wwPDB X-ray Structure Validation Summary Report (i)

Nov 19, 2023 – 10:13 PM JST

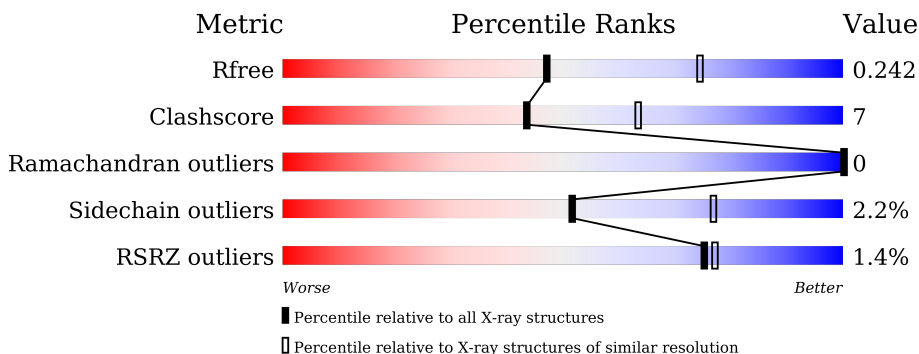|		
PDB ID	:	7BZZ
Title	:	Crystal structure of the SRCR domain of mouse SCARA5
Authors	:	Yu, B.; He, Y.
Deposited on	:	2020-04-29
Resolution	:	2.50 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.242
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		2.2%
RSRZ outliers		1.4%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	113	.% 86% 10% · ·
1	D	113	2% 88% 7% · ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2809 atoms, of which 1035 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 Scavenger receptor class A member 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	109	Total	C	H	N	O	S	0	0	0
			1333	522	484	159	159	9			
1	D	109	Total	C	H	N	O	S	0	0	0
			1404	525	551	161	158	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	490	SER	-	expression tag	UNP Q8K299
A	491	HIS	-	expression tag	UNP Q8K299
A	492	HIS	-	expression tag	UNP Q8K299
A	493	HIS	-	expression tag	UNP Q8K299
A	494	HIS	-	expression tag	UNP Q8K299
A	495	HIS	-	expression tag	UNP Q8K299
A	496	HIS	-	expression tag	UNP Q8K299
D	490	SER	-	expression tag	UNP Q8K299
D	491	HIS	-	expression tag	UNP Q8K299
D	492	HIS	-	expression tag	UNP Q8K299
D	493	HIS	-	expression tag	UNP Q8K299
D	494	HIS	-	expression tag	UNP Q8K299
D	495	HIS	-	expression tag	UNP Q8K299
D	496	HIS	-	expression tag	UNP Q8K299

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	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
3	A	3	Total 3	Ca 3	0	0
3	D	3	Total 3	Ca 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total 20	O 20	0	0
4	D	18	Total 18	O 18	0	0

3 Residue-property plots ⓘ

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: Scavenger receptor class A member 5

• Molecule 1: Scavenger receptor class A member 5

4　Data and refinement statistics　ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	39.80Å　　39.80Å　　132.17Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	27.14　–　2.50 27.15　–　2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (27.14-2.50) 99.5 (27.15-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.84 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.198　,　0.243 0.199　,　0.242	Depositor DCC
R_{free} test set	803 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 36.0	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l 0.487 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2809	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CA, NAG

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	0.54	1/870 (0.1%)	0.69	1/1173 (0.1%)
1	D	0.49	1/875 (0.1%)	0.62	0/1180
All	All	0.52	2/1745 (0.1%)	0.66	1/2353 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	GLN	CD-NE2	-5.91	1.18	1.32
1	D	469	GLN	CD-NE2	-5.73	1.18	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	472	LYS	CG-CD-CE	5.20	127.51	111.90

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	849	484	768	13	2
1	D	853	551	770	9	2
2	A	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	14	0	13	0	0
3	A	3	0	0	0	0
3	D	3	0	0	0	0
4	A	20	0	0	1	0
4	D	18	0	0	1	0
All	All	1774	1035	1564	22	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 7.

