



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2022 – 06:09 PM JST

PDB ID : 6LSC
Title : Structure of the E202Y mutant of the Cl⁻/H⁺ antiporter CLC-ec1 from E.coli:
a re-refined model of the 4FTP model
Authors : Lim, H.H.; Shane, T.; Miller, C.
Deposited on : 2020-01-17
Resolution : 3.21 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	:	2.27
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)	:	2.27

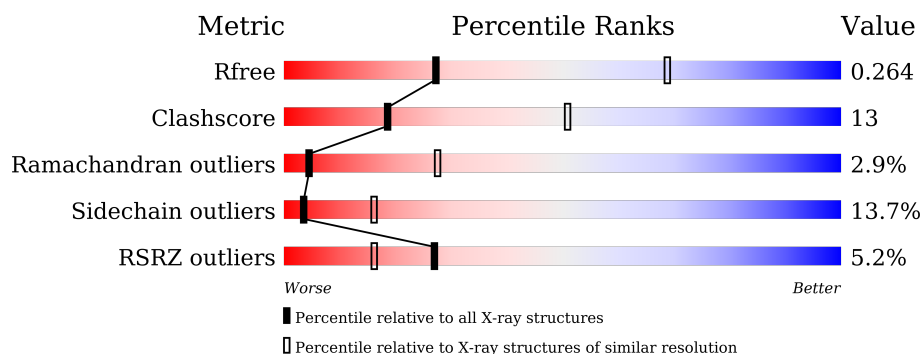
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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 $\leq 5\%$. 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	465	<div> <div>5%</div> <div> <div>57%</div> <div>29%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3144 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	423	Total	C	N	O	S	0	0	0
			3142	2076	515	531	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	TYR	GLU	engineered mutation	UNP P37019

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

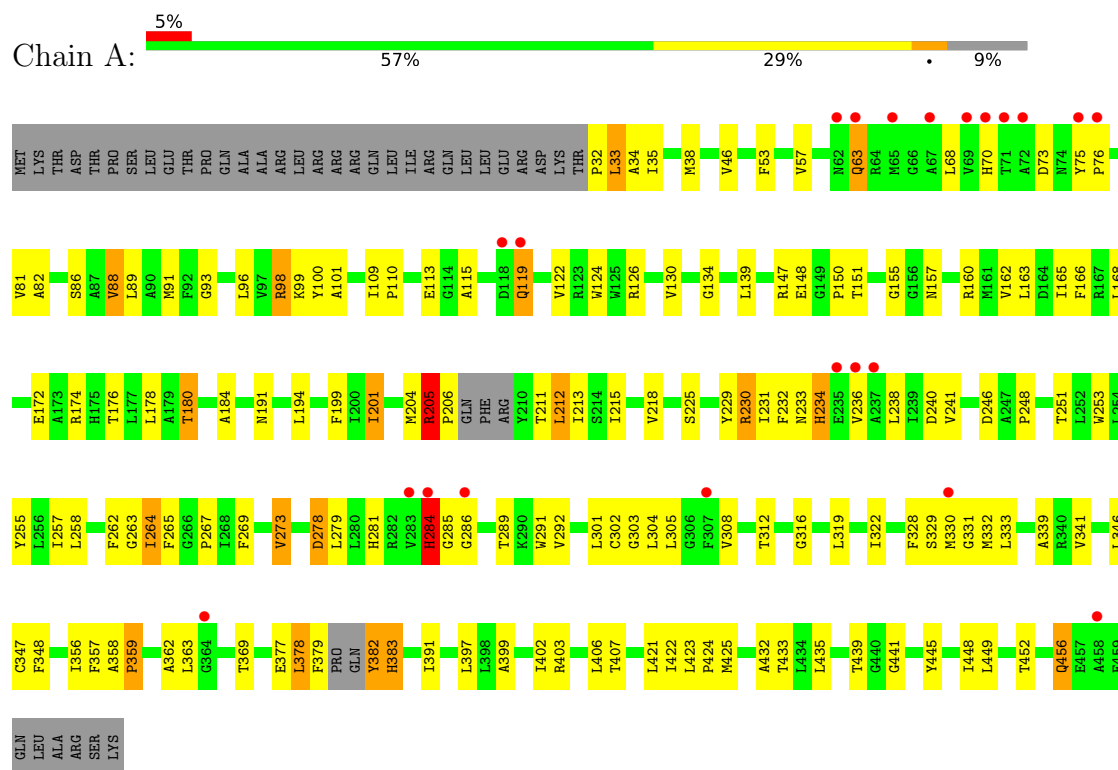
- Molecule 3 is water.

