



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:25 PM UTC

PDB ID : 2XR1 / pdb_00002xr1
Title : DIMERIC ARCHAEAL CLEAVAGE AND POLYADENYLATION SPECIFICITY FACTOR WITH N-TERMINAL KH DOMAINS (KH-CPSF) FROM METHANOSARCINA MAZEI
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Deposited on : 2010-09-08
Resolution : 2.59 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

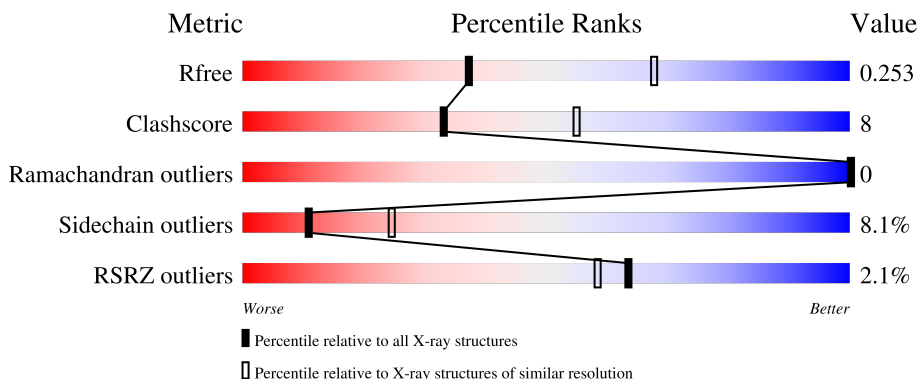
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

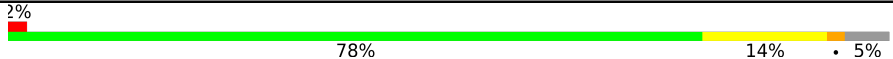
The reported resolution of this entry is 2.59 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	640	
1	B	640	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9391 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 CLEAVAGE AND POLYADENYLATION SPECIFICITY FACTOR 100 KD SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	1	0
			4640	2964	791	864	21			
1	B	611	Total	C	N	O	S	0	1	0
			4705	3008	797	875	25			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8PZ03
A	-1	SER	-	expression tag	UNP Q8PZ03
A	0	HIS	-	expression tag	UNP Q8PZ03
B	-2	GLY	-	expression tag	UNP Q8PZ03
B	-1	SER	-	expression tag	UNP Q8PZ03
B	0	HIS	-	expression tag	UNP Q8PZ03

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

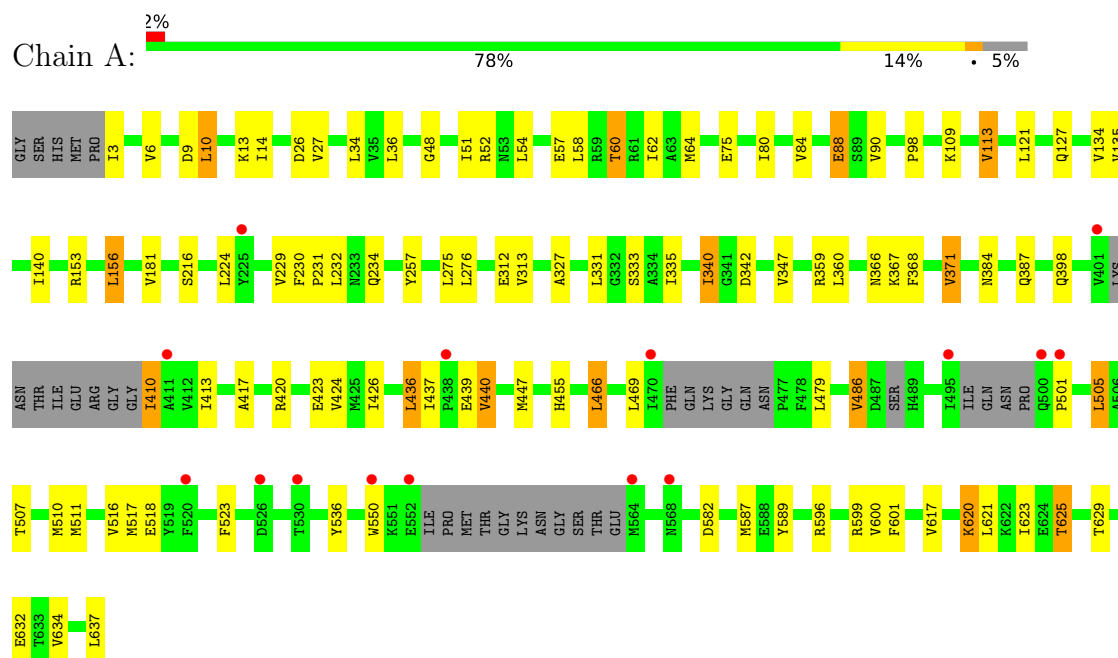
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	26	Total	O	0	0
			26	26		

