wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2026 – 08:15 PM JST

PDB ID	:	9XNI / pdb_00009xni
Title	:	Crystal structure of ASCT D62N mutant (modification by lysine succinylation) from Trypanosoma brucei.
Authors	:	Mochizuki, K.; Inaoka, D.K.; Fukuda, K.; Kurasawa, H.; Iyoda, K.; Nakai, U.; Harada, S.; Balogun, E.O.; Mazet, M.; Millerioux, Y.; Bringaud, F.; Boshart, M.; Hirayama, K.; Kita, K.; Shiba, T.
Deposited on	:	2025-11-12
Resolution	:	2.09 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 (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:

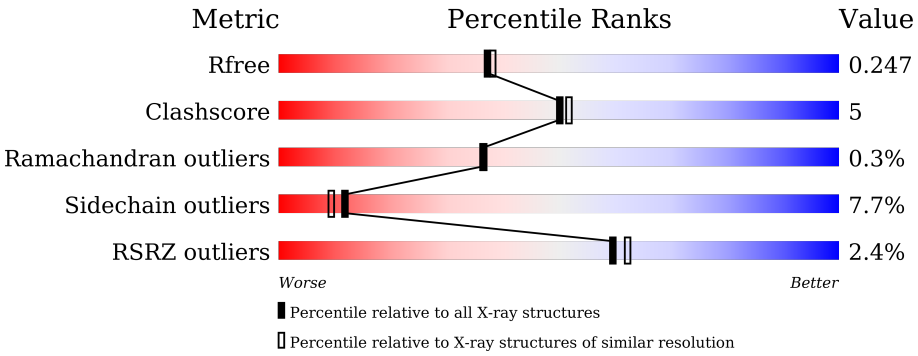
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.09 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 <=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	493	81% 12% • 5%
1	B	493	3% 81% 13% • •
1	C	493	77% 15% • •
1	D	493	4% 77% 14% • • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14456 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 Succinyl-CoA:3-ketoacid-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3546	2226	622	675	23			
1	B	472	Total	C	N	O	S	0	0	0
			3566	2241	626	676	23			
1	C	473	Total	C	N	O	S	0	0	0
			3569	2241	627	678	23			
1	D	470	Total	C	N	O	S	0	0	0
			3550	2229	624	674	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	ASN	ASP	engineered mutation	UNP Q386P1
A	419	ASN	SER	conflict	UNP Q386P1
B	62	ASN	ASP	engineered mutation	UNP Q386P1
B	419	ASN	SER	conflict	UNP Q386P1
C	62	ASN	ASP	engineered mutation	UNP Q386P1
C	419	ASN	SER	conflict	UNP Q386P1
D	62	ASN	ASP	engineered mutation	UNP Q386P1
D	419	ASN	SER	conflict	UNP Q386P1

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

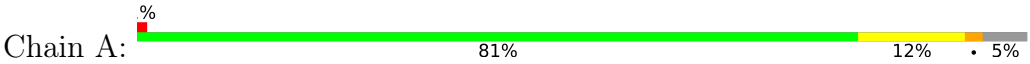
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	51	Total O 51 51	0	0
3	B	48	Total O 48 48	0	0
3	C	70	Total O 70 70	0	0
3	D	52	Total O 52 52	0	0

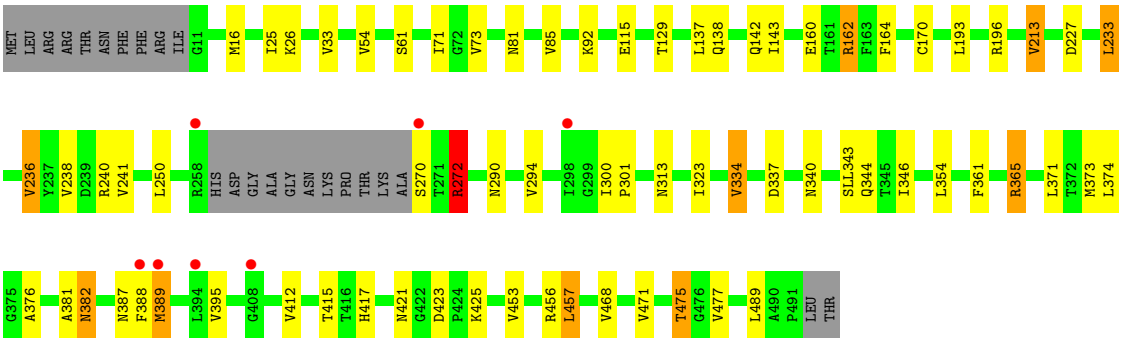
3 Residue-property plots (i)

