Full wwPDB X-ray Structure Validation Report (i)

Oct 28, 2021 – 08:07 AM JST

PDB ID	:	6K4E
Title	:	SiaA-PP2C domain of Pseudomonas aeruginosa
Authors	:	Lin, J.Q.; Lescar, J.
Deposited on	:	2019-05-23
Resolution	:	2.09 Å(reported)

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

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

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

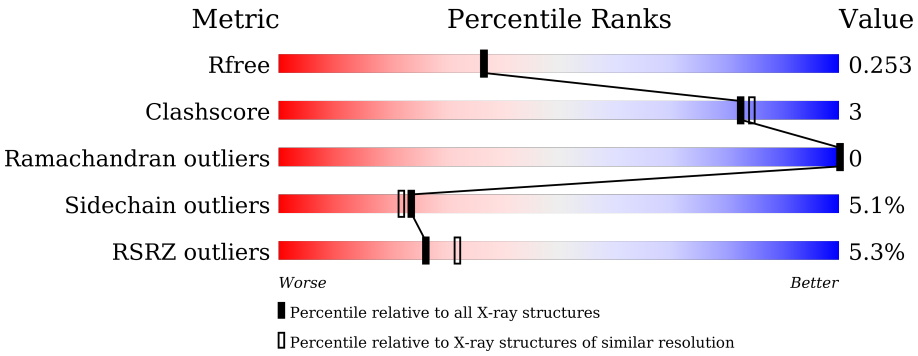
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.09 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 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	301	5% 75% 6% • 19%
1	B	301	4% 72% 9% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4099 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 Putative serine phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1906	1198	345	355	8			
1	B	246	Total	C	N	O	S	0	0	0
			1900	1193	342	357	8			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	363	MET	-	initiating methionine	UNP A0A4U9RCZ4
A	364	HIS	-	expression tag	UNP A0A4U9RCZ4
A	365	HIS	-	expression tag	UNP A0A4U9RCZ4
A	366	HIS	-	expression tag	UNP A0A4U9RCZ4
A	367	HIS	-	expression tag	UNP A0A4U9RCZ4
A	368	HIS	-	expression tag	UNP A0A4U9RCZ4
A	369	HIS	-	expression tag	UNP A0A4U9RCZ4
A	370	SER	-	expression tag	UNP A0A4U9RCZ4
A	371	SER	-	expression tag	UNP A0A4U9RCZ4
A	372	GLY	-	expression tag	UNP A0A4U9RCZ4
A	373	VAL	-	expression tag	UNP A0A4U9RCZ4
A	374	ASP	-	expression tag	UNP A0A4U9RCZ4
A	375	LEU	-	expression tag	UNP A0A4U9RCZ4
A	376	GLY	-	expression tag	UNP A0A4U9RCZ4
A	377	THR	-	expression tag	UNP A0A4U9RCZ4
A	378	GLU	-	expression tag	UNP A0A4U9RCZ4
A	379	ASN	-	expression tag	UNP A0A4U9RCZ4
A	380	LEU	-	expression tag	UNP A0A4U9RCZ4
A	381	TYR	-	expression tag	UNP A0A4U9RCZ4
A	382	PHE	-	expression tag	UNP A0A4U9RCZ4
A	383	GLN	-	expression tag	UNP A0A4U9RCZ4
A	384	SER	-	expression tag	UNP A0A4U9RCZ4
A	385	MET	-	expression tag	UNP A0A4U9RCZ4
B	363	MET	-	initiating methionine	UNP A0A4U9RCZ4
B	364	HIS	-	expression tag	UNP A0A4U9RCZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	365	HIS	-	expression tag	UNP A0A4U9RCZ4
B	366	HIS	-	expression tag	UNP A0A4U9RCZ4
B	367	HIS	-	expression tag	UNP A0A4U9RCZ4
B	368	HIS	-	expression tag	UNP A0A4U9RCZ4
B	369	HIS	-	expression tag	UNP A0A4U9RCZ4
B	370	SER	-	expression tag	UNP A0A4U9RCZ4
B	371	SER	-	expression tag	UNP A0A4U9RCZ4
B	372	GLY	-	expression tag	UNP A0A4U9RCZ4
B	373	VAL	-	expression tag	UNP A0A4U9RCZ4
B	374	ASP	-	expression tag	UNP A0A4U9RCZ4
B	375	LEU	-	expression tag	UNP A0A4U9RCZ4
B	376	GLY	-	expression tag	UNP A0A4U9RCZ4
B	377	THR	-	expression tag	UNP A0A4U9RCZ4
B	378	GLU	-	expression tag	UNP A0A4U9RCZ4
B	379	ASN	-	expression tag	UNP A0A4U9RCZ4
B	380	LEU	-	expression tag	UNP A0A4U9RCZ4
B	381	TYR	-	expression tag	UNP A0A4U9RCZ4
B	382	PHE	-	expression tag	UNP A0A4U9RCZ4
B	383	GLN	-	expression tag	UNP A0A4U9RCZ4
B	384	SER	-	expression tag	UNP A0A4U9RCZ4
B	385	MET	-	expression tag	UNP A0A4U9RCZ4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0
2	B	3	Total Mg 3 3	0	0

