



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:40 PM UTC

PDB ID : 1RO2 / pdb_00001ro2
Title : Bifunctional DNA primase/polymerase domain of ORF904 from the archaeal plasmid pRN1- Triple mutant F50M/L107M/L110M manganese soak
Authors : Lipps, G.; Weinzierl, A.O.; von Scheven, G.; Buchen, C.; Cramer, P.
Deposited on : 2003-12-01
Resolution : 1.60 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

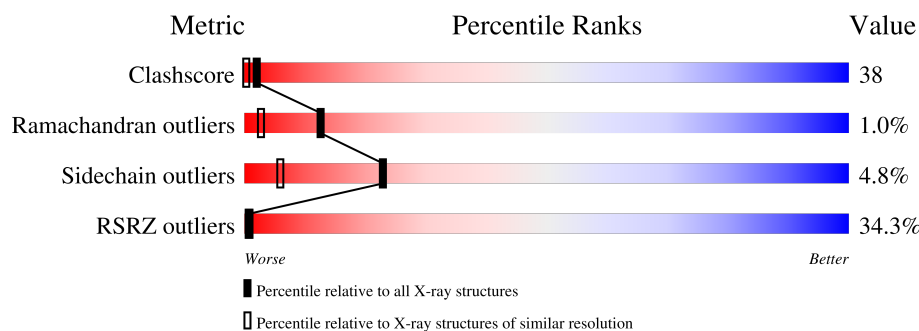
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	216	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1919 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 hypothetical protein ORF904.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1703	1090	285	317	11			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	PHE	engineered mutation	UNP Q54324
A	107	MET	LEU	engineered mutation	UNP Q54324
A	110	MET	LEU	engineered mutation	UNP Q54324
A	250	HIS	-	expression tag	UNP Q54324
A	251	HIS	-	expression tag	UNP Q54324
A	252	HIS	-	expression tag	UNP Q54324
A	253	HIS	-	expression tag	UNP Q54324
A	254	HIS	-	expression tag	UNP Q54324
A	255	HIS	-	expression tag	UNP Q54324

- 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		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

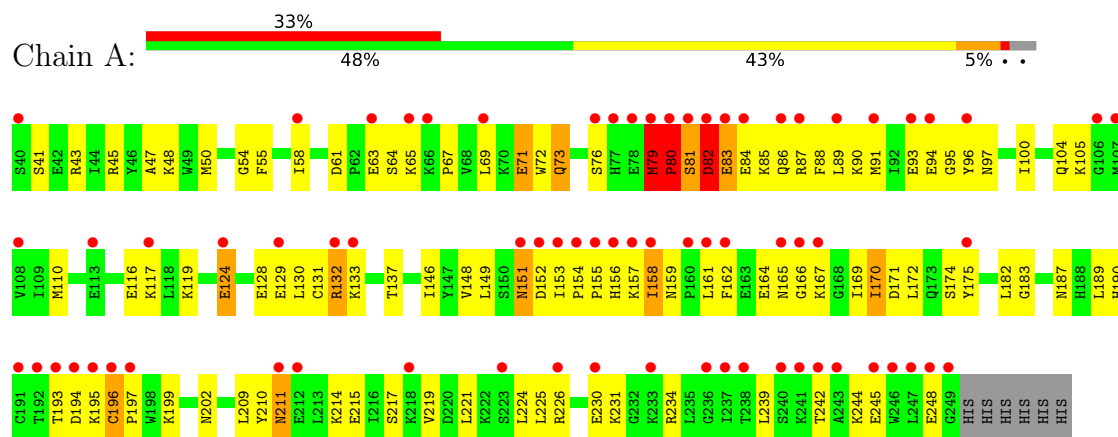
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total 213	O 213	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: hypothetical protein ORF904



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	45.81Å 119.91Å 41.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 20.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.60) 97.5 (20.00-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.265 0.262 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.5	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	0.92	EDS
Total number of atoms	1919	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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, MN

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	1.88	9/1743 (0.5%)	1.59	20/2348 (0.9%)

