



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 19, 2021 – 12:10 PM JST

PDB ID : 6LB7
Title : Crystal structure of the Ca²⁺-free and Ca²⁺-bound MICU1-MICU2 complex
Authors : Wu, W.; Shen, Q.; Zheng, J.; Jia, Z.
Deposited on : 2019-11-13
Resolution : 2.10 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 ⓘ 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 : 2.16
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) : 2.16

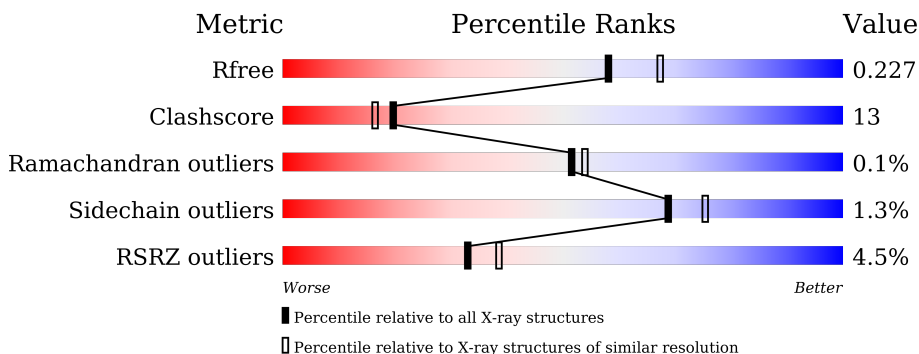
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


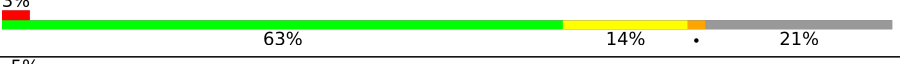
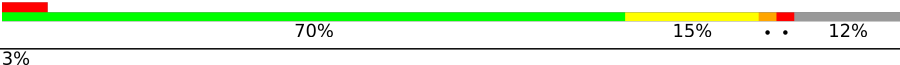

The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	377	 5% 67% 13% • 19%
1	C	377	 3% 63% 14% • 21%
2	B	330	 5% 70% 15% • • 12%
2	D	330	 3% 73% 19% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10993 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 Calcium uptake protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2468	1576	411	469	12			
1	C	298	Total	C	N	O	S	0	0	0
			2400	1532	400	454	14			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	expression tag	UNP Q9BPX6
A	77	GLY	-	expression tag	UNP Q9BPX6
A	78	SER	-	expression tag	UNP Q9BPX6
A	79	SER	-	expression tag	UNP Q9BPX6
A	80	HIS	-	expression tag	UNP Q9BPX6
A	81	HIS	-	expression tag	UNP Q9BPX6
A	82	HIS	-	expression tag	UNP Q9BPX6
A	83	HIS	-	expression tag	UNP Q9BPX6
A	84	HIS	-	expression tag	UNP Q9BPX6
A	85	HIS	-	expression tag	UNP Q9BPX6
A	86	SER	-	expression tag	UNP Q9BPX6
A	87	SER	-	expression tag	UNP Q9BPX6
A	88	GLY	-	expression tag	UNP Q9BPX6
A	89	LEU	-	expression tag	UNP Q9BPX6
A	90	VAL	-	expression tag	UNP Q9BPX6
A	91	PRO	-	expression tag	UNP Q9BPX6
A	92	ARG	-	expression tag	UNP Q9BPX6
A	93	GLY	-	expression tag	UNP Q9BPX6
A	94	SER	-	expression tag	UNP Q9BPX6
A	95	HIS	-	expression tag	UNP Q9BPX6
A	96	MET	-	expression tag	UNP Q9BPX6
A	445	GLY	-	expression tag	UNP Q9BPX6
A	446	SER	-	expression tag	UNP Q9BPX6
A	447	GLY	-	expression tag	UNP Q9BPX6
A	448	SER	-	expression tag	UNP Q9BPX6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	449	GLY	-	expression tag	UNP Q9BPX6
A	450	SER	-	expression tag	UNP Q9BPX6
A	451	GLY	-	expression tag	UNP Q9BPX6
A	452	SER	-	expression tag	UNP Q9BPX6
C	76	MET	-	expression tag	UNP Q9BPX6
C	77	GLY	-	expression tag	UNP Q9BPX6
C	78	SER	-	expression tag	UNP Q9BPX6
C	79	SER	-	expression tag	UNP Q9BPX6
C	80	HIS	-	expression tag	UNP Q9BPX6
C	81	HIS	-	expression tag	UNP Q9BPX6
C	82	HIS	-	expression tag	UNP Q9BPX6
C	83	HIS	-	expression tag	UNP Q9BPX6
C	84	HIS	-	expression tag	UNP Q9BPX6
C	85	HIS	-	expression tag	UNP Q9BPX6
C	86	SER	-	expression tag	UNP Q9BPX6
C	87	SER	-	expression tag	UNP Q9BPX6
C	88	GLY	-	expression tag	UNP Q9BPX6
C	89	LEU	-	expression tag	UNP Q9BPX6
C	90	VAL	-	expression tag	UNP Q9BPX6
C	91	PRO	-	expression tag	UNP Q9BPX6
C	92	ARG	-	expression tag	UNP Q9BPX6
C	93	GLY	-	expression tag	UNP Q9BPX6
C	94	SER	-	expression tag	UNP Q9BPX6
C	95	HIS	-	expression tag	UNP Q9BPX6
C	96	MET	-	expression tag	UNP Q9BPX6
C	445	GLY	-	expression tag	UNP Q9BPX6
C	446	SER	-	expression tag	UNP Q9BPX6
C	447	GLY	-	expression tag	UNP Q9BPX6
C	448	SER	-	expression tag	UNP Q9BPX6
C	449	GLY	-	expression tag	UNP Q9BPX6
C	450	SER	-	expression tag	UNP Q9BPX6
C	451	GLY	-	expression tag	UNP Q9BPX6
C	452	SER	-	expression tag	UNP Q9BPX6

