

wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2020 - 08:02 PM BST

PDB ID	:	6SV1
Title	:	Crystal structure of Rhodospirillum rubrum Rru_A0973 E34A variant
Authors	:	Marles-Wright, J.; He, D.
Deposited on	:	2019-09-17
Resolution	:	2.19 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.5
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)	:	2.14.5

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 2.19 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	4898 (2.20-2.20)
Ramachandran outliers	138981	5503(2.20-2.20)
Sidechain outliers	138945	5504(2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	
-		110	3%	
	A	116	78%	22%
	D	110	3%	
	В	116	78%	22%
	~		2%	
1	C	116	78%	22%
	_			
1	D	116	78%	22%
	_		2%	
1	E	116	78%	22%
			3%	
1	F	116	76% •	22%
			3%	
1	G	116	78%	22%



Mol	Chain	Length	Quality of chain		
1	тт	116	%		
	П	110	2%		23%
1	Ι	116	78%		• 22%
1	J	116	3%		23%
			2%		
1	K	116	78%		22%
1	L	116	72%		28%
1	М	116	75%	.	24%
			3%		
1	N	116	77%		23%
1	Ο	116	75%	•	24%
1	Р	116	4% 78%		22%
1	0	116	2%		
	Q	110	76% <u>3%</u>	•	23%
1	R	116	75%	•	24%
1	S	116	78%		• 22%
1	Т	116	78%		• 22%
	т.т.	110	2% 		
	U	116	76%	•	23%
1	V	116	78%		22%
1	W	116	78%		22%
1	v	116	2%		220/
1	<u> </u>	110	2%	•	2290
1	Y	116	78%		22%
1	Z	116	78%		22%
1	a	116	3% 		• 22%
-	1	110	6%		-
	d	110	77% 4%	•	22%
1	с	116	76%	<u> </u>	22%
1	d	116	78%		22%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 43828 atoms, of which 21068 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.

Mol	Chain	Residues			Aton	ıs			ZeroOcc	AltConf	Trace
1	А	90	Total	С	Н	N	0	S	0	0	0
			1440	459	704	131	144	2			
1	В	91	Total	С	Н	Ν	Ο	\mathbf{S}	0	0	0
		91	1450	462	708	132	146	2	0	0	0
1	C	91	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	Ο
	0	51	1450	462	708	132	146	2	0	0	0
1	п	01	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
⊥	D	91	1450	462	708	132	146	2	0	0	0
1	F	01	Total	С	Η	Ν	Ο	S	0	0	0
1		91	1450	462	708	132	146	2	0	0	0
1	Б	0.0	Total	С	Η	Ν	Ο	S	0	0	0
L	Г	90	1440	459	704	131	144	2	0	0	0
1	C	0.1	Total	С	Н	Ν	Ο	S	0	0	0
	G	91	1450	462	708	132	146	2	0		
1	и	89	Total	С	Η	Ν	Ο	S	0	0	0
	11		1430	456	699	130	143	2			U
1	т	0.1	Total	С	Η	Ν	Ο	S	0	0	0
	1	91	1450	462	708	132	146	2			
1	т	80	Total	С	Η	Ν	Ο	S	0	0	0
	J	09	1430	456	698	130	144	2	0	0	
1	IZ.	0.1	Total	С	Η	Ν	Ο	S	0	0	0
	I II	91	1450	462	708	132	146	2	0	0	U
1	т	0.4	Total	С	Η	Ν	Ο	S	0	0	0
		04	1361	434	664	125	136	2	0	0	U
1	м	00	Total	С	Η	Ν	Ο	S	0	0	0
	1V1	00	1420	453	694	129	142	2	0	0	0
1	N	80	Total	С	Η	Ν	Ο	S	0	0	0
		89	1430	456	698	130	144	2	0	0	0
1	0	00	Total	С	Н	Ν	Ο	S	0	0	0
		00	1419	453	693	129	142	2		U	U
1	р	0.0	Total	С	Η	Ν	Ο	S	0	0	0
	r	90	1440	459	703	131	145	2		U	U

• Molecule 1 is a protein called Encapsulated Ferritin.



Mol	Chain	Residues	5		Aton	ns			ZeroOcc	AltConf	Trace
1	0	20	Total	С	Η	Ν	Ο	S	0	0	0
	Q	89	1430	456	698	130	144	2	0	0	0
1	D	00	Total	С	Η	Ν	Ο	S	0	0	0
	R	88	1420	453	694	129	142	2	0	0	0
1	C	0.1	Total	С	Η	Ν	Ο	S	0	0	0
	G	91	1450	462	708	132	146	2	0	0	0
1	т	01	Total	С	Η	Ν	Ο	S	0	0	0
	L	91	1450	462	708	132	146	2	0	0	0
1	T	80	Total	С	Η	Ν	0	S	0	0	0
1	U	09	1430	456	698	130	144	2	0	0	
1	V	0.1	Total	С	Η	Ν	Ο	S	0	0	0
1	v	91	1450	462	708	132	146	2			U
1	W	90	Total	С	Η	Ν	Ο	S	0	0	0
1	vv		1440	459	704	131	144	2	0	0	0
1	v	01	Total	С	Η	Ν	Ο	\mathbf{S}	Ο	0	0
L	Λ	31	1450	462	708	132	146	2	0		
1	V	0.0	Total	С	Η	Ν	Ο	\mathbf{S}	Ο	0	0
1	L	30	1440	459	703	131	145	2	0	0	
1	7	01	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
		31	1450	462	708	132	146	2	0	0	
1	2	91	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
	a	51	1450	462	708	132	146	2	0	0	0
1	h	90	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1	D	30	1440	459	703	131	145	2	0	0	0
1	C	90	Total	С	Η	Ν	Ο	\mathbf{S}	0	Ο	0
1	C	50	1440	459	704	131	144	2	0	U	0
1	d	90	Total	C	H	N	0	S	0	0	
		90	1440	459	703	131	145	2	0	U	U

There are 630 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	34	ALA	GLU	engineered mutation	UNP Q2RVS1
А	97	ALA	-	expression tag	UNP Q2RVS1
A	98	ASN	-	expression tag	UNP Q2RVS1
A	99	SER	-	expression tag	UNP Q2RVS1
A	100	SER	-	expression tag	UNP Q2RVS1
A	101	SER	-	expression tag	UNP Q2RVS1
A	102	VAL	-	expression tag	UNP Q2RVS1
A	103	ASP	-	expression tag	UNP Q2RVS1
A	104	LYS	-	expression tag	UNP Q2RVS1
A	105	LEU	-	expression tag	UNP Q2RVS1
A	106	ALA	-	expression tag	UNP Q2RVS1



Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	_	expression tag	UNP Q2RVS1
A	108	ALA	_	expression tag	UNP Q2RVS1
A	109	LEU	-	expression tag	UNP Q2RVS1
A	110	GLU	_	expression tag	UNP Q2RVS1
A	111	HIS	_	expression tag	UNP Q2RVS1
A	112	HIS	_	expression tag	UNP Q2RVS1
A	113	HIS	_	expression tag	UNP Q2RVS1
A	114	HIS	_	expression tag	UNP Q2RVS1
A	115	HIS	_	expression tag	UNP Q2RVS1
A	116	HIS	-	expression tag	UNP Q2RVS1
В	34	ALA	GLU	engineered mutation	UNP Q2RVS1
В	97	ALA	_	expression tag	UNP Q2RVS1
В	98	ASN	_	expression tag	UNP Q2RVS1
В	99	SER	_	expression tag	UNP Q2RVS1
В	100	SER	-	expression tag	UNP Q2RVS1
В	101	SER	_	expression tag	UNP Q2RVS1
В	102	VAL	-	expression tag	UNP Q2RVS1
В	103	ASP	-	expression tag	UNP Q2RVS1
В	104	LYS	-	expression tag	UNP Q2RVS1
В	105	LEU	-	expression tag	UNP Q2RVS1
В	106	ALA	-	expression tag	UNP Q2RVS1
В	107	ALA	-	expression tag	UNP Q2RVS1
В	108	ALA	-	expression tag	UNP Q2RVS1
В	109	LEU	_	expression tag	UNP Q2RVS1
В	110	GLU	_	expression tag	UNP Q2RVS1
В	111	HIS	-	expression tag	UNP Q2RVS1
В	112	HIS	-	expression tag	UNP Q2RVS1
В	113	HIS	-	expression tag	UNP Q2RVS1
В	114	HIS	-	expression tag	UNP Q2RVS1
В	115	HIS	-	expression tag	UNP Q2RVS1
В	116	HIS	-	expression tag	UNP Q2RVS1
С	34	ALA	GLU	engineered mutation	UNP Q2RVS1
С	97	ALA	-	expression tag	UNP Q2RVS1
С	98	ASN	-	expression tag	UNP Q2RVS1
С	99	SER	-	expression tag	UNP Q2RVS1
C	100	SER	-	expression tag	UNP Q2RVS1
C	101	SER	-	expression tag	UNP Q2RVS1
C	102	VAL	-	expression tag	UNP Q2RVS1
C	103	ASP	-	expression tag	UNP Q2RVS1
C	104	LYS	-	expression tag	UNP Q2RVS1
C	105	LEU	-	expression tag	UNP Q2RVS1
C	106	ALA	-	expression tag	UNP Q2RVS1