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	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	PRO	N-CD	48.46	2.15	1.47
1	A	196	CYS	C-N	36.10	1.78	1.34
1	A	79	MET	C-N	-29.04	0.65	1.33
1	A	80	PRO	CA-CB	21.77	1.84	1.53
1	A	83	GLU	C-N	14.30	1.54	1.33
1	A	83	GLU	CB-CG	-12.66	1.14	1.52
1	A	195	LYS	C-N	12.26	1.58	1.33
1	A	81	SER	CB-OG	10.84	1.63	1.42
1	A	82	ASP	CB-CG	10.65	1.78	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	PRO	CA-N-CD	-30.15	69.79	112.00
1	A	80	PRO	N-CA-CB	24.48	128.95	103.25
1	A	79	MET	CA-C-N	24.22	150.11	119.84
1	A	79	MET	C-N-CA	24.22	150.11	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	MET	O-C-N	-15.95	99.94	121.64
1	A	195	LYS	O-C-N	14.07	142.98	122.43
1	A	81	SER	CA-CB-OG	-12.93	85.23	111.10
1	A	80	PRO	CA-CB-CG	-9.77	85.93	104.50
1	A	196	CYS	O-C-N	-9.07	110.89	121.32
1	A	76	SER	N-CA-C	-8.15	103.34	113.28
1	A	82	ASP	CB-CG-OD2	7.99	136.78	118.40
1	A	80	PRO	N-CD-CG	7.95	115.13	103.20
1	A	82	ASP	CB-CG-OD1	-7.61	100.91	118.40
1	A	151	ASN	N-CA-C	-6.41	104.29	111.28
1	A	83	GLU	CA-CB-CG	6.07	126.23	114.10
1	A	47	ALA	N-CA-C	-5.77	104.91	111.14
1	A	132	ARG	N-CA-C	-5.40	106.82	113.41
1	A	158	ILE	N-CA-C	5.38	114.55	106.42
1	A	97	ASN	N-CA-C	-5.26	103.66	110.19
1	A	159	ASN	N-CA-C	5.13	114.21	108.25

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	MET	Peptide,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	1703	0	1698	130	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	213	0	0	50	0
All	All	1919	0	1698	130	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 38.

