



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:58 AM UTC

PDB ID : 2AYU / pdb_00002ayu
Title : The structure of nucleosome assembly protein suggests a mechanism for histone binding and shuttling
Authors : Park, Y.J.; Luger, K.
Deposited on : 2005-09-08
Resolution : 3.00 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

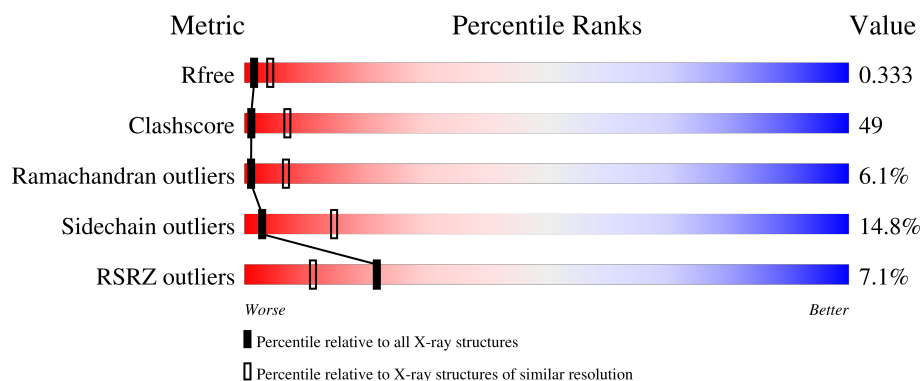
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	417	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2323 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 Nucleosome assembly protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	283	2323	1488	365	465	5	0	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.70Å 86.70Å 176.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 92.7 (50.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.280 0.315 , 0.333	Depositor DCC
R_{free} test set	1414 reflections (9.14%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2323	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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	1.10	7/2370 (0.3%)	1.51	32/3199 (1.0%)

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	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ILE	CB-CG1	33.12	2.19	1.53
1	A	328	GLU	C-N	-22.92	1.01	1.33
1	A	198	ILE	CB-CG2	-15.93	0.99	1.52
1	A	197	PRO	C-N	-10.40	1.19	1.33
1	A	198	ILE	C-N	-8.93	1.24	1.34
1	A	199	VAL	CB-CG2	-8.54	1.24	1.52
1	A	199	VAL	C-N	-5.03	1.26	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ILE	CA-CB-CG2	32.49	165.74	110.50
1	A	328	GLU	CA-C-N	20.64	160.97	121.54
1	A	328	GLU	C-N-CA	20.64	160.97	121.54
1	A	328	GLU	O-C-N	-19.98	96.34	123.11
1	A	198	ILE	CA-CB-CG1	-16.73	81.95	110.40
1	A	197	PRO	O-C-N	-11.15	107.59	122.64
1	A	199	VAL	CA-CB-CG2	11.05	129.18	110.40
1	A	197	PRO	CA-C-N	10.22	140.37	121.97
1	A	197	PRO	C-N-CA	10.22	140.37	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	PRO	CA-N-CD	-9.63	98.52	112.00
1	A	330	LEU	N-CA-C	-8.59	102.80	113.20
1	A	141	GLY	N-CA-C	-8.34	103.51	115.27
1	A	185	ILE	CA-C-N	8.19	128.24	119.89
1	A	185	ILE	C-N-CA	8.19	128.24	119.89
1	A	260	TYR	N-CA-C	-8.17	102.45	111.36
1	A	125	LEU	N-CA-C	-7.36	103.25	111.28
1	A	337	ARG	N-CA-C	-6.58	104.15	111.71
1	A	212	GLU	N-CA-C	-6.15	104.68	111.82
1	A	240	ASN	CA-C-N	6.07	125.46	118.85
1	A	240	ASN	C-N-CA	6.07	125.46	118.85
1	A	90	LYS	N-CA-C	-6.03	103.88	111.11
1	A	314	ASN	N-CA-C	-5.76	106.21	113.18
1	A	218	GLY	N-CA-C	5.74	120.02	111.18
1	A	199	VAL	CG1-CB-CG2	5.73	123.40	110.80
1	A	196	LEU	CA-C-N	-5.53	112.93	119.84
1	A	196	LEU	C-N-CA	-5.53	112.93	119.84
1	A	106	LEU	N-CA-C	-5.35	104.49	111.02
1	A	362	GLY	N-CA-C	-5.26	108.45	115.40
1	A	88	LEU	CA-C-N	5.10	125.38	119.92
1	A	88	LEU	C-N-CA	5.10	125.38	119.92
1	A	330	LEU	CB-CA-C	5.10	119.81	110.11
1	A	99	LEU	N-CA-C	-5.08	105.74	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	PRO	Mainchain,Peptide
1	A	328	GLU	Mainchain,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	2323	0	2237	224	1
All	All	2323	0	2237	224	1

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 49.

