Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 01:09 pm GMT

PDB ID	:	7BF1
Title	:	Ca2+-Calmodulin in complex with peptide from brain-type creatine kinase in extended 1:2 binding mode
Authors	:	Sprenger, J.; Akerfeldt, K.S.; Bredfelt, J.; Patel, N.; Rowlett, R.; Trifan, A.; Vanderbeck, A.; Lo Leggio, L.; Snogerup Linse, S.
Deposited on	:	2020-12-31
Resolution	:	1.24 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 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:

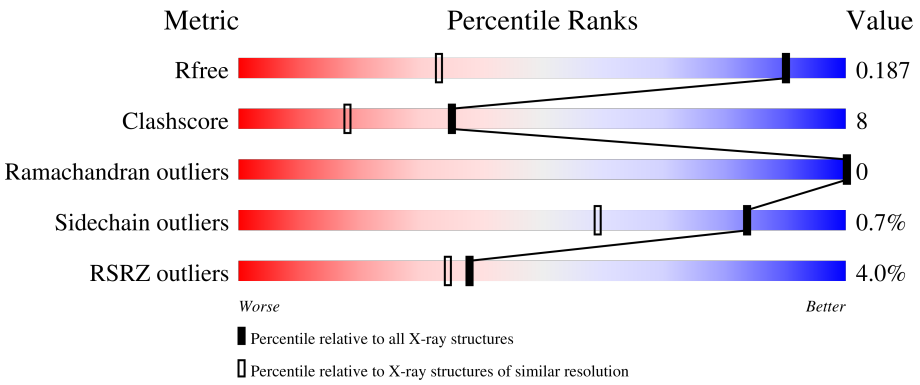
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

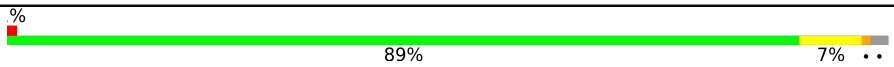
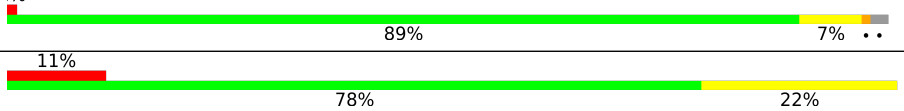
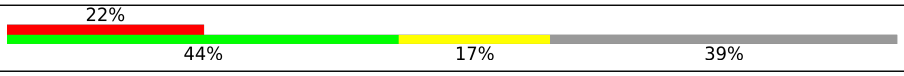
The reported resolution of this entry is 1.24 Å.

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	2024 (1.28-1.20)
Clashscore	141614	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)
RSRZ outliers	127900	1987 (1.28-1.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	AAA	149	
2	CCC	18	
2	DDD	18	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3087 atoms, of which 1448 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 Calmodulin-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	146	2374	748	1150	197	267	12	50	9	0

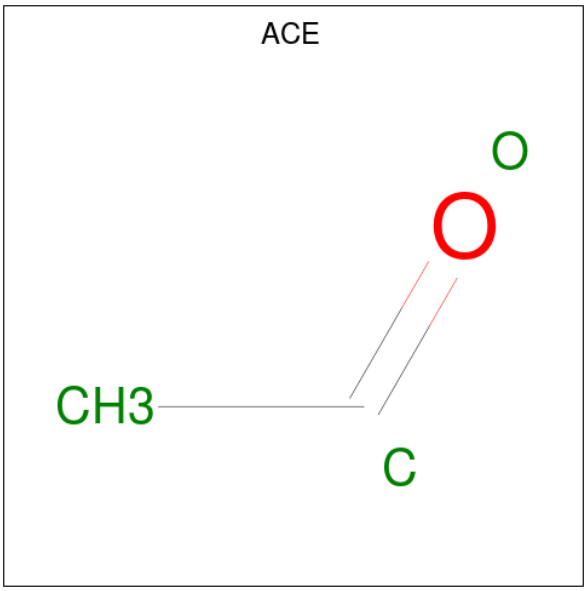
- Molecule 2 is a protein called Creatine kinase B-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	CCC	18	324	98	169	31	26	7	0	0
2	DDD	11	231	69	126	22	14	1	1	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	AAA	4	4	4	0	0

- Molecule 4 is ACETYL GROUP (three-letter code: ACE) (formula: C_2H_4O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	CCC	1	6	2	3	1	0	0

- Molecule 5 is water.

