WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 2, 2023 – 11:17 AM EDT

PDB ID	:	3PUF
Title	:	Crystal structure of human RNase H2 complex
Authors	:	Figiel, M.; Chon, H.; Cerritelli, S.M.; Cybulska, M.; Crouch, R.J.; Nowotny, M.
Deposited on	:	2010-12-04
Resolution	:	3.10 Å(reported)

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

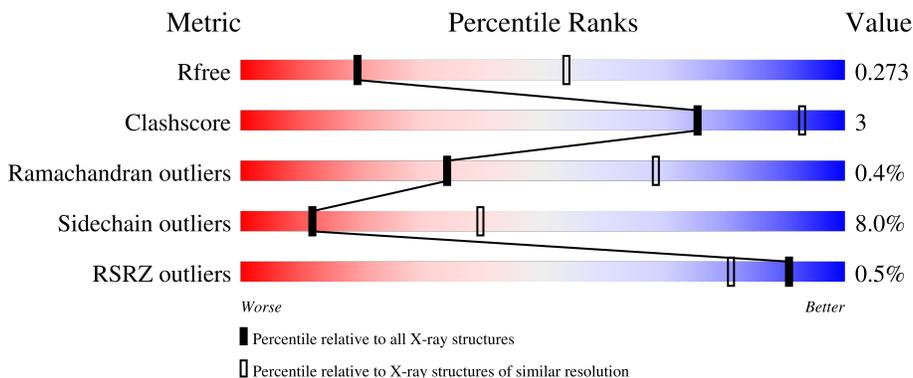|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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.
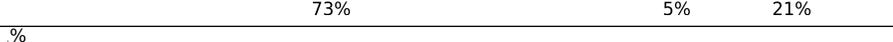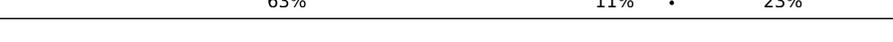
Metric	Percentile Ranks	Value
Rfree		0.273
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		8.0%
RSRZ outliers		0.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	302	73% 16% 11%
1	D	302	73% 17% • 9%
1	G	302	75% 12% • 12%
1	J	302	.% 77% 11% • 11%
1	M	302	82% 8% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	302	74% 11% • 14%
2	B	224	67% 14% • 17%
2	E	224	69% 11% • 19%
2	H	224	82% 8% • 10%
2	K	224	72% 9% 19%
2	N	224	74% 9% 17%
2	Q	224	73% 5% 21%
3	C	167	65% 10% • 24%
3	F	167	63% 11% • 23%
3	I	167	73% 11% 16%
3	L	167	61% 8% • 31%
3	O	167	64% 5% 31%
3	R	167	63% 5% 31%
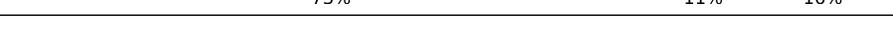
2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 25820 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 Ribonuclease H2 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2031	1300	340	380	11			
1	D	274	Total	C	N	O	S	0	0	0
			2040	1299	348	384	9			
1	G	266	Total	C	N	O	S	0	0	0
			1999	1274	334	382	9			
1	J	270	Total	C	N	O	S	0	0	0
			1965	1251	330	374	10			
1	M	272	Total	C	N	O	S	0	0	0
			1995	1273	333	381	8			
1	P	259	Total	C	N	O	S	0	0	0
			1895	1211	318	357	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O75792
A	-1	PRO	-	expression tag	UNP O75792
A	0	HIS	-	expression tag	UNP O75792
D	-2	GLY	-	expression tag	UNP O75792
D	-1	PRO	-	expression tag	UNP O75792
D	0	HIS	-	expression tag	UNP O75792
G	-2	GLY	-	expression tag	UNP O75792
G	-1	PRO	-	expression tag	UNP O75792
G	0	HIS	-	expression tag	UNP O75792
J	-2	GLY	-	expression tag	UNP O75792
J	-1	PRO	-	expression tag	UNP O75792
J	0	HIS	-	expression tag	UNP O75792
M	-2	GLY	-	expression tag	UNP O75792
M	-1	PRO	-	expression tag	UNP O75792
M	0	HIS	-	expression tag	UNP O75792
P	-2	GLY	-	expression tag	UNP O75792
P	-1	PRO	-	expression tag	UNP O75792

