

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 17, 2022 – 03:24 PM EDT

PDB ID : 3X00

Title: Crystal structure of the core streptavidin mutant V212 (Y22S/N23D/S27D/

S45N/Y83S/R84K/E101D/R103K/E116N) complexed with bis iminobiotin

long tail (Bis-IMNtail) at 1.3 A resolution

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T.; Sugiyama, A.

Deposited on : 2014-10-09

Resolution : 1.30 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.29

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) : 2.29

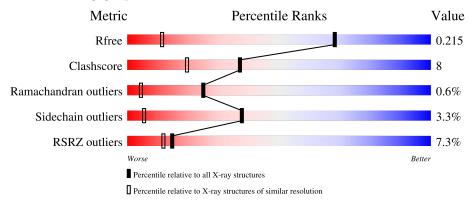


# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
$R_{free}$	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	A	147	71%	13%	·	16%		
1	В	147	72%	11%		16%		
1	С	147	7%	10%		16%		
1	D	147	73%	9%		16%		



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4405 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	${f Atoms}$		ZeroOcc	AltConf	Trace			
1	A	124	Total	С	N	О	0	12	0	
1	A	124	968	612	159	197	0	12	U	
1	В	124	Total	С	N	О	0	14	0	
1	Ъ	124	975	617	159	199	0	14	U	
1	С	124	Total	С	N	О	0	10	0	
1		124	959	603	159	197	0	10	U	
1	D	124	Total	С	N	О	0	10	0	
1	ש	124	961	605	160	196		10		

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P22629
A	0	ALA	-	expression tag	UNP P22629
A	1	SER	-	expression tag	UNP P22629
A	2	MET	-	expression tag	UNP P22629
A	3	THR	-	expression tag	UNP P22629
A	4	GLY	-	expression tag	UNP P22629
A	5	GLY	-	expression tag	UNP P22629
A	6	GLN	-	expression tag	UNP P22629
A	7	GLN	-	expression tag	UNP P22629
A	8	MET	-	expression tag	UNP P22629
A	9	GLY	-	expression tag	UNP P22629
A	10	ARG	_	expression tag	UNP P22629
A	11	GLY	-	expression tag	UNP P22629
A	12	SER	_	expression tag	UNP P22629
A	22	SER	TYR	engineered mutation	UNP P22629
A	23	ASP	ASN	engineered mutation	UNP P22629
A	27	ASP	SER	engineered mutation	UNP P22629
A	45	ASN	SER	engineered mutation	UNP P22629
A	83	SER	TYR	engineered mutation	UNP P22629
A	84	LYS	ARG	engineered mutation	UNP P22629
A	101	ASP	GLU	engineered mutation	UNP P22629

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Chain	Residue	Modelled	Actual	Comment	Reference
A	103	LYS	ARG	engineered mutation	UNP P22629
A	116	ASN	GLU	engineered mutation	UNP P22629
A	140	HIS	-	expression tag	UNP P22629
A	141	HIS	-	expression tag	UNP P22629
A	142	HIS	-	expression tag	UNP P22629
A	143	HIS	-	expression tag	UNP P22629
A	144	HIS	-	expression tag	UNP P22629
A	145	HIS	-	expression tag	UNP P22629
В	-1	MET	-	expression tag	UNP P22629
В	0	ALA	-	expression tag	UNP P22629
В	1	SER	-	expression tag	UNP P22629
В	2	MET	-	expression tag	UNP P22629
В	3	THR	-	expression tag	UNP P22629
В	4	GLY	-	expression tag	UNP P22629
В	5	GLY	-	expression tag	UNP P22629
В	6	GLN	-	expression tag	UNP P22629
В	7	GLN	-	expression tag	UNP P22629
В	8	MET	-	expression tag	UNP P22629
В	9	GLY	-	expression tag	UNP P22629
В	10	ARG	-	expression tag	UNP P22629
В	11	GLY	-	expression tag	UNP P22629
В	12	SER	-	expression tag	UNP P22629
В	22	SER	TYR	engineered mutation	UNP P22629
В	23	ASP	ASN	engineered mutation	UNP P22629
В	27	ASP	SER	engineered mutation	UNP P22629
В	45	ASN	SER	engineered mutation	UNP P22629
В	83	SER	TYR	engineered mutation	UNP P22629
В	84	LYS	ARG	engineered mutation	UNP P22629
В	101	ASP	GLU	engineered mutation	UNP P22629
В	103	LYS	ARG	engineered mutation	UNP P22629
В	116	ASN	GLU	engineered mutation	UNP P22629
В	140	HIS	-	expression tag	UNP P22629
В	141	HIS	-	expression tag	UNP P22629
В	142	HIS	-	expression tag	UNP P22629
В	143	HIS	-	expression tag	UNP P22629
В	144	HIS	-	expression tag	UNP P22629
В	145	HIS	-	expression tag	UNP P22629
С	-1	MET	-	expression tag	UNP P22629
С	0	ALA	-	expression tag	UNP P22629
С	1	SER	-	expression tag	UNP P22629
С	2	MET	-	expression tag	UNP P22629
С	3	THR	-	expression tag	UNP P22629