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

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.70Å 85.17Å 100.09Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	24.43 – 3.21 24.42 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.43-3.21) 99.2 (24.42-3.21)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.85 (at 3.23Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.210 , 0.263 0.216 , 0.264	Depositor DCC
R_{free} test set	637 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	103.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3144	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.67	0/3211	0.81	0/4360

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	THR	Peptide

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	A	3142	0	3278	85	0
2	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
All	All	3144	0	3278	85	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 13.

All (85) 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	1.48	0.79
1:A:204:MET:O	1:A:205:ARG:HB2	1.86	0.73
1:A:456:GLN:O	1:A:456:GLN:CG	2.40	0.69
1:A:165:ILE:HG22	1:A:166:PHE:CD1	2.32	0.65
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.28	0.64
1:A:91:MET:HG2	1:A:292:VAL:O	1.97	0.64
1:A:445:TYR:OH	2:A:501:CL:CL	2.53	0.62
1:A:263:GLY:HA2	1:A:432:ALA:O	2.00	0.61
1:A:176:THR:O	1:A:180:THR:HG23	2.01	0.61
1:A:456:GLN:O	1:A:456:GLN:HG3	2.00	0.61
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.36	0.60
1:A:122:VAL:HG21	1:A:178:LEU:HD11	1.84	0.60
1:A:184:ALA:HB1	1:A:225:SER:HB2	1.82	0.60
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.84	0.59
1:A:205:ARG:HD3	1:A:206:PRO:HD2	1.85	0.59
1:A:269:PHE:O	1:A:273:VAL:HG12	2.01	0.59
1:A:147:ARG:O	1:A:151:THR:HG23	2.05	0.56
1:A:53:PHE:O	1:A:57:VAL:HG23	2.05	0.56
1:A:382:TYR:O	1:A:383:HIS:HB2	2.07	0.55
1:A:356:ILE:O	1:A:356:ILE:HG23	2.06	0.55
1:A:148:GLU:HG3	1:A:357:PHE:HB3	1.88	0.54
1:A:180:THR:HB	1:A:218:VAL:HA	1.89	0.54
1:A:248:PRO:O	1:A:251:THR:HB	2.09	0.53
1:A:378:LEU:HB3	1:A:379:PHE:CE1	2.44	0.53
1:A:278:ASP:N	1:A:278:ASP:OD1	2.41	0.52
1:A:284:HIS:O	1:A:286:GLY:N	2.43	0.52
1:A:231:ILE:HG22	1:A:232:PHE:CD1	2.44	0.52
1:A:348:PHE:CD1	1:A:356:ILE:HB	2.45	0.52
1:A:258:LEU:HD11	1:A:262:PHE:HE2	1.74	0.52
1:A:93:GLY:HA2	1:A:134:GLY:HA2	1.93	0.51
1:A:163:LEU:HD22	1:A:174:ARG:HA	1.92	0.51
