



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:49 AM UTC

PDB ID : 7V97 / pdb_00007v97
Title : Arsenic-bound p53 DNA-binding domain mutant V272M
Authors : Lu, M.; Xing, Y.F.; Wang, Z.Y.; Ni, Y.; Song, H.X.
Deposited on : 2021-08-24
Resolution : 2.02 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 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:

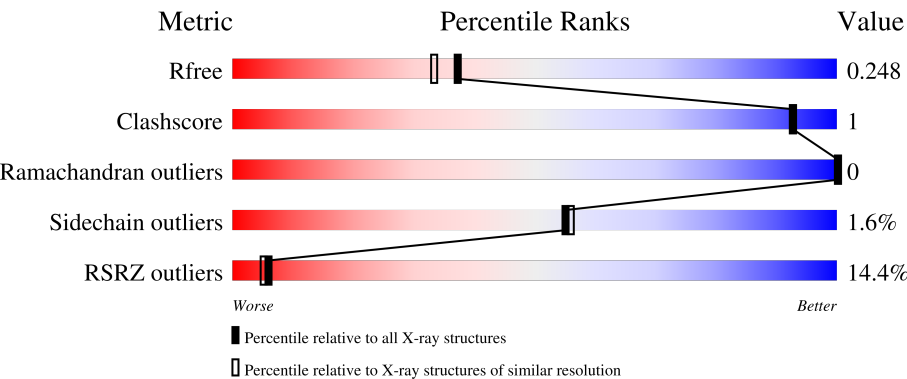
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	200	6% 90%6%
1	B	200	9% 90%6%
1	C	200	15% 92%6%
1	D	200	26% 94%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6196 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	2	0
			1533	944	282	289	18			
1	B	193	Total	C	N	O	S	0	4	0
			1547	953	287	289	18			
1	C	194	Total	C	N	O	S	0	2	0
			1533	944	282	289	18			
1	D	192	Total	C	N	O	S	0	1	0
			1514	933	279	285	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	MET	VAL	variant	UNP P04637
B	272	MET	VAL	variant	UNP P04637
C	272	MET	VAL	variant	UNP P04637
D	272	MET	VAL	variant	UNP P04637

- Molecule 2 is ARSENIC (CCD ID: ARS) (formula: As) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

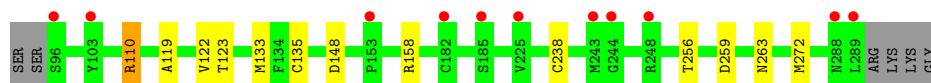
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	11	Total 11	O 11	0	0
4	C	16	Total 16	O 16	0	0
4	D	16	Total 16	O 16	0	0

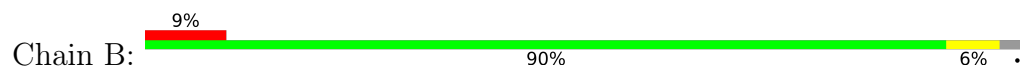
3 Residue-property plots [i](#)

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.

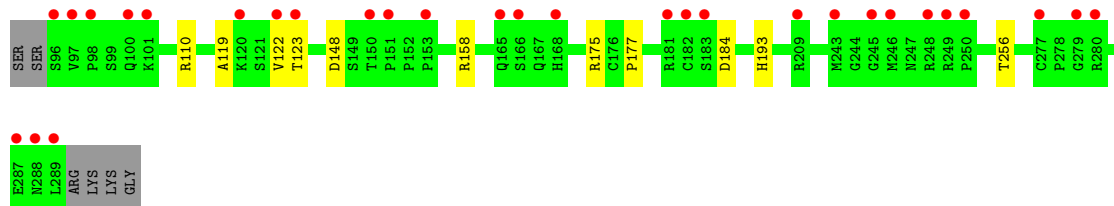
- Molecule 1: Cellular tumor antigen p53