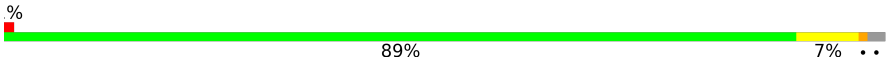
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	AAA	134	134	134	0	0
			Total	O		
5	CCC	8	8	8	0	0
			Total	O		
5	DDD	6	6	6	0	0

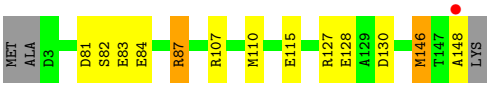
3 Residue-property plots (i)

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: Calmodulin-1

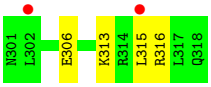
Chain AAA:





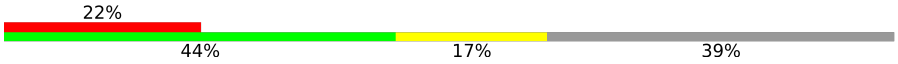
- Molecule 2: Creatine kinase B-type

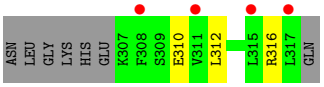
Chain CCC:



- Molecule 2: Creatine kinase B-type

Chain DDD:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	24.41Å 59.53Å 52.48Å 90.00° 98.34° 90.00°	Depositor
Resolution (Å)	39.16 – 1.24 39.13 – 1.24	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.16-1.24) 98.8 (39.13-1.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.24Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.135 , 0.186 0.136 , 0.187	Depositor DCC
R_{free} test set	2093 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	16.2	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	3087	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.71% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, CA

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	AAA	0.74	3/1245 (0.2%)	1.06	8/1669 (0.5%)
2	CCC	0.60	0/156	0.84	0/203
2	DDD	0.44	0/108	0.95	0/140
All	All	0.71	3/1509 (0.2%)	1.04	8/2012 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	128	GLU	CD-OE1	-6.35	1.18	1.25
1	AAA	87	ARG	NE-CZ	5.67	1.40	1.33
1	AAA	84	GLU	CD-OE2	5.61	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	87	ARG	NE-CZ-NH2	16.23	128.42	120.30
1	AAA	87	ARG	NE-CZ-NH1	-10.57	115.02	120.30
1	AAA	146[A]	MET	CG-SD-CE	-7.56	88.11	100.20
1	AAA	146[B]	MET	CG-SD-CE	-7.56	88.11	100.20
1	AAA	127[A]	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	AAA	127[B]	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	AAA	127[A]	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	AAA	127[B]	ARG	NE-CZ-NH2	-5.61	117.49	120.30

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	AAA	1224	1150	1142	19	0
2	CCC	155	169	167	9	0
2	DDD	105	126	126	3	0
3	AAA	4	0	0	0	0
4	CCC	3	3	3	0	0
5	AAA	134	0	0	4	0
5	CCC	8	0	0	1	0
5	DDD	6	0	0	1	0
All	All	1639	1448	1438	24	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 8.