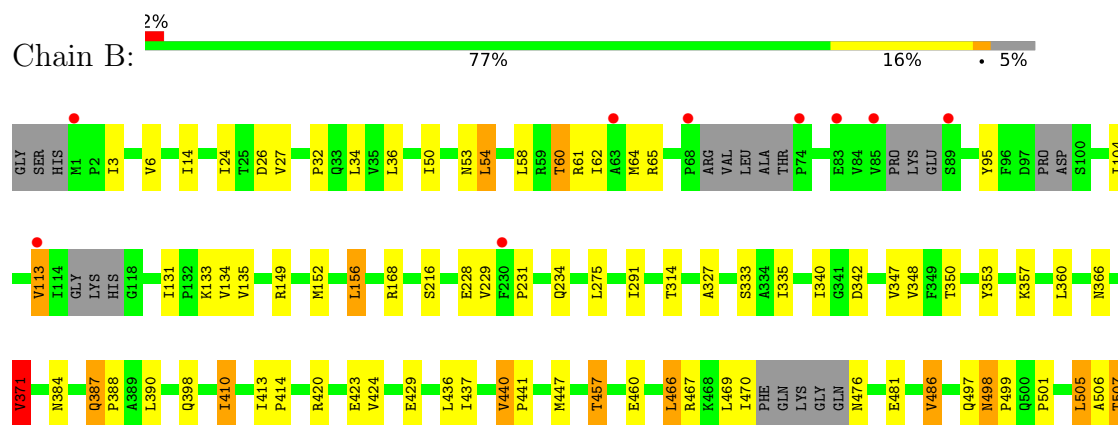
3 Residue-property plots

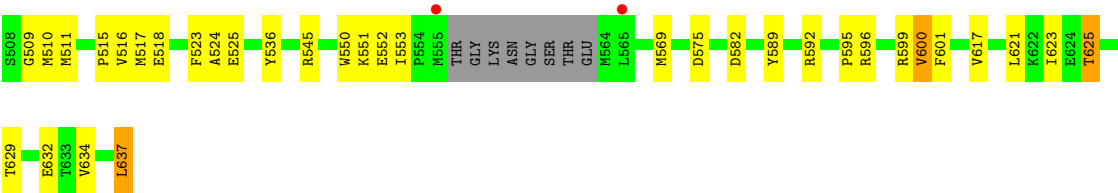
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CLEAVAGE AND POLYADENYLATION SPECIFICITY FACTOR 100 KD SUB-UNIT



• Molecule 1: CLEAVAGE AND POLYADENYLATION SPECIFICITY FACTOR 100 KD SUB-UNIT





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.66Å 97.72Å 90.72Å 90.00° 98.26° 90.00°	Depositor
Resolution (Å)	38.43 – 2.59 38.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.43-2.59) 98.9 (38.43-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.209 , 0.267 0.204 , 0.253	Depositor DCC
R_{free} test set	2023 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.8	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	0.94	EDS
Total number of atoms	9391	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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	0.84	0/4741	0.94	5/6450 (0.1%)
1	B	0.97	1/4807 (0.0%)	0.97	7/6529 (0.1%)
All	All	0.91	1/9548 (0.0%)	0.95	12/12979 (0.1%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	ILE	CA-CB	5.57	1.59	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	VAL	CB-CA-C	-7.36	99.23	111.29
1	B	498	ASN	CA-C-N	-7.26	112.31	119.78
1	B	498	ASN	C-N-CA	-7.26	112.31	119.78
1	A	371	VAL	CB-CA-C	-7.06	99.71	111.29
1	B	509	GLY	N-CA-C	6.39	121.49	114.40
1	B	65	ARG	N-CA-C	5.86	115.04	108.25
1	A	368	PHE	CA-C-N	-5.59	112.75	118.85
1	A	368	PHE	C-N-CA	-5.59	112.75	118.85
1	A	51	ILE	N-CA-C	5.51	116.24	110.62
1	B	387	GLN	CB-CA-C	5.33	117.13	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	437	ILE	N-CA-C	-5.14	102.14	107.84
1	A	313	VAL	CB-CA-C	-5.09	104.51	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	384	ASN	Peptide