Chain	Residue	Modelled	Actual	Comment	Reference
C	107	ALA	-	expression tag	UNP Q2RVS1
C	108	ALA	_	expression tag	UNP Q2RVS1
C	109	LEU	_	expression tag	UNP Q2RVS1
C	110	GLU	_	expression tag	UNP Q2RVS1
C	111	HIS	_	expression tag	UNP Q2RVS1
C	112	HIS	_	expression tag	UNP Q2RVS1
C	113	HIS	_	expression tag	UNP Q2RVS1
C	114	HIS	_	expression tag	UNP Q2RVS1
C	115	HIS	_	expression tag	UNP Q2RVS1
C	116	HIS	_	expression tag	UNP Q2RVS1
D	34	ALA	GLU	engineered mutation	UNP Q2RVS1
D	97	ALA	_	expression tag	UNP Q2RVS1
D	98	ASN	-	expression tag	UNP Q2RVS1
D	99	SER	_	expression tag	UNP Q2RVS1
D	100	SER	_	expression tag	UNP Q2RVS1
D	101	SER	-	expression tag	UNP Q2RVS1
D	102	VAL	-	expression tag	UNP Q2RVS1
D	103	ASP	-	expression tag	UNP Q2RVS1
D	104	LYS	-	expression tag	UNP Q2RVS1
D	105	LEU	-	expression tag	UNP Q2RVS1
D	106	ALA	-	expression tag	UNP Q2RVS1
D	107	ALA	-	expression tag	UNP Q2RVS1
D	108	ALA	-	expression tag	UNP Q2RVS1
D	109	LEU	-	expression tag	UNP Q2RVS1
D	110	GLU	-	expression tag	UNP Q2RVS1
D	111	HIS	-	expression tag	UNP Q2RVS1
D	112	HIS	-	expression tag	UNP Q2RVS1
D	113	HIS	-	expression tag	UNP Q2RVS1
D	114	HIS	-	expression tag	UNP Q2RVS1
D	115	HIS	-	expression tag	UNP Q2RVS1
D	116	HIS	-	expression tag	UNP Q2RVS1
E	34	ALA	GLU	engineered mutation	UNP Q2RVS1
Е	97	ALA	-	expression tag	UNP Q2RVS1
E	98	ASN	-	expression tag	UNP Q2RVS1
E	99	SER	-	expression tag	UNP Q2RVS1
E	100	SER	-	expression tag	UNP Q2RVS1
E	101	SER	-	expression tag	UNP Q2RVS1
E	102	VAL	-	expression tag	UNP Q2RVS1
E	103	ASP	-	expression tag	UNP Q2RVS1
E	104	LYS	-	expression tag	UNP Q2RVS1
E	105	LEU	-	expression tag	UNP Q2RVS1
E	106	ALA	-	expression tag	UNP Q2RVS1



Chain	Residue	Modelled	Actual	Comment	Reference
Е	107	ALA	_	expression tag	UNP Q2RVS1
Е	108	ALA	_	expression tag	UNP Q2RVS1
Е	109	LEU	-	expression tag	UNP Q2RVS1
Е	110	GLU	_	expression tag	UNP Q2RVS1
Е	111	HIS	-	expression tag	UNP Q2RVS1
Е	112	HIS	-	expression tag	UNP Q2RVS1
Е	113	HIS	-	expression tag	UNP Q2RVS1
Е	114	HIS	-	expression tag	UNP Q2RVS1
Е	115	HIS	-	expression tag	UNP Q2RVS1
Ε	116	HIS	-	expression tag	UNP Q2RVS1
F	34	ALA	GLU	engineered mutation	UNP Q2RVS1
F	97	ALA	_	expression tag	UNP Q2RVS1
F	98	ASN	_	expression tag	UNP Q2RVS1
F	99	SER	-	expression tag	UNP Q2RVS1
F	100	SER	_	expression tag	UNP Q2RVS1
F	101	SER	-	expression tag	UNP Q2RVS1
F	102	VAL	_	expression tag	UNP Q2RVS1
F	103	ASP	_	expression tag	UNP Q2RVS1
F	104	LYS	_	expression tag	UNP Q2RVS1
F	105	LEU	_	expression tag	UNP Q2RVS1
F	106	ALA	_	expression tag	UNP Q2RVS1
F	107	ALA	_	expression tag	UNP Q2RVS1
F	108	ALA	_	expression tag	UNP Q2RVS1
F	109	LEU	_	expression tag	UNP Q2RVS1
F	110	GLU	_	expression tag	UNP Q2RVS1
F	111	HIS	_	expression tag	UNP Q2RVS1
F	112	HIS	_	expression tag	UNP Q2RVS1
F	113	HIS	_	expression tag	UNP Q2RVS1
F	114	HIS	_	expression tag	UNP Q2RVS1
F	115	HIS	-	expression tag	UNP Q2RVS1
F	116	HIS	_	expression tag	UNP Q2RVS1
G	34	ALA	GLU	engineered mutation	UNP Q2RVS1
G	97	ALA	_	expression tag	UNP Q2RVS1
G	98	ASN	-	expression tag	UNP Q2RVS1
G	99	SER	_	expression tag	UNP Q2RVS1
G	100	SER	_	expression tag	UNP Q2RVS1
G	101	SER	_	expression tag	UNP Q2RVS1
G	102	VAL	-	expression tag	UNP Q2RVS1
G	103	ASP	-	expression tag	UNP Q2RVS1
G	104	LYS	-	expression tag	UNP Q2RVS1
G	105	LEU	-	expression tag	UNP Q2RVS1
G	106	ALA	_	expression tag	UNP Q2RVS1

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Chain | Residue | Modelled | Actual |

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	Residue	Modelled	Actual	Comment	Reference
G	107	ALA	_	expression tag	UNP Q2BVS1
G	108	ALA	_	expression tag	UNP Q2RVS1
G	109	LEU	_	expression tag	UNP Q2RVS1
G	110	GLU	_	expression tag	UNP Q2RVS1
G	111	HIS	_	expression tag	UNP Q2RVS1
G	112	HIS	_	expression tag	UNP Q2RVS1
G	113	HIS	_	expression tag	UNP Q2RVS1
G	114	HIS	_	expression tag	UNP Q2RVS1
G	115	HIS	_	expression tag	UNP Q2RVS1
G	116	HIS	-	expression tag	UNP Q2RVS1
Н	34	ALA	GLU	engineered mutation	UNP Q2RVS1
Н	97	ALA	-	expression tag	UNP Q2RVS1
Н	98	ASN	-	expression tag	UNP Q2RVS1
Н	99	SER	_	expression tag	UNP Q2RVS1
Н	100	SER	_	expression tag	UNP Q2RVS1
Н	101	SER	-	expression tag	UNP Q2RVS1
Н	102	VAL	-	expression tag	UNP Q2RVS1
Н	103	ASP	-	expression tag	UNP Q2RVS1
Н	104	LYS	-	expression tag	UNP Q2RVS1
Н	105	LEU	-	expression tag	UNP Q2RVS1
Н	106	ALA	-	expression tag	UNP Q2RVS1
Н	107	ALA	-	expression tag	UNP Q2RVS1
Н	108	ALA	-	expression tag	UNP Q2RVS1
Н	109	LEU	-	expression tag	UNP Q2RVS1
Н	110	GLU	-	expression tag	UNP Q2RVS1
Н	111	HIS	-	expression tag	UNP Q2RVS1
Н	112	HIS	-	expression tag	UNP Q2RVS1
Н	113	HIS	-	expression tag	UNP Q2RVS1
Н	114	HIS	-	expression tag	UNP Q2RVS1
Н	115	HIS	-	expression tag	UNP Q2RVS1
Н	116	HIS	-	expression tag	UNP Q2RVS1
I	34	ALA	GLU	engineered mutation	UNP Q2RVS1
Ι	97	ALA	-	expression tag	UNP Q2RVS1
I	98	ASN	-	expression tag	UNP Q2RVS1
I	99	SER	-	expression tag	UNP Q2RVS1
I	100	SER	-	expression tag	UNP Q2RVS1
I	101	SER	-	expression tag	UNP Q2RVS1
I	102	VAL	-	expression tag	UNP Q2RVS1
I	103	ASP	-	expression tag	UNP Q2RVS1
I	104	LYS	-	expression tag	UNP Q2RVS1
I	105	LEU	-	expression tag	UNP Q2RVS1
I	106	ALA	-	expression tag	UNP Q2RVS1