- Molecule 2 is a protein called Calcium uptake protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	290	Total	C	N	O	S	0	0	0
			2423	1558	411	438	16			
2	D	313	Total	C	N	O	S	0	0	0
			2602	1669	440	477	16			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	77	GLY	-	expression tag	UNP Q8IYU8
B	78	SER	-	expression tag	UNP Q8IYU8
B	79	GLY	-	expression tag	UNP Q8IYU8
B	80	SER	-	expression tag	UNP Q8IYU8
B	81	GLY	-	expression tag	UNP Q8IYU8
B	82	SER	-	expression tag	UNP Q8IYU8
B	83	GLY	-	expression tag	UNP Q8IYU8
D	77	GLY	-	expression tag	UNP Q8IYU8
D	78	SER	-	expression tag	UNP Q8IYU8
D	79	GLY	-	expression tag	UNP Q8IYU8
D	80	SER	-	expression tag	UNP Q8IYU8
D	81	GLY	-	expression tag	UNP Q8IYU8
D	82	SER	-	expression tag	UNP Q8IYU8
D	83	GLY	-	expression tag	UNP Q8IYU8

- 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	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

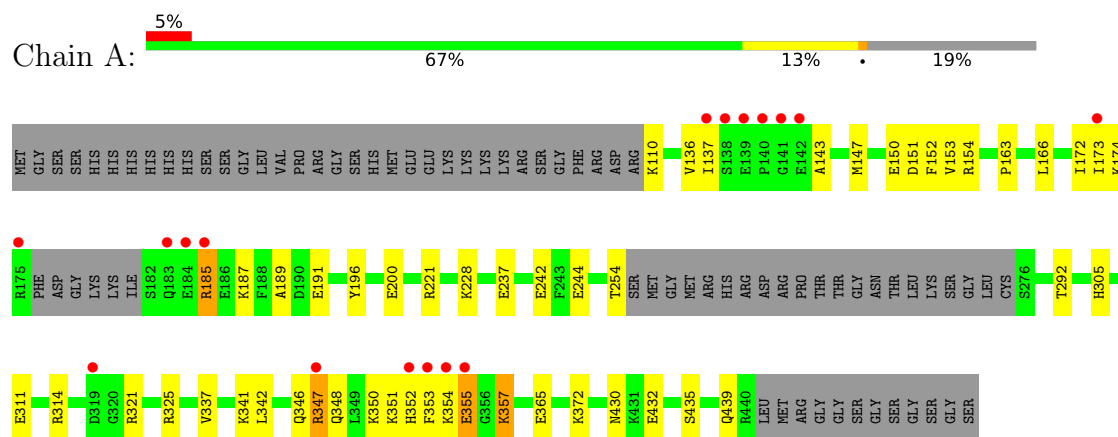
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	278	Total O 278 278	0	0
4	B	305	Total O 305 305	0	0
4	C	240	Total O 240 240	0	0
4	D	275	Total O 275 275	0	0