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Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
С	4	GLY	-	expression tag	UNP P22629
С	5	GLY	-	expression tag	UNP P22629
С	6	GLN	-	expression tag	UNP P22629
С	7	GLN	-	expression tag	UNP P22629
С	8	MET	-	expression tag	UNP P22629
С	9	GLY	-	expression tag	UNP P22629
С	10	ARG	-	expression tag	UNP P22629
С	11	GLY	-	expression tag	UNP P22629
С	12	SER	-	expression tag	UNP P22629
С	22	SER	TYR	engineered mutation	UNP P22629
С	23	ASP	ASN	engineered mutation	UNP P22629
С	27	ASP	SER	engineered mutation	UNP P22629
С	45	ASN	SER	engineered mutation	UNP P22629
С	83	SER	TYR	engineered mutation	UNP P22629
С	84	LYS	ARG	engineered mutation	UNP P22629
С	101	ASP	GLU	engineered mutation	UNP P22629
С	103	LYS	ARG	engineered mutation	UNP P22629
С	116	ASN	GLU	engineered mutation	UNP P22629
С	140	HIS	-	expression tag	UNP P22629
С	141	HIS	-	expression tag	UNP P22629
С	142	HIS	-	expression tag	UNP P22629
С	143	HIS	-	expression tag	UNP P22629
С	144	HIS	-	expression tag	UNP P22629
С	145	HIS	-	expression tag	UNP P22629
D	-1	MET	-	expression tag	UNP P22629
D	0	ALA	-	expression tag	UNP P22629
D	1	SER	-	expression tag	UNP P22629
D	2	MET	-	expression tag	UNP P22629
D	3	THR	-	expression tag	UNP P22629
D	4	GLY	-	expression tag	UNP P22629
D	5	GLY	-	expression tag	UNP P22629
D	6	GLN	-	expression tag	UNP P22629
D	7	GLN	-	expression tag	UNP P22629
D	8	MET	-	expression tag	UNP P22629
D	9	GLY	-	expression tag	UNP P22629
D	10	ARG	-	expression tag	UNP P22629
D	11	GLY	-	expression tag	UNP P22629
D	12	SER	-	expression tag	UNP P22629
D	22	SER	TYR	engineered mutation	UNP P22629
D	23	ASP	ASN	engineered mutation	UNP P22629
D	27	ASP	SER	engineered mutation	UNP P22629
D	45	ASN	SER	engineered mutation	UNP P22629