All (24) 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:AAA:110[A]:MET:SD	2:CCC:315:LEU:HD11	2.06	0.95
1:AAA:110[B]:MET:HE3	1:AAA:110[B]:MET:HA	1.61	0.81
2:DDD:316[A]:ARG:NH1	5:DDD:401:HOH:O	2.18	0.76
1:AAA:81:ASP:C	1:AAA:82[B]:SER:CA	2.53	0.75
1:AAA:110[B]:MET:HA	1:AAA:110[B]:MET:CE	2.19	0.72
1:AAA:82[B]:SER:CA	1:AAA:83:GLU:N	2.53	0.70
1:AAA:87:ARG:NH1	5:AAA:403:HOH:O	2.24	0.66
2:CCC:306:GLU:OE2	5:CCC:501:HOH:O	2.15	0.65
1:AAA:110[A]:MET:SD	2:CCC:315:LEU:CD1	2.84	0.65
1:AAA:148:ALA:HB3	5:AAA:475:HOH:O	1.96	0.65
1:AAA:130:ASP:O	5:AAA:401:HOH:O	2.16	0.60
1:AAA:110[A]:MET:CE	1:AAA:115:GLU:HB3	2.36	0.56
1:AAA:110[A]:MET:CE	2:CCC:315:LEU:HD11	2.37	0.54
1:AAA:110[B]:MET:CE	1:AAA:110[B]:MET:CA	2.82	0.54
2:CCC:313:LYS:O	2:CCC:316:ARG:HG2	2.09	0.52
1:AAA:146[B]:MET:HE3	1:AAA:146[B]:MET:HA	1.91	0.52
1:AAA:110[B]:MET:HE1	2:CCC:315:LEU:HD11	1.92	0.51
2:DDD:312:LEU:O	2:DDD:316[A]:ARG:HG3	2.12	0.50
1:AAA:110[A]:MET:HE1	2:CCC:315:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:110[B]:MET:CE	2:CCC:315:LEU:HD11	2.43	0.48
1:AAA:148:ALA:HB1	5:AAA:502:HOH:O	2.14	0.48
1:AAA:110[A]:MET:HE2	1:AAA:115:GLU:HB3	1.98	0.46
2:DDD:310:GLU:N	2:DDD:310:GLU:OE1	2.53	0.42
1:AAA:82[B]:SER:HB2	2:CCC:316:ARG:HH12	1.85	0.41

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	AAA	154/149 (103%)	152 (99%)	2 (1%)	0	100	100
2	CCC	16/18 (89%)	16 (100%)	0	0	100	100
2	DDD	10/18 (56%)	10 (100%)	0	0	100	100
All	All	180/185 (97%)	178 (99%)	2 (1%)	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	AAA	135/127 (106%)	134 (99%)	1 (1%)	84	59
2	CCC	17/17 (100%)	17 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DDD	12/17 (71%)	12 (100%)	0	100	100
All	All	164/161 (102%)	163 (99%)	1 (1%)	84	63

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	107	ARG

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

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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	ACE	CCC	401	2	1,2,2	0.02	0	1,1,1	0.30	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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	146/149 (97%)	-0.40	1 (0%)	87	84	13, 19, 32, 53	0
2	CCC	18/18 (100%)	0.53	2 (11%)	5	4	20, 28, 40, 44	0
2	DDD	11/18 (61%)	2.12	4 (36%)	0	0	27, 38, 50, 56	0
All	All	175/185 (94%)	-0.14	7 (4%)	38	34	13, 20, 39, 56	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	DDD	308	PHE	5.9
2	DDD	317	LEU	5.9
2	CCC	315	LEU	5.1
2	DDD	311	VAL	3.4
1	AAA	148	ALA	3.1
2	CCC	302	LEU	2.3
2	DDD	315	LEU	2.1

