



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:12 AM UTC

PDB ID : 6DEG / pdb_00006deg
Title : Crystal structure of a DNA polymerase III subunit beta DnaN sliding clamp from Bartonella birtlesii LL-WM9
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2018-05-11
Resolution : 2.45 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

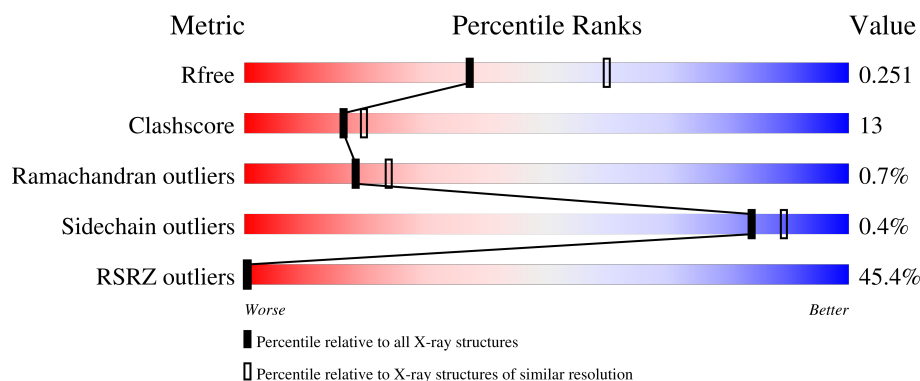
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	381	39% 66% 25% • 8%
1	B	381	44% 68% 24% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5161 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 Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	1	0
			2555	1622	435	486	12			
1	B	351	Total	C	N	O	S	0	1	0
			2571	1638	432	489	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP J1IY24
A	-6	ALA	-	expression tag	UNP J1IY24
A	-5	HIS	-	expression tag	UNP J1IY24
A	-4	HIS	-	expression tag	UNP J1IY24
A	-3	HIS	-	expression tag	UNP J1IY24
A	-2	HIS	-	expression tag	UNP J1IY24
A	-1	HIS	-	expression tag	UNP J1IY24
A	0	HIS	-	expression tag	UNP J1IY24
B	-7	MET	-	initiating methionine	UNP J1IY24
B	-6	ALA	-	expression tag	UNP J1IY24
B	-5	HIS	-	expression tag	UNP J1IY24
B	-4	HIS	-	expression tag	UNP J1IY24
B	-3	HIS	-	expression tag	UNP J1IY24
B	-2	HIS	-	expression tag	UNP J1IY24
B	-1	HIS	-	expression tag	UNP J1IY24
B	0	HIS	-	expression tag	UNP J1IY24

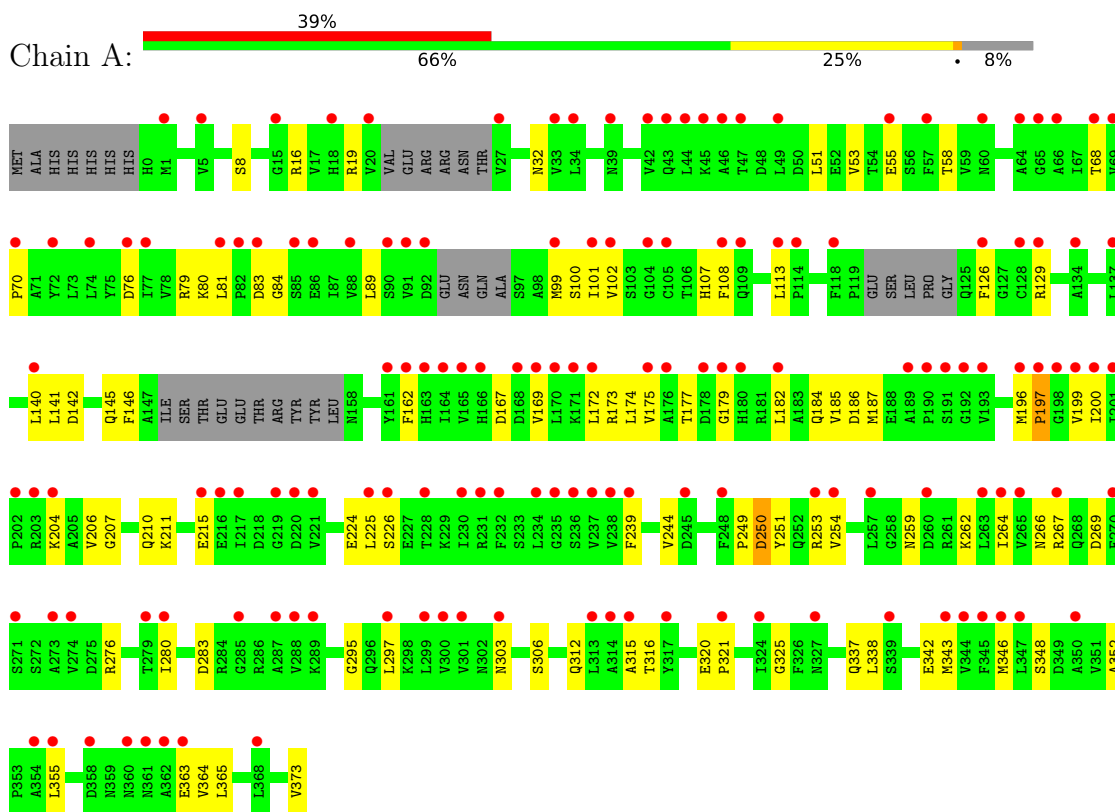
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	9	Total	O	0	0
			9	9		

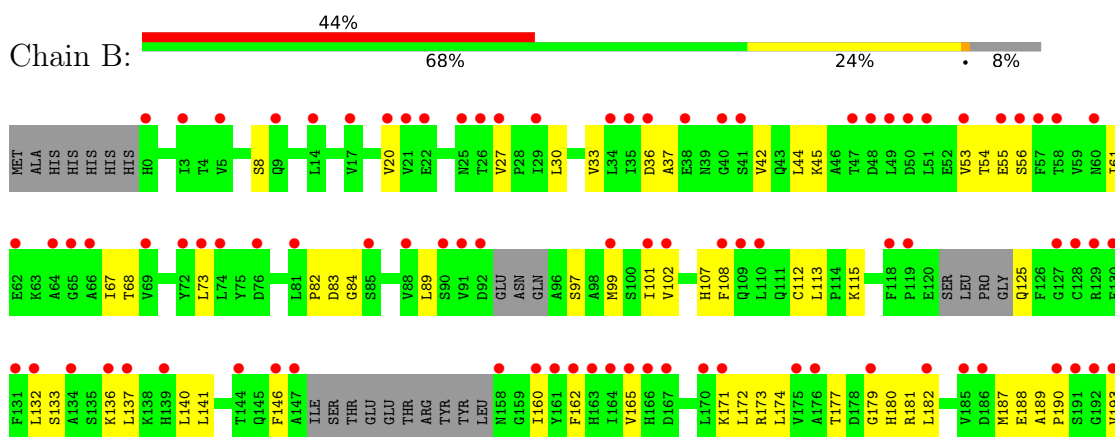
3 Residue-property plots

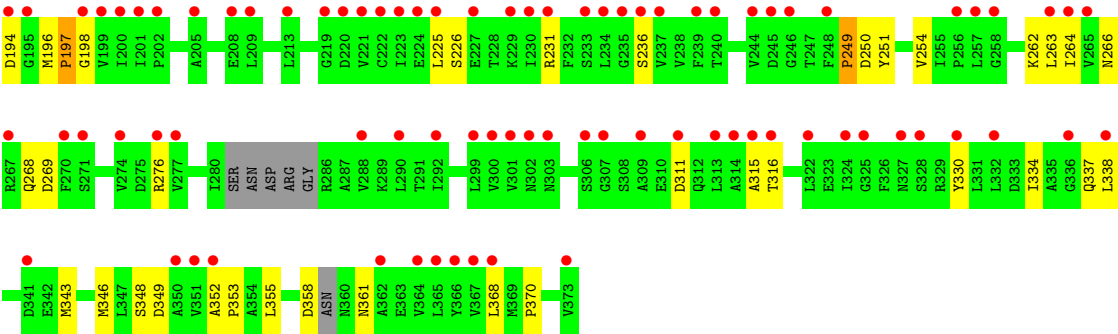
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Beta sliding clamp





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.51Å 157.67Å 53.54Å 90.00° 110.81° 90.00°	Depositor