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: Succinyl-CoA:3-ketoacid-coenzyme A transferase

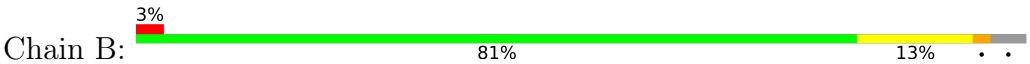
Chain A:

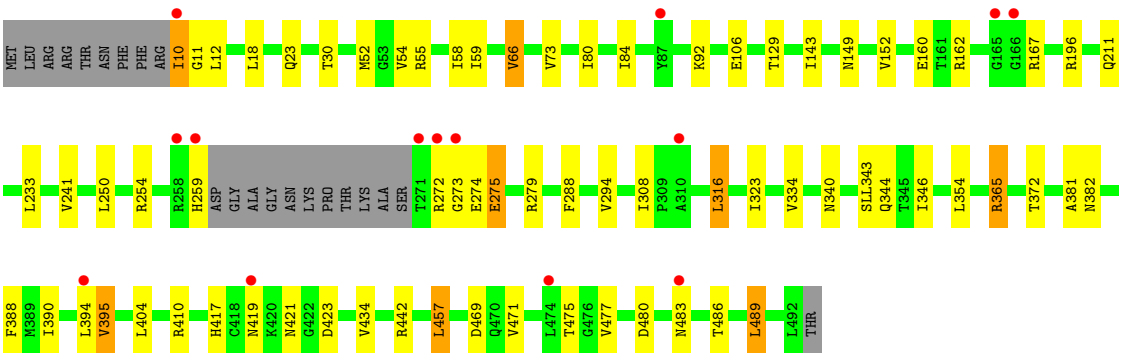




• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase

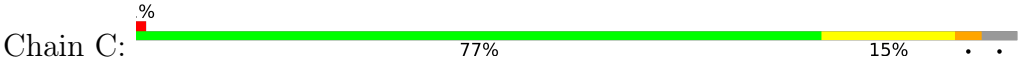
Chain B:



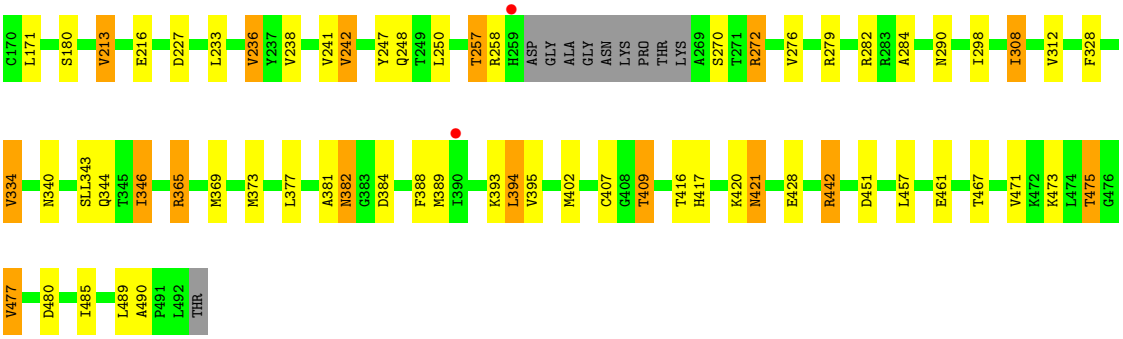


• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase

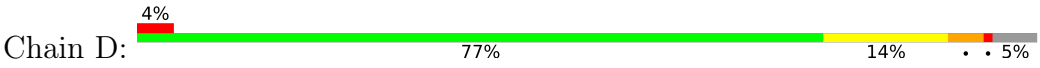
Chain C:

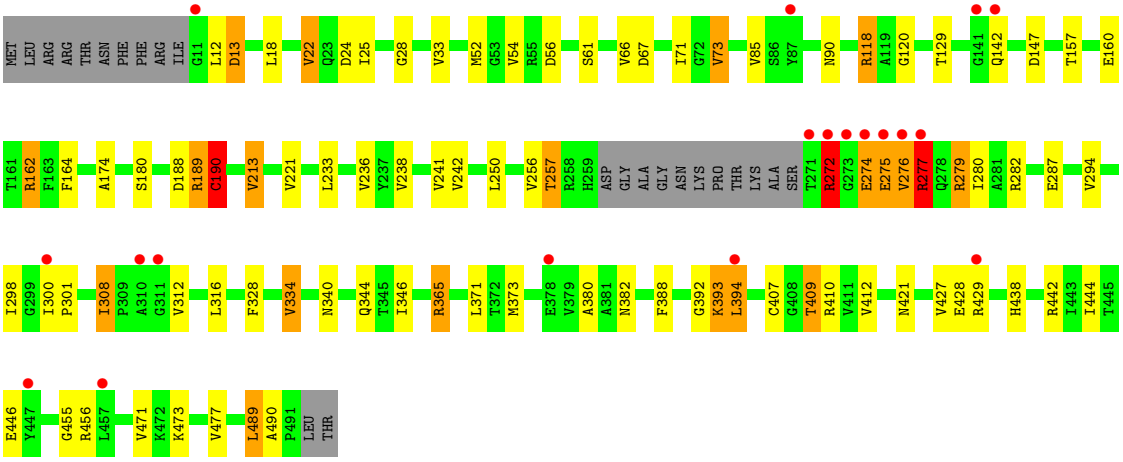






• Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.93Å 163.85Å 186.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.09 19.99 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.99-2.09) 99.5 (19.99-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.192 , 0.244 0.199 , 0.247	Depositor DCC
R_{free} test set	5480 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.5	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	0.95	EDS
Total number of atoms	14456	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

5.1 Standard geometry

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

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	0.61	0/3586	1.11	6/4851 (0.1%)
1	B	0.58	0/3607	1.08	4/4880 (0.1%)
1	C	0.61	0/3610	1.13	11/4884 (0.2%)
1	D	0.60	0/3591	1.15	10/4858 (0.2%)
All	All	0.60	0/14394	1.12	31/19473 (0.2%)

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	2
1	B	0	3
1	C	0	3
1	D	0	6
All	All	0	14

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	190	CYS	CB-CA-C	-9.15	92.22	110.42
1	D	334	VAL	N-CA-CB	7.64	122.05	110.13
1	C	22	VAL	N-CA-CB	-6.79	101.75	112.07
1	B	388	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	334	VAL	N-CA-CB	6.40	120.12	110.13

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	ARG	Sidechain
1	A	365	ARG	Sidechain
1	B	167	ARG	Sidechain
1	B	196	ARG	Sidechain
1	B	365	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	3546	0	3555	30	1
1	B	3566	0	3579	31	0
1	C	3569	0	3578	46	1
1	D	3550	0	3557	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	51	0	0	1	0
3	B	48	0	0	0	0
3	C	70	0	0	1	0
3	D	52	0	0	0	0
All	All	14456	0	14269	150	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 5.