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	0	HIS	-	expression tag	UNP O75792

- Molecule 2 is a protein called Ribonuclease H2 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	185	Total 1459	C 961	N 233	O 261	S 4	0	0	0
2	E	181	Total 1355	C 883	N 228	O 240	S 4	0	0	0
2	H	202	Total 1546	C 1010	N 249	O 281	S 6	0	0	0
2	K	182	Total 1357	C 891	N 222	O 240	S 4	0	0	0
2	N	186	Total 1387	C 906	N 227	O 250	S 4	0	0	0
2	Q	176	Total 1299	C 852	N 211	O 233	S 3	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLY	-	expression tag	UNP Q5TBB1
B	11	SER	-	expression tag	UNP Q5TBB1
B	12	HIS	-	expression tag	UNP Q5TBB1
B	13	MET	-	expression tag	UNP Q5TBB1
E	10	GLY	-	expression tag	UNP Q5TBB1
E	11	SER	-	expression tag	UNP Q5TBB1
E	12	HIS	-	expression tag	UNP Q5TBB1
E	13	MET	-	expression tag	UNP Q5TBB1
H	10	GLY	-	expression tag	UNP Q5TBB1
H	11	SER	-	expression tag	UNP Q5TBB1
H	12	HIS	-	expression tag	UNP Q5TBB1
H	13	MET	-	expression tag	UNP Q5TBB1
K	10	GLY	-	expression tag	UNP Q5TBB1
K	11	SER	-	expression tag	UNP Q5TBB1
K	12	HIS	-	expression tag	UNP Q5TBB1
K	13	MET	-	expression tag	UNP Q5TBB1
N	10	GLY	-	expression tag	UNP Q5TBB1
N	11	SER	-	expression tag	UNP Q5TBB1
N	12	HIS	-	expression tag	UNP Q5TBB1
N	13	MET	-	expression tag	UNP Q5TBB1
Q	10	GLY	-	expression tag	UNP Q5TBB1

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Q	11	SER	-	expression tag	UNP Q5TBB1
Q	12	HIS	-	expression tag	UNP Q5TBB1
Q	13	MET	-	expression tag	UNP Q5TBB1

• Molecule 3 is a protein called Ribonuclease H2 subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	127	Total 933	C 601	N 166	O 163	S 3	0	0	0
3	F	128	Total 952	C 609	N 176	O 164	S 3	0	0	0
3	I	140	Total 1048	C 669	N 193	O 183	S 3	0	0	0
3	L	116	Total 840	C 543	N 148	O 146	S 3	0	0	0
3	O	116	Total 828	C 537	N 145	O 143	S 3	0	0	0
3	R	115	Total 800	C 519	N 145	O 133	S 3	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q8TDP1
C	-1	SER	-	expression tag	UNP Q8TDP1
C	0	HIS	-	expression tag	UNP Q8TDP1
F	-2	GLY	-	expression tag	UNP Q8TDP1
F	-1	SER	-	expression tag	UNP Q8TDP1
F	0	HIS	-	expression tag	UNP Q8TDP1
I	-2	GLY	-	expression tag	UNP Q8TDP1
I	-1	SER	-	expression tag	UNP Q8TDP1
I	0	HIS	-	expression tag	UNP Q8TDP1
L	-2	GLY	-	expression tag	UNP Q8TDP1
L	-1	SER	-	expression tag	UNP Q8TDP1
L	0	HIS	-	expression tag	UNP Q8TDP1
O	-2	GLY	-	expression tag	UNP Q8TDP1
O	-1	SER	-	expression tag	UNP Q8TDP1
O	0	HIS	-	expression tag	UNP Q8TDP1
R	-2	GLY	-	expression tag	UNP Q8TDP1
R	-1	SER	-	expression tag	UNP Q8TDP1
R	0	HIS	-	expression tag	UNP Q8TDP1