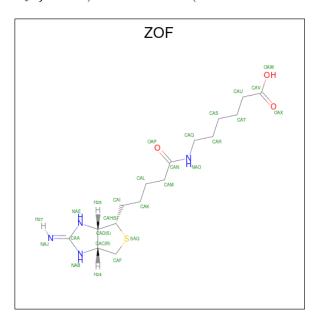
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Chain	Residue	Modelled	Actual Comment		Reference
D	83	SER	TYR	TYR engineered mutation	
D	84	LYS	ARG	engineered mutation	UNP P22629
D	101	ASP	GLU	engineered mutation	UNP P22629
D	103	LYS	ARG	engineered mutation	UNP P22629
D	116	ASN	GLU	engineered mutation	UNP P22629
D	140	HIS	_	expression tag	UNP P22629
D	141	HIS	-	expression tag	UNP P22629
D	142	HIS	-	expression tag	UNP P22629
D	143	HIS	-	- expression tag	
D	144	HIS	_	expression tag	UNP P22629
D	145	HIS	-	expression tag	UNP P22629

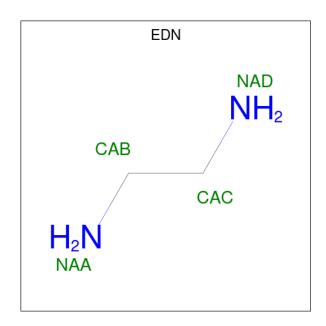
• Molecule 2 is 6-( $\{5-[(2E,3aS,4S,6aR)-2-iminohexahydro-1H-thieno[3,4-d]imidazol-4-yl]$ penta noyl $\}$ amino $\}$ hexanoic acid (three-letter code: ZOF) (formula:  $C_{16}H_{28}N_4O_3S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	А	1	Total	С	N	О	S	0	0
2	Λ	1	23	16	4	2	1	U	U
2	B	1	Total	С	N	О	S	0	0
2	Ъ	1	23	16	4	2	1	0	0
2	С	1	Total	С	N	О	S	0	0
2		1	23	16	4	2	1	0	U
9	D	1	Total	С	N	О	S	0	0
2	ש	1	23	16	4	2	1		U

• Molecule 3 is ETHANE-1,2-DIAMINE (three-letter code: EDN) (formula:  $C_2H_8N_2$ ).





Mo	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
3		В	1	Total C N 4 2 2	0	0
3		D	1	Total C N 4 2 2	0	0

#### • Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	128	Total O 128 128	0	0
4	В	122	Total O 122 122	0	0
4	С	100	Total O 100 100	0	0
4	D	92	Total O 92 92	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.



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	77.35Å 77.38Å 174.12Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	50.00 - 1.30	Depositor
rtesolution (A)	35.35 - 1.30	EDS
% Data completeness	99.5 (50.00-1.30)	Depositor
(in resolution range)	99.5 (35.35-1.30)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$< I/\sigma(I) > 1$	3.48 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
Ρ. Р.	0.146 , 0.188	Depositor
$R, R_{free}$	0.181 , $0.215$	DCC
$R_{free}$ test set	6384 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35 , 41.4	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.477 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4405	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: EDN, ZOF

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).

Mal Chain		Bo	nd lengths	Bond angles		
MIOI	Mol   Chain		# Z  > 5	RMSZ	# Z  > 5	
1	A	1.12	1/1026 (0.1%)	1.03	0/1402	
1	В	1.16	2/1039~(0.2%)	1.05	0/1420	
1	С	1.01	0/1011	1.01	5/1383 (0.4%)	
1	D	1.00	0/1013	1.00	4/1383 (0.3%)	
All	All	1.08	3/4089 (0.1%)	1.02	9/5588 (0.2%)	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$Ideal(\AA)$
1	В	50	ALA	C-O	8.33	1.39	1.23
1	В	13	ALA	CA-CB	6.70	1.66	1.52
1	A	13	ALA	CA-CB	6.30	1.65	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	D	53	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	С	53	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	D	53	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	С	53	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	С	27	ASP	CB-CG-OD1	5.29	123.06	118.30

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	968	0	944	21	0
1	В	975	0	956	18	0
1	С	959	0	920	10	0
1	D	961	0	930	14	0
2	A	23	0	27	0	0
2	В	23	0	27	0	0
2	С	23	0	27	0	0
2	D	23	0	27	0	0
3	В	4	0	5	0	0
3	D	4	0	5	0	0
4	A	128	0	0	2	0
4	В	122	0	0	4	0
4	С	100	0	0	0	0
4	D	92	0	0	2	0
All	All	4405	0	3868	61	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.