- Molecule 3 is water.

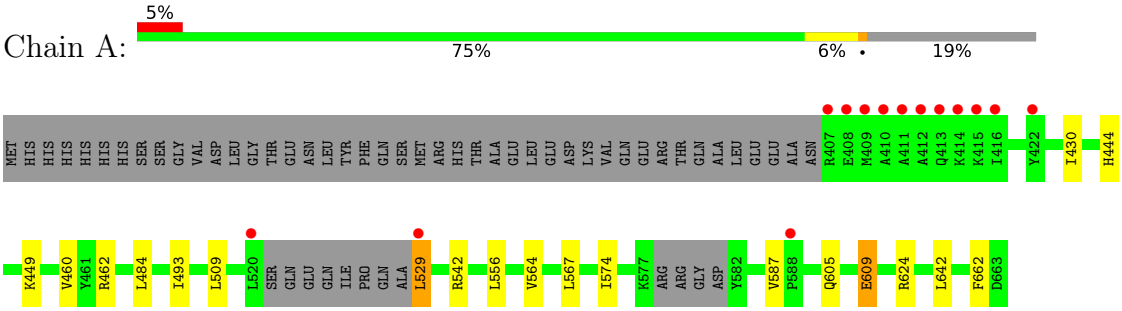
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	149	Total O 149 149	0	0
3	B	138	Total O 138 138	0	0

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.

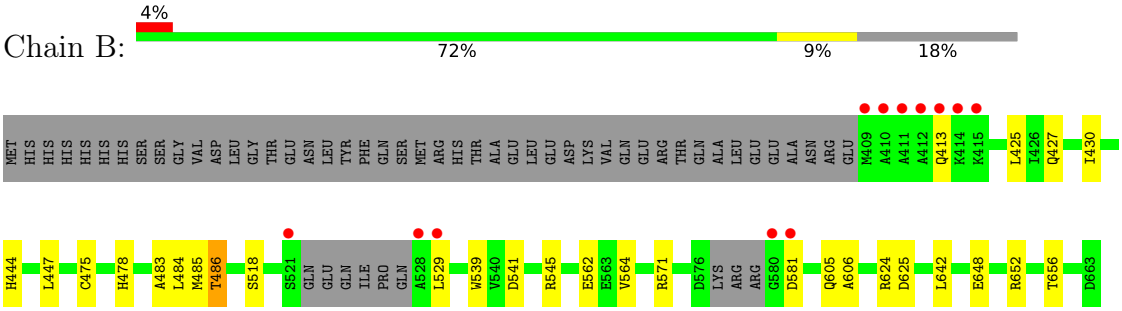
• Molecule 1: Putative serine phosphatase

Chain A:



• Molecule 1: Putative serine phosphatase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.17Å 110.48Å 111.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.09 49.81 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.81-2.09) 99.2 (49.81-2.09)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.212 , 0.241 0.217 , 0.253	Depositor DCC
R_{free} test set	1887 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 70.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4099	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.66% 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: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/1944	0.67	0/2623
1	B	0.52	0/1938	0.68	0/2617
All	All	0.51	0/3882	0.68	0/5240

