



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:59 pm BST

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)

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

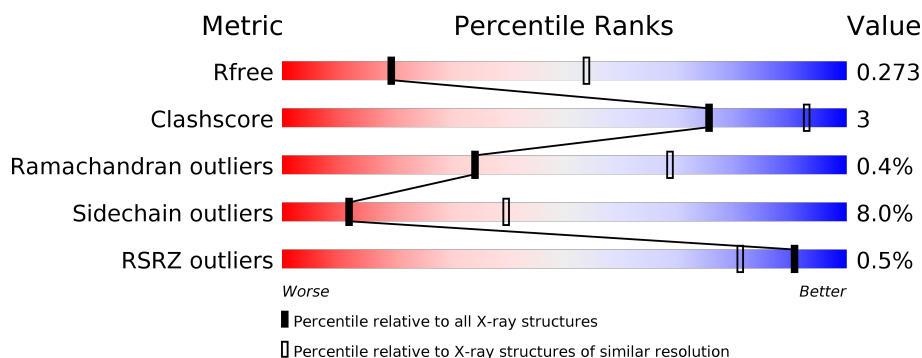
1 Overall quality at a glance

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	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 on 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	302	<div> <div style="width: 73%;"></div> <div style="width: 16%;"></div> <div style="width: 11%;"></div> </div>
1	D	302	<div> <div style="width: 73%;"></div> <div style="width: 17%;"></div> <div style="width: 9%;"></div> </div>
1	G	302	<div> <div style="width: 75%;"></div> <div style="width: 12%;"></div> <div style="width: 12%;"></div> </div>
1	J	302	<div> <div style="width: 77%;"></div> <div style="width: 11%;"></div> <div style="width: 11%;"></div> </div>
1	M	302	<div> <div style="width: 82%;"></div> <div style="width: 8%;"></div> <div style="width: 10%;"></div> </div>
1	P	302	<div> <div style="width: 74%;"></div> <div style="width: 11%;"></div> <div style="width: 14%;"></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	224	
2	E	224	
2	H	224	
2	K	224	
2	N	224	
2	Q	224	
3	C	167	
3	F	167	
3	I	167	
3	L	167	
3	O	167	
3	R	167	

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...

Continued from previous 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	C	N	O	S	0	0	0
			1459	961	233	261	4			
2	E	181	Total	C	N	O	S	0	0	0
			1355	883	228	240	4			
2	H	202	Total	C	N	O	S	0	0	0
			1546	1010	249	281	6			
2	K	182	Total	C	N	O	S	0	0	0
			1357	891	222	240	4			
2	N	186	Total	C	N	O	S	0	0	0
			1387	906	227	250	4			
2	Q	176	Total	C	N	O	S	0	0	0
			1299	852	211	233	3			

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 on next page...

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

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

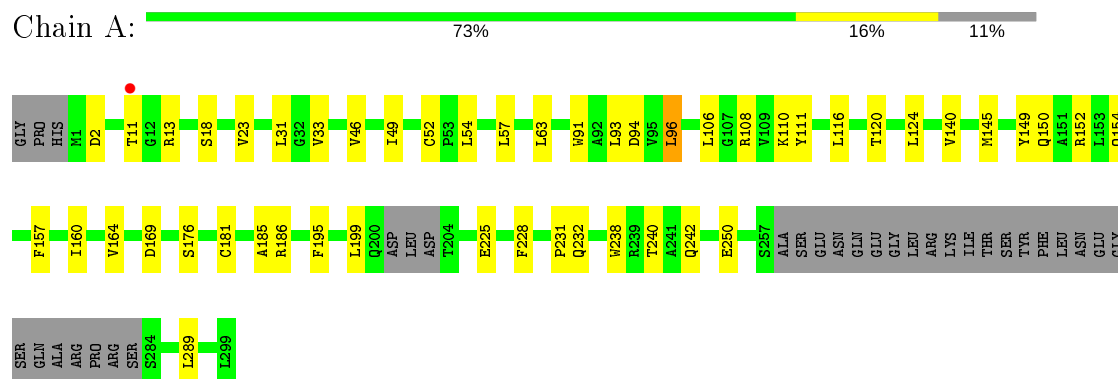
- Molecule 4 is water.