Continu	ed from pre	vious page			-
Chain	Residue	Modelled	Actual	Comment	Reference
I	107	ALA	-	expression tag	UNP Q2RVS1
I	108	ALA	-	expression tag	UNP Q2RVS1
I	109	LEU	-	expression tag	UNP Q2RVS1
I	110	GLU	-	expression tag	UNP Q2RVS1
I	111	HIS	-	expression tag	UNP Q2RVS1
I	112	HIS	-	expression tag	UNP Q2RVS1
Ι	113	HIS	_	expression tag	UNP Q2RVS1
Ι	114	HIS	-	expression tag	UNP Q2RVS1
Ι	115	HIS	-	expression tag	UNP Q2RVS1
Ι	116	HIS	-	expression tag	UNP Q2RVS1
J	34	ALA	GLU	engineered mutation	UNP Q2RVS1
J	97	ALA	-	expression tag	UNP Q2RVS1
J	98	ASN	-	expression tag	UNP Q2RVS1
J	99	SER	-	expression tag	UNP Q2RVS1
J	100	SER	-	expression tag	UNP Q2RVS1
J	101	SER	-	expression tag	UNP Q2RVS1
J	102	VAL	-	expression tag	UNP Q2RVS1
J	103	ASP	-	expression tag	UNP Q2RVS1
J	104	LYS	-	expression tag	UNP Q2RVS1
J	105	LEU	-	expression tag	UNP Q2RVS1
J	106	ALA	-	expression tag	UNP Q2RVS1
J	107	ALA	-	expression tag	UNP Q2RVS1
J	108	ALA	-	expression tag	UNP Q2RVS1
J	109	LEU	-	expression tag	UNP Q2RVS1
J	110	GLU	-	expression tag	UNP Q2RVS1
J	111	HIS	-	expression tag	UNP Q2RVS1
J	112	HIS	-	expression tag	UNP Q2RVS1
J	113	HIS	-	expression tag	UNP Q2RVS1
J	114	HIS	-	expression tag	UNP Q2RVS1
J	115	HIS	-	expression tag	UNP Q2RVS1
J	116	HIS	-	expression tag	UNP Q2RVS1
Κ	34	ALA	GLU	engineered mutation	UNP Q2RVS1
Κ	97	ALA	-	expression tag	UNP Q2RVS1
Κ	98	ASN	-	expression tag	UNP Q2RVS1
Κ	99	SER	-	expression tag	UNP Q2RVS1
K	100	SER	-	expression tag	UNP Q2RVS1
Κ	101	SER	-	expression tag	UNP Q2RVS1
Κ	102	VAL	-	expression tag	UNP Q2RVS1
Κ	103	ASP	-	expression tag	UNP Q2RVS1
Κ	104	LYS	-	expression tag	UNP Q2RVS1
Κ	105	LEU	-	expression tag	UNP Q2RVS1
K	106	ALA	-	expression tag	UNP Q2RVS1



Chain	Residue	Modelled	Actual	Comment	Reference
K	107	ALA	_	expression tag	UNP Q2RVS1
K	108	ALA	_	expression tag	UNP Q2RVS1
K	109	LEU	_	expression tag	UNP Q2RVS1
K	110	GLU	_	expression tag	UNP Q2RVS1
K	111	HIS	_	expression tag	UNP Q2RVS1
K	112	HIS	_	expression tag	UNP Q2RVS1
K	113	HIS	_	expression tag	UNP Q2RVS1
K	114	HIS	_	expression tag	UNP Q2RVS1
K	115	HIS	-	expression tag	UNP Q2RVS1
K	116	HIS	-	expression tag	UNP Q2RVS1
L	34	ALA	GLU	engineered mutation	UNP Q2RVS1
L	97	ALA	_	expression tag	UNP Q2RVS1
L	98	ASN	_	expression tag	UNP Q2RVS1
L	99	SER	_	expression tag	UNP Q2RVS1
L	100	SER	_	expression tag	UNP Q2RVS1
L	101	SER	_	expression tag	UNP Q2RVS1
L	102	VAL	-	expression tag	UNP Q2RVS1
L	103	ASP	-	expression tag	UNP Q2RVS1
L	104	LYS	-	expression tag	UNP Q2RVS1
L	105	LEU	-	expression tag	UNP Q2RVS1
L	106	ALA	-	expression tag	UNP Q2RVS1
L	107	ALA	-	expression tag	UNP Q2RVS1
L	108	ALA	-	expression tag	UNP Q2RVS1
L	109	LEU	_	expression tag	UNP Q2RVS1
L	110	GLU	_	expression tag	UNP Q2RVS1
L	111	HIS	-	expression tag	UNP Q2RVS1
L	112	HIS	-	expression tag	UNP Q2RVS1
L	113	HIS	-	expression tag	UNP Q2RVS1
L	114	HIS	-	expression tag	UNP Q2RVS1
L	115	HIS	-	expression tag	UNP Q2RVS1
L	116	HIS	-	expression tag	UNP Q2RVS1
М	34	ALA	GLU	engineered mutation	UNP Q2RVS1
М	97	ALA	-	expression tag	UNP Q2RVS1
М	98	ASN	-	expression tag	UNP Q2RVS1
М	99	SER	-	expression tag	UNP Q2RVS1
М	100	SER	-	expression tag	UNP Q2RVS1
М	101	SER	-	expression tag	UNP Q2RVS1
М	102	VAL	-	expression tag	UNP Q2RVS1
М	103	ASP	-	expression tag	UNP Q2RVS1
М	104	LYS	-	expression tag	UNP Q2RVS1
M	105	LEU	-	expression tag	UNP Q2RVS1
М	106	ALA	-	expression tag	UNP Q2RVS1



Chain	Residue	Modelled	Actual	Comment	Reference
М	107	ALA	_	expression tag	UNP Q2RVS1
М	108	ALA	_	expression tag	UNP Q2RVS1
М	109	LEU	_	expression tag	UNP Q2RVS1
М	110	GLU	_	expression tag	UNP Q2RVS1
М	111	HIS	-	expression tag	UNP Q2RVS1
М	112	HIS	-	expression tag	UNP Q2RVS1
М	113	HIS	-	expression tag	UNP Q2RVS1
М	114	HIS	_	expression tag	UNP Q2RVS1
М	115	HIS	-	expression tag	UNP Q2RVS1
М	116	HIS	-	expression tag	UNP Q2RVS1
N	34	ALA	GLU	engineered mutation	UNP Q2RVS1
N	97	ALA	-	expression tag	UNP Q2RVS1
N	98	ASN	-	expression tag	UNP Q2RVS1
N	99	SER	-	expression tag	UNP Q2RVS1
N	100	SER	-	expression tag	UNP Q2RVS1
N	101	SER	-	expression tag	UNP Q2RVS1
N	102	VAL	-	expression tag	UNP Q2RVS1
N	103	ASP	-	expression tag	UNP Q2RVS1
N	104	LYS	-	expression tag	UNP Q2RVS1
N	105	LEU	_	expression tag	UNP Q2RVS1
N	106	ALA	_	expression tag	UNP Q2RVS1
N	107	ALA	-	expression tag	UNP Q2RVS1
N	108	ALA	_	expression tag	UNP Q2RVS1
N	109	LEU	-	expression tag	UNP Q2RVS1
N	110	GLU	-	expression tag	UNP Q2RVS1
N	111	HIS	-	expression tag	UNP Q2RVS1
N	112	HIS	-	expression tag	UNP Q2RVS1
N	113	HIS	-	expression tag	UNP Q2RVS1
N	114	HIS	-	expression tag	UNP Q2RVS1
N	115	HIS	-	expression tag	UNP Q2RVS1
N .	116	HIS	-	expression tag	UNP Q2RVS1
0	34	ALA	GLU	engineered mutation	UNP Q2RVS1
0	97	ALA	-	expression tag	UNP Q2RVS1
0	98	ASN	-	expression tag	UNP Q2RVS1
0	99	SER	-	expression tag	UNP Q2RVS1
0	100	SER	-	expression tag	UNP Q2RVS1
0	101	SER	-	expression tag	UNP Q2RVS1
0	102	VAL	-	expression tag	UNP Q2RVS1
0	103	ASP	-	expression tag	UNP Q2RVS1
0	104	LYS	-	expression tag	UNP Q2RVS1
0	105		-	expression tag	UNP Q2RVS1
0	106	ALA	-	expression tag	UNP Q2RVS1



