wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 02:41 PM EDT

PDB ID	:	6RRE
Title	:	SidD, deAMPylase from Legionella pneumophila
Authors	:	Tascon, I.; Lucas, M.; Rojas, A.L.; Hierro, A.
Deposited on	:	2019-05-17
Resolution	:	3.59 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

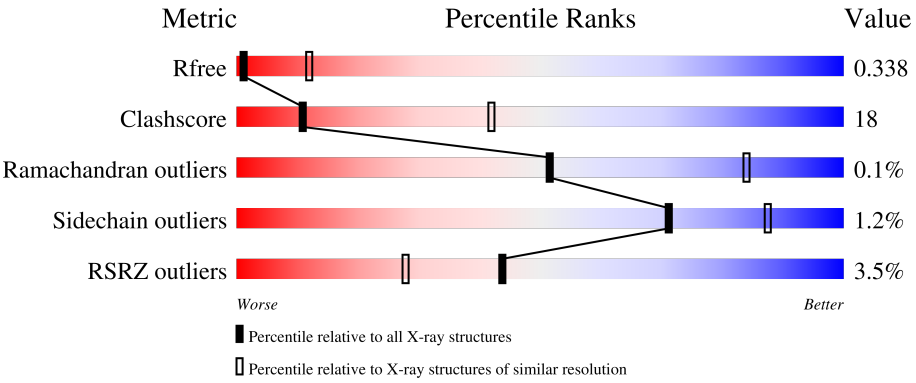
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.59 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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	471	3% 53% 34% 13%
1	B	471	3% 58% 31% • 10%
1	C	471	% 56% 32% • 11%
1	D	471	% 57% 33% • 9%
1	E	471	7% 50% 37% 13%

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Mol	Chain	Length	Quality of chain
1	F	471	

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
2	MG	B	601	-	-	-	X
2	MG	F	601	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19778 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 Adenosine monophosphate-protein hydrolase SidD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3262	2082	533	634	13			
1	B	422	Total	C	N	O	S	0	0	0
			3346	2133	554	646	13			
1	C	421	Total	C	N	O	S	0	0	0
			3334	2127	551	644	12			
1	D	427	Total	C	N	O	S	0	0	0
			3387	2161	560	654	12			
1	E	409	Total	C	N	O	S	0	0	0
			3223	2053	528	630	12			
1	F	407	Total	C	N	O	S	0	0	0
			3221	2054	528	627	12			

- 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	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

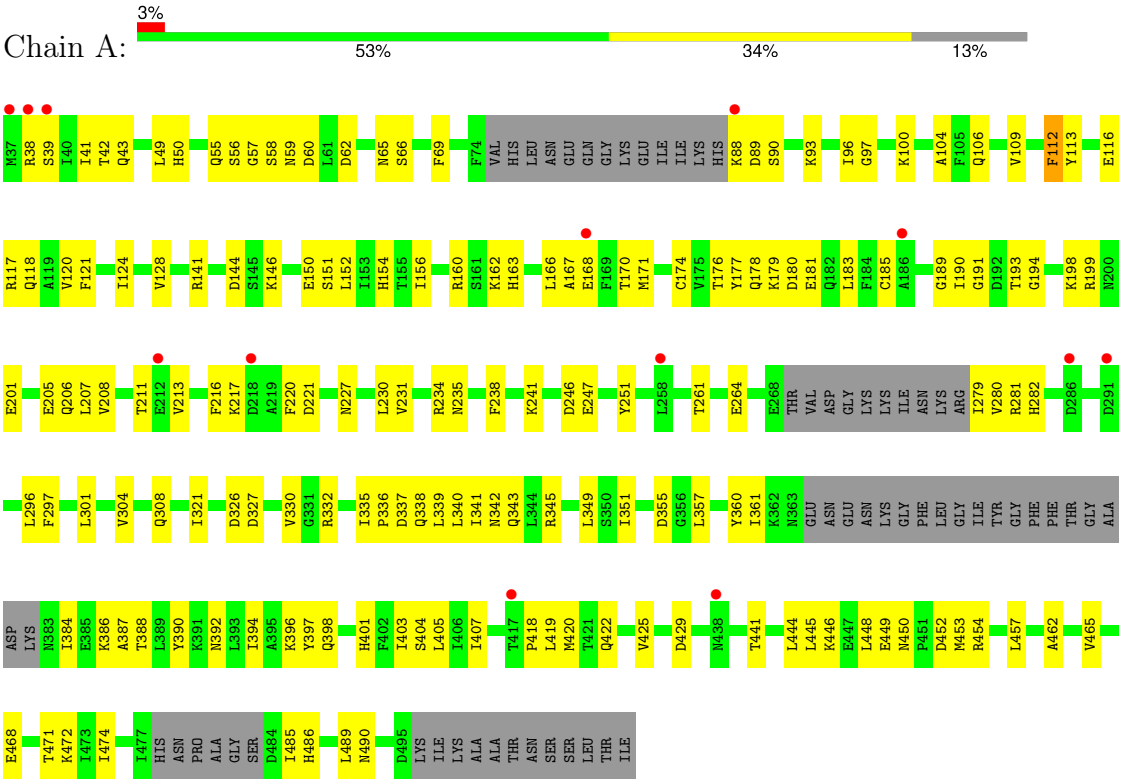
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	O	0	0
			1	1		

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.

