



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 02:31 PM UTC

PDB ID : 7V9P / pdb_00007v9p
Title : Crystal structure of the lanthipeptide zinc-metallopeptidase EryP from
saccharopolyspora erythraea in intermediate state
Authors : Zhao, C.; Zhao, N.L.; Bao, R.
Deposited on : 2021-08-26
Resolution : 1.80 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
Xtriage (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

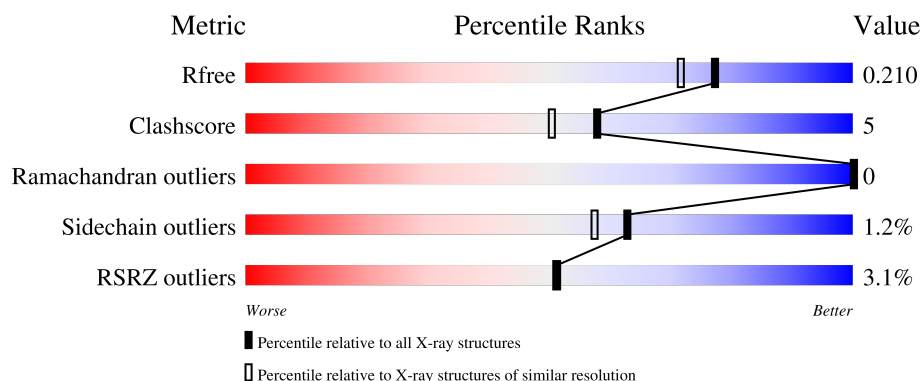
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	884	2% 83% 12% • •
1	B	884	4% 81% 13% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14378 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 Alanine aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	850	Total	C	N	O	S	0	5	0
			6689	4215	1172	1284	18			
1	B	845	Total	C	N	O	S	0	3	0
			6629	4180	1161	1271	17			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A4F9D7
A	-22	GLY	-	expression tag	UNP A4F9D7
A	-21	SER	-	expression tag	UNP A4F9D7
A	-20	SER	-	expression tag	UNP A4F9D7
A	-19	HIS	-	expression tag	UNP A4F9D7
A	-18	HIS	-	expression tag	UNP A4F9D7
A	-17	HIS	-	expression tag	UNP A4F9D7
A	-16	HIS	-	expression tag	UNP A4F9D7
A	-15	HIS	-	expression tag	UNP A4F9D7
A	-14	HIS	-	expression tag	UNP A4F9D7
A	-13	HIS	-	expression tag	UNP A4F9D7
A	-12	HIS	-	expression tag	UNP A4F9D7
A	-11	HIS	-	expression tag	UNP A4F9D7
A	-10	HIS	-	expression tag	UNP A4F9D7
A	-9	SER	-	expression tag	UNP A4F9D7
A	-8	SER	-	expression tag	UNP A4F9D7
A	-7	GLY	-	expression tag	UNP A4F9D7
A	-6	LEU	-	expression tag	UNP A4F9D7
A	-5	VAL	-	expression tag	UNP A4F9D7
A	-4	PRO	-	expression tag	UNP A4F9D7
A	-3	ARG	-	expression tag	UNP A4F9D7
A	-2	GLY	-	expression tag	UNP A4F9D7
A	-1	SER	-	expression tag	UNP A4F9D7
A	0	HIS	-	expression tag	UNP A4F9D7
A	1	VAL	-	expression tag	UNP A4F9D7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	initiating methionine	UNP A4F9D7
B	-22	GLY	-	expression tag	UNP A4F9D7
B	-21	SER	-	expression tag	UNP A4F9D7
B	-20	SER	-	expression tag	UNP A4F9D7
B	-19	HIS	-	expression tag	UNP A4F9D7
B	-18	HIS	-	expression tag	UNP A4F9D7
B	-17	HIS	-	expression tag	UNP A4F9D7
B	-16	HIS	-	expression tag	UNP A4F9D7
B	-15	HIS	-	expression tag	UNP A4F9D7
B	-14	HIS	-	expression tag	UNP A4F9D7
B	-13	HIS	-	expression tag	UNP A4F9D7
B	-12	HIS	-	expression tag	UNP A4F9D7
B	-11	HIS	-	expression tag	UNP A4F9D7
B	-10	HIS	-	expression tag	UNP A4F9D7
B	-9	SER	-	expression tag	UNP A4F9D7
B	-8	SER	-	expression tag	UNP A4F9D7
B	-7	GLY	-	expression tag	UNP A4F9D7
B	-6	LEU	-	expression tag	UNP A4F9D7
B	-5	VAL	-	expression tag	UNP A4F9D7
B	-4	PRO	-	expression tag	UNP A4F9D7
B	-3	ARG	-	expression tag	UNP A4F9D7
B	-2	GLY	-	expression tag	UNP A4F9D7
B	-1	SER	-	expression tag	UNP A4F9D7
B	0	HIS	-	expression tag	UNP A4F9D7
B	1	VAL	-	expression tag	UNP A4F9D7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	621	Total O 621 621	0	0
3	B	437	Total O 437 437	0	0