Chain	Residue	Modelled	Actual	Comment	Reference
0	107	ALA	_	expression tag	UNP Q2RVS1
0	108	ALA	_	expression tag	UNP Q2RVS1
0	109	LEU	_	expression tag	UNP Q2RVS1
0	110	GLU	_	expression tag	UNP Q2RVS1
0	111	HIS	_	expression tag	UNP Q2RVS1
0	112	HIS	_	expression tag	UNP Q2RVS1
0	113	HIS	_	expression tag	UNP Q2RVS1
0	114	HIS	_	expression tag	UNP Q2RVS1
0	115	HIS	_	expression tag	UNP Q2RVS1
0	116	HIS	_	expression tag	UNP Q2RVS1
Р	34	ALA	GLU	engineered mutation	UNP Q2RVS1
Р	97	ALA	_	expression tag	UNP Q2RVS1
Р	98	ASN	_	expression tag	UNP Q2RVS1
Р	99	SER	_	expression tag	UNP Q2RVS1
Р	100	SER	-	expression tag	UNP Q2RVS1
Р	101	SER	-	expression tag	UNP Q2RVS1
Р	102	VAL	-	expression tag	UNP Q2RVS1
Р	103	ASP	-	expression tag	UNP Q2RVS1
Р	104	LYS	-	expression tag	UNP Q2RVS1
Р	105	LEU	-	expression tag	UNP Q2RVS1
Р	106	ALA	-	expression tag	UNP Q2RVS1
Р	107	ALA	-	expression tag	UNP Q2RVS1
Р	108	ALA	-	expression tag	UNP Q2RVS1
Р	109	LEU	_	expression tag	UNP Q2RVS1
Р	110	GLU	-	expression tag	UNP Q2RVS1
Р	111	HIS	_	expression tag	UNP Q2RVS1
Р	112	HIS	_	expression tag	UNP Q2RVS1
Р	113	HIS	_	expression tag	UNP Q2RVS1
Р	114	HIS	-	expression tag	UNP Q2RVS1
Р	115	HIS	_	expression tag	UNP Q2RVS1
Р	116	HIS	-	expression tag	UNP Q2RVS1
Q	34	ALA	GLU	engineered mutation	UNP Q2RVS1
Q	97	ALA	-	expression tag	UNP Q2RVS1
Q	98	ASN	-	expression tag	UNP Q2RVS1
Q	99	SER	-	expression tag	UNP Q2RVS1
Q	100	SER	-	expression tag	UNP Q2RVS1
Q	101	SER	-	expression tag	UNP Q2RVS1
Q	102	VAL	-	expression tag	UNP Q2RVS1
Q	103	ASP	-	expression tag	UNP Q2RVS1
Q	104	LYS	-	expression tag	UNP Q2RVS1
Q	105	LEU	-	expression tag	UNP Q2RVS1
Q	106	ALA	-	expression tag	UNP Q2RVS1



Chain	Residue	Modelled	Actual	Comment	Reference
Q	107	ALA	_	expression tag	UNP Q2RVS1
Q	108	ALA	_	expression tag	UNP Q2RVS1
Q	109	LEU	_	expression tag	UNP Q2RVS1
Q	110	GLU	_	expression tag	UNP Q2RVS1
Q	111	HIS	_	expression tag	UNP Q2RVS1
Q	112	HIS	-	expression tag	UNP Q2RVS1
Q	113	HIS	-	expression tag	UNP Q2RVS1
Q	114	HIS	-	expression tag	UNP Q2RVS1
Q	115	HIS	-	expression tag	UNP Q2RVS1
Q	116	HIS	_	expression tag	UNP Q2RVS1
R	34	ALA	GLU	engineered mutation	UNP Q2RVS1
R	97	ALA	_	expression tag	UNP Q2RVS1
R	98	ASN	_	expression tag	UNP Q2RVS1
R	99	SER	_	expression tag	UNP Q2RVS1
R	100	SER	_	expression tag	UNP Q2RVS1
R	101	SER	-	expression tag	UNP Q2RVS1
R	102	VAL	-	expression tag	UNP Q2RVS1
R	103	ASP	-	expression tag	UNP Q2RVS1
R	104	LYS	-	expression tag	UNP Q2RVS1
R	105	LEU	-	expression tag	UNP Q2RVS1
R	106	ALA	-	expression tag	UNP Q2RVS1
R	107	ALA	-	expression tag	UNP Q2RVS1
R	108	ALA	_	expression tag	UNP Q2RVS1
R	109	LEU	-	expression tag	UNP Q2RVS1
R	110	GLU	-	expression tag	UNP Q2RVS1
R	111	HIS	-	expression tag	UNP Q2RVS1
R	112	HIS	-	expression tag	UNP Q2RVS1
R	113	HIS	-	expression tag	UNP Q2RVS1
R	114	HIS	-	expression tag	UNP Q2RVS1
R	115	HIS	-	expression tag	UNP Q2RVS1
R	116	HIS	-	expression tag	UNP Q2RVS1
S	34	ALA	GLU	engineered mutation	UNP Q2RVS1
S	97	ALA	-	expression tag	UNP Q2RVS1
S	98	ASN	-	expression tag	UNP Q2RVS1
S	99	SER	-	expression tag	UNP Q2RVS1
S	100	SER	-	expression tag	UNP Q2RVS1
S	101	SER	_	expression tag	UNP Q2RVS1
S	102	VAL	-	expression tag	UNP Q2RVS1
S	103	ASP	-	expression tag	UNP Q2RVS1
S	104	LYS	-	expression tag	UNP Q2RVS1
S	105	LEU	-	expression tag	UNP Q2RVS1
S	106	ALA	-	expression tag	UNP Q2RVS1



	Residue	Modelled	Actual	Comment	Reference
S	107	ALA		expression tag	UNP O2RVS1
S	101	ALA	_	expression tag	UNP O2RVS1
S	100	LEU	_	expression tag	UNP O2RVS1
S	109	GLU	_	expression tag	UNP O2RVS1
S	110	HIS		expression tag	UNP O2RVS1
S	111	HIS	_	expression tag	UNP O2RVS1
S S	112	HIS	_	expression tag	UNP O2RVS1
S	110	HIS	_	expression tag	UNP O2RVS1
S	114	HIS	_	expression tag	UNP O2RVS1
S S	116	HIS		expression tag	UNP O2RVS1
	34		CLU	ongineered mutation	UNP O2RVS1
	97		GLU	ovpression tag	UNP O2RVS1
	91	ADA	-	expression tag	UNP O2RVS1
	98	CED ADN	-	expression tag	UNI Q2RV51
	99	SER	-	expression tag	UNF Q2RV51
	100		-	expression tag	UNF Q2RV51
	101	SER VAL	-	expression tag	UNP Q2RV51
	102		-	expression tag	UNP Q2RVSI
	103	ASP	-	expression tag	UNP Q2RVSI
	104		-	expression tag	UNP Q2RVSI
	105		-	expression tag	UNP Q2RVSI
	106	ALA	-	expression tag	UNP Q2RVS1
	107	ALA	-	expression tag	UNP Q2RVS1
	108	ALA	-	expression tag	UNP Q2RVS1
	109	LEU	-	expression tag	UNP Q2RVS1
T	110	GLU	-	expression tag	UNP Q2RVS1
<u> </u>	111	HIS	-	expression tag	UNP Q2RVS1
T	112	HIS	-	expression tag	UNP Q2RVS1
T	113	HIS	-	expression tag	UNP Q2RVS1
T	114	HIS	-	expression tag	UNP Q2RVS1
T	115	HIS	-	expression tag	UNP Q2RVS1
T	116	HIS	-	expression tag	UNP Q2RVS1
U	34	ALA	GLU	engineered mutation	UNP Q2RVS1
U	97	ALA	-	expression tag	UNP Q2RVS1
U	98	ASN	-	expression tag	UNP Q2RVS1
U	99	SER	-	expression tag	UNP Q2RVS1
U	100	SER	_	expression tag	UNP Q2RVS1
U	101	SER	_	expression tag	UNP Q2RVS1
U	102	VAL	-	expression tag	UNP Q2RVS1
U	103	ASP	-	expression tag	UNP Q2RVS1
U	104	LYS	-	expression tag	UNP Q2RVS1
U	105	LEU	-	expression tag	UNP Q2RVS1
U	106	ALA	-	expression tag	UNP Q2RVS1