All (130) 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:80:PRO:CA	1:A:80:PRO:CB	1.84	1.53
1:A:82:ASP:CB	1:A:82:ASP:CG	1.78	1.51
1:A:81:SER:OG	1:A:81:SER:CB	1.63	1.45
1:A:196:CYS:C	1:A:197:PRO:N	1.78	1.40
1:A:80:PRO:CA	1:A:80:PRO:CD	2.15	1.23
1:A:239:LEU:HD23	4:A:473:HOH:O	1.39	1.20
1:A:221:LEU:HG	4:A:489:HOH:O	1.43	1.17
1:A:80:PRO:CA	1:A:80:PRO:CG	2.28	1.12
1:A:80:PRO:CD	1:A:80:PRO:N	2.15	1.09
1:A:209:LEU:HA	4:A:510:HOH:O	1.55	1.05
1:A:81:SER:OG	1:A:81:SER:CA	2.14	0.95
1:A:214:LYS:HG3	4:A:501:HOH:O	1.68	0.94
1:A:158:ILE:O	1:A:158:ILE:HG13	1.70	0.91
1:A:88:PHE:HA	1:A:91:MET:HE3	1.54	0.90
1:A:87:ARG:HG2	1:A:91:MET:HE2	1.55	0.88
1:A:149:LEU:HD22	4:A:487:HOH:O	1.73	0.88
1:A:80:PRO:CB	1:A:80:PRO:HA	2.01	0.87
1:A:90:LYS:O	1:A:94:GLU:HG3	1.75	0.87
1:A:161:LEU:O	4:A:473:HOH:O	1.95	0.85
1:A:151:ASN:HB2	4:A:408:HOH:O	1.81	0.81
1:A:182:LEU:HD21	4:A:510:HOH:O	1.80	0.79
1:A:79:MET:C	1:A:80:PRO:CD	2.49	0.78
1:A:54:GLY:C	4:A:426:HOH:O	2.27	0.78
1:A:137:THR:HG22	4:A:510:HOH:O	1.83	0.77
1:A:81:SER:OG	1:A:81:SER:C	2.28	0.76
1:A:119:LYS:HE3	1:A:124:GLU:HB3	1.67	0.75
1:A:128:GLU:OE2	1:A:210:TYR:OH	2.05	0.74
1:A:43:ARG:NH1	4:A:393:HOH:O	2.19	0.73
1:A:82:ASP:CB	1:A:82:ASP:OD1	2.36	0.73
1:A:86:GLN:HB2	4:A:415:HOH:O	1.89	0.72
1:A:211:ASN:HB3	4:A:320:HOH:O	1.89	0.71
1:A:155:PRO:HG2	1:A:156:HIS:ND1	2.06	0.70
1:A:187:ASN:ND2	1:A:189:LEU:HB2	2.07	0.69
1:A:239:LEU:HA	4:A:473:HOH:O	1.93	0.69
1:A:245:GLU:HB2	4:A:462:HOH:O	1.93	0.69
1:A:199:LYS:HE2	4:A:382:HOH:O	1.92	0.68
1:A:54:GLY:O	1:A:105:LYS:HE3	1.95	0.67
1:A:55:PHE:CD1	4:A:426:HOH:O	2.49	0.66
1:A:124:GLU:O	1:A:128:GLU:HG2	1.96	0.65
1:A:225:LEU:HG	4:A:489:HOH:O	1.95	0.64
1:A:83:GLU:C	4:A:415:HOH:O	2.39	0.64
1:A:81:SER:CB	1:A:81:SER:HG	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:HE2	4:A:391:HOH:O	1.99	0.62
1:A:55:PHE:CG	4:A:426:HOH:O	2.53	0.62
1:A:155:PRO:HG2	1:A:156:HIS:CE1	2.34	0.62
1:A:165:ASN:HB3	4:A:370:HOH:O	2.00	0.62
1:A:225:LEU:CD1	4:A:489:HOH:O	2.48	0.61
1:A:71:GLU:H	1:A:71:GLU:CD	2.10	0.60
1:A:86:GLN:HB3	4:A:496:HOH:O	2.01	0.59
1:A:190:HIS:HD2	4:A:411:HOH:O	1.85	0.59
1:A:50:MET:HE2	1:A:100:ILE:HG12	1.84	0.59
1:A:244:LYS:HE2	1:A:248:GLU:OE2	2.02	0.58
1:A:69:LEU:HB3	1:A:71:GLU:OE2	2.03	0.57
1:A:89:LEU:O	1:A:93:GLU:HG3	2.03	0.57
1:A:196:CYS:C	1:A:197:PRO:CA	2.75	0.57
1:A:117:LYS:NZ	1:A:164:GLU:OE1	2.39	0.56
1:A:170:ILE:C	1:A:170:ILE:HD13	2.30	0.56
1:A:189:LEU:HG	1:A:202:ASN:HA	1.88	0.56
1:A:221:LEU:C	4:A:489:HOH:O	2.48	0.56
1:A:117:LYS:NZ	1:A:169:ILE:HG21	2.21	0.56
1:A:73:GLN:NE2	1:A:73:GLN:H	2.04	0.56
1:A:193:THR:O	1:A:196:CYS:HB2	2.06	0.56
1:A:50:MET:HE2	1:A:100:ILE:CG1	2.35	0.55
1:A:91:MET:HB3	1:A:96:TYR:CD1	2.42	0.55
1:A:231:LYS:HD3	1:A:234:ARG:NH2	2.21	0.55
1:A:43:ARG:CZ	4:A:393:HOH:O	2.51	0.55