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1906	0	1852	9	0
1	B	1900	0	1837	12	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	149	0	0	0	0
3	B	138	0	0	1	0
All	All	4099	0	3689	19	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (19) 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:427:GLN:HE21	1:B:486:THR:HG21	1.03	1.16
1:B:427:GLN:NE2	1:B:486:THR:HG21	1.77	0.99
1:A:529:LEU:HD21	1:B:425:LEU:HB3	1.59	0.85
1:A:484:LEU:HD23	1:B:484:LEU:HD23	1.84	0.58
1:A:556:LEU:HD23	1:A:567:LEU:HD22	1.84	0.58
1:B:478:HIS:HD2	3:B:918:HOH:O	1.87	0.55
1:A:509:LEU:HD22	1:A:574:ILE:HD11	1.88	0.54
1:B:564:VAL:CG2	1:B:624:ARG:HB2	2.39	0.52
1:B:483:ALA:O	1:B:486:THR:HG22	2.10	0.50
1:A:542:ARG:HD3	1:A:662:PHE:HE1	1.78	0.48
1:A:564:VAL:CG2	1:A:624:ARG:HB2	2.46	0.46
1:A:609:GLU:CD	1:A:609:GLU:H	2.19	0.46
1:A:605:GLN:HB3	1:A:642:LEU:HD11	1.98	0.45
1:B:605:GLN:HB3	1:B:642:LEU:HD11	1.99	0.44
1:B:539:TRP:NE1	1:B:541:ASP:HB2	2.32	0.44
1:B:606:ALA:HB2	1:B:652:ARG:HH11	1.85	0.41
1:A:460:VAL:HG11	1:A:493:ILE:HG21	2.03	0.41
1:B:447:LEU:O	1:B:656:THR:HA	2.20	0.41
1:B:475:CYS:HB3	1:B:485:MET:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/301 (79%)	232 (97%)	7 (3%)	0	100	100
1	B	240/301 (80%)	236 (98%)	4 (2%)	0	100	100
All	All	479/602 (80%)	468 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/237 (79%)	181 (96%)	7 (4%)	34	35
1	B	187/237 (79%)	175 (94%)	12 (6%)	17	14
All	All	375/474 (79%)	356 (95%)	19 (5%)	24	22

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	430	ILE
1	A	444	HIS
1	A	449	LYS
1	A	462	ARG
1	A	529	LEU
1	A	587	VAL
1	A	609	GLU
1	B	413	GLN
1	B	430	ILE
1	B	444	HIS
1	B	486	THR
1	B	518	SER
1	B	529	LEU
1	B	545	ARG
1	B	562	GLU
1	B	571	ARG
1	B	581	ASP
1	B	625	ASP
1	B	648	GLU

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

Mol	Chain	Res	Type
1	A	464	GLN
1	B	443	HIS
1	B	565	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	245/301 (81%)	0.28	14 (5%)	23 29	33, 47, 82, 169	0
1	B	246/301 (81%)	0.21	12 (4%)	29 35	33, 48, 83, 126	0
All	All	491/602 (81%)	0.25	26 (5%)	26 32	33, 48, 83, 169	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	MET	5.7
1	B	411	ALA	5.4
1	B	409	MET	5.3
1	A	407	ARG	5.2
1	A	529	LEU	4.9
1	A	413	GLN	4.7
1	A	410	ALA	4.5
1	B	410	ALA	4.2
1	B	529	LEU	3.9
1	A	411	ALA	3.9
1	B	413	GLN	3.8
1	B	521	SER	3.7
1	A	414	LYS	3.6
1	B	414	LYS	3.4
1	B	580	GLY	2.9
1	B	528	ALA	2.7
1	B	415	LYS	2.6
1	A	408	GLU	2.6
1	B	412	ALA	2.5
1	A	416	ILE	2.3
1	A	588	PRO	2.3
1	A	415	LYS	2.2
1	B	581	ASP	2.1
1	A	422	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	412	ALA	2.0
1	A	520	LEU	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)

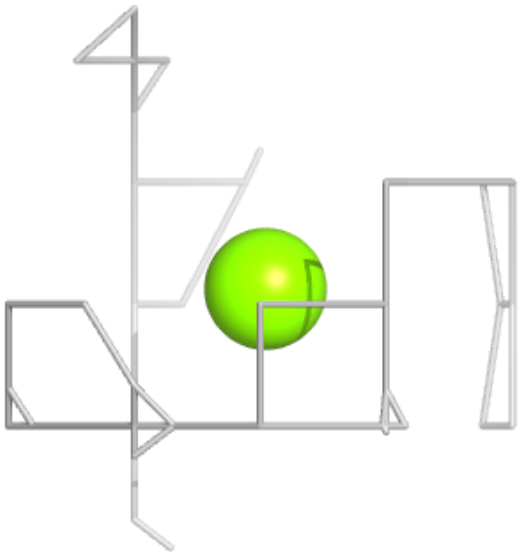
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