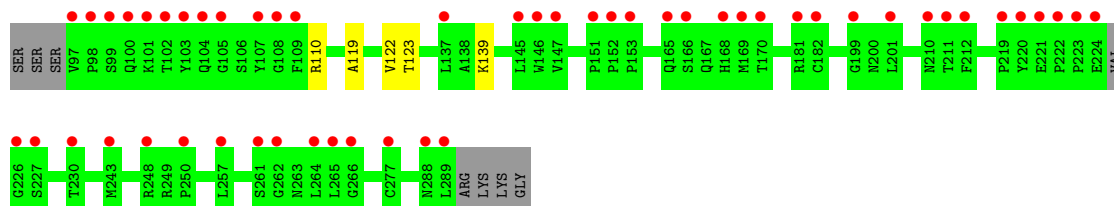
- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.84Å 71.52Å 84.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.80 – 2.02 42.80 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.3 (42.80-2.02) 99.8 (42.80-2.02)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.234 , 0.251 0.233 , 0.248	Depositor DCC
R_{free} test set	2593 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l 0.018 for k,h,-l 0.110 for h,-k,-l	Xtriage
Reported twinning fraction	0.568 for H, K, L 0.432 for -h,-k,l	Depositor
Outliers	0 of 54021 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6196	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.89% 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: ZN, ARS

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	1.02	0/1571	1.29	0/2130
1	B	1.03	0/1585	1.29	0/2147
1	C	1.04	0/1571	1.29	0/2129
1	D	1.03	0/1551	1.28	0/2100
All	All	1.03	0/6278	1.29	0/8506

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 [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	1533	0	1487	7	0
1	B	1547	0	1506	4	0
1	C	1533	0	1486	7	0
1	D	1514	0	1467	2	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	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	18	0	0	0	0
4	B	11	0	0	0	0
4	C	16	0	0	0	0
4	D	16	0	0	0	0
All	All	6196	0	5946	18	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 1.

All (18) 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:263:ASN:HD21	1:C:177:PRO:HB2	1.11	1.08
1:A:263:ASN:ND2	1:C:177:PRO:HB2	1.94	0.82
1:B:119:ALA:O	1:B:122:VAL:HG22	1.94	0.68
1:A:110:ARG:NH1	1:A:148:ASP:OD1	2.42	0.52
1:C:175:ARG:NH2	1:C:184:ASP:OD2	2.47	0.47
1:C:110:ARG:NH1	1:C:148:ASP:OD1	2.48	0.47
1:D:123:THR:CG2	1:D:139:LYS:HB3	2.45	0.47
1:B:100:GLN:OE1	1:B:162:ILE:HD11	2.15	0.46
1:A:259:ASP:OD1	1:A:259:ASP:C	2.59	0.45
1:A:119:ALA:O	1:A:122:VAL:HG22	2.17	0.45
1:B:175:ARG:HD3	1:B:191:PRO:O	2.17	0.45
1:A:158:ARG:HB3	1:A:256:THR:OG1	2.17	0.44
1:D:119:ALA:O	1:D:122:VAL:HG22	2.18	0.44
1:C:158:ARG:HB3	1:C:256:THR:OG1	2.20	0.42
1:C:119:ALA:O	1:C:122:VAL:HG22	2.21	0.41
1:A:133:MET:HB3	1:A:272:MET:SD	2.61	0.41
1:B:164[B]:LYS:HE3	1:B:250:PRO:HB2	2.01	0.41
1:C:175:ARG:HD2	1:C:193:HIS:O	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	194/200 (97%)	191 (98%)	3 (2%)	0	100	100
1	B	195/200 (98%)	192 (98%)	3 (2%)	0	100	100
1	C	194/200 (97%)	192 (99%)	2 (1%)	0	100	100
1	D	189/200 (94%)	183 (97%)	6 (3%)	0	100	100
All	All	772/800 (96%)	758 (98%)	14 (2%)	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	176/179 (98%)	172 (98%)	4 (2%)	44	43
1	B	177/179 (99%)	172 (97%)	5 (3%)	38	35
1	C	176/179 (98%)	175 (99%)	1 (1%)	78	79
1	D	173/179 (97%)	172 (99%)	1 (1%)	78	79
All	All	702/716 (98%)	691 (98%)	11 (2%)	55	56