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

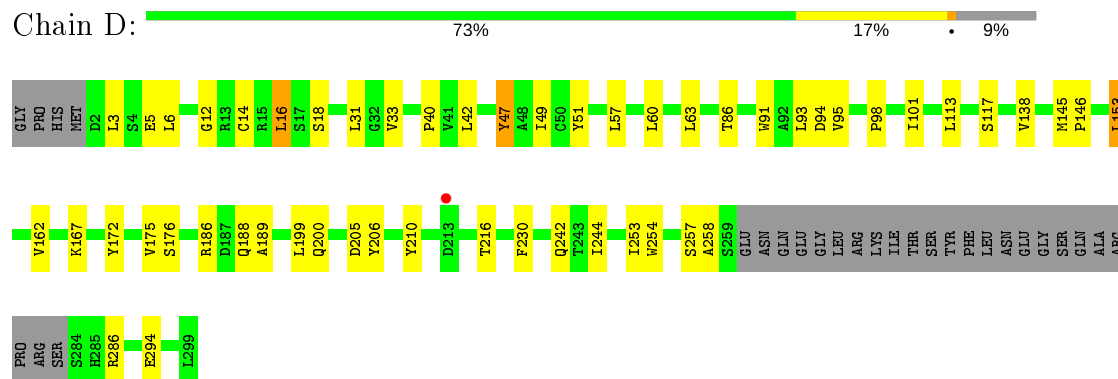
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

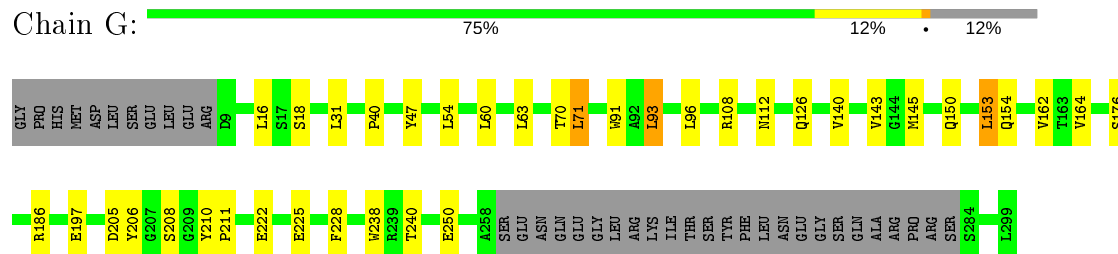
- Molecule 1: Ribonuclease H2 subunit A



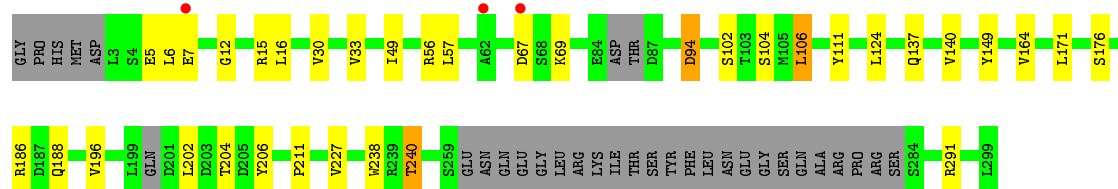
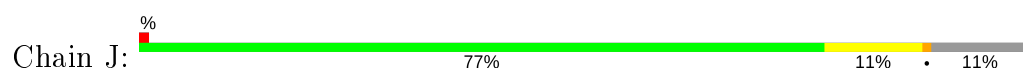
- Molecule 1: Ribonuclease H2 subunit A



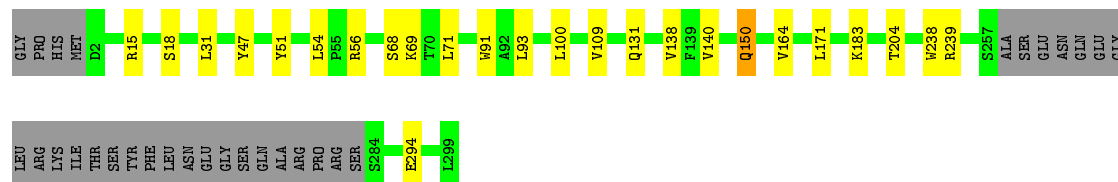
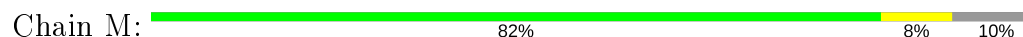
- Molecule 1: Ribonuclease H2 subunit A