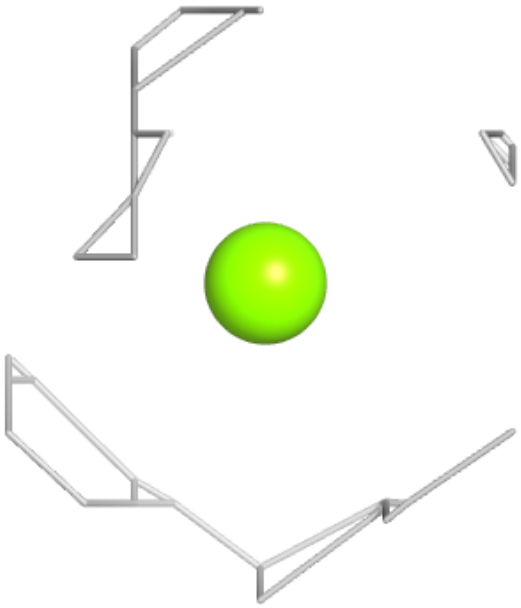
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	701	1/1	0.89	0.04	49,49,49,49	0
2	MG	B	703	1/1	0.94	0.12	43,43,43,43	0
2	MG	B	702	1/1	0.96	0.06	31,31,31,31	0
2	MG	A	701	1/1	0.97	0.08	38,38,38,38	0
2	MG	A	703	1/1	0.98	0.20	47,47,47,47	0
2	MG	A	702	1/1	0.98	0.04	33,33,33,33	0

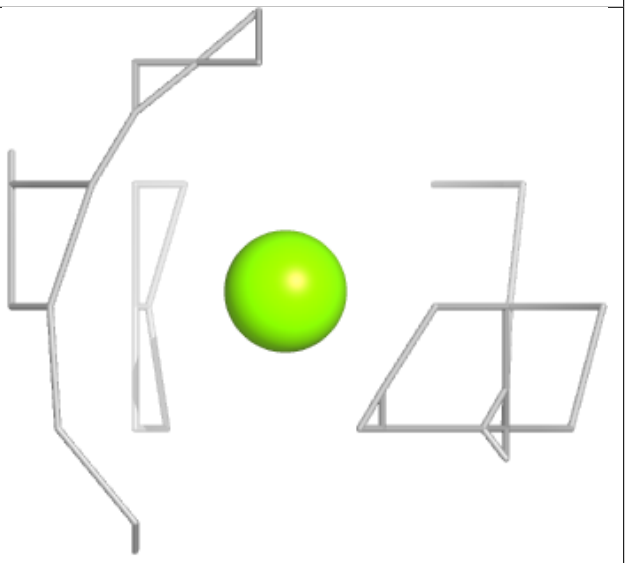
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MG B 701:

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

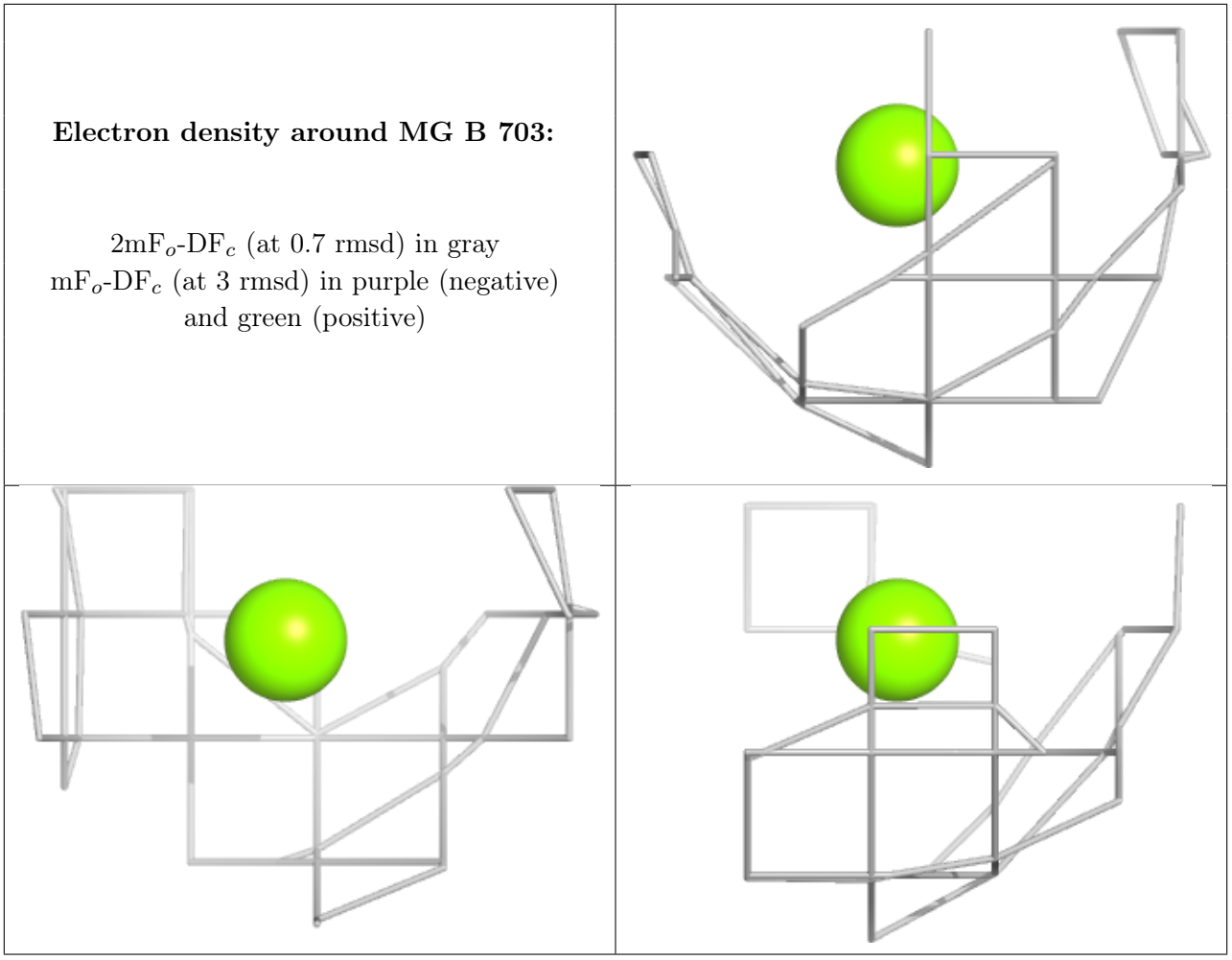






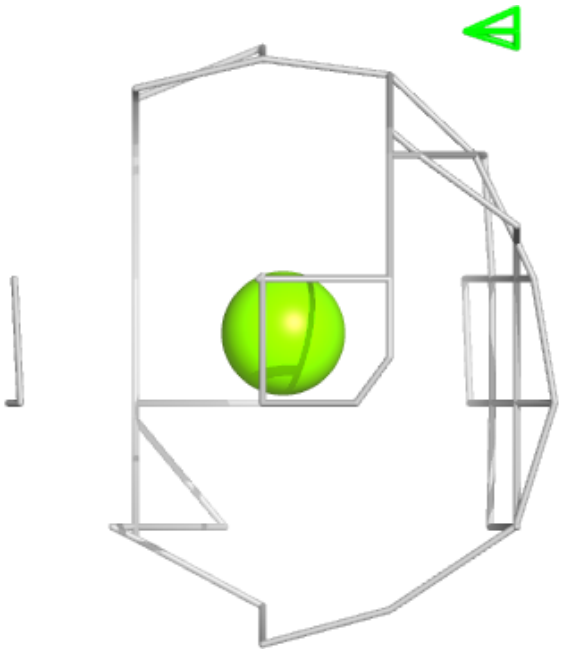
Electron density around MG B 703:

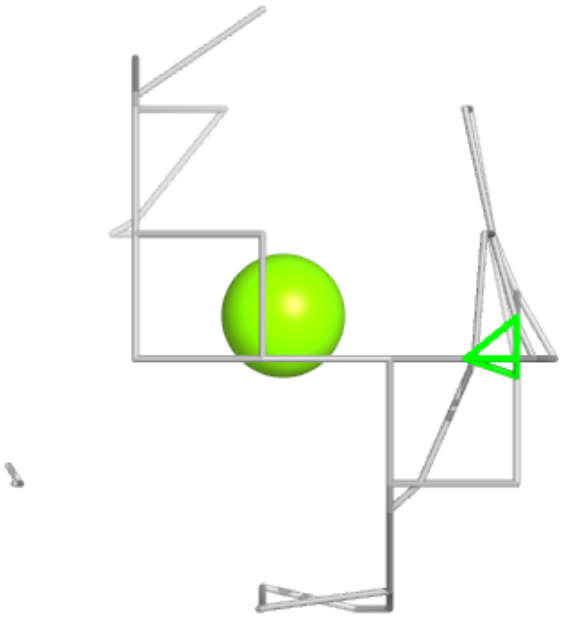
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