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	4640	0	4523	68	0
1	B	4705	0	4597	76	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	16	0	0	0	0
3	B	26	0	0	0	0
All	All	9391	0	9120	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (144) 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:410:ILE:HG22	1:B:501:PRO:HA	1.42	1.00
1:A:360:LEU:HD23	1:A:466:LEU:HD12	1.57	0.86
1:B:413:ILE:HB	1:B:505:LEU:HD12	1.61	0.80
1:A:360:LEU:HD23	1:A:466:LEU:CD1	2.14	0.77
1:B:360:LEU:HD23	1:B:466:LEU:CD1	2.16	0.76
1:B:360:LEU:HD23	1:B:466:LEU:HD12	1.68	0.75
1:B:511:MET:HE2	1:B:517:MET:HE1	1.68	0.75
1:A:510:MET:HE2	1:A:536:TYR:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLN:NE2	1:A:436:LEU:HD23	2.06	0.71
1:A:587:MET:HE3	1:A:620:LYS:HE2	1.74	0.70
1:A:413:ILE:HB	1:A:505:LEU:HD12	1.72	0.70
1:B:231:PRO:HD2	1:B:234:GLN:NE2	2.09	0.68
1:A:360:LEU:CD2	1:A:466:LEU:HD12	2.23	0.68
1:B:231:PRO:HD2	1:B:234:GLN:HE21	1.59	0.66
1:A:231:PRO:HD2	1:A:234:GLN:NE2	2.10	0.66
1:A:231:PRO:HD2	1:A:234:GLN:HE21	1.60	0.66
1:A:156:LEU:HD22	1:A:156:LEU:O	1.96	0.65
1:A:410:ILE:HG22	1:A:501:PRO:HA	1.78	0.64
1:B:440:VAL:HG22	1:B:441:PRO:HD2	1.79	0.64
1:B:64:MET:HE3	1:B:131:ILE:HD11	1.79	0.64
1:A:98:PRO:HB2	1:A:156:LEU:HD21	1.82	0.62
1:B:516:VAL:HG13	1:B:517:MET:HE3	1.81	0.62
1:A:275:LEU:CD1	1:A:447:MET:HE3	2.31	0.61
1:B:113:VAL:CG1	1:B:134:VAL:HG11	2.30	0.61
1:A:398:GLN:CD	1:A:436:LEU:HD23	2.24	0.61
1:A:3:ILE:O	1:A:6:VAL:HG22	2.01	0.61
1:B:507:THR:HG22	1:B:515:PRO:HD2	1.83	0.61
1:B:516:VAL:HG13	1:B:517:MET:CE	2.31	0.60
1:A:275:LEU:HD11	1:A:447:MET:HE3	1.84	0.60
1:A:516:VAL:HG13	1:A:517:MET:HE3	1.84	0.60
1:A:601:PHE:CZ	1:A:634:VAL:HG11	2.36	0.60
1:A:511:MET:HE2	1:A:517:MET:HE1	1.85	0.59
1:B:27:VAL:HG13	1:B:34:LEU:HD11	1.85	0.59
1:B:113:VAL:HG13	1:B:134:VAL:HG11	1.86	0.58
1:A:439:GLU:O	1:A:440:VAL:HG23	2.04	0.58
1:B:511:MET:CE	1:B:517:MET:HE1	2.34	0.58
1:B:552:GLU:C	1:B:553:ILE:HD12	2.28	0.57
1:A:58:LEU:O	1:A:60:THR:HG23	2.04	0.57
1:A:88:GLU:O	1:A:90:VAL:HG23	2.05	0.56
1:A:360:LEU:CD2	1:A:466:LEU:CD1	2.82	0.56
1:B:3:ILE:O	1:B:6:VAL:HG22	2.05	0.56
1:B:601:PHE:CZ	1:B:634:VAL:HG11	2.41	0.56
1:A:623:ILE:O	1:A:625:THR:HG23	2.05	0.56
1:A:14:ILE:HG12	1:A:54:LEU:HD21	1.87	0.55
1:A:48:GLY:HA3	1:A:52:ARG:NH2	2.22	0.55
1:A:587:MET:CE	1:A:620:LYS:HE2	2.36	0.54
1:A:516:VAL:HG13	1:A:517:MET:CE	2.38	0.54
1:B:50:ILE:HG22	1:B:54:LEU:HD22	1.89	0.53
1:A:410:ILE:HD11	1:A:523:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LEU:O	1:B:60:THR:HG22	2.09	0.53
1:B:510:MET:HE2	1:B:536:TYR:O	2.08	0.53
1:A:617:VAL:CG1	1:A:625:THR:HG21	2.39	0.53
1:B:524:ALA:CB	1:B:569:MET:HE2	2.39	0.52
1:B:3:ILE:HG21	1:B:168:ARG:HD3	1.92	0.52
1:A:113:VAL:CG1	1:A:134:VAL:HG11	2.40	0.52
1:A:398:GLN:HE22	1:A:436:LEU:HD23	1.73	0.52
1:B:420:ARG:O	1:B:424:VAL:HG23	2.09	0.52
1:B:617:VAL:CG1	1:B:625:THR:HG21	2.40	0.51
1:B:64:MET:CE	1:B:131:ILE:HD11	2.40	0.51
1:B:410:ILE:HG22	1:B:501:PRO:CA	2.28	0.51
1:A:58:LEU:HD12	1:A:62:ILE:HD11	1.92	0.51
1:B:156:LEU:HD22	1:B:156:LEU:O	2.11	0.51
1:A:517:MET:HE2	1:A:517:MET:HA	1.94	0.50
1:A:335:ILE:HD13	1:A:589:TYR:OH	2.11	0.50
1:B:623:ILE:O	1:B:625:THR:HG23	2.11	0.50
1:B:360:LEU:HD23	1:B:466:LEU:HD11	1.92	0.49
1:A:420:ARG:O	1:A:424:VAL:HG23	2.12	0.49
1:B:32:PRO:HB3	1:B:314:THR:HG23	1.94	0.49
1:A:623:ILE:O	1:A:625:THR:CG2	2.61	0.49
1:B:457:THR:O	1:B:457:THR:CG2	2.59	0.49
1:B:617:VAL:HG13	1:B:621:LEU:HD12	1.94	0.49
1:B:14:ILE:HG21	1:B:24:ILE:HD13	1.95	0.49