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total 11	O 11	0	0
4	B	5	Total 5	O 5	0	0
4	C	6	Total 6	O 6	0	0
4	D	4	Total 4	O 4	0	0
4	E	3	Total 3	O 3	0	0
4	F	7	Total 7	O 7	0	0
4	G	7	Total 7	O 7	0	0
4	H	8	Total 8	O 8	0	0
4	I	9	Total 9	O 9	0	0
4	J	11	Total 11	O 11	0	0
4	K	4	Total 4	O 4	0	0
4	L	3	Total 3	O 3	0	0
4	M	1	Total 1	O 1	0	0
4	N	2	Total 2	O 2	0	0
4	O	3	Total 3	O 3	0	0
4	P	4	Total 4	O 4	0	0
4	Q	2	Total 2	O 2	0	0
4	R	1	Total 1	O 1	0	0

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: Ribonuclease H2 subunit A

Chain A:

- Molecule 1: Ribonuclease H2 subunit A

Chain D:

- Molecule 1: Ribonuclease H2 subunit A

Chain G:

- Molecule 1: Ribonuclease H2 subunit A

Chain J:

Chain J residue map:
GLY PRO HIS MET ASP L3 S4 E5 L6 E7 G12 R15 L16 V30 V33 I49 R56 L57 A62 D67 S68 K69 E84 ASP THR D87 D94 S102 T103 S104 M105 L106 Y111 L124 Q137 V140 Y149 V164 L171 S176

R186 D187 Q188 V196 L199 GLN D201 L202 D203 T204 D205 Y206 P211 V227 W238 R239 T240 S259 GLU ASN GLN GLU GLY LEU ARG LYS ILE THR SER TYR PHE LEU ASN GLU GLY SER GLN ALA ARG PRO ARG SER S284 R291 L299

• Molecule 1: Ribonuclease H2 subunit A

Chain M:

Chain M residue map:
GLY PRO HIS MET D2 R15 S18 L31 Y47 Y51 L54 P55 R56 S68 K69 T70 L71 W91 A92 L93 L100 V109 Q131 V138 F139 V140 Q150 V164 L171 K183 T204 W238 R239 S257 ALA SER GLU ASN GLN GLU GLY

LEU ARG LYS ILE THR SER TYR PHE LEU ASN GLU GLY SER GLN ALA ARG PRO ARG SER S284 E294 L299

• Molecule 1: Ribonuclease H2 subunit A

Chain P:

Chain P residue map:
GLY PRO HIS MET ASP LEU SER E5 S18 E27 V30 R38 V41 L42 Y47 P53 L57 L60 L63 L71 R76 V89 G90 W91 A92 L93 D94 P98 I101 L113 N114 S115 L116 L153 V162 T163 D169 V174 W193

E197 LYS LEU GLN ASP LEU ASP THR ASP TYR G207 P211 T216 E222 P226 W238 R239 T240 A249 W254 S257 ALA SER GLU ASN GLN GLU GLY LEU ARG LYS ILE THR SER TYR PHE LEU ASN GLU GLY SER GLN ALA ARG PRO ARG SER SER H285 F288

L299

• Molecule 2: Ribonuclease H2 subunit B

Chain B:

Chain B residue map:
GLY SER HIS M13 R14 L19 E22 Y23 L24 LYS ASP ALA SER LYS LYS MET LYS ASN GLY L35 M36 F37 V38 K39 P43 M55 C56 F66 W73 F74 Q80 L85 V91 L101 D105 K109 F110 L113 D114 L129 K130 V141 T142 E143 E144

