



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 07:02 PM BST

PDB ID : 7A9C
Title : Human serum albumin (HSA) crystallized in the presence of yttrium (III) chloride
Authors : Zocher, G.; Stehle, T.
Deposited on : 2020-09-01
Resolution : 2.75 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 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	:	2.20
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)	:	2.20

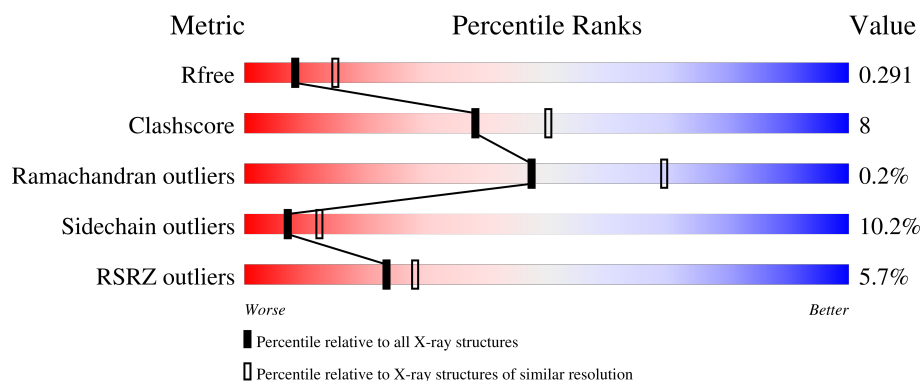
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	AAA	585	<div> <div>6%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4537 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 Albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	582	Total	C	N	O	S	0	0	0
			4535	2871	764	859	41			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	521	GLU	ARG	conflict	UNP P02768

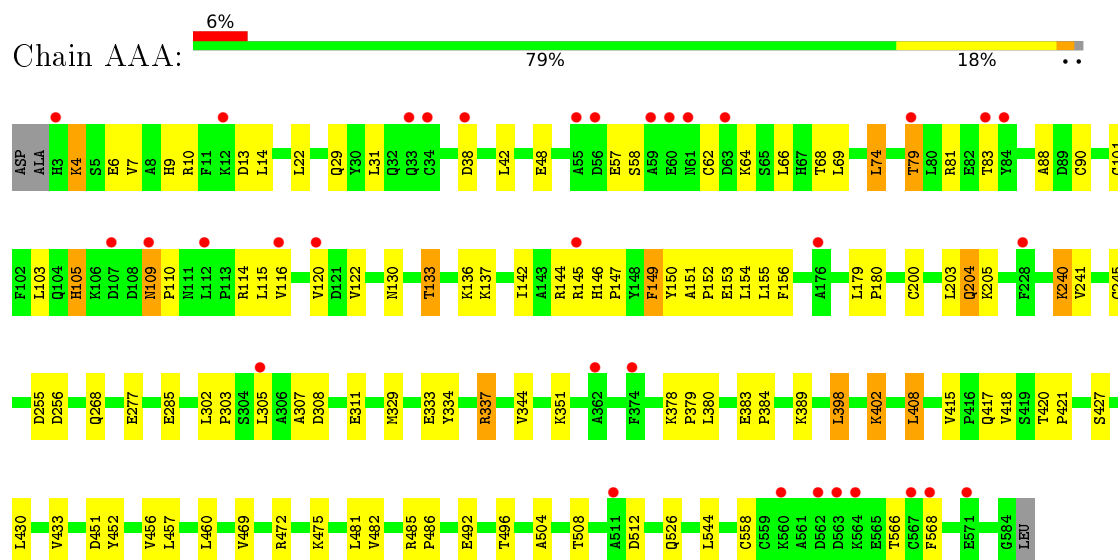
- Molecule 2 is YTTRIUM (III) ION (three-letter code: YT3) (formula: Y) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	2	Total	Y	0	0
			2	2		

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: Albumin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.27Å 71.93Å 180.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 39.41 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.75) 99.4 (39.41-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0232 2018/13/08	Depositor
R, R_{free}	0.238 , 0.295 0.240 , 0.291	Depositor DCC
R_{free} test set	1541 reflections (8.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4537	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: YT3

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	0.65	0/4624	0.71	0/6251

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	AAA	4535	0	4376	68	1
2	AAA	2	0	0	0	1
All	All	4537	0	4376	68	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 8.