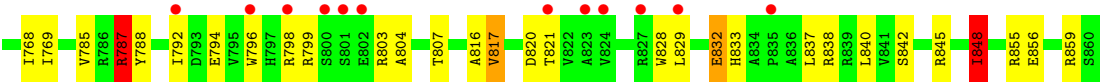
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

Chain A:

Amino Acid	Count
W359	1
V359	1
W351	1
T351	1
T548	1
P813	1
S814	1
W815	1
P835	1
A836	1
L837	1
L840	1
R855	1
S860	1
W360	1
D379	1
A382	1
V383	1
GLU	1
VAL	1
ASN	1
PHE	1
ASP	1
GLY	1
Q616	1
P632	1
L646	1
L647	1
L667	1
Q676	1
M680	1
R681	1
G686	1
P689	1
T697	1
L703	1
E717	1
A728	1
T729	1
G730	1
E735	1
Q773	1
R778	1
R786	1
L792	1
E802	1
R803	1
A804	1
Q805	1
D806	1
W360	1
D379	1
A382	1
V383	1
GLU	1
VAL	1
ASN	1
PHE	1
ASP	1
GLY	1
Q616	1
P632	1
L646	1
L647	1
L667	1
Q676	1
M680	1
R681	1
G686	1
P689	1
T697	1
L703	1
E717	1
A728	1
T729	1
G730	1
E735	1
Q773	1
R778	1
R786	1
L792	1
E802	1
R803	1
A804	1
Q805	1
D806	1
W360	1
D379	1
A382	1
V383	1
GLU	1
VAL	1
ASN	1
PHE	1
ASP	1
GLY	1
Q616	1
P632	1
L646	1
L647	1
L667	1
Q676	1
M680	1
R681	1
G686	1
P689	1
T697	1
L703	1
E717	1
A728	1
T729	1
G730	1
E735	1
Q773	1
R778	1
R786	1
L792	1
E802	1
R803	1
A804	1
Q805	1
D806	1
W360	1
D379	1
A382	1
V383	1
GLU	1
VAL	1
ASN	1
PHE	1
ASP	1
GLY	1
Q616	1
P632	1
L646	1
L647	1
L667	1
Q676	1
M680	1
R681	1
G686	1
P689	1
T697	1
L703	1
E717	1
A728	1
T729	1
G730	1
E735	1
Q773	1
R778	1
R786	1
L792	1
E802	1
R803	1
A804	1
Q805	1
D806	1
W360	1
D379	1
A382	1
V383	1
GLU	1
VAL	1
ASN	1
PHE	1
ASP	1
GLY	1
Q616	1
P632	1
L646	1
L647	1
L667	1
Q676	1
M680	1
R681	1
G686	1
P689	1
T697	1
L703	1
E717	1
A728	1
T729	1
G730	1
E735	1
Q773	1
R778	1
R786	1
L792	1
E802	1
R803	1
A804	1
Q805	1
D806	1
W360	1
D379	1
A382	1
V383	1
GLU	1
VAL	1
ASN	1
PHE	1
ASP	1
GLY	1
Q616	1
P632	1
L646	1
L647	1
L667	1
Q676	1
M680	1
R681	1
G686	1
P689	1
T697	1
L703	1
E717	1
A728	1
T729	1

Chain B:

Amino Acid	Frequency (%)
MET	4%
GLY	81%
13%	13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.42Å 66.63Å 153.74Å 90.00° 93.41° 90.00°	Depositor
Resolution (Å)	31.06 – 1.80 31.06 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (31.06-1.80) 92.8 (31.06-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.190 , 0.210 0.191 , 0.210	Depositor DCC
R_{free} test set	1989 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14378	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0383e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.90	39/6846 (0.6%)	0.78	15/9325 (0.2%)
1	B	0.98	49/6785 (0.7%)	0.82	18/9246 (0.2%)
All	All	0.94	88/13631 (0.6%)	0.80	33/18571 (0.2%)