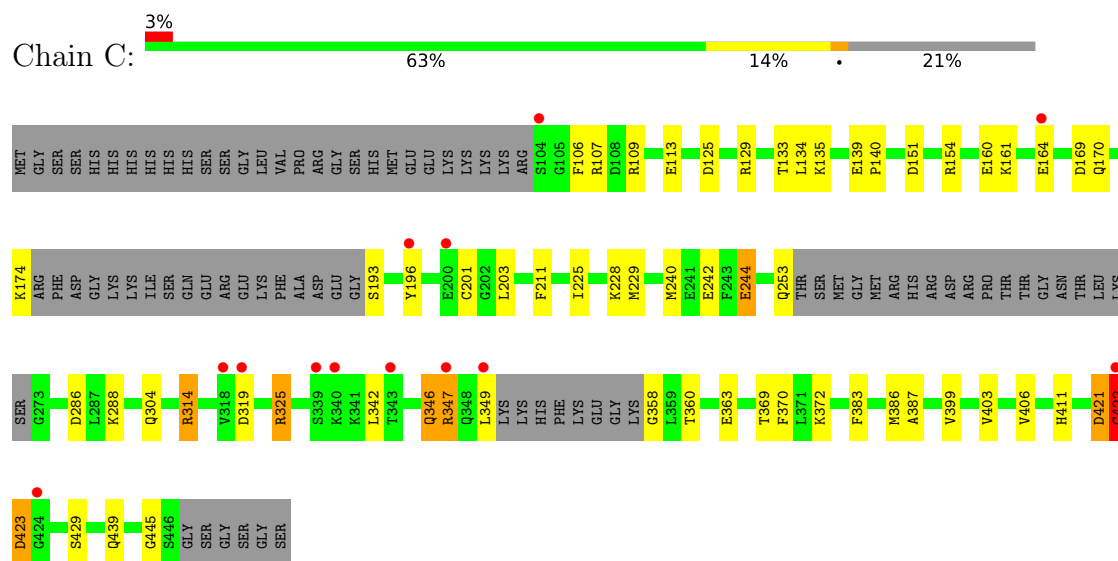
3 Residue-property plots [i](#)

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: Calcium uptake protein 1, mitochondrial

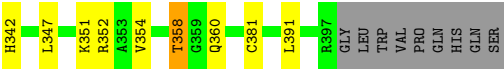
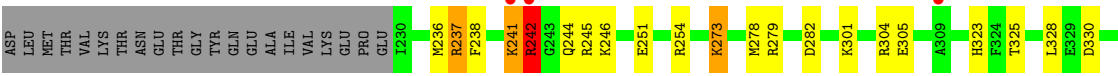
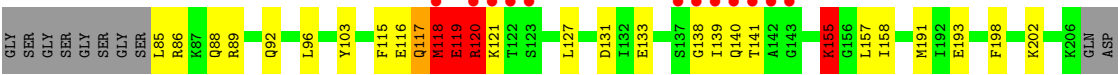


- Molecule 1: Calcium uptake protein 1, mitochondrial

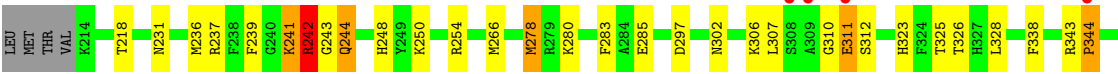
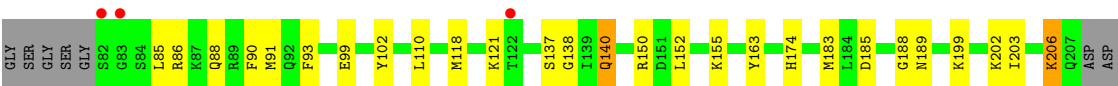
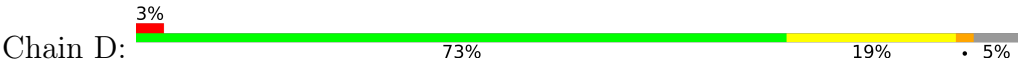