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	123	THR

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Mol	Chain	Res	Type
1	A	135	CYS
1	A	238	CYS
1	B	110	ARG
1	B	123	THR
1	B	135	CYS
1	B	238	CYS
1	B	268	ASN
1	C	123	THR
1	D	110	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	263	ASN
1	A	288	ASN
1	B	131	ASN
1	B	168	HIS
1	B	235	ASN
1	B	239	ASN
1	C	100	GLN
1	C	115	HIS
1	C	168	HIS
1	C	210	ASN
1	C	239	ASN
1	C	288	ASN
1	D	100	GLN
1	D	165	GLN
1	D	168	HIS

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 oligosaccharides 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 [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, 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	194/200 (97%)	0.47	11 (5%) 29 28	12, 22, 32, 47	2 (1%)
1	B	193/200 (96%)	0.85	18 (9%) 14 13	13, 26, 40, 48	4 (2%)
1	C	194/200 (97%)	1.08	30 (15%) 5 4	14, 26, 46, 57	2 (1%)
1	D	192/200 (96%)	1.32	52 (27%) 1 1	16, 29, 49, 56	1 (0%)
All	All	773/800 (96%)	0.93	111 (14%) 6 5	12, 25, 45, 57	9 (1%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	97	VAL	5.1
1	D	265	LEU	4.7
1	C	183	SER	4.6
1	C	289	LEU	4.5
1	B	226	GLY	4.3
1	C	280	ARG	4.3
1	D	105	GLY	4.2
1	C	166	SER	4.2
1	B	289	LEU	4.2
1	D	153	PRO	4.2
1	C	153	PRO	4.1
1	C	248	ARG	4.0
1	D	243	MET	4.0
1	A	289	LEU	3.9
1	D	100	GLN	3.8
1	D	289	LEU	3.7
1	D	264	LEU	3.6
1	D	166	SER	3.6
1	D	103	TYR	3.6
1	D	226	GLY	3.5
1	C	243	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	225	VAL	3.5
1	B	227	SER	3.4
1	C	182[A]	CYS	3.3
1	D	102	THR	3.3
1	B	225	VAL	3.2
1	D	169	MET	3.2
1	D	221	GLU	3.2
1	A	153	PRO	3.1
1	B	243	MET	3.1
1	D	107	TYR	3.1
1	D	151	PRO	3.1
1	C	277	CYS	3.0
1	C	150	THR	3.0
1	C	168	HIS	3.0
1	C	100	GLN	3.0
1	C	165	GLN	2.9
1	D	146	TRP	2.9
1	C	245	GLY	2.9
1	B	122	VAL	2.9
1	D	152	PRO	2.8
1	B	120	LYS	2.8
1	C	97	VAL	2.8
1	C	246	MET	2.7
1	D	230	THR	2.7
1	D	288	ASN	2.7
1	C	96	SER	2.7
1	D	248	ARG	2.7
1	C	288	ASN	2.7
1	D	211	THR	2.6
1	C	250	PRO	2.6
1	A	96	SER	2.6
1	D	182	CYS	2.6
1	D	104	GLN	2.6
1	D	168	HIS	2.6
1	A	244	GLY	2.6
1	D	98	PRO	2.6
1	C	287	GLU	2.5
1	D	277	CYS	2.5
1	C	249	ARG	2.5
1	D	101	LYS	2.5
1	C	181	ARG	2.5
1	D	250	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	97	VAL	2.5
1	C	101	LYS	2.5
1	B	248	ARG	2.5
1	D	210	ASN	2.4
1	D	224	GLU	2.4
1	D	227	SER	2.4
1	D	261	SER	2.4
1	D	223	PRO	2.4
1	C	279	GLY	2.4
1	B	183	SER	2.4
1	C	120	LYS	2.3
1	D	181	ARG	2.3
1	C	122	VAL	2.3
1	C	123	THR	2.3
1	C	151	PRO	2.3
1	B	187	GLY	2.3
1	C	209	ARG	2.3
1	D	201	LEU	2.3
1	D	220	TYR	2.3
1	D	212	PHE	2.3
1	C	98	PRO	2.3
1	D	99	SER	2.2
1	D	170	THR	2.2
1	A	248	ARG	2.2
1	A	288	ASN	2.2
1	D	257	LEU	2.2
1	B	182	CYS	2.2
1	B	209	ARG	2.2
1	B	223	PRO	2.1
1	D	108	GLY	2.1
1	D	222	PRO	2.1
1	D	145	LEU	2.1
1	D	109	PHE	2.1
1	B	245	GLY	2.1
1	D	199	GLY	2.1
1	D	147	VAL	2.1
1	A	185	SER	2.1
1	D	137	LEU	2.0
1	B	210	ASN	2.0
1	D	165	GLN	2.0
1	D	262	GLY	2.0
1	D	266	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	243	MET	2.0
1	B	100	GLN	2.0
1	B	264	LEU	2.0
1	A	182	CYS	2.0
1	D	219	PRO	2.0
1	A	103	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