All (68) 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:90:CYS:SG	1:AAA:105:HIS:NE2	2.14	1.20
1:AAA:90:CYS:SG	1:AAA:105:HIS:CD2	2.51	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:101:CYS:SG	1:AAA:105:HIS:NE2	2.41	0.93
1:AAA:81:ARG:HB3	1:AAA:88:ALA:CB	2.14	0.75
1:AAA:558:CYS:HB2	1:AAA:568:PHE:CZ	2.24	0.73
1:AAA:303:PRO:O	1:AAA:337:ARG:NH1	2.23	0.71
1:AAA:240:LYS:CE	1:AAA:256:ASP:OD2	2.40	0.70
1:AAA:4:LYS:HD2	1:AAA:58:SER:OG	1.92	0.69
1:AAA:558:CYS:HB2	1:AAA:568:PHE:CE1	2.30	0.67
1:AAA:333:GLU:OE1	1:AAA:337:ARG:NH2	2.28	0.66
1:AAA:240:LYS:HE2	1:AAA:256:ASP:OD2	1.97	0.65
1:AAA:200:CYS:O	1:AAA:204:GLN:HG2	1.97	0.64
1:AAA:109:ASN:N	1:AAA:110:PRO:CD	2.62	0.63
1:AAA:472:ARG:NH2	1:AAA:492:GLU:O	2.35	0.60
1:AAA:14:LEU:HD21	1:AAA:22:LEU:HD12	1.84	0.58
1:AAA:79:THR:OG1	1:AAA:79:THR:O	2.21	0.58
1:AAA:156:PHE:HZ	1:AAA:285:GLU:HA	1.70	0.56
1:AAA:240:LYS:HE3	1:AAA:256:ASP:OD2	2.05	0.56
1:AAA:6:GLU:HG2	1:AAA:66:LEU:HD11	1.88	0.55
1:AAA:241:VAL:O	1:AAA:245:CYS:SG	2.65	0.55
1:AAA:417:GLN:HB3	1:AAA:469:VAL:CG1	2.38	0.54
1:AAA:81:ARG:HB3	1:AAA:88:ALA:HB3	1.89	0.54
1:AAA:29:GLN:HG2	1:AAA:147:PRO:HA	1.91	0.53
1:AAA:241:VAL:HG22	1:AAA:256:ASP:HB3	1.90	0.53
1:AAA:504:ALA:O	1:AAA:508:THR:HG23	2.09	0.53
1:AAA:9:HIS:O	1:AAA:13:ASP:N	2.43	0.52
1:AAA:398:LEU:HB3	1:AAA:402:LYS:HB3	1.92	0.52
1:AAA:329:MET:O	1:AAA:333:GLU:HG2	2.11	0.51
1:AAA:151:ALA:HB3	1:AAA:152:PRO:HD3	1.93	0.51
1:AAA:430:LEU:HD13	1:AAA:456:VAL:HG11	1.92	0.50
1:AAA:420:THR:N	1:AAA:421:PRO:HD2	2.26	0.50
1:AAA:109:ASN:H	1:AAA:110:PRO:HD3	1.77	0.50
1:AAA:156:PHE:CZ	1:AAA:285:GLU:HA	2.47	0.49
1:AAA:64:LYS:HB2	1:AAA:69:LEU:HD21	1.94	0.49
1:AAA:485:ARG:HB3	1:AAA:486:PRO:HD3	1.94	0.49
1:AAA:10:ARG:NH2	1:AAA:255:ASP:OD1	2.46	0.48
1:AAA:344:VAL:HG23	1:AAA:482:VAL:HA	1.96	0.48
1:AAA:142:ILE:HG22	1:AAA:154:LEU:HD21	1.94	0.48
1:AAA:415:VAL:HG12	1:AAA:418:VAL:HG23	1.96	0.48
1:AAA:4:LYS:HB2	1:AAA:57:GLU:OE1	2.13	0.47
1:AAA:408:LEU:HD13	1:AAA:427:SER:CB	2.45	0.47
1:AAA:142:ILE:CG2	1:AAA:154:LEU:HD11	2.46	0.46
1:AAA:433:VAL:HG22	1:AAA:452:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:408:LEU:CD1	1:AAA:427:SER:HB2	2.45	0.46
1:AAA:241:VAL:HG22	1:AAA:256:ASP:CB	2.45	0.46
1:AAA:66:LEU:HD12	1:AAA:66:LEU:H	1.81	0.45
1:AAA:9:HIS:CE1	1:AAA:13:ASP:OD1	2.70	0.45
1:AAA:378:LYS:N	1:AAA:379:PRO:HD2	2.32	0.45
1:AAA:146:HIS:HB3	1:AAA:149:PHE:HB2	1.99	0.45
1:AAA:14:LEU:HD21	1:AAA:22:LEU:CD1	2.47	0.45
1:AAA:130:ASN:CG	1:AAA:133:THR:OG1	2.55	0.45
1:AAA:9:HIS:O	1:AAA:13:ASP:HB2	2.17	0.45
1:AAA:155:LEU:HD12	1:AAA:155:LEU:HA	1.85	0.44
1:AAA:383:GLU:HB3	1:AAA:384:PRO:CD	2.47	0.44
1:AAA:408:LEU:HD21	1:AAA:526:GLN:HB3	1.99	0.44
1:AAA:109:ASN:H	1:AAA:110:PRO:CD	2.31	0.43
1:AAA:64:LYS:O	1:AAA:69:LEU:HD11	2.19	0.43
1:AAA:307:ALA:HA	1:AAA:311:GLU:HB2	2.01	0.42
1:AAA:179:LEU:N	1:AAA:180:PRO:HD2	2.34	0.42
1:AAA:383:GLU:HB3	1:AAA:384:PRO:HD3	2.02	0.42
1:AAA:4:LYS:HD2	1:AAA:58:SER:HG	1.83	0.42
1:AAA:302:LEU:HD23	1:AAA:302:LEU:HA	1.89	0.42
1:AAA:74:LEU:HD12	1:AAA:74:LEU:O	2.19	0.42
1:AAA:142:ILE:HG21	1:AAA:154:LEU:HD11	2.02	0.41
1:AAA:408:LEU:CD1	1:AAA:427:SER:CB	2.98	0.41
1:AAA:408:LEU:HD12	1:AAA:408:LEU:HA	1.87	0.41
1:AAA:344:VAL:CG2	1:AAA:482:VAL:HA	2.51	0.40
1:AAA:150:TYR:CZ	1:AAA:152:PRO:HG2	2.56	0.40