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,

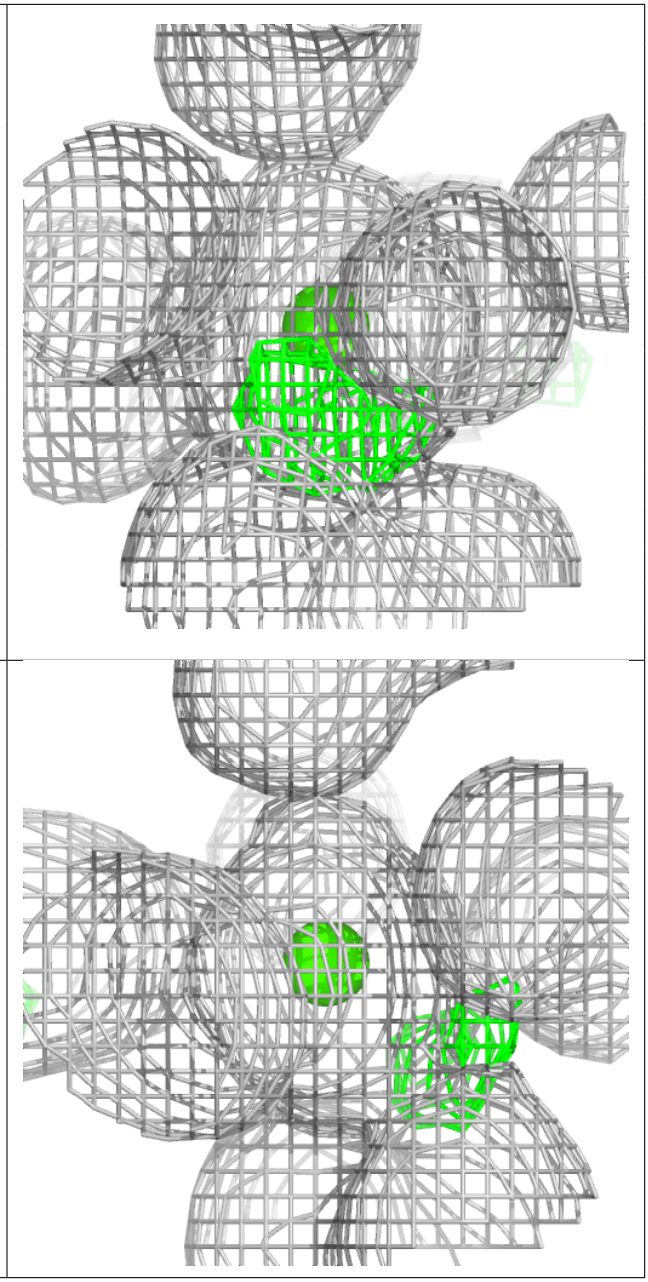
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACE	CCC	401	3/3	0.83	0.18	60,61,63,64	0
3	CA	AAA	302	1/1	1.00	0.06	16,16,16,16	0
3	CA	AAA	303	1/1	1.00	0.08	13,13,13,13	0
3	CA	AAA	304	1/1	1.00	0.06	14,14,14,14	0
3	CA	AAA	301	1/1	1.00	0.08	12,12,12,12	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.

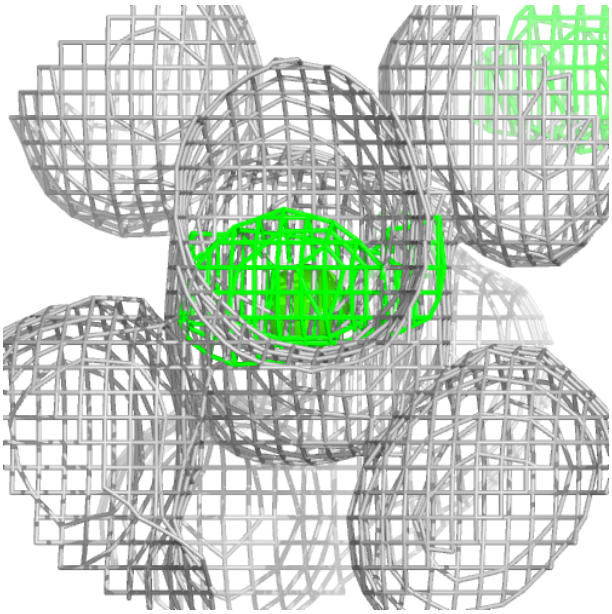
Electron density around CA AAA 302:

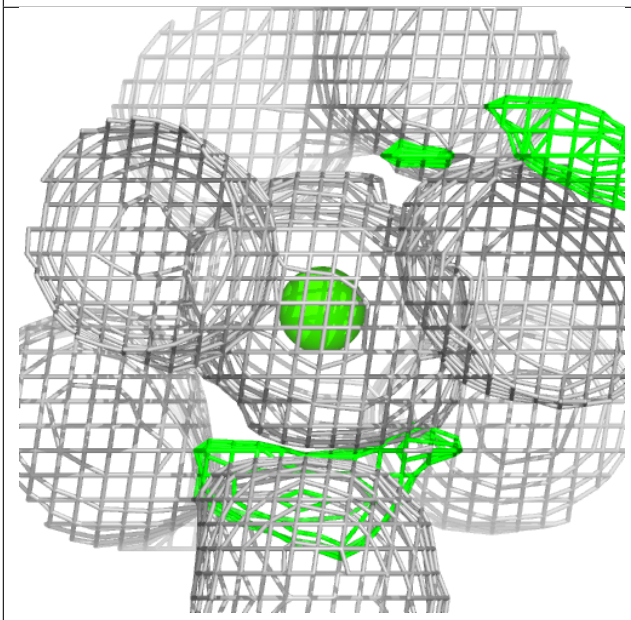
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