All (224) 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:198:ILE:N	1:A:198:ILE:CG1	2.00	1.24
1:A:198:ILE:CG1	1:A:198:ILE:CB	2.19	1.20
1:A:198:ILE:CD1	1:A:347:GLN:HG3	1.76	1.13
1:A:207:ASP:HB3	1:A:283:VAL:HG11	1.32	1.10
1:A:198:ILE:HD11	1:A:347:GLN:CG	1.82	1.08
1:A:320:LYS:HG2	1:A:323:ASN:HD21	1.19	1.05
1:A:198:ILE:HD11	1:A:347:GLN:HG3	1.37	1.02
1:A:245:ASN:HD21	1:A:275:SER:HB2	1.28	0.98
1:A:198:ILE:HD11	1:A:347:GLN:CD	1.88	0.98
1:A:198:ILE:N	1:A:198:ILE:HG12	1.79	0.97
1:A:282:ASN:OD1	1:A:284:THR:HG22	1.68	0.94
1:A:250:LYS:HE3	1:A:318:PRO:HG3	1.49	0.93
1:A:90:LYS:HG3	1:A:91:ASN:H	1.34	0.92
1:A:199:VAL:HG22	1:A:344:ILE:HG23	1.53	0.89
1:A:198:ILE:CG1	1:A:198:ILE:CA	2.51	0.89
1:A:329:GLU:O	1:A:333:ASP:HB3	1.73	0.87
1:A:198:ILE:CG1	1:A:198:ILE:CG2	2.52	0.87
1:A:198:ILE:HD12	1:A:347:GLN:HG3	1.57	0.86
1:A:245:ASN:ND2	1:A:275:SER:HB2	1.94	0.83
1:A:234:ARG:HE	1:A:247:ILE:HD11	1.44	0.82
1:A:90:LYS:HG3	1:A:91:ASN:N	1.92	0.82
1:A:113:PHE:CZ	1:A:117:MET:HE3	2.15	0.82
1:A:197:PRO:O	1:A:198:ILE:HG13	1.79	0.81
1:A:118:PHE:CZ	1:A:221:TYR:HB3	2.17	0.80
1:A:198:ILE:CD1	1:A:347:GLN:CG	2.50	0.80
1:A:198:ILE:CG1	1:A:198:ILE:HG23	2.13	0.78
1:A:319:PRO:HB2	1:A:338:LEU:HG	1.66	0.77
1:A:215:GLN:NE2	1:A:236:ASP:HA	1.99	0.77
1:A:198:ILE:N	1:A:198:ILE:HG13	1.98	0.77
1:A:81:ASP:O	1:A:85:VAL:HG12	1.84	0.76
1:A:256:LYS:HE3	1:A:256:LYS:H	1.51	0.75
1:A:237:SER:HB2	1:A:246:ASP:OD2	1.87	0.74
1:A:210:VAL:HG21	1:A:283:VAL:HG21	1.68	0.74
1:A:245:ASN:HD21	1:A:275:SER:CB	1.99	0.74
1:A:197:PRO:C	1:A:198:ILE:CG1	2.61	0.73
1:A:278:ASP:HB3	1:A:281:HIS:HB2	1.71	0.73
1:A:287:LEU:HD11	1:A:304:GLU:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:O	1:A:194:GLU:HG2	1.89	0.73
1:A:255:GLN:HG2	1:A:267:ASP:HB2	1.71	0.73
1:A:259:GLY:HA2	1:A:265:ILE:HD11	1.69	0.72
1:A:249:CYS:C	1:A:272:CYS:SG	2.73	0.72
1:A:120:LEU:O	1:A:120:LEU:HD23	1.90	0.71
1:A:132:TRP:O	1:A:135:ARG:HG3	1.90	0.70
1:A:114:GLN:HG3	1:A:258:LEU:HD21	1.71	0.70
1:A:198:ILE:CD1	1:A:198:ILE:HG23	2.22	0.70
1:A:185:ILE:HD11	1:A:188:PHE:HD1	1.56	0.70
1:A:363:ALA:HB1	1:A:367:PHE:CE1	2.28	0.69
1:A:303:ILE:HD12	1:A:304:GLU:H	1.58	0.69
1:A:266:TYR:HB3	1:A:342:TYR:CE2	2.27	0.69
1:A:256:LYS:H	1:A:256:LYS:CE	2.05	0.68
1:A:248:LEU:HD22	1:A:274:ILE:HG12	1.76	0.68
1:A:203:ILE:HD12	1:A:203:ILE:O	1.93	0.67
1:A:240:ASN:HD22	1:A:241:PRO:CD	2.06	0.67
1:A:320:LYS:CG	1:A:323:ASN:HD21	2.03	0.67
1:A:245:ASN:N	1:A:245:ASN:HD22	1.92	0.67
