



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:39 PM UTC

PDB ID : 7V9Q / pdb_00007v9q
Title : Crystal structure of the lanthipeptide zinc-metallopeptidase EryP from
saccharopolyspora erythraea in open state
Authors : Zhao, C.; Zhao, N.L.; Bao, R.
Deposited on : 2021-08-26
Resolution : 2.67 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

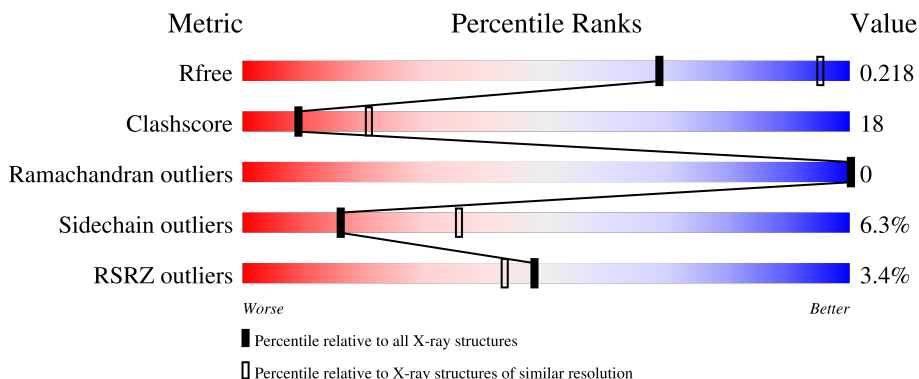
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6852 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	859	Total	C	N	O	S	0	0	0
			6720	4235	1171	1297	17			

There are 25 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

- 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 1	Zn 1	0	0

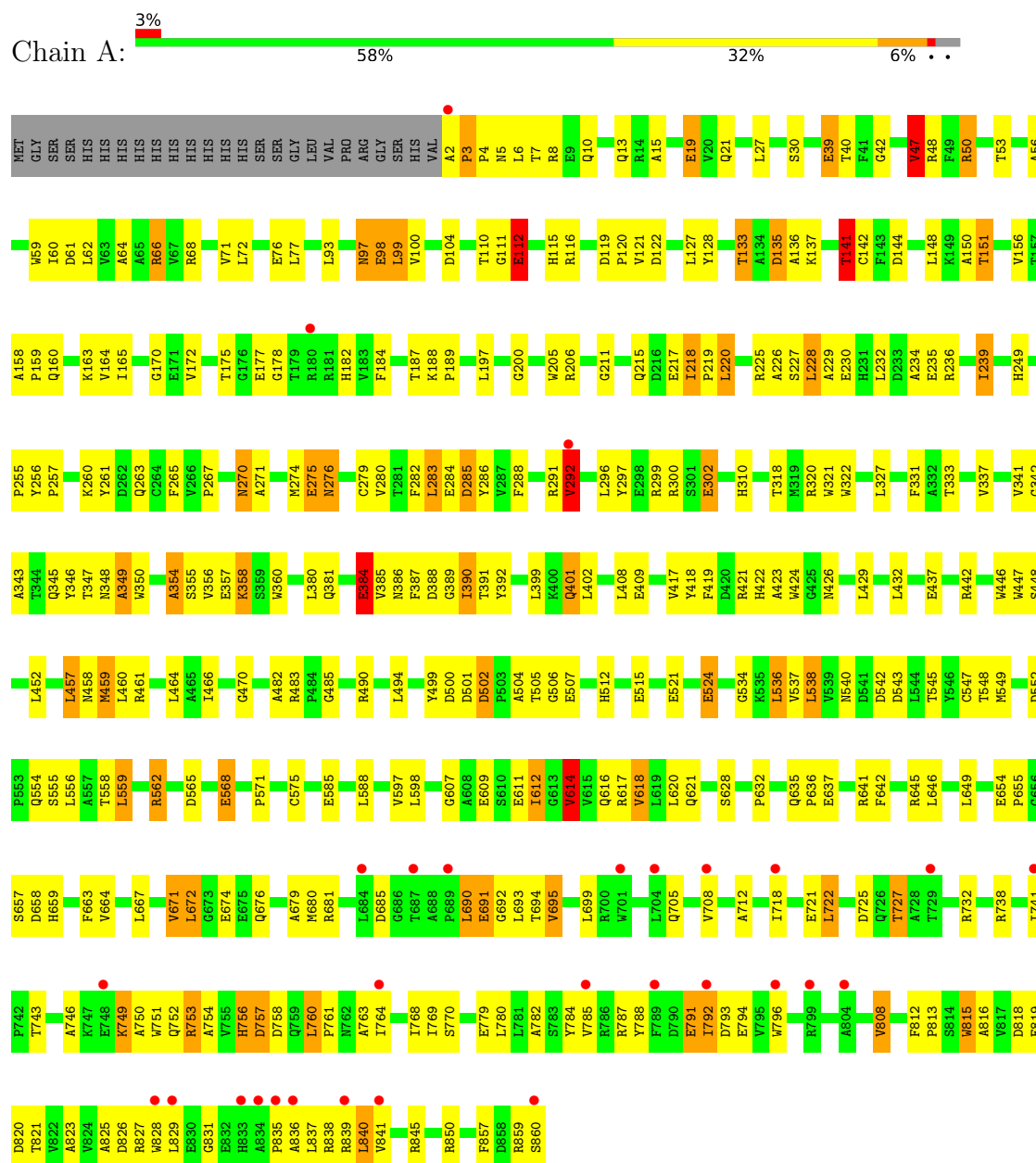
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0

