



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2AYU
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

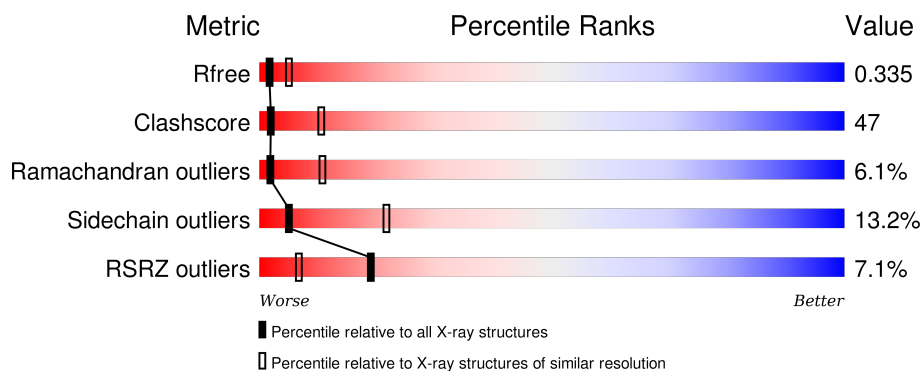
1 Overall quality at a glance

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

Chain A:

5% 26% 32% 9% 32%

MET	ALA	E133	A208	V283	I348
SER	ASN	Q134	E209	V285	L352
ASP	GLN	R135	V210	L286	I353
PRO	PRO	S136	E211	L287	P354
ILE	LEU	I139	E212	K291	V357
ARG	LEU	K146	E214	Q292	D358
THR	GLN	K149	D215	ARG	K359
LYS	LYS	Q149	D216	ASN	F360
PRO	PRO	I150	Y221	LYS	A363
SER	SER	Q154	K230	THR	A364
MET	MET	V157	L231	LYS	L365
GLN	GLN	L160	L232	VAL	E366
ILE	ILE	N161	F233	ARG	F367
ASP	ASP	E162	R234	T302	E368
ASN	ALA	T163	F235	I303	F369
ALA	ALA	E164	D236	I304	E370
THR	THR	L165	S237	K305	ASP
PRO	PRO	L166	N240	I306	GLU
HIS	HIS	V167	P241	I309	GLU
ASN	ASN	D168	F242	E310	GLU
THR	THR	E169	F243	S311	GLU
ALA	ALA	E170	T244	N314	ASP
SER	SER	E171	N245	F315	GLU
VAL	VAL	L175	D246	P318	GLU
LEU	LEU	ALA	T247	F319	ASP
ASN	ASN	GLN	L248	K320	GLU
PRO	PRO	ASP	K250	I321	GLU
SER	SER	ASP	F253	K322	ASP
TYR	TYR	GLU	Y254	N323	ASP
LYS	LYS	GLU	Q255	E324	HIS
ASN	ASN	GLU	K256	N325	GLY
GLY	GLY	Q181	E257	Q326	LEU
ASN	ASN	V182	L258	D327	GLU
PRO	PRO	E185	G259	K328	ASP
VAL	VAL	F186	D263	E329	ASP
ARG	ARG	S187	F264	L330	ASP
ALA	ALA	F188	L265	E331	GLY
GLN	GLN	W189	Y266	E332	GLU
GLU	GLU	L190	D267	D333	SER
GLN	GLN	E194	H268	L334	ALA
ASP	ASP	P197	A269	E385	GLU
LYS	LYS	P198	C272	E386	GLU
ILE	ILE	V199	E273	R337	GLN
GLY	GLY	C200	L274	L338	ASP
THR	THR	D201	S275	A339	ASP
ILE	ILE	T202	N276	D341	PHE
ASN	ASN	L203	K277	E342	ALA
GLU	GLU	D204	N279	S343	GLY
ASP	ASP	T205	A280	I344	ARG
TYR	TYR	P206	E281	G345	PRO
ILE	ILE	R207	N282	F346	GLU
LEU	LEU	K208	V283	I347	ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.70 Å 86.70 Å 176.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 48.61 – 2.84	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 86.7 (48.61-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 2.86 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.280 0.317 , 0.335	Depositor DCC
R_{free} test set	1340 reflections (10.24%)	DCC
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 4.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 15466 reflections	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.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.89	5/2370 (0.2%)	1.08	12/3199 (0.4%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ILE	CB-CG1	23.44	2.19	1.54
1	A	198	ILE	CB-CG2	-17.05	0.99	1.52
1	A	328	GLU	C-N	-14.11	1.01	1.34
1	A	199	VAL	CB-CG2	-13.57	1.24	1.52
1	A	197	PRO	C-N	-6.33	1.19	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ILE	CA-CB-CG2	27.42	165.74	110.90
1	A	328	GLU	O-C-N	-16.47	96.34	122.70
1	A	328	GLU	C-N-CA	15.71	160.97	121.70
1	A	198	ILE	CA-CB-CG1	-15.29	81.95	111.00
1	A	199	VAL	CA-CB-CG2	12.19	129.18	110.90
1	A	328	GLU	CA-C-N	11.14	141.71	117.20
1	A	197	PRO	O-C-N	-9.45	107.59	122.70
1	A	197	PRO	CA-N-CD	-9.27	98.52	111.50
1	A	199	VAL	CG1-CB-CG2	7.81	123.40	110.90
1	A	197	PRO	C-N-CA	7.47	140.37	121.70
1	A	198	ILE	CG1-CB-CG2	-6.44	97.23	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	LEU	CB-CA-C	5.06	119.81	110.20