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)
1:AAA:277:GLU:OE2	2:AAA:601:YT3:Y[4_445]	1.98	0.22

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	AAA	580/585 (99%)	544 (94%)	35 (6%)	1 (0%)	47 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	109	ASN

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	AAA	480/511 (94%)	431 (90%)	49 (10%)	7 12

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	4	LYS
1	AAA	7	VAL
1	AAA	31	LEU
1	AAA	38	ASP
1	AAA	42	LEU
1	AAA	48	GLU
1	AAA	62	CYS
1	AAA	68	THR
1	AAA	74	LEU
1	AAA	79	THR
1	AAA	83	THR
1	AAA	103	LEU
1	AAA	105	HIS
1	AAA	114	ARG
1	AAA	115	LEU
1	AAA	116	VAL
1	AAA	120	VAL
1	AAA	122	VAL

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Mol	Chain	Res	Type
1	AAA	133	THR
1	AAA	136	LYS
1	AAA	137	LYS
1	AAA	144	ARG
1	AAA	145	ARG
1	AAA	149	PHE
1	AAA	153	GLU
1	AAA	203	LEU
1	AAA	204	GLN
1	AAA	205	LYS
1	AAA	240	LYS
1	AAA	268	GLN
1	AAA	305	LEU
1	AAA	308	ASP
1	AAA	334	TYR
1	AAA	337	ARG
1	AAA	351	LYS
1	AAA	380	LEU
1	AAA	389	LYS
1	AAA	398	LEU
1	AAA	402	LYS
1	AAA	408	LEU
1	AAA	451	ASP
1	AAA	457	LEU
1	AAA	460	LEU
1	AAA	475	LYS
1	AAA	481	LEU
1	AAA	496	THR
1	AAA	512	ASP
1	AAA	544	LEU
1	AAA	566	THR