1:A:378:LEU:HB3	1:A:379:PHE:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:HD11	1:A:369:THR:HG22	1.93	0.49
1:A:205:ARG:HD3	1:A:206:PRO:CD	2.43	0.49
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.94	0.49
1:A:119:GLN:HE21	1:A:119:GLN:HA	1.77	0.49
1:A:251:THR:HG22	1:A:255:TYR:HE2	1.77	0.49
1:A:329:SER:O	1:A:332:MET:N	2.46	0.49
1:A:34:ALA:O	1:A:38:MET:HG2	2.13	0.48
1:A:99:LYS:HG2	1:A:100:TYR:CE1	2.47	0.48
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.94	0.48
1:A:199:PHE:HB2	1:A:407:THR:HG21	1.94	0.48
1:A:100:TYR:O	1:A:126:ARG:HD3	2.14	0.48
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.96	0.48
1:A:316:GLY:HA3	1:A:362:ALA:HB2	1.94	0.48
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.49	0.47
1:A:423:LEU:N	1:A:424:PRO:HD2	2.30	0.47
1:A:229:TYR:CE1	1:A:233:ASN:ND2	2.83	0.47
1:A:253:TRP:CE3	1:A:257:ILE:CD1	2.99	0.46
1:A:148:GLU:CG	1:A:357:PHE:HB3	2.46	0.46
1:A:205:ARG:HB3	1:A:206:PRO:HD2	1.96	0.46
1:A:267:PRO:HB3	1:A:441:GLY:HA3	1.98	0.46
1:A:301:LEU:O	1:A:304:LEU:HB3	2.16	0.46
1:A:358:ALA:HB3	1:A:359:PRO:CD	2.46	0.45
1:A:35:ILE:HG21	1:A:176:THR:HG21	1.97	0.45
1:A:201:ILE:HD12	1:A:215:ILE:HG23	1.98	0.45
1:A:264:ILE:HG22	1:A:435:LEU:HD12	1.99	0.44
1:A:421:LEU:O	1:A:425:MET:HG3	2.16	0.44
1:A:130:VAL:O	1:A:134:GLY:N	2.40	0.44
1:A:322:ILE:HG22	1:A:328:PHE:CE2	2.52	0.44
1:A:63:GLN:HE21	1:A:63:GLN:N	2.16	0.44
1:A:346:LEU:HD12	1:A:346:LEU:HA	1.90	0.43
1:A:86:SER:CB	1:A:303:GLY:HA3	2.49	0.43
1:A:148:GLU:HG3	1:A:357:PHE:CB	2.48	0.43
1:A:329:SER:O	1:A:331:GLY:N	2.52	0.43
1:A:341:VAL:HG22	1:A:363:LEU:HD13	2.00	0.43
1:A:109:ILE:N	1:A:110:PRO:CD	2.82	0.43
1:A:110:PRO:O	1:A:449:LEU:HD13	2.19	0.43
1:A:201:ILE:CD1	1:A:215:ILE:HA	2.48	0.43
1:A:263:GLY:HA3	1:A:435:LEU:HB2	2.01	0.42
1:A:101:ALA:HB3	1:A:130:VAL:HG11	2.01	0.42
1:A:253:TRP:CZ3	1:A:257:ILE:CD1	3.03	0.42
1:A:174:ARG:O	1:A:178:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HD21	1:A:82:ALA:HB2	2.02	0.42
1:A:88:VAL:HG12	1:A:89:LEU:N	2.35	0.42
1:A:194:LEU:HA	1:A:194:LEU:HD23	1.78	0.41
1:A:312:THR:HG22	1:A:339:ALA:CB	2.50	0.41
1:A:75:TYR:HB3	1:A:76:PRO:HD3	2.03	0.41
1:A:148:GLU:H	1:A:148:GLU:CD	2.24	0.41
1:A:399:ALA:O	1:A:403:ARG:HA	2.21	0.41
1:A:115:ALA:HB1	1:A:178:LEU:HD21	2.02	0.41
1:A:110:PRO:HG2	1:A:448:ILE:HG21	2.02	0.41
1:A:302:CYS:SG	1:A:347:CYS:SG	3.17	0.41
1:A:264:ILE:HG13	1:A:265:PHE:N	2.36	0.40
1:A:267:PRO:HG2	1:A:439:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

