



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2023 – 01:12 pm GMT

PDB ID : 8BOZ
Title : structure of the Adherent-Invasive Escherichia coli Tle3/Tli3 T6SS effector/immunity complex
Authors : Cambillau, C.; Roussel, A.
Deposited on : 2022-11-15
Resolution : 3.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

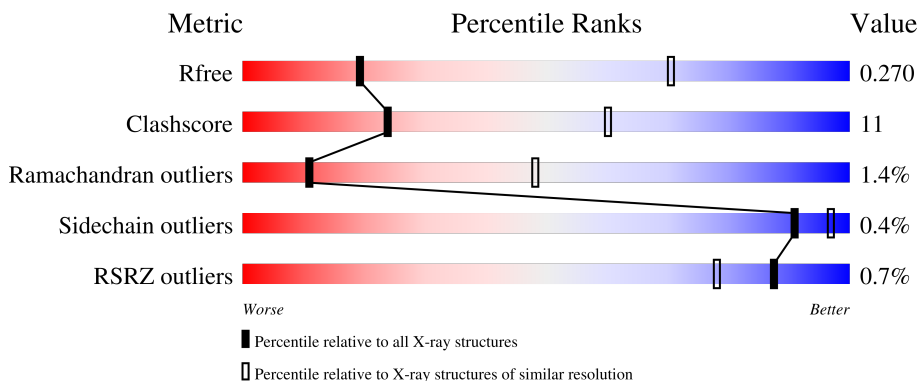
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.













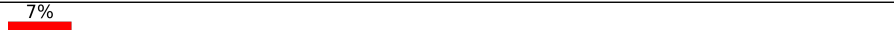
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 $\leq 5\%$. 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	658	
1	C	658	
1	E	658	
1	G	658	
1	I	658	

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Mol	Chain	Length	Quality of chain
1	K	658	 62% 20% 17%
1	M	658	 59% 20% 19%
1	O	658	 59% 20% 21%
2	B	274	 66% 13% 22%
2	D	274	 62% 14% 23%
2	F	274	 54% 23% 22%
2	H	274	 60% 17% 23%
2	J	274	 60% 19% 21%
2	L	274	 57% 19% 25%
2	N	274	 56% 19% 25%
2	P	274	 51% 23% 26%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 45234 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 Transmembrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	541	Total 4072	C 2577	N 705	O 781	S 9	0	0	0
1	C	530	Total 3989	C 2529	N 681	O 770	S 9	0	0	0
1	E	553	Total 4127	C 2614	N 710	O 794	S 9	0	0	0
1	G	558	Total 4143	C 2619	N 713	O 802	S 9	0	0	0
1	I	543	Total 4042	C 2559	N 698	O 776	S 9	0	0	0
1	K	546	Total 4079	C 2580	N 703	O 787	S 9	0	0	0
1	M	530	Total 3978	C 2519	N 686	O 764	S 9	0	0	0
1	O	521	Total 3900	C 2466	N 672	O 754	S 8	0	0	0

- Molecule 2 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	215	Total 1655	C 1051	N 281	O 313	S 10	0	0	0
2	D	210	Total 1615	C 1023	N 278	O 304	S 10	0	0	0
2	F	213	Total 1628	C 1032	N 277	O 309	S 10	0	0	0
2	H	211	Total 1609	C 1020	N 273	O 306	S 10	0	0	0
2	J	216	Total 1651	C 1043	N 283	O 315	S 10	0	0	0
2	L	206	Total 1586	C 1004	N 273	O 299	S 10	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	206	Total	C	N	O	S	0	0	0
			1580	1001	271	298	10			
2	P	204	Total	C	N	O	S	0	0	0
			1572	994	271	297	10			

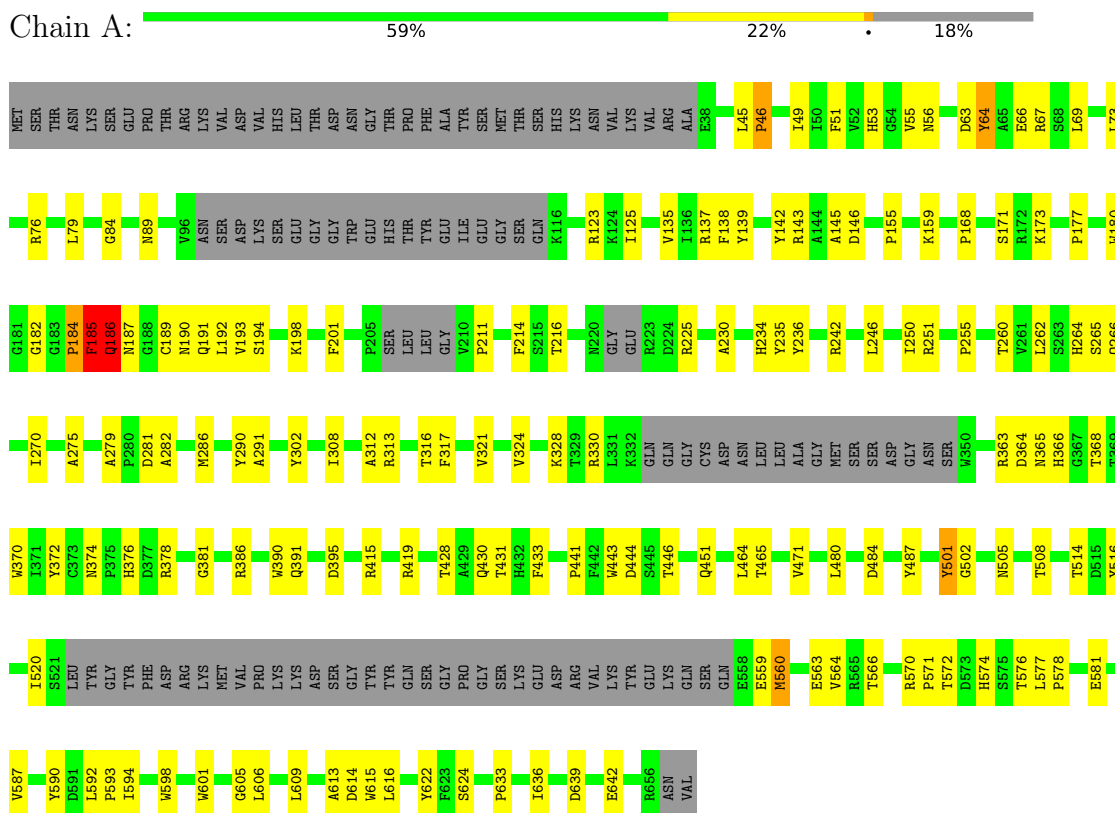
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		
3	M	1	Total	Ca	0	0
			1	1		
3	O	1	Total	Ca	0	0
			1	1		

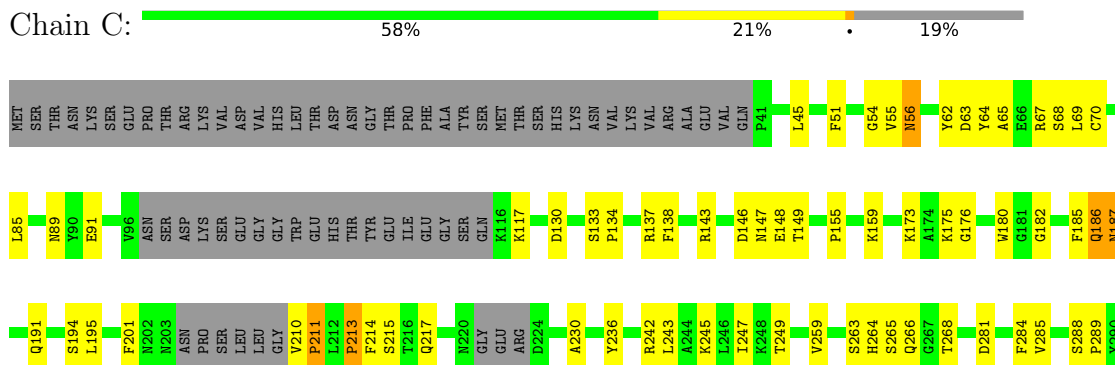
3 Residue-property plots [i](#)