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	ILE	C-O	-9.24	1.14	1.24
1	A	392	TYR	C-O	-8.98	1.13	1.24
1	B	393	ALA	C-O	-7.85	1.15	1.24
1	B	787	ARG	C-O	-7.75	1.15	1.24
1	A	537	VAL	C-O	-7.44	1.16	1.24
1	B	91	PRO	C-N	-7.17	1.25	1.33
1	B	754	ALA	C-O	-7.04	1.16	1.24
1	A	181	ARG	C-O	-7.03	1.15	1.24
1	B	563	ILE	C-O	-6.92	1.16	1.24
1	A	280	VAL	C-O	-6.90	1.16	1.24
1	A	786	ARG	C-O	-6.86	1.16	1.24
1	B	461	ARG	C-O	-6.84	1.16	1.24
1	A	461	ARG	C-O	-6.84	1.16	1.24
1	A	393	ALA	C-O	-6.83	1.16	1.24
1	B	785	VAL	C-O	-6.83	1.16	1.24
1	B	360	TRP	C-O	-6.82	1.16	1.24
1	B	358	LYS	C-O	-6.82	1.16	1.24
1	B	92	GLU	C-N	6.72	1.42	1.33
1	B	311	MET	C-O	-6.69	1.16	1.24
1	B	501	ASP	C-O	-6.63	1.16	1.23
1	B	598	LEU	C-O	-6.48	1.16	1.24
1	A	527	ASP	C-O	-6.47	1.16	1.24
1	A	505	THR	C-O	-6.41	1.15	1.24
1	A	164	VAL	C-O	-6.40	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	ILE	C-O	-6.37	1.17	1.24
1	A	396	ALA	C-O	-6.36	1.16	1.24
1	B	61	ASP	C-O	-6.32	1.16	1.23
1	A	409	GLU	C-O	-6.32	1.16	1.24
1	B	210	PRO	C-O	-6.21	1.16	1.23
1	B	755	VAL	C-O	-6.17	1.16	1.24
1	B	832	GLU	N-CA	-6.04	1.38	1.46
1	A	117	PHE	C-O	-5.98	1.16	1.23
1	B	363	ARG	C-O	-5.93	1.17	1.24
1	A	167	ASN	C-O	-5.93	1.17	1.24
1	B	416	LYS	C-O	-5.91	1.17	1.24
1	B	641	ARG	C-O	-5.91	1.17	1.24
1	B	746	ALA	C-O	-5.90	1.17	1.24
1	A	730	GLY	C-O	-5.88	1.16	1.23
1	B	601	SER	C-O	-5.88	1.16	1.24
1	A	467	ASP	C-O	-5.87	1.17	1.23
1	B	409	GLU	C-O	-5.84	1.17	1.24
1	A	166	SER	C-O	-5.80	1.17	1.24
1	B	277	ALA	C-O	-5.79	1.17	1.24
1	A	235	GLU	C-O	-5.76	1.17	1.24
1	B	381	GLN	C-O	-5.76	1.17	1.24
1	B	519	THR	C-O	-5.75	1.16	1.23
1	B	276	ASN	C-O	-5.69	1.17	1.23
1	B	505	THR	C-O	-5.68	1.16	1.24
1	A	728	ALA	C-O	-5.66	1.17	1.24
1	B	817	VAL	CA-C	-5.65	1.47	1.53
1	B	271	ALA	C-O	-5.57	1.16	1.24
1	B	359	SER	C-O	-5.55	1.17	1.24
1	A	165	ILE	C-O	-5.53	1.18	1.24
1	B	540	ASN	C-O	-5.50	1.15	1.23
1	B	748	GLU	C-O	-5.49	1.17	1.24
1	A	521	GLU	C-O	-5.48	1.17	1.24
1	B	396	ALA	C-O	-5.47	1.17	1.24
1	B	745	GLU	CA-C	-5.46	1.45	1.52
1	A	501	ASP	C-O	-5.42	1.17	1.23
1	A	355	SER	C-O	-5.41	1.17	1.24
1	A	360	TRP	C-O	-5.41	1.17	1.24
1	B	382	ALA	C-O	-5.39	1.17	1.24
1	A	503	PRO	C-O	-5.38	1.17	1.24
1	A	523	THR	C-O	-5.37	1.17	1.24
1	B	362	TYR	C-O	-5.37	1.17	1.24
1	A	260	LYS	C-O	-5.32	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	680	MET	C-O	-5.26	1.18	1.24
1	A	139	MET	C-O	-5.26	1.16	1.23
1	A	567	GLN	C-O	-5.22	1.18	1.24
1	A	735	GLU	C-O	-5.18	1.18	1.24
1	A	278	GLY	C-O	-5.17	1.17	1.24
1	A	561	ASP	C-O	-5.16	1.18	1.24
1	A	394	LYS	C-O	-5.14	1.18	1.24
1	A	778	ARG	C-O	-5.14	1.18	1.24
1	B	356	VAL	C-O	-5.14	1.18	1.24
1	B	848	ILE	C-O	-5.13	1.18	1.24
1	B	753	ARG	C-O	-5.13	1.18	1.24
1	B	840	LEU	C-O	-5.12	1.18	1.24
1	A	502	ASP	C-O	-5.11	1.17	1.24
1	B	751	TRP	C-O	-5.10	1.18	1.24
1	B	392	TYR	C-O	-5.08	1.17	1.24
1	B	503	PRO	C-O	-5.07	1.17	1.24
1	A	697	THR	C-O	-5.04	1.18	1.24
1	A	835	PRO	C-O	-5.03	1.17	1.24
1	B	756	HIS	C-O	-5.03	1.17	1.24
1	B	726	GLN	CA-C	-5.02	1.47	1.53
1	B	567	GLN	C-O	-5.02	1.18	1.24
1	A	281	THR	C-O	-5.00	1.18	1.23