1:A:50:MET:HE2	1:A:100:ILE:HD13	1.89	0.54
1:A:154:PRO:HB2	4:A:400:HOH:O	2.08	0.54
1:A:41:SER:CB	4:A:393:HOH:O	2.55	0.53
1:A:50:MET:HE2	1:A:100:ILE:CD1	2.37	0.53
1:A:80:PRO:HG2	1:A:85:LYS:HG3	1.90	0.53
1:A:71:GLU:O	1:A:71:GLU:HG2	2.09	0.53
1:A:194:ASP:C	1:A:196:CYS:N	2.66	0.52
1:A:130:LEU:HD12	1:A:133:LYS:HE3	1.91	0.52
1:A:79:MET:CA	1:A:80:PRO:CD	2.87	0.52
1:A:64:SER:O	1:A:65:LYS:HB2	2.09	0.51
1:A:137:THR:HA	4:A:510:HOH:O	2.09	0.51
1:A:157:LYS:HB3	4:A:365:HOH:O	2.09	0.51
1:A:194:ASP:C	1:A:196:CYS:H	2.10	0.49
1:A:63:GLU:HA	1:A:63:GLU:OE1	2.13	0.48
1:A:131:CYS:O	4:A:501:HOH:O	2.19	0.48
1:A:217:SER:HA	4:A:471:HOH:O	2.13	0.48
1:A:41:SER:HB2	4:A:338:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASP:HB3	4:A:383:HOH:O	2.12	0.48
1:A:87:ARG:HG2	1:A:91:MET:CE	2.36	0.48
1:A:85:LYS:HE2	4:A:354:HOH:O	2.13	0.48
1:A:73:GLN:H	1:A:73:GLN:HE21	1.60	0.47
1:A:187:ASN:HD21	1:A:189:LEU:HB2	1.78	0.47
1:A:110:MET:HE1	1:A:224:LEU:HD21	1.96	0.47
1:A:165:ASN:O	1:A:167:LYS:N	2.47	0.47
1:A:190:HIS:HB2	4:A:361:HOH:O	2.15	0.46
1:A:153:ILE:O	1:A:154:PRO:C	2.56	0.46
1:A:242:THR:O	1:A:245:GLU:HB3	2.16	0.46
1:A:43:ARG:NH2	1:A:95:GLY:HA2	2.31	0.46
1:A:154:PRO:HG2	1:A:172:LEU:HD23	1.97	0.45
1:A:165:ASN:C	1:A:167:LYS:N	2.74	0.45
1:A:61:ASP:HB3	1:A:64:SER:OG	2.17	0.45
1:A:149:LEU:HB3	4:A:487:HOH:O	2.16	0.45
1:A:48:LYS:NZ	4:A:495:HOH:O	2.50	0.44
1:A:43:ARG:HA	1:A:183:GLY:HA3	1.99	0.44
1:A:170:ILE:HD13	1:A:171:ASP:N	2.32	0.44
1:A:110:MET:HE3	1:A:146:ILE:HB	1.98	0.44
1:A:162:PHE:CG	4:A:473:HOH:O	2.69	0.44
1:A:116:GLU:HG3	4:A:333:HOH:O	2.18	0.43
1:A:130:LEU:CD1	1:A:133:LYS:HE3	2.48	0.43
1:A:154:PRO:HB3	4:A:374:HOH:O	2.18	0.43
1:A:129:GLU:O	1:A:132:ARG:HB3	2.19	0.43
1:A:225:LEU:CG	4:A:489:HOH:O	2.58	0.43
1:A:187:ASN:HD22	1:A:189:LEU:HB2	1.81	0.43
1:A:148:VAL:HB	1:A:219:VAL:HG22	1.99	0.42
1:A:157:LYS:HG2	4:A:398:HOH:O	2.18	0.42
1:A:58:ILE:HD13	1:A:67:PRO:HB3	2.01	0.42
1:A:244:LYS:O	1:A:245:GLU:C	2.61	0.42
1:A:154:PRO:HD2	4:A:400:HOH:O	2.19	0.42
1:A:234:ARG:NH1	4:A:436:HOH:O	2.53	0.42
1:A:80:PRO:HB2	1:A:84:GLU:HB2	2.02	0.42
1:A:162:PHE:CE2	4:A:473:HOH:O	2.72	0.42
1:A:225:LEU:HD12	4:A:489:HOH:O	2.16	0.42
1:A:58:ILE:HD13	1:A:72:TRP:HB3	2.01	0.42
1:A:153:ILE:HG21	1:A:175:TYR:CE1	2.55	0.42
1:A:117:LYS:HZ3	1:A:169:ILE:CG2	2.33	0.41
1:A:226:ARG:O	1:A:230:GLU:HG3	2.20	0.41
1:A:80:PRO:HG2	1:A:85:LYS:CG	2.50	0.41
1:A:58:ILE:CD1	1:A:72:TRP:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:HIS:CD2	4:A:374:HOH:O	2.74	0.41
1:A:174:SER:OG	1:A:175:TYR:N	2.53	0.41
1:A:165:ASN:C	1:A:167:LYS:H	2.29	0.41
1:A:71:GLU:O	1:A:71:GLU:CG	2.68	0.40
1:A:104:GLN:O	1:A:105:LYS:C	2.64	0.40
1:A:55:PHE:N	4:A:426:HOH:O	2.50	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	208/216 (96%)	194 (93%)	12 (6%)	2 (1%)	12 3

