



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 01:02 PM UTC

PDB ID : 2QKK / pdb_00002qkk
Title : Human RNase H catalytic domain mutant D210N in complex with 14-mer RNA/DNA hybrid
Authors : Nowotny, M.; Gaidamakov, S.A.; Ghirlando, R.; Cerritelli, S.M.; Crouch, R.J.; Yang, W.
Deposited on : 2007-07-11
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul : 2022.3.0, CSD as543be (2022)
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

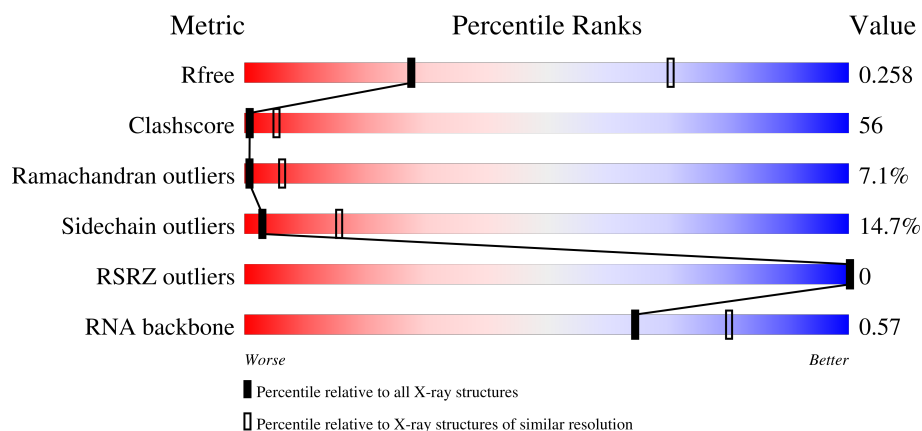
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



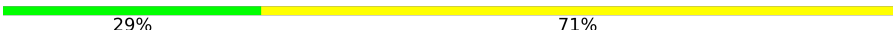
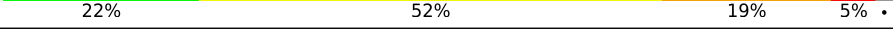
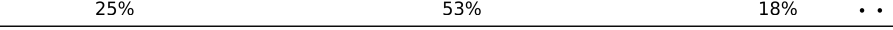
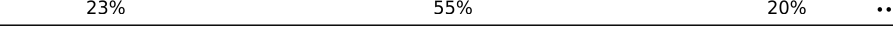
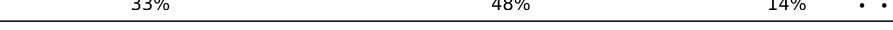
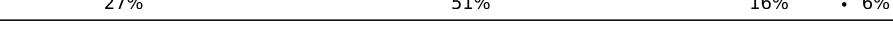
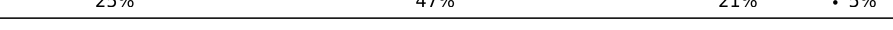
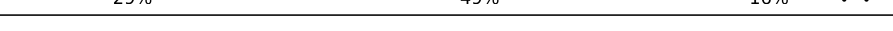
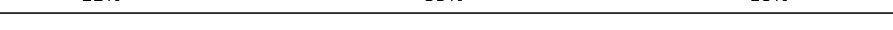
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	C	14	
1	G	14	
1	K	14	
1	O	14	

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Mol	Chain	Length	Quality of chain
1	T	14	
1	X	14	
2	D	14	
2	H	14	
2	L	14	
2	P	14	
2	U	14	
2	Z	14	
3	A	154	
3	B	154	
3	E	154	
3	F	154	
3	I	154	
3	J	154	
3	M	154	
3	N	154	
3	R	154	
3	S	154	
3	W	154	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 16231 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 RNA chain called 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	14	Total	C	N	O	P	0	0	0
			289	131	49	96	13			
1	G	14	Total	C	N	O	P	0	0	0
			289	131	49	96	13			
1	K	14	Total	C	N	O	P	0	0	0
			289	131	49	96	13			
1	O	14	Total	C	N	O	P	0	0	0
			289	131	49	96	13			
1	T	14	Total	C	N	O	P	0	0	0
			289	131	49	96	13			
1	X	13	Total	C	N	O	P	0	0	0
			269	122	46	89	12			