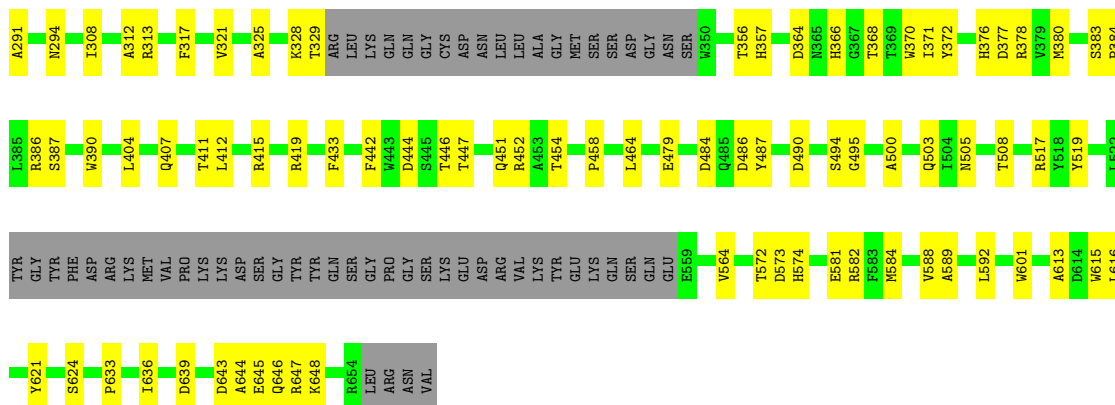
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Transmembrane protein