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ASP	CA-C-N	10.67	130.90	119.05
1	A	119	ASP	C-N-CA	10.67	130.90	119.05
1	B	271	ALA	N-CA-C	10.07	125.65	113.16
1	A	35	GLY	CA-C-N	9.23	129.44	119.28
1	A	35	GLY	C-N-CA	9.23	129.44	119.28
1	A	392	TYR	N-CA-C	-7.79	102.86	111.36
1	A	561	ASP	N-CA-C	7.54	119.58	111.36
1	A	112	GLU	N-CA-C	-7.39	96.27	108.76
1	B	561	ASP	N-CA-C	7.39	119.41	111.36
1	A	697	THR	N-CA-C	6.81	118.71	111.28
1	B	756	HIS	N-CA-C	6.76	122.36	113.30
1	B	567	GLN	N-CA-C	6.73	118.41	111.14
1	A	356	VAL	N-CA-C	6.67	118.01	111.67
1	A	567	GLN	N-CA-C	6.23	117.87	111.14
1	B	562	ARG	N-CA-C	6.21	120.03	111.71
1	A	562	ARG	N-CA-C	6.20	118.35	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ASN	N-CA-C	-6.16	104.25	112.94
1	A	392	TYR	N-CA-CB	6.12	119.22	110.16
1	B	109	ASN	N-CA-C	-5.97	104.52	112.94
1	B	213	ASP	N-CA-C	5.72	119.29	111.39
1	B	755	VAL	N-CA-C	5.68	116.45	110.72
1	B	131	PHE	N-CA-C	5.56	120.34	113.50
1	B	383	VAL	CB-CA-C	-5.44	101.06	111.40
1	B	355	SER	N-CA-C	5.40	117.25	111.36
1	B	379	ASP	N-CA-C	5.35	115.61	108.38
1	B	785	VAL	CB-CA-C	-5.31	105.17	111.97
1	B	469	GLU	N-CA-C	5.28	119.59	113.20
1	B	758	ASP	N-CA-C	5.22	119.28	113.01
1	A	778	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	723	GLU	N-CA-C	-5.11	105.71	111.28
1	A	505	THR	N-CA-C	5.10	120.89	114.31
1	B	820	ASP	N-CA-C	5.08	116.82	111.28
1	B	687	THR	N-CA-C	5.05	116.79	111.28