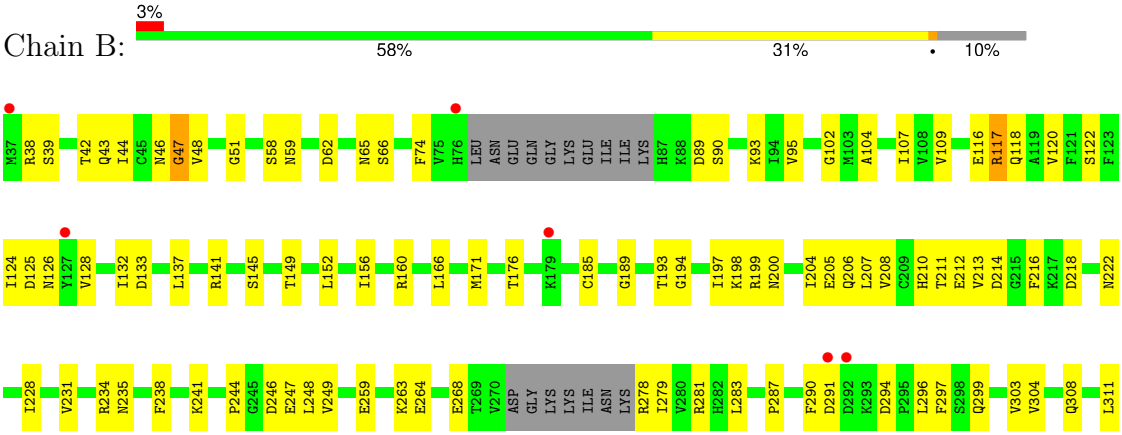
• Molecule 1: Adenosine monophosphate-protein hydrolase SidD

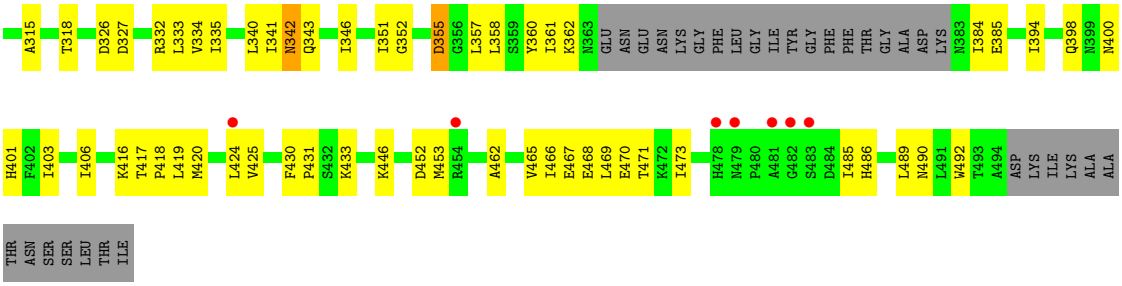
Chain A:



• Molecule 1: Adenosine monophosphate-protein hydrolase SidD

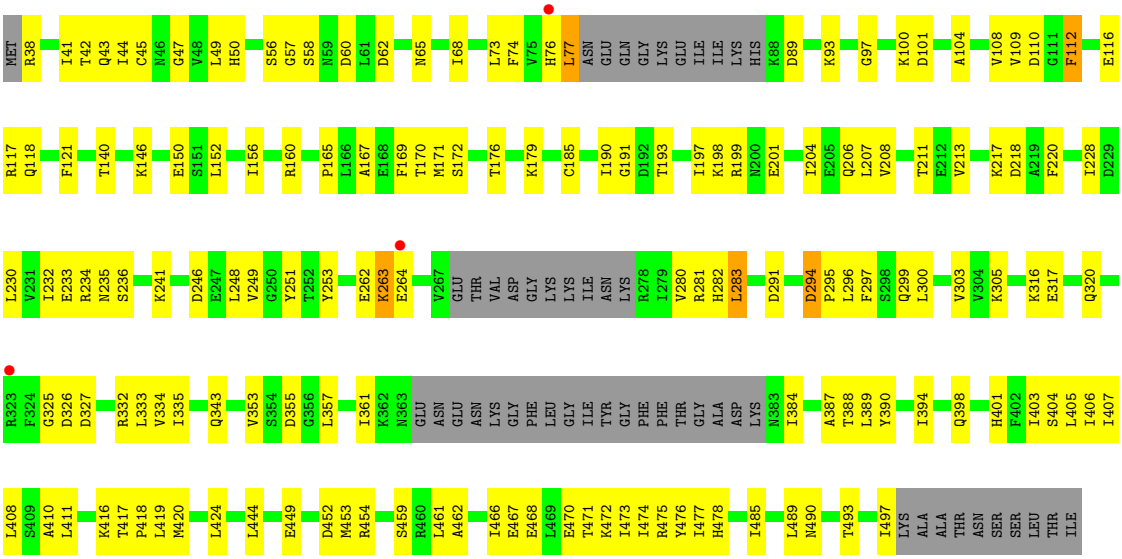
Chain B:





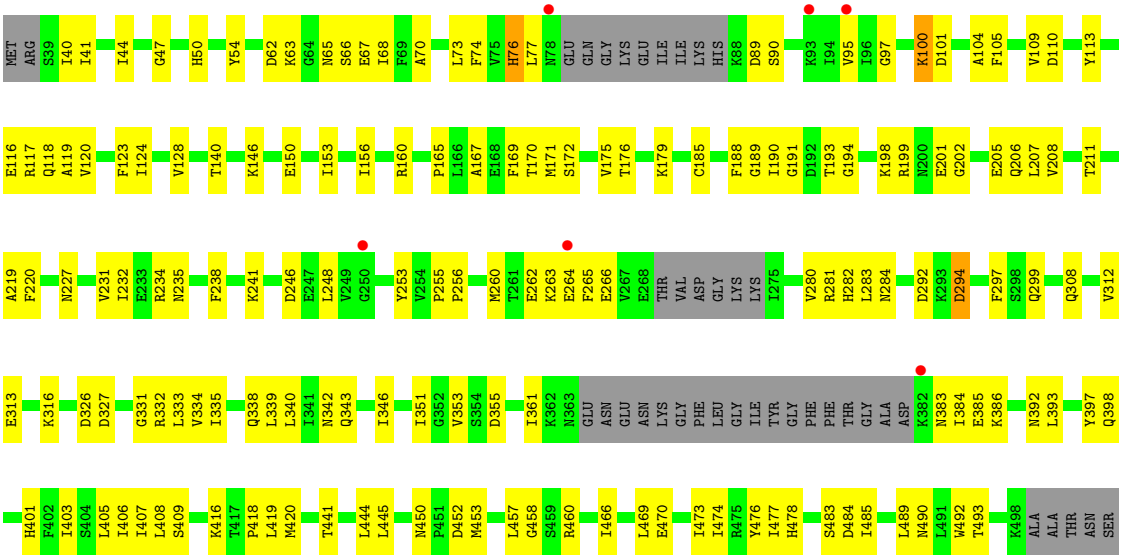
• Molecule 1: Adenosine monophosphate-protein hydrolase SidD

Chain C:



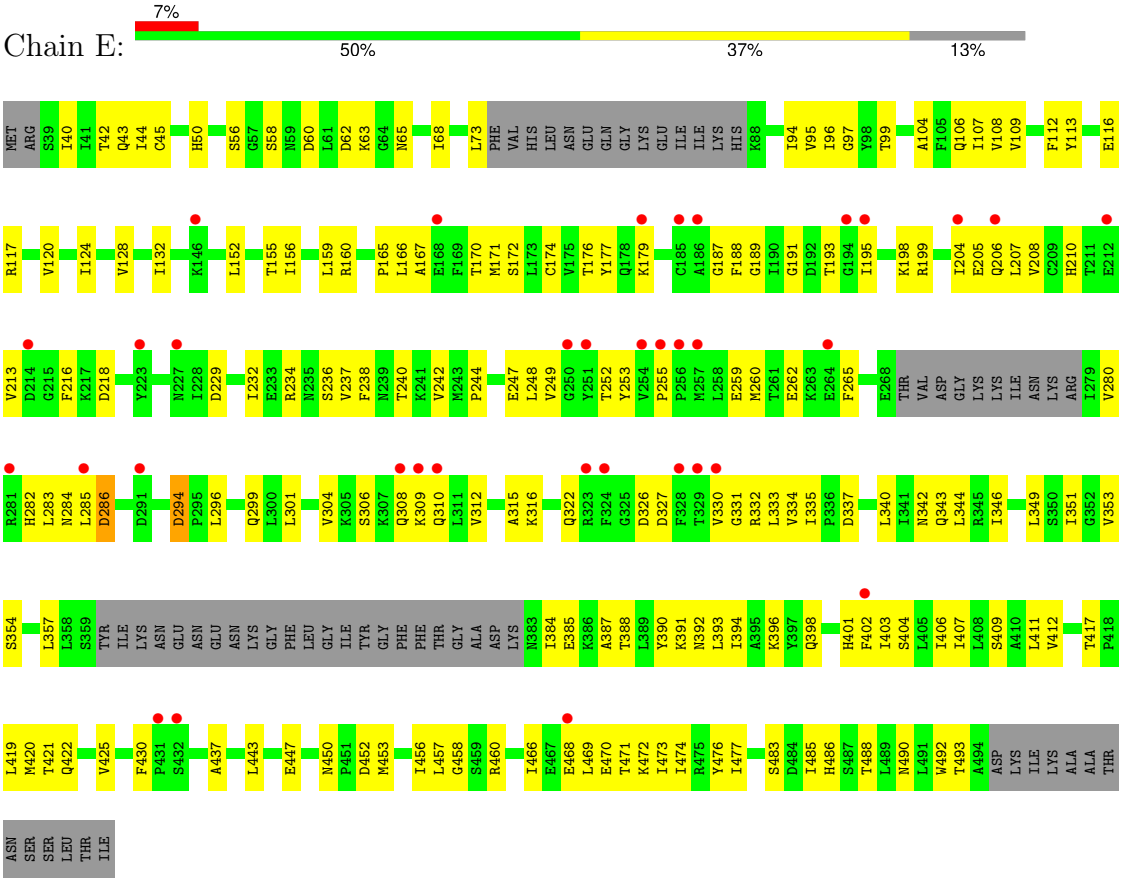
• Molecule 1: Adenosine monophosphate-protein hydrolase SidD

Chain D:



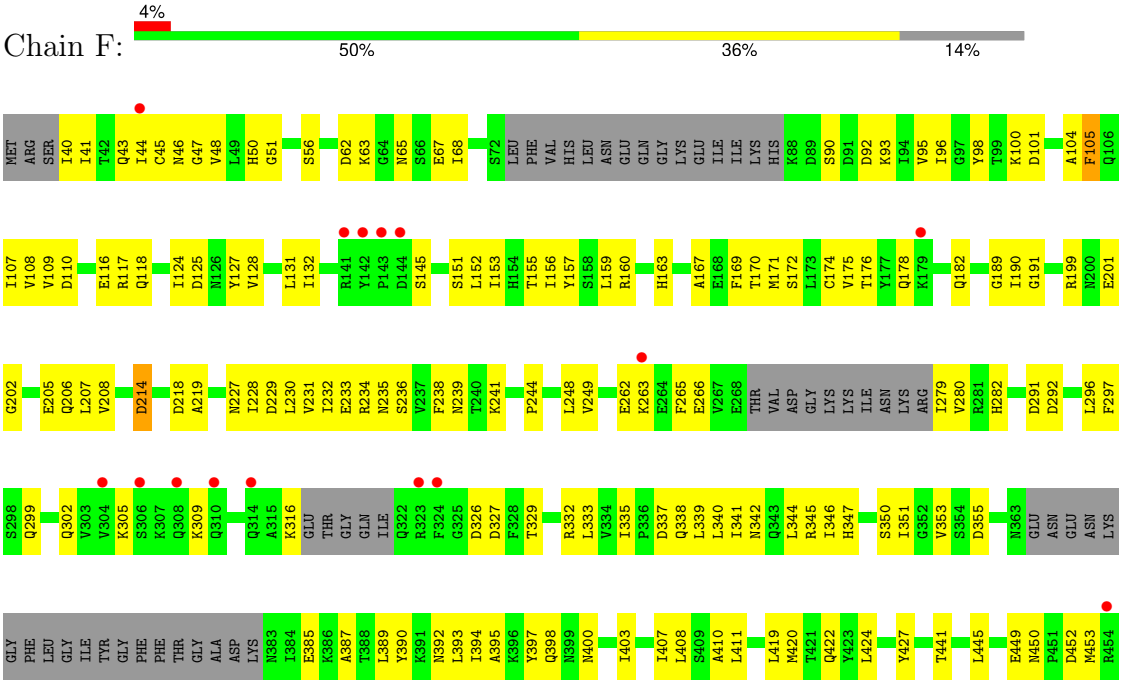
• Molecule 1: Adenosine monophosphate-protein hydrolase SidD