- Molecule 2: Calcium uptake protein 2, mitochondrial





● Molecule 2: Calcium uptake protein 2, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.48Å 107.72Å 170.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 2.10 47.30 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.30-2.10) 98.4 (47.30-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.194 , 0.227 0.194 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10993	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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:
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	A	1.00	21/2514 (0.8%)	0.63	2/3374 (0.1%)
1	C	0.82	12/2443 (0.5%)	0.69	4/3280 (0.1%)
2	B	1.23	26/2474 (1.1%)	0.73	5/3303 (0.2%)
2	D	1.96	25/2657 (0.9%)	0.93	3/3551 (0.1%)
All	All	1.34	84/10088 (0.8%)	0.75	14/13508 (0.1%)

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
1	C	0	4
2	B	0	3
2	D	0	1
All	All	0	9

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	344	PRO	N-CD	84.81	2.66	1.47
2	B	242	ARG	NE-CZ	-19.57	1.07	1.33
1	A	150	GLU	CD-OE1	-18.91	1.04	1.25
2	B	242	ARG	CZ-NH1	-17.87	1.09	1.33
2	B	242	ARG	CZ-NH2	-17.64	1.10	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	344	PRO	N-CD-CG	-29.33	59.20	103.20
2	D	344	PRO	CA-N-CD	-26.16	74.87	111.50
1	C	422	CYS	O-C-N	-16.86	95.72	122.70
2	B	358	THR	N-CA-C	10.05	138.13	111.00
1	C	421	ASP	C-N-CA	-9.07	99.03	121.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ARG	Sidechain
2	B	118	MET	Mainchain
2	B	119	GLU	Mainchain
2	B	120	ARG	Sidechain
1	C	107	ARG	Sidechain

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	2468	0	2430	41	0
1	C	2400	0	2364	52	0
2	B	2423	0	2405	82	0
2	D	2602	0	2572	82	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	278	0	0	8	0
4	B	305	0	0	11	1
4	C	240	0	0	16	0
4	D	275	0	0	12	1
All	All	10993	0	9771	249	1

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.

The worst 5 of 249 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:C:325:ARG:HD3	1:C:346:GLN:NE2	1.30	1.45
1:C:325:ARG:CD	1:C:346:GLN:NE2	1.80	1.44
1:C:421:ASP:O	1:C:422:CYS:CB	1.69	1.30
1:C:325:ARG:NE	1:C:346:GLN:HE22	1.29	1.27
1:C:325:ARG:CD	1:C:346:GLN:HE21	1.42	1.24

All (1) 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)
4:B:754:HOH:O	4:D:759:HOH:O[2_594]	1.95	0.25

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	298/377 (79%)	294 (99%)	4 (1%)	0	100	100
1	C	290/377 (77%)	284 (98%)	5 (2%)	1 (0%)	41	41
2	B	286/330 (87%)	278 (97%)	8 (3%)	0	100	100
2	D	309/330 (94%)	299 (97%)	10 (3%)	0	100	100
All	All	1183/1414 (84%)	1155 (98%)	27 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	422	CYS

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	271/331 (82%)	270 (100%)	1 (0%)	91	94
1	C	264/331 (80%)	258 (98%)	6 (2%)	50	55
2	B	265/298 (89%)	261 (98%)	4 (2%)	65	71
2	D	284/298 (95%)	281 (99%)	3 (1%)	73	79
All	All	1084/1258 (86%)	1070 (99%)	14 (1%)	69	75

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	174	LYS
1	C	319	ASP
2	D	206	LYS
1	C	135	LYS
1	C	423	ASP