Resolution (Å)	47.70 – 2.45 47.70 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.70-2.45) 98.3 (47.70-2.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.45Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.257 0.216 , 0.251	Depositor DCC
R_{free} test set	2115 reflections (6.97%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 177.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.246 for l,-k,h	Xtriage
Reported twinning fraction	0.290 for l,-k,h	Depositor
Outliers	0 of 29944 reflections	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	5161	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.17	0/2597	0.38	0/3533
1	B	0.18	0/2613	0.40	0/3553
All	All	0.18	0/5210	0.39	0/7086

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	249	PRO	Peptide

5.2 Too-close contacts [i](#)

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	2555	0	2453	70	0
1	B	2571	0	2475	65	0
2	A	26	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9	0	0	0	0
All	All	5161	0	4928	131	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 13.

All (131) 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:190:PRO:HD2	1:B:193:VAL:HG21	1.60	0.83
1:A:346:MET:HB2	1:A:355:LEU:HB3	1.64	0.80
1:A:280:ILE:HD12	1:A:280:ILE:O	1.88	0.73
1:A:355:LEU:HD11	1:A:365:LEU:HD11	1.69	0.72
1:B:346:MET:HB2	1:B:355:LEU:HB3	1.72	0.72
1:B:67:ILE:HD11	1:B:97:SER:H	1.55	0.72
1:B:89:LEU:HB3	1:B:99:MET:HE2	1.70	0.71
1:B:262:LYS:HD2	1:B:346:MET:HE1	1.74	0.70
1:B:132:LEU:HD23	1:B:133:SER:N	2.06	0.69
1:A:89:LEU:HB3	1:A:99:MET:HE2	1.74	0.68
1:A:253:ARG:NH1	2:A:405:HOH:O	2.26	0.67
1:B:97:SER:HA	1:B:112:CYS:HB2	1.78	0.66
1:A:186:ASP:OD2	2:A:402:HOH:O	2.15	0.64
1:A:58:THR:O	2:A:401:HOH:O	2.15	0.63
1:A:79:ARG:NH2	2:A:408:HOH:O	2.31	0.63
1:B:146:PHE:CE1	1:B:337:GLN:HG3	2.33	0.63
1:B:181:ARG:HH22	1:B:334:ILE:HD11	1.64	0.61
1:A:173:ARG:NE	1:A:186:ASP:OD1	2.22	0.60
1:B:37:ALA:HB1	1:B:61:ILE:HD11	1.84	0.60
1:A:211:LYS:O	1:A:215:GLU:HG2	2.02	0.60