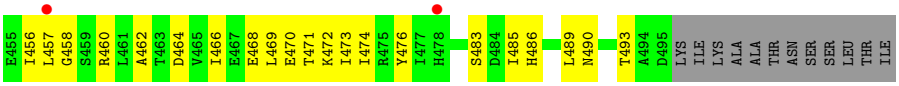
Chain E:



• Molecule 1: Adenosine monophosphate-protein hydrolase SidD

Chain F:




E455
I456
L457
G458
S459
R460
L461
A462
T463
D464
V465
I466
E467
E468
L469
E470
T471
K472
I473
I474
R475
Y476
I477
H478
S483
D484
I485
H486
L489
N490
T493
A494
D495
LYS
ILE
LYS
ALA
ALA
THR
ASN
SER
SER
LEU
THR
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.57Å 141.64Å 234.30Å 90.00° 92.75° 90.00°	Depositor
Resolution (Å)	46.81 – 3.59 47.52 – 3.59	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.81-3.59) 98.8 (47.52-3.59)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.295 , 0.338 0.298 , 0.338	Depositor DCC
R_{free} test set	2445 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	134.3	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 79.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19778	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4725e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.26	0/3315	0.48	0/4479
1	B	0.26	0/3404	0.48	0/4603
1	C	0.26	0/3391	0.48	0/4586
1	D	0.26	0/3444	0.48	0/4654
1	E	0.26	0/3277	0.48	0/4434
1	F	0.26	0/3275	0.50	0/4428
All	All	0.26	0/20106	0.48	0/27184

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	3262	0	3260	125	0
1	B	3346	0	3342	102	0
1	C	3334	0	3332	120	0
1	D	3387	0	3398	121	0
1	E	3223	0	3209	131	0
1	F	3221	0	3211	138	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
3	C	1	0	0	0	0
All	All	19778	0	19752	720	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 18.

The worst 5 of 720 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:F:389:LEU:O	1:F:393:LEU:HD22	1.56	1.05
1:A:180:ASP:OD1	1:A:181:GLU:OE2	1.87	0.92
1:F:124:ILE:HA	1:F:128:VAL:HG12	1.51	0.91
1:E:208:VAL:HG23	1:E:236:SER:HB2	1.57	0.87
1:F:45:CYS:HB2	1:F:68:ILE:HD12	1.57	0.83

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	401/471 (85%)	375 (94%)	26 (6%)	0	100	100
1	B	414/471 (88%)	379 (92%)	33 (8%)	2 (0%)	29	67
1	C	413/471 (88%)	377 (91%)	36 (9%)	0	100	100
1	D	419/471 (89%)	385 (92%)	34 (8%)	0	100	100
1	E	401/471 (85%)	371 (92%)	30 (8%)	0	100	100
1	F	397/471 (84%)	362 (91%)	34 (9%)	1 (0%)	41	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2445/2826 (86%)	2249 (92%)	193 (8%)	3 (0%)	51 84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	47	GLY
1	F	47	GLY
1	B	117	ARG

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	369/418 (88%)	367 (100%)	2 (0%)	88 95
1	B	378/418 (90%)	372 (98%)	6 (2%)	62 83
1	C	376/418 (90%)	368 (98%)	8 (2%)	53 79
1	D	383/418 (92%)	379 (99%)	4 (1%)	76 89
1	E	364/418 (87%)	361 (99%)	3 (1%)	81 92
1	F	364/418 (87%)	360 (99%)	4 (1%)	73 88
All	All	2234/2508 (89%)	2207 (99%)	27 (1%)	71 87

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	305	LYS
1	D	76	HIS
1	F	201	GLU
1	D	74	PHE
1	D	100	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	182	GLN
1	F	43	GLN
1	D	486	HIS
1	F	50	HIS
1	C	200	ASN

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 4 ligands modelled in this entry, 4 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	411/471 (87%)	-0.01	13 (3%)	47	31	84, 138, 189, 201	0
1	B	422/471 (89%)	-0.01	13 (3%)	49	31	67, 122, 176, 200	0
1	C	421/471 (89%)	-0.06	3 (0%)	87	77	84, 125, 173, 207	0
1	D	427/471 (90%)	-0.04	6 (1%)	75	59	76, 117, 166, 188	0
1	E	409/471 (86%)	0.24	35 (8%)	10	6	104, 151, 182, 202	0
1	F	407/471 (86%)	0.15	17 (4%)	36	22	99, 141, 178, 203	0
All	All	2497/2826 (88%)	0.04	87 (3%)	44	28	67, 134, 180, 207	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	212	GLU	7.4
1	A	39	SER	5.5
1	E	250	GLY	5.1
1	A	38	ARG	4.7
1	E	251	TYR	4.7

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)