The worst 5 of 150 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:274:GLU:OE2	1:D:277:ARG:HD3	1.69	0.93
1:D:340:ASN:HD21	1:D:344:GLN:HE21	1.25	0.85
1:D:274:GLU:OE2	1:D:277:ARG:CD	2.26	0.83
1:D:407:CYS:SG	1:D:409:THR:HB	2.20	0.81
1:B:417:HIS:NE2	1:B:475:THR:HG22	1.97	0.79

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ARG:NH1	1:C:87:TYR:OH[3_545]	2.11	0.09

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	465/493 (94%)	452 (97%)	12 (3%)	1 (0%)	43	44
1	B	467/493 (95%)	452 (97%)	13 (3%)	2 (0%)	30	28
1	C	468/493 (95%)	456 (97%)	12 (3%)	0	100	100
1	D	465/493 (94%)	454 (98%)	8 (2%)	3 (1%)	21	18
All	All	1865/1972 (95%)	1814 (97%)	45 (2%)	6 (0%)	36	36

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	394	LEU
1	B	273	GLY
1	D	392	GLY
1	A	389	MET
1	B	395	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	377/396 (95%)	350 (93%)	27 (7%)	13 11
1	B	379/396 (96%)	352 (93%)	27 (7%)	13 11
1	C	379/396 (96%)	346 (91%)	33 (9%)	9 7
1	D	377/396 (95%)	347 (92%)	30 (8%)	11 8
All	All	1512/1584 (96%)	1395 (92%)	117 (8%)	12 9

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	93	ILE
1	D	409	THR
1	C	290	ASN
1	D	382	ASN
1	D	257	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	344	GLN
1	D	110	GLN
1	C	348	HIS
1	C	483	ASN
1	D	295	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\|>2$
1	SLL	B	343	1	14,15,16	0.69	0	12,17,19	1.48	2 (16%)
1	SLL	D	343	1	14,15,16	0.67	0	12,17,19	0.98	0
1	SLL	A	343	1	14,15,16	0.74	0	12,17,19	1.28	3 (25%)
1	SLL	C	343	1	14,15,16	0.77	0	12,17,19	1.38	3 (25%)

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
1	SLL	B	343	1	-	4/14/15/17	-
1	SLL	D	343	1	-	1/14/15/17	-
1	SLL	A	343	1	-	3/14/15/17	-
1	SLL	C	343	1	-	4/14/15/17	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	343	SLL	CK-CL-CP	-3.56	105.94	113.60
1	C	343	SLL	CE-NZ-CX	2.78	127.99	122.84
1	A	343	SLL	CE-NZ-CX	2.65	127.75	122.84
1	C	343	SLL	OP1-CP-CL	-2.35	115.54	123.08
1	A	343	SLL	OP1-CP-CL	-2.18	116.06	123.08

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	343	SLL	O-C-CA-CB
1	A	343	SLL	N-CA-CB-CG
1	B	343	SLL	CG-CD-CE-NZ
1	B	343	SLL	CK-CL-CP-OP2
1	A	343	SLL	CK-CL-CP-OP2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 (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

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, 95^{th} 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	469/493 (95%)	-0.14	7 (1%) 72 74	21, 31, 50, 98	0
1	B	471/493 (95%)	0.08	14 (2%) 52 55	21, 35, 64, 127	0
1	C	472/493 (95%)	-0.10	5 (1%) 78 80	21, 31, 53, 86	0
1	D	469/493 (95%)	0.19	19 (4%) 41 43	22, 35, 68, 120	0
All	All	1881/1972 (95%)	0.00	45 (2%) 59 62	21, 33, 63, 127	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	ILE	4.4
1	D	141	GLY	3.5
1	A	394	LEU	3.4
1	D	276	VAL	3.4
1	A	408	GLY	3.1

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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
1	SLL	B	343	16/17	0.85	0.11	31,42,50,50	0
1	SLL	C	343	16/17	0.91	0.10	24,36,58,59	0
1	SLL	D	343	16/17	0.91	0.09	28,39,49,50	0
1	SLL	A	343	16/17	0.92	0.09	27,45,58,58	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