3 Residue-property plots

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: Alanine aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.82Å 111.58Å 156.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.18 – 2.67 36.18 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.18-2.67) 99.5 (36.18-2.67)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.202 , 0.216 0.202 , 0.218	Depositor DCC
R_{free} test set	1995 reflections (6.61%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6852	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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

5.1 Standard geometry

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	1.35	74/6880 (1.1%)	1.16	56/9378 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	MET	C-O	-8.76	1.14	1.23
1	A	226	ALA	C-O	8.52	1.34	1.24
1	A	482	ALA	C-O	-8.46	1.13	1.23
1	A	485	GLY	C-O	-8.34	1.12	1.23
1	A	568	GLU	C-O	-8.13	1.13	1.23
1	A	230	GLU	N-CA	8.04	1.56	1.46
1	A	19	GLU	C-O	-7.97	1.15	1.23
1	A	230	GLU	CA-C	7.74	1.63	1.52
1	A	357	GLU	C-O	-7.66	1.15	1.24
1	A	280	VAL	C-O	-7.52	1.15	1.24
1	A	390	ILE	C-O	-7.00	1.16	1.24
1	A	554	GLN	C-O	-6.96	1.16	1.24
1	A	100	VAL	C-O	-6.95	1.17	1.24
1	A	483	ARG	C-O	-6.92	1.16	1.24
1	A	392	TYR	C-O	-6.80	1.16	1.24
1	A	276	ASN	C-O	-6.79	1.15	1.23
1	A	354	ALA	C-O	-6.75	1.16	1.24
1	A	391	THR	C-O	-6.68	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	ASP	C-O	-6.35	1.15	1.23
1	A	757	ASP	N-CA	-6.33	1.38	1.46
1	A	408	LEU	C-O	-6.28	1.16	1.24
1	A	48	ARG	C-O	-6.26	1.16	1.24
1	A	565	ASP	C-O	-6.24	1.15	1.24
1	A	409	GLU	C-O	-6.12	1.17	1.24
1	A	360	TRP	C-O	-6.09	1.17	1.24
1	A	385	VAL	C-O	-6.05	1.18	1.24
1	A	68	ARG	C-O	-6.02	1.17	1.24
1	A	229	ALA	CA-C	-6.02	1.44	1.52
1	A	98	GLU	C-O	-6.00	1.17	1.24
1	A	60	ILE	C-O	-5.99	1.17	1.24
1	A	614	VAL	C-O	-5.96	1.17	1.24
1	A	387	PHE	C-O	-5.93	1.17	1.24
1	A	757	ASP	CA-C	-5.86	1.45	1.52
1	A	389	GLY	C-O	-5.82	1.16	1.23
1	A	388	ASP	C-O	-5.82	1.16	1.24
1	A	524	GLU	CA-C	-5.75	1.45	1.52
1	A	59	TRP	C-O	-5.75	1.16	1.23
1	A	537	VAL	C-O	-5.68	1.18	1.24
1	A	355	SER	C-O	-5.67	1.16	1.24
1	A	356	VAL	C-O	-5.65	1.17	1.24
1	A	350	TRP	C-O	-5.60	1.17	1.24
1	A	386	ASN	C-O	-5.59	1.16	1.24
1	A	228	LEU	C-O	-5.59	1.16	1.24
1	A	597	VAL	C-O	-5.58	1.17	1.24
1	A	524	GLU	C-O	-5.54	1.17	1.23
1	A	218	ILE	C-O	-5.53	1.18	1.23
1	A	482	ALA	CA-C	-5.52	1.45	1.52
1	A	3	PRO	C-O	-5.50	1.20	1.25
1	A	618	VAL	C-O	-5.49	1.17	1.24
1	A	141	THR	C-O	-5.47	1.17	1.24
1	A	333	THR	C-O	-5.47	1.17	1.24
1	A	679	ALA	C-O	-5.46	1.17	1.24
1	A	617	ARG	C-O	-5.44	1.17	1.24
1	A	658	ASP	C-O	-5.42	1.17	1.24
1	A	50	ARG	C-O	-5.39	1.17	1.23
1	A	349	ALA	C-O	-5.37	1.17	1.24
1	A	135	ASP	C-O	-5.34	1.17	1.24
1	A	620	LEU	C-O	-5.32	1.17	1.24
1	A	384	GLU	C-O	-5.31	1.17	1.24
1	A	142	CYS	C-O	-5.30	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	ILE	CA-C	-5.28	1.48	1.52
1	A	346	TYR	C-O	-5.26	1.17	1.23
1	A	358	LYS	C-O	-5.24	1.17	1.24
1	A	136	ALA	C-O	-5.22	1.18	1.24
1	A	507	GLU	C-O	-5.21	1.17	1.23
1	A	558	THR	C-O	-5.20	1.18	1.24
1	A	506	GLY	C-O	-5.19	1.16	1.23
1	A	99	LEU	C-O	-5.19	1.18	1.24
1	A	612	ILE	C-O	-5.18	1.18	1.24
1	A	343	ALA	C-O	-5.17	1.16	1.24
1	A	13	GLN	C-O	-5.10	1.18	1.24
1	A	276	ASN	CA-C	-5.09	1.46	1.52
1	A	348	ASN	C-O	-5.04	1.17	1.24
1	A	504	ALA	C-O	-5.02	1.18	1.24