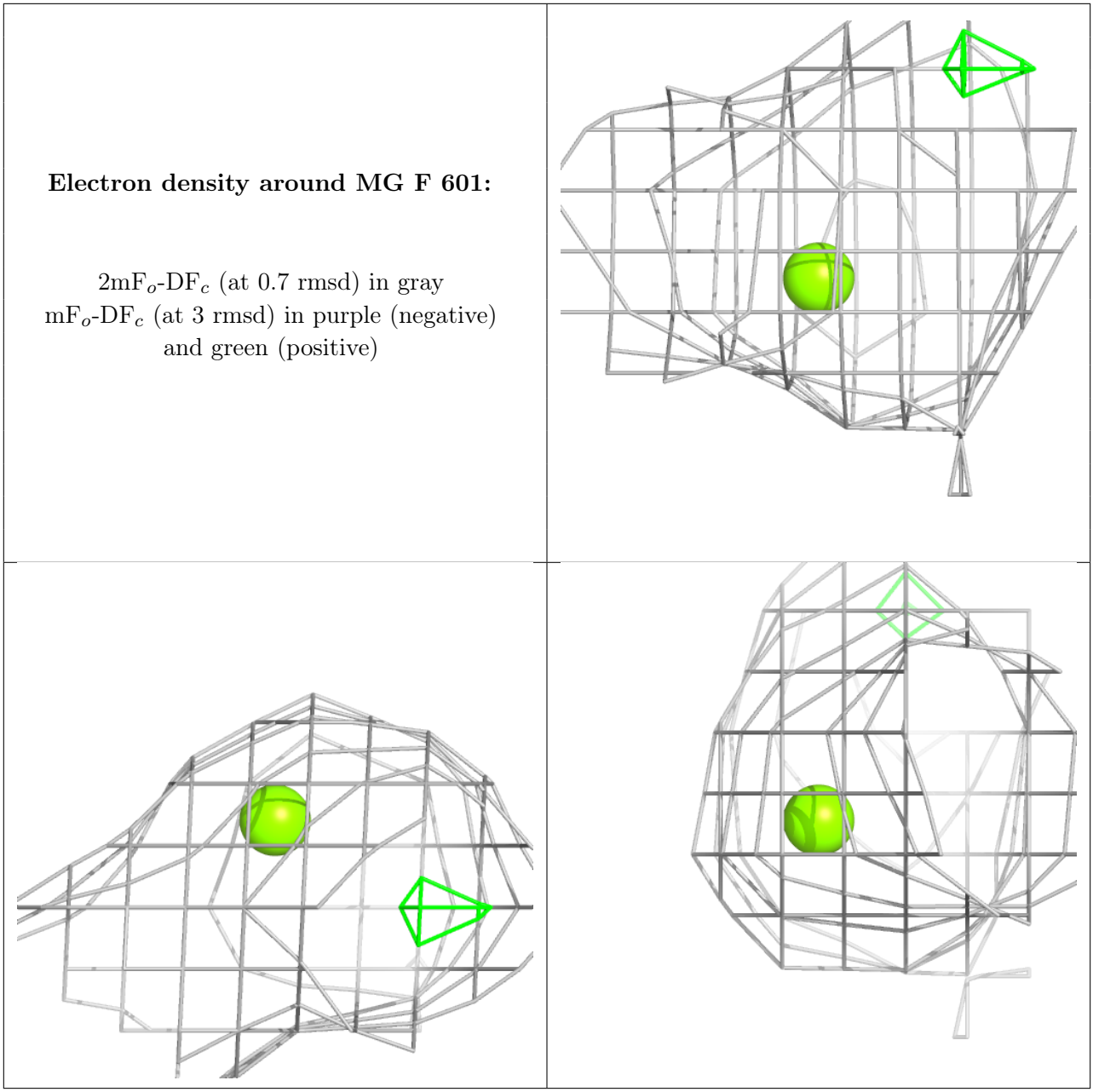
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MG	F	601	1/1	0.62	0.93	128,128,128,128	0
2	MG	B	601	1/1	0.64	0.58	101,101,101,101	0
2	MG	C	601	1/1	0.90	0.18	121,121,121,121	0
2	MG	D	601	1/1	0.94	0.26	120,120,120,120	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.