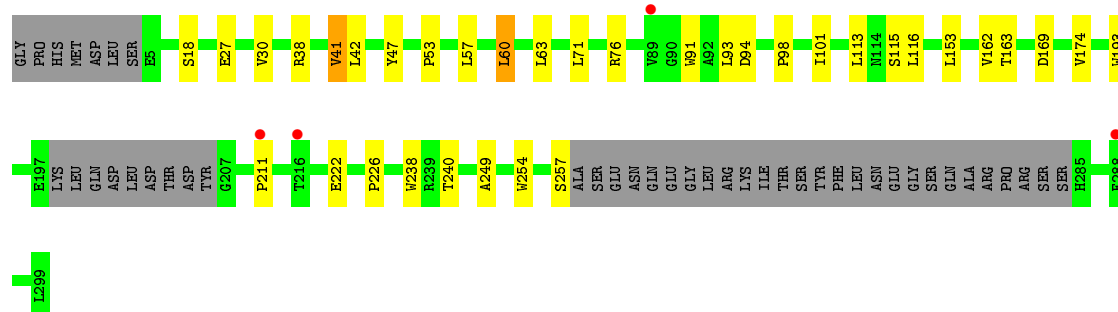
- Molecule 1: Ribonuclease H2 subunit A



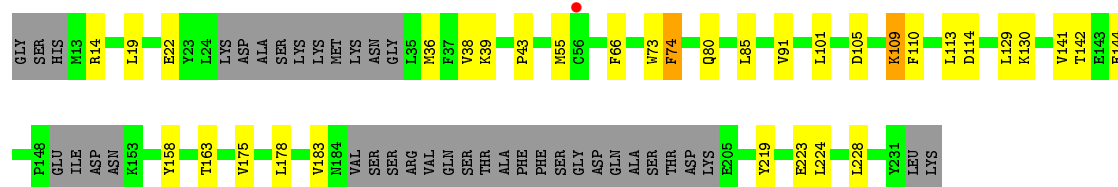
• Molecule 1: Ribonuclease H2 subunit A



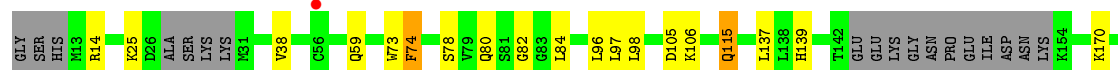
• Molecule 1: Ribonuclease H2 subunit A

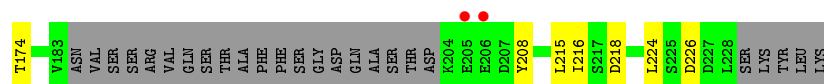


• Molecule 2: Ribonuclease H2 subunit B



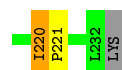
• Molecule 2: Ribonuclease H2 subunit B





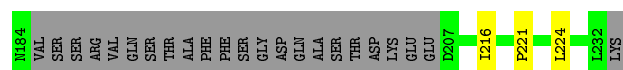
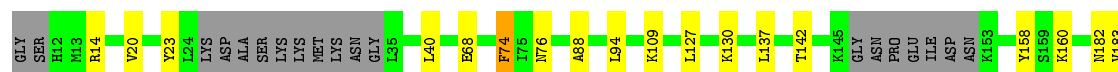
- Molecule 2: Ribonuclease H2 subunit B

Chain H: 82% 8% 10%



- Molecule 2: Ribonuclease H2 subunit B

Chain K: 72% 9% 19%



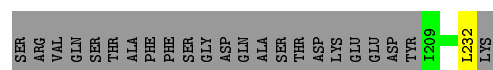
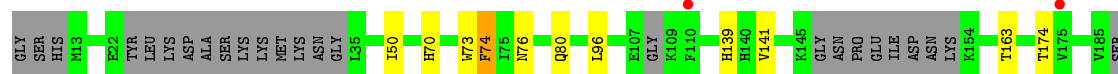
- Molecule 2: Ribonuclease H2 subunit B

