Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2025 – 04:07 pm BST

PDB ID	:	9HNB / pdb_00009hnb
Title	:	X-ray structure of the adduct formed upon reaction of the diiodido analogue of picoplatin with human serum albumin
Authors	:	Ferraro, G.; Merlino, A.
Deposited on	:	2024-12-10
Resolution	:	3.90 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:

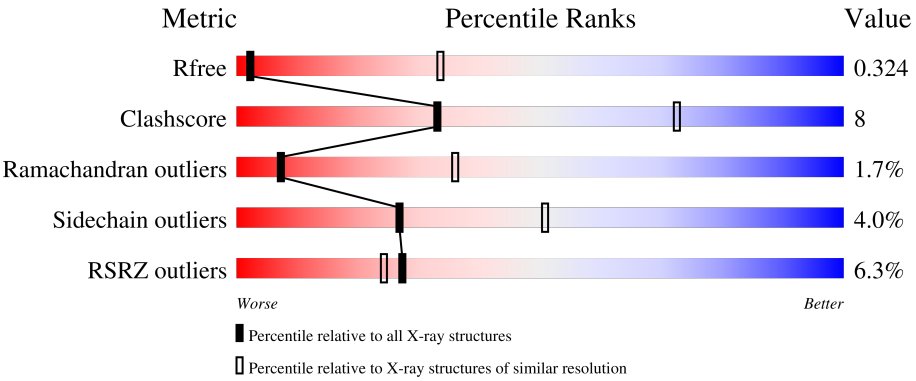
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.90 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}	164625	1157 (4.10-3.70)
Clashscore	180529	1219 (4.10-3.70)
Ramachandran outliers	177936	1177 (4.10-3.70)
Sidechain outliers	177891	1169 (4.10-3.70)
RSRZ outliers	164620	1157 (4.10-3.70)

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	AAA	585	6% 72% 20% · 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4198 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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	543	4195	2656	705	794	40	0	0	0

- Molecule 2 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt) (labeled as "Ligand of Interest" by depositor).

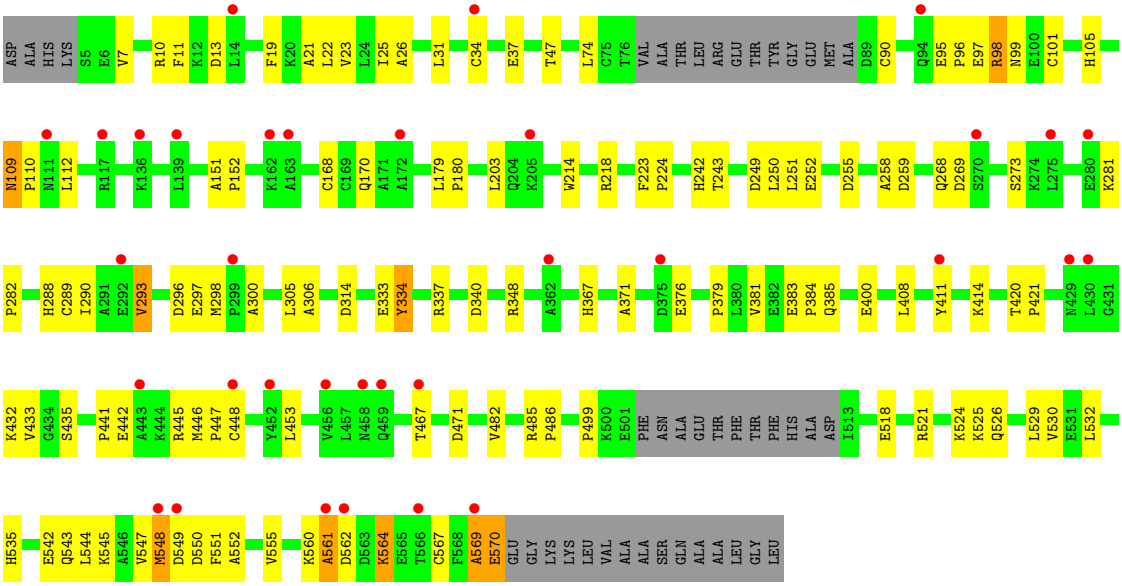
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Pt		
2	AAA	3	3	3	0	0