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

Mol	Chain	Res	Type
2	B	92	GLN
1	C	170	GLN
1	C	346	GLN
2	D	231	ASN
2	D	295	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 2 ligands modelled in this entry, 2 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	304/377 (80%)	0.13	17 (5%) 24 29	13, 34, 65, 123	0
1	C	298/377 (79%)	-0.01	13 (4%) 34 40	20, 36, 66, 81	0
2	B	290/330 (87%)	-0.04	15 (5%) 27 32	12, 27, 68, 104	0
2	D	313/330 (94%)	0.04	9 (2%) 51 57	13, 29, 65, 84	0
All	All	1205/1414 (85%)	0.03	54 (4%) 33 38	12, 32, 66, 123	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	PRO	11.6
2	D	309	ALA	5.7
2	B	139	ILE	5.6
2	B	138	GLY	5.1
1	C	349	LEU	4.8

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](#)

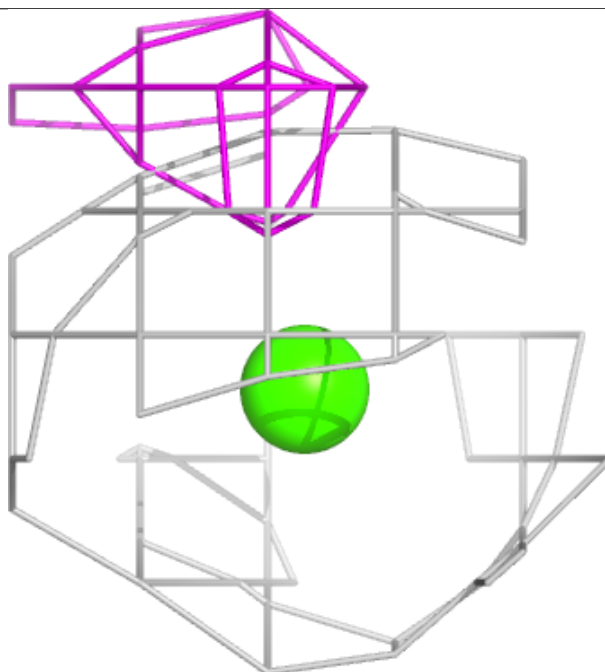
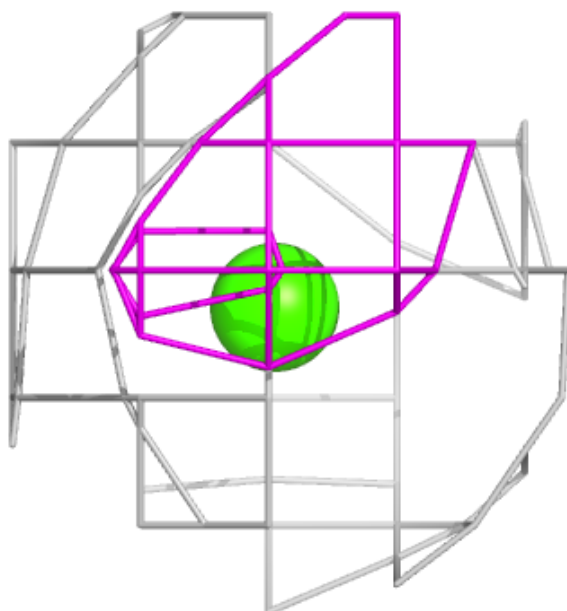
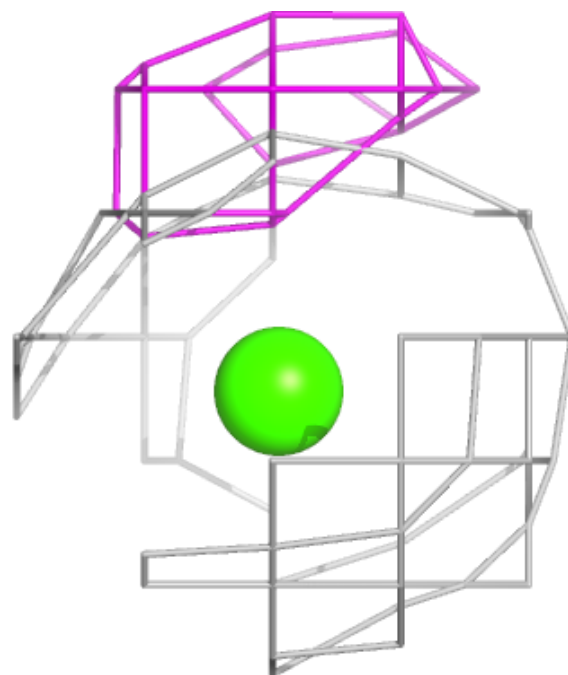
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

