



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:48 AM UTC

PDB ID : 6TIP / pdb\_00006tip  
Title : Engineered streptavidin variant (YNAFM) in complex with the Strep-tag II peptide  
Authors : Skerra, A.; Eichinger, A.  
Deposited on : 2019-11-22  
Resolution : 2.10 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

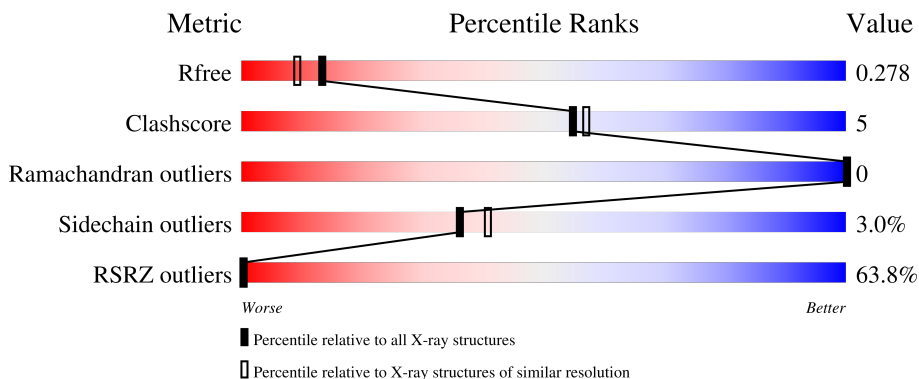
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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  $\geq 3$ , 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	127	 27% 83% 13% ..
1	B	127	 95% 95% 5%
2	P	10	 30% 80% 20%
2	Q	10	 80% 80% 20%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1189 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 Streptavidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	123	932	584	161	185	2	0	1	0
1	B	121	Total	C				0	0	121
			121	121						

There are 14 discrepancies between the modelled and reference sequences:

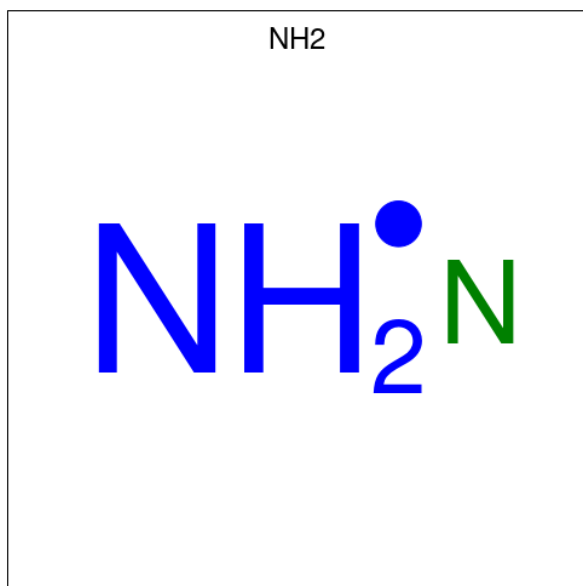
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	initiating methionine	UNP P22629
A	44	VAL	GLU	engineered mutation	UNP P22629
A	45	THR	SER	engineered mutation	UNP P22629
A	47	ARG	VAL	engineered mutation	UNP P22629
A	117	TYR	ALA	engineered mutation	UNP P22629
A	120	PHE	TRP	engineered mutation	UNP P22629
A	121	MET	LYS	engineered mutation	UNP P22629
B	13	MET	-	initiating methionine	UNP P22629
B	44	VAL	GLU	engineered mutation	UNP P22629
B	45	THR	SER	engineered mutation	UNP P22629
B	47	ARG	VAL	engineered mutation	UNP P22629
B	117	TYR	ALA	engineered mutation	UNP P22629
B	120	PHE	TRP	engineered mutation	UNP P22629
B	121	MET	LYS	engineered mutation	UNP P22629

- Molecule 2 is a protein called Strep-tag II peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	8	75	50	13	12	0	0	0
2	Q	8	Total	C			0	0	8
			8	8					

- Molecule 3 is AMINO GROUP (CCD ID: NH2) (formula: H<sub>2</sub>N) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total N 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	51	Total O 51 51	0	0
4	P	1	Total O 1 1	0	0