Chain	Residue	Modelled	Actual	Comment	Reference
U	107	ALA	_	expression tag	UNP Q2BVS1
U	108	ALA	_	expression tag	UNP Q2RVS1
U	109	LEU	_	expression tag	UNP Q2RVS1
U	110	GLU	_	expression tag	UNP Q2RVS1
U	111	HIS	_	expression tag	UNP Q2RVS1
U	112	HIS	_	expression tag	UNP Q2RVS1
U	113	HIS	_	expression tag	UNP Q2RVS1
U	114	HIS	_	expression tag	UNP Q2RVS1
U	115	HIS	_	expression tag	UNP Q2RVS1
U	116	HIS	-	expression tag	UNP Q2RVS1
V	34	ALA	GLU	engineered mutation	UNP Q2RVS1
V	97	ALA	_	expression tag	UNP Q2RVS1
V	98	ASN	_	expression tag	UNP Q2RVS1
V	99	SER	_	expression tag	UNP Q2RVS1
V	100	SER	-	expression tag	UNP Q2RVS1
V	101	SER	-	expression tag	UNP Q2RVS1
V	102	VAL	-	expression tag	UNP Q2RVS1
V	103	ASP	-	expression tag	UNP Q2RVS1
V	104	LYS	-	expression tag	UNP Q2RVS1
V	105	LEU	-	expression tag	UNP Q2RVS1
V	106	ALA	-	expression tag	UNP Q2RVS1
V	107	ALA	-	expression tag	UNP Q2RVS1
V	108	ALA	-	expression tag	UNP Q2RVS1
V	109	LEU	-	expression tag	UNP Q2RVS1
V	110	GLU	-	expression tag	UNP Q2RVS1
V	111	HIS	-	expression tag	UNP Q2RVS1
V	112	HIS	-	expression tag	UNP Q2RVS1
V	113	HIS	-	expression tag	UNP Q2RVS1
V	114	HIS	-	expression tag	UNP Q2RVS1
V	115	HIS	-	expression tag	UNP Q2RVS1
V	116	HIS	-	expression tag	UNP Q2RVS1
W	34	ALA	GLU	engineered mutation	UNP Q2RVS1
W	97	ALA	-	expression tag	UNP Q2RVS1
W	98	ASN	-	expression tag	UNP Q2RVS1
W	99	SER	-	expression tag	UNP Q2RVS1
W	100	SER	-	expression tag	UNP $Q2\overline{RVS1}$
W	101	SER		expression tag	UNP Q2RVS1
W	102	VAL	-	expression tag	UNP Q2RVS1
W	103	ASP	-	expression tag	UNP Q2RVS1
W	104	LYS	-	expression tag	UNP Q2RVS1
W	105	LEU	-	expression tag	UNP Q2RVS1
W	106	ALA	-	expression tag	UNP Q2RVS1



	Residue	Modelled	Actual	Comment	Reference
W	107	ALA	-	expression tag	UNP O2RVS1
W	107	ALA	_	expression tag	UNP O2RVS1
W	100	LEU	_	expression tag	UNP O2RVS1
W	105	GLU	_	expression tag	UNP O2RVS1
W	110	HIS	_	expression tag	UNP O2RVS1
W	112	HIS	_	expression tag	UNP O2RVS1
W	112	HIS	_	expression tag	UNP O2RVS1
W	110	HIS	_	expression tag	UNP Q2RVS1
W	115	HIS	_	expression tag	UNP Q2RVS1
W	116	HIS	_	expression tag	UNP Q2RVS1
X	34	ALA	GLU	engineered mutation	UNP Q2RVS1
X	97	ALA	-	expression tag	UNP Q2RVS1
X	98	ASN	_	expression tag	UNP Q2RVS1
X	99	SEB	_	expression tag	UNP Q2RVS1
X	100	SER	_	expression tag	UNP Q2RVS1
X	101	SER	_	expression tag	UNP Q2RVS1
X	102	VAL	_	expression tag	UNP Q2RVS1
X	103	ASP	_	expression tag	UNP Q2RVS1
X	104	LYS	_	expression tag	UNP Q2RVS1
X	105	LEU	_	expression tag	UNP Q2RVS1
X	106	ALA	_	expression tag	UNP Q2RVS1
X	107	ALA	-	expression tag	UNP Q2RVS1
X	108	ALA	-	expression tag	UNP Q2RVS1
X	109	LEU	_	expression tag	UNP Q2RVS1
X	110	GLU	_	expression tag	UNP Q2RVS1
X	111	HIS	-	expression tag	UNP Q2RVS1
Х	112	HIS	-	expression tag	UNP Q2RVS1
Х	113	HIS	-	expression tag	UNP Q2RVS1
Х	114	HIS	-	expression tag	UNP Q2RVS1
Х	115	HIS	-	expression tag	UNP Q2RVS1
Х	116	HIS	-	expression tag	UNP Q2RVS1
Y	34	ALA	GLU	engineered mutation	UNP Q2RVS1
Y	97	ALA	_	expression tag	UNP Q2RVS1
Y	98	ASN	-	expression tag	UNP Q2RVS1
Y	99	SER	_	expression tag	UNP Q2RVS1
Y	100	SER	_	expression tag	UNP Q2RVS1
Y	101	SER	-	expression tag	UNP Q2RVS1
Y	102	VAL	-	expression tag	UNP Q2RVS1
Y	103	ASP	-	expression tag	UNP Q2RVS1
Y	104	LYS	-	expression tag	UNP Q2RVS1
Y	105	LEU	-	expression tag	UNP Q2RVS1
Y	106	ALA	-	expression tag	UNP Q2RVS1



	Besidue	Modelled	Actual	Comment	Reference
V	107			expression tag	UNP O2RVS1
V	107	ALA	_	expression tag	UNP O2RVS1
V I	100	LEU	_	expression tag	UNP Q2RVS1
V	110	GLU	_	expression tag	UNP O2RVS1
V I	110	HIS	_	expression tag	UNP Q2RVS1
Y	112	HIS	_	expression tag	UNP Q2RVS1
Y	112	HIS	_	expression tag	UNP Q2RVS1
Y	114	HIS	_	expression tag	UNP Q2RVS1
Y	115	HIS	_	expression tag	UNP Q2RVS1
Y	116	HIS	_	expression tag	UNP Q2RVS1
Z	34	ALA	GLU	engineered mutation	UNP Q2RVS1
 Z	97	ALA	-	expression tag	UNP Q2RVS1
Z	98	ASN	_	expression tag	UNP Q2RVS1
Z	99	SER	_	expression tag	UNP Q2RVS1
Z	100	SER	-	expression tag	UNP Q2RVS1
Z	101	SER	-	expression tag	UNP Q2RVS1
Z	102	VAL	_	expression tag	UNP Q2RVS1
Z	103	ASP	_	expression tag	UNP Q2RVS1
Z	104	LYS	_	expression tag	UNP Q2RVS1
Z	105	LEU	-	expression tag	UNP Q2RVS1
Z	106	ALA	-	expression tag	UNP Q2RVS1
Z	107	ALA	-	expression tag	UNP Q2RVS1
Z	108	ALA	-	expression tag	UNP Q2RVS1
Z	109	LEU	-	expression tag	UNP Q2RVS1
Z	110	GLU	-	expression tag	UNP Q2RVS1
Ζ	111	HIS	-	expression tag	UNP Q2RVS1
Z	112	HIS	-	expression tag	UNP Q2RVS1
Ζ	113	HIS	-	expression tag	UNP Q2RVS1
Z	114	HIS	-	expression tag	UNP Q2RVS1
Z	115	HIS	-	expression tag	UNP Q2RVS1
Z	116	HIS	-	expression tag	UNP Q2RVS1
a	34	ALA	GLU	engineered mutation	UNP Q2RVS1
a	97	ALA	-	expression tag	UNP Q2RVS1
a	98	ASN	-	expression tag	UNP Q2RVS1
a	99	SER	-	expression tag	UNP Q2RVS1
a	100	SER	-	expression tag	UNP Q2RVS1
a	101	SER	-	expression tag	UNP Q2RVS1
a	102	VAL	-	expression tag	UNP Q2RVS1
a	103	ASP	-	expression tag	UNP Q2RVS1
a	104	LYS	-	expression tag	UNP Q2RVS1
a	105		-	expression tag	UNP Q2RVS1
a	106	ALA	-	expression tag	UNP Q2RVS1