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: Serum albumin

Chain AAA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.07Å 86.55Å 59.50Å 90.00° 102.55° 90.00°	Depositor
Resolution (Å)	47.42 – 3.90 47.42 – 3.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (47.42-3.90) 93.4 (47.42-3.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.292 , 0.328 0.293 , 0.324	Depositor DCC
R_{free} test set	277 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å^2)	129.5	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.057 for l,-k,h	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	4198	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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: PT

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	AAA	0.82	0/4277	1.07	1/5793 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	255	ASP	N-CA-C	-5.27	105.22	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	AAA	4195	0	4006	63	0
2	AAA	3	0	0	1	0
All	All	4198	0	4006	63	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 8.

All (63) 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:AAA:298:MET:SD	2:AAA:603:PT:PT	1.19	1.21
1:AAA:95:GLU:OE2	1:AAA:99:ASN:HB2	1.90	0.72
1:AAA:333:GLU:OE1	1:AAA:337:ARG:NH2	2.29	0.65
1:AAA:90:CYS:SG	1:AAA:105:HIS:CD2	2.92	0.62
1:AAA:98:ARG:O	1:AAA:101:CYS:HB3	2.00	0.61
1:AAA:485:ARG:HB3	1:AAA:486:PRO:HD3	1.83	0.59
1:AAA:179:LEU:HB2	1:AAA:180:PRO:HD3	1.85	0.59
1:AAA:524:LYS:O	1:AAA:525:LYS:C	2.45	0.59
1:AAA:383:GLU:HB3	1:AAA:384:PRO:HD3	1.85	0.59
1:AAA:400:GLU:OE1	1:AAA:435:SER:OG	2.22	0.58
1:AAA:290:ILE:O	1:AAA:293:VAL:HG22	2.06	0.56
1:AAA:249:ASP:O	1:AAA:252:GLU:HG2	2.07	0.55
1:AAA:151:ALA:HB3	1:AAA:152:PRO:HD3	1.89	0.54
1:AAA:109:ASN:HD22	1:AAA:109:ASN:C	2.17	0.53
1:AAA:560:LYS:O	1:AAA:561:ALA:HB3	2.09	0.53
1:AAA:543:GLN:O	1:AAA:547:VAL:HG23	2.10	0.52
1:AAA:525:LYS:CE	1:AAA:548:MET:HE3	2.39	0.52
1:AAA:296:ASP:OD1	1:AAA:297:GLU:N	2.42	0.51
1:AAA:432:LYS:O	1:AAA:433:VAL:C	2.53	0.50