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	214	1
All	All	2323	0	2237	214	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 47.

All (214) 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: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:198:ILE:HD11	1:A:347:GLN:CD	1.88	0.93
1:A:90:LYS:HG3	1:A:91:ASN:H	1.34	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG23	1:A:198:ILE:CG1	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:H	1:A:256:LYS:HE3	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:287:LEU:HD11	1:A:304:GLU:HB2	1.70	0.73
1:A:278:ASP:HB3	1:A:281:HIS:HB2	1.71	0.73
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: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:198:ILE:CD1	1:A:198:ILE:HG23	2.22	0.70
1:A:114:GLN:HG3	1:A:258:LEU:HD21	1.71	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:197:PRO:C	1:A:198:ILE:CG1	2.61	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:O	1:A:203:ILE:HD12	1.93	0.67
1:A:240:ASN:HD22	1:A:241:PRO:CD	2.06	0.67
1:A:249:CYS:C	1:A:272:CYS:SG	2.73	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H	1:A:245:ASN:HD22	1.45	0.63
1:A:309:ILE:HG22	1:A:310:GLU:N	2.13	0.63
1:A:185:ILE:HG12	1:A:185:ILE:O	1.97	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:O	1:A:70:ILE:HG22	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: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:O	1:A:302:THR:HG22	2.00	0.60
1:A:90:LYS:CG	1:A:91:ASN:H	2.12	0.60
1:A:197:PRO:C	1:A:198:ILE:HG13	2.21	0.60
1:A:249:CYS:H	1:A:272:CYS:HB2	1.67	0.60
1:A:154:GLN:NE2	1:A:167:VAL:H	1.99	0.60
1:A:348:LEU:HD22	1:A:348:LEU:H	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:70:ILE:C	1:A:72:ASP:H	2.07	0.57
1:A:215:GLN:NE2	1:A:236:ASP:CA	2.66	0.57
1:A:190:LEU:C	1:A:190:LEU:HD13	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:C	1:A:74:LEU:H	2.08	0.56
1:A:120:LEU:HD23	1:A:120:LEU:C	2.26	0.56
1:A:94:GLU:HA	1:A:97:LEU:HD23	1.88	0.56
1:A:70:ILE:N	1:A:70:ILE:HD12	2.22	0.55
1:A:240:ASN:HD22	1:A:241:PRO:HD2	1.71	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:157:VAL:HG13	1:A:162:GLU:O	2.09	0.53
1:A:129:LYS:HB2	1:A:130:PRO:HD3	1.90	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
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:168:ASP:O	1:A:169:GLU:C	2.49	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:323:ASN:N	1:A:323:ASN:HD22	2.09	0.51
1:A:274:ILE:HB	1:A:276:TRP:CZ3	2.45	0.51
1:A:285:VAL:CG2	1:A:306:ILE:HG23	2.40	0.51
1:A:234:ARG:NE	1:A:247:ILE:HD11	2.20	0.51
1:A:133:GLU:O	1:A:136:SER:HB3	2.11	0.50
1:A:321:ILE:O	1:A:322:GLN:C	2.50	0.50
1:A:203:ILE:C	1:A:203:ILE:HD12	2.32	0.50
1:A:113:PHE:CZ	1:A:117:MET:HE2	2.46	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:256:LYS:N	1:A:256:LYS:HD2	2.28	0.49