1:B:146:PHE:HE1	1:B:337:GLN:HG3	1.66	0.59
1:A:186:ASP:N	1:A:363:GLU:O	2.23	0.59
1:A:264:ILE:HB	1:A:316:THR:HB	1.85	0.58
1:B:263:LEU:HD11	1:B:315:ALA:HB1	1.85	0.58
1:A:348:SER:HB3	1:A:352:ALA:HB3	1.84	0.58
1:B:249:PRO:O	1:B:251:TYR:N	2.37	0.58
1:B:162:PHE:CE1	1:B:172:LEU:HD11	2.38	0.58
1:A:146:PHE:CE1	1:A:337:GLN:HG3	2.40	0.56
1:A:162:PHE:HB3	1:A:199:VAL:HG23	1.87	0.56
1:A:140:LEU:HB3	1:A:174:LEU:HD13	1.87	0.56
1:A:342:GLU:N	1:A:342:GLU:OE2	2.40	0.55
1:A:185:VAL:HA	1:A:364:VAL:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLN:O	1:B:226:SER:HB2	2.06	0.55
1:B:338:LEU:HD12	1:B:343:MET:HG3	1.89	0.55
1:A:16:ARG:NH1	1:A:55:GLU:OE2	2.39	0.55
1:A:267:ARG:HG3	1:A:343:MET:HG3	1.88	0.55
1:B:276:ARG:NH2	1:B:311:ASP:OD2	2.36	0.54
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.40	0.54
1:B:353:PRO:HA	1:B:370:PRO:HD3	1.91	0.53
1:B:68:THR:OG1	1:B:113:LEU:O	2.23	0.53
1:B:165:VAL:HG23	1:B:171:LYS:HB2	1.89	0.53
1:A:16:ARG:HD2	1:A:55:GLU:HG3	1.92	0.52
1:B:180:HIS:NE2	1:B:254:VAL:O	2.41	0.52
1:A:200:ILE:HB	1:A:244:VAL:HB	1.92	0.52
1:A:177:THR:HB	1:A:182:LEU:HD12	1.92	0.51
1:A:280:ILE:HD12	1:A:280:ILE:C	2.35	0.51
1:A:199:VAL:HG21	1:A:225:LEU:HD11	1.92	0.51
1:B:182:LEU:HD11	1:B:251:TYR:HB2	1.92	0.51
1:A:32:ASN:HD22	1:A:68:THR:HG22	1.76	0.51
1:B:83:ASP:OD1	1:B:84:GLY:N	2.45	0.50
1:A:206:VAL:O	1:A:210:GLN:HG2	2.11	0.50
1:A:32:ASN:HA	1:A:70:PRO:HA	1.93	0.50
1:B:68:THR:O	1:B:112:CYS:HB3	2.12	0.50
1:A:101:ILE:HB	1:A:108:PHE:HB2	1.93	0.50
1:B:180:HIS:HA	1:B:254:VAL:HG13	1.94	0.50
1:B:225:LEU:HD23	1:B:226:SER:O	2.13	0.49
1:B:37:ALA:HB1	1:B:61:ILE:CD1	2.41	0.49
1:A:51:LEU:HD11	1:A:204:LYS:HG2	1.94	0.49
1:A:142:ASP:HA	1:A:145:GLN:HG2	1.94	0.49
1:A:303:ASN:HB3	1:A:306:SER:HB2	1.94	0.49
1:B:36:ASP:OD2	1:B:115:LYS:NZ	2.29	0.49
1:A:167:ASP:O	1:A:169:VAL:N	2.42	0.48
1:A:325:GLY:HA3	1:A:373:VAL:HG11	1.94	0.48
