



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1DVB / pdb_00001dvb
Title : RUBRERYTHRIN
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Deposited on : 2000-01-20
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
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

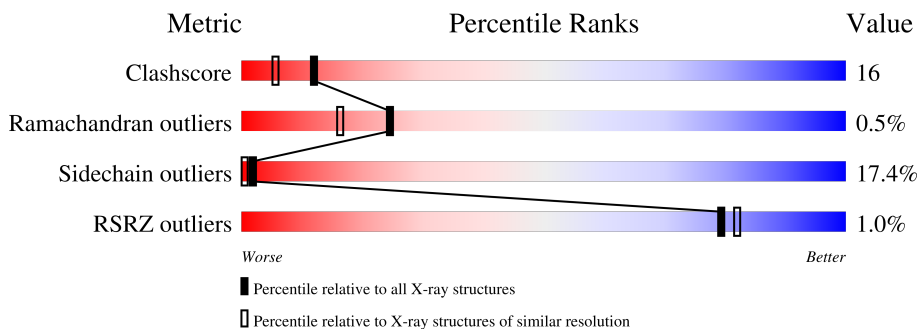
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	A	191	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1740 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 RUBRERYTHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	191	1572	983	291	292	6	0	15	0

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

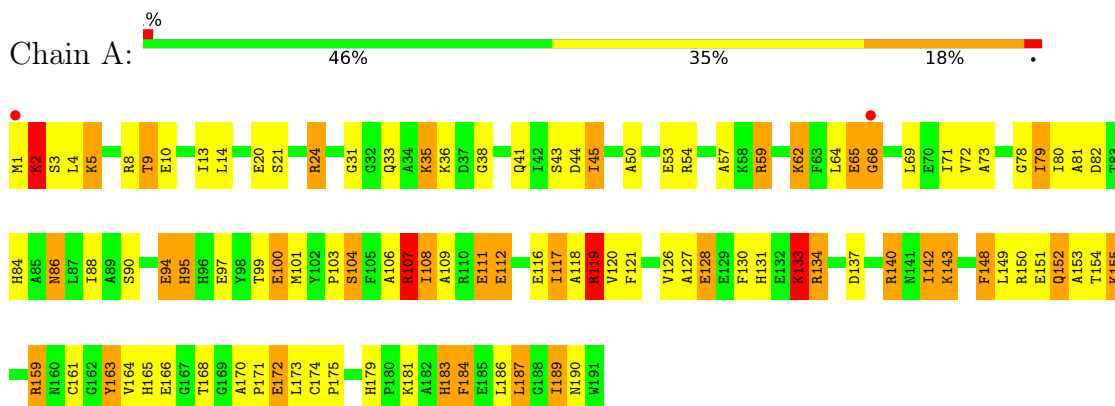
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	165	Total	O	0	0
			165	165		

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: RUBRERYTHRIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	50.63Å 81.55Å 100.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	83.0 (20.00-1.90) 93.6 (20.00-1.91)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.91Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.176 , 0.255 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtrriage
Anisotropy	0.496	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 113.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1740	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.04% 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: ZN, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.82	0/1696	2.31	99/2272 (4.4%)

There are no bond length outliers.