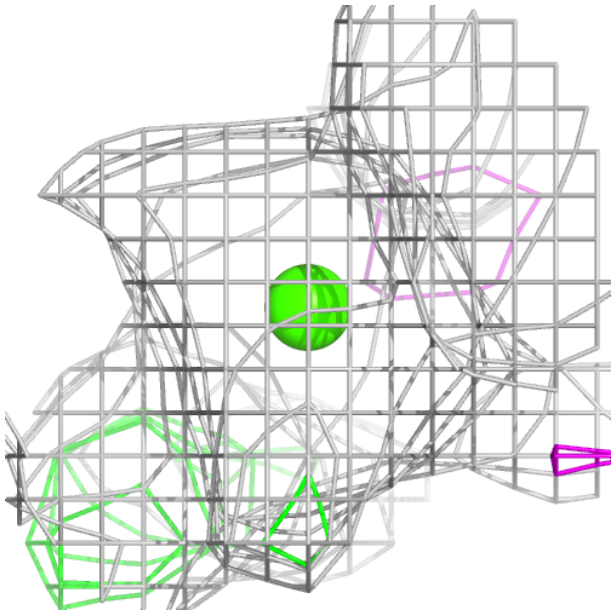
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

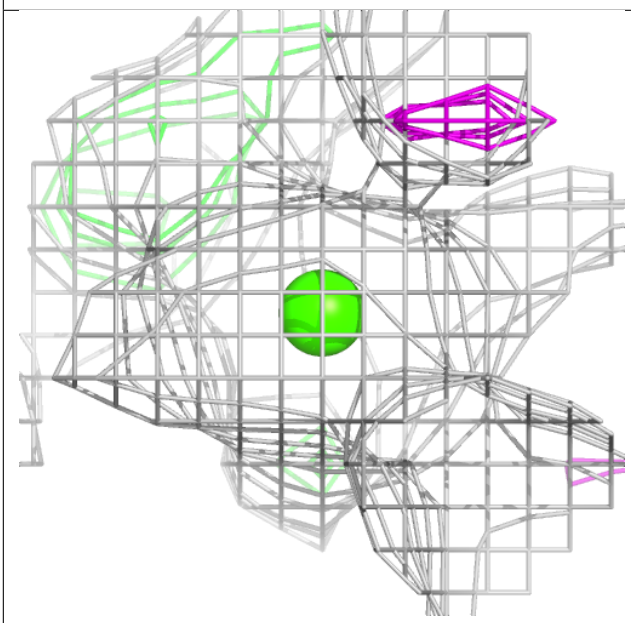
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	C	501	1/1	0.84	0.09	64,64,64,64	0
2	CA	B	501	1/1	0.91	0.08	52,52,52,52	0
2	CA	A	501	1/1	0.95	0.04	48,48,48,48	0
2	CA	D	501	1/1	0.98	0.05	49,49,49,49	0

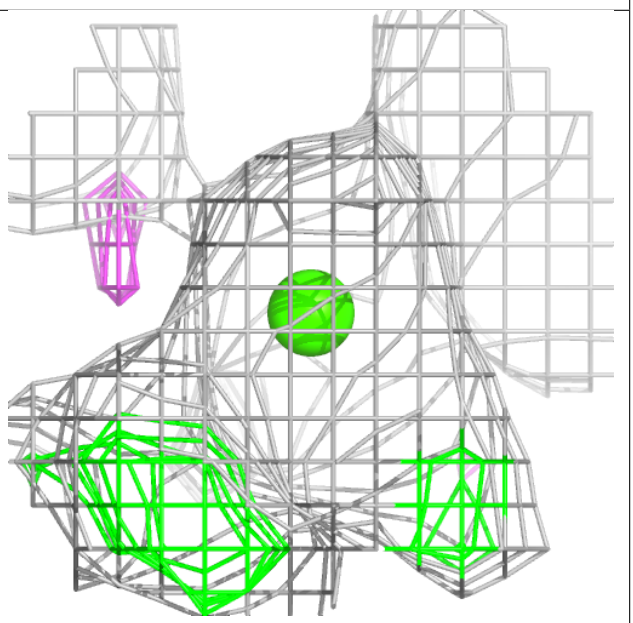
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CA C 501:

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

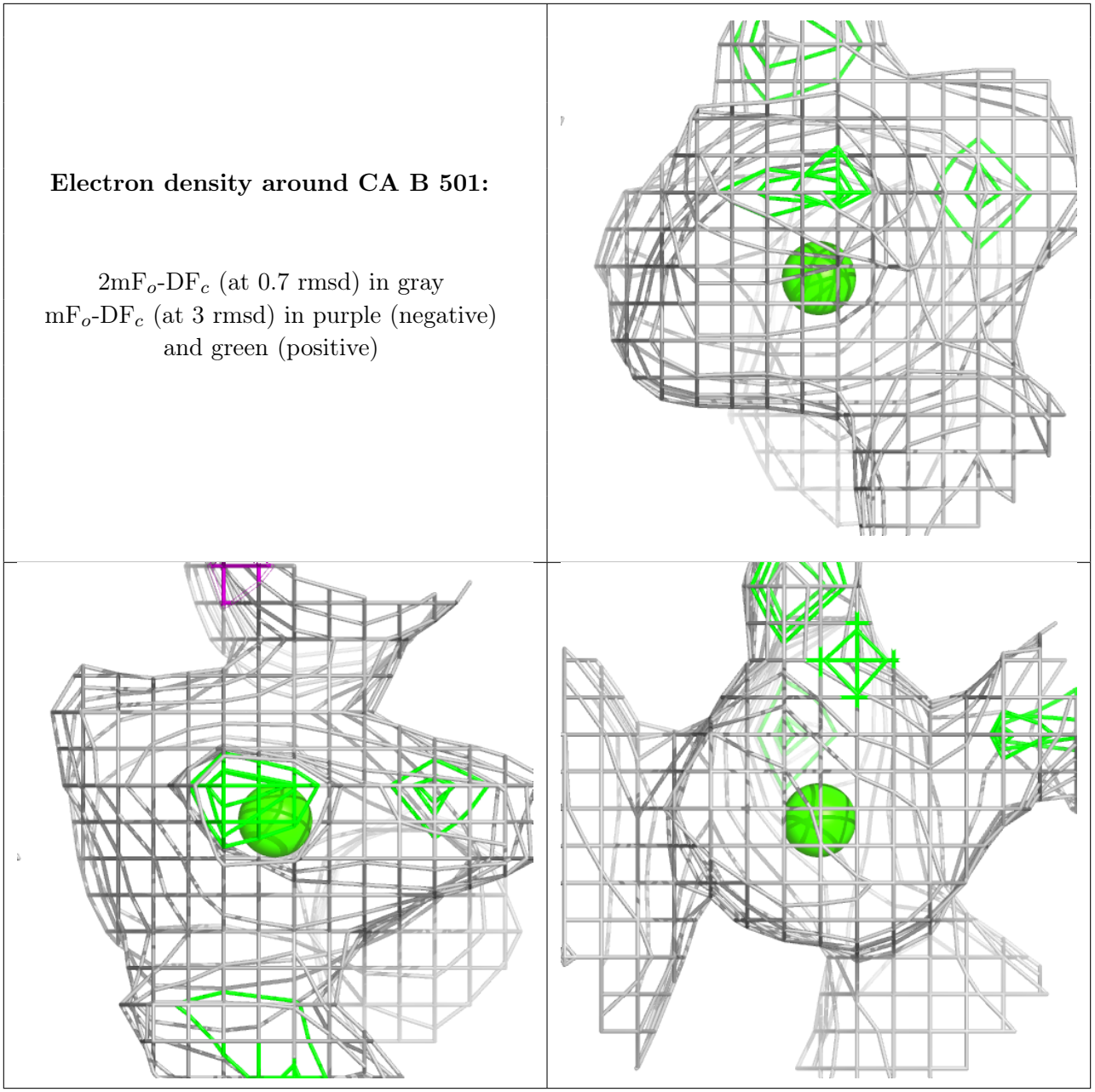