1:A:274:ILE:HD12	1:A:276:TRP:CH2	2.31	0.66
1:A:320:LYS:HG2	1:A:323:ASN:ND2	2.03	0.66
1:A:185:ILE:HD11	1:A:188:PHE:CD1	2.31	0.65
1:A:311:SER:H	1:A:314:ASN:ND2	1.95	0.65
1:A:353:ILE:HB	1:A:354:PRO:HD3	1.78	0.65
1:A:197:PRO:C	1:A:198:ILE:HG13	2.21	0.65
1:A:194:GLU:O	1:A:200:CYS:HB3	1.96	0.64
1:A:163:THR:HG23	1:A:166:LEU:HD12	1.79	0.64
1:A:245:ASN:HD22	1:A:245:ASN:H	1.45	0.63
1:A:309:ILE:HG22	1:A:310:GLU:N	2.13	0.63
1:A:70:ILE:C	1:A:72:ASP:H	2.07	0.62
1:A:185:ILE:HG12	1:A:185:ILE:O	1.97	0.62
1:A:190:LEU:C	1:A:190:LEU:HD13	2.25	0.62
1:A:250:LYS:HE3	1:A:318:PRO:CG	2.26	0.62
1:A:366:GLU:HG2	1:A:370:GLU:OE1	2.00	0.62
1:A:70:ILE:HG22	1:A:70:ILE:O	2.01	0.61
1:A:331:GLU:OE1	1:A:332:GLU:HG3	2.01	0.61
1:A:266:TYR:OH	1:A:346:GLU:HG2	2.00	0.61
1:A:72:ASP:C	1:A:74:LEU:H	2.08	0.61
1:A:120:LEU:HD23	1:A:120:LEU:C	2.26	0.60
1:A:285:VAL:HG21	1:A:306:ILE:HG23	1.83	0.60
1:A:90:LYS:O	1:A:94:GLU:HG3	2.02	0.60
1:A:302:THR:HG22	1:A:302:THR:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:CG	1:A:91:ASN:H	2.12	0.60
1:A:154:GLN:NE2	1:A:167:VAL:H	1.99	0.60
1:A:249:CYS:H	1:A:272:CYS:HB2	1.67	0.60
1:A:348:LEU:H	1:A:348:LEU:HD22	1.65	0.60
1:A:249:CYS:O	1:A:272:CYS:SG	2.61	0.58
1:A:210:VAL:HG22	1:A:242:PHE:CE2	2.39	0.58
1:A:113:PHE:CZ	1:A:117:MET:CE	2.87	0.58
1:A:215:GLN:NE2	1:A:236:ASP:CA	2.66	0.57
1:A:328:GLU:HG2	1:A:332:GLU:OE2	2.04	0.57
1:A:111:LYS:O	1:A:115:VAL:HG23	2.03	0.57
1:A:200:CYS:O	1:A:203:ILE:HG13	2.05	0.57
1:A:198:ILE:HG23	1:A:198:ILE:HD13	1.86	0.57
1:A:215:GLN:HE21	1:A:236:ASP:CB	2.17	0.57
1:A:215:GLN:HE21	1:A:236:ASP:HB2	1.68	0.57
1:A:259:GLY:CA	1:A:265:ILE:HD11	2.35	0.57
1:A:199:VAL:CG1	1:A:199:VAL:O	2.53	0.57
1:A:363:ALA:HB1	1:A:367:PHE:HE1	1.70	0.57
1:A:115:VAL:HG12	1:A:119:GLU:OE2	2.05	0.57
1:A:363:ALA:O	1:A:367:PHE:HD1	1.88	0.56
1:A:237:SER:CB	1:A:246:ASP:OD2	2.54	0.56
1:A:168:ASP:O	1:A:169:GLU:C	2.49	0.56
1:A:94:GLU:HA	1:A:97:LEU:HD23	1.88	0.56
1:A:70:ILE:HD12	1:A:70:ILE:N	2.22	0.55
1:A:240:ASN:HD22	1:A:241:PRO:HD2	1.71	0.55
1:A:203:ILE:HD12	1:A:203:ILE:C	2.32	0.55
1:A:321:ILE:O	1:A:322:GLN:C	2.50	0.55
1:A:240:ASN:HD22	1:A:241:PRO:N	2.05	0.54
1:A:117:MET:HG3	1:A:121:GLU:OE2	2.07	0.54
1:A:291:LYS:HG2	1:A:302:THR:HA	1.90	0.54
1:A:231:LEU:O	1:A:249:CYS:HA	2.08	0.54
1:A:215:GLN:HE22	1:A:236:ASP:HA	1.71	0.54
1:A:320:LYS:HZ3	1:A:323:ASN:CG	2.15	0.54
1:A:129:LYS:HB2	1:A:130:PRO:HD3	1.90	0.53
1:A:157:VAL:HG13	1:A:162:GLU:O	2.09	0.53