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PRO	CA-C-N	11.00	131.09	119.76
1	A	3	PRO	C-N-CA	11.00	131.09	119.76
1	A	121	VAL	N-CA-C	10.36	120.27	110.53
1	A	756	HIS	CA-C-N	-10.15	107.50	122.41
1	A	756	HIS	C-N-CA	-10.15	107.50	122.41
1	A	230	GLU	N-CA-C	9.40	123.78	111.75
1	A	112	GLU	N-CA-C	9.02	123.22	110.50
1	A	2	ALA	CA-C-N	8.81	126.09	119.66
1	A	2	ALA	C-N-CA	8.81	126.09	119.66
1	A	791	GLU	N-CA-C	8.59	120.72	111.36
1	A	226	ALA	N-CA-C	8.48	120.60	111.36
1	A	291	ARG	N-CA-C	-8.13	97.99	110.10
1	A	230	GLU	CA-C-N	8.04	135.51	122.65
1	A	230	GLU	C-N-CA	8.04	135.51	122.65
1	A	229	ALA	CA-C-N	-7.96	108.75	120.38
1	A	229	ALA	C-N-CA	-7.96	108.75	120.38
1	A	390	ILE	CB-CA-C	-7.90	101.47	112.14
1	A	225	ARG	O-C-N	-7.85	113.42	122.68
1	A	292	VAL	CB-CA-C	7.67	122.64	110.82
1	A	672	LEU	N-CA-C	7.44	121.67	110.14
1	A	271	ALA	N-CA-C	7.29	121.49	112.59
1	A	342	GLY	N-CA-C	7.00	121.74	112.77
1	A	392	TYR	N-CA-C	6.94	118.93	111.36
1	A	542	ASP	CB-CA-C	6.90	123.53	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	GLU	N-CA-C	6.86	120.21	110.68
1	A	226	ALA	CA-C-O	6.82	127.65	120.42
1	A	270	ASN	N-CA-C	6.74	118.70	111.36
1	A	408	LEU	N-CA-C	6.67	118.21	111.07
1	A	349	ALA	N-CA-C	6.66	118.54	111.28
1	A	655	PRO	N-CA-C	6.62	122.74	113.53
1	A	692	GLY	N-CA-C	-6.39	107.48	115.08
1	A	97	ASN	N-CA-C	6.17	119.60	109.85
1	A	562	ARG	N-CA-C	6.13	120.64	112.30
1	A	749	LYS	N-CA-C	-6.11	104.53	111.07
1	A	597	VAL	N-CA-C	6.06	116.84	110.72
1	A	691	GLU	N-CA-C	5.96	118.90	109.96
1	A	756	HIS	N-CA-C	5.93	119.48	112.72
1	A	628	SER	N-CA-C	5.91	121.36	114.04
1	A	815	TRP	CA-C-N	-5.69	114.94	122.85
1	A	815	TRP	C-N-CA	-5.69	114.94	122.85
1	A	502	ASP	N-CA-C	-5.58	102.61	109.65
1	A	284	GLU	N-CA-C	5.55	119.32	112.54
1	A	343	ALA	N-CA-C	5.43	121.11	113.02
1	A	211	GLY	N-CA-C	5.41	117.69	111.36
1	A	291	ARG	CA-C-N	-5.37	113.65	122.67
1	A	291	ARG	C-N-CA	-5.37	113.65	122.67
1	A	357	GLU	N-CA-C	5.37	117.21	111.36
1	A	705	GLN	N-CA-C	-5.26	105.55	111.28
1	A	39	GLU	CB-CA-C	5.21	117.82	109.27
1	A	292	VAL	CA-CB-CG1	5.18	119.21	110.40
1	A	47	VAL	N-CA-C	5.16	115.33	108.11
1	A	399	LEU	N-CA-C	-5.15	105.85	111.82
1	A	218	ILE	CB-CA-C	-5.05	105.06	110.16
1	A	358	LYS	N-CA-C	5.05	116.87	111.36
1	A	840	LEU	N-CA-C	5.04	116.58	111.14
1	A	690	LEU	N-CA-C	-5.03	101.77	109.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	THR	Mainchain

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	6720	0	6449	239	0
2	A	1	0	0	0	0
3	A	131	0	0	9	0
All	All	6852	0	6449	239	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 18.