1:AAA:96:PRO:O	1:AAA:97:GLU:C	2.55	0.49
1:AAA:564:LYS:O	1:AAA:567:CYS:HB3	2.12	0.49
1:AAA:549:ASP:O	1:AAA:550:ASP:C	2.56	0.49
1:AAA:25:ILE:O	1:AAA:26:ALA:C	2.56	0.49
1:AAA:10:ARG:O	1:AAA:11:PHE:C	2.55	0.49
1:AAA:408:LEU:HD22	1:AAA:530:VAL:HG22	1.95	0.48
1:AAA:348:ARG:HG3	1:AAA:482:VAL:CG1	2.44	0.47
1:AAA:381:VAL:O	1:AAA:384:PRO:HD2	2.13	0.47
1:AAA:525:LYS:HE3	1:AAA:548:MET:HE3	1.97	0.47
1:AAA:518:GLU:OE2	1:AAA:521:ARG:NH1	2.47	0.47
1:AAA:21:ALA:O	1:AAA:22:LEU:C	2.57	0.47
1:AAA:340:ASP:O	1:AAA:447:PRO:HD3	2.15	0.46
1:AAA:420:THR:HB	1:AAA:421:PRO:HD3	1.98	0.46
1:AAA:560:LYS:O	1:AAA:561:ALA:CB	2.64	0.46
1:AAA:411:TYR:HA	1:AAA:414:LYS:HD3	1.97	0.45
1:AAA:168:CYS:C	1:AAA:170:GLN:H	2.24	0.45
1:AAA:305:LEU:HD13	1:AAA:334:TYR:CD2	2.51	0.44
1:AAA:499:PRO:HB3	1:AAA:535:HIS:O	2.17	0.44
1:AAA:288:HIS:O	1:AAA:289:CYS:C	2.61	0.44
1:AAA:110:PRO:C	1:AAA:112:LEU:H	2.26	0.44
1:AAA:223:PHE:N	1:AAA:224:PRO:HD3	2.33	0.44
1:AAA:19:PHE:CE1	1:AAA:23:VAL:HG21	2.53	0.43
1:AAA:90:CYS:SG	1:AAA:105:HIS:HD2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:281:LYS:HB2	1:AAA:282:PRO:CD	2.49	0.43
1:AAA:544:LEU:O	1:AAA:545:LYS:C	2.62	0.43
1:AAA:214:TRP:CH2	1:AAA:218:ARG:HD3	2.53	0.43
1:AAA:445:ARG:O	1:AAA:448:CYS:HB3	2.19	0.43
1:AAA:367:HIS:O	1:AAA:371:ALA:HB2	2.18	0.43
1:AAA:376:GLU:O	1:AAA:379:PRO:HD2	2.20	0.42
1:AAA:441:PRO:O	1:AAA:442:GLU:C	2.62	0.42
1:AAA:525:LYS:HE2	1:AAA:548:MET:HE3	2.01	0.42
1:AAA:242:HIS:O	1:AAA:243:THR:C	2.62	0.42
1:AAA:552:ALA:O	1:AAA:555:VAL:HG12	2.20	0.42
1:AAA:446:MET:N	1:AAA:447:PRO:HD2	2.35	0.41
1:AAA:569:ALA:O	1:AAA:570:GLU:HB2	2.21	0.41
1:AAA:433:VAL:HG21	1:AAA:453:LEU:HD21	2.02	0.41
1:AAA:214:TRP:CZ3	1:AAA:218:ARG:HD3	2.56	0.41
1:AAA:151:ALA:HB3	1:AAA:152:PRO:CD	2.50	0.40
1:AAA:31:LEU:HD12	1:AAA:74:LEU:HD22	2.03	0.40
1:AAA:250:LEU:O	1:AAA:251:LEU:C	2.64	0.40
1:AAA:526:GLN:O	1:AAA:529:LEU:HB3	2.22	0.40
1:AAA:214:TRP:CH2	1:AAA:218:ARG:CD	3.04	0.40
1:AAA:258:ALA:O	1:AAA:259:ASP:C	2.64	0.40
1:AAA:203:LEU:HD13	1:AAA:243:THR:HA	2.03	0.40