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	6689	0	6433	53	0
1	B	6629	0	6363	65	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	621	0	0	10	0
3	B	437	0	0	6	0
All	All	14378	0	12796	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (118) 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:B:829:LEU:O	1:B:838:ARG:NH1	1.60	1.31
1:B:748:GLU:OE1	1:B:787:ARG:NH2	1.98	0.96
1:B:392:TYR:HB2	3:B:1386:HOH:O	1.69	0.92
1:A:50:ARG:HG2	1:A:96:ASP:OD1	1.70	0.91
1:A:235:GLU:HG3	3:A:1269:HOH:O	1.72	0.89
1:B:817:VAL:HA	1:B:848:ILE:CD1	2.05	0.86
1:B:748:GLU:CD	1:B:787:ARG:HH22	1.87	0.81
1:A:697:THR:HG23	3:A:1322:HOH:O	1.82	0.78
1:B:788:TYR:O	1:B:792:ILE:HG12	1.83	0.78
1:B:548:THR:HG23	3:B:1364:HOH:O	1.84	0.77
1:B:391:THR:HG22	1:B:394:LYS:H	1.51	0.74
1:A:338:LEU:HD12	3:A:1205:HOH:O	1.87	0.72
1:B:828:TRP:O	1:B:833:HIS:NE2	2.26	0.69
1:B:761:PRO:HG2	1:B:764:ILE:CG2	2.23	0.68
1:A:379:ASP:OD1	1:A:382:ALA:HB2	1.94	0.68
1:A:809:ILE:HD11	1:A:840:LEU:HD22	1.75	0.67
1:B:761:PRO:O	1:B:764:ILE:HG22	1.96	0.66
1:B:391:THR:HG23	3:B:1323:HOH:O	1.96	0.65
1:A:34:GLY:O	1:A:116:ARG:NH1	2.29	0.65
1:B:253:GLY:HA3	1:B:416:LYS:HD3	1.79	0.63
1:B:459:MET:HG2	1:B:548:THR:HB	1.82	0.62
1:B:57:GLU:OE1	1:B:89:ARG:CD	2.47	0.62
1:B:788:TYR:CE1	1:B:792:ILE:HD11	2.37	0.60
1:B:761:PRO:HG2	1:B:764:ILE:HG22	1.82	0.59
1:A:498:ILE:HD12	1:A:537:VAL:HG22	1.84	0.59
1:A:647:LEU:HD22	1:A:676:GLN:HG3	1.86	0.58
1:A:585[A]:GLU:OE2	1:A:585[A]:GLU:HA	2.03	0.58
1:B:749:LYS:O	1:B:753:ARG:HG3	2.03	0.57
1:A:133:THR:HG22	1:A:134:ALA:N	2.18	0.57
1:A:680[A]:MET:HG3	1:A:703:LEU:HD22	1.87	0.57
1:B:348[B]:ASN:ND2	1:B:348[B]:ASN:H	2.02	0.56
1:B:57:GLU:OE1	1:B:89:ARG:CG	2.54	0.56
1:A:616:GLN:NE2	3:A:1014:HOH:O	2.37	0.54
1:A:792:ILE:HG23	1:A:837:LEU:HD21	1.90	0.54
1:B:792:ILE:HG22	1:B:837:LEU:HD21	1.89	0.53
1:A:422:HIS:HE1	3:A:1279:HOH:O	1.91	0.53
1:B:794:GLU:O	1:B:798:ARG:HG3	2.08	0.53
1:B:348[B]:ASN:H	1:B:348[B]:ASN:HD22	1.57	0.53
1:A:681:ARG:NH2	1:A:717:GLU:OE1	2.35	0.52
1:A:416:LYS:HE3	1:A:420:ASP:OD2	2.10	0.52
1:A:459:MET:HG2	1:A:548:THR:HB	1.90	0.51
1:B:15:ALA:HA	1:B:148:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLU:HG3	1:B:91:PRO:HA	1.93	0.51
1:A:646:LEU:HB3	1:A:667:LEU:HG	1.93	0.51
1:A:57:GLU:HG3	1:A:91:PRO:HA	1.94	0.50
1:B:817:VAL:HA	1:B:848:ILE:HD12	1.93	0.50
1:B:698[B]:ASP:OD1	1:B:733:ARG:NH1	2.45	0.50
1:B:362:TYR:CD1	1:B:457:LEU:HD21	2.48	0.49
1:B:799:ARG:HB2	1:B:804:ALA:HB2	1.93	0.49
1:B:461:ARG:HB3	1:B:550:ARG:HB2	1.95	0.49
1:B:845:ARG:NH1	3:B:1005:HOH:O	2.34	0.49
1:A:539:VAL:HG22	3:A:1236:HOH:O	2.13	0.49
1:A:478:LEU:HD22	1:A:522:ARG:HG3	1.94	0.49
1:A:478:LEU:CD2	1:A:522:ARG:HG3	2.43	0.49
1:B:210:PRO:HA	1:B:217:GLU:HG2	1.94	0.48
1:A:50:ARG:CG	1:A:96:ASP:OD1	2.54	0.47
1:A:60:ILE:HB	1:A:90:LEU:HD11	1.97	0.47
1:B:680:MET:HE3	1:B:680:MET:HB2	1.72	0.47
1:B:816:ALA:CB	1:B:821:THR:HG21	2.45	0.47