All (239) 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:835:PRO:O	1:A:839:ARG:HG3	1.55	1.05
1:A:784:TYR:HA	1:A:787:ARG:HG2	1.44	0.97
1:A:672:LEU:HD22	1:A:676:GLN:HB3	1.42	0.96
1:A:637:GLU:OE2	1:A:641:ARG:HD2	1.74	0.88
1:A:681:ARG:NH2	1:A:712:ALA:HB1	1.93	0.84
1:A:825:ALA:O	1:A:829:LEU:HG	1.78	0.83
1:A:818:ASP:HB3	1:A:821:THR:HG22	1.60	0.82
1:A:757:ASP:HB3	1:A:760:LEU:HB2	1.60	0.81
1:A:288:PHE:CG	1:A:292:VAL:HG11	2.16	0.81
1:A:732:ARG:HH21	1:A:763:ALA:HB1	1.45	0.81
1:A:288:PHE:HB3	1:A:292:VAL:HG11	1.60	0.80
1:A:753:ARG:O	1:A:757:ASP:HB2	1.81	0.79
1:A:188:LYS:HD3	1:A:424:TRP:CH2	2.19	0.77
1:A:836:ALA:HA	1:A:839:ARG:HD2	1.66	0.77
1:A:288:PHE:CB	1:A:292:VAL:HG11	2.16	0.76
1:A:752:GLN:O	1:A:756:HIS:HB2	1.86	0.76
1:A:61:ASP:HB3	1:A:137:LYS:HE3	1.69	0.75
1:A:672:LEU:CD2	1:A:680:MET:HE1	2.17	0.75
1:A:235:GLU:O	1:A:239:ILE:HG13	1.86	0.75
1:A:816:ALA:O	1:A:821:THR:HG21	1.88	0.74
1:A:754:ALA:HB2	1:A:768:ILE:CG2	2.19	0.73
1:A:512:HIS:HE1	3:A:1023:HOH:O	1.72	0.72
1:A:732:ARG:HD3	1:A:763:ALA:HB1	1.71	0.70
1:A:791:GLU:O	1:A:794:GLU:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:TRP:CD2	1:A:837:LEU:HD13	2.26	0.70
1:A:19:GLU:OE1	1:A:50:ARG:NH1	2.25	0.69
1:A:62:LEU:HB2	1:A:141:THR:HG23	1.74	0.69
1:A:609:GLU:HG2	1:A:614:VAL:HG22	1.73	0.69
1:A:285:ASP:OD1	1:A:285:ASP:N	2.25	0.69
1:A:72:LEU:HB3	1:A:77:LEU:HD21	1.75	0.68
1:A:27:LEU:HA	1:A:42:GLY:O	1.92	0.68
1:A:749:LYS:O	1:A:753:ARG:HG3	1.93	0.68
1:A:667:LEU:HD22	1:A:680:MET:HE2	1.75	0.68
1:A:828:TRP:CE3	1:A:829:LEU:HD23	2.29	0.68
1:A:690:LEU:HD23	1:A:693:LEU:HB2	1.76	0.68
1:A:828:TRP:HE3	1:A:829:LEU:HD23	1.57	0.68
1:A:172:VAL:HG22	1:A:182:HIS:CD2	2.29	0.68
1:A:792:ILE:HD11	1:A:808:VAL:HB	1.76	0.67
1:A:384:GLU:O	1:A:384:GLU:HG2	1.92	0.67
1:A:286:TYR:CD1	1:A:300:ARG:HG3	2.31	0.66
1:A:646:LEU:HB3	1:A:667:LEU:HG	1.79	0.65
1:A:236:ARG:HA	1:A:239:ILE:HD12	1.78	0.65
1:A:458:ASN:OD1	1:A:490:ARG:HG3	1.97	0.64
1:A:612:ILE:O	1:A:616:GLN:HG3	1.97	0.64
1:A:754:ALA:HB2	1:A:768:ILE:HG21	1.79	0.64
1:A:727:THR:HG22	3:A:1093:HOH:O	1.97	0.64
1:A:119:ASP:HB3	1:A:122:ASP:OD1	1.98	0.64
1:A:796:TRP:CE3	1:A:837:LEU:CD1	2.81	0.63
1:A:826:ASP:HA	1:A:829:LEU:HD12	1.80	0.62
1:A:784:TYR:HA	1:A:787:ARG:CG	2.27	0.62
1:A:540:ASN:HD21	1:A:545:THR:H	1.46	0.62
1:A:151:THR:HB	1:A:187:THR:O	2.00	0.61
1:A:857:PHE:O	1:A:860:SER:HB3	2.00	0.61
1:A:421:ARG:HG2	1:A:422:HIS:CE1	2.35	0.61
1:A:828:TRP:HZ2	1:A:837:LEU:HD23	1.66	0.61
1:A:727:THR:CG2	3:A:1093:HOH:O	2.48	0.61
1:A:419:PHE:O	1:A:423:ALA:HB2	2.01	0.61
1:A:654:GLU:HB2	1:A:657:SER:HB3	1.83	0.61
1:A:260:LYS:HD2	1:A:260:LYS:C	2.26	0.60
1:A:56:ALA:O	1:A:93:LEU:HD12	2.02	0.60
1:A:796:TRP:CG	1:A:837:LEU:HD13	2.36	0.60
1:A:757:ASP:OD2	1:A:760:LEU:HD22	2.01	0.60
1:A:836:ALA:HA	1:A:839:ARG:CD	2.32	0.60
1:A:218:ILE:HG22	1:A:220:LEU:HD23	1.83	0.60
1:A:708:VAL:HG11	1:A:718:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:GLU:HB2	1:A:614:VAL:HG13	1.82	0.59
1:A:672:LEU:HD22	1:A:680:MET:HE1	1.84	0.59
1:A:144:ASP:HB3	3:A:1003:HOH:O	2.02	0.59
1:A:215:GLN:HG3	1:A:255:PRO:HB3	1.84	0.59
1:A:691:GLU:O	1:A:691:GLU:HG2	2.02	0.59
1:A:754:ALA:HB2	1:A:768:ILE:HG22	1.84	0.59
1:A:837:LEU:O	1:A:841:VAL:HG23	2.03	0.59
1:A:828:TRP:CZ2	1:A:837:LEU:HD23	2.37	0.59
1:A:672:LEU:HD22	1:A:680:MET:CE	2.32	0.59
1:A:757:ASP:CB	1:A:760:LEU:HB2	2.29	0.59
1:A:751:TRP:HH2	1:A:788:TYR:HB2	1.68	0.58
1:A:559:LEU:HD11	1:A:575:CYS:HB3	1.84	0.58
1:A:8:ARG:HD2	3:A:1075:HOH:O	2.04	0.57
1:A:172:VAL:CG2	1:A:182:HIS:CD2	2.86	0.57
1:A:672:LEU:HD22	1:A:676:GLN:CB	2.25	0.57