1:A:196:MET:HG3	1:A:197:PRO:HD2	1.95	0.48
1:B:42:VAL:O	1:B:56:SER:HA	2.13	0.48
1:A:126:PHE:CE1	1:A:226:SER:HB3	2.49	0.47
1:B:140:LEU:HB3	1:B:174:LEU:HD12	1.96	0.47
1:A:79:ARG:HH21	1:A:80:LYS:NZ	2.13	0.47
1:B:8:SER:HB3	1:B:83:ASP:OD1	2.14	0.47
1:A:276:ARG:HH21	1:B:82:PRO:HD3	1.79	0.47
1:B:136:LYS:HE3	1:B:187:MET:SD	2.53	0.47
1:B:102:VAL:HG22	1:B:107[B]:HIS:ND1	2.30	0.47
1:A:295:GLY:HA2	1:A:315:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:VAL:HG22	1:A:107[B]:HIS:HD2	1.80	0.46
1:A:187:MET:HE2	1:A:187:MET:HB3	1.71	0.46
1:B:330:TYR:HD2	1:B:368:LEU:HD11	1.80	0.46
1:A:162:PHE:CE1	1:A:172:LEU:HD11	2.51	0.46
1:A:262:LYS:HE2	1:A:264:ILE:HD11	1.98	0.46
1:B:44:LEU:O	1:B:54:THR:HA	2.16	0.46
1:B:348:SER:HB3	1:B:352:ALA:HB3	1.96	0.46
1:A:68:THR:HB	1:A:113:LEU:O	2.15	0.46
1:B:193:VAL:HG13	1:B:196:MET:HE3	1.98	0.45
1:A:207:GLY:HA2	1:A:210:GLN:HE21	1.81	0.45
1:B:101:ILE:HB	1:B:108:PHE:HB2	1.98	0.45
1:B:264:ILE:HA	1:B:343:MET:O	2.17	0.45
1:A:129:ARG:HB2	1:A:224:GLU:HG2	1.99	0.45
1:B:194:ASP:OD2	1:B:194:ASP:N	2.48	0.45
1:B:165:VAL:HG11	1:B:173:ARG:NH1	2.32	0.45
1:A:53:VAL:HG22	1:A:239:PHE:CD1	2.51	0.45
1:B:132:LEU:HD22	1:B:133:SER:O	2.17	0.45
1:B:136:LYS:O	1:B:140:LEU:HG	2.17	0.44
1:B:181:ARG:HD2	1:B:182:LEU:N	2.32	0.44
1:B:20:VAL:HG21	1:B:53:VAL:HG23	1.99	0.44
1:A:266:ASN:HB3	1:A:269:ASP:HB2	2.00	0.44
1:A:320:GLU:HG2	1:A:321:PRO:HD2	2.00	0.44
1:A:280:ILE:HG23	1:B:108:PHE:HE2	1.81	0.44
1:A:283:ASP:OD1	1:A:283:ASP:N	2.38	0.44
1:A:269:ASP:OD1	2:A:403:HOH:O	2.21	0.43
1:A:83:ASP:OD1	1:A:84:GLY:N	2.51	0.43
1:A:325:GLY:HA3	1:A:373:VAL:CG1	2.47	0.43
1:B:180:HIS:CE1	1:B:353:PRO:HG2	2.54	0.43
1:A:177:THR:HA	1:A:182:LEU:HA	2.01	0.42
1:A:297:LEU:O	1:A:312:GLN:HA	2.19	0.42
1:A:126:PHE:CD1	1:A:226:SER:HB3	2.54	0.42
1:B:266:ASN:HB3	1:B:269:ASP:HB2	2.00	0.42
1:A:8:SER:O	2:A:404:HOH:O	2.21	0.42
1:B:187:MET:HG2	1:B:188:GLU:N	2.33	0.42