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ARG	CD-NE-CZ	-11.61	108.15	124.40
1	A	159	ARG	NE-CZ-NH1	-10.40	111.09	121.50
1	A	50	ALA	CA-C-O	9.54	131.61	120.92
1	A	21	SER	CA-C-O	9.49	130.61	120.55
1	A	78	GLY	N-CA-C	-9.28	99.83	111.70
1	A	107	ARG	CD-NE-CZ	9.06	137.08	124.40
1	A	137	ASP	CA-CB-CG	-8.44	104.16	112.60
1	A	134	ARG	CD-NE-CZ	-8.20	112.91	124.40
1	A	134	ARG	NE-CZ-NH2	8.19	126.57	119.20
1	A	119	ARG	CD-NE-CZ	7.92	135.49	124.40
1	A	43	SER	CA-C-O	7.80	129.01	120.82
1	A	53	GLU	CA-C-O	7.76	128.78	120.55
1	A	84	HIS	CA-CB-CG	-7.60	106.20	113.80
1	A	66	GLY	N-CA-C	7.58	122.96	112.57
1	A	189	ILE	CA-C-O	-7.33	112.71	120.48
1	A	161	CYS	CA-C-O	-7.29	110.79	119.03
1	A	133[A]	LYS	O-C-N	7.28	129.66	122.09
1	A	133[B]	LYS	O-C-N	7.28	129.66	122.09
1	A	154	THR	CA-C-N	-7.20	112.50	122.93
1	A	154	THR	C-N-CA	-7.20	112.50	122.93
1	A	131	HIS	CA-CB-CG	7.15	120.95	113.80
1	A	172[A]	GLU	CA-C-N	7.08	133.67	121.64
1	A	172[A]	GLU	C-N-CA	7.08	133.67	121.64
1	A	172[B]	GLU	CA-C-N	7.08	133.67	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172[B]	GLU	C-N-CA	7.08	133.67	121.64
1	A	90	SER	CA-C-O	6.97	127.94	120.55
1	A	159	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	A	128	GLU	CA-C-N	-6.85	110.56	120.29
1	A	128	GLU	C-N-CA	-6.85	110.56	120.29
1	A	97	GLU	N-CA-C	6.69	118.23	111.07
1	A	126	VAL	CA-C-O	6.54	128.10	121.17
1	A	165	HIS	CA-C-O	-6.48	113.37	120.24
1	A	94	GLU	OE1-CD-OE2	-6.45	107.43	122.90
1	A	121	PHE	CA-CB-CG	6.40	120.20	113.80
1	A	151	GLU	CA-C-N	-6.38	111.69	122.92
1	A	151	GLU	C-N-CA	-6.38	111.69	122.92
1	A	163	TYR	O-C-N	6.34	130.67	122.87
1	A	163	TYR	CA-C-O	-6.33	114.22	121.19
1	A	43	SER	O-C-N	-6.26	115.62	122.07
1	A	108	ILE	CB-CA-C	-6.22	103.74	112.14
1	A	127	ALA	CA-C-N	-6.21	110.34	120.72
1	A	127	ALA	C-N-CA	-6.21	110.34	120.72
1	A	2	LYS	CA-C-N	6.21	133.19	122.64
1	A	2	LYS	C-N-CA	6.21	133.19	122.64
1	A	187	LEU	CA-C-O	-6.20	113.68	120.81
1	A	82[A]	ASP	CA-CB-CG	-6.15	106.45	112.60
1	A	82[B]	ASP	CA-CB-CG	-6.15	106.45	112.60
1	A	186	LEU	CA-C-N	-6.10	112.40	120.95
1	A	186	LEU	C-N-CA	-6.10	112.40	120.95
1	A	38	GLY	CA-C-N	5.99	132.47	123.24
1	A	38	GLY	C-N-CA	5.99	132.47	123.24
1	A	164	VAL	CA-C-N	5.97	131.19	122.77
1	A	164	VAL	C-N-CA	5.97	131.19	122.77
1	A	33	GLN	O-C-N	-5.95	115.37	122.15
1	A	3[A]	SER	CA-C-O	-5.92	114.30	121.28
1	A	3[B]	SER	CA-C-O	-5.92	114.30	121.28
1	A	100	GLU	CB-CA-C	-5.88	101.53	110.83
1	A	69	LEU	CA-C-N	5.87	129.90	121.50
1	A	69	LEU	C-N-CA	5.87	129.90	121.50
1	A	21	SER	O-C-N	-5.86	115.91	122.12
1	A	50	ALA	O-C-N	-5.77	115.47	122.11
1	A	155	LYS	CA-C-N	5.77	130.68	122.72
1	A	155	LYS	C-N-CA	5.77	130.68	122.72
1	A	104	SER	CB-CA-C	-5.74	101.80	110.92
1	A	20	GLU	O-C-N	-5.72	116.06	122.12
1	A	100	GLU	N-CA-C	5.65	119.88	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ILE	N-CA-C	5.61	116.35	110.62
1	A	112	GLU	O-C-N	-5.60	115.62	122.34
1	A	2	LYS	O-C-N	5.59	130.03	122.59
1	A	101	MET	CA-C-O	5.51	126.27	120.42
1	A	57	ALA	CA-C-O	5.50	126.38	120.55
1	A	31	GLY	O-C-N	-5.50	116.91	122.19
1	A	88	ILE	CB-CA-C	-5.47	104.91	112.24
1	A	24	ARG	CA-C-O	5.47	126.75	120.90
1	A	95	HIS	CA-CB-CG	-5.41	108.39	113.80
1	A	94	GLU	N-CA-C	-5.38	105.42	111.28
1	A	184	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	179	HIS	CA-C-O	5.33	126.13	120.64
1	A	104	SER	N-CA-C	5.30	117.49	111.02
1	A	183	HIS	CA-CB-CG	-5.29	108.51	113.80
1	A	142	ILE	N-CA-CB	5.29	117.34	110.57
1	A	86	ASN	CA-C-O	5.26	126.12	120.55
1	A	134	ARG	CA-C-O	5.21	126.48	120.90
1	A	106	ALA	CA-C-N	5.19	128.00	120.79
1	A	106	ALA	C-N-CA	5.19	128.00	120.79
1	A	14	LEU	CA-C-O	5.17	125.94	120.10
1	A	174	CYS	CA-C-O	5.12	124.92	119.80
1	A	148	PHE	CA-C-N	5.11	129.86	121.58
1	A	148	PHE	C-N-CA	5.11	129.86	121.58
1	A	143	LYS	O-C-N	-5.08	116.73	122.12
1	A	82[A]	ASP	O-C-N	-5.08	116.80	122.75
1	A	82[B]	ASP	O-C-N	-5.08	116.80	122.75
1	A	62	LYS	CA-C-N	-5.08	112.25	121.14
1	A	62	LYS	C-N-CA	-5.08	112.25	121.14
1	A	111	GLU	CA-C-N	-5.07	114.54	122.65
1	A	111	GLU	C-N-CA	-5.07	114.54	122.65
1	A	130	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	78	GLY	CA-C-O	-5.04	117.27	122.26
1	A	117	ILE	N-CA-C	-5.01	105.50	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1572	0	1492	49	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	165	0	0	7	0
All	All	1740	0	1492	49	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 16.