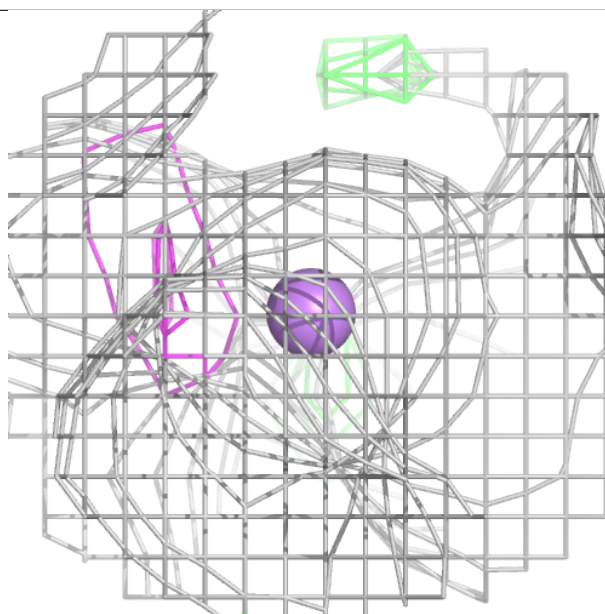
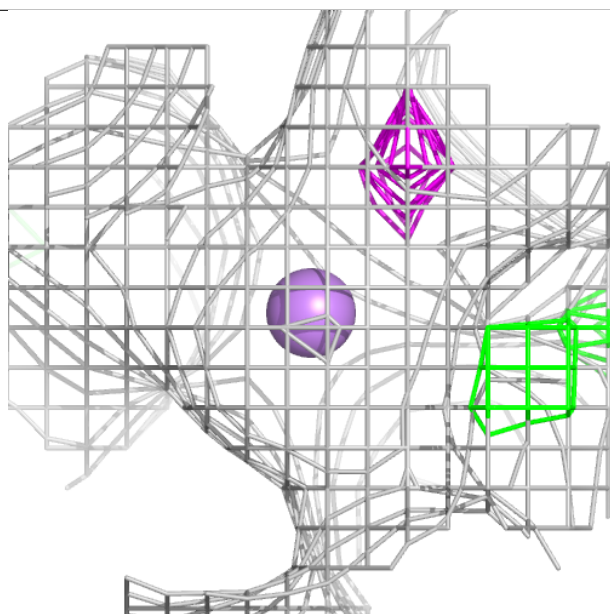
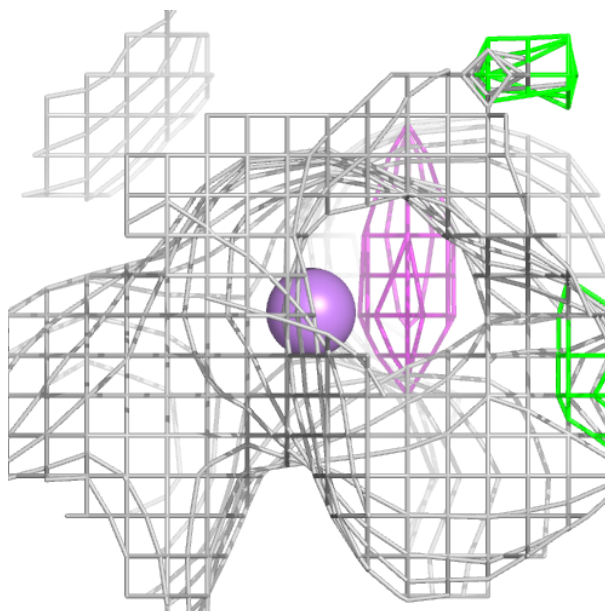
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ARS	C	301	1/1	0.91	0.10	29,29,29,29	1
2	ARS	B	301	1/1	0.95	0.05	29,29,29,29	1
2	ARS	A	301	1/1	0.95	0.06	21,21,21,21	1
2	ARS	D	301	1/1	0.95	0.08	23,23,23,23	1
3	ZN	C	302	1/1	0.96	0.05	22,22,22,22	1
3	ZN	D	302	1/1	0.97	0.04	21,21,21,21	1
3	ZN	B	302	1/1	0.98	0.04	22,22,22,22	1
3	ZN	A	302	1/1	0.99	0.03	20,20,20,20	1