The worst 5 of 22 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:D:439:TYR:CD2	1:D:443:ARG:HG3	2.12	0.84
1:A:407:ASP:O	1:A:408:ARG:HB2	1.79	0.81
1:A:443:ARG:O	1:A:443:ARG:HD2	1.85	0.75
1:A:439:TYR:CD2	1:A:443:ARG:HG3	2.24	0.72
1:A:439:TYR:CD2	1:A:443:ARG:CG	2.74	0.71

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:A:440:ARG:HH12	1:D:436:GLU:OE1[2_555]	1.47	0.13
1:A:416:ASP:OD2	1:D:420:LYS:NZ[2_555]	2.15	0.05

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	107/113 (95%)	98 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	107/113 (95%)	99 (92%)	8 (8%)	0	100	100
All	All	214/226 (95%)	197 (92%)	17 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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	89/95 (94%)	88 (99%)	1 (1%)	73	89
1	D	89/95 (94%)	86 (97%)	3 (3%)	37	63
All	All	178/190 (94%)	174 (98%)	4 (2%)	52	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	ARG
1	D	420	LYS
1	D	443	ARG
1	D	492	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	#$|Z| > 2$
2	NAG	A	501	1	14,14,15	0.72	1 (7%)	17,19,21	0.77	0
2	NAG	D	501	1	14,14,15	0.69	1 (7%)	17,19,21	0.77	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
2	NAG	A	501	1	-	2/6/23/26	0/1/1/1
2	NAG	D	501	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAG	O5-C1	-2.39	1.39	1.43
2	D	501	NAG	O5-C1	-2.39	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	NAG	O5-C5-C6-O6
2	A	501	NAG	O5-C5-C6-O6
2	D	501	NAG	C4-C5-C6-O6
2	A	501	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	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, 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	A	109/113 (96%)	-0.16	1 (0%)	84	86	33, 47, 72, 101	0
1	D	109/113 (96%)	-0.18	2 (1%)	68	71	33, 47, 72, 91	0
All	All	218/226 (96%)	-0.17	3 (1%)	75	77	33, 47, 80, 101	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	PHE	3.0
1	D	386	PHE	3.0
1	D	433	HIS	2.4

