



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:58 PM BST

PDB ID : 6V2J
Title : Crystal structure of ClC-ec1 triple mutant (E113Q, E148Q, E203Q)
Authors : Maduke, M.; Mathews, I.I.; Chavan, T.S.
Deposited on : 2019-11-24
Resolution : 2.62 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 ⓘ symbol.

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

MolProbity : 4.02b-467
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

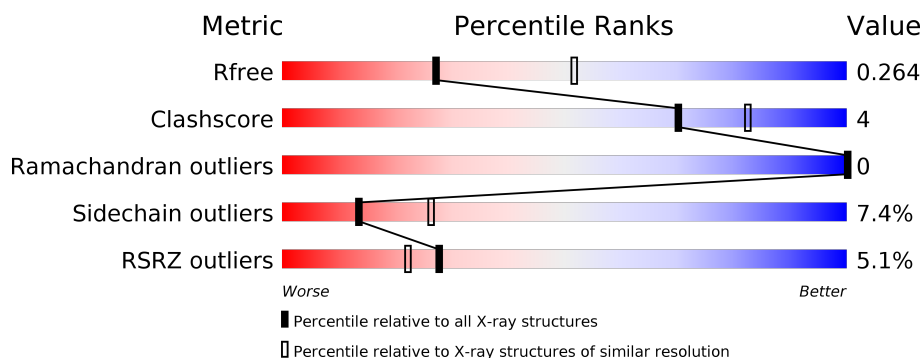
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 $\leq 5\%$. 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	489	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3310 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 H(+)/Cl(-) exchange transporter ClcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	1	0
			3252	2141	544	547	20			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLN	GLU	engineered mutation	UNP P37019
A	148	GLN	GLU	engineered mutation	UNP P37019
A	203	GLN	GLU	engineered mutation	UNP P37019
A	469	LYS	-	expression tag	UNP P37019
A	470	GLY	-	expression tag	UNP P37019
A	471	SER	-	expression tag	UNP P37019
A	472	GLY	-	expression tag	UNP P37019
A	473	THR	-	expression tag	UNP P37019
A	474	LEU	-	expression tag	UNP P37019
A	475	VAL	-	expression tag	UNP P37019
A	476	PRO	-	expression tag	UNP P37019
A	477	ARG	-	expression tag	UNP P37019
A	478	GLY	-	expression tag	UNP P37019
A	479	SER	-	expression tag	UNP P37019
A	480	GLY	-	expression tag	UNP P37019
A	481	GLY	-	expression tag	UNP P37019
A	482	LEU	-	expression tag	UNP P37019
A	483	GLU	-	expression tag	UNP P37019
A	484	HIS	-	expression tag	UNP P37019
A	485	HIS	-	expression tag	UNP P37019
A	486	HIS	-	expression tag	UNP P37019
A	487	HIS	-	expression tag	UNP P37019
A	488	HIS	-	expression tag	UNP P37019
A	489	HIS	-	expression tag	UNP P37019

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cl	0	0
			3	3		

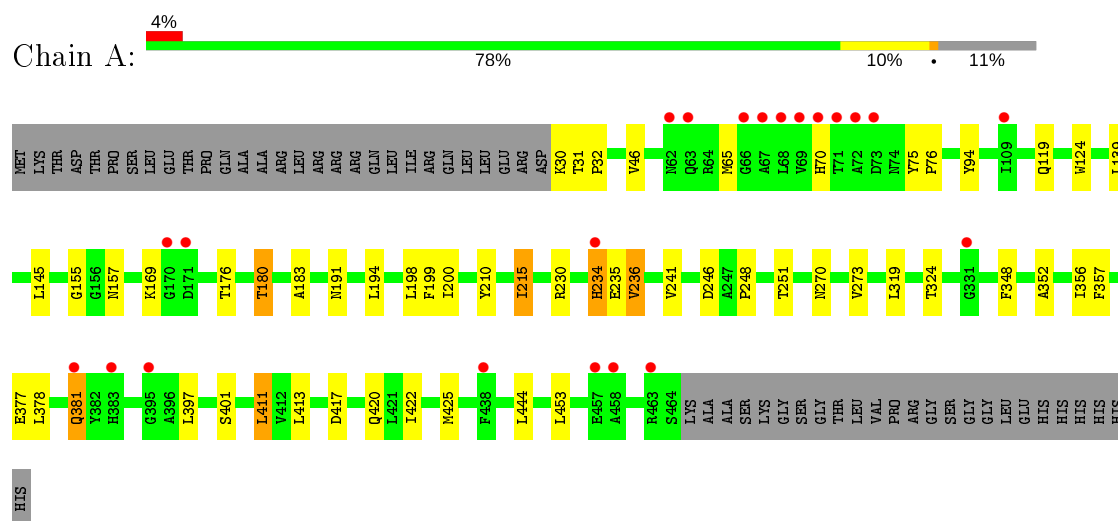
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		