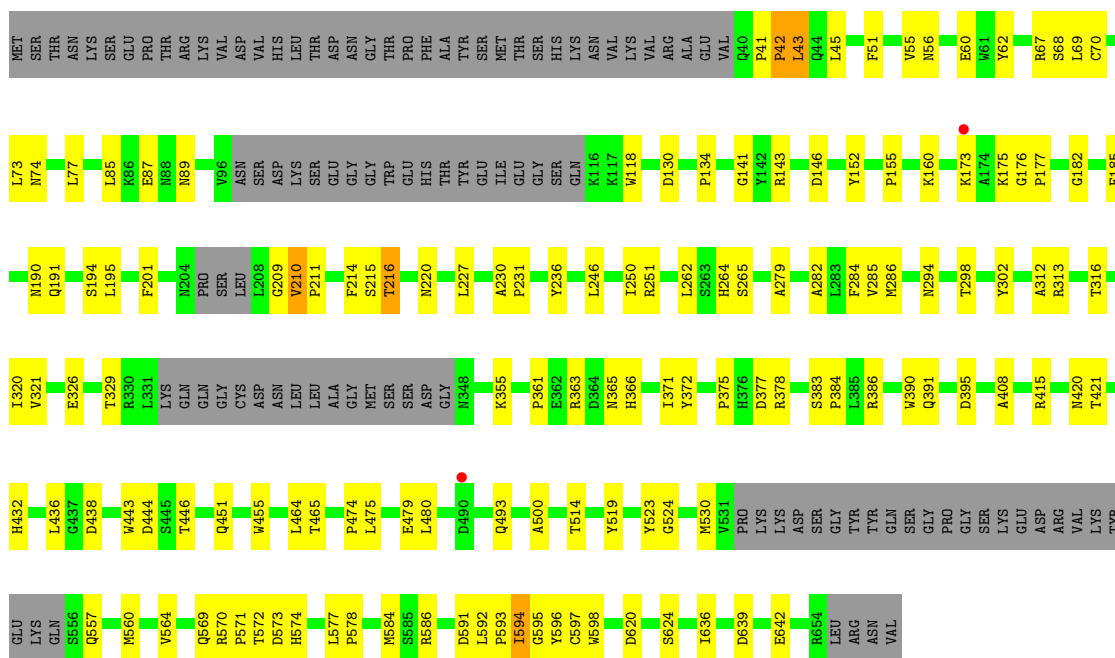
- Molecule 1: Transmembrane protein





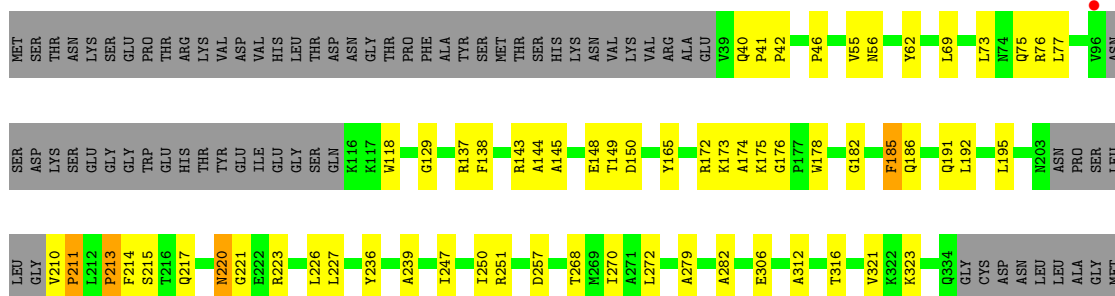
- Molecule 1: Transmembrane protein

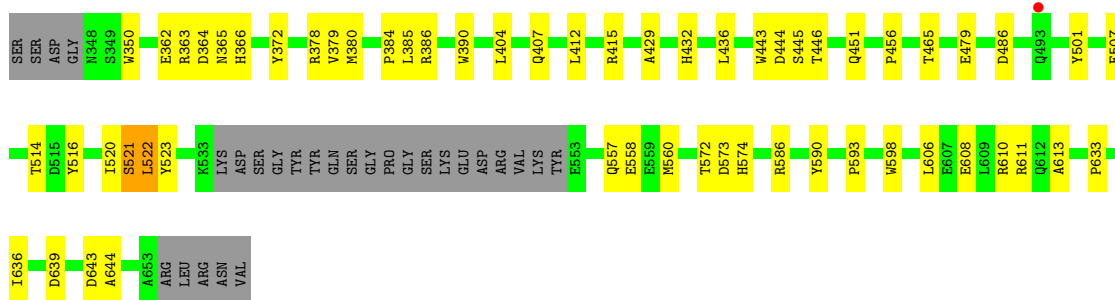
Chain E: 63% 20% 16%



- Molecule 1: Transmembrane protein

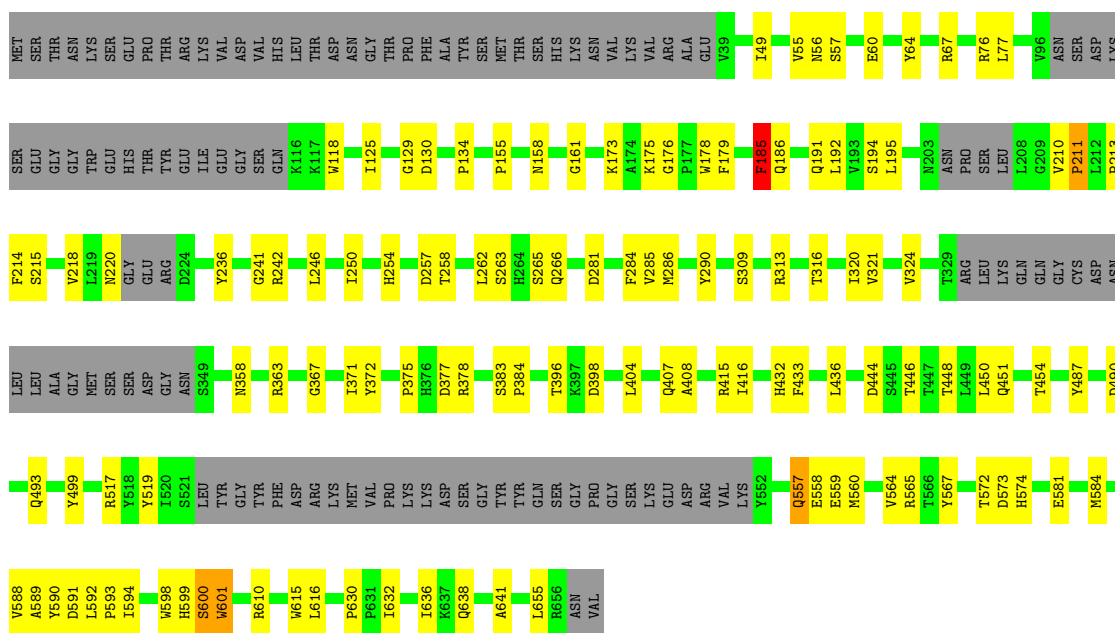
Chain G: 67% 17% 15%





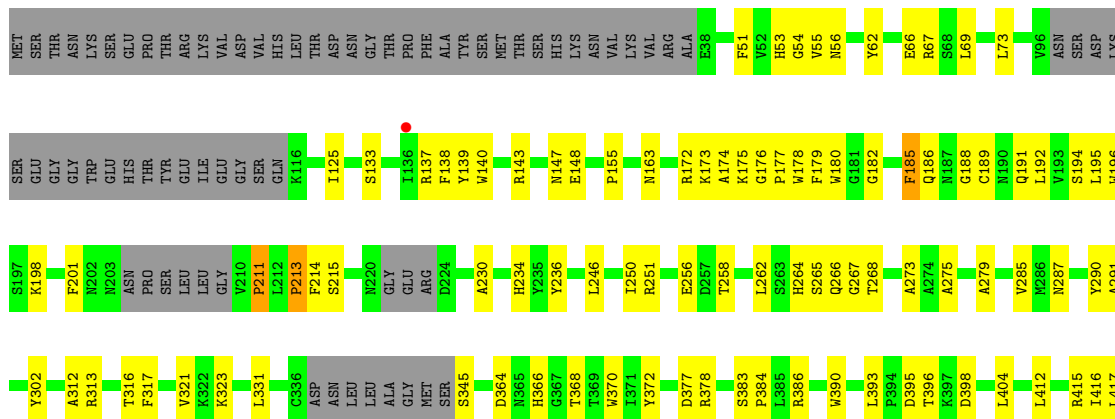
- Molecule 1: Transmembrane protein

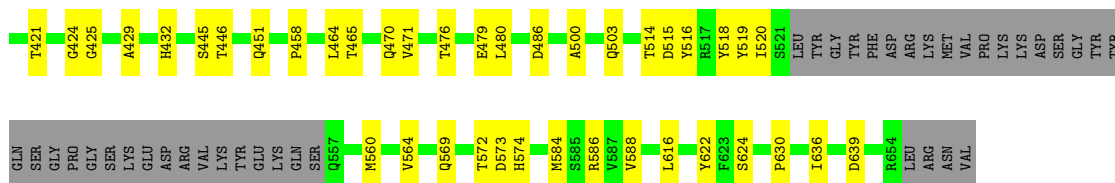
Chain I: 64% 18% 17%



- Molecule 1: Transmembrane protein

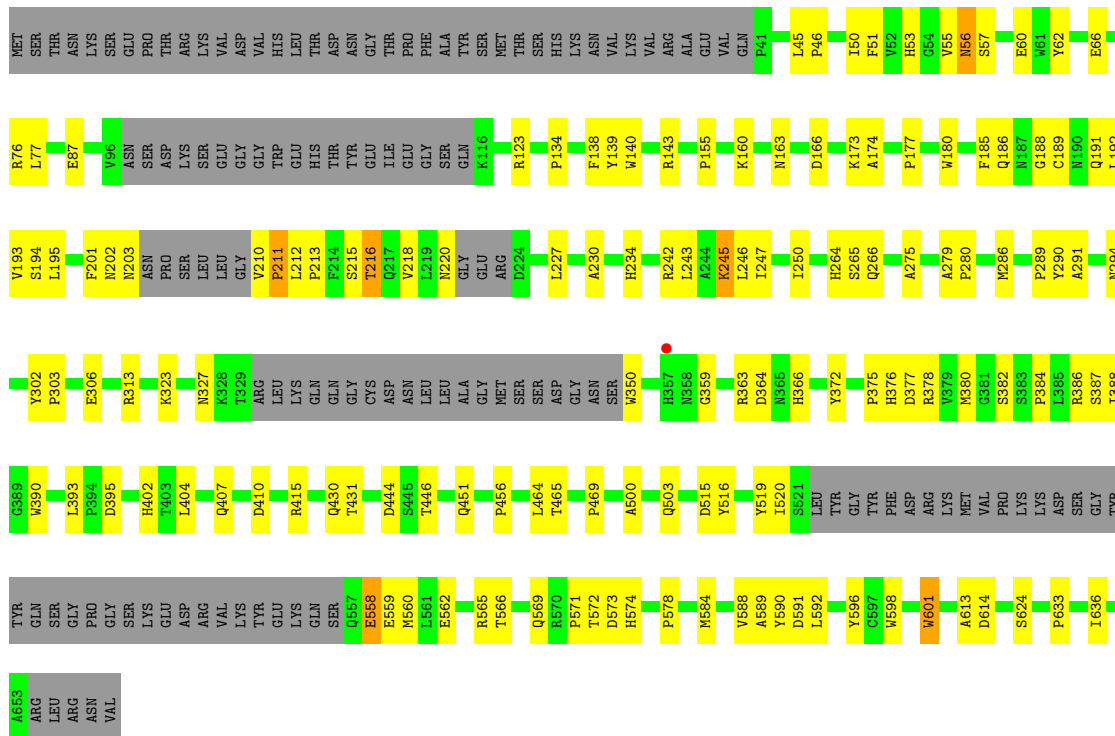
Chain K: 62% 20% 17%





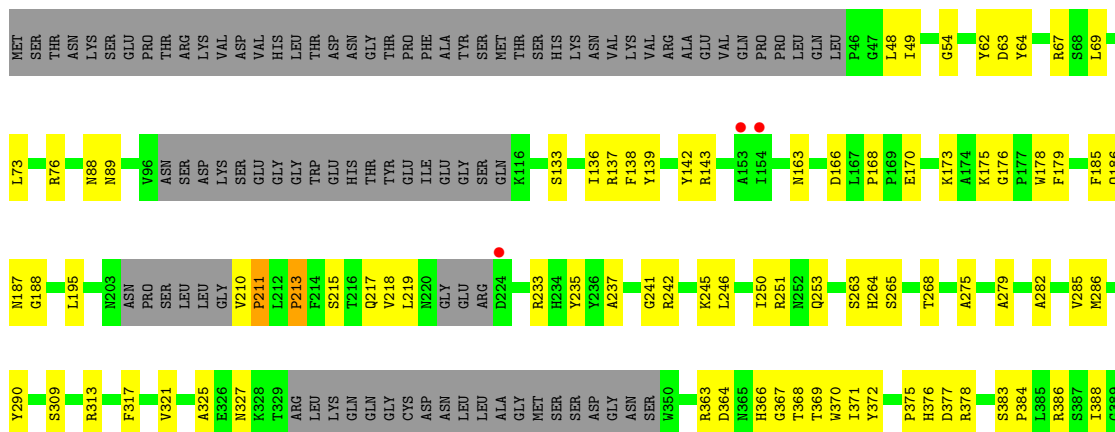
- Molecule 1: Transmembrane protein

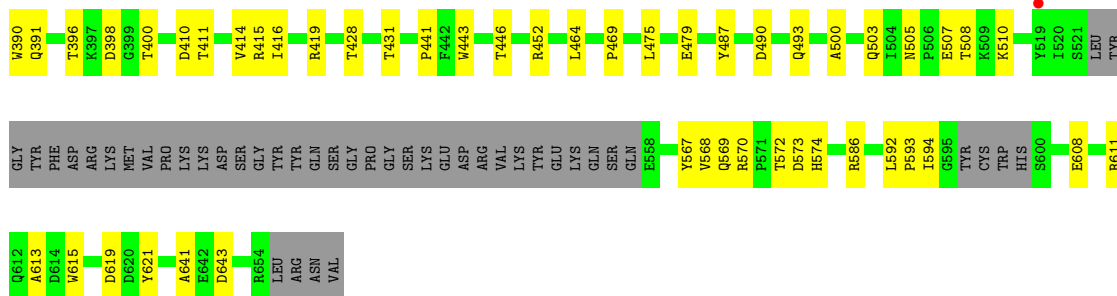
Chain M: 59% 20% 19%



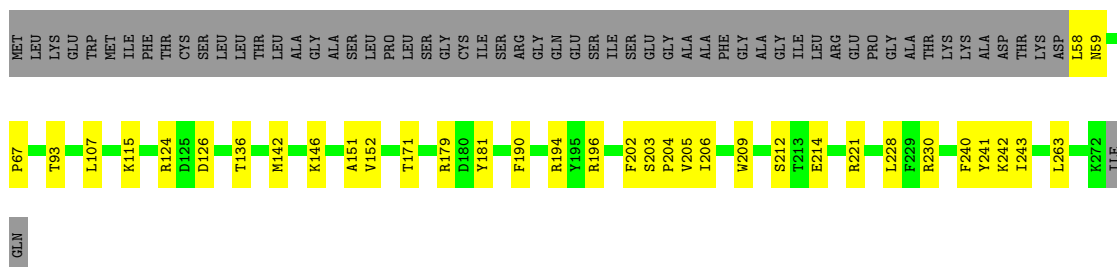
- Molecule 1: Transmembrane protein

Chain O: 59% 20% 21%

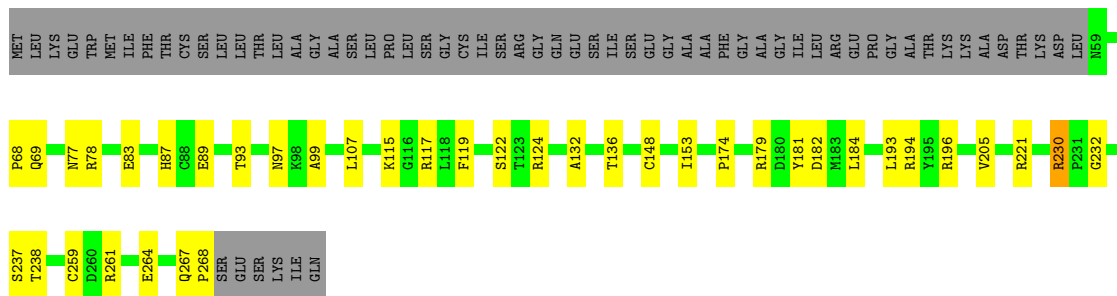




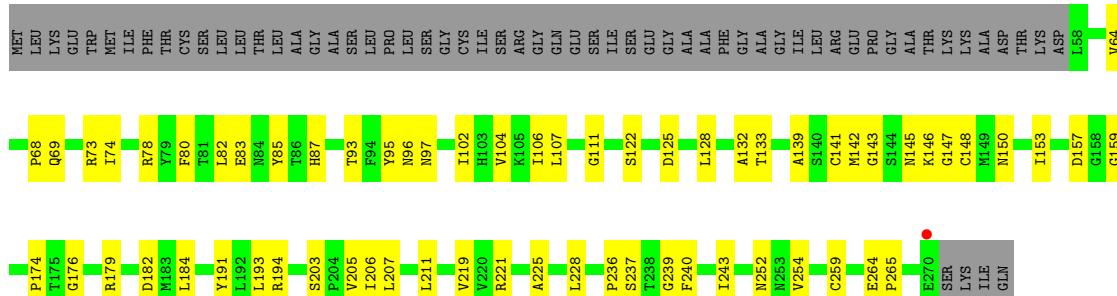
• Molecule 2: Lipoprotein



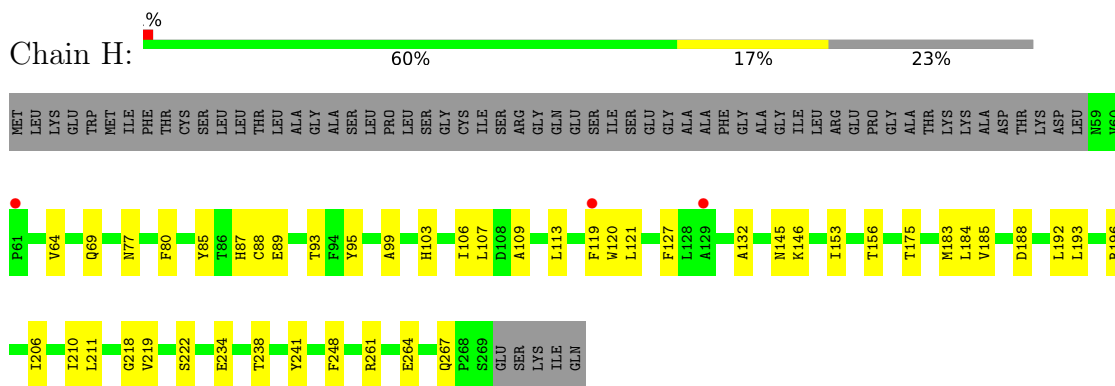
• Molecule 2: Lipoprotein



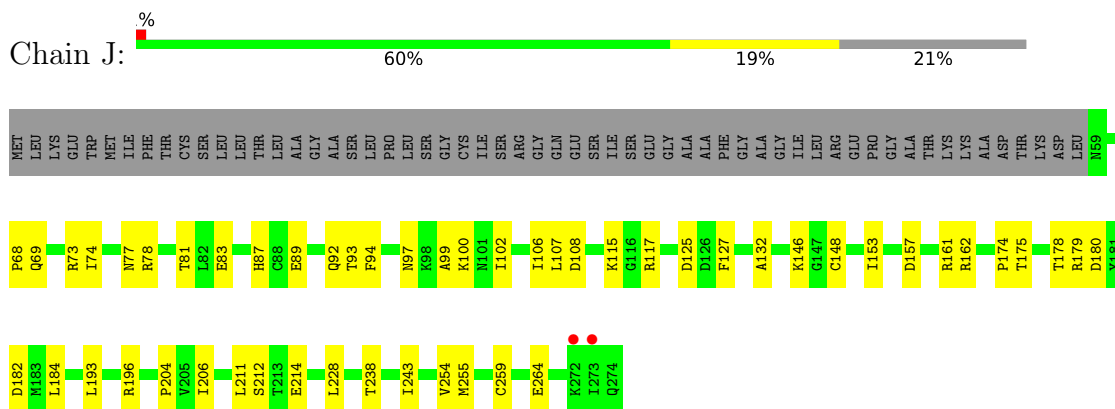
• Molecule 2: Lipoprotein



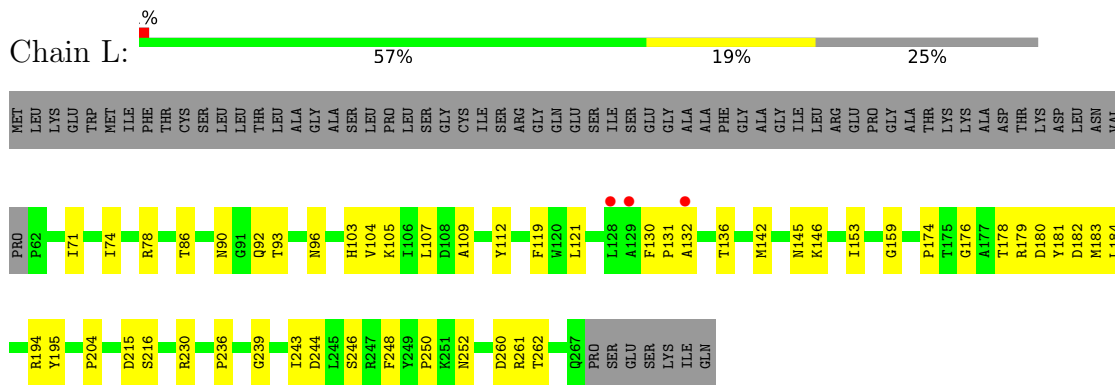
• Molecule 2: Lipoprotein



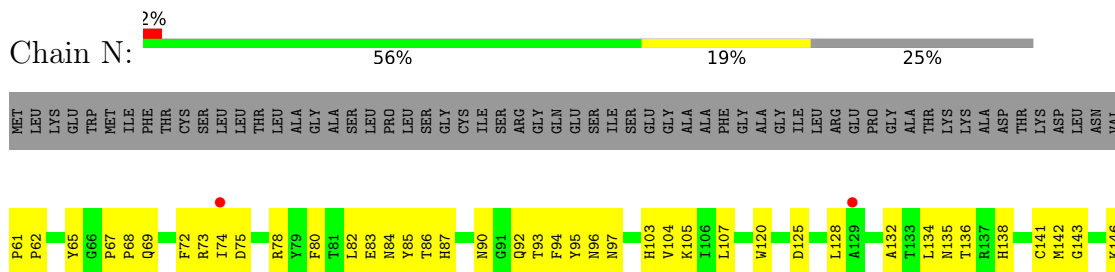
• Molecule 2: Lipoprotein



• Molecule 2: Lipoprotein

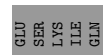
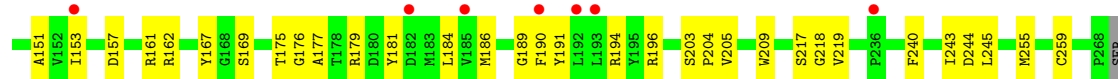
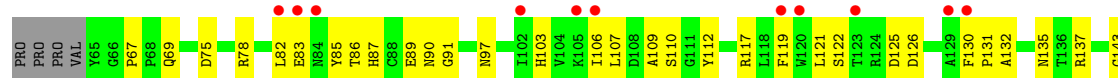
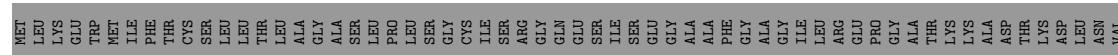


• Molecule 2: Lipoprotein





● Molecule 2: Lipoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.86Å 449.07Å 116.23Å 90.00° 93.18° 90.00°	Depositor
Resolution (Å)	48.74 – 3.60 48.74 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.74-3.60) 98.9 (48.74-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.57Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.233 , 0.268 0.234 , 0.270	Depositor DCC