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 ⓘ

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
2	NAG	A	501	14/15	0.84	0.17	64,73,78,82	0
2	NAG	D	501	14/15	0.89	0.15	63,73,78,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	A	502	1/1	0.94	0.14	43,43,43,43	0
3	CA	D	504	1/1	0.94	0.10	58,58,58,58	0
3	CA	A	504	1/1	0.95	0.14	52,52,52,52	0
3	CA	D	503	1/1	0.96	0.13	43,43,43,43	0
3	CA	A	503	1/1	0.97	0.13	42,42,42,42	0
3	CA	D	502	1/1	0.97	0.12	40,40,40,40	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 A 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
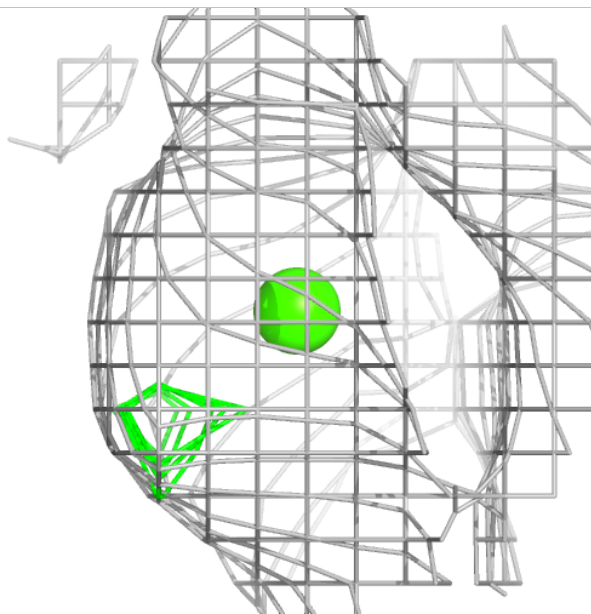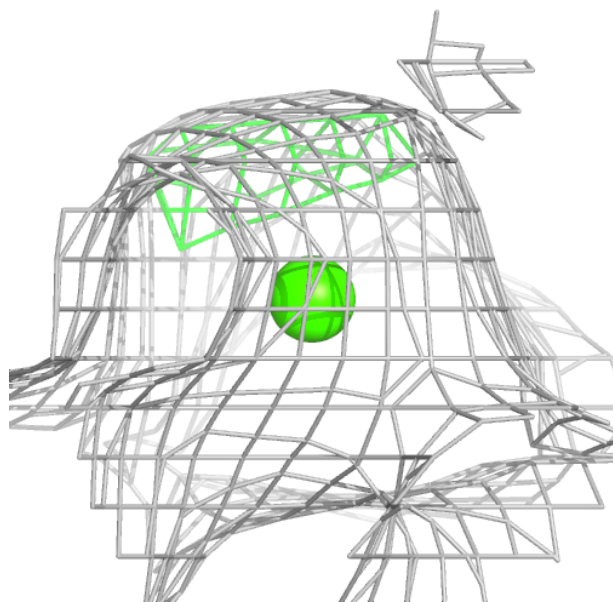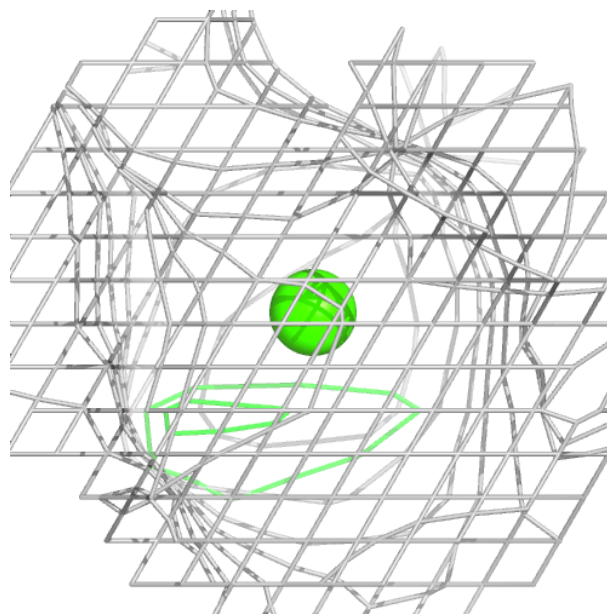
Electron density around CA D 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
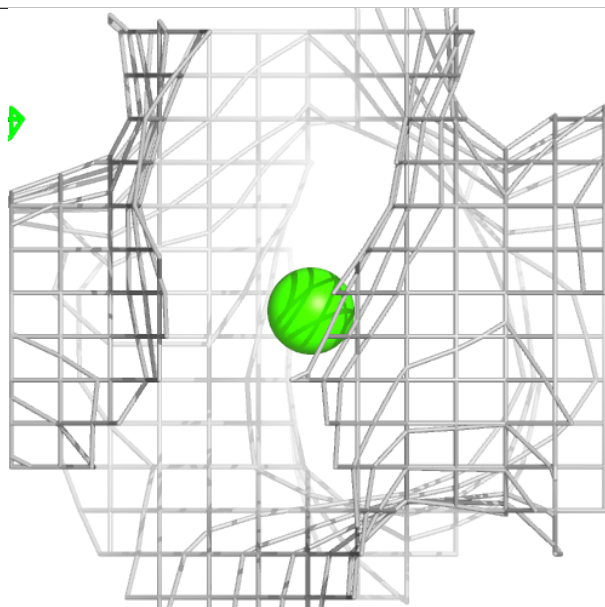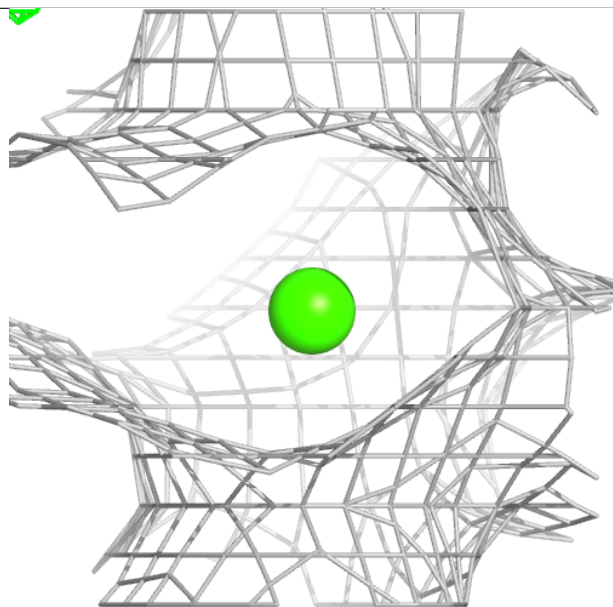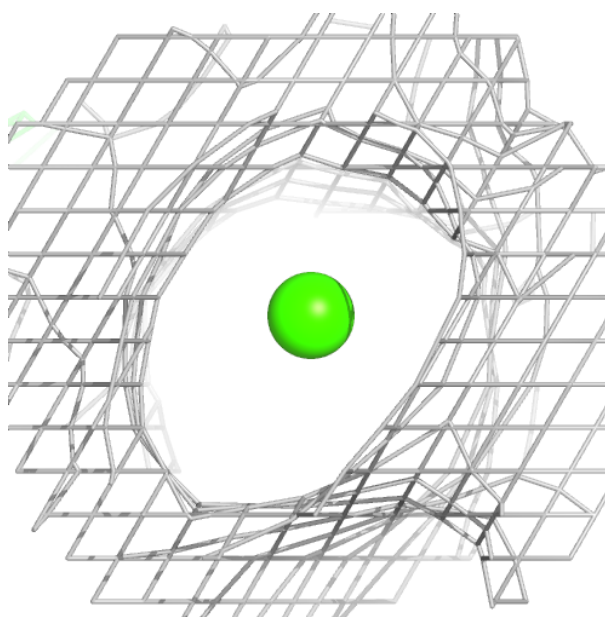and