1:A:494:LEU:C	1:A:494:LEU:HD12	2.30	0.57
1:A:585:GLU:OE2	1:A:850:ARG:NH1	2.36	0.57
1:A:327:LEU:HD22	1:A:429:LEU:HD13	1.86	0.57
1:A:111:GLY:HA3	1:A:270:ASN:OD1	2.06	0.55
1:A:15:ALA:HA	1:A:148:LEU:HD21	1.88	0.55
1:A:30:SER:HA	1:A:159:PRO:HD3	1.87	0.55
1:A:61:ASP:CB	1:A:137:LYS:HE3	2.35	0.55
1:A:133:THR:HG23	1:A:322:TRP:CE2	2.42	0.55
1:A:331:PHE:CD1	1:A:331:PHE:C	2.85	0.54
1:A:188:LYS:CD	1:A:424:TRP:CH2	2.88	0.54
1:A:672:LEU:CD1	1:A:680:MET:HE1	2.38	0.54
1:A:288:PHE:HB3	1:A:292:VAL:CG1	2.33	0.54
1:A:275:GLU:O	1:A:275:GLU:HG2	2.07	0.54
1:A:236:ARG:NH1	1:A:297:TYR:CG	2.76	0.53
1:A:672:LEU:CD2	1:A:676:GLN:HB3	2.27	0.53
1:A:524:GLU:HG3	3:A:1090:HOH:O	2.09	0.53
1:A:165:ILE:HD12	1:A:165:ILE:N	2.23	0.53
1:A:276:ASN:HB2	1:A:279:CYS:O	2.08	0.53
1:A:743:THR:HG23	1:A:746:ALA:H	1.73	0.52
1:A:664:VAL:HG21	1:A:693:LEU:HD22	1.92	0.52
1:A:722:LEU:HD12	1:A:738:ARG:HH22	1.74	0.52
1:A:788:TYR:OH	1:A:808:VAL:HG23	2.10	0.52
1:A:645:ARG:HG3	1:A:649:LEU:HD12	1.90	0.52
1:A:156:VAL:HG21	1:A:197:LEU:HD21	1.92	0.52
1:A:646:LEU:CB	1:A:667:LEU:HG	2.39	0.52
1:A:769:ILE:O	1:A:770:SER:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ALA:HB1	1:A:104:ASP:O	2.09	0.51
1:A:722:LEU:HD12	1:A:738:ARG:NH2	2.25	0.51
1:A:708:VAL:HG21	1:A:718:ILE:HG12	1.92	0.51
1:A:760:LEU:HG	1:A:761:PRO:HD2	1.92	0.51
1:A:672:LEU:HD21	1:A:680:MET:HE1	1.92	0.51
1:A:749:LYS:C	1:A:753:ARG:HG3	2.35	0.51
1:A:21:GLN:NE2	1:A:50:ARG:HG3	2.26	0.51
1:A:607:GLY:CA	1:A:649:LEU:HD21	2.40	0.51
1:A:341:VAL:HG23	1:A:349:ALA:HB3	1.94	0.50
1:A:228:LEU:N	1:A:228:LEU:HD23	2.25	0.50
1:A:341:VAL:CG2	1:A:349:ALA:HB3	2.41	0.50
1:A:446:TRP:H	1:A:446:TRP:CD1	2.30	0.50
1:A:466:ILE:HD12	1:A:470:GLY:HA2	1.93	0.50
1:A:236:ARG:NH1	1:A:297:TYR:CD1	2.80	0.50
1:A:215:GLN:OE1	1:A:249:HIS:HB3	2.13	0.49
1:A:732:ARG:HH21	1:A:763:ALA:CB	2.21	0.49
1:A:659:HIS:O	1:A:663:PHE:CD2	2.65	0.49
1:A:681:ARG:NH2	1:A:712:ALA:CB	2.71	0.49
1:A:823:ALA:O	1:A:827:ARG:HG3	2.13	0.49
1:A:71:VAL:HG22	1:A:76:GLU:HG3	1.95	0.48
1:A:21:GLN:HE22	1:A:50:ARG:HG3	1.79	0.48
1:A:205:TRP:O	1:A:206:ARG:HD2	2.13	0.48
1:A:464:LEU:HD12	1:A:464:LEU:C	2.38	0.48
1:A:757:ASP:CG	1:A:760:LEU:HB2	2.37	0.48
1:A:812:PHE:CD1	1:A:813:PRO:HD2	2.49	0.48
1:A:112:GLU:HB3	1:A:135:ASP:OD2	2.13	0.48
1:A:750:ALA:O	1:A:751:TRP:C	2.55	0.48
1:A:499:TYR:HB2	1:A:536:LEU:HB3	1.96	0.48
1:A:695:VAL:HG23	1:A:695:VAL:O	2.12	0.48
1:A:796:TRP:CE3	1:A:837:LEU:HD12	2.49	0.48
1:A:318:THR:O	1:A:426:ASN:HA	2.13	0.47
1:A:607:GLY:HA3	1:A:649:LEU:HD21	1.96	0.47
1:A:796:TRP:CD2	1:A:837:LEU:CD1	2.97	0.47
1:A:738:ARG:O	1:A:741:ILE:HG13	2.15	0.47
1:A:556:LEU:HD21	1:A:588:LEU:HD13	1.97	0.47
1:A:815:TRP:HB3	3:A:1041:HOH:O	2.14	0.47
1:A:275:GLU:HG3	1:A:310:HIS:HB3	1.96	0.47
1:A:819:GLU:CD	1:A:819:GLU:H	2.23	0.47
1:A:93:LEU:HD23	1:A:97:ASN:ND2	2.30	0.47
1:A:133:THR:CG2	1:A:380:LEU:HD22	2.45	0.46
1:A:607:GLY:HA2	1:A:649:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:THR:HG22	1:A:53:THR:O	2.15	0.46
1:A:788:TYR:O	1:A:792:ILE:HB	2.16	0.46
1:A:119:ASP:OD1	1:A:120:PRO:HD2	2.16	0.46
1:A:552:ASP:OD1	1:A:555:SER:OG	2.27	0.46
1:A:502:ASP:OD2	1:A:505:THR:OG1	2.26	0.46
1:A:808:VAL:HG22	1:A:840:LEU:HD13	1.98	0.45
1:A:421:ARG:HG2	1:A:422:HIS:ND1	2.31	0.45
1:A:459:MET:HE1	1:A:461:ARG:HB2	1.98	0.45
1:A:540:ASN:ND2	1:A:545:THR:H	2.14	0.45
1:A:792:ILE:CG2	1:A:793:ASP:N	2.78	0.45
1:A:825:ALA:CB	1:A:845:ARG:HD2	2.47	0.45
1:A:110:THR:O	1:A:115:HIS:ND1	2.40	0.45
1:A:150:ALA:O	1:A:189:PRO:HA	2.16	0.45
1:A:158:ALA:HB3	1:A:182:HIS:CE1	2.51	0.45
1:A:568:GLU:HB2	1:A:571:PRO:HG2	1.98	0.45