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: H(+)/Cl(-) exchange transporter ClcA



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	80.97Å 120.44Å 122.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.65 – 2.62 28.64 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.2 (28.65-2.62) 97.4 (28.64-2.62)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.193 , 0.262 0.198 , 0.264	Depositor DCC
R_{free} test set	962 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3310	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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:
CL

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	0.64	0/3324	0.70	0/4514

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	3252	0	3401	24	0
2	A	3	0	0	1	0
3	A	55	0	0	1	0
All	All	3310	0	3401	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 4.

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:A:124:TRP:HA	1:A:157:ASN:HD22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLN:HE21	1:A:381:GLN:H	1.50	0.59
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.41	0.56
1:A:183:ALA:HB2	1:A:200:ILE:HD13	1.87	0.56
1:A:357:PHE:CZ	1:A:411:LEU:HD13	2.42	0.54
1:A:357:PHE:HB3	2:A:503:CL:CL	2.47	0.51
1:A:31:THR:N	1:A:32:PRO:CD	2.74	0.51
1:A:241:VAL:HG21	1:A:324:THR:HG21	1.92	0.50
1:A:139:LEU:HD22	1:A:145:LEU:HB2	1.96	0.48
1:A:176:THR:O	1:A:180:THR:HG23	2.15	0.47
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.97	0.46
1:A:241:VAL:CG2	1:A:324:THR:HG21	2.45	0.46
1:A:124:TRP:CA	1:A:157:ASN:HD22	2.28	0.46
1:A:199:PHE:CD2	1:A:200:ILE:HD12	2.53	0.43
1:A:199:PHE:HD2	1:A:200:ILE:HD12	1.83	0.43
1:A:169:LYS:HA	3:A:650:HOH:O	2.18	0.43
1:A:413:LEU:HD21	1:A:425:MET:HE3	2.01	0.42
1:A:270:ASN:HD21	1:A:401:SER:HB3	1.85	0.42
1:A:210:TYR:CZ	1:A:215:ILE:HG13	2.56	0.41
1:A:248:PRO:O	1:A:251:THR:HB	2.21	0.41
1:A:234:HIS:O	1:A:236:VAL:HG22	2.20	0.41
1:A:191:ASN:HD21	1:A:235:GLU:HG2	1.86	0.41
1:A:348:PHE:CD2	1:A:356:ILE:HD12	2.55	0.41
1:A:75:TYR:N	1:A:76:PRO:CD	2.85	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	434/489 (89%)	418 (96%)	16 (4%)	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	326/370 (88%)	302 (93%)	24 (7%)	13	26

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	65	MET
1	A	70	HIS
1	A	119	GLN
1	A	180	THR
1	A	194	LEU
1	A	198	LEU
1	A	215	ILE
1	A	230	ARG
1	A	234	HIS
1	A	236	VAL
1	A	246	ASP
1	A	273	VAL
1	A	319	LEU
1	A	377	GLU
1	A	378	LEU
1	A	381	GLN
1	A	397	LEU
1	A	411	LEU
1	A	417	ASP
1	A	420	GLN
1	A	422	ILE
1	A	444	LEU
1	A	453	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN

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Mol	Chain	Res	Type
1	A	153	GLN
1	A	157	ASN
1	A	270	ASN
1	A	277	GLN
1	A	327	ASN
1	A	381	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 3 ligands modelled in this entry, 3 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 [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	A	435/489 (88%)	0.06	22 (5%) 28 22	45, 61, 89, 123	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	VAL	5.2
1	A	70	HIS	5.2
1	A	72	ALA	4.5
1	A	73	ASP	4.3
1	A	66	GLY	4.1
1	A	71	THR	4.1
1	A	438	PHE	3.5
1	A	458	ALA	3.2
1	A	63	GLN	2.9
1	A	67	ALA	2.9
1	A	234	HIS	2.8
1	A	62	ASN	2.8
1	A	331	GLY	2.6
1	A	68	LEU	2.6
1	A	383	HIS	2.4
1	A	109	ILE	2.4
1	A	171	ASP	2.3
1	A	395	GLY	2.3
1	A	381	GLN	2.2
1	A	170	GLY	2.1
1	A	463	ARG	2.1
1	A	457	GLU	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

There are no monosaccharides in this entry.