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	AAA	537/585 (92%)	466 (87%)	62 (12%)	9 (2%)	7 36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	561	ALA
1	AAA	562	ASP
1	AAA	569	ALA
1	AAA	268	GLN
1	AAA	300	ALA
1	AAA	293	VAL
1	AAA	564	LYS
1	AAA	306	ALA
1	AAA	7	VAL

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	AAA	445/511 (87%)	427 (96%)	18 (4%)	27 51

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	13	ASP
1	AAA	34	CYS
1	AAA	37	GLU
1	AAA	47	THR
1	AAA	98	ARG
1	AAA	109	ASN
1	AAA	269	ASP
1	AAA	273	SER
1	AAA	314	ASP
1	AAA	334	TYR
1	AAA	385	GLN
1	AAA	467	THR
1	AAA	471	ASP
1	AAA	532	LEU
1	AAA	542	GLU
1	AAA	548	MET
1	AAA	551	PHE
1	AAA	570	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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

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	AAA	543/585 (92%)	0.36	34 (6%)	27	24	63, 120, 187, 251	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	456	VAL	10.7
1	AAA	458	ASN	4.5
1	AAA	566	THR	4.5
1	AAA	549	ASP	4.3
1	AAA	562	ASP	4.3
1	AAA	275	LEU	4.2
1	AAA	270	SER	4.2
1	AAA	430	LEU	4.2
1	AAA	429	ASN	3.9
1	AAA	292	GLU	3.9
1	AAA	163	ALA	3.7
1	AAA	111	ASN	3.4
1	AAA	205	LYS	3.1
1	AAA	561	ALA	3.0
1	AAA	280	GLU	3.0
1	AAA	569	ALA	2.8
1	AAA	162	LYS	2.7
1	AAA	117	ARG	2.6
1	AAA	34	CYS	2.6
1	AAA	452	TYR	2.6
1	AAA	443	ALA	2.6
1	AAA	139	LEU	2.6
1	AAA	299	PRO	2.5
1	AAA	362	ALA	2.4
1	AAA	467	THR	2.4
1	AAA	548	MET	2.4
1	AAA	411	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	448	CYS	2.2
1	AAA	375	ASP	2.2
1	AAA	136	LYS	2.2
1	AAA	459	GLN	2.1
1	AAA	172	ALA	2.0
1	AAA	94	GLN	2.0
1	AAA	14	LEU	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)

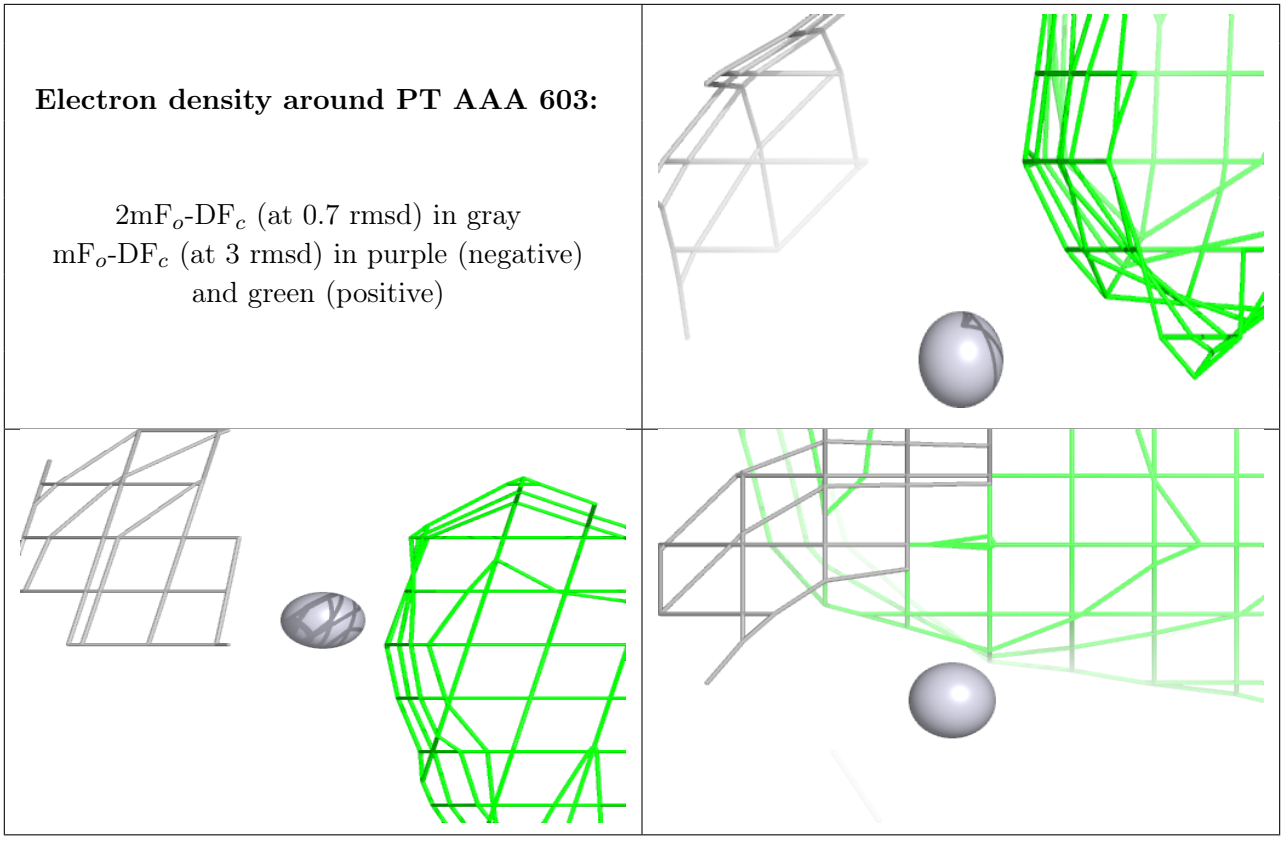
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	PT	AAA	603	1/1	0.92	0.13	110,110,110,110	1
2	PT	AAA	602	1/1	0.96	0.11	86,86,86,86	1
2	PT	AAA	601	1/1	0.96	0.14	75,75,75,75	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.