Chain N: 74% 9% 17%



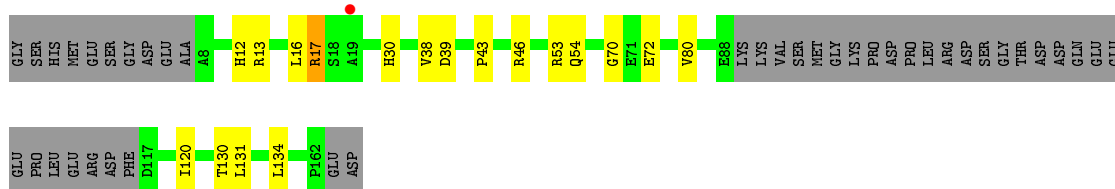
- Molecule 2: Ribonuclease H2 subunit B

Chain Q: 73% 5% 21%



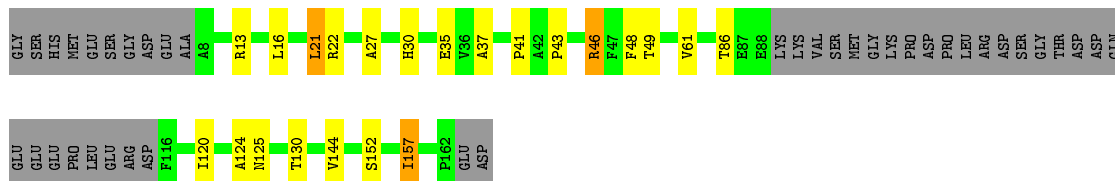
- Molecule 3: Ribonuclease H2 subunit C

Chain C: 65% 10% 24%



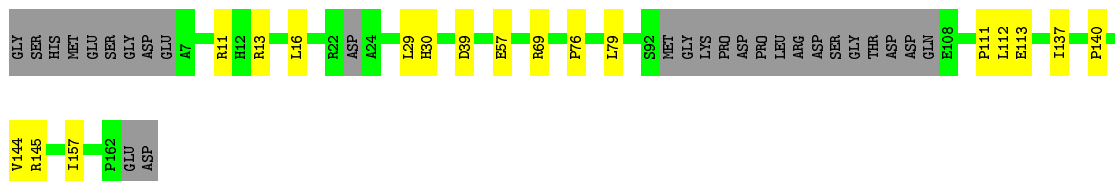
- Molecule 3: Ribonuclease H2 subunit C

Chain F: 63% 11% • 23%



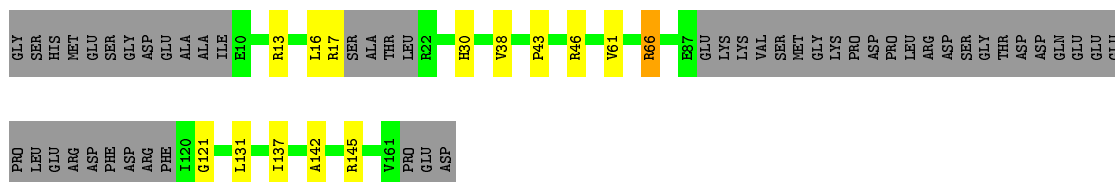
- Molecule 3: Ribonuclease H2 subunit C

Chain I:  73% 11% 16%



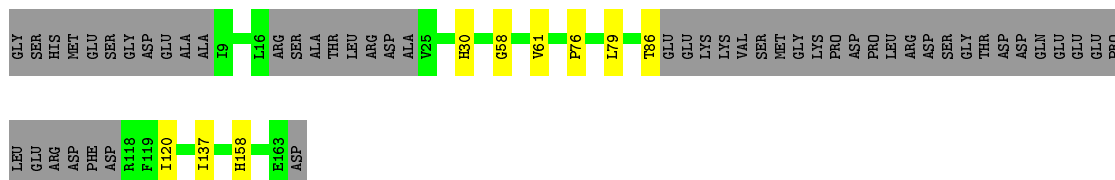
- Molecule 3: Ribonuclease H2 subunit C

Chain L:  61% 8% • 31%



- Molecule 3: Ribonuclease H2 subunit C

Chain 0: 64% 5% 31%



- Molecule 3: Ribonuclease H2 subunit C

Chain R:  63% 5% 31%

GLY	SER	HIS	GLU	SER	GLY	ASP	GLU	ALA	ALA	ILE	E10	R17	SER	ALA	THR	ARG	LEU	ASP	ALA	W25	H30	T49	I52	V61	T86	GLU	GLU	LYS	LYS	VAL	SER	SER	MET	GLY	LYS	PRO	ASP	ARG	ASP	SER	GLY	THR	GLN	GLU	GLU	GLU	PRO	LEU	LEU	LEU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------------	------------	-----	-----	-----	-----	-----	-----	-----	------------	------------	------------	------------	------------	------------	------------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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.