1:B:33:VAL:HG23	1:B:45:LYS:O	2.20	0.42
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.81	0.41
1:B:137:LEU:O	1:B:141:LEU:HD12	2.20	0.41
1:B:197:PRO:HB2	1:B:198:GLY:H	1.73	0.41
1:A:280:ILE:HA	1:B:73:LEU:HD11	2.02	0.41
1:A:259:ASN:HD22	1:A:346:MET:C	2.26	0.41
1:A:179:GLY:O	1:A:254:VAL:HG11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:PRO:O	1:A:250:ASP:C	2.63	0.41
1:A:19:ARG:HH21	1:A:215:GLU:HG3	1.85	0.41
1:B:189:ALA:HA	1:B:190:PRO:HD3	1.84	0.41
1:B:264:ILE:HB	1:B:316:THR:HB	2.02	0.41
1:A:175:VAL:HG22	1:A:184:GLN:HB2	2.01	0.41
1:B:160:ILE:HD12	1:B:174:LEU:HD22	2.03	0.41
1:B:349:ASP:OD1	1:B:349:ASP:N	2.52	0.41
1:B:55:GLU:HA	1:B:236:SER:O	2.21	0.40
1:B:132:LEU:HD23	1:B:133:SER:H	1.84	0.40
1:B:177:THR:HA	1:B:182:LEU:HA	2.02	0.40
1:B:231:ARG:HE	1:B:231:ARG:HB2	1.59	0.40
1:A:141:LEU:O	1:A:145:GLN:N	2.49	0.40
1:B:27:VAL:HB	1:B:30:LEU:HD12	2.04	0.40
1:A:182:LEU:HD11	1:A:251:TYR:HB2	2.03	0.40
1:A:276:ARG:NH2	1:B:82:PRO:HD3	2.37	0.40
1:A:338:LEU:HD12	1:A:343:MET:HG2	2.04	0.40
1:B:358:ASP:HB3	1:B:361:ASN:H	1.85	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	340/381 (89%)	323 (95%)	15 (4%)	2 (1%)	21	27
1	B	340/381 (89%)	326 (96%)	11 (3%)	3 (1%)	14	17
All	All	680/762 (89%)	649 (95%)	26 (4%)	5 (1%)	18	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	ASP

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Mol	Chain	Res	Type
1	B	250	ASP
1	B	197	PRO
1	A	197	PRO
1	B	179	GLY

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	265/335 (79%)	264 (100%)	1 (0%)	84	89
1	B	267/335 (80%)	266 (100%)	1 (0%)	84	89
All	All	532/670 (79%)	530 (100%)	2 (0%)	84	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	B	268	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	210	GLN
1	A	302	ASN
1	B	294	HIS
1	B	302	ASN
1	B	312	GLN
1	B	327	ASN
1	B	337	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	349/381 (91%)	1.95	150 (42%)  	34, 66, 98, 131	1 (0%)