Chain	Residue	Modelled	Actual	Comment	Reference
a	107	ALA	_	expression tag	UNP Q2RVS1
a	108	ALA	_	expression tag	UNP Q2RVS1
a	109	LEU	_	expression tag	UNP Q2RVS1
a	110	GLU	_	expression tag	UNP Q2RVS1
a	111	HIS	_	expression tag	UNP Q2RVS1
a	112	HIS	_	expression tag	UNP Q2RVS1
a	113	HIS	_	expression tag	UNP Q2RVS1
a	114	HIS	-	expression tag	UNP Q2RVS1
a	115	HIS	-	expression tag	UNP Q2RVS1
a	116	HIS	-	expression tag	UNP Q2RVS1
b	34	ALA	GLU	engineered mutation	UNP Q2RVS1
b	97	ALA	_	expression tag	UNP Q2RVS1
b	98	ASN	-	expression tag	UNP Q2RVS1
b	99	SER	_	expression tag	UNP Q2RVS1
b	100	SER	_	expression tag	UNP Q2RVS1
b	101	SER	_	expression tag	UNP Q2RVS1
b	102	VAL	-	expression tag	UNP Q2RVS1
b	103	ASP	_	expression tag	UNP Q2RVS1
b	104	LYS	-	expression tag	UNP Q2RVS1
b	105	LEU	-	expression tag	UNP Q2RVS1
b	106	ALA	-	expression tag	UNP Q2RVS1
b	107	ALA	-	expression tag	UNP Q2RVS1
b	108	ALA	-	expression tag	UNP Q2RVS1
b	109	LEU	-	expression tag	UNP Q2RVS1
b	110	GLU	-	expression tag	UNP Q2RVS1
b	111	HIS	-	expression tag	UNP Q2RVS1
b	112	HIS	-	expression tag	UNP Q2RVS1
b	113	HIS	-	expression tag	UNP Q2RVS1
b	114	HIS	-	expression tag	UNP Q2RVS1
b	115	HIS	-	expression tag	UNP Q2RVS1
b	116	HIS	-	expression tag	UNP Q2RVS1
с	34	ALA	GLU	engineered mutation	UNP Q2RVS1
с	97	ALA	-	expression tag	UNP Q2RVS1
с	98	ASN	-	expression tag	UNP Q2RVS1
с	99	SER	-	expression tag	UNP Q2RVS1
с	100	SER	-	expression tag	UNP Q2RVS1
с	101	SER	-	expression tag	UNP Q2RVS1
с	102	VAL	-	expression tag	UNP Q2RVS1
c	103	ASP	-	expression tag	UNP Q2RVS1
с	104	LYS	-	expression tag	UNP Q2RVS1
с	105	LEU	-	expression tag	UNP Q2RVS1
с	106	ALA	-	expression tag	UNP Q2RVS1



Chain	Residue	Modelled	Actual	Comment	Reference
с	107	ALA	-	expression tag	UNP Q2RVS1
с	108	ALA	-	expression tag	UNP Q2RVS1
с	109	LEU	-	expression tag	UNP Q2RVS1
с	110	GLU	-	expression tag	UNP Q2RVS1
с	111	HIS	-	expression tag	UNP Q2RVS1
с	112	HIS	-	expression tag	UNP Q2RVS1
с	113	HIS	-	expression tag	UNP Q2RVS1
с	114	HIS	-	expression tag	UNP Q2RVS1
с	115	HIS	-	expression tag	UNP Q2RVS1
с	116	HIS	-	expression tag	UNP Q2RVS1
d	34	ALA	GLU	engineered mutation	UNP Q2RVS1
d	97	ALA	-	expression tag	UNP Q2RVS1
d	98	ASN	-	expression tag	UNP Q2RVS1
d	99	SER	-	expression tag	UNP Q2RVS1
d	100	SER	-	expression tag	UNP Q2RVS1
d	101	SER	-	expression tag	UNP Q2RVS1
d	102	VAL	-	expression tag	UNP Q2RVS1
d	103	ASP	-	expression tag	UNP Q2RVS1
d	104	LYS	-	expression tag	UNP Q2RVS1
d	105	LEU	-	expression tag	UNP Q2RVS1
d	106	ALA	-	expression tag	UNP Q2RVS1
d	107	ALA	-	expression tag	UNP Q2RVS1
d	108	ALA	-	expression tag	UNP Q2RVS1
d	109	LEU	_	expression tag	UNP Q2RVS1
d	110	GLU	-	expression tag	UNP Q2RVS1
d	111	HIS	-	expression tag	UNP Q2RVS1
d	112	HIS	-	expression tag	UNP Q2RVS1
d	113	HIS	-	expression tag	UNP Q2RVS1
d	114	HIS	-	expression tag	UNP Q2RVS1
d	115	HIS	-	expression tag	UNP Q2RVS1
d	116	HIS	-	expression tag	UNP Q2RVS1

• Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Р	1	Total Fe 1 1	0	0
2	Κ	1	Total Fe 1 1	0	0
2	В	1	Total Fe 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	с	1	Total Fe 1 1	0	0
2	W	1	Total Fe 1 1	0	0
2	Ν	1	Total Fe 1 1	0	0
2	Х	1	Total Fe 1 1	0	0
2	S	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0
2	Е	1	Total Fe 1 1	0	0
2	b	1	Total Fe 1 1	0	0
2	V	1	Total Fe 1 1	0	0
2	А	1	Total Fe 1 1	0	0
2	R	1	Total Fe 1 1	0	0
2	М	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	Ι	1	Total Fe 1 1	0	0
2	Ζ	1	Total Fe 1 1	0	0
2	a	1	Total Fe 1 1	0	0
2	U	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	Q	1	Total Fe 1 1	0	0
2	d	1	Total Fe 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Н	1	Total Fe 1 1	0	0
2	С	1	Total Fe 1 1	0	0
2	Т	1	Total Fe 1 1	0	0
2	Ο	1	Total Fe 1 1	0	0
2	Υ	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	2	Total Ca 2 2	0	0
3	Q	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	К	1	Total Ca 1 1	0	0
3	b	1	Total Ca 1 1	0	0
3	Η	2	Total Ca 2 2	0	0
3	В	1	Total Ca 1 1	0	0
3	Ι	1	Total Ca 1 1	0	0
3	С	1	Total Ca 1 1	0	0
3	V	1	Total Ca 1 1	0	0
3	с	1	Total Ca 1 1	0	0
3	Z	1	Total Ca 1 1	0	0
3	Т	1	Total Ca 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Х	1	Total Ca 1 1	0	0
3	L	1	Total Ca 1 1	0	0
3	S	1	Total Ca 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	24	$\begin{array}{ccc} \text{Total} & \text{O} \\ 24 & 24 \end{array}$	0	0
4	В	33	Total O 33 33	0	0
4	С	24	Total O 24 24	0	0
4	D	31	Total O 31 31	0	0
4	Е	28	Total O 28 28	0	0
4	F	29	Total O 29 29	0	0
4	G	32	Total O 32 32	0	0
4	Н	29	Total O 29 29	0	0
4	Ι	30	Total O 30 30	0	0
4	J	22	Total O 22 22	0	0
4	К	22	$\begin{array}{ccc} \text{Total} & \text{O} \\ 22 & 22 \end{array}$	0	0
4	L	24	$\begin{array}{ccc} \text{Total} & \text{O} \\ 24 & 24 \end{array}$	0	0
4	М	18	Total O 18 18	0	0
4	Ν	14	Total O 14 14	0	0
4	О	7	Total O 7 7	0	0
4	Р	3	Total O 3 3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Q	13	Total O 13 13	0	0
4	R	12	Total O 12 12	0	0
4	S	22	$\begin{array}{ccc} \text{Total} & \text{O} \\ 22 & 22 \end{array}$	0	0
4	Т	23	Total O 23 23	0	0
4	U	16	Total O 16 16	0	0
4	V	12	Total O 12 12	0	0
4	W	23	Total O 23 23	0	0
4	Х	25	$\begin{array}{ccc} \text{Total} & \text{O} \\ 25 & 25 \end{array}$	0	0
4	Y	31	Total O 31 31	0	0
4	Z	32	$\begin{array}{cc} \text{Total} & \text{O} \\ 32 & 32 \end{array}$	0	0
4	a	14	Total O 14 14	0	0
4	b	19	Total O 19 19	0	0
4	С	10	Total O 10 10	0	0
4	d	18	Total O 18 18	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: Encapsulated Ferritin