1:A:256:LYS:CD	1:A:256:LYS:H	2.25	0.49
1:A:205:ASP:OD2	1:A:205:ASP:N	2.45	0.49
1:A:348:LEU:HD22	1:A:348:LEU:N	2.28	0.49
1:A:369:PHE:CD1	1:A:369:PHE:N	2.80	0.48
1:A:357:VAL:O	1:A:360:PHE:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:278:ASP:HB3	1:A:281:HIS:H	1.77	0.48
1:A:213:TYR:CZ	1:A:241:PRO:HD3	2.49	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:CD	1:A:256:LYS:N	2.76	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:249:CYS:H	1:A:272:CYS:CB	2.25	0.48
1:A:256:LYS:HD2	1:A:257:GLU:H	1.79	0.48
1:A:344:ILE:O	1:A:348:LEU:CD2	2.63	0.47
1:A:160:LEU:HD13	1:A:367:PHE:CE2	2.49	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:320:LYS:HZ1	1:A:334:LEU:HD22	1.80	0.47
1:A:210:VAL:HG13	1:A:242:PHE:CD1	2.50	0.47
1:A:320:LYS:HZ3	1:A:323:ASN:CG	2.18	0.46
1:A:113:PHE:CZ	1:A:117:MET:HE3	2.48	0.46
1:A:185:ILE:CG1	1:A:185:ILE:O	2.63	0.46
1:A:242:PHE:CD1	1:A:242:PHE:N	2.83	0.46
1:A:135:ARG:O	1:A:139:ILE:HG13	2.16	0.46
1:A:146:LYS:HG2	1:A:149:GLN:CD	2.36	0.46
1:A:215:GLN:O	1:A:216:ASP:HB2	2.16	0.46
1:A:358:ASP:HB3	1:A:364:ALA:HB2	1.98	0.45
1:A:74:LEU:O	1:A:78:VAL:HB	2.16	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:72:ASP:C	1:A:74:LEU:N	2.70	0.44
1:A:291:LYS:HE2	1:A:302:THR:OG1	2.18	0.44
1:A:240:ASN:C	1:A:240:ASN:HD22	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:234:ARG:HA	1:A:247:ILE:HG12	2.01	0.43
1:A:73:ARG:O	1:A:77:LEU:HB2	2.19	0.43
1:A:287:LEU:HD13	1:A:306:ILE:CD1	2.49	0.43
1:A:161:ASN:C	1:A:161:ASN:HD22	2.21	0.43
1:A:70:ILE:N	1:A:70:ILE:CD1	2.82	0.43
1:A:146:LYS:HD3	1:A:146:LYS:N	2.34	0.42
1:A:209:GLU:O	1:A:212:GLU:HB2	2.20	0.42
1:A:232:LEU:N	1:A:232:LEU:HD12	2.33	0.42
1:A:331:GLU:O	1:A:335:GLU:HB2	2.19	0.42
1:A:344:ILE:HG22	1:A:348:LEU:HD21	2.01	0.42
1:A:334:LEU:HA	1:A:337:ARG:NH1	2.34	0.42
1:A:250:LYS:NZ	1:A:341:ASP:OD1	2.42	0.42
1:A:311:SER:H	1:A:314:ASN:HD22	1.66	0.42
1:A:150:ILE:HD13	1:A:150:ILE:HA	1.89	0.42
1:A:366:GLU:C	1:A:368:GLU:N	2.74	0.42
1:A:328:GLU:C	1:A:330:LEU:H	2.21	0.42
1:A:199:VAL:O	1:A:199:VAL:HG12	2.20	0.41
1:A:331:GLU:CD	1:A:332:GLU:N	2.74	0.41
1:A:348:LEU:HD12	1:A:352:LEU:HD12	2.02	0.41
1:A:96:LEU:HA	1:A:99:LEU:HB2	2.02	0.41
1:A:190:LEU:HD11	1:A:194:GLU:OE2	2.20	0.41
1:A:320:LYS:HD2	1:A:323:ASN:OD1	2.20	0.41
1:A:250:LYS:HG2	1:A:315:PHE:CE2	2.56	0.41
1:A:268:HIS:CD2	1:A:269:ALA:N	2.89	0.41
1:A:325:ASP:N	1:A:325:ASP:OD2	2.54	0.41
1:A:71:GLN:HE21	1:A:71:GLN:HB2	1.55	0.41
1:A:340:LEU:O	1:A:344:ILE:HG13	2.22	0.40
1:A:282:ASN:HB3	1:A:285:VAL:HG12	2.03	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:88:LEU:HA	1:A:89:PRO:HD3	1.95	0.40
1:A:150:ILE:HG22	1:A:170:GLU:OE1	2.22	0.40
1:A:161:ASN:O	1:A:161:ASN:ND2	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 [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	277/417 (66%)	237 (86%)	23 (8%)	17 (6%)	2 11