R_{free} test set	3949 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtrriage
Anisotropy	0.370	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	45234	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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	0.26	0/4188	0.50	0/5736
1	C	0.26	0/4102	0.50	0/5618
1	E	0.26	0/4246	0.49	0/5819
1	G	0.27	0/4259	0.50	0/5838
1	I	0.25	0/4157	0.50	0/5700
1	K	0.26	0/4193	0.50	0/5745
1	M	0.27	0/4091	0.50	0/5604
1	O	0.26	0/4008	0.49	0/5486
2	B	0.26	0/1699	0.51	0/2316
2	D	0.26	0/1657	0.53	0/2258
2	F	0.26	0/1670	0.51	0/2277
2	H	0.26	0/1651	0.50	0/2252
2	J	0.26	0/1693	0.50	0/2307
2	L	0.25	0/1626	0.51	0/2212
2	N	0.25	0/1621	0.52	0/2208
2	P	0.27	0/1611	0.54	0/2191
All	All	0.26	0/46472	0.50	0/63567

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	64	TYR	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	4072	0	3708	113	0
1	C	3989	0	3645	114	0
1	E	4127	0	3709	84	0
1	G	4143	0	3713	66	0
1	I	4042	0	3646	75	0
1	K	4079	0	3693	105	0
1	M	3978	0	3627	92	0
1	O	3900	0	3540	90	0
2	B	1655	0	1537	24	0
2	D	1615	0	1505	29	0
2	F	1628	0	1510	42	0
2	H	1609	0	1488	27	0
2	J	1651	0	1525	36	0
2	L	1586	0	1477	30	0
2	N	1580	0	1465	32	0
2	P	1572	0	1460	45	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
All	All	45234	0	41248	960	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 11.

The worst 5 of 960 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:K:331:LEU:HD12	1:K:366:HIS:CD2	1.36	1.57
1:K:331:LEU:CD1	1:K:366:HIS:CD2	2.05	1.38
1:K:331:LEU:CD1	1:K:366:HIS:HD2	1.33	1.37
1:C:185:PHE:CZ	1:C:217:GLN:NE2	2.19	1.10
1:K:258:THR:HG22	1:K:331:LEU:HD11	1.48	0.96

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	529/658 (80%)	475 (90%)	45 (8%)	9 (2%)	9 45