1:B:470:ILE:HA	1:B:476:ASN:ND2	2.26	0.49
1:A:224:LEU:O	1:A:230:PHE:CE1	2.66	0.49
1:B:517:MET:HA	1:B:517:MET:HE2	1.95	0.48
1:B:553:ILE:HD12	1:B:553:ILE:N	2.27	0.48
1:B:348:VAL:HG23	1:B:371:VAL:HG13	1.96	0.48
1:B:387:GLN:HG2	1:B:582:ASP:HB3	1.95	0.48
1:A:113:VAL:HG13	1:A:134:VAL:HG11	1.94	0.48
1:B:486:VAL:HG22	1:B:486:VAL:O	2.14	0.48
1:A:410:ILE:HD11	1:A:523:PHE:CE2	2.49	0.48
1:B:410:ILE:HD11	1:B:523:PHE:CE1	2.49	0.48
1:B:600:VAL:HG22	1:B:625:THR:HB	1.96	0.48
1:A:366:ASN:HB3	1:A:589:TYR:CE1	2.48	0.48
1:A:387:GLN:HG2	1:A:582:ASP:HB3	1.96	0.47
1:A:617:VAL:HG13	1:A:621:LEU:HD12	1.96	0.47
1:B:58:LEU:CD1	1:B:62:ILE:HD11	2.44	0.47
1:A:9:ASP:O	1:A:13:LYS:HB2	2.14	0.47
1:A:331:LEU:HD22	1:A:455:HIS:CG	2.49	0.47
1:B:275:LEU:HD11	1:B:447:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:O	1:A:156:LEU:CD2	2.63	0.47
1:A:327:ALA:HB3	1:A:333:SER:OG	2.15	0.47
1:B:366:ASN:HB3	1:B:589:TYR:CE1	2.49	0.47
1:A:27:VAL:HG13	1:A:34:LEU:HD11	1.96	0.47
1:A:80:ILE:O	1:A:84:VAL:HG23	2.15	0.47
1:A:232:LEU:HD12	1:A:257:TYR:O	2.15	0.46
1:B:231:PRO:CD	1:B:234:GLN:HE21	2.28	0.46
1:A:10:LEU:HD22	1:A:14:ILE:HD11	1.97	0.46
1:A:181:VAL:HG11	1:A:340:ILE:HD12	1.96	0.46
1:A:398:GLN:OE1	1:A:436:LEU:HD23	2.15	0.46
1:B:360:LEU:CD2	1:B:466:LEU:HD12	2.42	0.46
1:B:104:ILE:HD13	1:B:133:LYS:HB2	1.97	0.46
1:B:228:GLU:OE1	1:B:228:GLU:N	2.49	0.46
1:A:510:MET:HE1	1:A:536:TYR:CE2	2.51	0.46
1:B:371:VAL:HG23	1:B:595:PRO:HD2	1.99	0.45
1:B:524:ALA:HA	1:B:569:MET:HE2	1.99	0.45
1:A:466:LEU:HD23	1:A:466:LEU:HA	1.74	0.45
1:A:98:PRO:HB2	1:A:156:LEU:CD2	2.47	0.45
1:A:629:THR:HB	1:A:632:GLU:HG3	1.99	0.45
1:A:64:MET:SD	1:A:64:MET:C	3.00	0.44
1:A:276:LEU:HD21	1:A:417:ALA:HB3	2.00	0.44
1:A:587:MET:HE3	1:A:620:LYS:CE	2.45	0.44
1:B:360:LEU:CD2	1:B:466:LEU:CD1	2.93	0.44
1:B:64:MET:C	1:B:64:MET:SD	3.01	0.44
1:A:27:VAL:HG22	1:A:36:LEU:CD2	2.48	0.44
1:B:95:TYR:CE1	1:B:149:ARG:HB3	2.52	0.43
1:B:152:MET:HE2	1:B:152:MET:HA	2.00	0.43
1:B:27:VAL:HG22	1:B:36:LEU:CD2	2.49	0.43
1:A:511:MET:CE	1:A:517:MET:HE1	2.48	0.43
1:B:457:THR:O	1:B:457:THR:HG22	2.17	0.43
1:B:58:LEU:HD12	1:B:62:ILE:HD11	1.99	0.43
1:B:335:ILE:HD13	1:B:589:TYR:OH	2.18	0.43
1:B:60:THR:OG1	1:B:61:ARG:N	2.52	0.42
1:B:414:PRO:HA	1:B:506:ALA:O	2.18	0.42
1:B:623:ILE:O	1:B:625:THR:CG2	2.67	0.42
1:B:637:LEU:HD22	1:B:637:LEU:O	2.20	0.42
1:A:140:ILE:HG12	1:A:479:LEU:HD21	2.02	0.42
1:B:53:ASN:HD22	1:B:53:ASN:HA	1.68	0.42
1:B:498:ASN:O	1:B:499:PRO:C	2.61	0.42
1:B:398:GLN:NE2	1:B:436:LEU:HD23	2.34	0.42
1:A:27:VAL:HG22	1:A:36:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:HB3	1:B:333:SER:OG	2.20	0.41
1:B:440:VAL:CG2	1:B:501:PRO:O	2.68	0.41
1:B:32:PRO:HB3	1:B:314:THR:CG2	2.50	0.41
1:B:350:THR:HB	1:B:353:TYR:CD1	2.55	0.41
1:B:275:LEU:CD1	1:B:447:MET:HE3	2.51	0.41
1:A:275:LEU:HD12	1:A:447:MET:HE3	2.03	0.41
1:A:359:ARG:HG2	1:A:426:ILE:HG21	2.03	0.41
1:B:50:ILE:O	1:B:54:LEU:N	2.52	0.41
1:B:388:PRO:HD2	1:B:575:ASP:O	2.21	0.41
1:A:486:VAL:O	1:A:486:VAL:HG22	2.21	0.41
1:B:629:THR:HB	1:B:632:GLU:HG3	2.02	0.41
1:A:156:LEU:HD22	1:A:156:LEU:C	2.46	0.40
1:B:95:TYR:CZ	1:B:149:ARG:HG2	2.57	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	594/640 (93%)	567 (96%)	27 (4%)	0	100	100
1	B	598/640 (93%)	570 (95%)	28 (5%)	0	100	100
All	All	1192/1280 (93%)	1137 (95%)	55 (5%)	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	487/560 (87%)	447 (92%)	40 (8%)	10	24
1	B	495/560 (88%)	456 (92%)	39 (8%)	11	26
All	All	982/1120 (88%)	903 (92%)	79 (8%)	11	25