All (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
1:P:153:LEU:HB3	1:P:162:VAL:HG11	1.76	0.67
1:D:230:PHE:HZ	1:D:244:ILE:HD11	1.61	0.66
2:E:73:TRP:HB2	2:E:80:GLN:HB3	1.77	0.65
2:H:174:THR:HG22	3:I:157:ILE:HG12	1.79	0.64
1:A:250:GLU:HG2	3:C:38:VAL:HB	1.81	0.62
2:H:73:TRP:HB2	2:H:80:GLN:HB3	1.82	0.62
2:N:142:THR:HG22	2:N:158:TYR:HA	1.83	0.61
1:D:31:LEU:HD12	1:D:51:TYR:HB3	1.82	0.60
1:D:63:LEU:HD21	1:D:86:THR:HG21	1.82	0.60
1:G:16:LEU:HB2	1:G:93:LEU:HB2	1.83	0.60
1:A:33:VAL:HG22	1:A:49:ILE:HG22	1.84	0.60
2:K:94:LEU:HD21	2:K:137:LEU:HB2	1.83	0.60
1:G:70:THR:O	1:G:71:LEU:HB2	2.01	0.60
2:K:74:PHE:HB2	3:L:30:HIS:HB2	1.84	0.59
2:Q:74:PHE:HB2	3:R:30:HIS:HB2	1.84	0.59
2:B:73:TRP:HB2	2:B:80:GLN:HB3	1.84	0.58
1:J:67:ASP:H	1:J:176:SER:HB3	1.67	0.58
1:J:33:VAL:HB	1:J:140:VAL:HB	1.86	0.57
1:D:200:GLN:HB2	3:F:46:ARG:HH11	1.68	0.57
1:A:49:ILE:HG12	1:A:124:LEU:HB3	1.86	0.57
1:M:31:LEU:HB3	1:M:138:VAL:HG22	1.85	0.57
2:B:74:PHE:HB2	3:C:30:HIS:HB2	1.86	0.56
2:Q:174:THR:HG22	3:R:157:ILE:HG12	1.87	0.56
1:M:31:LEU:HD23	1:M:51:TYR:HB3	1.88	0.56
3:O:86:THR:HA	3:O:120:ILE:HG22	1.87	0.56
1:G:153:LEU:HB3	1:G:162:VAL:HG11	1.88	0.56
2:N:92:ASP:H	3:O:158:HIS:CD2	2.25	0.55
2:B:22:GLU:HA	3:C:80:VAL:HG23	1.88	0.54
1:P:98:PRO:HA	1:P:101:ILE:HD12	1.90	0.54
2:Q:73:TRP:HB2	2:Q:80:GLN:HB3	1.90	0.54
2:B:39:LYS:HB3	3:C:12:HIS:HD2	1.73	0.53
1:A:108:ARG:NH2	3:C:134:LEU:O	2.40	0.53
1:G:140:VAL:HB	1:G:164:VAL:HG12	1.90	0.53
2:E:74:PHE:HB2	3:F:30:HIS:HB2	1.89	0.53
1:J:104:SER:HB3	1:J:111:TYR:HD2	1.73	0.52
1:P:41:VAL:HG13	1:P:211:PRO:HG3	1.91	0.52
2:H:74:PHE:HB2	3:I:30:HIS:HB2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PHE:CE2	1:A:231:PRO:HB2	2.45	0.52
1:A:96:LEU:HD11	1:A:120:THR:HG21	1.91	0.52
3:O:76:PRO:HB2	3:O:79:LEU:HD13	1.91	0.52
1:P:30:VAL:HG11	1:P:57:LEU:HD13	1.92	0.52
3:C:43:PRO:HB2	3:C:46:ARG:HB2	1.92	0.51
2:N:141:VAL:HB	2:N:163:THR:HG22	1.92	0.51
1:A:31:LEU:HD11	1:A:49:ILE:HB	1.92	0.51
2:K:221:PRO:HD2	2:K:224:LEU:HD12	1.91	0.51
3:I:111:PRO:HB3	3:I:113:GLU:HG2	1.91	0.51
2:N:92:ASP:H	3:O:158:HIS:HD2	1.58	0.50
1:J:5:GLU:HB2	1:J:16:LEU:HD21	1.93	0.50
1:J:106:LEU:O	3:L:66:ARG:HD3	2.11	0.50
1:D:18:SER:HB3	1:D:91:TRP:CE2	2.46	0.50