P148 GLU ILE ASP ASN K153 Y158 T163 V175 L178 N184 VAL SER ARG VAL GLN SER THR ALA PHE PHE SER GLY ASP GLN ALA SER THR ASP LYS E205 Y219 E223 L224 L228 Y231 LEU LYS

• Molecule 2: Ribonuclease H2 subunit B

Chain E:

Chain E residue map:
GLY SER HIS R14 K25 D26 ALA SER LYS LYS M31 V38 C56 Q59 W73 F74 S78 V79 Q80 S81 G82 G83 L84 L96 L97 L98 D105 K106 Q115 L137 L138 H139 T142 GLU GLU LYS GLY ASN PRO GLU ILE ASP ASN LYS K154 K170

T174 V183 ASN VAL SER ARG VAL GLN SER THR ALA PHE PHE SER GLY ASP GLN ALA SER THR ASP K204 E205 E206 D207 Y208 L215 I216 S217 D218 L224 S225 D226 D227 L228 SER LYS TYR LEU LYS

● Molecule 2: Ribonuclease H2 subunit B

Chain H:

| 82% | | 8% | • | 10% |

GLY SER H12 V17 V20 V38 N54 Q59 K67 W73 F74 Q80 L84 E107 E135 K136 G146 ASN PRO GLU ILE ASP N152 T174 V189 GLN SER THR ALA PHE PHE SER GLY ASP GLN ALA SER THR ASP K204 Y208 L215 I216 S217

I220 P221 L232 LYS

● Molecule 2: Ribonuclease H2 subunit B

Chain K:

| 72% | | 9% | 19% |

GLY SER H12 M13 R14 V20 Y23 L24 LYS ASP ALA SER LYS LYS MET LYS ASN GLY L35 L40 E68 F74 I75 N76 A88 L94 K109 L127 K130 L137 T142 K145 GLY ASN PRO GLU ILE ASP ASN K153 Y158 S159 K160 N182 V183

N184 VAL SER SER ARG VAL GLN SER THR ALA PHE PHE SER GLY ASP GLN ALA SER THR ASP LYS GLU GLU D207 I216 P221 L224 L232 LYS

● Molecule 2: Ribonuclease H2 subunit B

Chain N:

| 74% | | 9% | 17% |

GLY SER HIS M13 L24 K25 ASP ALA SER LYS LYS MET LYS ASN GLY L35 E47 L52 F61 K67 F74 D92 L101 L131 V141 T142 E143 E144 K145 GLY ASN PRO GLU ILE D151 Y158 K162 T163 L164 N172 V175 V183 S187 ARG

VAL GLN SER THR ALA PHE PHE SER GLY ASP GLN ALA SER THR ASP LYS GLU GLU E206 K230 TYR LEU LYS

● Molecule 2: Ribonuclease H2 subunit B

Chain Q:

%

| 73% | | 5% | 21% |

GLY SER HIS M13 E22 TYR LEU LYS ASP ALA SER LYS LYS MET LYS ASN GLY L35 I50 H70 W73 F74 I75 N76 Q80 L96 E107 GLY K109 F110 H139 H140 V141 K145 GLY ASN PRO GLU ILE ASP ASN LYS K154 T163 T174 V175 V185 SER

SER ARG VAL GLN SER THR ALA PHE PHE SER GLY ASP GLN ALA SER THR ASP LYS GLU GLU ASP TYR I209 L232 LYS

● Molecule 3: Ribonuclease H2 subunit C

Chain C:

%

| 65% | | 10% | • | 24% |

GLY SER HIS MET GLU SER GLY ASP GLU ALA **A8** **H12** **R13** **L16** **R17** **S18** **A19** **H30** **V38** **D39** **P43** **R46** **R53** **Q54** **G70** **E71** **E72** **V80** **E88** LYS LYS VAL SER MET GLY LYS PRO ASP PRO LEU ARG ASP SER GLY THR ASP ASP GLN GLU GLU