1:A:139:ILE:HD13	1:A:188:PHE:CD2	2.44	0.52
1:A:126:GLN:O	1:A:130:PRO:HD3	2.09	0.52
1:A:319:PRO:HD2	1:A:338:LEU:HD23	1.92	0.52
1:A:189:TRP:NE1	1:A:216:ASP:HA	2.25	0.52
1:A:94:GLU:O	1:A:97:LEU:HB2	2.09	0.52
1:A:364:ALA:O	1:A:368:GLU:HG3	2.09	0.52
1:A:253:PHE:O	1:A:267:ASP:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:O	1:A:126:GLN:HG2	2.10	0.51
1:A:210:VAL:HG22	1:A:242:PHE:CZ	2.45	0.51
1:A:340:LEU:HD23	1:A:341:ASP:N	2.26	0.51
1:A:198:ILE:HD11	1:A:347:GLN:OE1	2.08	0.51
1:A:274:ILE:HB	1:A:276:TRP:CZ3	2.45	0.51
1:A:323:ASN:N	1:A:323:ASN:HD22	2.09	0.51
1:A:146:LYS:HG2	1:A:149:GLN:CD	2.36	0.51
1:A:234:ARG:NE	1:A:247:ILE:HD11	2.20	0.51
1:A:285:VAL:CG2	1:A:306:ILE:HG23	2.40	0.51
1:A:133:GLU:O	1:A:136:SER:HB3	2.11	0.50
1:A:269:ALA:HB2	1:A:342:TYR:HE1	1.76	0.50
1:A:369:PHE:HD1	1:A:369:PHE:N	2.10	0.49
1:A:106:LEU:O	1:A:110:GLU:HG3	2.13	0.49
1:A:240:ASN:HD22	1:A:240:ASN:C	2.20	0.49
1:A:256:LYS:HD2	1:A:256:LYS:N	2.28	0.49
1:A:205:ASP:OD2	1:A:205:ASP:N	2.45	0.49
1:A:256:LYS:H	1:A:256:LYS:CD	2.25	0.49
1:A:348:LEU:HD22	1:A:348:LEU:N	2.28	0.49
1:A:357:VAL:O	1:A:360:PHE:HB3	2.13	0.48
1:A:369:PHE:N	1:A:369:PHE:CD1	2.80	0.48
1:A:70:ILE:O	1:A:72:ASP:N	2.39	0.48
1:A:102:LEU:HD12	1:A:105:GLU:OE1	2.13	0.48
1:A:112:GLU:OE2	1:A:116:GLU:HG3	2.13	0.48
1:A:213:TYR:CZ	1:A:241:PRO:HD3	2.49	0.48
1:A:278:ASP:HB3	1:A:281:HIS:H	1.77	0.48
1:A:366:GLU:O	1:A:368:GLU:N	2.46	0.48
1:A:323:ASN:O	1:A:325:ASP:N	2.47	0.48
1:A:344:ILE:O	1:A:348:LEU:HD22	2.13	0.48
1:A:256:LYS:N	1:A:256:LYS:CD	2.76	0.48
1:A:249:CYS:H	1:A:272:CYS:CB	2.25	0.48
1:A:250:LYS:HG2	1:A:315:PHE:CZ	2.49	0.48
1:A:266:TYR:HB3	1:A:342:TYR:CD2	2.48	0.48
1:A:256:LYS:HD2	1:A:257:GLU:H	1.79	0.48
1:A:160:LEU:HD13	1:A:367:PHE:CE2	2.49	0.47
1:A:161:ASN:C	1:A:161:ASN:HD22	2.21	0.47
1:A:344:ILE:O	1:A:348:LEU:CD2	2.63	0.47
1:A:72:ASP:C	1:A:74:LEU:N	2.70	0.47
1:A:120:LEU:O	1:A:123:LYS:HB3	2.15	0.47
1:A:243:PHE:CZ	1:A:248:LEU:HD11	2.50	0.47
1:A:309:ILE:CG2	1:A:310:GLU:N	2.77	0.47
1:A:210:VAL:HG13	1:A:242:PHE:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:O	1:A:185:ILE:CG1	2.63	0.46
1:A:331:GLU:CD	1:A:332:GLU:N	2.74	0.46
1:A:242:PHE:CD1	1:A:242:PHE:N	2.83	0.46
1:A:328:GLU:C	1:A:330:LEU:H	2.21	0.46
1:A:135:ARG:O	1:A:139:ILE:HG13	2.16	0.46
1:A:215:GLN:O	1:A:216:ASP:HB2	2.16	0.46
1:A:320:LYS:HZ1	1:A:334:LEU:HD22	1.82	0.45
1:A:366:GLU:C	1:A:368:GLU:N	2.74	0.45
1:A:74:LEU:O	1:A:78:VAL:HB	2.16	0.45