The worst 5 of 61 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & & & & & & & & & & & & & & & & & & &$	Clash overlap (Å)
1:A:43[B]:TYR:CE2	1:A:45[B]:ASN:OD1	1.73	1.39
1:A:43[B]:TYR:CZ	1:A:45[B]:ASN:OD1	1.91	1.23
1:C:43[B]:TYR:OH	1:C:45[B]:ASN:OD1	1.53	1.22
1:D:43[B]:TYR:OH	1:D:45[B]:ASN:OD1	1.70	1.09
1:A:43[B]:TYR:OH	1:A:45[B]:ASN:OD1	1.86	0.94

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	Perce	ntiles
1	A	134/147 (91%)	130 (97%)	4 (3%)	0	100	100
1	В	136/147 (92%)	132 (97%)	3 (2%)	1 (1%)	22	3
1	С	132/147 (90%)	130 (98%)	1 (1%)	1 (1%)	19	2
1	D	132/147 (90%)	129 (98%)	2 (2%)	1 (1%)	19	2
All	All	534/588 (91%)	521 (98%)	10 (2%)	3 (1%)	25	4

#### All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	49	ASN
1	D	49	ASN
1	В	49	ASN

#### 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	102/107~(95%)	100 (98%)	2 (2%)	55	17	
1	В	104/107 (97%)	103 (99%)	1 (1%)	76	48	
1	С	100/107 (94%)	96 (96%)	4 (4%)	31	3	
1	D	100/107 (94%)	92 (92%)	8 (8%)	12	0	
All	All	406/428 (95%)	391 (96%)	15 (4%)	38	3	

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	12	SER
1	D	73	LEU
1	D	40[A]	THR
1	D	134	LYS
1	D	43[B]	TYR



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	49	ASN
1	D	95	GLN
1	D	116	ASN

#### 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)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	ol Type Chain I		Dag	T inle	Link Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ZOF	С	201	3	24,24,25	2.20	6 (25%)	27,30,32	2.95	13 (48%)
2	ZOF	D	201	3	24,24,25	2.31	6 (25%)	27,30,32	2.69	12 (44%)
2	ZOF	В	201	3	24,24,25	1.33	3 (12%)	27,30,32	2.69	8 (29%)
3	EDN	В	202	2	3,3,3	0.22	0	2,2,2	0.40	0
3	EDN	D	202	2	3,3,3	0.31	0	2,2,2	0.41	0
2	ZOF	A	201	3	24,24,25	1.34	3 (12%)	27,30,32	2.56	9 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
2	ZOF	С	201	3	-	0/14/36/37	0/2/2/2
2	ZOF	D	201	3	-	0/14/36/37	0/2/2/2
2	ZOF	В	201	3	-	0/14/36/37	0/2/2/2
3	EDN	В	202	2	-	0/1/1/1	-
3	EDN	D	202	2	-	0/1/1/1	-
2	ZOF	A	201	3	-	0/14/36/37	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
2	D	201	ZOF	CAD-NAE	-6.51	1.34	1.45
2	D	201	ZOF	CAA-NAE	5.55	1.43	1.35
2	С	201	ZOF	CAA-NAE	5.36	1.43	1.35
2	С	201	ZOF	CAD-NAE	-4.69	1.37	1.45
2	С	201	ZOF	CAA-NAB	4.35	1.41	1.35

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
2	В	201	ZOF	CAC-CAF-SAG	8.40	113.50	106.31
2	С	201	ZOF	NAE-CAA-NAB	-8.13	100.85	109.20
2	A	201	ZOF	CAC-CAF-SAG	7.81	113.00	106.31
2	D	201	ZOF	NAE-CAA-NAB	-7.45	101.55	109.20
2	В	201	ZOF	CAF-CAC-NAB	-6.40	104.90	113.03

There are no chirality outliers.

There are no torsion outliers.