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	26	ASP
1	A	57	GLU
1	A	60	THR
1	A	75	GLU
1	A	88	GLU
1	A	109	LYS
1	A	113	VAL
1	A	121	LEU
1	A	127	GLN
1	A	135	VAL
1	A	153	ARG
1	A	156	LEU
1	A	216	SER
1	A	229	VAL
1	A	312	GLU
1	A	340	ILE
1	A	342	ASP
1	A	347	VAL
1	A	367	LYS
1	A	371	VAL
1	A	384	ASN
1	A	410	ILE
1	A	423	GLU
1	A	436	LEU
1	A	437	ILE
1	A	440	VAL
1	A	466	LEU
1	A	469	LEU
1	A	486	VAL
1	A	505	LEU
1	A	507	THR
1	A	518	GLU

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Mol	Chain	Res	Type
1	A	550	TRP
1	A	596	ARG
1	A	599	ARG
1	A	600	VAL
1	A	620	LYS
1	A	625	THR
1	A	637	LEU
1	B	26	ASP
1	B	54	LEU
1	B	60	THR
1	B	113	VAL
1	B	135	VAL
1	B	156	LEU
1	B	216	SER
1	B	229	VAL
1	B	340	ILE
1	B	342	ASP
1	B	347	VAL
1	B	357	LYS
1	B	371	VAL
1	B	390	LEU
1	B	410	ILE
1	B	423	GLU
1	B	429	GLU
1	B	440	VAL
1	B	457	THR
1	B	460	GLU
1	B	466	LEU
1	B	467	ARG
1	B	469	LEU
1	B	481	GLU
1	B	486	VAL
1	B	497	GLN
1	B	505	LEU
1	B	507	THR
1	B	518	GLU
1	B	525	GLU
1	B	545	ARG
1	B	550	TRP
1	B	551	LYS
1	B	592	ARG
1	B	596	ARG