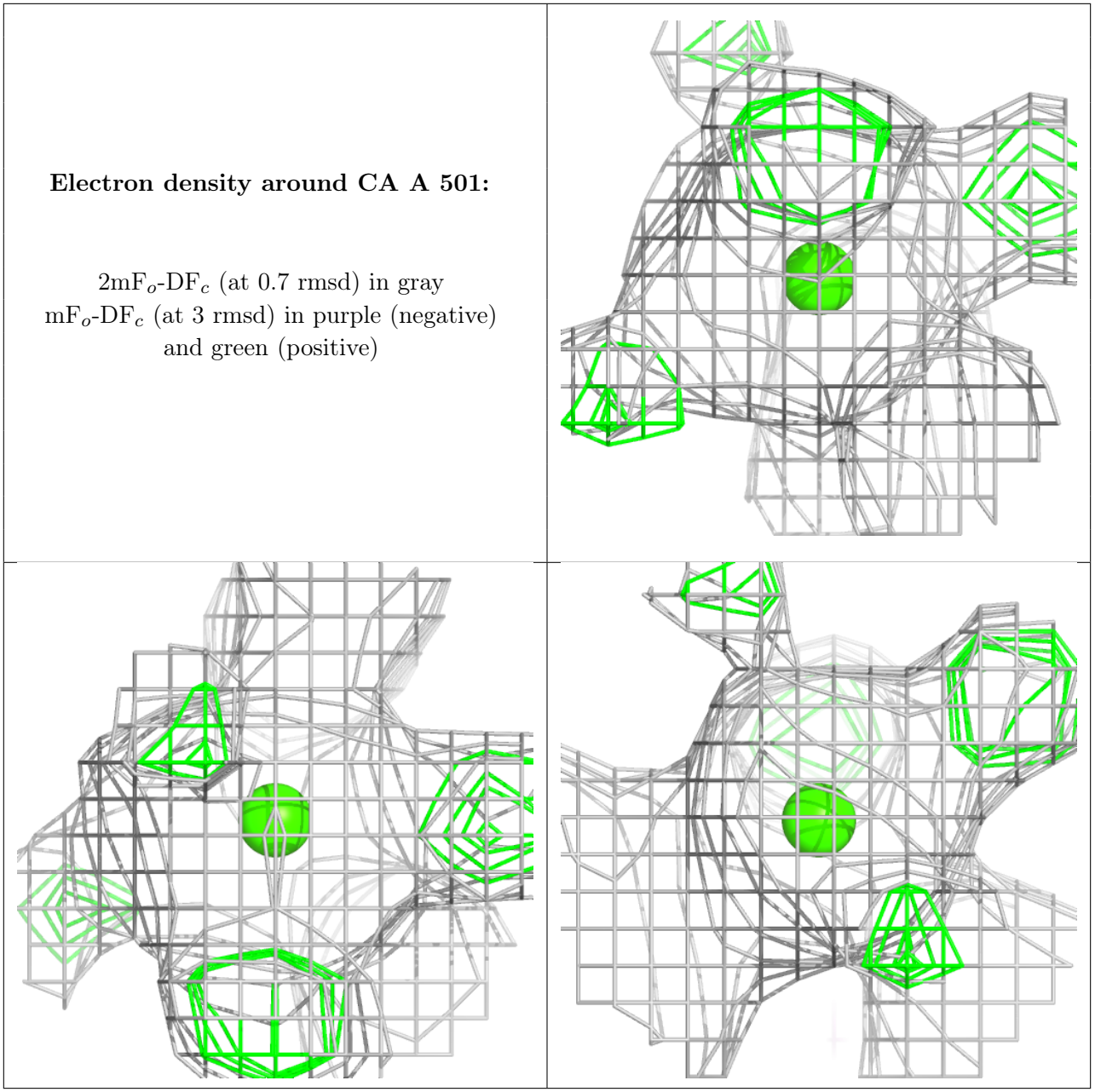
Electron density around CA B 501:

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



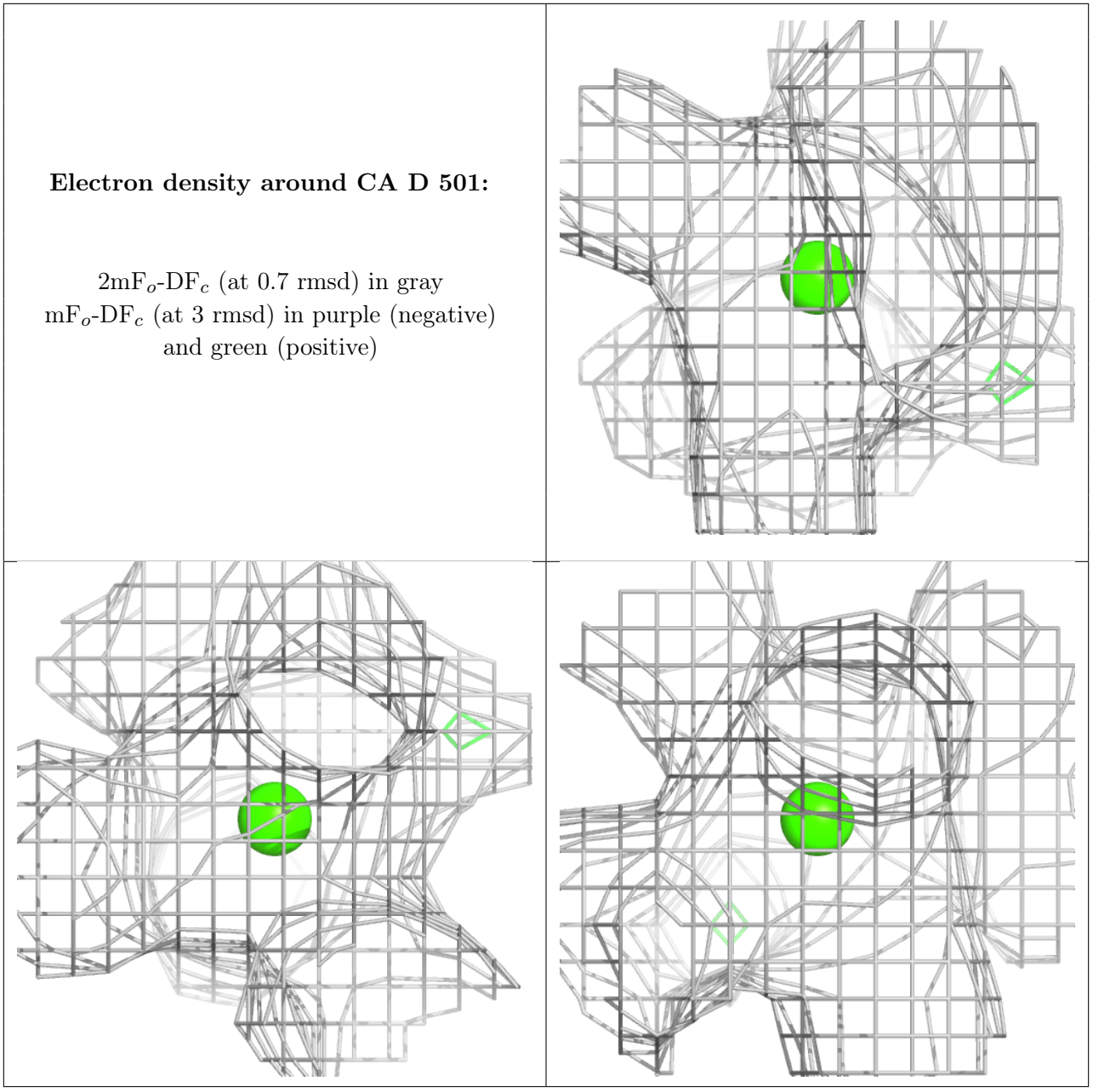
Electron density around CA A 501:

$2mF_o$-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 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.