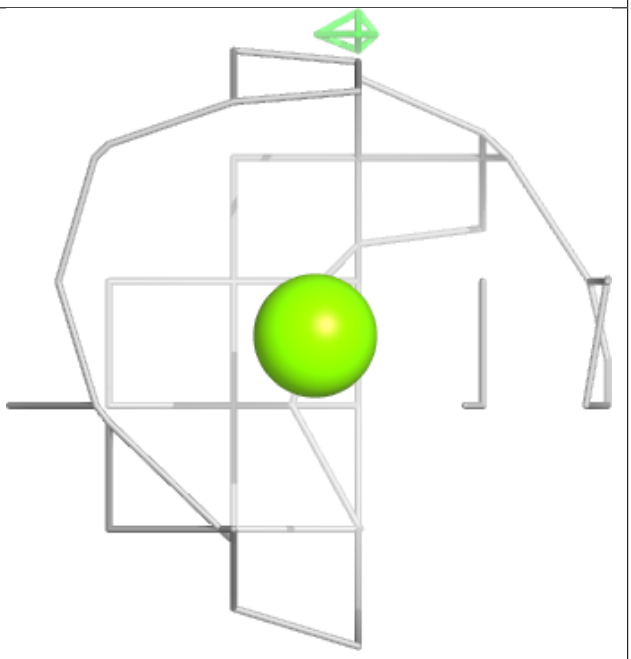


Electron density around MG B 702:

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

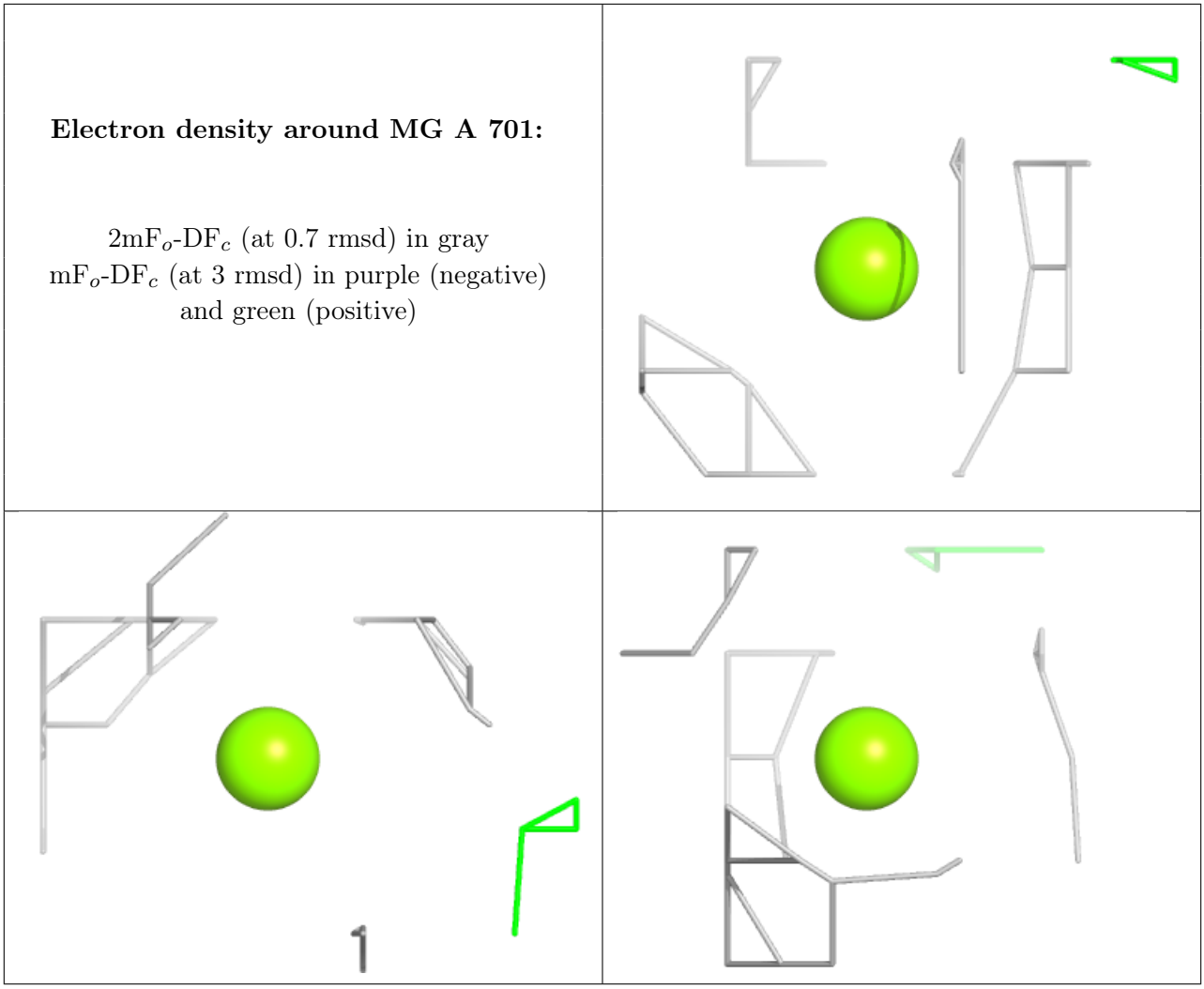






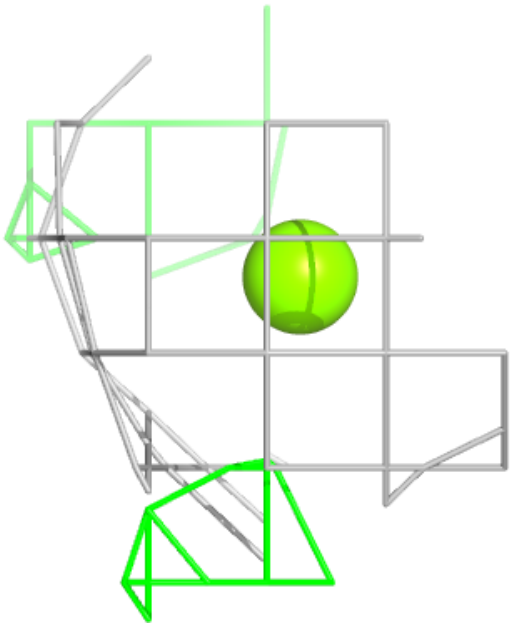
Electron density around MG A 701:

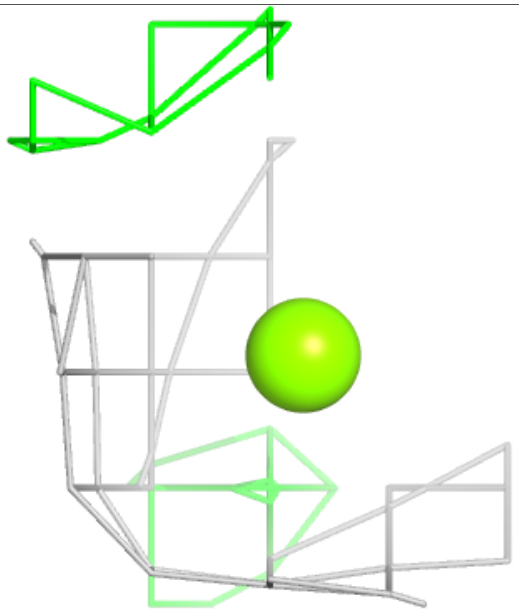
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

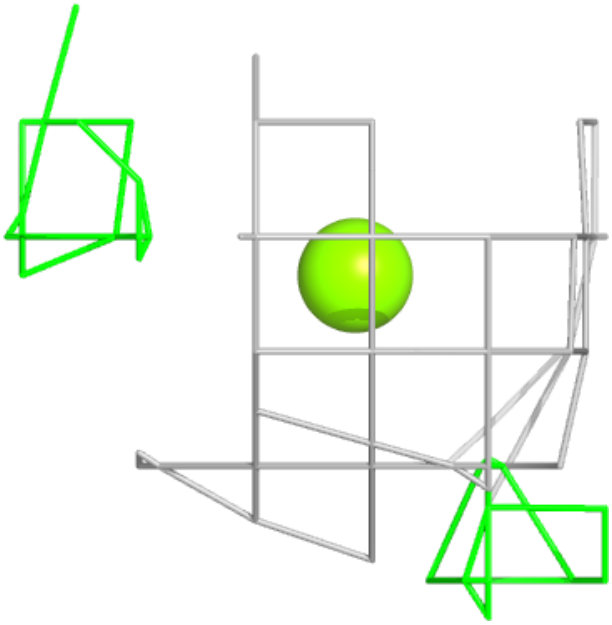


Electron density around MG A 703:

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

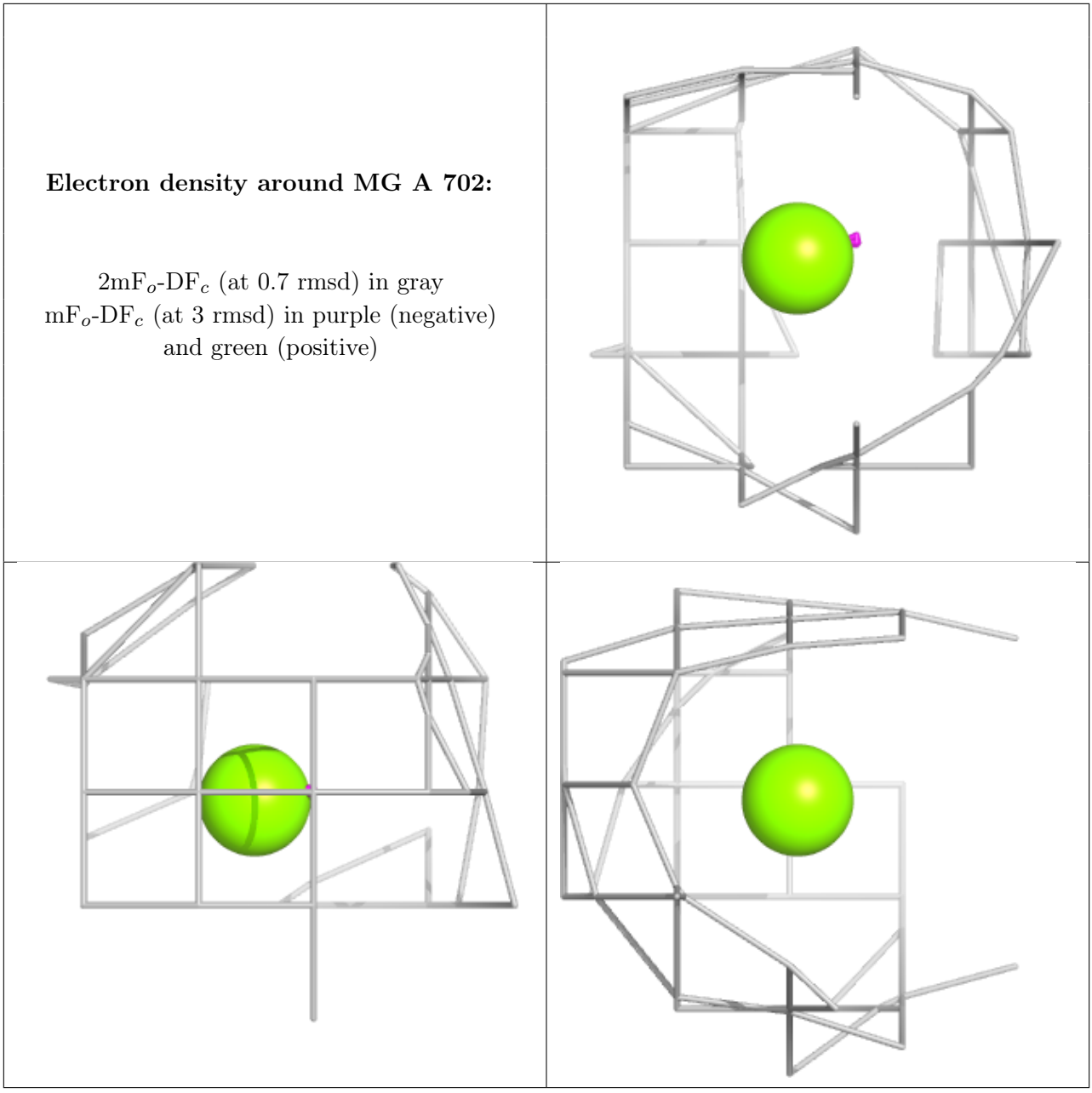






Electron density around MG A 702:

$2mF_o$-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.