1:A:664:VAL:HG11	1:A:699:LEU:HD11	1.98	0.45
1:A:796:TRP:CE3	1:A:837:LEU:HD13	2.49	0.45
1:A:760:LEU:HD12	1:A:760:LEU:HA	1.76	0.45
1:A:632:PRO:O	1:A:636:PRO:HD3	2.17	0.44
1:A:796:TRP:HZ2	1:A:836:ALA:HB3	1.82	0.44
1:A:232:LEU:HD23	1:A:234:ALA:HB2	2.00	0.44
1:A:598:LEU:HD21	1:A:642:PHE:HD1	1.83	0.44
1:A:671:VAL:O	1:A:671:VAL:HG12	2.16	0.44
1:A:128:TYR:HE2	1:A:267:PRO:O	2.01	0.44
1:A:3:PRO:CB	1:A:4:PRO:HD2	2.47	0.44
1:A:8:ARG:HD3	1:A:321:TRP:CD1	2.53	0.44
1:A:792:ILE:HG23	1:A:793:ASP:N	2.33	0.44
1:A:464:LEU:HD12	1:A:464:LEU:O	2.17	0.44
1:A:6:LEU:HD12	1:A:10:GLN:OE1	2.17	0.43
1:A:164:VAL:CG1	1:A:197:LEU:HD11	2.47	0.43
1:A:219:PRO:O	1:A:260:LYS:HB2	2.18	0.43
1:A:538:LEU:HD23	1:A:538:LEU:HA	1.80	0.43
1:A:618:VAL:HA	1:A:621:GLN:HG2	2.01	0.43
1:A:112:GLU:HB3	1:A:135:ASP:CG	2.44	0.43
1:A:796:TRP:CZ2	1:A:836:ALA:HB3	2.53	0.43
1:A:116:ARG:HG3	1:A:127:LEU:CD2	2.48	0.43
1:A:128:TYR:CD1	1:A:128:TYR:C	2.96	0.43
1:A:390:ILE:HG21	1:A:390:ILE:HD13	1.70	0.43
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.84	0.43
1:A:500:ASP:OD2	1:A:534:GLY:HA2	2.19	0.43
1:A:859:ARG:O	1:A:860:SER:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD23	1:A:283:LEU:O	2.19	0.43
1:A:437:GLU:HG2	1:A:442:ARG:O	2.18	0.43
1:A:459:MET:HB3	1:A:459:MET:HE2	1.47	0.43
1:A:585:GLU:CD	1:A:850:ARG:HH12	2.24	0.42
1:A:607:GLY:HA2	1:A:649:LEU:HD21	2.01	0.42
1:A:66:ARG:O	1:A:66:ARG:HG3	2.12	0.42
1:A:664:VAL:HG21	1:A:693:LEU:CD2	2.48	0.42
1:A:635:GLN:N	1:A:636:PRO:CD	2.82	0.42
1:A:47:VAL:HG13	1:A:99:LEU:HB3	2.00	0.42
1:A:170:GLY:HA2	1:A:184:PHE:HA	2.01	0.42
1:A:402:LEU:HB2	1:A:447:TRP:CZ2	2.54	0.42
1:A:7:THR:OG1	1:A:10:GLN:HG3	2.19	0.42
1:A:457:LEU:N	1:A:457:LEU:HD12	2.34	0.42
1:A:782:ALA:O	1:A:785:VAL:HG23	2.19	0.42
1:A:837:LEU:HD12	1:A:837:LEU:HA	1.73	0.42
1:A:197:LEU:HA	1:A:197:LEU:HD12	1.60	0.42
1:A:302:GLU:OE1	3:A:1001:HOH:O	2.21	0.42
1:A:681:ARG:HH21	1:A:712:ALA:HB1	1.75	0.42
1:A:693:LEU:HD11	1:A:699:LEU:CD2	2.50	0.42
1:A:831:GLY:O	1:A:838:ARG:NH1	2.53	0.42
1:A:536:LEU:HD21	1:A:559:LEU:HD23	2.01	0.42
1:A:160:GLN:HG2	1:A:178:GLY:O	2.19	0.42
1:A:175:THR:O	1:A:177:GLU:HG3	2.20	0.42
1:A:236:ARG:NH2	1:A:345:GLN:HE22	2.18	0.41
1:A:265:PHE:CD1	1:A:282:PHE:HB2	2.55	0.41
1:A:818:ASP:CG	1:A:820:ASP:HB2	2.45	0.41
1:A:39:GLU:HG3	1:A:40:THR:HG23	2.02	0.41
1:A:708:VAL:CG1	1:A:741:ILE:HG12	2.50	0.41
1:A:760:LEU:HG	1:A:761:PRO:CD	2.50	0.41
1:A:261:TYR:HE2	1:A:263:GLN:OE1	2.02	0.41
1:A:512:HIS:CE1	3:A:1023:HOH:O	2.58	0.41
1:A:721:GLU:O	1:A:721:GLU:HG3	2.20	0.41
1:A:460:LEU:HD12	1:A:547:CYS:SG	2.60	0.41
1:A:296:LEU:N	1:A:296:LEU:HD23	2.33	0.41
1:A:175:THR:HG22	1:A:177:GLU:CD	2.46	0.41
1:A:337:VAL:HG13	1:A:349:ALA:HB1	2.03	0.41
1:A:354:ALA:HA	1:A:358:LYS:HB2	2.03	0.41
1:A:446:TRP:CE3	1:A:447:TRP:HA	2.55	0.41
1:A:5:ASN:CG	1:A:381:GLN:HG3	2.46	0.41
1:A:116:ARG:HG3	1:A:127:LEU:HD21	2.01	0.41
1:A:401:GLN:HA	1:A:401:GLN:HE21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:PRO:HD2	1:A:764:ILE:HB	2.02	0.40
1:A:664:VAL:CG1	1:A:699:LEU:HD11	2.51	0.40
1:A:163:LYS:N	1:A:200:GLY:O	2.51	0.40
1:A:215:GLN:HG3	1:A:255:PRO:CB	2.50	0.40
1:A:256:TYR:HA	1:A:257:PRO:HD3	1.91	0.40
1:A:418:TYR:CE2	1:A:432:LEU:HB2	2.55	0.40
1:A:501:ASP:OD1	1:A:562:ARG:NH1	2.48	0.40
1:A:695:VAL:O	1:A:695:VAL:CG2	2.69	0.40
1:A:417:VAL:O	1:A:421:ARG:HB3	2.22	0.40
1:A:448:SER:CB	1:A:452:LEU:HD12	2.52	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	857/884 (97%)	840 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	693/717 (97%)	649 (94%)	44 (6%)	16	35