1:A:358:ASP:HB3	1:A:364:ALA:HB2	1.98	0.45
1:A:198:ILE:CD1	1:A:198:ILE:CG2	2.89	0.45
1:A:258:LEU:HD11	1:A:264:PHE:CD2	2.51	0.45
1:A:131:ILE:O	1:A:134:GLN:HB2	2.17	0.45
1:A:74:LEU:N	1:A:74:LEU:HD23	2.31	0.45
1:A:303:ILE:HD12	1:A:304:GLU:N	2.28	0.45
1:A:287:LEU:CD1	1:A:304:GLU:HB2	2.43	0.44
1:A:83:GLY:O	1:A:84:TYR:C	2.61	0.44
1:A:197:PRO:C	1:A:198:ILE:HG12	2.32	0.44
1:A:291:LYS:HE2	1:A:302:THR:OG1	2.18	0.44
1:A:70:ILE:O	1:A:70:ILE:CG2	2.65	0.44
1:A:241:PRO:O	1:A:277:LYS:HD3	2.17	0.44
1:A:215:GLN:NE2	1:A:236:ASP:CB	2.80	0.44
1:A:321:ILE:O	1:A:323:ASN:ND2	2.50	0.44
1:A:328:GLU:HA	1:A:332:GLU:OE2	2.18	0.44
1:A:235:PHE:CE1	1:A:248:LEU:HD12	2.53	0.43
1:A:287:LEU:HD11	1:A:304:GLU:CB	2.44	0.43
1:A:73:ARG:O	1:A:77:LEU:HB2	2.19	0.43
1:A:234:ARG:HA	1:A:247:ILE:HG12	2.01	0.43
1:A:289:MET:HE3	1:A:304:GLU:HB3	2.01	0.43
1:A:287:LEU:HD13	1:A:306:ILE:CD1	2.49	0.43
1:A:70:ILE:N	1:A:70:ILE:CD1	2.82	0.43
1:A:366:GLU:C	1:A:368:GLU:H	2.27	0.43
1:A:146:LYS:N	1:A:146:LYS:HD3	2.34	0.42
1:A:209:GLU:O	1:A:212:GLU:HB2	2.20	0.42
1:A:232:LEU:HD12	1:A:232:LEU:N	2.33	0.42
1:A:331:GLU:O	1:A:335:GLU:HB2	2.19	0.42
1:A:204:THR:O	1:A:205:ASP:C	2.63	0.42
1:A:340:LEU:HD23	1:A:340:LEU:C	2.44	0.42
1:A:344:ILE:HG22	1:A:348:LEU:HD21	2.01	0.42
1:A:250:LYS:NZ	1:A:341:ASP:OD1	2.42	0.42
1:A:334:LEU:HA	1:A:337:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:O	1:A:197:PRO:C	2.56	0.42
1:A:150:ILE:HD13	1:A:150:ILE:HA	1.89	0.42
1:A:311:SER:H	1:A:314:ASN:HD22	1.66	0.42
1:A:199:VAL:O	1:A:199:VAL:HG12	2.20	0.41
1:A:96:LEU:HA	1:A:99:LEU:HB2	2.02	0.41
1:A:348:LEU:HD12	1:A:352:LEU:HD12	2.02	0.41
1:A:120:LEU:C	1:A:120:LEU:CD2	2.93	0.41
1:A:331:GLU:O	1:A:332:GLU:C	2.63	0.41
1:A:190:LEU:HD11	1:A:194:GLU:OE2	2.20	0.41
1:A:250:LYS:HG2	1:A:315:PHE:CE2	2.56	0.41
1:A:320:LYS:HD2	1:A:323:ASN:OD1	2.20	0.41
1:A:268:HIS:CD2	1:A:269:ALA:N	2.89	0.41
1:A:71:GLN:HE21	1:A:71:GLN:HB2	1.55	0.41
1:A:146:LYS:O	1:A:147:PRO:C	2.64	0.41
1:A:325:ASP:N	1:A:325:ASP:OD2	2.54	0.41
1:A:329:GLU:C	1:A:331:GLU:H	2.29	0.41
1:A:340:LEU:O	1:A:344:ILE:HG13	2.22	0.40
1:A:88:LEU:HA	1:A:89:PRO:HD3	1.95	0.40
1:A:230:LYS:HA	1:A:250:LYS:O	2.21	0.40
1:A:240:ASN:HA	1:A:241:PRO:HD3	1.71	0.40
1:A:282:ASN:HB3	1:A:285:VAL:HG12	2.03	0.40
1:A:150:ILE:HG22	1:A:170:GLU:OE1	2.22	0.40
1:A:161:ASN:ND2	1:A:161:ASN:O	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:MET:SD	1:A:117:MET:SD[8_665]	1.98	0.22