1	C	518/658 (79%)	463 (89%)	49 (10%)	6 (1%)	13 51
1	E	543/658 (82%)	481 (89%)	49 (9%)	13 (2%)	6 37
1	G	548/658 (83%)	480 (88%)	55 (10%)	13 (2%)	6 37
1	I	531/658 (81%)	473 (89%)	48 (9%)	10 (2%)	8 42
1	K	534/658 (81%)	493 (92%)	38 (7%)	3 (1%)	25 64
1	M	518/658 (79%)	472 (91%)	34 (7%)	12 (2%)	6 38
1	O	507/658 (77%)	464 (92%)	35 (7%)	8 (2%)	9 46
2	B	213/274 (78%)	193 (91%)	18 (8%)	2 (1%)	17 57
2	D	208/274 (76%)	191 (92%)	16 (8%)	1 (0%)	29 68
2	F	211/274 (77%)	197 (93%)	13 (6%)	1 (0%)	29 68
2	H	209/274 (76%)	192 (92%)	15 (7%)	2 (1%)	15 55
2	J	214/274 (78%)	191 (89%)	23 (11%)	0	100 100
2	L	204/274 (74%)	188 (92%)	15 (7%)	1 (0%)	29 68
2	N	204/274 (74%)	189 (93%)	15 (7%)	0	100 100
2	P	202/274 (74%)	180 (89%)	22 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5893/7456 (79%)	5322 (90%)	490 (8%)	81 (1%)	11	48

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	PRO
1	A	211	PRO
1	A	501	TYR
1	A	560	MET
1	E	211	PRO

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	402/559 (72%)	398 (99%)	4 (1%)	76	88
1	C	396/559 (71%)	395 (100%)	1 (0%)	92	97
1	E	398/559 (71%)	397 (100%)	1 (0%)	92	97
1	G	400/559 (72%)	396 (99%)	4 (1%)	76	88
1	I	393/559 (70%)	392 (100%)	1 (0%)	92	97
1	K	399/559 (71%)	398 (100%)	1 (0%)	92	97
1	M	392/559 (70%)	389 (99%)	3 (1%)	81	91
1	O	382/559 (68%)	382 (100%)	0	100	100
2	B	174/234 (74%)	174 (100%)	0	100	100
2	D	169/234 (72%)	169 (100%)	0	100	100
2	F	170/234 (73%)	169 (99%)	1 (1%)	86	94
2	H	168/234 (72%)	168 (100%)	0	100	100
2	J	172/234 (74%)	172 (100%)	0	100	100
2	L	165/234 (70%)	165 (100%)	0	100	100
2	N	164/234 (70%)	164 (100%)	0	100	100
2	P	163/234 (70%)	163 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4507/6344 (71%)	4491 (100%)	16 (0%)	91 97