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	66	ARG
1	A	98	GLU
1	A	112	GLU
1	A	133	THR
1	A	141	THR
1	A	151	THR
1	A	217	GLU
1	A	220	LEU
1	A	227	SER
1	A	239	ILE
1	A	283	LEU
1	A	285	ASP
1	A	292	VAL
1	A	299	ARG
1	A	302	GLU
1	A	320	ARG
1	A	384	GLU
1	A	401	GLN
1	A	457	LEU
1	A	459	MET
1	A	515	GLU
1	A	521	GLU
1	A	536	LEU
1	A	538	LEU
1	A	548	THR
1	A	549	MET
1	A	559	LEU
1	A	614	VAL
1	A	671	VAL
1	A	674	GLU
1	A	685	ASP
1	A	694	THR
1	A	695	VAL
1	A	722	LEU
1	A	725	ASP
1	A	727	THR
1	A	753	ARG
1	A	758	ASP
1	A	760	LEU
1	A	779	GLU
1	A	780	LEU

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Mol	Chain	Res	Type
1	A	792	ILE
1	A	808	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	182	HIS
1	A	270	ASN
1	A	310	HIS
1	A	345	GLN
1	A	366	GLN
1	A	512	HIS
1	A	540	ASN
1	A	554	GLN
1	A	616	GLN
1	A	660	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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	859/884 (97%)	0.15	29 (3%)	48 43	20, 45, 102, 124	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	764	ILE	3.7
1	A	704	LEU	3.5
1	A	835	PRO	3.4
1	A	718	ILE	3.3
1	A	836	ALA	3.0
1	A	799	ARG	3.0
1	A	708	VAL	2.9
1	A	829	LEU	2.8
1	A	789	PHE	2.8
1	A	792	ILE	2.7
1	A	785	VAL	2.6
1	A	804	ALA	2.6
1	A	701	TRP	2.4
1	A	748	GLU	2.4
1	A	741	ILE	2.4
1	A	828	TRP	2.3
1	A	729	THR	2.3
1	A	292	VAL	2.2
1	A	834	ALA	2.2
1	A	860	SER	2.2
1	A	841	VAL	2.2
1	A	833	HIS	2.2
1	A	689	PRO	2.2
1	A	839	ARG	2.1
1	A	180	ARG	2.1
1	A	687	THR	2.1
1	A	684	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	2.1
1	A	796	TRP	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](#)