2:H:38:VAL:HG12	3:I:13:ARG:HG2	1.93	0.49
1:J:30:VAL:HG23	1:J:137:GLN:HG3	1.93	0.49
1:J:211:PRO:HB3	1:J:240:THR:HG21	1.95	0.49
2:K:127:LEU:HD21	3:L:13:ARG:HH21	1.77	0.49
1:D:14:CYS:HB3	1:D:95:VAL:HB	1.93	0.49
2:K:142:THR:HG22	2:K:158:TYR:HA	1.95	0.49
1:P:254:TRP:H	1:P:257:SER:HB3	1.76	0.49
3:I:140:PRO:HA	3:I:145:ARG:HD2	1.94	0.49
3:F:86:THR:HB	3:F:120:ILE:HD12	1.95	0.48
1:D:253:ILE:HG22	3:F:35:GLU:HB3	1.96	0.48
1:D:98:PRO:HA	1:D:101:ILE:HD12	1.96	0.48
1:G:60:LEU:HA	1:G:63:LEU:HD12	1.95	0.48
1:P:71:LEU:HD23	1:P:76:ARG:HG3	1.95	0.48
1:M:18:SER:HB3	1:M:91:TRP:CE2	2.48	0.48
1:P:60:LEU:HA	1:P:63:LEU:HD12	1.96	0.48
2:B:105:ASP:HB2	2:B:158:TYR:HB3	1.96	0.47
3:C:16:LEU:HA	3:C:120:ILE:O	2.15	0.47
1:A:11:THR:HG23	1:A:232:GLN:HE22	1.80	0.47
3:C:70:GLY:HA3	3:C:131:LEU:O	2.15	0.47
3:L:43:PRO:HB2	3:L:46:ARG:HB2	1.97	0.47
2:B:142:THR:HG22	2:B:158:TYR:HA	1.97	0.47
1:D:31:LEU:HB3	1:D:138:VAL:HG22	1.97	0.47
1:J:49:ILE:HG12	1:J:124:LEU:HB3	1.96	0.47
1:J:6:LEU:HD13	1:J:188:GLN:HB3	1.97	0.46
2:E:115:GLN:HE21	2:E:115:GLN:HB2	1.61	0.46
2:N:74:PHE:HB2	3:O:30:HIS:HB2	1.97	0.46
1:D:31:LEU:HD11	1:D:49:ILE:HD12	1.96	0.46
3:F:16:LEU:HD23	3:F:120:ILE:HG23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:SER:HB3	1:G:91:TRP:CE2	2.51	0.46
1:P:226:PRO:HA	1:P:249:ALA:HA	1.98	0.46
1:A:150:GLN:HE21	1:A:154:GLN:HE22	1.64	0.46
2:N:101:LEU:HD22	2:N:142:THR:HG21	1.98	0.46
2:N:52:LEU:HB3	2:N:61:PHE:HB2	1.97	0.46
1:A:169:ASP:O	1:A:176:SER:OG	2.29	0.45
3:F:16:LEU:HD11	3:F:21:LEU:HD21	1.99	0.45
3:C:72:GLU:HA	3:C:130:THR:HA	1.98	0.45
3:L:142:ALA:HB3	3:L:145:ARG:HG3	1.98	0.45
2:H:17:VAL:HG11	2:H:73:TRP:NE1	2.31	0.45
1:D:254:TRP:H	1:D:257:SER:HB2	1.82	0.45
1:G:211:PRO:HB3	1:G:240:THR:HG21	1.99	0.45
3:L:17:ARG:HA	3:L:121:GLY:HA2	1.97	0.45
3:O:58:GLY:HA3	3:O:137:ILE:HD11	1.99	0.45
2:E:25:LYS:HA	3:F:21:LEU:HD12	1.98	0.45
3:C:17:ARG:HG2	3:C:17:ARG:H	1.60	0.44
2:B:114:ASP:HA	2:B:129:LEU:HD21	2.00	0.44
2:B:175:VAL:HA	2:B:178:LEU:HD12	1.99	0.44
1:J:94:ASP:HB2	1:J:124:LEU:HD11	2.00	0.44
2:N:24:LEU:HD12	2:N:35:LEU:HD21	1.99	0.44
2:Q:141:VAL:HG12	2:Q:163:THR:HA	1.99	0.44
2:E:78:SER:HA	3:F:41:PRO:HA	2.00	0.44
2:H:220:ILE:HG13	2:H:221:PRO:HD2	1.98	0.44