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	AAA	582/585 (99%)	0.40	33 (5%) 23 28	43, 84, 137, 169	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	511	ALA	6.2
1	AAA	112	LEU	5.2
1	AAA	564	LYS	5.0
1	AAA	3	HIS	4.4
1	AAA	560	LYS	4.3
1	AAA	55	ALA	4.2
1	AAA	61	ASN	4.1
1	AAA	567	CYS	4.1
1	AAA	60	GLU	4.0
1	AAA	79	THR	3.7
1	AAA	571	GLU	3.7
1	AAA	228	PHE	3.5
1	AAA	568	PHE	3.4
1	AAA	374	PHE	2.8
1	AAA	56	ASP	2.8
1	AAA	63	ASP	2.8
1	AAA	83	THR	2.7
1	AAA	116	VAL	2.6
1	AAA	84	TYR	2.5
1	AAA	59	ALA	2.5
1	AAA	34	CYS	2.5
1	AAA	562	ASP	2.3
1	AAA	145	ARG	2.3
1	AAA	120	VAL	2.3
1	AAA	107	ASP	2.3
1	AAA	563	ASP	2.3
1	AAA	33	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	12	LYS	2.1
1	AAA	176	ALA	2.1
1	AAA	305	LEU	2.1
1	AAA	109	ASN	2.0
1	AAA	38	ASP	2.0
1	AAA	362	ALA	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](#)

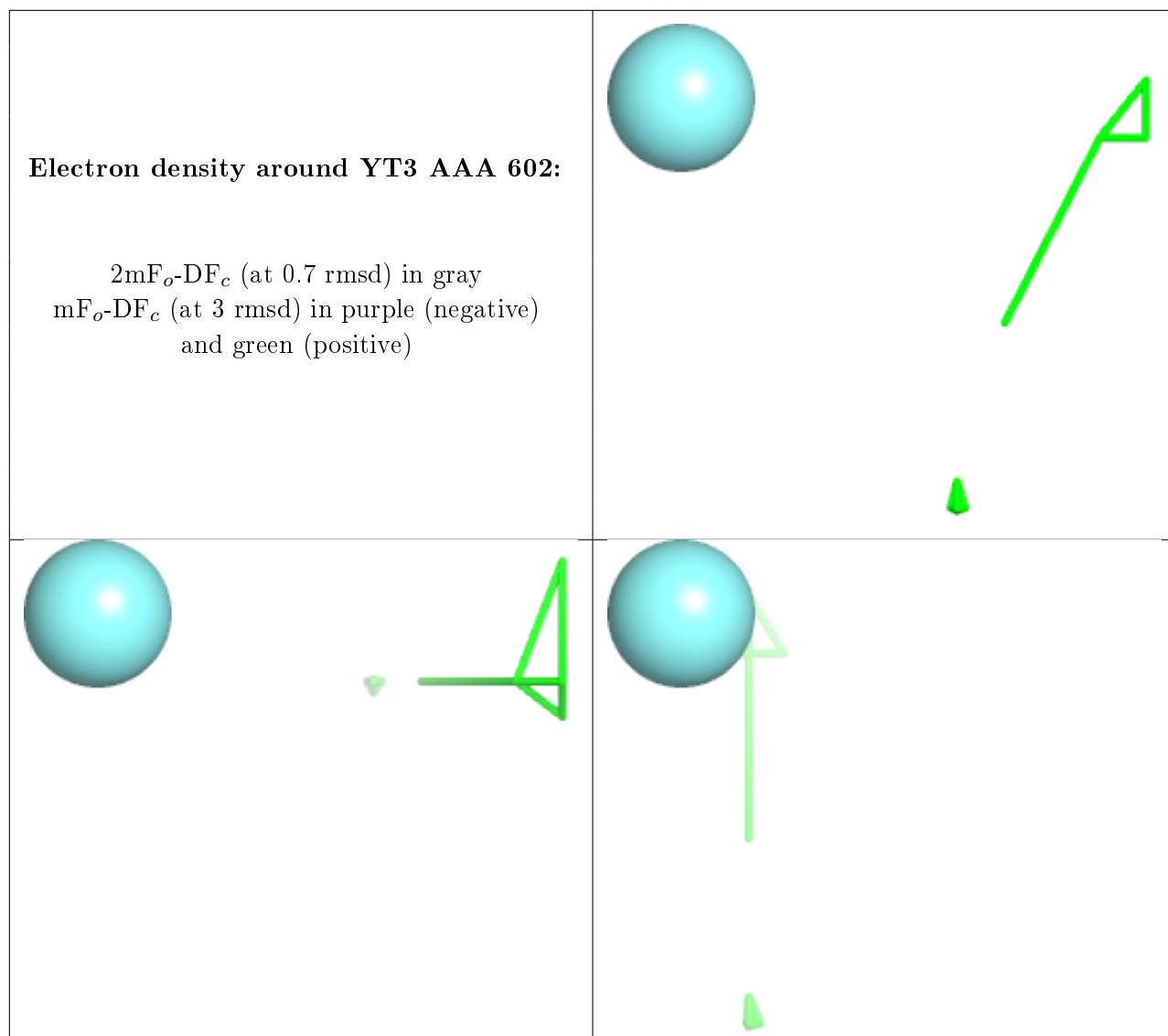
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