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	417/465 (90%)	338 (81%)	67 (16%)	12 (3%)	4	27

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ARG
1	A	212	LEU
1	A	330	MET
1	A	234	HIS
1	A	452	THR
1	A	33	LEU
1	A	285	GLY
1	A	383	HIS
1	A	284	HIS

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Mol	Chain	Res	Type
1	A	391	ILE
1	A	150	PRO
1	A	241	VAL

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	314/353 (89%)	271 (86%)	43 (14%)	3	16

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PRO
1	A	33	LEU
1	A	63	GLN
1	A	70	HIS
1	A	73	ASP
1	A	81	VAL
1	A	88	VAL
1	A	96	LEU
1	A	98	ARG
1	A	113	GLU
1	A	119	GLN
1	A	139	LEU
1	A	160	ARG
1	A	162	VAL
1	A	172	GLU
1	A	180	THR
1	A	201	ILE
1	A	205	ARG
1	A	212	LEU
1	A	213	ILE
1	A	230	ARG
1	A	234	HIS
1	A	236	VAL

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Mol	Chain	Res	Type
1	A	238	LEU
1	A	240	ASP
1	A	246	ASP
1	A	264	ILE
1	A	273	VAL
1	A	278	ASP
1	A	279	LEU
1	A	284	HIS
1	A	289	THR
1	A	319	LEU
1	A	359	PRO
1	A	377	GLU
1	A	378	LEU
1	A	382	TYR
1	A	397	LEU
1	A	402	ILE
1	A	406	LEU
1	A	422	ILE
1	A	433	THR
1	A	456	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	63	GLN
1	A	119	GLN
1	A	157	ASN
1	A	270	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [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	A	423/465 (90%)	-0.06	22 (5%) 27 16	62, 98, 148, 189	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ALA	7.0
1	A	72	ALA	4.5
1	A	118	ASP	4.2
1	A	71	THR	3.4
1	A	307	PHE	3.4
1	A	75	TYR	3.2
1	A	65	MET	3.1
1	A	235	GLU	3.0
1	A	70	HIS	3.0
1	A	236	VAL	2.7
1	A	286	GLY	2.7
1	A	119	GLN	2.6
1	A	283	VAL	2.6
1	A	67	ALA	2.5
1	A	284	HIS	2.4
1	A	62	ASN	2.3
1	A	76	PRO	2.2
1	A	364	GLY	2.2
1	A	69	VAL	2.2
1	A	63	GLN	2.0
1	A	458	ALA	2.0
1	A	330	MET	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](#)

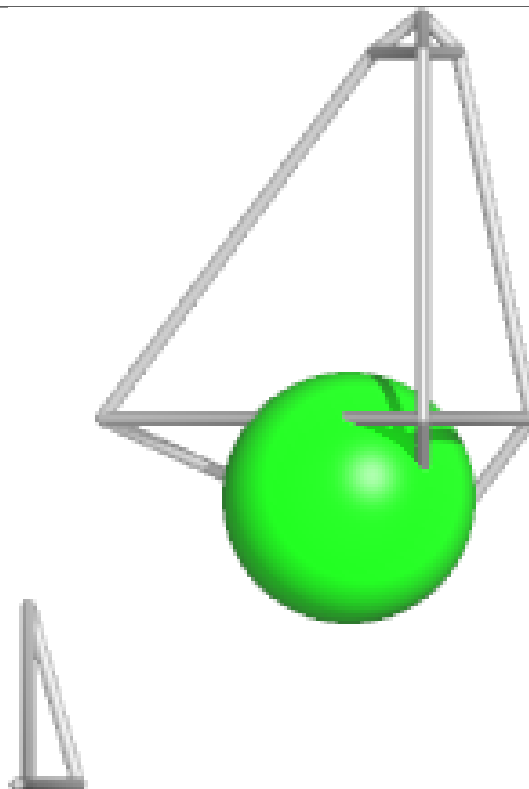
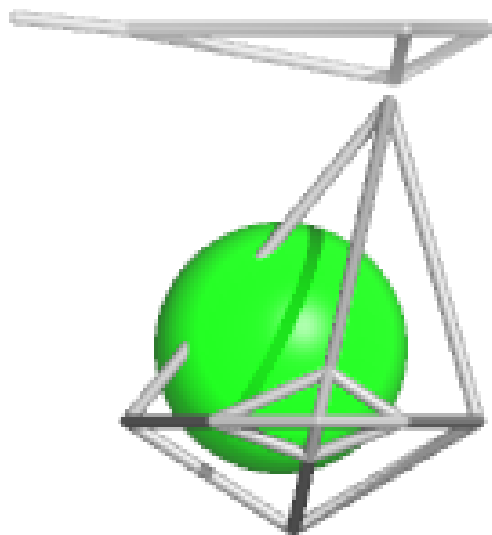
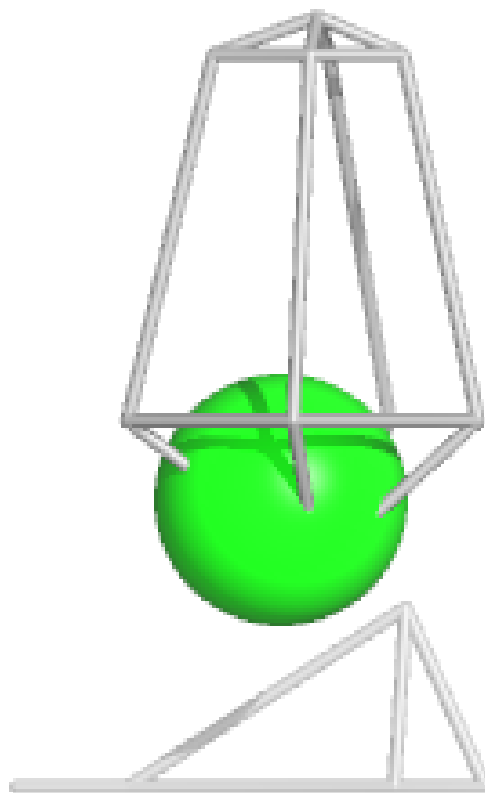
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	501	1/1	0.87	0.43	113,113,113,113	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 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.