- Molecule 2 is a DNA chain called 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	14	Total	C	N	O	P	0	0	0
			290	138	57	82	13			
2	H	14	Total	C	N	O	P	0	0	0
			290	138	57	82	13			
2	L	14	Total	C	N	O	P	0	0	0
			290	138	57	82	13			
2	P	14	Total	C	N	O	P	0	0	0
			290	138	57	82	13			
2	U	14	Total	C	N	O	P	0	0	0
			290	138	57	82	13			
2	Z	11	Total	C	N	O	P	0	0	0
			229	109	47	63	10			

- Molecule 3 is a protein called Ribonuclease H1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	154	Total	C	N	O	S	0	0	0
			1186	737	222	220	7			
3	B	151	Total	C	N	O	S	1	0	0
			1175	731	223	214	7			
3	E	149	Total	C	N	O	S	0	0	0
			1147	715	217	209	6			
3	F	152	Total	C	N	O	S	3	0	0
			1175	733	219	216	7			
3	I	149	Total	C	N	O	S	6	0	0
			1133	706	213	208	6			
3	J	151	Total	C	N	O	S	5	0	0
			1166	728	218	213	7			
3	M	145	Total	C	N	O	S	3	0	0
			1117	700	208	203	6			
3	N	146	Total	C	N	O	S	0	0	0
			1121	701	208	206	6			
3	R	148	Total	C	N	O	S	0	0	0
			1144	714	215	208	7			
3	S	148	Total	C	N	O	S	7	0	0
			1126	704	210	206	6			
3	W	148	Total	C	N	O	S	9	0	0
			1141	716	211	207	7			

There are 44 discrepancies between the modelled and reference sequences:

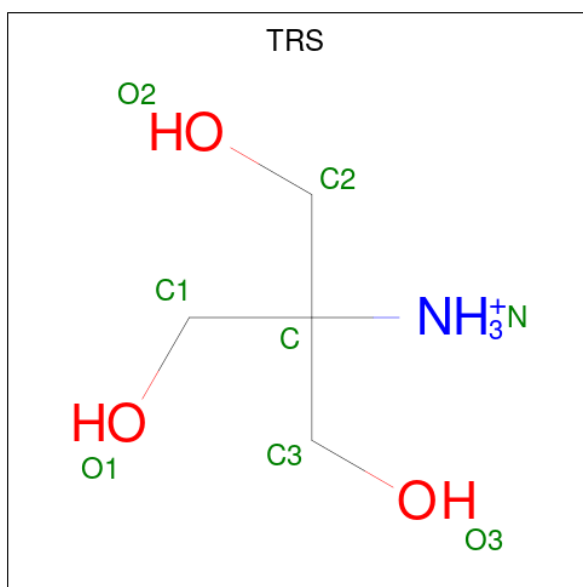
Chain	Residue	Modelled	Actual	Comment	Reference
A	133	GLY	-	expression tag	UNP O60930
A	134	SER	-	expression tag	UNP O60930
A	135	HIS	-	expression tag	UNP O60930
A	210	ASN	ASP	engineered mutation	UNP O60930
B	133	GLY	-	expression tag	UNP O60930
B	134	SER	-	expression tag	UNP O60930
B	135	HIS	-	expression tag	UNP O60930
B	210	ASN	ASP	engineered mutation	UNP O60930
E	133	GLY	-	expression tag	UNP O60930
E	134	SER	-	expression tag	UNP O60930
E	135	HIS	-	expression tag	UNP O60930
E	210	ASN	ASP	engineered mutation	UNP O60930
F	133	GLY	-	expression tag	UNP O60930
F	134	SER	-	expression tag	UNP O60930
F	135	HIS	-	expression tag	UNP O60930
F	210	ASN	ASP	engineered mutation	UNP O60930
I	133	GLY	-	expression tag	UNP O60930
I	134	SER	-	expression tag	UNP O60930