1:B:422:HIS:HE1	3:B:1249:HOH:O	1.98	0.46
1:A:140:PHE:CE2	1:A:142:CYS:HB3	2.51	0.46
1:B:514:VAL:HG21	1:B:527:ASP:HB3	1.98	0.46
1:B:728:ALA:O	1:B:732:ARG:HG3	2.16	0.46
1:A:805:GLN:HB3	1:A:806:PRO:HD3	1.98	0.46
1:B:83:ASP:O	1:B:86:THR:HG22	2.15	0.46
1:B:647:LEU:HD22	1:B:676:GLN:HG3	1.98	0.46
1:A:802:GLU:HG3	1:A:803:ARG:N	2.32	0.45
1:A:773:GLN:NE2	3:A:1030:HOH:O	2.48	0.45
1:A:676:GLN:O	1:A:680[B]:MET:HG3	2.17	0.45
1:A:813:PRO:HA	1:A:815:TRP:CE3	2.52	0.45
1:A:686:GLY:O	1:A:689:PRO:HD3	2.17	0.45
1:A:813:PRO:HA	1:A:815:TRP:CZ3	2.51	0.45
1:B:391:THR:CG2	1:B:394:LYS:H	2.26	0.45
1:A:296:LEU:HD23	1:A:296:LEU:HA	1.67	0.45
1:B:817:VAL:HA	1:B:848:ILE:HD11	1.97	0.45
1:B:685:ASP:OD1	1:B:687:THR:HB	2.17	0.45
1:A:110:THR:HG23	1:A:112:GLU:HB2	1.99	0.44
1:B:548:THR:HG22	1:B:550:ARG:NH1	2.32	0.44
1:B:856:GLU:OE2	1:B:859:ARG:NH1	2.45	0.44
1:B:816:ALA:HB3	1:B:821:THR:HG21	2.00	0.44
1:B:769:ILE:HD13	1:B:807:THR:HA	2.00	0.44
1:A:117:PHE:CD1	1:A:117:PHE:C	2.96	0.43
1:A:527:ASP:HB2	3:A:1498:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLU:OE1	1:B:89:ARG:HD3	2.18	0.43
1:A:459:MET:HE3	1:A:459:MET:HB3	1.90	0.43
1:B:794:GLU:HB3	1:B:798:ARG:NH1	2.34	0.43
1:B:39:GLU:O	1:B:106:GLN:HA	2.18	0.43
1:B:816:ALA:O	1:B:821:THR:HG21	2.18	0.43
1:A:337:VAL:HG11	1:A:350:TRP:CE3	2.54	0.43
1:B:845:ARG:O	1:B:848:ILE:CG2	2.66	0.43
1:A:126:TYR:CZ	1:A:201:PRO:HG2	2.53	0.43
1:B:799:ARG:NH1	1:B:803:ARG:O	2.51	0.43
1:A:117:PHE:HD2	1:A:268:GLU:CD	2.27	0.42
1:B:606:ILE:HD12	1:B:606:ILE:HA	1.92	0.42
1:A:190:MET:HE2	1:A:190:MET:HB3	1.90	0.42
1:B:796:TRP:CE3	1:B:837:LEU:HD13	2.54	0.42
1:A:256:TYR:HA	1:A:257:PRO:HD3	1.81	0.42
1:B:323:ASP:HA	1:B:377:ILE:HG13	2.01	0.42
1:B:735:GLU:HG2	1:B:764:ILE:HG13	2.02	0.42
1:A:680[A]:MET:HB2	1:A:680[A]:MET:HE3	1.60	0.42
1:B:437:GLU:HG3	1:B:444:LEU:HD12	2.01	0.42
1:B:696:ASP:O	1:B:700:ARG:HG3	2.19	0.42
1:A:792:ILE:HA	1:A:792:ILE:HD12	1.75	0.42
1:B:105:CYS:HB3	3:B:1142:HOH:O	2.20	0.42
1:A:253:GLY:O	1:A:416:LYS:NZ	2.49	0.42
1:A:351:THR:HG23	1:A:573:ALA:HB2	2.02	0.42
1:A:588:LEU:HD12	3:A:1080:HOH:O	2.20	0.41
1:A:348:ASN:HB2	3:A:1481:HOH:O	2.20	0.41
1:B:735:GLU:HG3	1:B:768:ILE:HG12	2.02	0.41
1:B:735:GLU:HG3	1:B:768:ILE:CG1	2.51	0.41
1:B:160:GLN:HA	1:B:180:ARG:HG3	2.02	0.41
1:B:303:THR:O	1:B:307:GLU:HG2	2.21	0.41
1:A:632:PRO:HG3	1:A:855:ARG:NH1	2.36	0.41
1:B:632:PRO:HG3	1:B:855:ARG:NH1	2.35	0.41
1:A:498:ILE:CD1	1:A:537:VAL:HG22	2.50	0.41
1:A:559:LEU:HD23	1:A:559:LEU:C	2.46	0.40
1:B:276:ASN:HB2	1:B:279:CYS:O	2.21	0.40
1:A:222:ILE:HA	1:A:263:GLN:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	849/884 (96%)	838 (99%)	11 (1%)	0	100	100
1	B	842/884 (95%)	824 (98%)	18 (2%)	0	100	100
All	All	1691/1768 (96%)	1662 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	690/717 (96%)	684 (99%)	6 (1%)	70	67
1	B	682/717 (95%)	672 (98%)	10 (2%)	57	49
All	All	1372/1434 (96%)	1356 (99%)	16 (1%)	63	57