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 [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	257/376 (68%)	223 (87%)	34 (13%)	5	22

All (34) 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	97	LEU
1	A	102	LEU
1	A	106	LEU
1	A	134	GLN
1	A	135	ARG
1	A	150	ILE
1	A	161	ASN
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	240	ASN
1	A	245	ASN
1	A	255	GLN
1	A	256	LYS
1	A	263	ASP
1	A	268	HIS
1	A	273	GLU
1	A	279	ASN
1	A	285	VAL
1	A	321	ILE
1	A	322	GLN
1	A	327	ASP
1	A	332	GLU
1	A	335	GLU
1	A	340	LEU
1	A	352	LEU
1	A	357	VAL

Some 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	154	GLN
1	A	161	ASN
1	A	195	ASN
1	A	215	GLN
1	A	240	ASN
1	A	245	ASN
1	A	255	GLN
1	A	314	ASN
1	A	322	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 [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%)	0.48	20 (7%) 19 7	15, 15, 15, 15	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	GLN	5.7
1	A	330	LEU	5.0
1	A	70	ILE	4.3
1	A	322	GLN	4.0
1	A	326	GLN	3.9
1	A	72	ASP	3.6
1	A	327	ASP	3.5
1	A	325	ASP	3.3
1	A	291	LYS	3.3
1	A	170	GLU	3.1
1	A	182	VAL	3.0
1	A	74	LEU	3.0
1	A	171	GLU	3.0
1	A	73	ARG	3.0
1	A	302	THR	2.9
1	A	303	ILE	2.8
1	A	328	GLU	2.8
1	A	71	GLN	2.4
1	A	334	LEU	2.3
1	A	323	ASN	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 carbohydrates 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.