GLU PRO LEU GLU ARG ASP PHE **D117** **I120** **T130** **L131** **L134** **P162** GLU ASP

• Molecule 3: Ribonuclease H2 subunit C

Chain F: 63%   11%   •   23%

GLY SER HIS MET GLU SER GLY ASP GLU ALA **A8** **R13** **L16** **L21** **R22** **A27** **H30** **E35** **V36** **A37** **P41** **A42** **P43** **R46** **F47** **F48** **T49** **V61** **T86** **E87** **E88** LYS LYS VAL SER MET GLY LYS PRO ASP PRO LEU ARG ASP SER GLY THR ASP ASP GLN

GLU GLU GLU PRO LEU GLU ARG ASP **F116** **I120** **A124** **N125** **T130** **V144** **S152** **I157** **P162** GLU ASP

• Molecule 3: Ribonuclease H2 subunit C

Chain I: 73%   11%   16%

GLY SER HIS MET GLU SER GLY ASP GLU **A7** **R11** **H12** **R13** **L16** **R22** ASP **A24** **L29** **H30** **D39** **E57** **R69** **P76** **L79** **S92** MET GLY LYS PRO ASP PRO LEU ARG ASP SER GLY THR ASP ASP GLN **E108** **P111** **L112** **E113** **I137** **P140**

V144 **R145** **I157** **P162** GLU ASP

• Molecule 3: Ribonuclease H2 subunit C

Chain L: 61%   8%   •   31%

GLY SER HIS MET GLU SER GLY ASP GLU ALA ALA ILE **E10** **R13** **L16** **R17** SER ALA THR LEU **R22** **H30** **V38** **P43** **R46** **V61** **R66** **E87** GLU LYS LYS VAL SER MET GLY LYS PRO ASP PRO LEU ARG ASP SER GLY THR ASP ASP GLN GLU GLU GLU

PRO LEU GLU ARG ASP PHE ARG ASP PHE **I120** **G121** **L131** **I137** **A142** **R145** **V161** PRO GLU ASP

• Molecule 3: Ribonuclease H2 subunit C

Chain O: 64%   5%   31%

GLY SER HIS MET GLU SER GLY ASP GLU ALA ALA **I9** **L16** ARG SER ALA THR LEU ARG ASP ALA **V25** **H30** **G58** **V61** **P76** **L79** **T86** GLU GLU LYS LYS VAL SER MET GLY LYS PRO ASP PRO LEU ARG ASP SER GLY THR ASP ASP GLN GLU GLU GLU PRO

LEU GLU ARG ASP PHE ASP **R118** **F119** **I120** **I137** **H158** **E163** ASP

• Molecule 3: Ribonuclease H2 subunit C

Chain R: 63%   5%   31%

GLY SER HIS MET GLU SER GLY ASP GLU ALA ALA ILE **E10** **R17** SER ALA THR LEU ARG ASP ALA **V25** **H30** **T49** **I52** **V61** **T86** GLU GLU LYS LYS VAL SER MET GLY LYS PRO ASP PRO LEU ARG ASP SER GLY THR ASP ASP GLN GLU GLU GLU PRO LEU GLU

ARG ASP PHE **D117** **F129** **T136** **P140** **R145** **I157** **V161** PRO GLU ASP

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.07Å 108.37Å 114.26Å 105.90° 103.71° 111.42°	Depositor
Resolution (Å)	44.10 – 3.10 44.10 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.10-3.10) 97.1 (44.10-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.203 , 0.255 0.216 , 0.273	Depositor DCC
R_{free} test set	3207 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	63.1	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 63.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	25820	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.99% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.40	0/2075	0.64	0/2830
1	D	0.41	0/2084	0.63	0/2851
1	G	0.41	0/2044	0.64	0/2797
1	J	0.40	0/2008	0.60	0/2748
1	M	0.40	0/2039	0.63	0/2795
1	P	0.39	0/1937	0.60	0/2656
2	B	0.38	0/1494	0.64	0/2028
2	E	0.39	0/1385	0.61	0/1887
2	H	0.39	0/1581	0.62	0/2148
2	K	0.39	0/1391	0.62	0/1899
2	N	0.39	0/1421	0.63	0/1938
2	Q	0.37	0/1329	0.57	0/1815
3	C	0.40	0/958	0.61	0/1312
3	F	0.40	0/977	0.64	0/1335
3	I	0.40	0/1074	0.66	0/1465
3	L	0.41	0/862	0.68	0/1181
3	O	0.39	0/850	0.62	0/1166
3	R	0.41	0/821	0.60	0/1127
All	All	0.40	0/26330	0.62	0/35978