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	133	THR
1	A	171	GLU
1	A	522	ARG
1	A	697	THR
1	A	792	ILE
1	B	76	GLU
1	B	381	GLN

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Mol	Chain	Res	Type
1	B	391	THR
1	B	421	ARG
1	B	463	LYS
1	B	687	THR
1	B	787	ARG
1	B	832	GLU
1	B	842	SER
1	B	848	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	243	GLN
1	A	422	HIS
1	A	426	ASN
1	A	532	HIS
1	A	726	GLN
1	A	756	HIS
1	A	759	GLN
1	A	773	GLN
1	B	13	GLN
1	B	249	HIS
1	B	263	GLN
1	B	453	GLN
1	B	752	GLN
1	B	762	ASN
1	B	797	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	850/884 (96%)	0.20	18 (2%) 63 64	14, 38, 62, 79	5 (0%)
1	B	845/884 (95%)	0.36	34 (4%) 42 41	14, 42, 68, 83	3 (0%)
All	All	1695/1768 (95%)	0.28	52 (3%) 51 51	14, 40, 66, 83	8 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	ALA	4.9
1	B	176	GLY	4.2
1	A	391	THR	4.1
1	B	175	THR	4.0
1	B	38	VAL	3.8
1	B	824	VAL	3.7
1	B	111	GLY	3.6
1	B	271	ALA	3.6
1	A	36	PRO	3.4
1	A	121	VAL	3.2
1	A	34	GLY	3.1
1	A	118	ILE	3.1
1	B	392	TYR	3.1
1	A	120	PRO	2.9
1	B	823	ALA	2.9
1	B	829	LEU	2.9
1	A	270	ASN	2.8
1	A	212	ASP	2.8
1	B	360	TRP	2.7
1	B	796	TRP	2.6
1	A	383	VAL	2.6
1	B	764	ILE	2.5
1	B	802	GLU	2.5
1	B	729	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	821	THR	2.5
1	B	213	ASP	2.5
1	A	82	TYR	2.5
1	B	827	ARG	2.4
1	B	86	THR	2.4
1	B	835	PRO	2.4
1	B	792	ILE	2.4
1	B	391	THR	2.4
1	B	722	LEU	2.4
1	A	360	TRP	2.4
1	A	792	ILE	2.3
1	B	457	LEU	2.3
1	B	801	SER	2.3
1	A	124	GLY	2.3
1	A	392	TYR	2.2
1	B	719	ASP	2.2
1	B	383	VAL	2.2
1	B	761	PRO	2.2
1	B	178	GLY	2.2
1	B	798	ARG	2.1
1	A	96	ASP	2.1
1	B	800	SER	2.1
1	A	446	TRP	2.1
1	B	348[A]	ASN	2.1
1	B	214	GLY	2.0
1	B	272	GLY	2.0
1	B	759	GLN	2.0
1	A	86	THR	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.

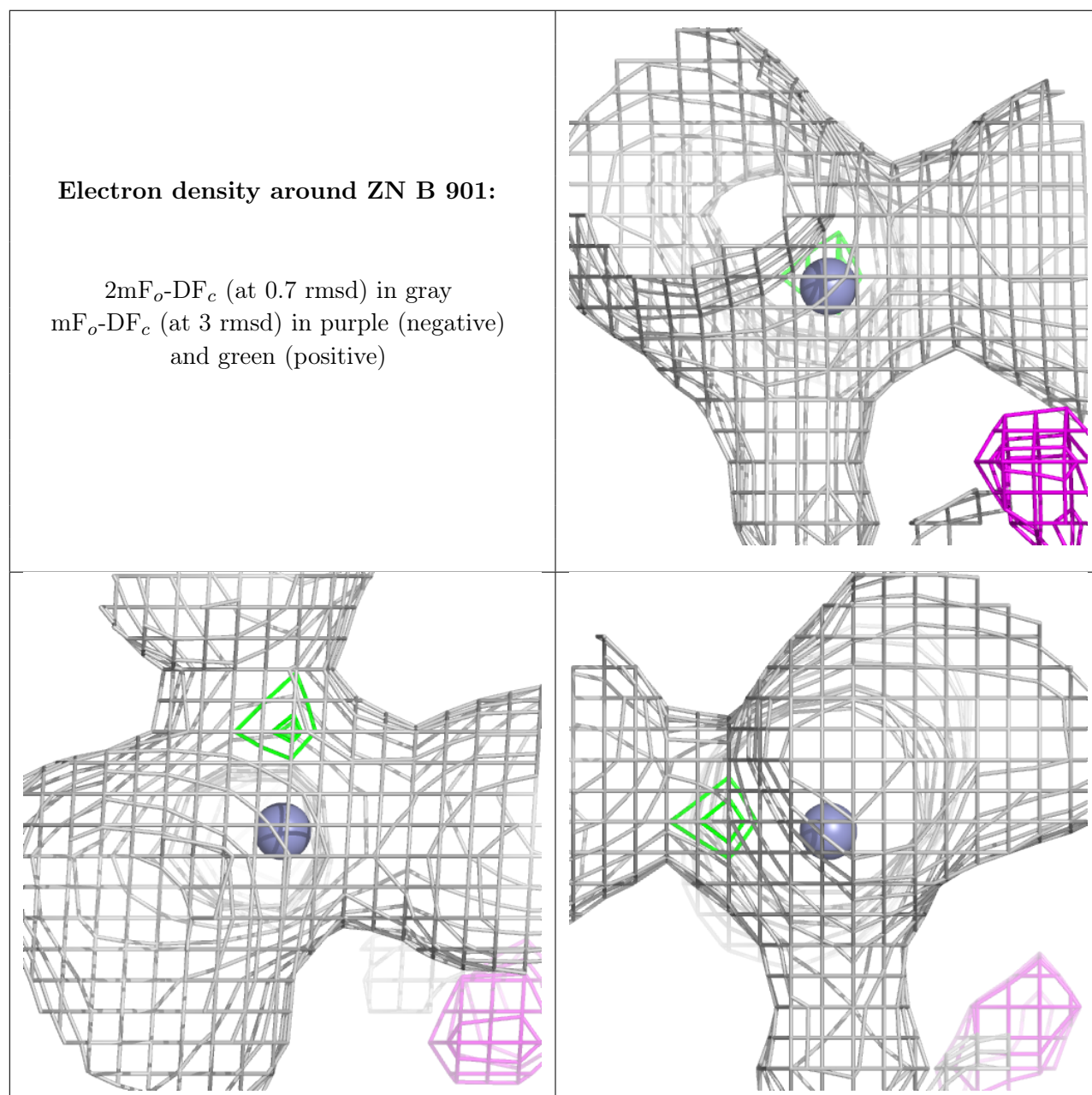
6.4 Ligands [i](#)