1	B	351/381 (92%)	2.13	168 (47%)  	35, 67, 102, 178	1 (0%)
All	All	700/762 (91%)	2.04	318 (45%)  	34, 66, 101, 178	2 (0%)

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	HIS	11.7
1	A	287	ALA	9.0
1	B	257	LEU	7.4
1	A	27	VAL	7.2
1	B	175	VAL	6.7
1	B	314	ALA	6.6
1	A	45	LYS	6.6
1	B	328	SER	6.3
1	B	185	VAL	6.1
1	A	171	LYS	6.0
1	A	236	SER	5.9
1	B	327	ASN	5.9
1	B	49	LEU	5.6
1	B	332	LEU	5.6
1	B	277	VAL	5.4
1	B	234	LEU	5.2
1	B	362	ALA	5.1
1	B	73	LEU	5.1
1	B	17	VAL	4.9
1	B	146	PHE	4.9
1	B	147	ALA	4.9
1	A	350	ALA	4.8
1	B	366	TYR	4.8
1	B	131	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	161	TYR	4.7
1	B	263	LEU	4.7
1	A	235	GLY	4.6
1	A	60	ASN	4.6
1	B	265	VAL	4.6
1	B	276	ARG	4.6
1	B	301	VAL	4.5
1	A	288	VAL	4.4
1	A	172	LEU	4.3
1	A	248	PHE	4.2
1	B	368	LEU	4.2
1	A	47	THR	4.2
1	B	57	PHE	4.2
1	B	108	PHE	4.2
1	A	168	ASP	4.2
1	A	34	LEU	4.2
1	B	170	LEU	4.2
1	B	166	HIS	4.0
1	B	201	ILE	3.9
1	A	165	VAL	3.9
1	A	178	ASP	3.9
1	B	55	GLU	3.9
1	B	60	ASN	3.8
1	A	297	LEU	3.8
1	A	197	PRO	3.8
1	B	191	SER	3.8
1	B	307	GLY	3.8
1	A	69	VAL	3.8
1	A	314	ALA	3.8
1	A	216	GLU	3.8
1	B	221	VAL	3.8
1	A	239	PHE	3.8
1	B	53	VAL	3.7
1	B	132	LEU	3.7
1	A	72	TYR	3.7
1	B	26	THR	3.7
1	B	306	SER	3.7
1	A	179	GLY	3.7
1	B	351	VAL	3.6
1	A	126	PHE	3.6
1	A	182	LEU	3.6
1	B	190	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	324	ILE	3.6
1	A	362	ALA	3.6
1	B	209	LEU	3.6
1	B	258	GLY	3.6
1	A	321	PRO	3.6
1	A	260	ASP	3.6
1	B	85	SER	3.5
1	B	179	GLY	3.5
1	A	279	THR	3.5
1	B	271	SER	3.5
1	A	219	GLY	3.5
1	B	300	VAL	3.5
1	A	189	ALA	3.5
1	A	180	HIS	3.5
1	B	290	LEU	3.4
1	A	90	SER	3.4
1	A	201	ILE	3.4
1	B	9	GLN	3.4
1	B	365	LEU	3.4
1	B	352	ALA	3.4
1	A	215	GLU	3.4
1	A	317	TYR	3.4
1	B	129	ARG	3.4
1	A	128	CYS	3.3
1	A	245	ASP	3.3
1	A	191	SER	3.3
1	A	43	GLN	3.3
1	B	35	ILE	3.3
1	B	64	ALA	3.3
1	B	101	ILE	3.3
1	B	239	PHE	3.3
1	B	3	ILE	3.3
1	B	118	PHE	3.2
1	A	263	LEU	3.2