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	277/417 (66%)	237 (86%)	23 (8%)	17 (6%)	1 7

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ILE
1	A	273	GLU
1	A	325	ASP
1	A	327	ASP
1	A	329	GLU
1	A	169	GLU
1	A	320	LYS
1	A	322	GLN
1	A	324	GLU
1	A	326	GLN
1	A	367	PHE
1	A	71	GLN
1	A	168	ASP
1	A	197	PRO
1	A	272	CYS
1	A	318	PRO
1	A	303	ILE

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	257/376 (68%)	219 (85%)	38 (15%)	3 15

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	74	LEU
1	A	77	LEU
1	A	85	VAL

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Mol	Chain	Res	Type
1	A	97	LEU
1	A	102	LEU
1	A	103	GLN
1	A	106	LEU
1	A	134	GLN
1	A	147	PRO
1	A	150	ILE
1	A	157	VAL
1	A	165	LEU
1	A	185	ILE
1	A	187	SER
1	A	197	PRO
1	A	198	ILE
1	A	202	THR
1	A	205	ASP
1	A	245	ASN
1	A	255	GLN
1	A	256	LYS
1	A	258	LEU
1	A	263	ASP
1	A	268	HIS
1	A	273	GLU
1	A	285	VAL
1	A	305	LYS
1	A	306	ILE
1	A	321	ILE
1	A	322	GLN
1	A	323	ASN
1	A	327	ASP
1	A	332	GLU
1	A	335	GLU
1	A	340	LEU
1	A	352	LEU
1	A	357	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	122	ASN
1	A	154	GLN
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	195	ASN
1	A	215	GLN
1	A	240	ASN
1	A	245	ASN
1	A	255	GLN
1	A	322	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](#)

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](#)

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	197:PRO	C	198:ILE	N	1.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	328:GLU	C	329:GLU	N	1.01

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	283/417 (67%)	0.31	20 (7%) 22 11	15, 15, 15, 15	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	GLU	5.5
1	A	330	LEU	5.2
1	A	325	ASP	4.6
1	A	321	ILE	4.4
1	A	322	GLN	4.2
1	A	326	GLN	4.1
1	A	292	GLN	4.1
1	A	272	CYS	3.5
1	A	72	ASP	3.4
1	A	327	ASP	3.4
1	A	303	ILE	3.1
1	A	171	GLU	3.0
1	A	323	ASN	2.9
1	A	331	GLU	2.8
1	A	334	LEU	2.7
1	A	329	GLU	2.5
1	A	328	GLU	2.3
1	A	335	GLU	2.2
1	A	324	GLU	2.0
1	A	70	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.