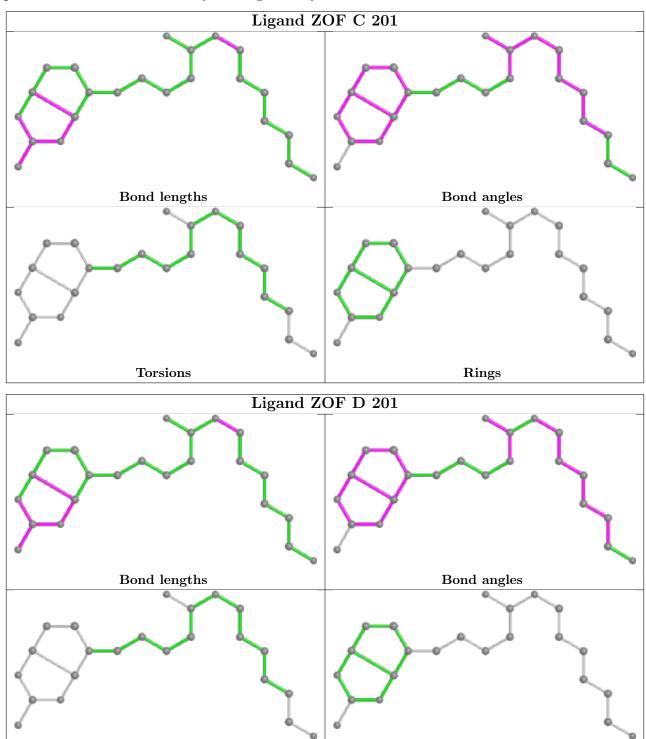
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and



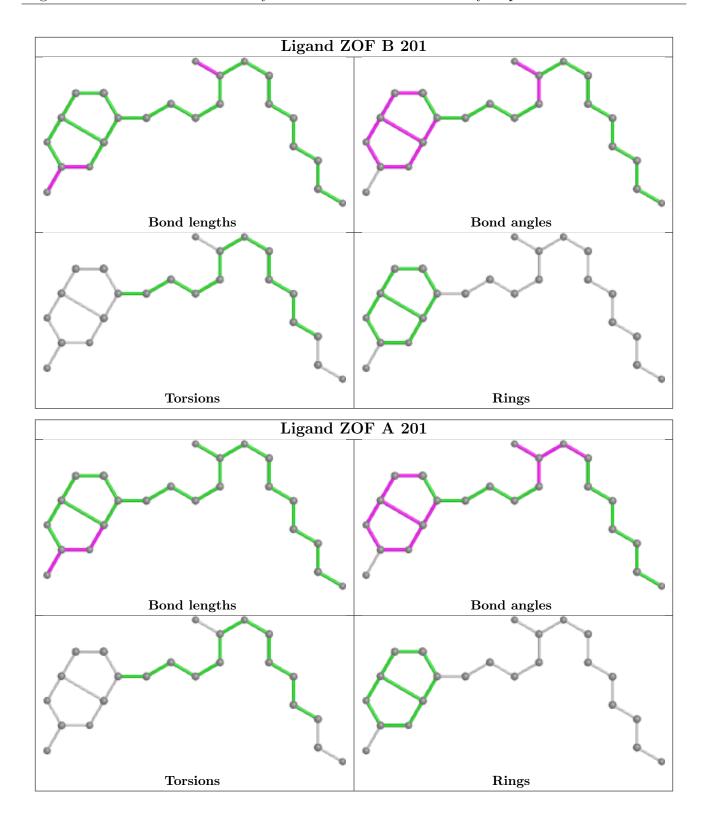
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Rings

Torsions



# 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 (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,  $95^{th}$  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>		# RSRZ >	·2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	A	124/147 (84%)	-0.02	9 (7%) 15	12	8, 15, 53, 86	0
1	В	124/147 (84%)	0.09	9 (7%) 15	12	9, 16, 53, 85	0
1	С	124/147 (84%)	0.31	10 (8%) 12	9	11, 19, 54, 102	0
1	D	124/147 (84%)	0.23	8 (6%) 18	16	11, 20, 56, 91	0
All	All	496/588 (84%)	0.15	36 (7%) 15	12	8, 18, 59, 102	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	ALA	9.1
1	С	47	VAL	8.6
1	A	47	VAL	8.3
1	D	47	VAL	8.1
1	В	46	ALA	7.7