1	A	169	VAL	3.2
1	A	354	ALA	3.2
1	A	55	GLU	3.2
1	A	74	LEU	3.2
1	B	51	LEU	3.2
1	A	254	VAL	3.2
1	A	88	VAL	3.1
1	A	280	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	47	THR	3.1
1	B	160	ILE	3.1
1	A	265	VAL	3.1
1	B	109	GLN	3.1
1	A	118	PHE	3.1
1	A	345	PHE	3.1
1	B	48	ASP	3.1
1	B	130	PHE	3.1
1	B	186	ASP	3.1
1	B	341	ASP	3.1
1	B	14	LEU	3.0
1	A	109	GLN	3.0
1	B	58	THR	3.0
1	B	144	THR	3.0
1	B	245	ASP	3.0
1	A	327	ASN	3.0
1	B	195	GLY	3.0
1	A	238	VAL	3.0
1	A	217	ILE	3.0
1	A	134	ALA	3.0
1	A	203	ARG	3.0
1	B	127	GLY	3.0
1	B	165	VAL	2.9
1	A	339	SER	2.9
1	A	104	GLY	2.9
1	B	229	LYS	2.9
1	B	162	PHE	2.9
1	A	129	ARG	2.9
1	B	330	TYR	2.9
1	B	236	SER	2.9
1	A	161	TYR	2.9
1	A	198	GLY	2.9
1	B	233	SER	2.8
1	B	171	LYS	2.8
1	A	199	VAL	2.8
1	A	237	VAL	2.8
1	A	344	VAL	2.8
1	A	347	LEU	2.8
1	B	192	GLY	2.8
1	B	91	VAL	2.8
1	B	27	VAL	2.8
1	B	167	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	194	ASP	2.8
1	A	39	ASN	2.8
1	B	20	VAL	2.8
1	A	313	LEU	2.8
1	B	267	ARG	2.8
1	B	237	VAL	2.7
1	B	213	LEU	2.7
1	B	322	LEU	2.7
1	B	66	ALA	2.7
1	B	36	ASP	2.7
1	B	302	ASN	2.7
1	A	221	VAL	2.7
1	A	44	LEU	2.7
1	B	34	LEU	2.7
1	B	225	LEU	2.7
1	A	64	ALA	2.7
1	A	163	HIS	2.7
1	A	65	GLY	2.7
1	A	91	VAL	2.7
1	A	301	VAL	2.7
1	B	56	SER	2.7
1	A	273	ALA	2.7
1	A	232	PHE	2.7
1	A	361	ASN	2.7
1	B	299	LEU	2.7
1	A	76	ASP	2.6
1	B	40	GLY	2.6
1	B	223	ILE	2.6
1	B	230	ILE	2.6
1	B	22	GLU	2.6
1	A	228	THR	2.6
1	B	72	TYR	2.6
1	A	83	ASP	2.6
1	B	198	GLY	2.6
1	A	114	PRO	2.6
1	A	49	LEU	2.6
1	A	299	LEU	2.6
1	A	289	LYS	2.6
1	B	76	ASP	2.6
1	A	358	ASP	2.6
1	B	200	ILE	2.6
1	A	137	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	42	VAL	2.6
1	B	25	ASN	2.6
1	B	222	CYS	2.6
1	A	196	MET	2.5
1	B	246	GLY	2.5
1	A	140	LEU	2.5
1	B	316	THR	2.5
1	A	5	VAL	2.5
1	B	367	VAL	2.5
1	A	226	SER	2.5
1	B	41	SER	2.5
1	A	190	PRO	2.5
1	B	256	PRO	2.5
1	A	92	ASP	2.5
1	B	21	VAL	2.5
1	B	139	HIS	2.5
1	B	336	GLY	2.5