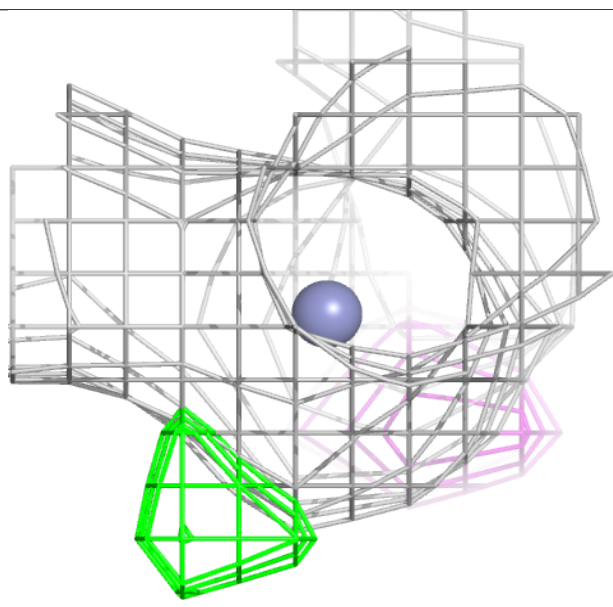
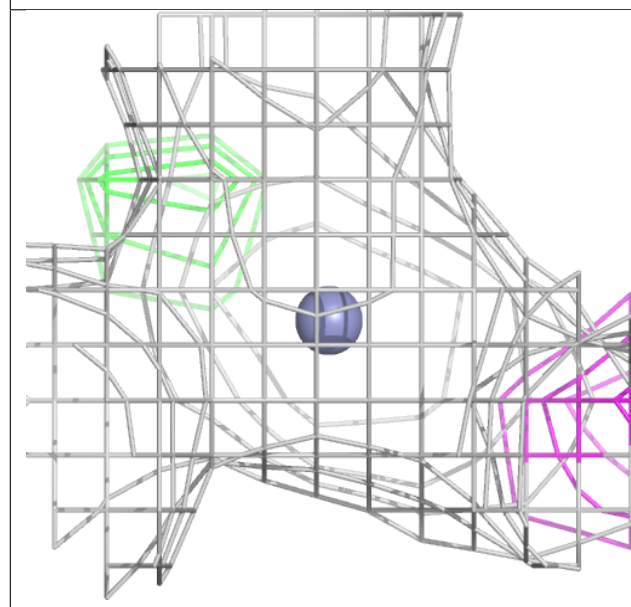
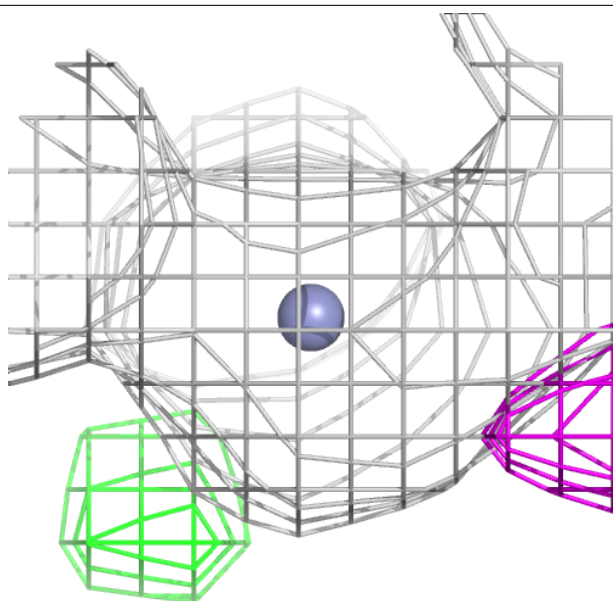
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	901	1/1	0.91	0.08	32,32,32,32	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.