## 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.

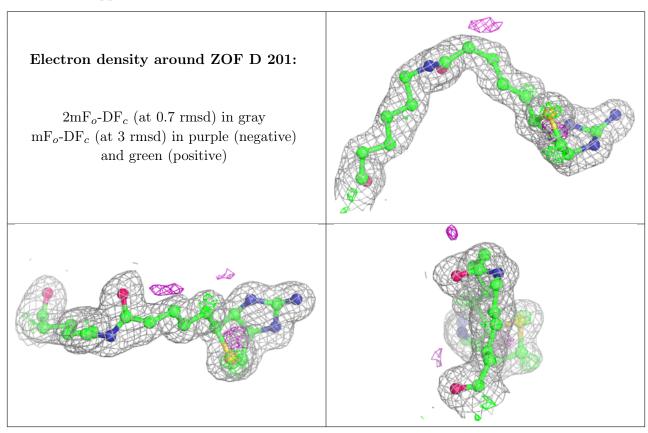
## 6.4 Ligands (i)

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.

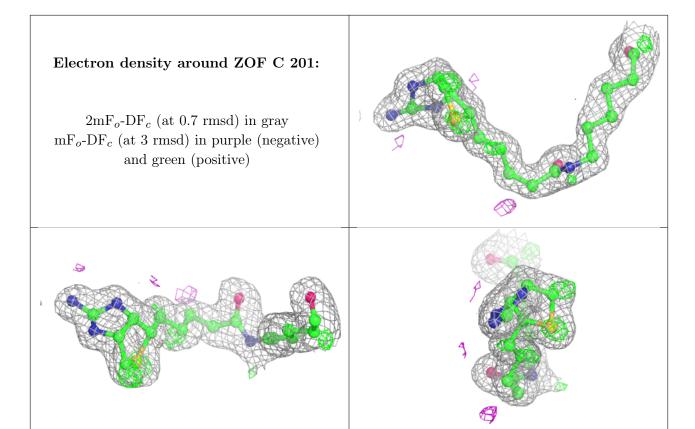


Mol	$\mathbf{Type}$	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	EDN	В	202	4/4	0.94	0.10	23,26,29,30	0
3	EDN	D	202	4/4	0.95	0.11	23,25,28,30	0
2	ZOF	D	201	23/24	0.96	0.09	19,24,33,36	0
2	ZOF	С	201	23/24	0.97	0.10	19,24,32,35	0
2	ZOF	A	201	23/24	0.97	0.11	15,19,27,31	0
2	ZOF	В	201	23/24	0.98	0.10	15,19,26,29	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.

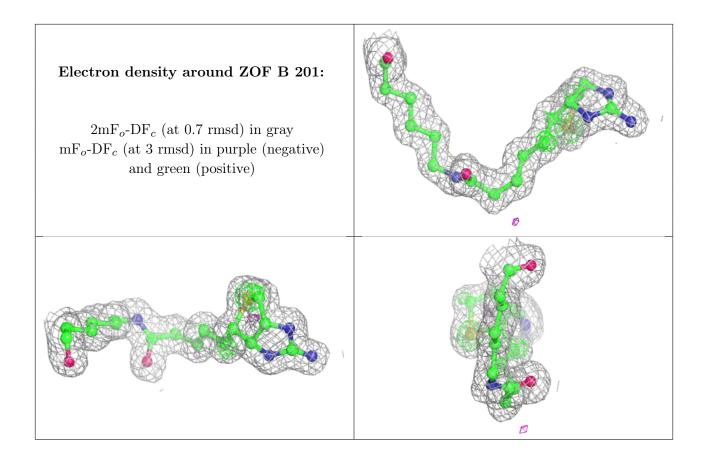






# Electron density around ZOF A 201: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)





# 6.5 Other polymers (i)

There are no such residues in this entry.