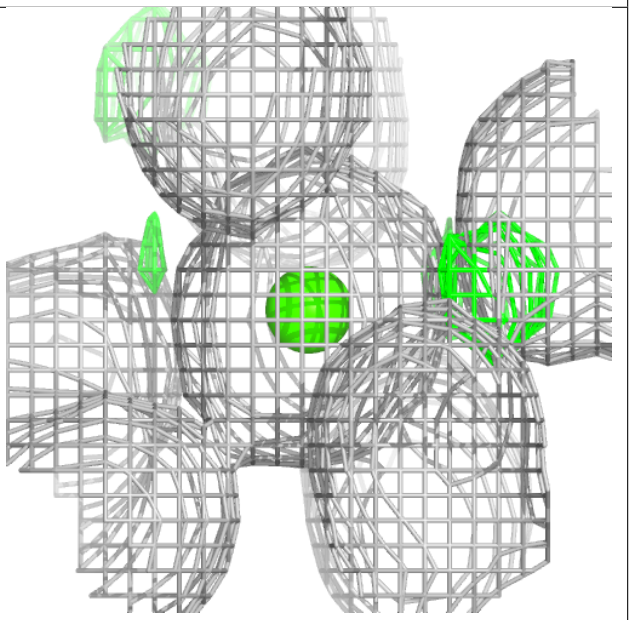


Electron density around CA AAA 303:

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

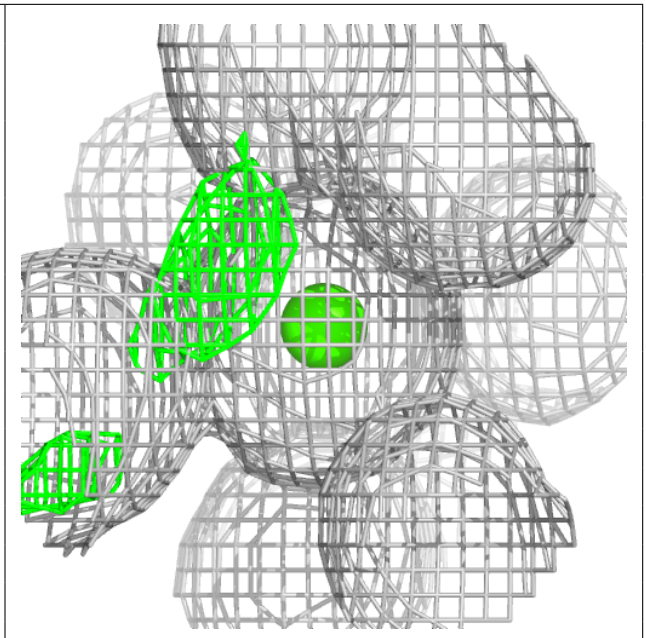


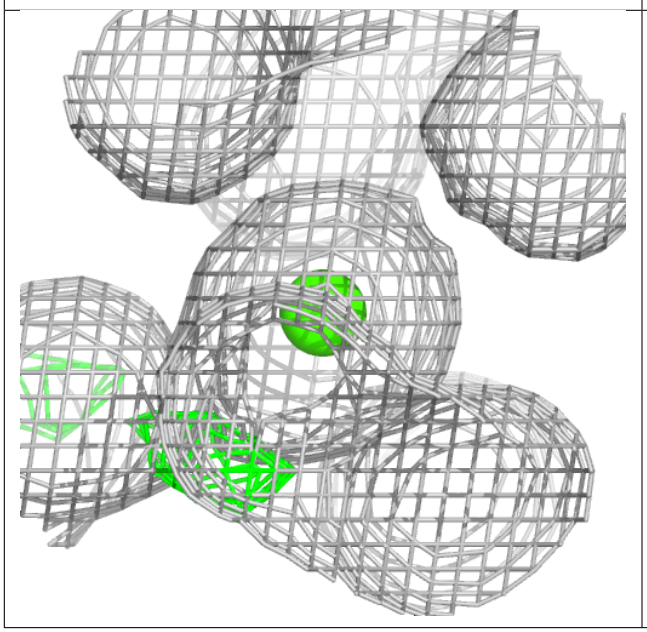


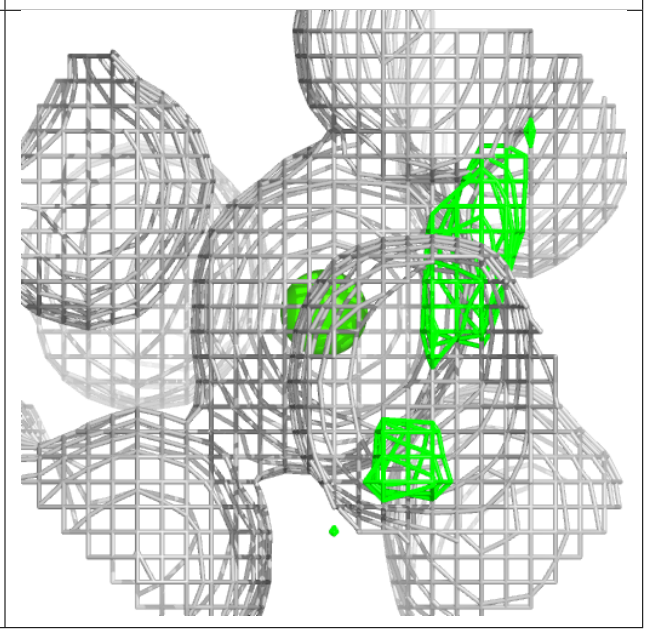


Electron density around CA AAA 304:

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

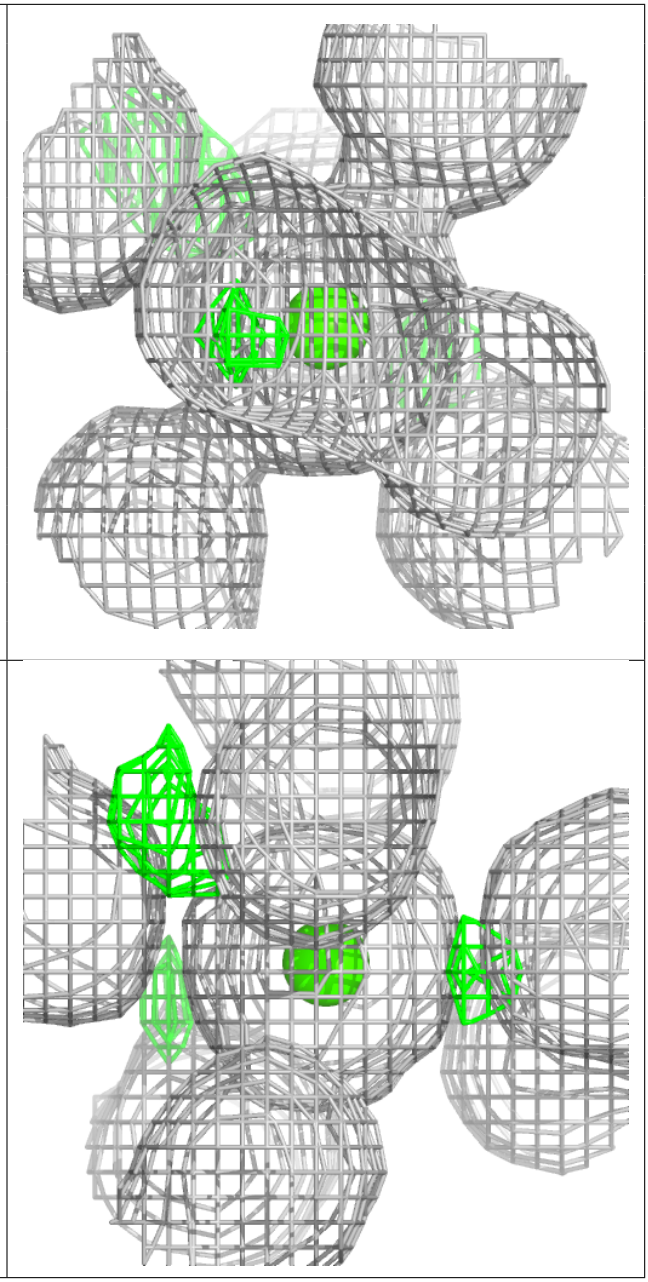






Electron density around CA AAA 301:

$2mF_o$-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 (i)

There are no such residues in this entry.