All (49) 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:59[A]:ARG:HD2	4:A:296:HOH:O	1.83	0.76
1:A:5:LYS:HE2	1:A:10:GLU:OE2	1.87	0.75
1:A:79:ILE:HB	4:A:266:HOH:O	1.91	0.70
1:A:79:ILE:HD13	1:A:80:ILE:N	2.11	0.66
1:A:1:MET:HE3	1:A:4:LEU:HD11	1.78	0.65
1:A:119:ARG:HH11	1:A:119:ARG:HG2	1.63	0.64
1:A:65:GLU:HB2	4:A:302:HOH:O	2.02	0.60
1:A:107:ARG:HG2	4:A:336:HOH:O	2.04	0.58
1:A:153:ALA:N	1:A:168:THR:HG22	2.19	0.57
1:A:79:ILE:HD13	1:A:80:ILE:H	1.68	0.57
1:A:148:PHE:HB3	1:A:181:LYS:HD2	1.86	0.57
1:A:41:GLN:O	1:A:45:ILE:HD12	2.09	0.53
1:A:1:MET:HE3	1:A:4:LEU:CD1	2.38	0.53
1:A:152:GLN:C	1:A:168:THR:HG22	2.33	0.52
1:A:5:LYS:HE3	1:A:66:GLY:HA2	1.92	0.51
1:A:104:SER:O	1:A:107:ARG:HB3	2.12	0.50
1:A:59[A]:ARG:HG2	1:A:59[A]:ARG:HH11	1.77	0.49
1:A:163:TYR:CE2	1:A:175:PRO:HG2	2.48	0.49
1:A:170:ALA:HB1	1:A:171:PRO:HD2	1.94	0.49
1:A:94:GLU:OE1	1:A:128:GLU:HB3	2.14	0.48
1:A:5:LYS:HE3	1:A:66:GLY:CA	2.44	0.47
1:A:8[A]:ARG:HG3	1:A:112:GLU:OE2	2.15	0.46
1:A:140[B]:ARG:NH2	4:A:241:HOH:O	2.49	0.46
1:A:13:ILE:HD11	1:A:117:ILE:HD13	1.99	0.45
1:A:72:VAL:O	1:A:73:ALA:HB2	2.17	0.45
1:A:95:HIS:NE2	1:A:99:THR:HG21	2.32	0.45
1:A:150:ARG:HA	1:A:150:ARG:HD3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:O	1:A:112:GLU:HG3	2.16	0.45
1:A:108:ILE:O	1:A:112:GLU:N	2.50	0.44
1:A:172[B]:GLU:HG3	4:A:305:HOH:O	2.17	0.43
1:A:9:THR:OG1	1:A:109:ALA:HA	2.19	0.43
1:A:159:ARG:HG3	1:A:183:HIS:O	2.18	0.43
1:A:71:ILE:HD13	1:A:71:ILE:HG21	1.70	0.42
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.69	0.42
1:A:187:LEU:HD21	1:A:189:ILE:HD11	2.02	0.41
1:A:81:ALA:O	1:A:86:ASN:ND2	2.53	0.41
1:A:24:ARG:HD2	1:A:54:ARG:HB2	2.02	0.41
1:A:79:ILE:HG12	4:A:229:HOH:O	2.20	0.41
1:A:171:PRO:HG2	1:A:184:PHE:CE2	2.56	0.40
1:A:142:ILE:HD13	1:A:142:ILE:HG21	1.76	0.40
1:A:13:ILE:HD13	1:A:13:ILE:HG21	1.81	0.40
1:A:44:ASP:OD2	1:A:159:ARG:NH1	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	204/191 (107%)	197 (97%)	6 (3%)	1 (0%)	24 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LYS