green (positive)
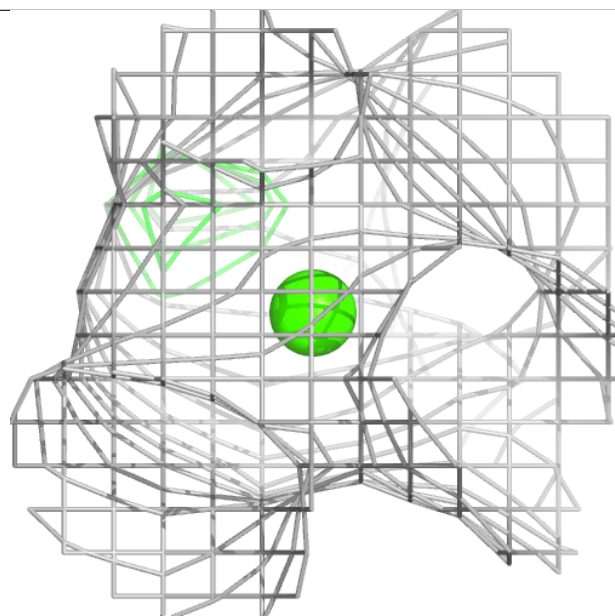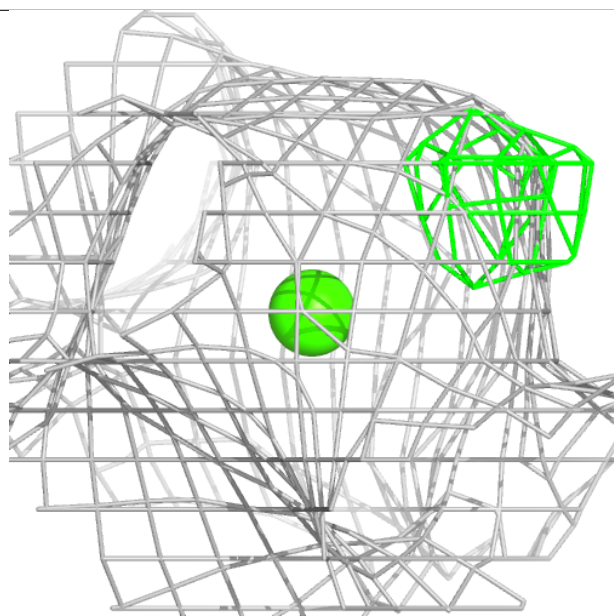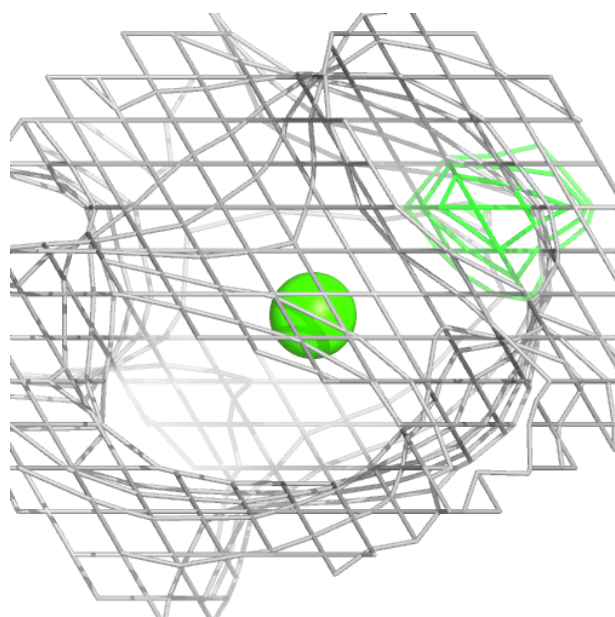
Electron density around CA A 504:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
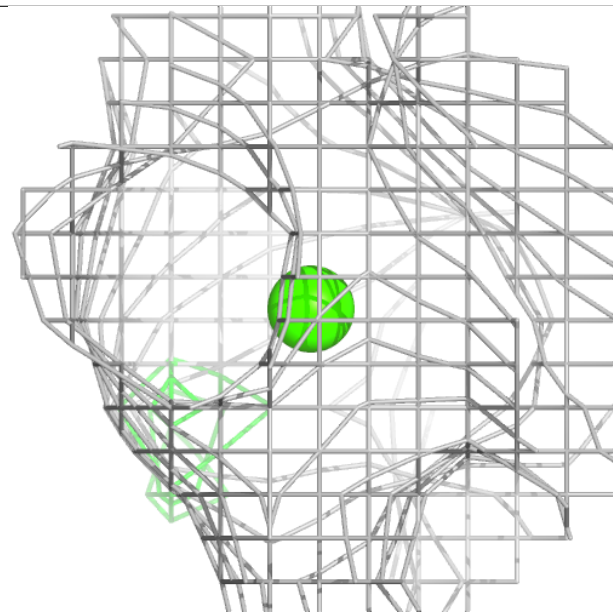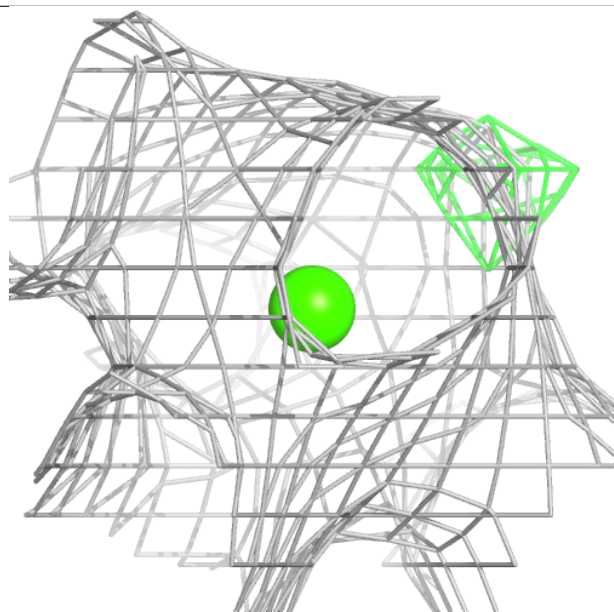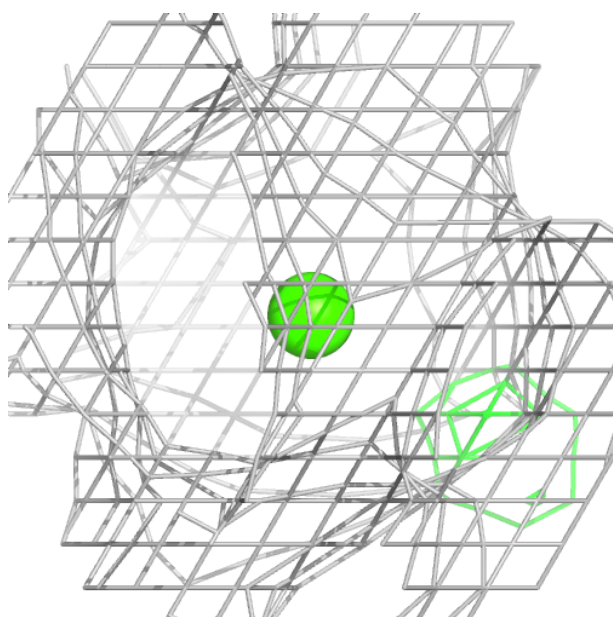
Electron density around CA D 503:

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

Electron density around CA A 503:
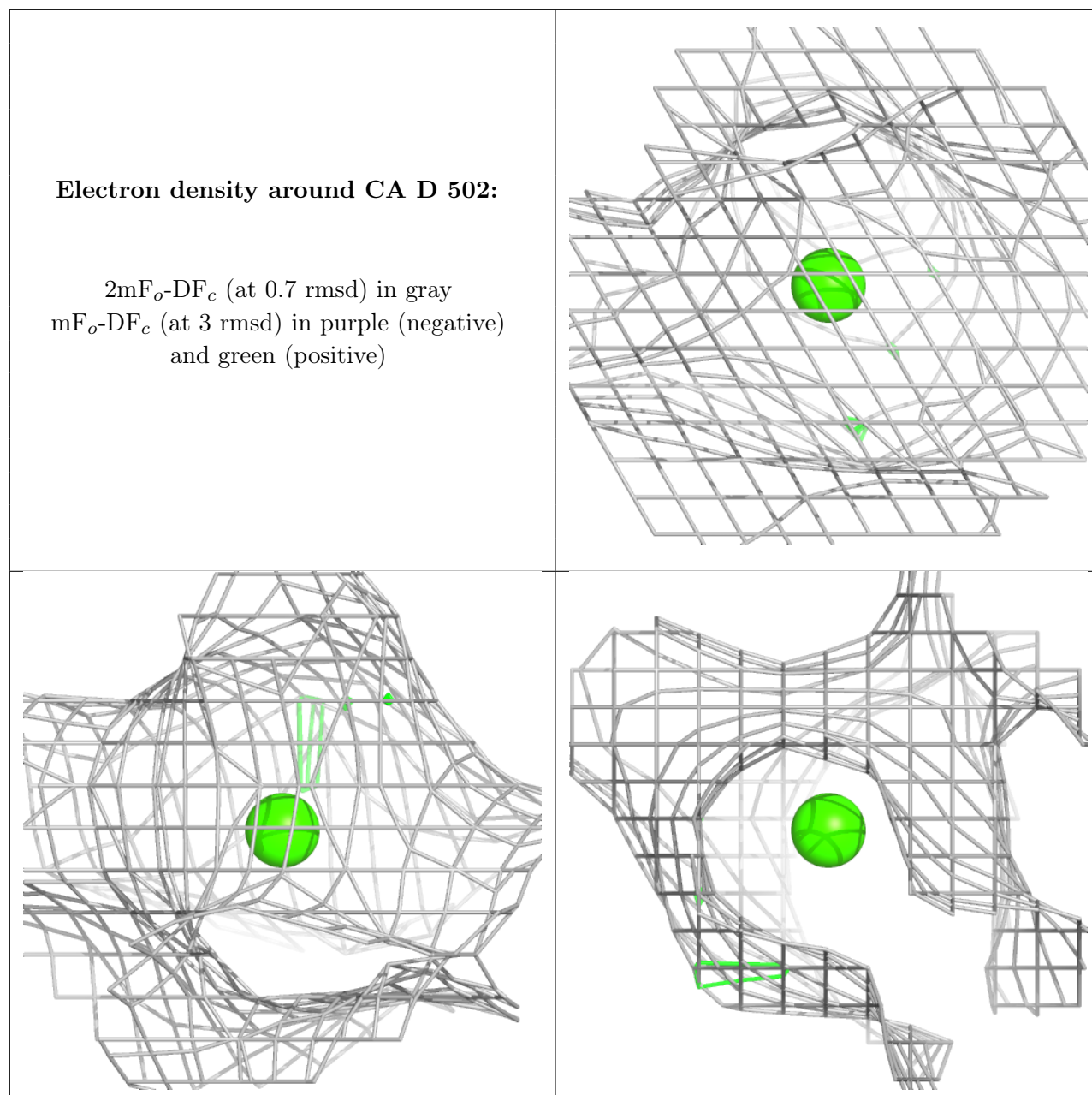
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CA D 502:

