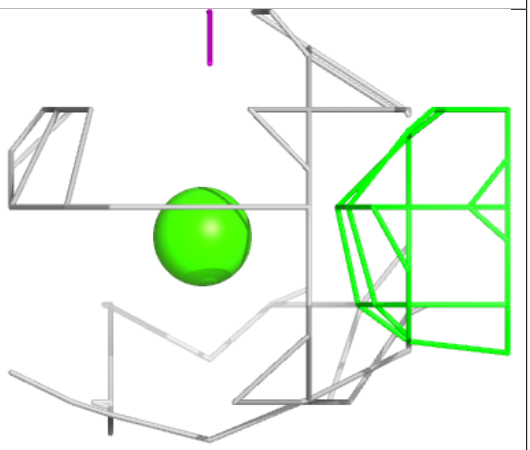


Electron density around CA C 301:

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

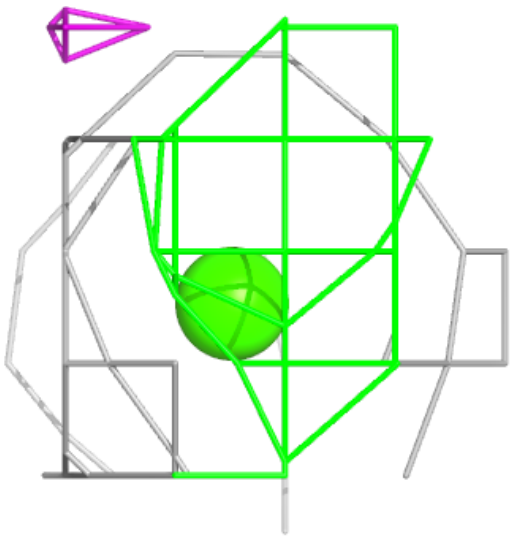


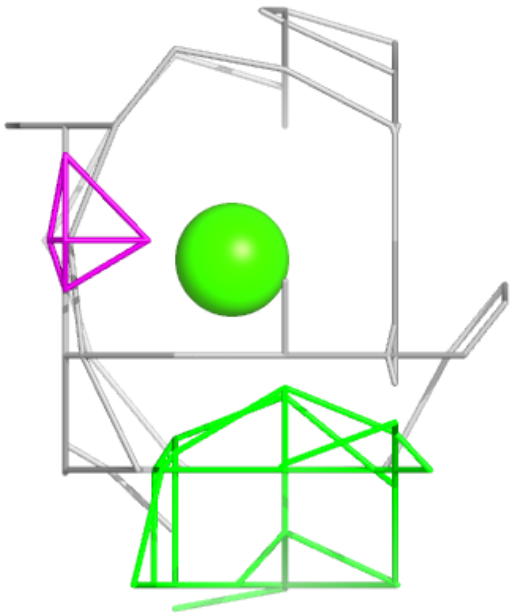


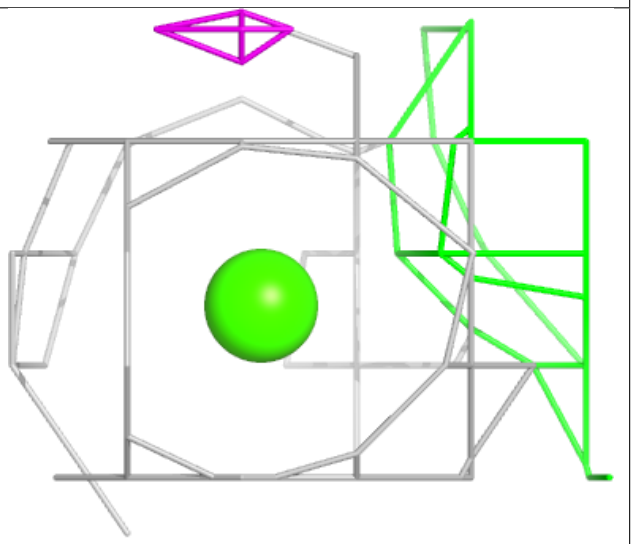


Electron density around CA E 302:

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

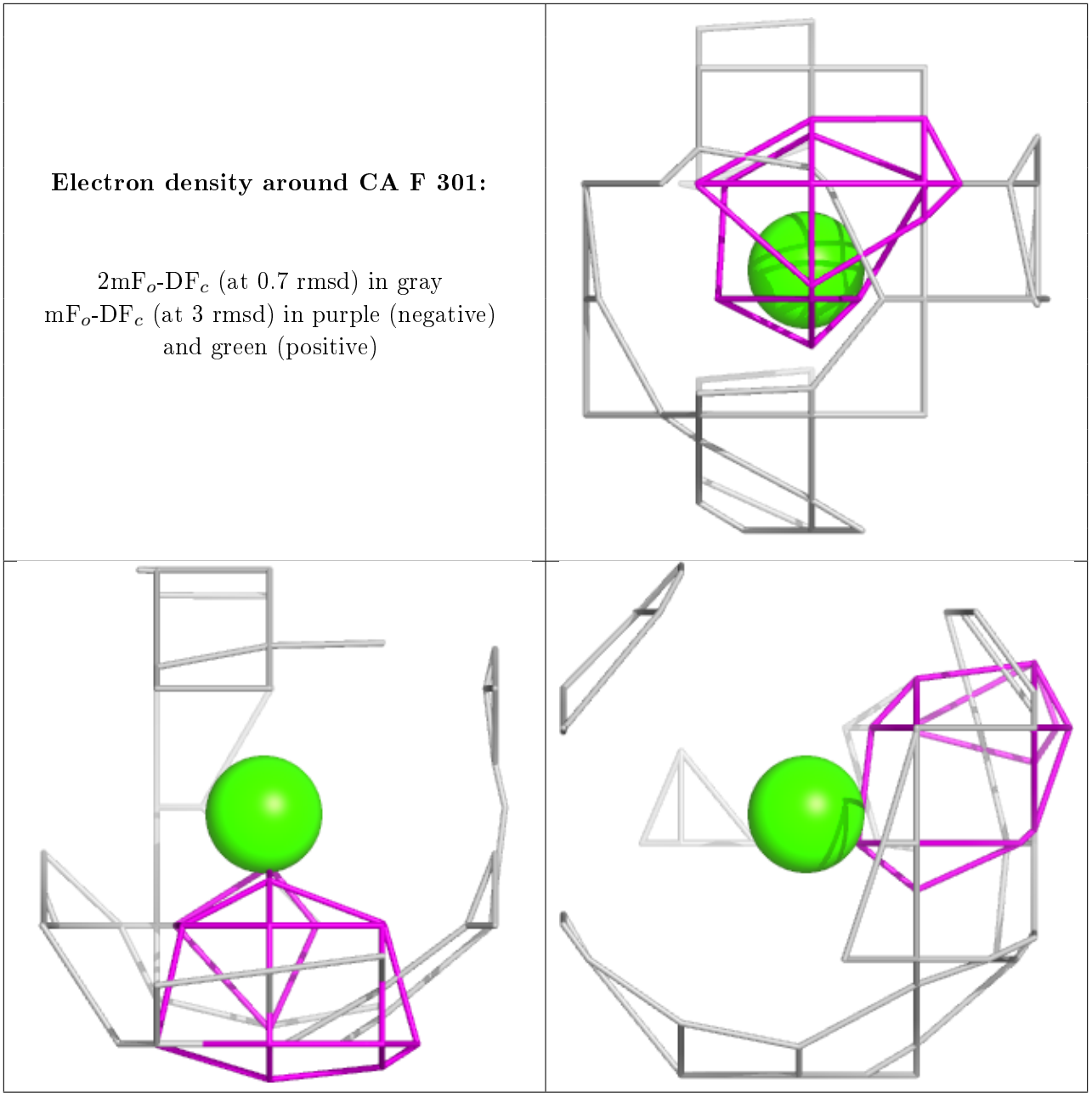






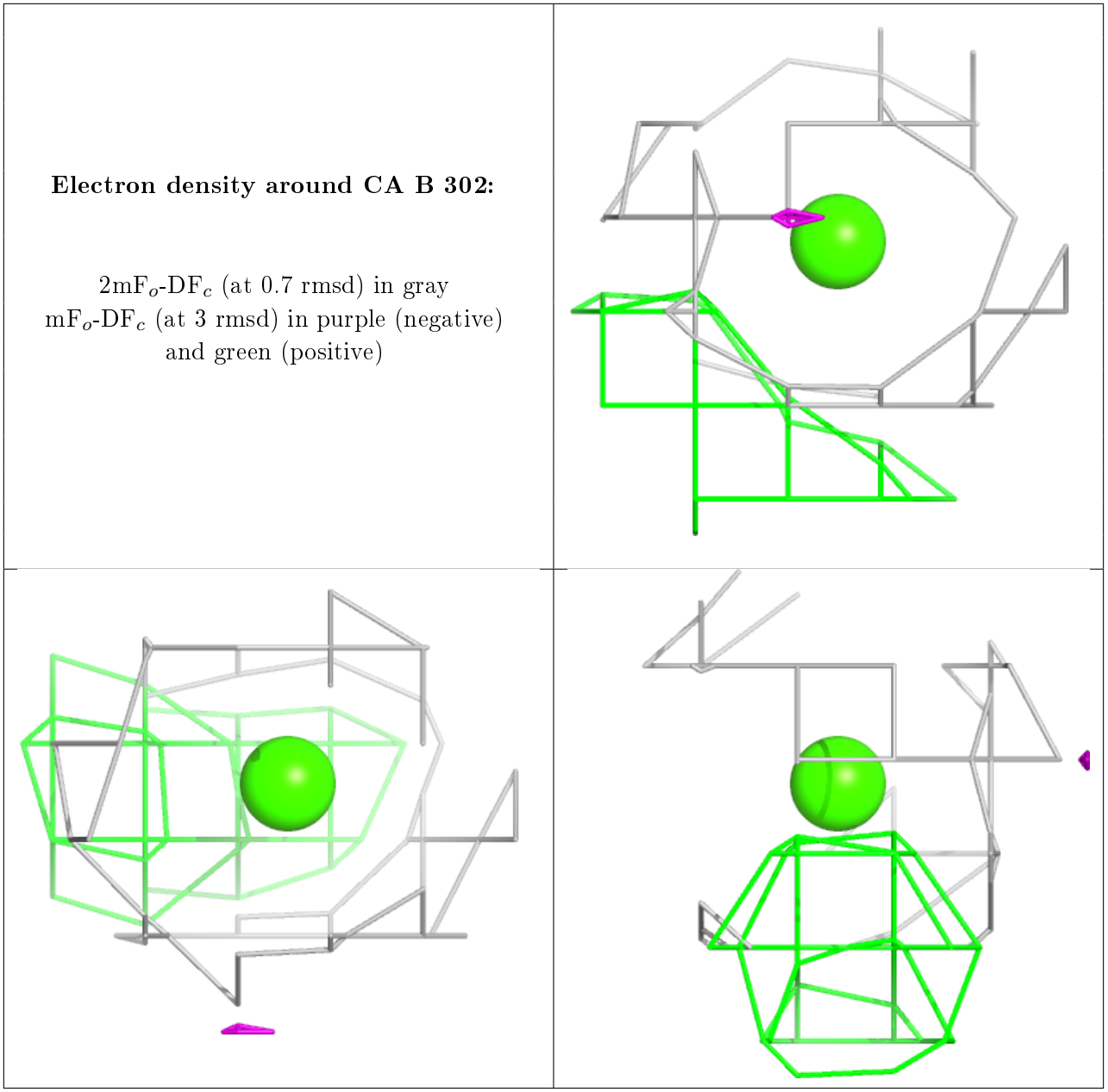