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2031	0	1951	17	0
1	D	2040	0	1932	21	0
1	G	1999	0	1886	10	0
1	J	1965	0	1800	14	0
1	M	1995	0	1850	5	0
1	P	1895	0	1766	11	0
2	B	1459	0	1402	15	0
2	E	1355	0	1248	8	0
2	H	1546	0	1448	8	0
2	K	1357	0	1212	6	0
2	N	1387	0	1235	9	0
2	Q	1299	0	1160	4	0
3	C	933	0	921	12	0
3	F	952	0	945	14	0
3	I	1048	0	1032	9	0
3	L	840	0	821	7	0
3	O	828	0	804	6	0
3	R	800	0	764	4	0
4	A	11	0	0	0	0
4	B	5	0	0	0	0
4	C	6	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	7	0	0	0	0
4	G	7	0	0	0	0
4	H	8	0	0	0	0
4	I	9	0	0	0	0
4	J	11	0	0	0	0
4	K	4	0	0	0	0
4	L	3	0	0	0	0
4	M	1	0	0	0	0
4	N	2	0	0	0	0
4	O	3	0	0	0	0
4	P	4	0	0	0	0
4	Q	2	0	0	0	0
4	R	1	0	0	0	0
All	All	25820	0	24177	153	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 3.

The worst 5 of 153 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)
2:E:174:THR:HG22	3:F:157:ILE:HB	1.60	0.84
3:I:111:PRO:HA	3:I:112:LEU:HB3	1.64	0.78
3:I:111:PRO:HA	3:I:112:LEU:CB	2.22	0.69
1:D:153:LEU:HB3	1:D:162:VAL:HG11	1.75	0.69
1:M:150:GLN:HG2	1:M:164:VAL:HG12	1.74	0.68

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	264/302 (87%)	255 (97%)	9 (3%)	0	100	100
1	D	270/302 (89%)	255 (94%)	13 (5%)	2 (1%)	22	57
1	G	262/302 (87%)	252 (96%)	9 (3%)	1 (0%)	34	69
1	J	262/302 (87%)	250 (95%)	10 (4%)	2 (1%)	19	54
1	M	268/302 (89%)	255 (95%)	13 (5%)	0	100	100
1	P	253/302 (84%)	244 (96%)	9 (4%)	0	100	100
2	B	177/224 (79%)	165 (93%)	10 (6%)	2 (1%)	14	46
2	E	173/224 (77%)	160 (92%)	12 (7%)	1 (1%)	25	59
2	H	196/224 (88%)	185 (94%)	11 (6%)	0	100	100
2	K	174/224 (78%)	163 (94%)	7 (4%)	4 (2%)	6	28
2	N	178/224 (80%)	166 (93%)	11 (6%)	1 (1%)	25	59
2	Q	166/224 (74%)	161 (97%)	4 (2%)	1 (1%)	25	59
3	C	123/167 (74%)	119 (97%)	4 (3%)	0	100	100
3	F	124/167 (74%)	119 (96%)	4 (3%)	1 (1%)	19	54
3	I	134/167 (80%)	129 (96%)	5 (4%)	0	100	100
3	L	110/167 (66%)	103 (94%)	7 (6%)	0	100	100

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	110/167 (66%)	106 (96%)	4 (4%)	0	100	100
3	R	109/167 (65%)	102 (94%)	7 (6%)	0	100	100
All	All	3353/4158 (81%)	3189 (95%)	149 (4%)	15 (0%)	34	69