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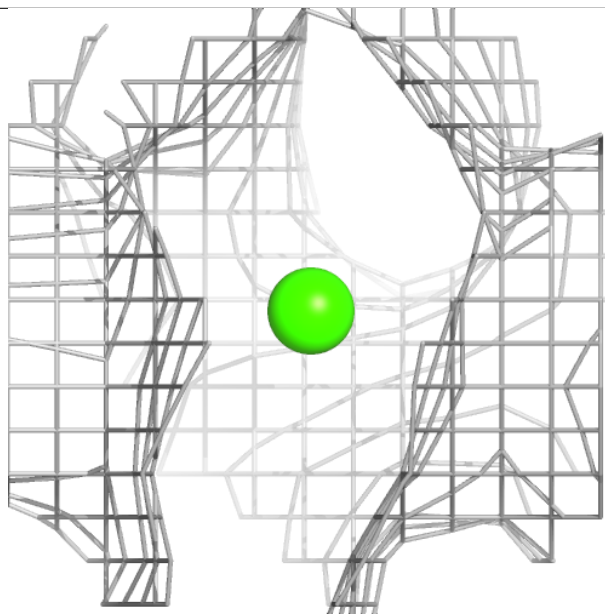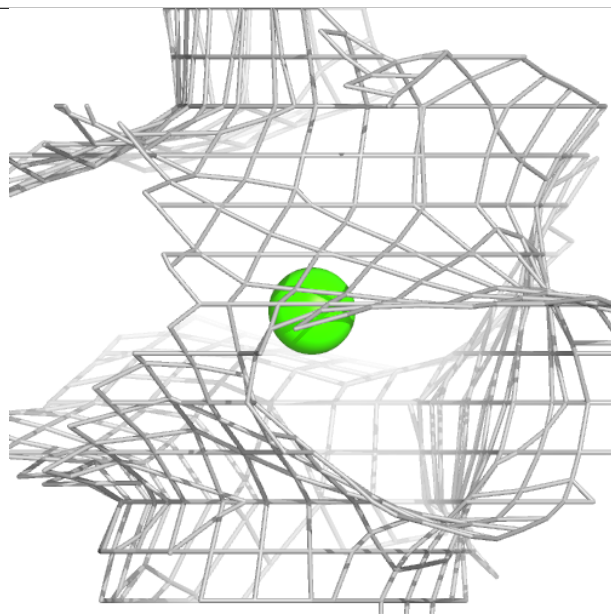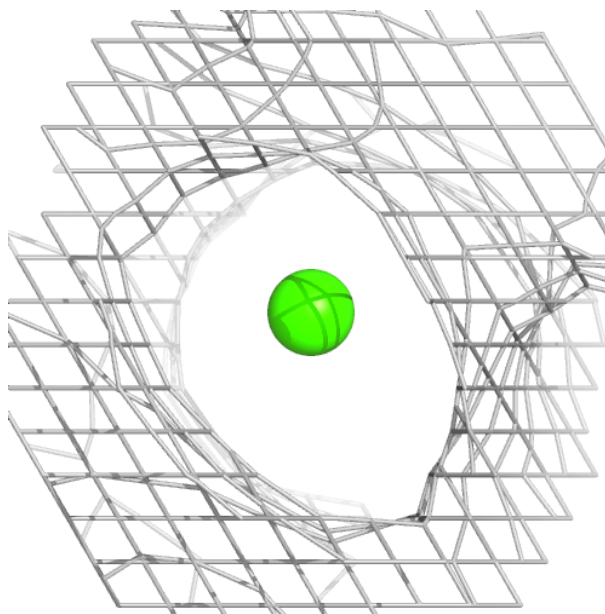
6.5 Other polymers (i)

There are no such residues in this entry.