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	430	GLN
1	M	245	LYS
1	G	251	ARG
1	K	185	PHE
1	G	185	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	638	GLN
2	L	96	ASN
1	K	264	HIS
1	M	53	HIS
1	C	264	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 8 ligands modelled in this entry, 8 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	541/658 (82%)	-0.50	0 100 100	54, 89, 117, 138	0
1	C	530/658 (80%)	-0.46	0 100 100	49, 83, 114, 142	0
1	E	553/658 (84%)	-0.49	2 (0%) 92 86	51, 95, 123, 143	0
1	G	558/658 (84%)	-0.44	2 (0%) 92 86	49, 93, 125, 173	0
1	I	543/658 (82%)	-0.49	0 100 100	49, 97, 126, 148	0
1	K	546/658 (82%)	-0.43	1 (0%) 95 91	53, 95, 129, 152	0
1	M	530/658 (80%)	-0.41	1 (0%) 95 91	75, 106, 140, 165	0
1	O	521/658 (79%)	-0.33	4 (0%) 86 75	83, 133, 169, 183	0
2	B	215/274 (78%)	-0.48	0 100 100	74, 93, 141, 172	0
2	D	210/274 (76%)	-0.46	0 100 100	64, 93, 124, 163	0
2	F	213/274 (77%)	-0.36	1 (0%) 91 83	68, 97, 132, 155	0
2	H	211/274 (77%)	-0.42	3 (1%) 75 61	77, 123, 145, 175	0
2	J	216/274 (78%)	-0.36	2 (0%) 84 73	64, 95, 146, 191	0
2	L	206/274 (75%)	-0.21	3 (1%) 73 60	79, 115, 141, 156	0
2	N	206/274 (75%)	-0.20	6 (2%) 51 35	83, 129, 150, 161	0
2	P	204/274 (74%)	0.10	18 (8%) 10 6	117, 181, 204, 221	0
All	All	6003/7456 (80%)	-0.41	43 (0%) 87 78	49, 100, 155, 221	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	128	LEU	5.1
2	L	129	ALA	5.0
2	P	120	TRP	4.6
2	J	273	ILE	4.2
1	O	154	ILE	3.9

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](#)

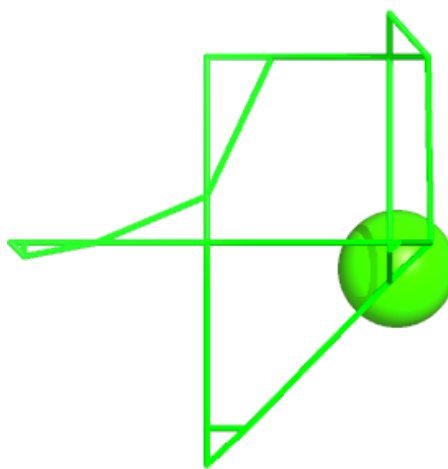
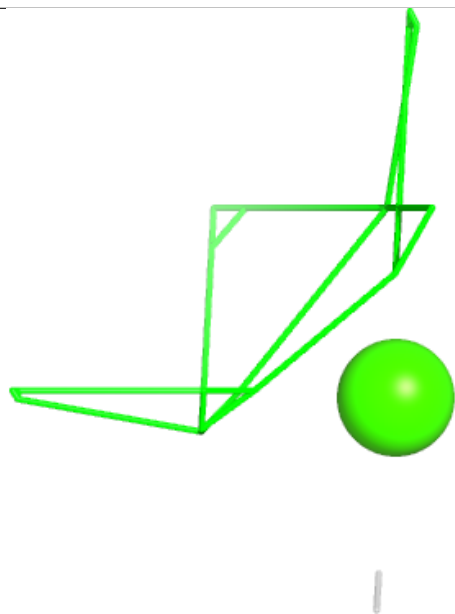
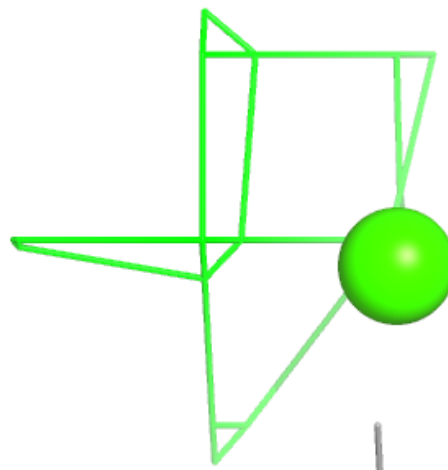
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	A	701	1/1	0.86	0.19	83,83,83,83	0
3	CA	K	701	1/1	0.94	0.19	81,81,81,81	0
3	CA	M	701	1/1	0.94	0.21	91,91,91,91	0
3	CA	C	701	1/1	0.97	0.22	72,72,72,72	0
3	CA	G	701	1/1	0.98	0.10	83,83,83,83	0
3	CA	I	701	1/1	0.98	0.19	70,70,70,70	0
3	CA	E	701	1/1	0.99	0.13	76,76,76,76	0
3	CA	O	701	1/1	0.99	0.17	106,106,106,106	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.

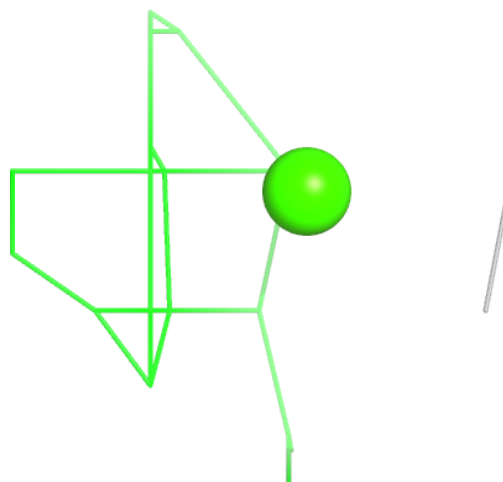
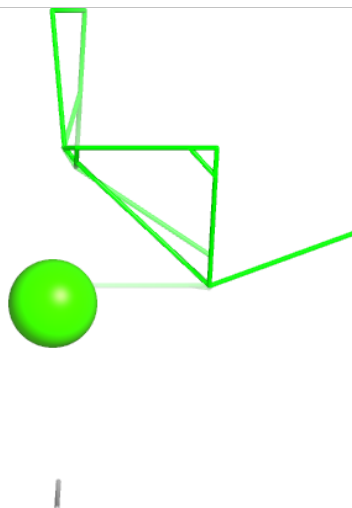
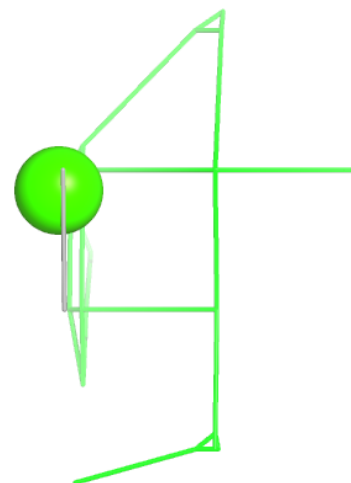
Electron density around CA A 701:

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



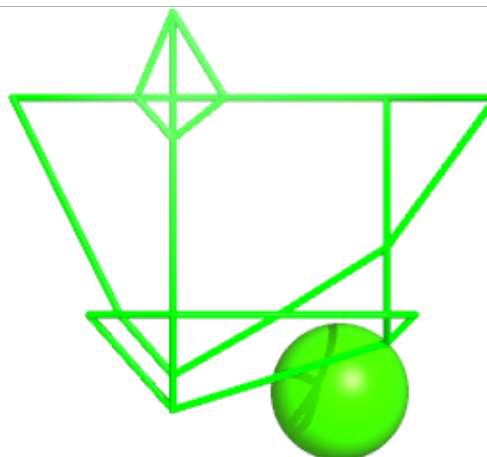
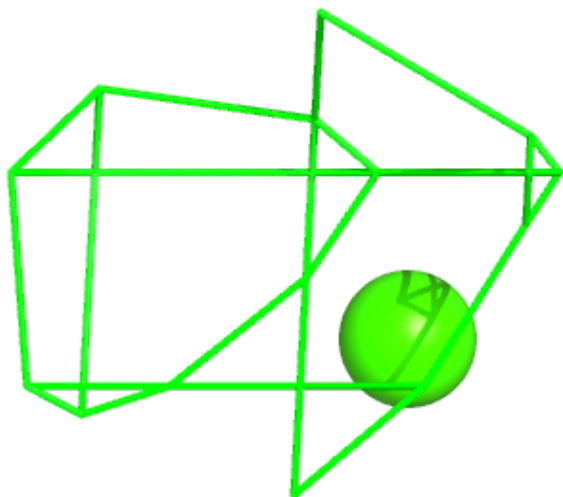
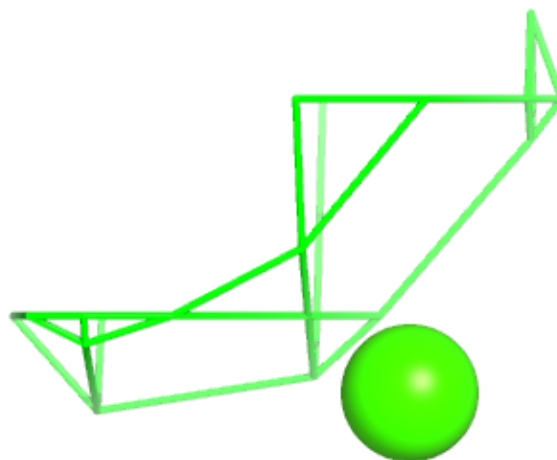
Electron density around CA K 701:

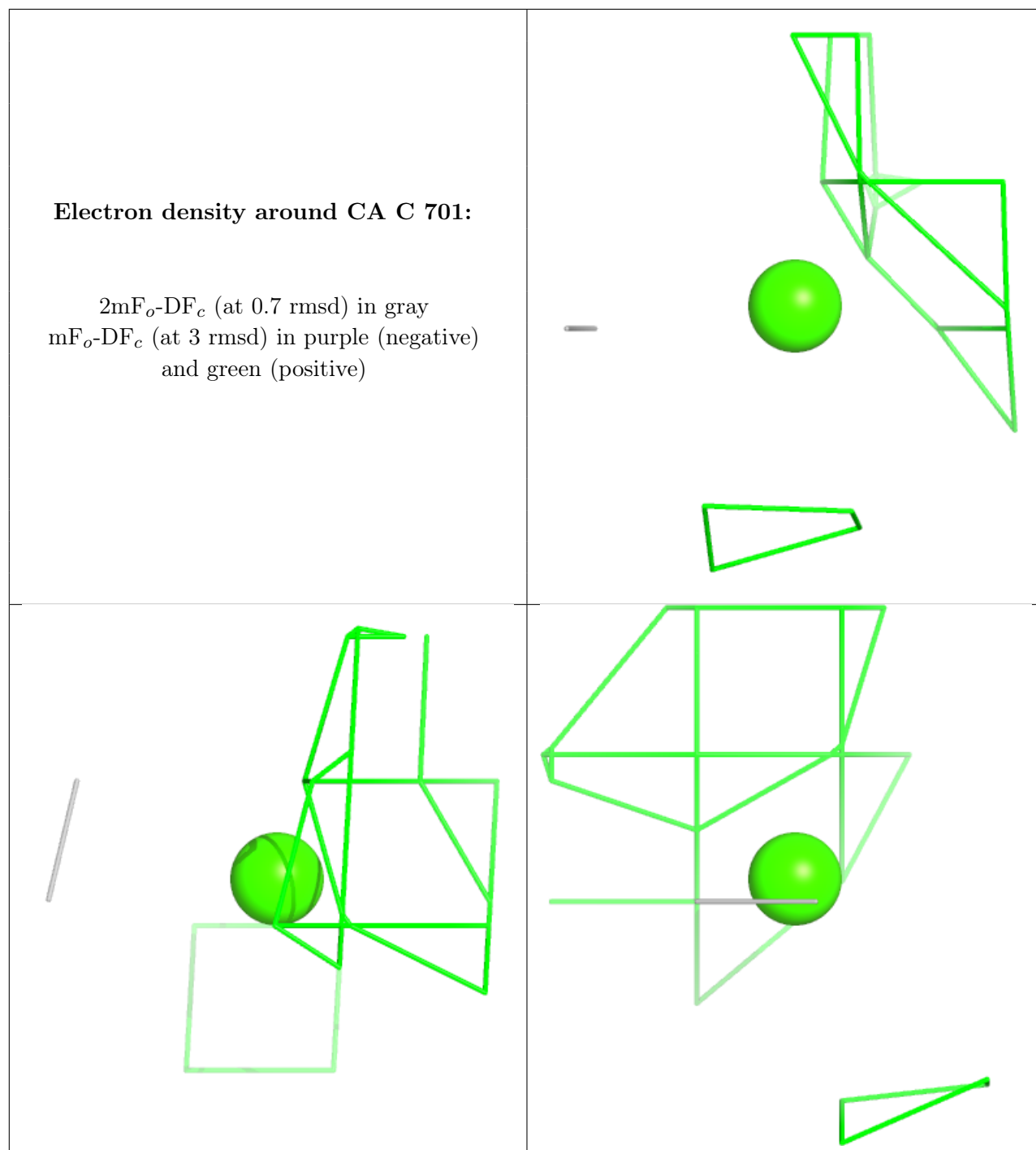
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA M 701:

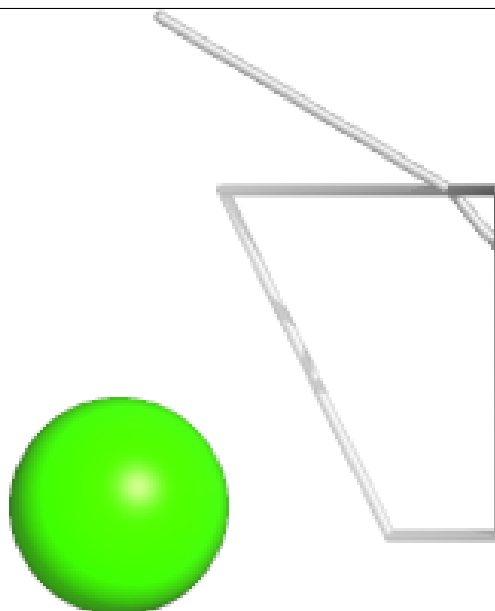
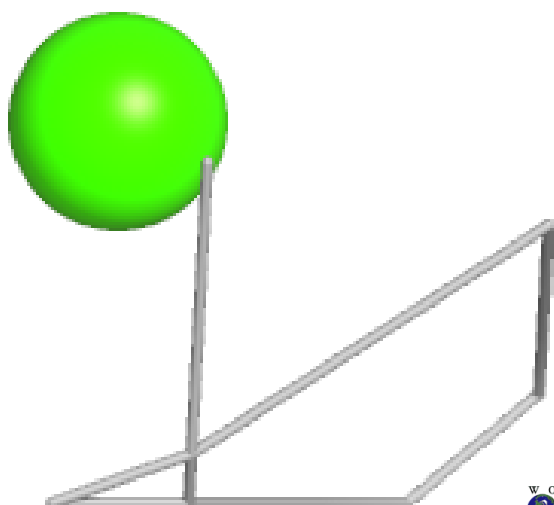
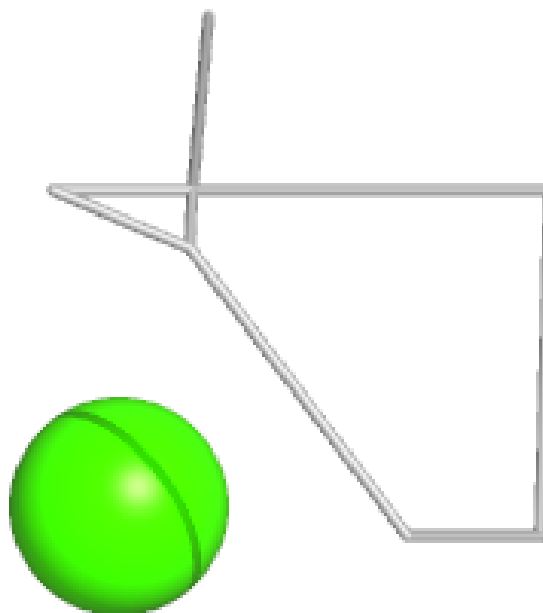
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