SER	●
ALA	●
W3	●
S4	●
H5	●
P6	●
Q7	●
F8	●
E9	●
K10	●

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.56Å 57.56Å 181.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.63 – 2.10 57.63 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (57.63-2.10) 99.6 (57.63-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.97 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.200 , 0.228 0.234 , 0.278	Depositor DCC
$R_{free}$ test set	939 reflections (3.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtrriage
Anisotropy	1.033	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 462.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	1189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NH2

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	1.14	2/958 (0.2%)	1.40	5/1309 (0.4%)
2	P	1.13	0/79	1.16	0/106
All	All	1.14	2/1037 (0.2%)	1.38	5/1415 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLY	C-O	5.75	1.29	1.23
1	A	125	VAL	C-O	5.36	1.29	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	THR	N-CA-C	-6.52	104.02	112.23
1	A	119	ALA	CA-C-N	5.94	129.55	121.05
1	A	119	ALA	C-N-CA	5.94	129.55	121.05
1	A	33	ALA	CA-C-O	-5.40	114.81	120.58
1	A	29	PHE	CB-CA-C	5.10	118.32	110.62

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	932	0	879	10	0
1	B	121	0	0	0	0
2	P	75	0	64	0	0
2	Q	8	0	0	0	0
3	P	1	0	0	0	0
4	A	51	0	0	1	0
4	P	1	0	0	0	0
All	All	1189	0	943	10	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 5.

All (10) 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:121:MET:HG3	1:A:121:MET:O	1.92	0.69
1:A:120:PHE:O	1:A:121:MET:HG2	2.04	0.57
1:A:73:LEU:O	1:A:73:LEU:HD12	2.04	0.57
1:A:56:LEU:HD12	1:A:56:LEU:C	2.31	0.56
1:A:36:ASP:HB2	4:A:235:HOH:O	2.09	0.51
1:A:73:LEU:HD12	1:A:73:LEU:C	2.34	0.51
1:A:24:GLN:HA	1:A:135:PRO:HG3	1.95	0.48
1:A:23:ASN:HB3	1:A:130:PHE:CE1	2.52	0.45
1:A:21:TRP:HB3	1:A:130:PHE:HB3	2.01	0.43
1:A:121:MET:O	1:A:121:MET:CG	2.64	0.41

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	122/127 (96%)	116 (95%)	6 (5%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	6/10 (60%)	5 (83%)	1 (17%)	0	100	100
All	All	128/137 (93%)	121 (94%)	7 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	93/94 (99%)	90 (97%)	3 (3%)	34	38
2	P	8/9 (89%)	8 (100%)	0	100	100
All	All	101/103 (98%)	98 (97%)	3 (3%)	36	41