• Molecule 1: Encapsulated Ferritin









• Molecule 1: Encapsulated Ferritin	
Chain M: 75% .	24%
MET ALA SER SER SER SER SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 1: Encapsulated Ferritin	
Chain N: 77%	23%
MET ALA ALA SER AS SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 1: Encapsulated Ferritin	
Chain O: 75% .	24%
MET ALLA SER SER SER SER SER R SER F SER C SER ALLA ALLA ALLA ALLA ALLA ALLA ALLA AL	
• Molecule 1: Encapsulated Ferritin	
Chain P: 78%	22%
MET ALA CLIM SER SER SER ASN ASN ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 1: Encapsulated Ferritin	
Chain Q: 76%	23%
MET ALIA SER SER SER ASN ASN ASS ASN ASS ALA ALA ALA ALA ALA ALA ALA ALA ALA	
• Molecule 1: Encapsulated Ferritin	
Chain R: 75% .	24%
MET ALA ALA ALA ASIN ASIN ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 1: Encapsulated Ferritin	
Chain S: 78%	22%





• Molecule 1: Encapsulated Ferritin







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	97.79Å 120.14Å 139.34Å	Depositor
a, b, c, α , β , γ	90.00° 95.20° 90.00°	Depositor
Bosolution (Å)	48.73 - 2.19	Depositor
Resolution (A)	49.43 - 2.19	EDS
$\% { m Data \ completeness}$	96.4 (48.73-2.19)	Depositor
(in resolution range)	88.3 (49.43-2.19)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.69 (at 2.18 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R R.	0.171 , 0.207	Depositor
Π, Π_{free}	0.176 , 0.210	DCC
R_{free} test set	7821 reflections $(4.95%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	28.9	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.42 , 40.8	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	43828	wwPDB-VP
Average B, all atoms $(Å^2)$	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.

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.



 $^{^1 {\}rm Intensities}$ 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: CA, FE

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	Bond lengths		Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.67	0/752	0.61	0/1024	
1	В	0.61	0/758	0.59	0/1032	
1	С	0.67	0/758	0.63	0/1032	
1	D	0.71	0/758	0.60	0/1032	
1	Е	0.72	0/758	0.62	0/1032	
1	F	0.72	1/752~(0.1%)	0.62	0/1024	
1	G	0.76	0/758	0.69	0/1032	
1	Н	0.67	0/747	0.61	0/1017	
1	Ι	0.68	0/758	0.64	1/1032~(0.1%)	
1	J	0.67	0/748	0.61	0/1018	
1	K	0.69	0/758	0.60	0/1032	
1	L	0.64	0/712	0.56	0/968	
1	М	0.59	0/742	0.54	0/1010	
1	N	0.57	0/748	0.58	0/1018	
1	0	0.50	0/742	0.51	0/1010	
1	Р	0.53	0/753	0.50	0/1025	
1	Q	0.64	1/748~(0.1%)	0.56	0/1018	
1	R	0.54	0/742	0.56	0/1010	
1	S	0.66	1/758~(0.1%)	0.58	0/1032	
1	Т	0.60	0/758	0.61	1/1032~(0.1%)	
1	U	0.58	0/748	0.55	0/1018	
1	V	0.58	0/758	0.53	0/1032	
1	W	0.64	0/752	0.59	0/1024	
1	Х	0.68	0/758	0.63	2/1032~(0.2%)	
1	Y	0.70	0/753	0.63	0/1025	
1	Ζ	0.73	0/758	0.63	0/1032	
1	a	0.63	0/758	0.56	0/1032	
1	b	0.82	2/753~(0.3%)	0.64	0/1025	
1	с	0.56	0/752	0.55	0/1024	
1	d	0.59	0/753	0.56	0/1025	
All	All	0.65	5/22551~(0.0%)	0.59	4/30699~(0.0%)	



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	38	TRP	CG-CD1	-13.04	1.18	1.36
1	b	38	TRP	CD1-NE1	7.09	1.50	1.38
1	S	38	TRP	CG-CD1	-6.56	1.27	1.36
1	Q	38	TRP	CG-CD1	-5.34	1.29	1.36
1	F	38	TRP	CG-CD1	-5.29	1.29	1.36

All (5) bond length outliers are listed below:

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Т	59	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	Х	22	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	Ι	24	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	Х	24	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	А	88/116 (76%)	88~(100%)	0	0	100	100
1	В	89/116~(77%)	88~(99%)	1 (1%)	0	100	100
1	С	89/116~(77%)	88~(99%)	1 (1%)	0	100	100
1	D	89/116~(77%)	89~(100%)	0	0	100	100
1	Е	89/116~(77%)	89~(100%)	0	0	100	100



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Mol	Chain	Analysed	alysed Favoured		Outliers	Percentiles	
1	F	88/116~(76%)	88~(100%)	0	0	100	100
1	G	89/116~(77%)	89 (100%)	0	0	100	100
1	Н	87/116~(75%)	87~(100%)	0	0	100	100
1	Ι	89/116~(77%)	88~(99%)	1 (1%)	0	100	100
1	J	87/116 (75%)	87~(100%)	0	0	100	100
1	K	89/116~(77%)	88~(99%)	1 (1%)	0	100	100
1	L	82/116 (71%)	82 (100%)	0	0	100	100
1	М	86/116 (74%)	86 (100%)	0	0	100	100
1	Ν	87/116 (75%)	87 (100%)	0	0	100	100
1	Ο	86/116 (74%)	86 (100%)	0	0	100	100
1	Р	88/116 (76%)	88 (100%)	0	0	100	100
1	Q	87/116 (75%)	87 (100%)	0	0	100	100
1	R	86/116 (74%)	86 (100%)	0	0	100	100
1	S	89/116~(77%)	88 (99%)	1 (1%)	0	100	100
1	Т	89/116~(77%)	89 (100%)	0	0	100	100
1	U	87/116 (75%)	87 (100%)	0	0	100	100
1	V	89/116~(77%)	89 (100%)	0	0	100	100
1	W	88/116 (76%)	88 (100%)	0	0	100	100
1	Х	89/116~(77%)	89 (100%)	0	0	100	100
1	Y	88/116~(76%)	88 (100%)	0	0	100	100
1	Z	89/116~(77%)	89 (100%)	0	0	100	100
1	a	89/116~(77%)	89 (100%)	0	0	100	100
1	b	88/116 (76%)	87~(99%)	1 (1%)	0	100	100
1	с	88/116~(76%)	88 (100%)	0	0	100	100
1	d	88/116 (76%)	88 (100%)	0	0	100	100
All	All	2636/3480~(76%)	2630 (100%)	6 (0%)	0	100	100

There are no Ramachandran outliers to report.

Protein sidechains (i) 5.3.2

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.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	77/99~(78%)	77 (100%)	0	100	100
1	В	78/99~(79%)	78 (100%)	0	100	100
1	С	78/99~(79%)	78 (100%)	0	100	100
1	D	78/99~(79%)	78 (100%)	0	100	100
1	Е	78/99~(79%)	77 (99%)	1 (1%)	69	81
1	F	77/99~(78%)	76 (99%)	1 (1%)	69	81
1	G	78/99~(79%)	78 (100%)	0	100	100
1	Н	77/99~(78%)	77 (100%)	0	100	100
1	Ι	78/99~(79%)	78 (100%)	0	100	100
1	J	78/99~(79%)	78 (100%)	0	100	100
1	K	78/99~(79%)	78 (100%)	0	100	100
1	L	74/99~(75%)	74 (100%)	0	100	100
1	М	77/99~(78%)	76 (99%)	1 (1%)	69	81
1	Ν	78/99~(79%)	78 (100%)	0	100	100
1	О	77/99~(78%)	76 (99%)	1 (1%)	69	81
1	Р	78/99~(79%)	78 (100%)	0	100	100
1	Q	78/99~(79%)	78 (100%)	0	100	100
1	R	77/99~(78%)	76 (99%)	1 (1%)	69	81
1	S	78/99~(79%)	78 (100%)	0	100	100
1	Т	78/99~(79%)	78 (100%)	0	100	100
1	U	78/99~(79%)	77 (99%)	1 (1%)	69	81
1	V	78/99~(79%)	78 (100%)	0	100	100
1	W	77/99~(78%)	77 (100%)	0	100	100
1	Х	78/99~(79%)	78 (100%)	0	100	100
1	Y	78/99~(79%)	78 (100%)	0	100	100
1	Z	78/99~(79%)	78 (100%)	0	100	100
1	a	78/99~(79%)	77 (99%)	1 (1%)	69	81
1	b	78/99~(79%)	78 (100%)	0	100	100
1	с	77/99~(78%)	75 (97%)	2 (3%)	46	58