1	A	270	PHE	2.5
1	A	303	ASN	2.5
1	B	193	VAL	2.5
1	A	315	ALA	2.5
1	A	77	ILE	2.4
1	A	324	ILE	2.4
1	B	81	LEU	2.4
1	A	274	VAL	2.4
1	A	70	PRO	2.4
1	A	113	LEU	2.4
1	A	368	LEU	2.4
1	B	88	VAL	2.4
1	A	66	ALA	2.4
1	A	176	ALA	2.4
1	A	204	LYS	2.4
1	A	234	LEU	2.4
1	B	313	LEU	2.4
1	A	20	VAL	2.4
1	A	343	MET	2.4
1	B	199	VAL	2.4
1	B	134	ALA	2.4
1	B	176	ALA	2.4
1	B	136	LYS	2.4
1	B	224	GLU	2.4
1	A	101	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	292	ILE	2.4
1	A	166	HIS	2.4
1	A	175	VAL	2.4
1	B	69	VAL	2.4
1	B	119	PRO	2.3
1	A	85	SER	2.3
1	B	65	GLY	2.3
1	B	270	PHE	2.3
1	B	205	ALA	2.3
1	A	202	PRO	2.3
1	A	267	ARG	2.3
1	A	108	PHE	2.3
1	A	86	GLU	2.3
1	A	360	ASN	2.3
1	A	271	SER	2.3
1	A	285	GLY	2.3
1	B	90	SER	2.3
1	B	163	HIS	2.3
1	B	182	LEU	2.3
1	A	102	VAL	2.3
1	B	62	GLU	2.3
1	B	244	VAL	2.3
1	A	231	ARG	2.3
1	A	81	LEU	2.3
1	A	225	LEU	2.3
1	A	264	ILE	2.3
1	A	220	ASP	2.3
1	A	57	PHE	2.3
1	B	38	GLU	2.3
1	A	193	VAL	2.3
1	A	82	PRO	2.3
1	B	350	ALA	2.2
1	B	264	ILE	2.2
1	B	5	VAL	2.2
1	B	274	VAL	2.2
1	A	192	GLY	2.2
1	B	235	GLY	2.2
1	A	170	LEU	2.2
1	A	355	LEU	2.2
1	B	29	ILE	2.2
1	A	99	MET	2.2
1	B	315	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	346	MET	2.2
1	A	68	THR	2.2
1	B	128	CYS	2.2
1	B	208	GLU	2.2
1	A	257	LEU	2.1
1	B	110	LEU	2.1
1	A	164	ILE	2.1
1	B	202	PRO	2.1
1	A	33	VAL	2.1
1	B	102	VAL	2.1
1	B	288	VAL	2.1
1	A	1	MET	2.1
1	B	99	MET	2.1
1	B	158	ASN	2.1
1	B	231	ARG	2.1
1	B	50	ASP	2.1
1	B	92	ASP	2.1
1	A	18	HIS	2.1
1	A	300	VAL	2.1
1	B	373	VAL	2.1
1	B	303	ASN	2.1
1	A	15	GLY	2.1
1	A	253	ARG	2.1
1	A	363	GLU	2.1
1	A	162	PHE	2.1
1	B	364	VAL	2.1
1	B	74	LEU	2.1
1	B	338	LEU	2.1
1	B	325	GLY	2.1
1	A	230	ILE	2.1
1	B	309	ALA	2.0
1	B	219	GLY	2.0
1	A	200	ILE	2.0
1	B	240	THR	2.0
1	B	311	ASP	2.0
1	A	105	CYS	2.0
1	B	248	PHE	2.0
1	A	46	ALA	2.0
1	B	137	LEU	2.0
1	B	227	GLU	2.0
1	B	164	ILE	2.0
1	B	220	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.