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	56	LEU
1	A	118	ASN

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

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is modelled with single atom - 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	123/127 (96%)	1.56	34 (27%) <b>1</b> <b>1</b>	11, 33, 83, 127	1 (0%)
1	B	121/127 (95%)	16.02	121 (100%) <b>0</b> <b>0</b>	101, 134, 169, 221	0
2	P	8/10 (80%)	2.39	3 (37%) <b>1</b> <b>1</b>	26, 37, 80, 132	0
2	Q	8/10 (80%)	13.64	8 (100%) <b>0</b> <b>0</b>	79, 121, 150, 160	0
All	All	260/274 (94%)	8.69	166 (63%) <b>0</b> <b>0</b>	11, 104, 159, 221	1 (0%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	PHE	53.8
1	B	132	LYS	34.0
1	B	117	TYR	33.1
1	B	26	GLY	31.8
1	B	79	TRP	31.7
1	B	66	THR	29.3
1	B	72	ALA	28.3
1	B	131	THR	26.7
1	B	99	GLY	26.2
1	B	121	MET	26.1
1	B	100	ALA	25.2
1	B	67	ASP	25.0
1	B	23	ASN	24.5
1	B	65	ALA	23.7
1	B	91	THR	23.3
1	B	95	GLN	22.0
1	B	39	LEU	21.7
1	B	34	GLY	21.4
1	B	104	ILE	20.8
1	B	78	ALA	20.7
2	Q	9	GLU	20.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	51	GLU	20.0
1	B	15	ALA	19.8
1	B	52	SER	19.8
2	Q	3	TRP	19.6
1	B	89	ALA	19.5
1	B	25	LEU	19.5
1	B	22	TYR	19.5
1	B	73	LEU	19.4
1	B	83	TYR	19.0
1	B	126	GLY	18.8
1	B	46	ALA	18.7
2	Q	4	SER	18.5
1	B	129	THR	18.5
1	B	37	GLY	18.2
1	B	68	GLY	18.1
1	B	113	GLY	18.1
1	B	118	ASN	17.8
1	B	21	TRP	17.8
1	B	16	GLY	17.6
1	B	108	TRP	17.5
1	B	71	THR	17.5
1	B	54	TYR	17.3
1	B	70	GLY	17.3
1	B	102	ALA	17.1
1	B	115	THR	16.9
1	B	45	THR	16.8
1	B	122	SER	16.7
1	B	97	VAL	16.6
1	B	90	THR	16.4
1	B	29	PHE	16.3
1	B	62	SER	16.2
2	Q	8	PHE	16.2
1	B	28	THR	16.1
1	B	57	THR	16.1
1	B	61	ASP	16.0
1	B	43	TYR	16.0
1	B	106	THR	15.8
1	B	114	THR	15.6
1	B	116	GLU	15.4
1	B	44	VAL	15.2
1	B	105	ASN	15.2
1	B	74	GLY	15.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	111	THR	14.8
1	B	76	THR	14.6
1	B	48	GLY	14.5
1	B	86	ALA	14.4
1	B	119	ALA	14.1
1	B	94	GLY	14.0
1	B	124	LEU	13.9
1	B	96	TYR	13.9
1	B	60	TYR	13.8
1	B	81	ASN	13.7
1	B	110	LEU	13.7
1	B	18	THR	13.7
1	B	40	THR	13.6
1	B	123	THR	13.5
1	B	56	LEU	13.4
1	B	88	SER	13.4
1	B	92	TRP	13.4
1	B	109	LEU	13.3
1	B	125	VAL	13.3
1	B	127	HIS	13.1
1	B	107	GLN	12.9
1	B	27	SER	12.9
1	B	85	ASN	12.7
1	B	58	GLY	12.7
1	B	63	ALA	12.7
1	B	31	VAL	12.4
1	B	75	TRP	12.1
1	B	120	PHE	12.1
1	B	50	ALA	12.0
1	B	32	THR	11.9
1	B	112	SER	11.8
1	B	64	PRO	11.7
1	B	30	ILE	11.5
1	B	103	ARG	11.3
1	B	87	HIS	11.2
1	B	98	GLY	11.2
1	B	80	LYS	11.2
1	B	84	ARG	11.2
1	B	55	VAL	11.0
1	A	121	MET	10.8
1	B	53	ARG	10.7
1	B	77	VAL	10.6

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Mol	Chain	Res	Type	RSRZ
1	B	69	SER	10.5
1	B	38	ALA	10.5
2	Q	6	PRO	10.4
1	B	59	ARG	10.2
1	B	42	THR	10.2
1	B	49	ASN	9.9
1	B	93	SER	9.6
1	B	17	ILE	9.5
1	B	19	GLY	9.4
1	B	35	ALA	9.4
1	B	33	ALA	9.2
1	B	41	GLY	9.1
1	B	20	THR	9.0
2	Q	5	HIS	8.9
1	B	47	ARG	8.4
1	B	134	LYS	8.3
1	B	133	VAL	8.3
1	A	135	PRO	8.2
1	B	128	ASP	8.2
1	B	101	GLU	8.2
1	B	36	ASP	8.2
1	B	82	ASN	7.9
2	Q	10	LYS	7.8
1	B	24	GLN	7.1
2	Q	7	GLN	7.1
2	P	3	TRP	5.8
1	A	115	THR	5.7
1	A	119	ALA	5.6
1	A	14	GLU	5.6
1	A	118	ASN	5.6
1	A	15	ALA	5.4
1	A	47	ARG	5.4
2	P	10	LYS	4.9
1	B	135	PRO	4.9
1	A	116	GLU	4.8
1	A	25	LEU	4.7
1	A	69	SER	4.7
1	A	13	MET	4.7
2	P	4	SER	4.2
1	A	112	SER	4.2
1	A	24	GLN	4.0
1	A	120	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	29	PHE	3.8
1	A	67	ASP	3.7
1	A	114	THR	3.7
1	A	100	ALA	3.2
1	A	103	ARG	3.0
1	A	113	GLY	2.9
1	A	66	THR	2.9
1	A	51	GLU	2.7
1	A	117	TYR	2.7
1	A	133	VAL	2.6
1	A	45	THR	2.6
1	A	99	GLY	2.5
1	A	46	ALA	2.4
1	A	68	GLY	2.4
1	A	101	GLU	2.3
1	A	44	VAL	2.3
1	A	97	VAL	2.3
1	A	30	ILE	2.3
1	A	50	ALA	2.2