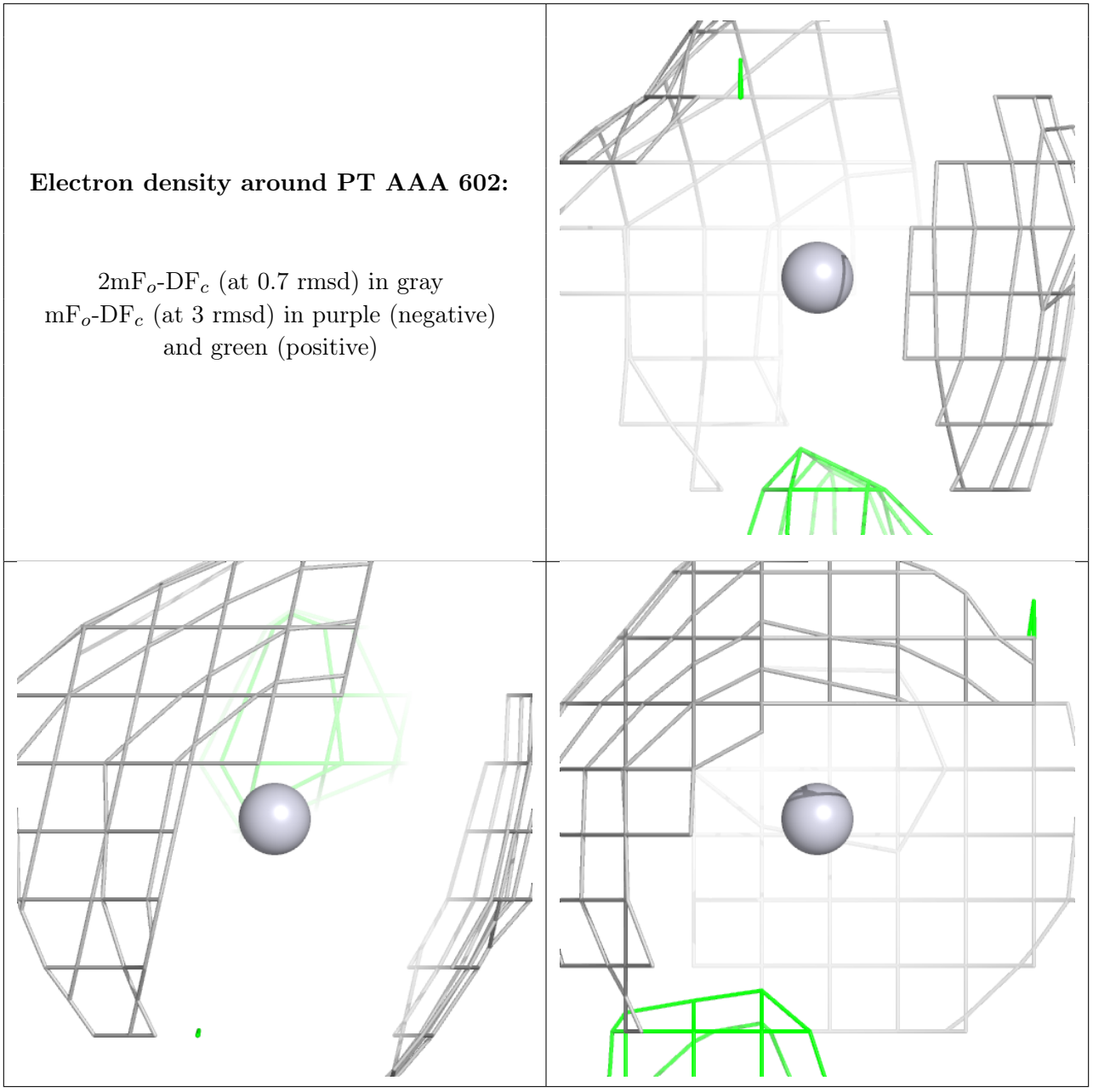
Electron density around PT AAA 603:

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



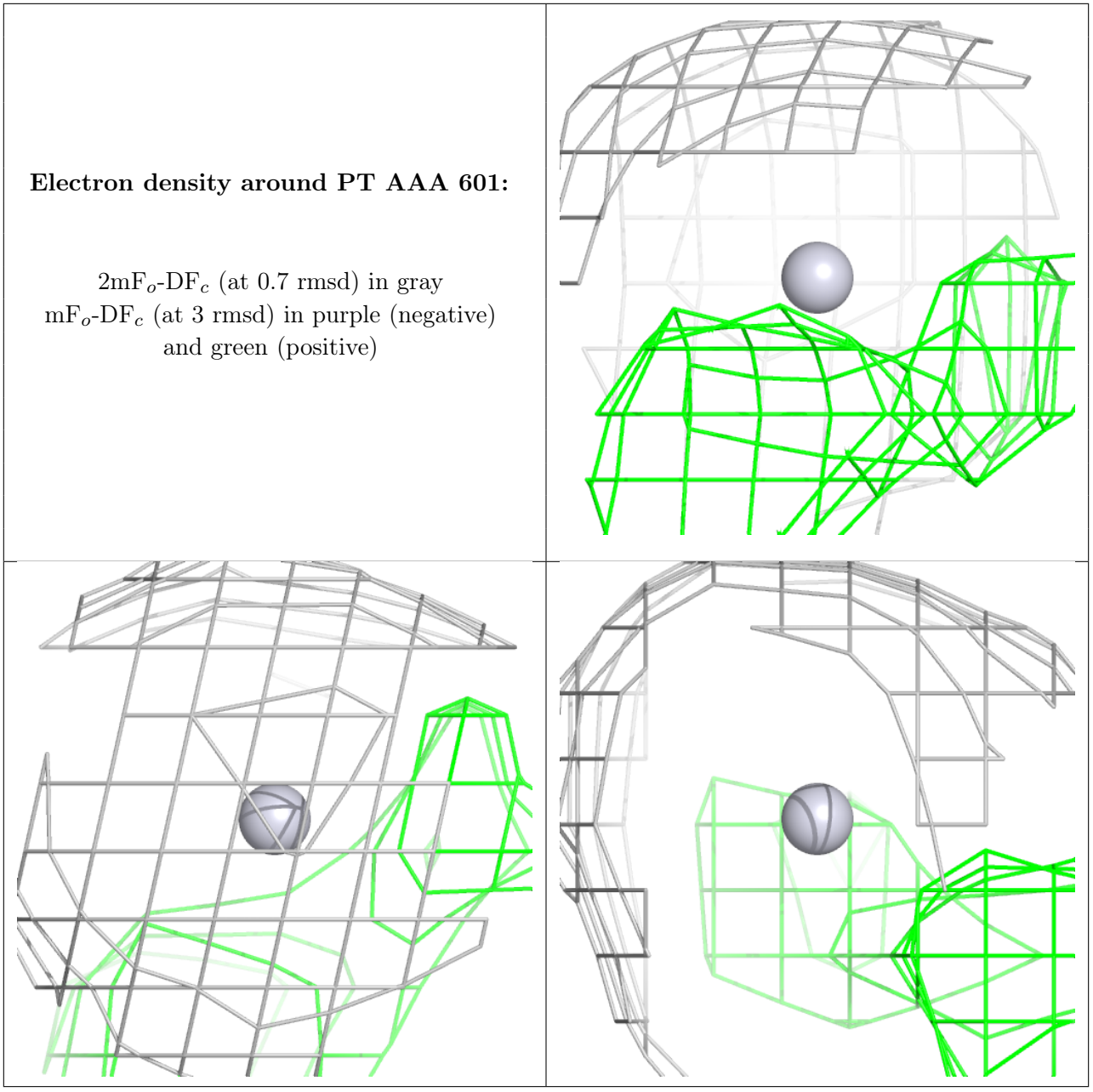
Electron density around PT AAA 602:

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



Electron density around PT AAA 601:

$2mF_o$-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.