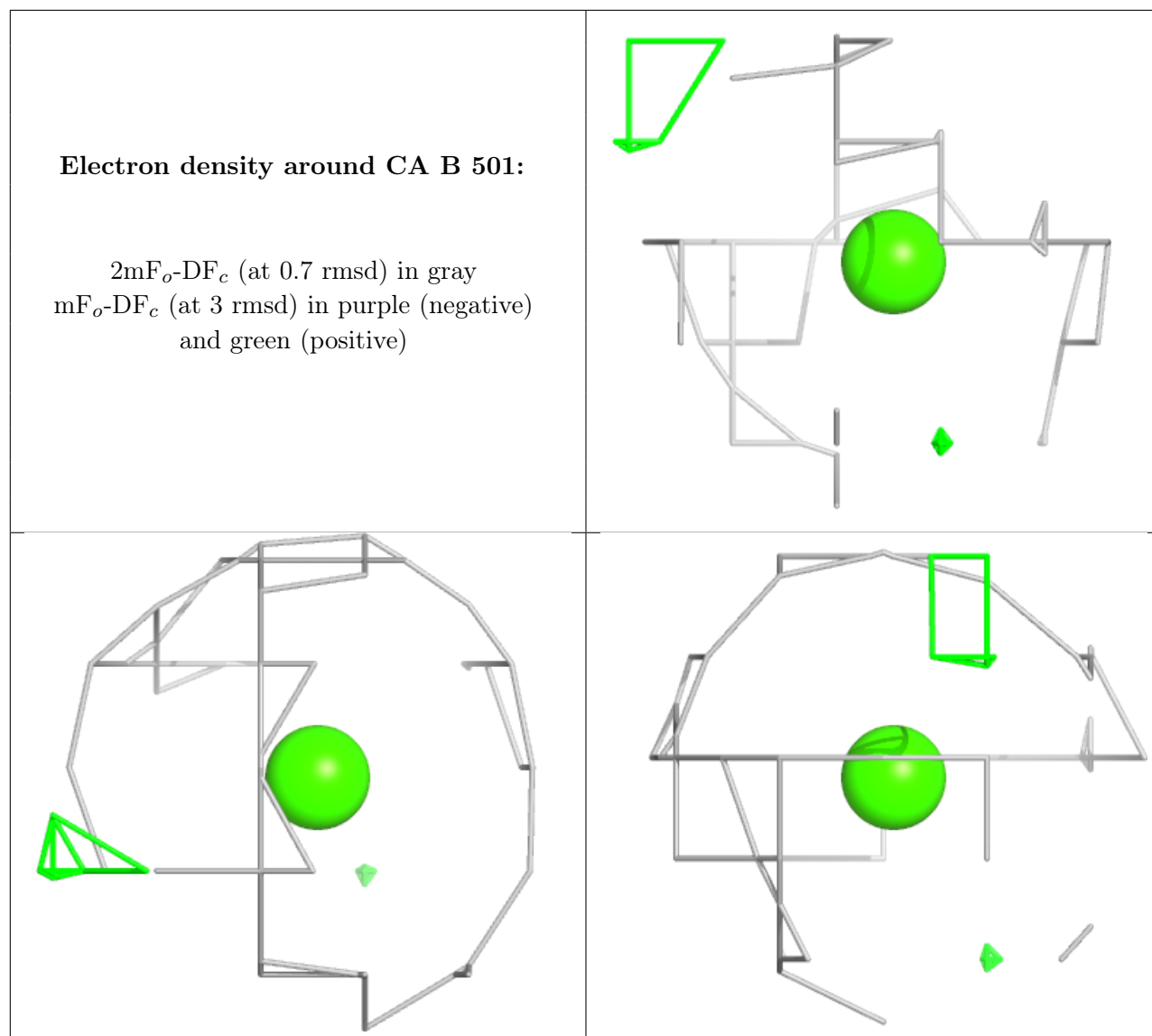
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	A	501	1/1	0.97	0.08	34,34,34,34	0
3	CA	B	501	1/1	0.99	0.13	22,22,22,22	0

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 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 ⓘ

There are no such residues in this entry.