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.

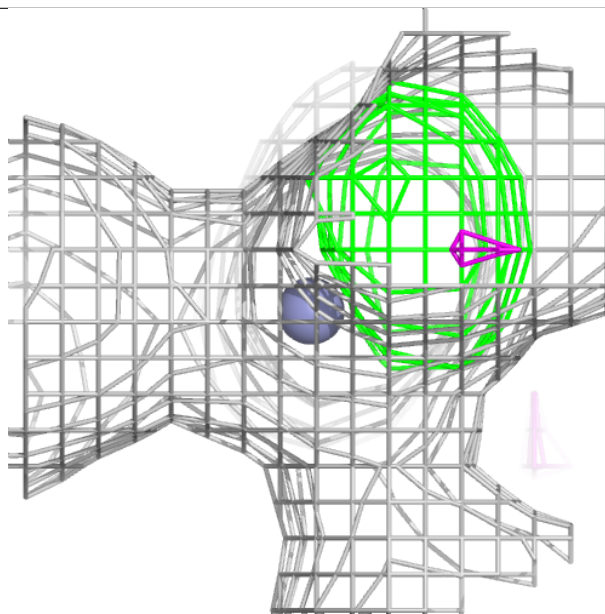
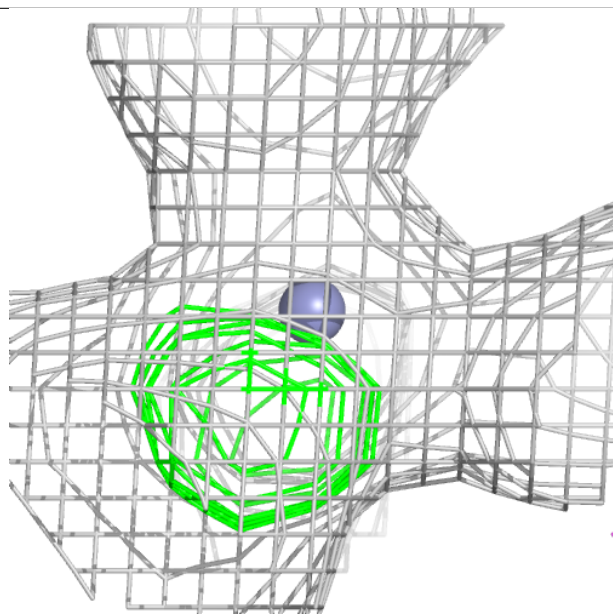
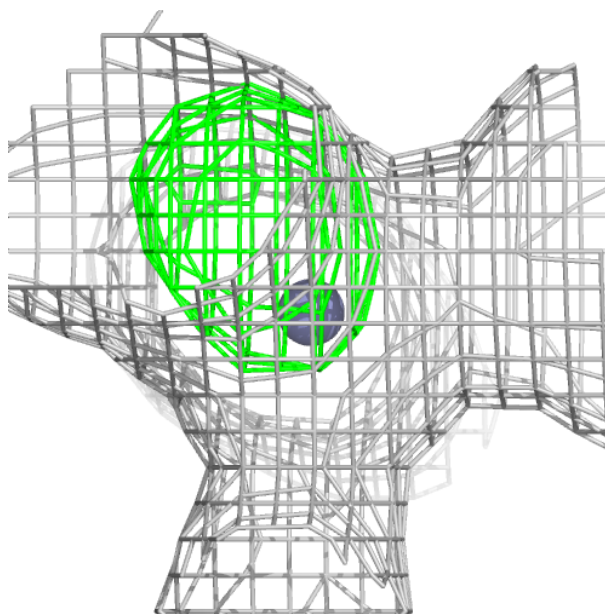
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	901	1/1	0.89	0.09	37,37,37,37	1
2	ZN	A	901	1/1	0.91	0.09	37,37,37,37	1

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 ZN A 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.