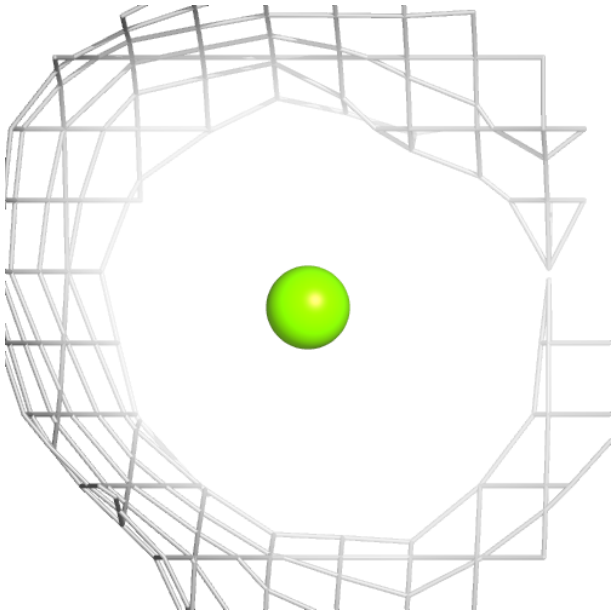
Electron density around MG F 601:

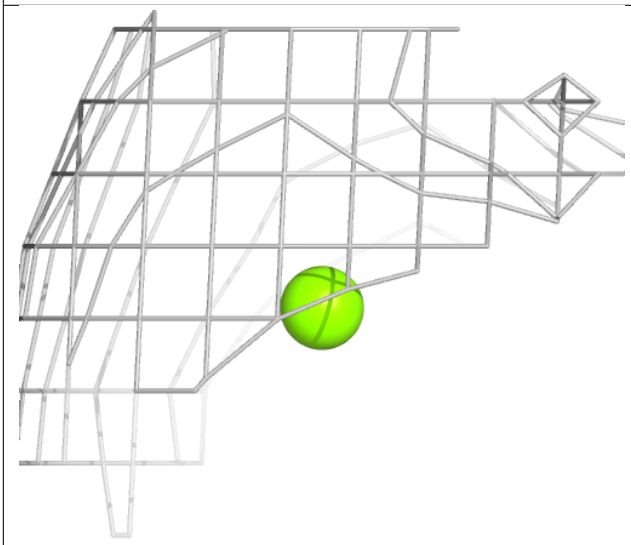
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

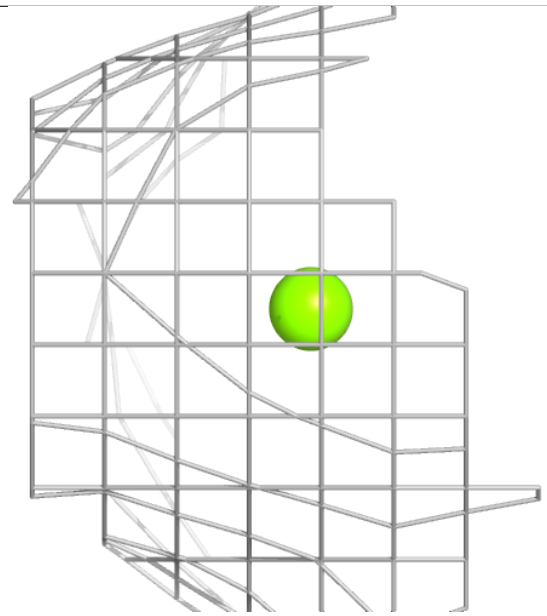


Electron density around MG B 601:

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

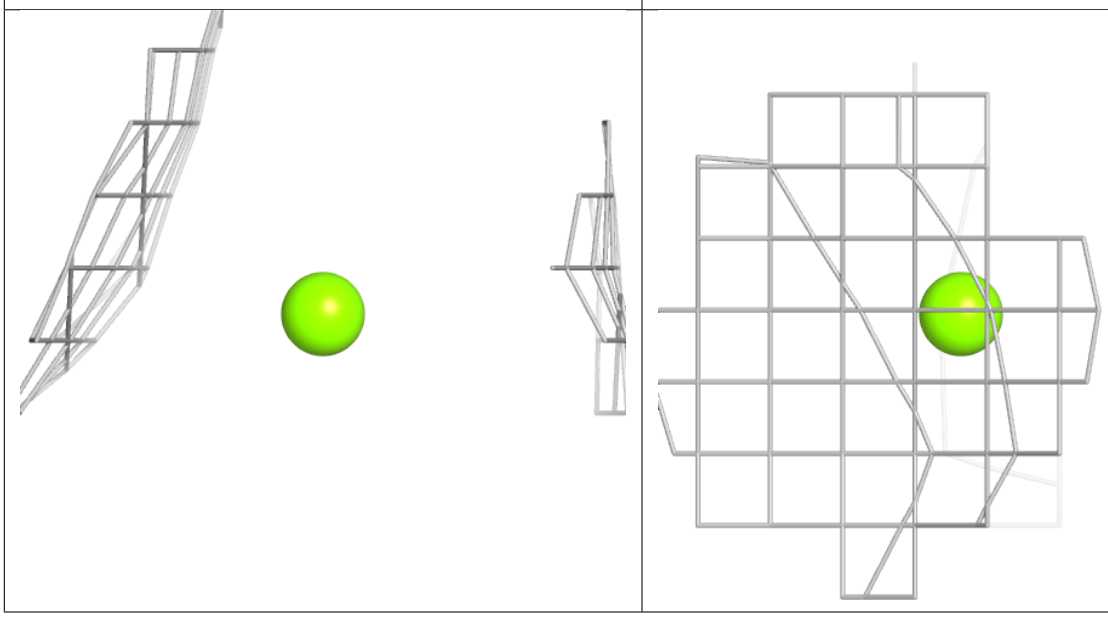






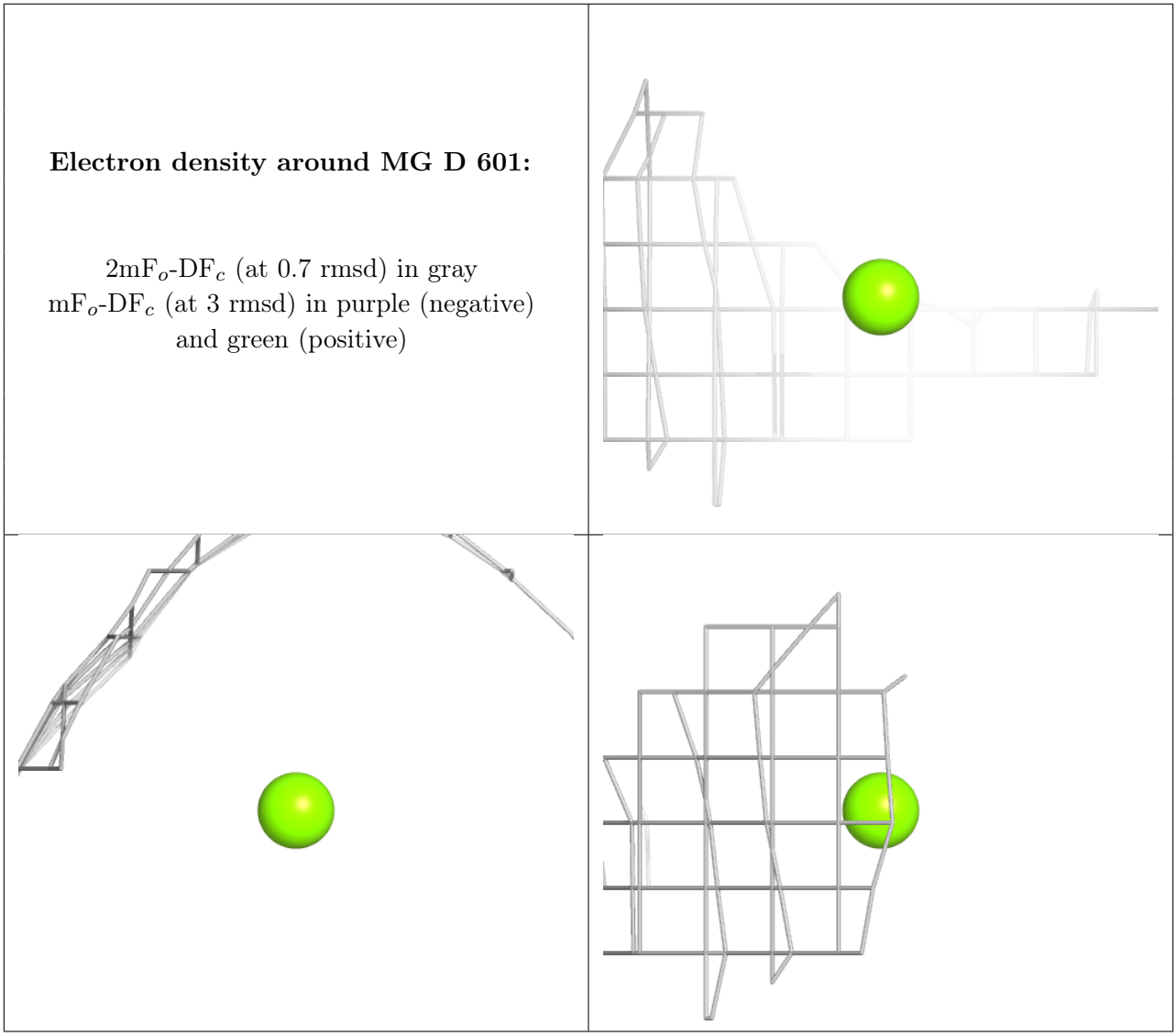
Electron density around MG C 601:

$2mF_o$-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 D 601:

$2mF_o$-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.