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	164/149 (110%)	131 (80%)	33 (20%)	1 0

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	5	LYS
1	A	9	THR
1	A	35[A]	LYS
1	A	35[B]	LYS
1	A	36[A]	LYS
1	A	36[B]	LYS
1	A	45	ILE
1	A	59[A]	ARG
1	A	59[B]	ARG
1	A	62	LYS
1	A	65	GLU
1	A	79	ILE
1	A	100	GLU
1	A	103	PRO
1	A	107	ARG
1	A	111	GLU
1	A	116[A]	GLU
1	A	116[B]	GLU
1	A	119	ARG
1	A	133[A]	LYS
1	A	133[B]	LYS
1	A	134	ARG
1	A	140[A]	ARG
1	A	140[B]	ARG
1	A	143	LYS
1	A	149	LEU
1	A	152	GLN
1	A	155	LYS
1	A	166[A]	GLU

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Mol	Chain	Res	Type
1	A	166[B]	GLU
1	A	173	LEU
1	A	190	ASN

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

Mol	Chain	Res	Type
1	A	12	ASN
1	A	28	ASN
1	A	141	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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, 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	A	191/191 (100%)	-0.08	2 (1%) 79 82	9, 24, 48, 108	13 (6%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.5
1	A	66	GLY	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 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, 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(Å ²)	Q<0.9
2	FE	A	193	1/1	0.98	0.13	35,35,35,35	0
3	ZN	A	194	1/1	0.99	0.29	20,20,20,20	0
2	FE	A	192	1/1	1.00	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.