6.4 Ligands

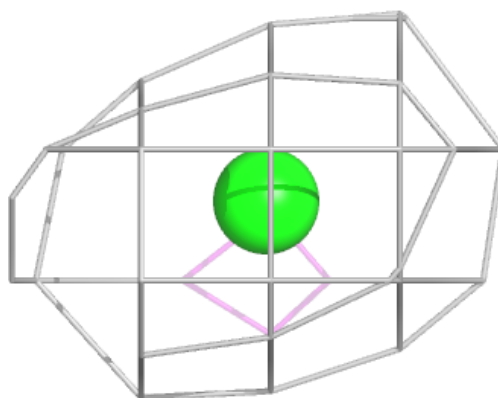
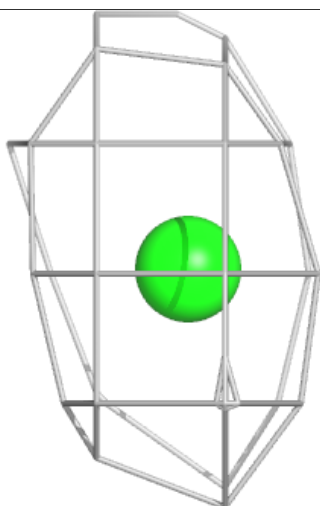
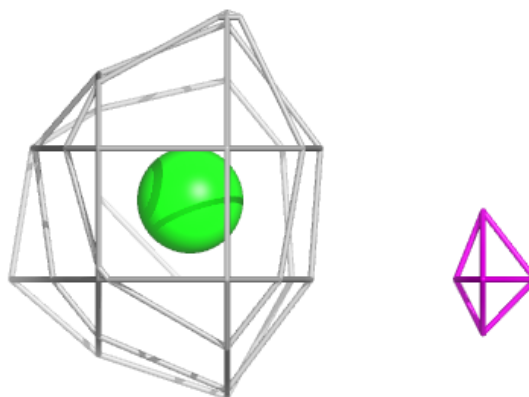
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	A	502	1/1	0.87	0.66	95,95,95,95	0
2	CL	A	503	1/1	0.93	0.22	75,75,75,75	0
2	CL	A	501	1/1	0.96	0.45	80,80,80,80	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.

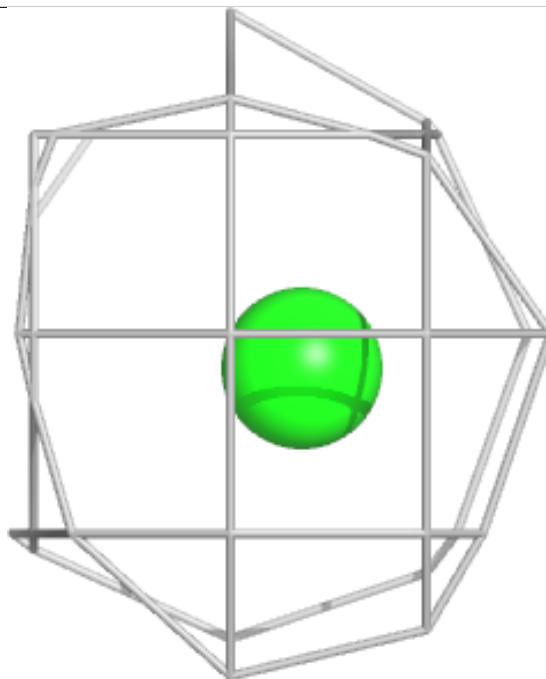
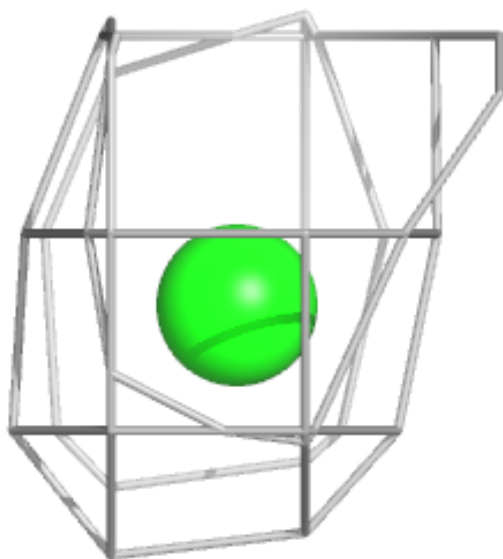
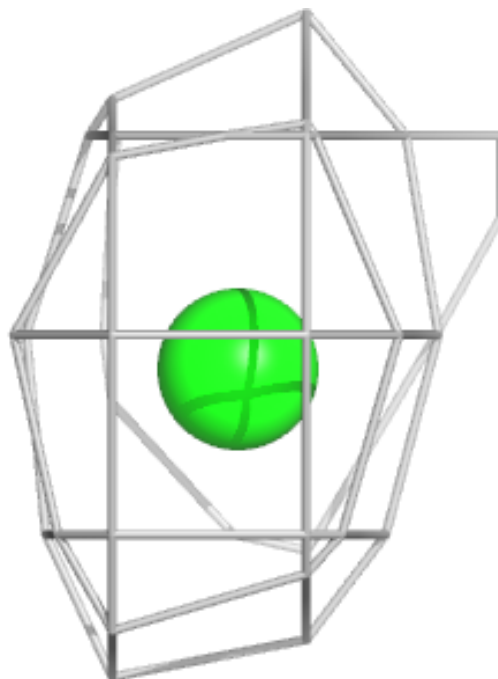
Electron density around CL A 502:

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



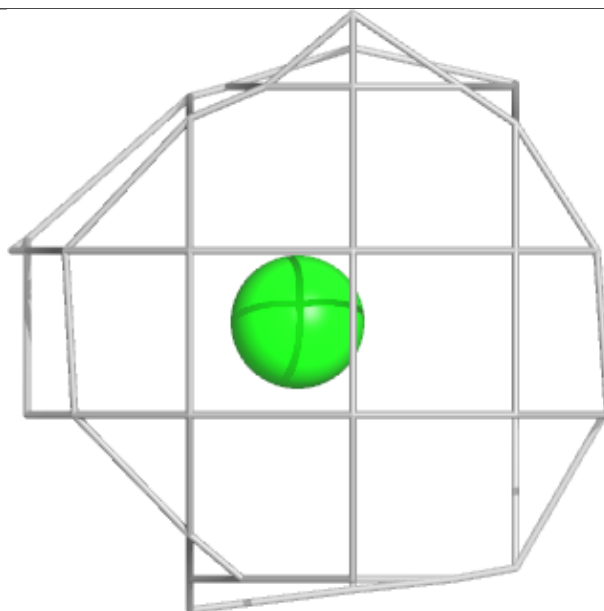
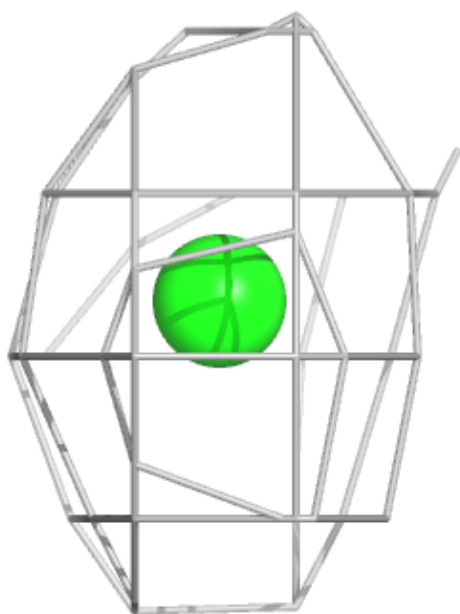
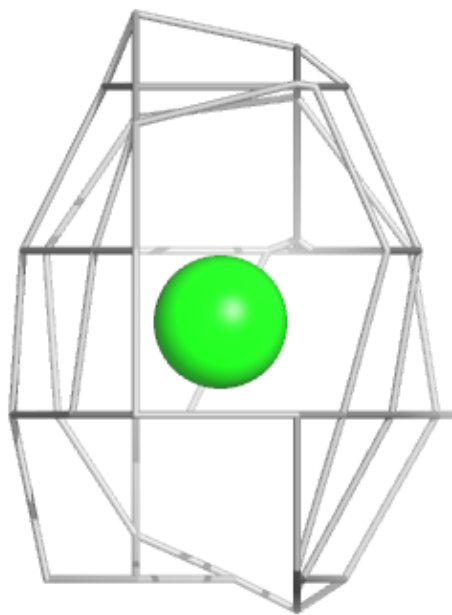
Electron density around CL A 503:

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



Electron density around CL A 501:

$2mF_o-DF_c$ (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.