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	78/99~(79%)	78~(100%)	0	100	100
All	All	2328/2970~(78%)	2319 (100%)	9~(0%)	91	96

 $5~{\rm of}~9$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	R	85	ARG
1	с	70	LEU
1	a	27	VAL
1	М	9	HIS
1	U	27	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	Р	9	HIS
1	a	9	HIS
1	Х	9	HIS
1	N	9	HIS
1	W	9	HIS

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)

Of 48 ligands modelled in this entry, 48 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 (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>2	$OWAB(Å^2)$	Q<0.9
1	А	90/116~(77%)	0.14	3 (3%) 46 44	25, 35, 60, 71	0
1	В	91/116~(78%)	0.19	4 (4%) 34 32	27, 34, 58, 70	0
1	С	91/116~(78%)	0.04	2 (2%) 62 59	28, 32, 56, 71	0
1	D	91/116~(78%)	0.12	0 100 100	25, 32, 58, 64	0
1	Е	91/116~(78%)	0.16	2 (2%) 62 59	25, 33, 55, 61	0
1	F	90/116~(77%)	0.33	3 (3%) 46 44	24, 30, 57, 67	0
1	G	91/116~(78%)	0.19	4 (4%) 34 32	25, 30, 56, 67	0
1	Н	89/116~(76%)	0.13	1 (1%) 80 79	23, 30, 50, 66	0
1	Ι	91/116~(78%)	0.05	2 (2%) 62 59	25, 32, 59, 76	0
1	J	89/116~(76%)	0.11	3 (3%) 45 43	25, 32, 52, 67	0
1	K	91/116~(78%)	0.11	2 (2%) 62 59	26, 36, 62, 69	0
1	L	84/116~(72%)	0.11	5 (5%) 21 20	27, 35, 60, 74	0
1	М	88/116~(75%)	0.33	5 (5%) 23 22	30, 39, 65, 86	0
1	Ν	89/116~(76%)	0.17	3 (3%) 45 43	32, 43, 62, 77	0
1	Ο	88/116~(75%)	0.53	6 (6%) 17 16	37, 53, 71, 78	0
1	Р	90/116~(77%)	0.46	5 (5%) 24 23	41, 51, 77, 82	0
1	Q	89/116~(76%)	0.31	2 (2%) 62 59	30, 40, 61, 76	0
1	R	88/116~(75%)	0.29	3 (3%) 45 43	34, 45, 66, 79	0
1	S	91/116~(78%)	0.36	5 (5%) 25 24	28, 38, 63, 75	0
1	Т	91/116~(78%)	0.32	3 (3%) 46 44	26, 35, 58, 73	0
1	U	89/116~(76%)	0.15	2 (2%) 62 59	32, 38, 62, 74	0
1	V	91/116~(78%)	0.09	3 (3%) 46 44	30, 38, 61, 76	0
1	W	90/116~(77%)	0.09	3 (3%) 46 44	27, 34, 57, 70	0
1	X	91/116~(78%)	0.07	2 (2%) 62 59	26, 34, 58, 70	0

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Mol	Chain	Analysed	<RSRZ $>$	$\# RSRZ {>}2$	$OWAB(A^2)$	Q<0.9
1	Y	90/116~(77%)	0.14	2 (2%) 62 59	25, 30, 54, 67	0
1	Z	91/116 (78%)	0.13	2 (2%) 62 59	25, 33, 51, 60	0
1	a	91/116~(78%)	0.43	4 (4%) 34 32	28, 43, 66, 72	0
1	b	90/116~(77%)	0.43	7 (7%) 13 11	28, 37, 75, 83	0
1	с	90/116~(77%)	0.45	5 (5%) 24 23	35, 43, 67, 79	0
1	d	90/116~(77%)	0.22	2 (2%) 62 59	30, 41, 64, 75	0
All	All	2696/3480 (77%)	0.22	95 (3%) 44 42	23, 37, 64, 86	0

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The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	с	97	ALA	5.8
1	G	96	ALA	5.2
1	F	96	ALA	4.8
1	F	97	ALA	4.8
1	М	13	GLU	4.8

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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
3	CA	J	202	1/1	0.69	0.09	72,72,72,72	0
3	CA	с	202	1/1	0.69	0.16	87,87,87,87	0
3	CA	В	202	1/1	0.74	0.07	84,84,84,84	0
3	CA	Х	202	1/1	0.76	0.11	$79,\!79,\!79,\!79$	0

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	nuea fro	m previoi	is page	Atoma	DECC	DCD	D footoma(λ^2)	$\Omega < 0.0$
	Type		Res		RSCC	R5R	\mathbf{B} -factors(\mathbf{A}^{-})	Q<0.9
<u>う</u>	CA		202		0.79	0.08	07,07,07,07	0
<u>う</u>	CA		202		0.80	0.11		0
<u>う</u>	CA		202		0.81	0.19		0
<u>う</u>	CA	V T	202		0.87	0.11		0
3	CA		202		0.88	0.12	69,69,69,69	0
3	CA	J	203		0.88	0.10		0
3	CA	b	202		0.88	0.08	77,77,77,77	0
3	CA	K	202		0.91	0.16	72,72,72,72	0
3	CA	C	202		0.93	0.08	56,56,56,56	0
3	CA	<u>'</u>]'	202	1/1	0.93	0.11	73,73,73,73	0
2	FE	W	201	1/1	0.95	0.09	30,30,30,30	0
2	FE	R	201	1/1	0.95	0.08	42,42,42,42	0
3	CA	H	203	1/1	0.95	0.09	69,69,69,69	0
2	FE	0	201	1/1	0.95	0.10	40,40,40,40	0
3	CA	H	202	1/1	0.95	0.18	66,66,66,66	0
3	CA	Q	202	1/1	0.96	0.07	70,70,70,70	0
2	FE	A	201	1/1	0.96	0.07	$26,\!26,\!26,\!26$	0
2	FE	P	201	1/1	0.96	0.12	39,39,39,39	0
3	CA	D	202	1/1	0.96	0.06	$53,\!53,\!53,\!53$	0
2	FE	U	201	1/1	0.96	0.12	$35,\!35,\!35,\!35$	0
2	FE	I	201	1/1	0.97	0.11	$25,\!25,\!25,\!25$	0
2	FE	V	201	1/1	0.97	0.06	$30,\!30,\!30,\!30,\!30$	0
2	FE	Q	201	1/1	0.97	0.09	$29,\!29,\!29,\!29$	0
2	FE	В	201	1/1	0.97	0.09	$30,\!30,\!30,\!30$	0
2	FE	L	201	1/1	0.97	0.10	$31,\!31,\!31,\!31$	0
2	FE	Н	201	1/1	0.98	0.07	$26,\!26,\!26,\!26$	0
2	FE	С	201	1/1	0.98	0.05	27,27,27,27	0
2	FE	Z	201	1/1	0.98	0.10	$25,\!25,\!25,\!25$	0
2	FE	J	201	1/1	0.98	0.05	27,27,27,27	0
2	FE	F	201	1/1	0.98	0.04	$26,\!26,\!26,\!26$	0
2	FE	d	201	1/1	0.98	0.12	33,33,33,33	0
2	FE	G	201	1/1	0.98	0.09	24,24,24,24	0
2	FE	b	201	1/1	0.98	0.10	28,28,28,28	0
2	FE	N	201	1/1	0.98	0.08	39,39,39,39	0
2	FE	с	201	1/1	0.98	0.04	36,36,36,36	0
2	FE	Т	201	1/1	0.99	0.06	25,25,25,25	0
2	FE	М	201	1/1	0.99	0.08	30,30,30,30	0
2	FE	Y	201	1/1	0.99	0.10	27,27,27,27	0
2	FE	Е	201	1/1	0.99	0.06	22,22,22,22	1
2	FE	X	201	1/1	0.99	0.05	27,27,27,27	0
2	FE	S	201	1/1	0.99	0.07	28,28.28.28	0
2	FE	a	201	1/1	0.99	0.10	36,36,36,36	0
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	FE	Κ	201	1/1	0.99	0.05	$25,\!25,\!25,\!25$	0
2	FE	D	201	1/1	0.99	0.06	24,24,24,24	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.