Electron density around CA F 301:

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



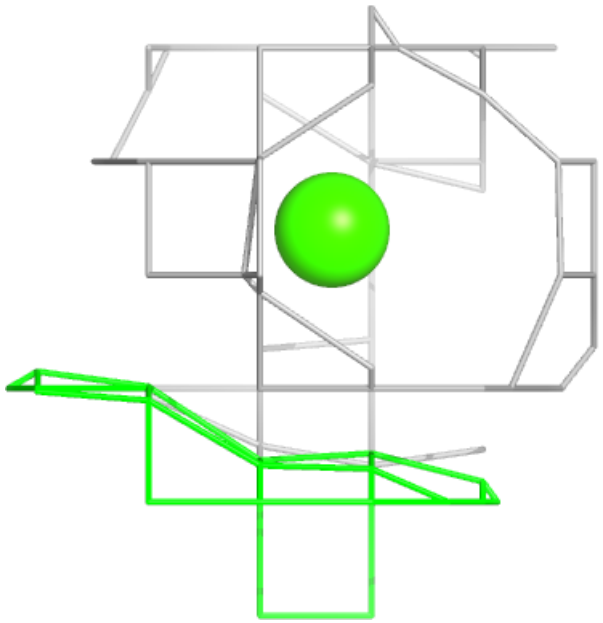
Electron density around CA B 302:

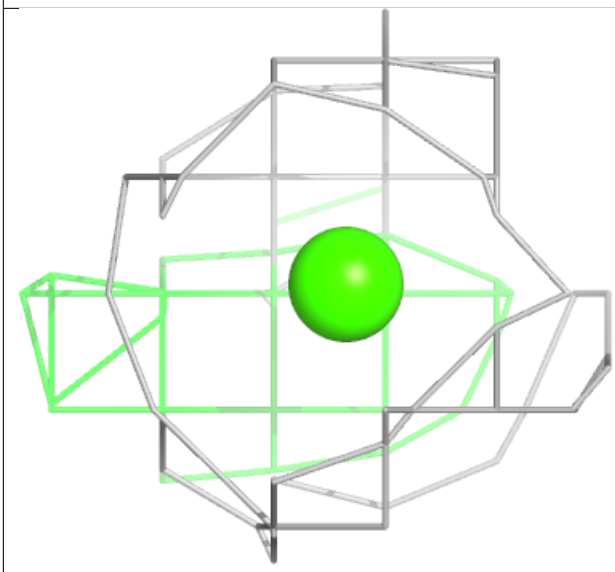
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

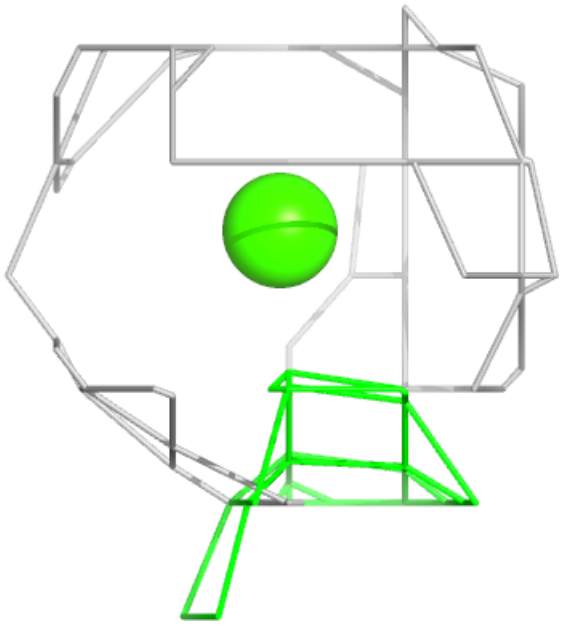


Electron density around CA B 301:

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

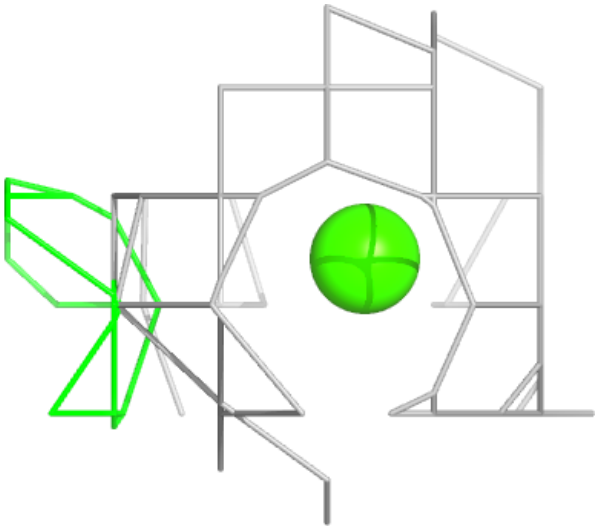


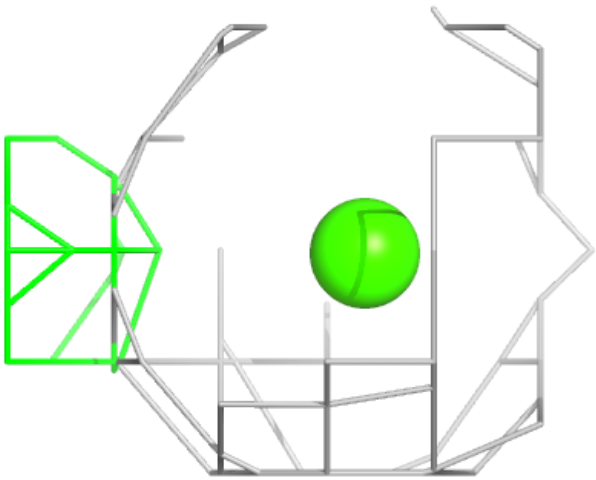


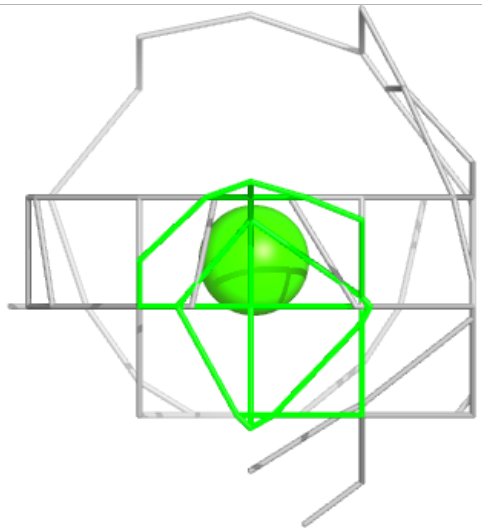


Electron density around CA D 302:

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

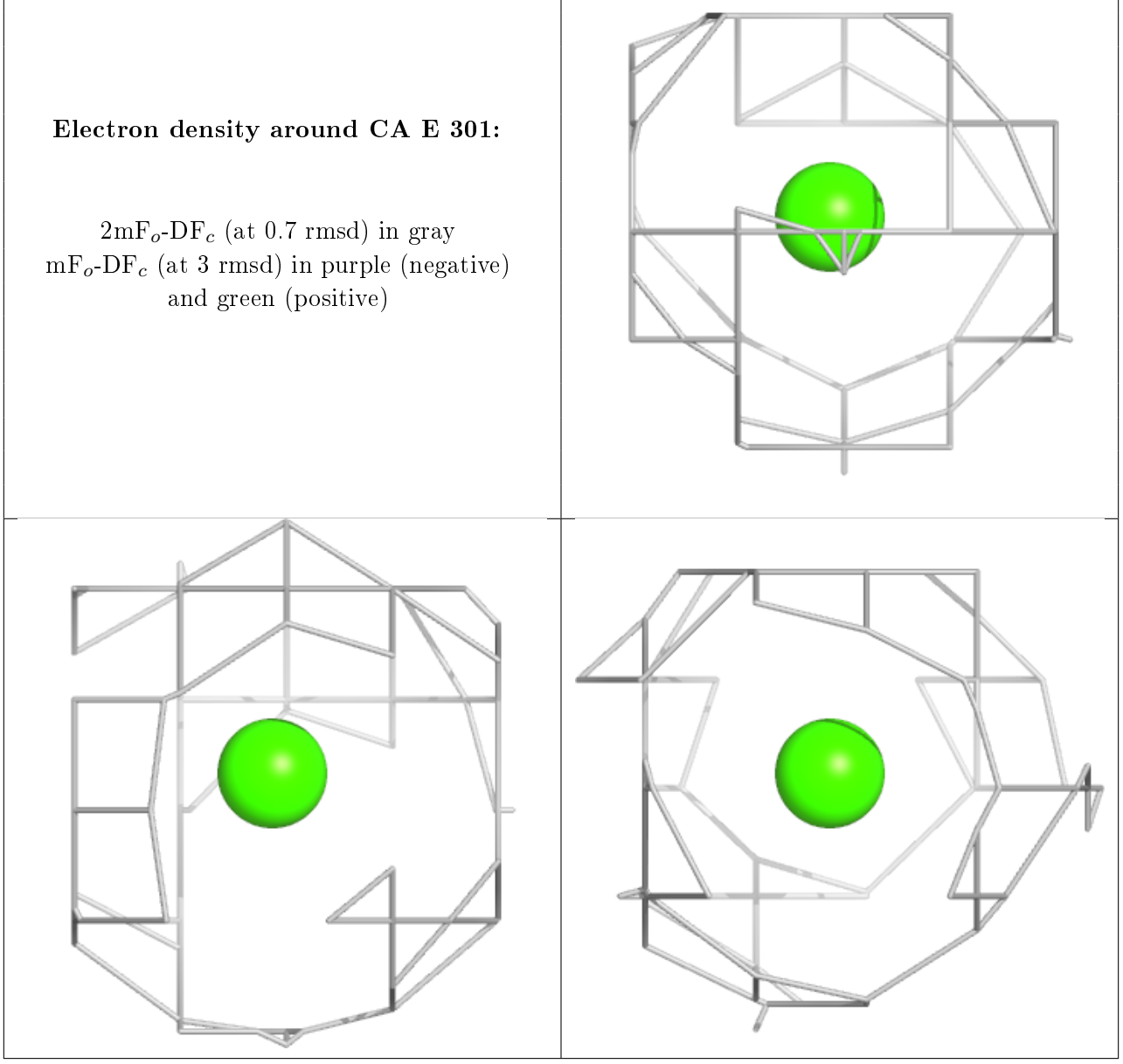






Electron density around CA E 301:

$2mF_o$-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.