## 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.

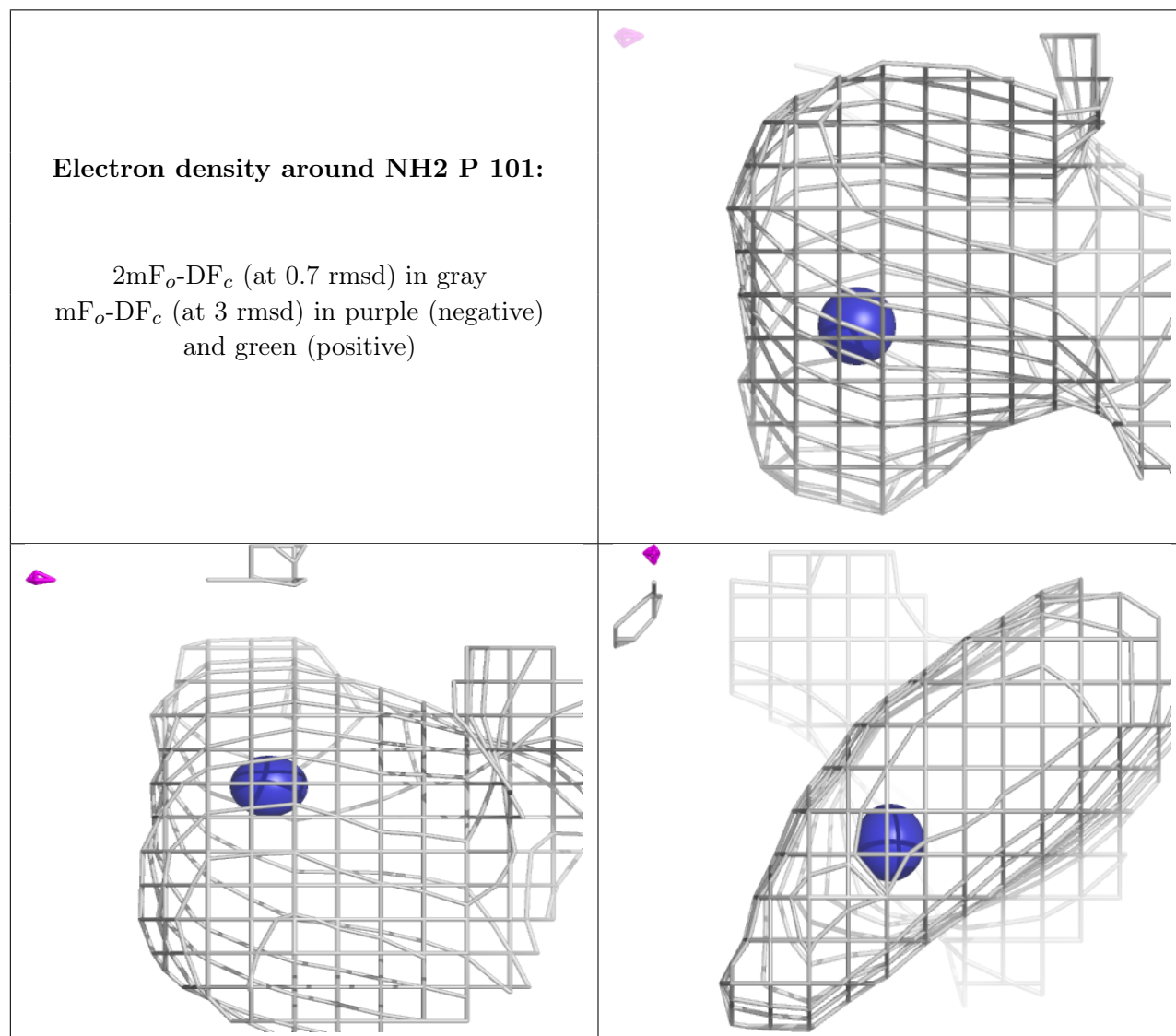
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NH2	P	101	1/1	0.91	0.18	60,60,60,60	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.