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	110	PHE
2	E	82	GLY
3	F	37	ALA
2	B	183	VAL
1	D	12	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	207/259 (80%)	186 (90%)	21 (10%)	7	28
1	D	205/259 (79%)	186 (91%)	19 (9%)	9	32
1	G	203/259 (78%)	182 (90%)	21 (10%)	7	27
1	J	190/259 (73%)	174 (92%)	16 (8%)	11	38
1	M	196/259 (76%)	179 (91%)	17 (9%)	10	36
1	P	187/259 (72%)	171 (91%)	16 (9%)	10	37
2	B	151/204 (74%)	139 (92%)	12 (8%)	12	40
2	E	130/204 (64%)	112 (86%)	18 (14%)	3	16
2	H	154/204 (76%)	142 (92%)	12 (8%)	12	40
2	K	126/204 (62%)	118 (94%)	8 (6%)	18	48
2	N	130/204 (64%)	123 (95%)	7 (5%)	22	53
2	Q	122/204 (60%)	116 (95%)	6 (5%)	25	57
3	C	92/134 (69%)	88 (96%)	4 (4%)	29	62
3	F	94/134 (70%)	85 (90%)	9 (10%)	8	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	104/134 (78%)	98 (94%)	6 (6%)	20	51
3	L	81/134 (60%)	76 (94%)	5 (6%)	18	49
3	O	79/134 (59%)	78 (99%)	1 (1%)	69	87
3	R	71/134 (53%)	68 (96%)	3 (4%)	30	62
All	All	2522/3582 (70%)	2321 (92%)	201 (8%)	12	40

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	220	ILE
2	K	130	LYS
3	R	129	PHE
3	I	39	ASP
1	J	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	184	ASN
3	O	160	GLN
2	Q	42	ASN
1	P	154	GLN
3	O	158	HIS

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 monosaccharides 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 ⓘ

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(Å²)	Q<0.9
1	A	270/302 (89%)	-0.54	1 (0%)	92	84	21, 48, 76, 104	0
1	D	274/302 (90%)	-0.44	1 (0%)	92	84	34, 59, 88, 106	0
1	G	266/302 (88%)	-0.56	0	100	100	24, 45, 77, 90	0
1	J	270/302 (89%)	-0.27	3 (1%)	80	64	33, 74, 106, 121	0
1	M	272/302 (90%)	-0.42	0	100	100	40, 68, 95, 109	0
1	P	259/302 (85%)	-0.29	4 (1%)	73	54	46, 76, 101, 109	0
2	B	185/224 (82%)	-0.49	1 (0%)	91	81	38, 59, 80, 95	0
2	E	181/224 (80%)	-0.34	3 (1%)	70	49	33, 77, 105, 117	0
2	H	202/224 (90%)	-0.50	0	100	100	31, 60, 85, 107	0
2	K	182/224 (81%)	-0.48	0	100	100	44, 73, 96, 127	0
2	N	186/224 (83%)	-0.33	0	100	100	44, 79, 109, 137	0
2	Q	176/224 (78%)	-0.31	2 (1%)	80	64	55, 81, 99, 118	0
3	C	127/167 (76%)	-0.50	1 (0%)	86	72	28, 56, 89, 104	0
3	F	128/167 (76%)	-0.60	0	100	100	34, 52, 78, 95	0
3	I	140/167 (83%)	-0.63	0	100	100	26, 44, 75, 95	0
3	L	116/167 (69%)	-0.43	0	100	100	32, 63, 100, 119	0
3	O	116/167 (69%)	-0.46	0	100	100	39, 66, 85, 102	0
3	R	115/167 (68%)	-0.41	0	100	100	54, 75, 90, 110	0
All	All	3465/4158 (83%)	-0.44	16 (0%)	91	81	21, 64, 96, 137	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	7	GLU	6.7
2	E	56	CYS	3.3
2	E	205	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Q	110	PHE	2.6
1	A	11	THR	2.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.