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.

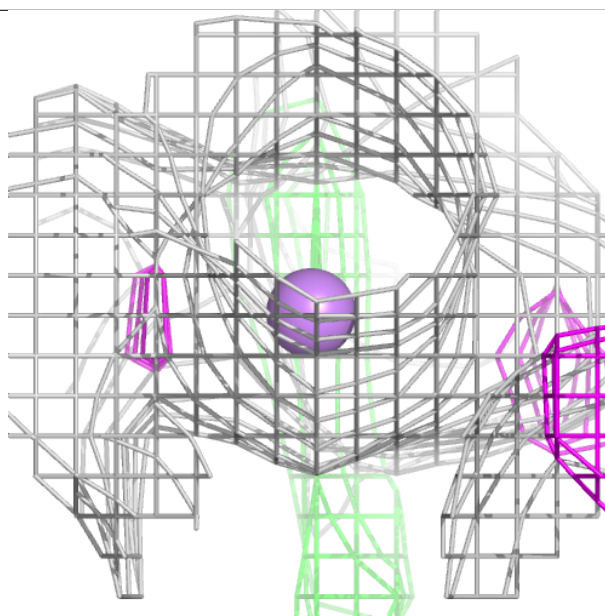
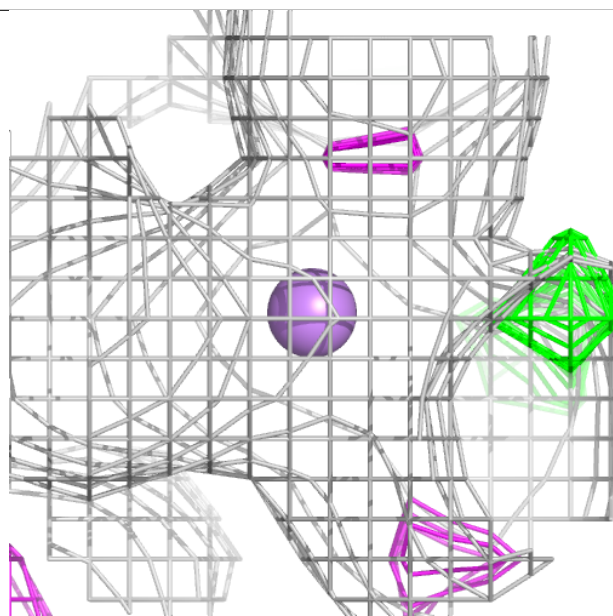
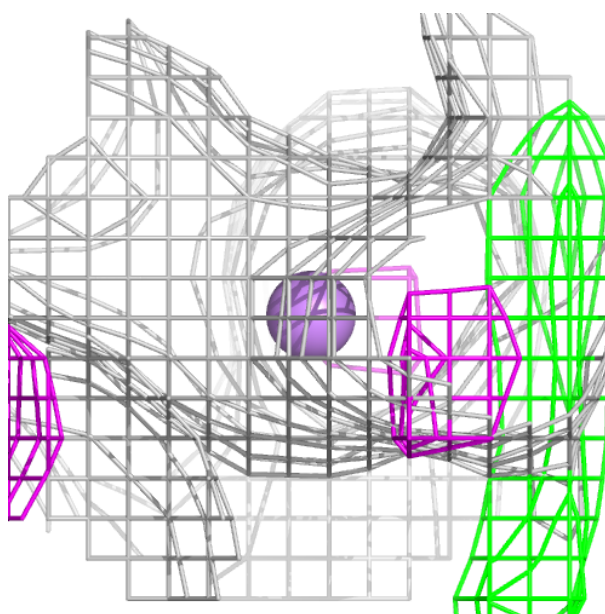
Electron density around ARS C 301:

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



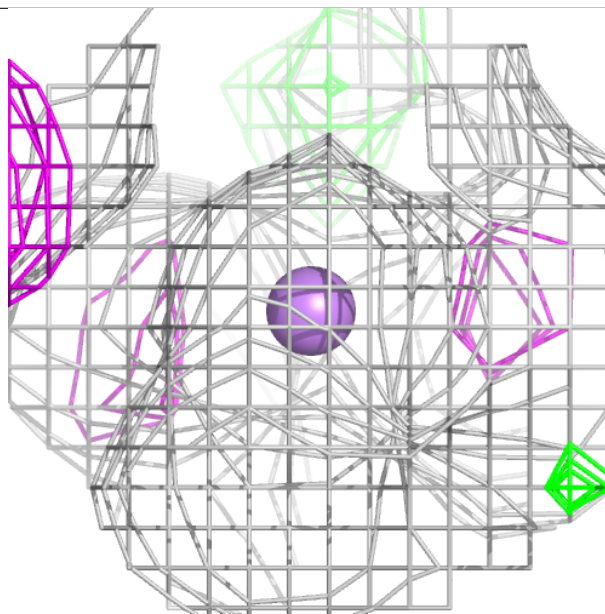
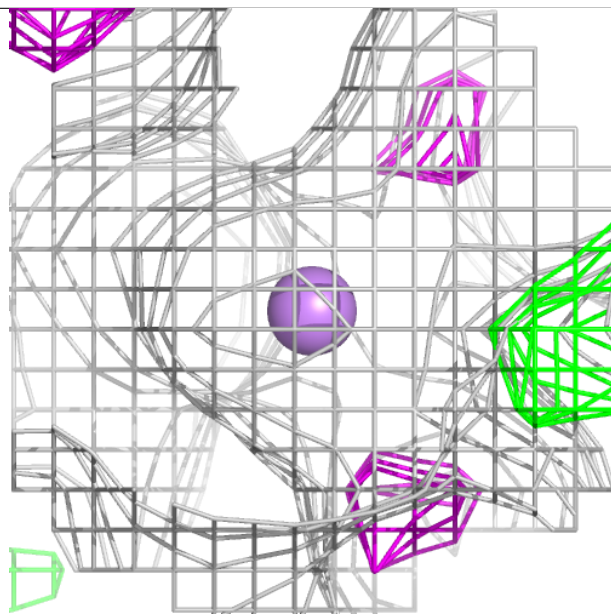
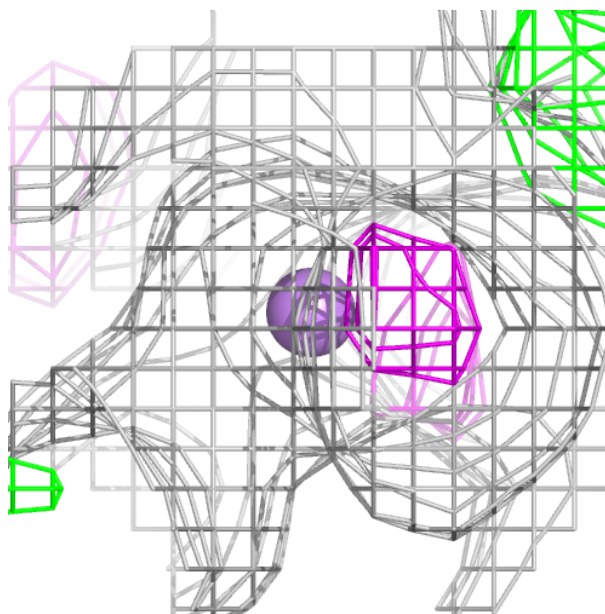
Electron density around ARS B 301:

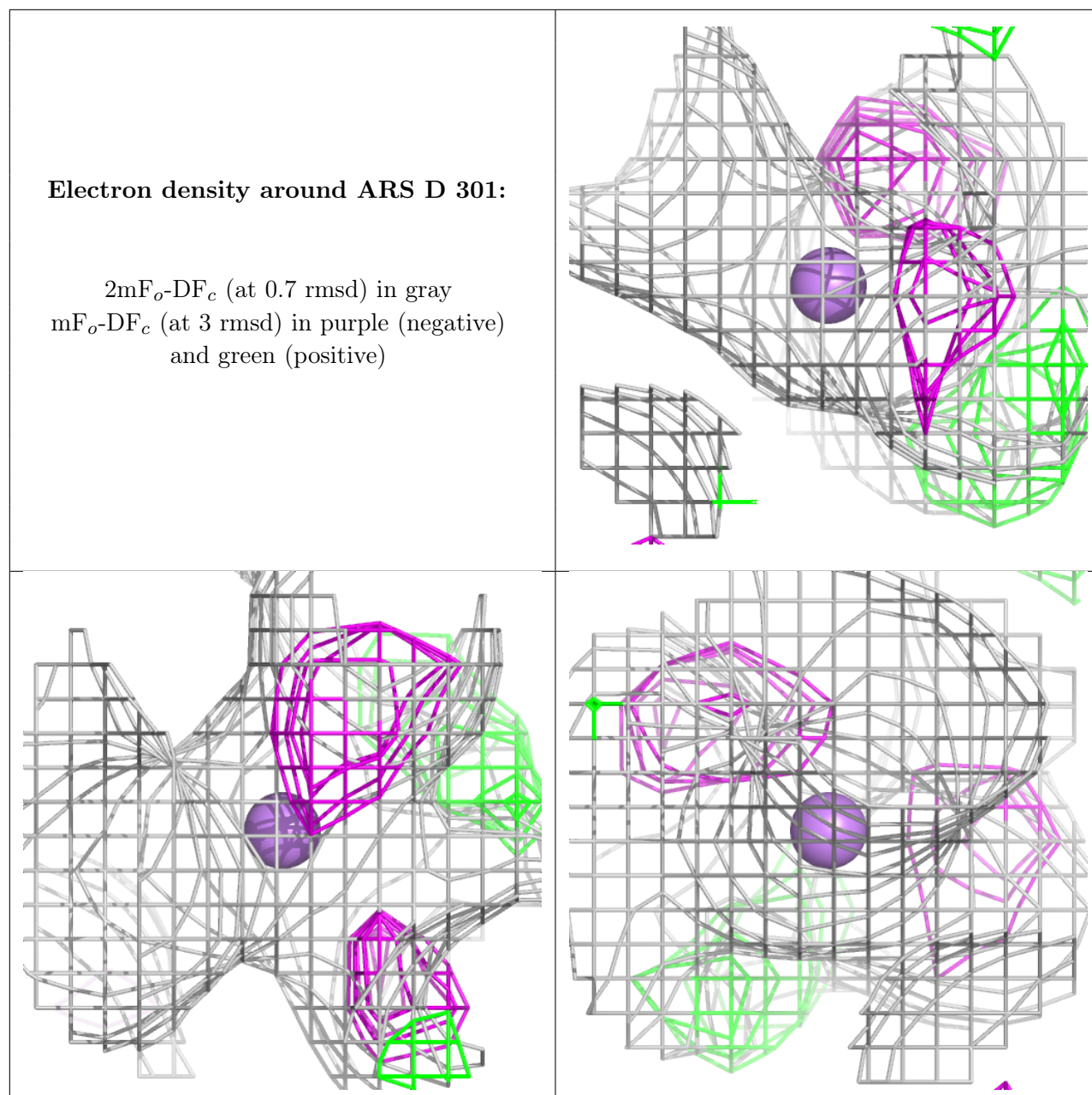
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ARS A 301:

$2mF_o-DF_c$ (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.