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Mol	Chain	Res	Type
1	B	599	ARG
1	B	600	VAL
1	B	625	THR
1	B	637	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	384	ASN
1	A	547	GLN
1	B	53	ASN
1	B	384	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 4 ligands modelled in this entry, 4 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	605/640 (94%)	0.11	15 (2%) 58 52	28, 60, 121, 158	1 (0%)
1	B	611/640 (95%)	-0.04	11 (1%) 67 63	22, 46, 93, 119	1 (0%)
All	All	1216/1280 (95%)	0.03	26 (2%) 63 58	22, 55, 107, 158	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225[A]	TYR	3.8
1	A	564	MET	3.5
1	B	565	LEU	3.4
1	A	401	VAL	3.3
1	A	552	GLU	3.2
1	A	411	ALA	3.2
1	A	568	ASN	3.2
1	B	1	MET	3.1
1	A	520	PHE	2.9
1	A	438	PRO	2.9
1	A	500	GLN	2.8
1	B	85	VAL	2.8
1	B	63	ALA	2.8
1	B	74	PRO	2.5
1	A	530	THR	2.3
1	B	89	SER	2.3
1	B	68	PRO	2.3
1	A	495	ILE	2.2
1	B	230	PHE	2.2
1	A	550	TRP	2.2
1	B	555	MET	2.1
1	B	113	VAL	2.1
1	A	501	PRO	2.1
1	B	83	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	526	ASP	2.0
1	A	470	ILE	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	1638	1/1	0.99	0.05	49,49,49,49	0
2	ZN	B	1638	1/1	0.99	0.05	34,34,34,34	0
2	ZN	B	1639	1/1	0.99	0.04	35,35,35,35	0
2	ZN	A	1639	1/1	1.00	0.03	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.