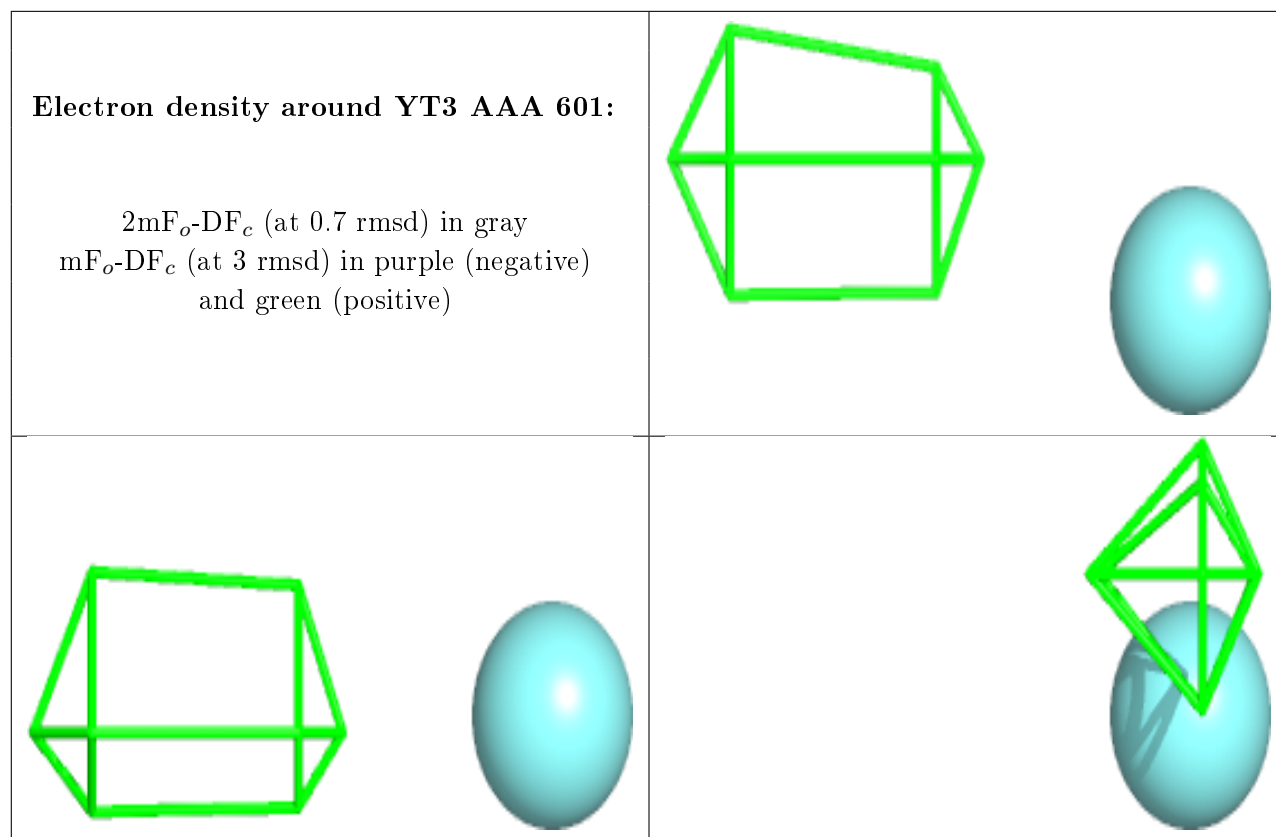
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	YT3	AAA	602	1/1	0.94	0.19	116,116,116,116	0
2	YT3	AAA	601	1/1	0.98	0.17	90,90,90,90	0

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 YT3 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.