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	PRO
1	A	166	GLY

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	189/195 (97%)	180 (95%)	9 (5%)	23 6

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	71	GLU
1	A	73	GLN
1	A	80	PRO
1	A	82	ASP
1	A	124	GLU
1	A	170	ILE
1	A	211	ASN
1	A	215	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	190	HIS
1	A	201	GLN
1	A	211	ASN

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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	196:CYS	C	197:PRO	N	1.78
1	A	79:MET	C	80:PRO	N	0.65

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	210/216 (97%)	1.60	72 (34%) ⓘ ⓘ	13, 24, 48, 55	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	158	ILE	7.5
1	A	152	ASP	6.3
1	A	157	LYS	6.2
1	A	155	PRO	6.0
1	A	165	ASN	5.7
1	A	81	SER	5.1
1	A	83	GLU	4.9
1	A	194	ASP	4.6
1	A	249	GLY	4.4
1	A	156	HIS	4.4
1	A	151	ASN	4.3
1	A	246	TRP	4.2
1	A	132	ARG	4.1
1	A	82	ASP	3.9
1	A	153	ILE	3.8
1	A	195	LYS	3.7
1	A	197	PRO	3.5
1	A	233	LYS	3.5
1	A	196	CYS	3.5
1	A	154	PRO	3.4
1	A	175	TYR	3.2
1	A	243	ALA	3.2
1	A	160	PRO	3.2
1	A	192	THR	3.2
1	A	238	THR	3.1
1	A	40	SER	3.1
1	A	193	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	66	LYS	3.0
1	A	84	GLU	3.0
1	A	129	GLU	3.0
1	A	167	LYS	3.0
1	A	63	GLU	3.0
1	A	94	GLU	3.0
1	A	161	LEU	2.9
1	A	191	CYS	2.8
1	A	240	SER	2.8
1	A	80	PRO	2.8
1	A	133	LYS	2.8
1	A	226	ARG	2.7
1	A	93	GLU	2.7
1	A	79	MET	2.7
1	A	69	LEU	2.7
1	A	87	ARG	2.7
1	A	166	GLY	2.7
1	A	65	LYS	2.7
1	A	211	ASN	2.6
1	A	241	LYS	2.6
1	A	117	LYS	2.6
1	A	248	GLU	2.6
1	A	212	GLU	2.5
1	A	230	GLU	2.5
1	A	242	THR	2.5
1	A	245	GLU	2.5
1	A	76	SER	2.5
1	A	223	SER	2.4
1	A	89	LEU	2.4
1	A	113	GLU	2.3
1	A	218	LYS	2.3
1	A	77	HIS	2.3
1	A	106	GLY	2.3
1	A	108	VAL	2.3
1	A	124	GLU	2.2
1	A	247	LEU	2.2
1	A	162	PHE	2.2
1	A	236	GLY	2.2
1	A	96	TYR	2.2
1	A	237	ILE	2.2
1	A	58	ILE	2.2
1	A	78	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	107	MET	2.1
1	A	86	GLN	2.1
1	A	91	MET	2.1

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	301	1/1	0.92	0.27	44,44,44,44	0
3	MN	A	303	1/1	0.93	0.15	26,26,26,26	0
2	ZN	A	302	1/1	0.94	0.09	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.