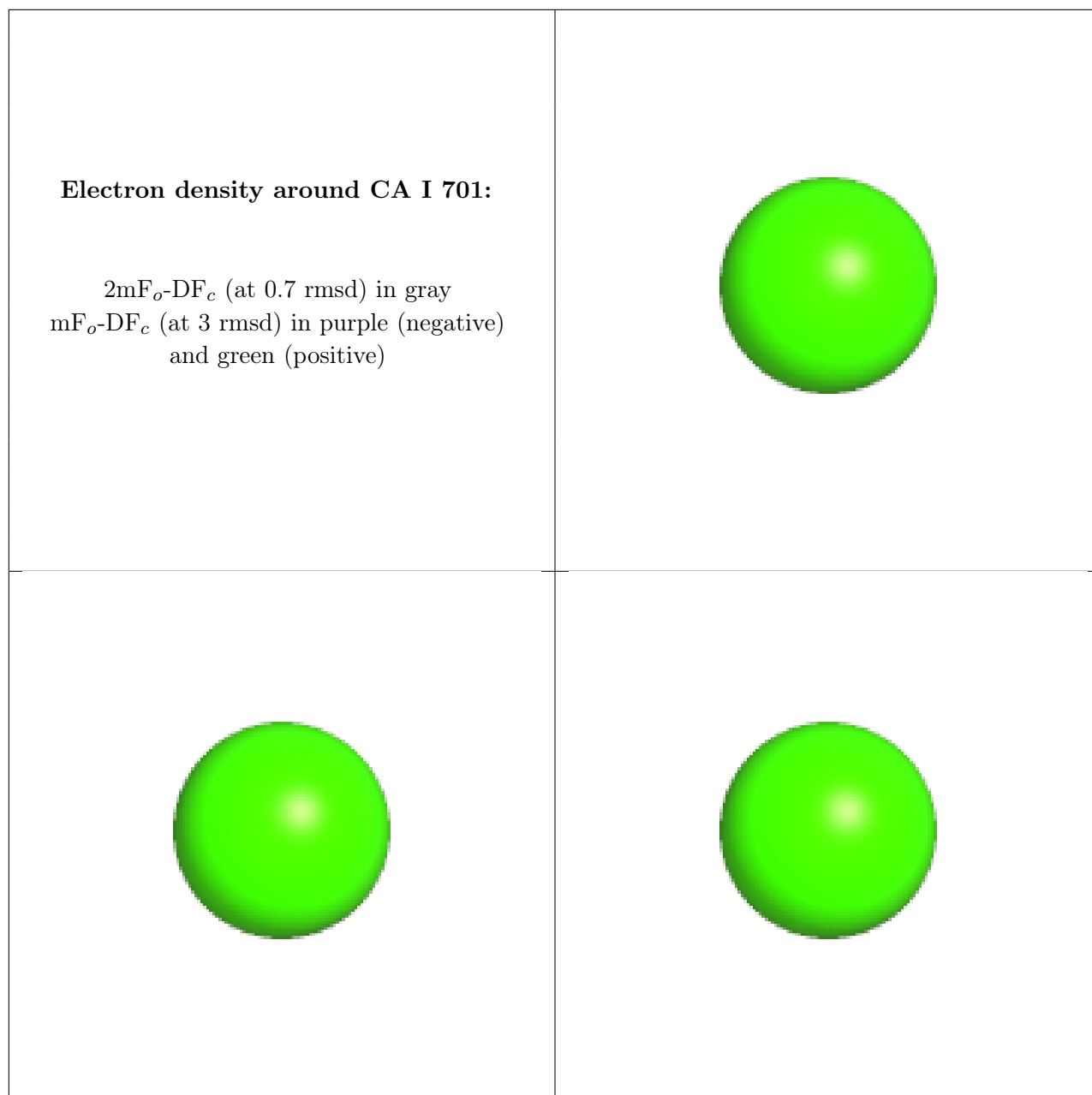




Electron density around CA G 701:

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

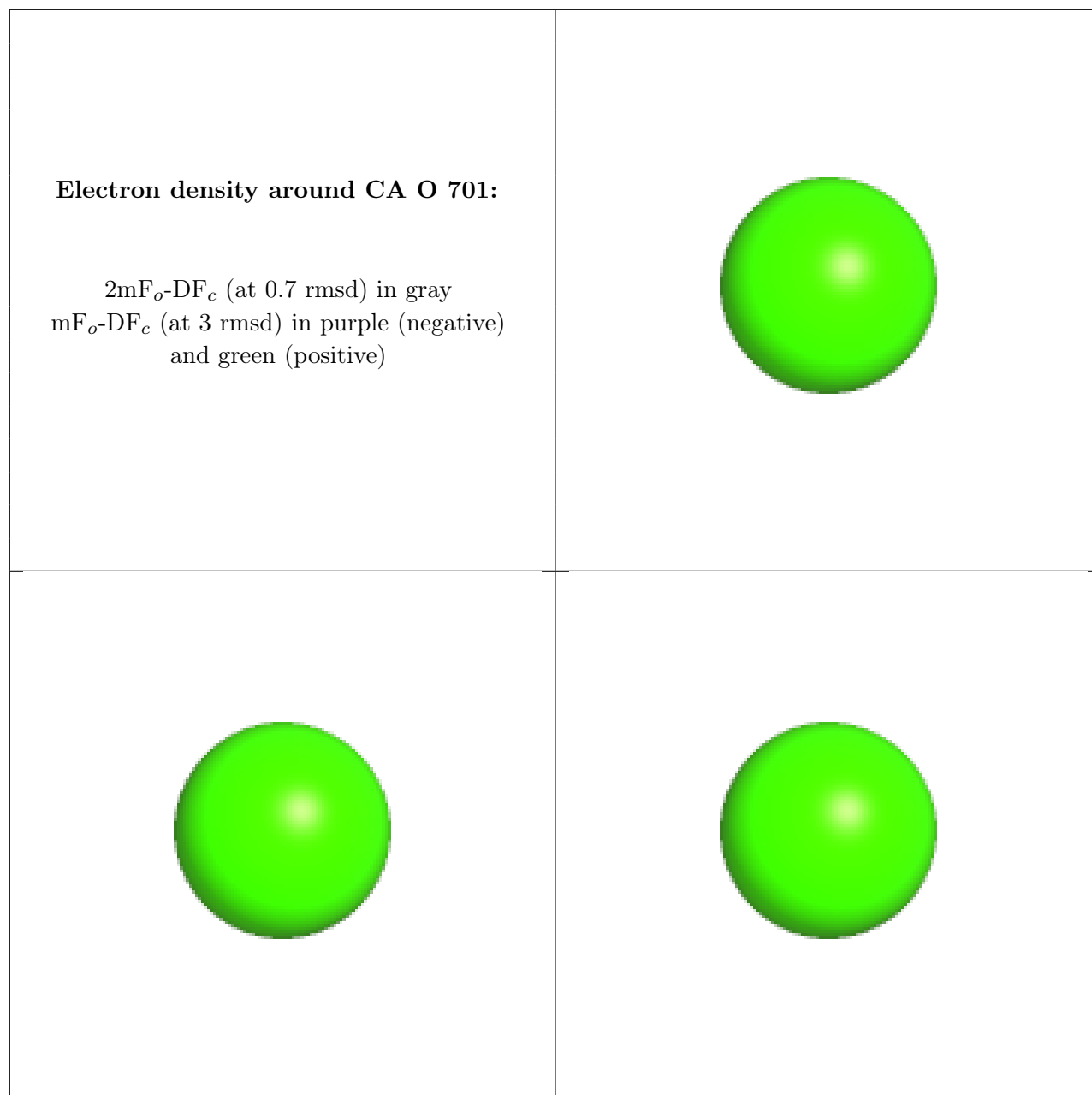




Electron density around CA E 701:

$2mF_o-DF_c$ (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.