1:A:199:LEU:HD23	3:C:46:ARG:HB3	2.00	0.44
1:M:68:SER:HA	1:M:71:LEU:HD12	1.99	0.43
1:A:93:LEU:HD11	1:A:181:CYS:HB3	2.00	0.43
2:H:217:SER:HA	2:H:220:ILE:HG22	2.00	0.43
1:J:140:VAL:HG22	1:J:164:VAL:HG13	2.01	0.43
1:A:157:PHE:HB3	1:A:160:ILE:HD12	2.00	0.43
1:D:253:ILE:CG2	3:F:35:GLU:HB3	2.48	0.43
1:D:33:VAL:HG22	1:D:49:ILE:HG22	2.00	0.43
1:A:225:GLU:HG3	1:A:228:PHE:H	1.85	0.42
1:D:42:LEU:HD22	1:D:216:THR:HG23	2.01	0.42
1:G:225:GLU:HG3	1:G:228:PHE:H	1.84	0.42
1:J:227:VAL:HG22	3:L:38:VAL:HG11	2.01	0.42
1:P:30:VAL:HG13	1:P:174:VAL:HG11	2.02	0.42
3:R:140:PRO:HA	3:R:145:ARG:HD2	2.02	0.42
2:B:141:VAL:HG12	2:B:163:THR:HA	2.02	0.42
2:E:38:VAL:HG23	3:F:13:ARG:HB3	2.01	0.42
1:A:140:VAL:HB	1:A:164:VAL:HG22	2.01	0.42
2:B:38:VAL:HG12	3:C:13:ARG:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:GLN:HG2	1:G:162:VAL:HB	2.01	0.42
1:J:33:VAL:HG22	1:J:49:ILE:HG22	2.02	0.42
2:B:66:PHE:HB3	2:B:85:LEU:HB3	2.02	0.41
1:P:27:GLU:HG3	1:P:53:PRO:HB3	2.02	0.41
3:R:49:THR:HA	3:R:52:ILE:HD12	2.02	0.41
1:D:172:TYR:HB2	1:D:175:VAL:HG23	2.02	0.41
2:B:109:LYS:HB3	2:B:109:LYS:HE2	1.90	0.41
1:D:47:TYR:OH	1:D:117:SER:HB3	2.20	0.41
2:E:170:LYS:O	2:E:174:THR:HG23	2.19	0.41
3:F:27:ALA:HB2	3:F:124:ALA:HB1	2.01	0.41
1:P:18:SER:HB3	1:P:91:TRP:CE2	2.56	0.41
3:F:43:PRO:HB2	3:F:46:ARG:HB2	2.01	0.41
2:N:172:ASN:HA	2:N:175:VAL:HG22	2.01	0.41
1:D:5:GLU:HB2	1:D:16:LEU:HD21	2.03	0.41
1:D:40:PRO:HD3	1:D:210:TYR:CZ	2.56	0.41
3:I:69:ARG:HH21	3:I:137:ILE:HD11	1.86	0.41
1:D:145:MET:HA	1:D:146:PRO:HD3	1.96	0.41
1:A:18:SER:HB3	1:A:91:TRP:CE2	2.55	0.41
2:B:19:LEU:HD13	2:B:85:LEU:HD11	2.02	0.41
3:I:76:PRO:HB2	3:I:79:LEU:HD12	2.03	0.41
2:K:20:VAL:HA	2:K:88:ALA:HB3	2.02	0.41
1:A:46:VAL:HG11	1:A:185:ALA:HB3	2.02	0.40
2:B:43:PRO:HB2	2:B:219:TYR:O	2.22	0.40
1:D:6:LEU:HD13	1:D:189:ALA:HB2	2.03	0.40
1:J:102:SER:O	1:J:106:LEU:HB2	2.21	0.40
3:F:48:PHE:CZ	3:F:61:VAL:HG11	2.57	0.40
1:G:40:PRO:HG3	1:G:210:TYR:CZ	2.56	0.40
2:H:17:VAL:HG11	2:H:73:TRP:CE2	2.57	0.40
2:B:101:LEU:HD22	2:B:142:THR:HG21	2.04	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	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
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

All (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
1	G	71	LEU
1	J	204	THR
2	K	76	ASN
2	K	182	ASN
2	Q	76	ASN
1	D	258	ALA
2	N	183	VAL
2	K	109	LYS
1	J	12	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	183	VAL

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
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

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	13	ARG
1	A	23	VAL
1	A	52	CYS
1	A	54	LEU
1	A	57	LEU
1	A	63	LEU
1	A	94	ASP
1	A	96	LEU
1	A	106	LEU
1	A	110	LYS
1	A	111	TYR
1	A	116	LEU
1	A	145	MET
1	A	149	TYR
1	A	152	ARG
1	A	186	ARG
1	A	238	TRP
1	A	240	THR
1	A	242	GLN
1	A	289	LEU
2	B	14	ARG
2	B	36	MET
2	B	55	MET
2	B	74	PHE
2	B	91	VAL
2	B	109	LYS
2	B	113	LEU
2	B	130	LYS
2	B	144	GLU
2	B	223	GLU
2	B	224	LEU
2	B	228	LEU
3	C	17	ARG
3	C	39	ASP
3	C	53	ARG
3	C	54	GLN
1	D	3	LEU
1	D	16	LEU
1	D	47	TYR
1	D	57	LEU
1	D	60	LEU
1	D	93	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	94	ASP
1	D	113	LEU
1	D	153	LEU
1	D	167	LYS
1	D	176	SER
1	D	186	ARG
1	D	188	GLN
1	D	199	LEU
1	D	205	ASP
1	D	206	TYR
1	D	242	GLN
1	D	286	ARG
1	D	294	GLU
2	E	14	ARG
2	E	59	GLN
2	E	74	PHE
2	E	84	LEU
2	E	96	LEU
2	E	97	LEU
2	E	98	LEU
2	E	105	ASP
2	E	106	LYS
2	E	115	GLN
2	E	137	LEU
2	E	139	HIS
2	E	208	TYR
2	E	215	LEU
2	E	216	ILE
2	E	218	ASP
2	E	224	LEU
2	E	226	ASP
3	F	21	LEU
3	F	22	ARG
3	F	46	ARG
3	F	49	THR
3	F	125	ASN
3	F	130	THR
3	F	144	VAL
3	F	152	SER
3	F	157	ILE
1	G	31	LEU
1	G	47	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	54	LEU
1	G	93	LEU
1	G	96	LEU
1	G	108	ARG
1	G	112	ASN
1	G	126	GLN
1	G	143	VAL
1	G	145	MET
1	G	150	GLN
1	G	153	LEU
1	G	176	SER
1	G	186	ARG
1	G	197	GLU
1	G	205	ASP
1	G	206	TYR
1	G	208	SER
1	G	222	GLU
1	G	238	TRP
1	G	250	GLU
2	H	17	VAL
2	H	20	VAL
2	H	54	ASN
2	H	59	GLN
2	H	67	LYS
2	H	84	LEU
2	H	107	GLU
2	H	135	GLU
2	H	136	LYS
2	H	208	TYR
2	H	215	LEU
2	H	220	ILE
3	I	11	ARG
3	I	16	LEU
3	I	29	LEU
3	I	39	ASP
3	I	57	GLU
3	I	144	VAL
1	J	7	GLU
1	J	15	ARG
1	J	56	ARG
1	J	57	LEU
1	J	69	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	94	ASP
1	J	106	LEU
1	J	149	TYR
1	J	171	LEU
1	J	186	ARG
1	J	196	VAL
1	J	202	LEU
1	J	206	TYR
1	J	238	TRP
1	J	240	THR
1	J	291	ARG
2	K	14	ARG
2	K	23	TYR
2	K	40	LEU
2	K	68	GLU
2	K	74	PHE
2	K	130	LYS
2	K	160	LYS
2	K	216	ILE
3	L	16	LEU
3	L	61	VAL
3	L	66	ARG
3	L	131	LEU
3	L	137	ILE
1	M	15	ARG
1	M	47	TYR
1	M	54	LEU
1	M	56	ARG
1	M	69	LYS
1	M	93	LEU
1	M	100	LEU
1	M	109	VAL
1	M	131	GLN
1	M	140	VAL
1	M	150	GLN
1	M	171	LEU
1	M	183	LYS
1	M	204	THR
1	M	238	TRP
1	M	239	ARG
1	M	294	GLU
2	N	47	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	67	LYS
2	N	131	LEU
2	N	144	GLU
2	N	162	LYS
2	N	164	LEU
2	N	230	LYS
3	O	61	VAL
1	P	38	ARG
1	P	41	VAL
1	P	42	LEU
1	P	47	TYR
1	P	60	LEU
1	P	93	LEU
1	P	94	ASP
1	P	113	LEU
1	P	115	SER
1	P	116	LEU
1	P	163	THR
1	P	169	ASP
1	P	193	TRP
1	P	222	GLU
1	P	238	TRP
1	P	240	THR
2	Q	50	ILE
2	Q	70	HIS
2	Q	74	PHE
2	Q	96	LEU
2	Q	139	HIS
2	Q	232	LEU
3	R	61	VAL
3	R	129	PHE
3	R	136	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	232	GLN
3	C	12	HIS
1	D	112	ASN
2	E	42	ASN
2	E	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	115	GLN
1	G	112	ASN
1	G	114	ASN
1	G	242	GLN
1	J	131	GLN
2	K	77	GLN
2	K	80	GLN
2	K	173	GLN
2	K	184	ASN
1	M	154	GLN
3	O	158	HIS
3	O	160	GLN
1	P	154	GLN
2	Q	15	GLN
2	Q	42	ASN

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 carbohydrates 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	270/302 (89%)	-0.54	1 (0%) 92 84	21, 48, 77, 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

All (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
1	P	89	VAL	2.5
1	P	216	THR	2.4
3	C	19	ALA	2.4
1	J	62	ALA	2.3
1	D	213	ASP	2.3
1	J	67	ASP	2.2
1	P	288	PHE	2.1
2	B	56	CYS	2.1
2	Q	175	VAL	2.1
1	P	211	PRO	2.1
2	E	206	GLU	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 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.