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Chain	Residue	Modelled	Actual	Comment	Reference
I	135	HIS	-	expression tag	UNP O60930
I	210	ASN	ASP	engineered mutation	UNP O60930
J	133	GLY	-	expression tag	UNP O60930
J	134	SER	-	expression tag	UNP O60930
J	135	HIS	-	expression tag	UNP O60930
J	210	ASN	ASP	engineered mutation	UNP O60930
M	133	GLY	-	expression tag	UNP O60930
M	134	SER	-	expression tag	UNP O60930
M	135	HIS	-	expression tag	UNP O60930
M	210	ASN	ASP	engineered mutation	UNP O60930
N	133	GLY	-	expression tag	UNP O60930
N	134	SER	-	expression tag	UNP O60930
N	135	HIS	-	expression tag	UNP O60930
N	210	ASN	ASP	engineered mutation	UNP O60930
R	133	GLY	-	expression tag	UNP O60930
R	134	SER	-	expression tag	UNP O60930
R	135	HIS	-	expression tag	UNP O60930
R	210	ASN	ASP	engineered mutation	UNP O60930
S	133	GLY	-	expression tag	UNP O60930
S	134	SER	-	expression tag	UNP O60930
S	135	HIS	-	expression tag	UNP O60930
S	210	ASN	ASP	engineered mutation	UNP O60930
W	133	GLY	-	expression tag	UNP O60930
W	134	SER	-	expression tag	UNP O60930
W	135	HIS	-	expression tag	UNP O60930
W	210	ASN	ASP	engineered mutation	UNP O60930

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).

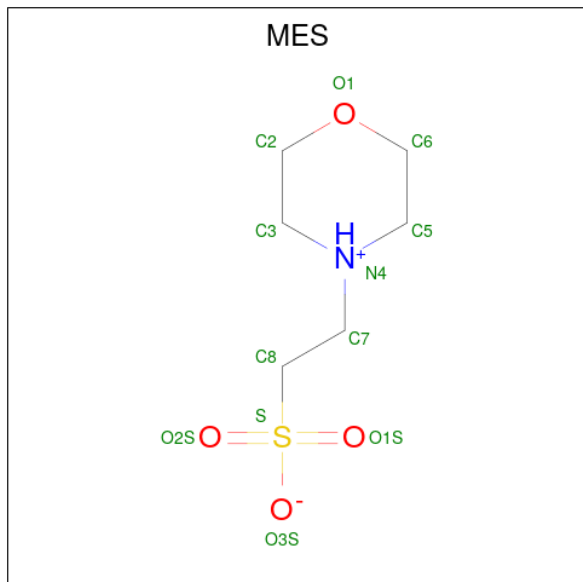


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	B	1	Total	Ca	0	0
			1	1		
5	E	2	Total	Ca	0	0
			2	2		
5	F	1	Total	Ca	0	0
			1	1		
5	I	1	Total	Ca	0	0
			1	1		
5	J	1	Total	Ca	0	0
			1	1		
5	M	2	Total	Ca	0	0
			2	2		
5	N	1	Total	Ca	0	0
			1	1		
5	R	1	Total	Ca	0	0
			1	1		
5	S	1	Total	Ca	0	0
			1	1		
5	W	1	Total	Ca	0	0
			1	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	2	Total	O	0	0
			2	2		
8	D	5	Total	O	0	0
			5	5		
8	G	8	Total	O	0	0
			8	8		
8	H	9	Total	O	0	0
			9	9		
8	K	4	Total	O	0	0
			4	4		
8	L	4	Total	O	0	0
			4	4		

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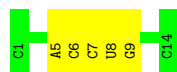
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	O	4	Total O 4 4	0	0
8	P	6	Total O 6 6	0	0
8	T	3	Total O 3 3	0	0
8	U	3	Total O 3 3	0	0
8	X	5	Total O 5 5	0	0
8	Z	3	Total O 3 3	0	0
8	A	16	Total O 16 16	0	0
8	B	15	Total O 15 15	0	0
8	E	16	Total O 16 16	0	0
8	F	13	Total O 13 13	0	0
8	I	3	Total O 3 3	0	0
8	J	12	Total O 12 12	0	0
8	M	6	Total O 6 6	0	0
8	N	7	Total O 7 7	0	0
8	R	7	Total O 7 7	0	0
8	S	11	Total O 11 11	0	0
8	W	10	Total O 10 10	0	0

3 Residue-property plots [i](#)

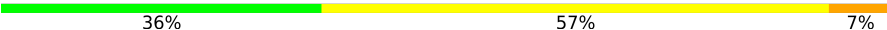
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'

Chain C: 

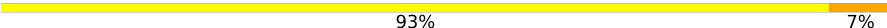


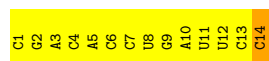
- Molecule 1: 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'

Chain G: 

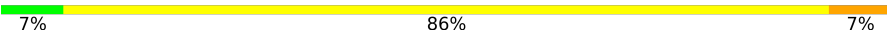


- Molecule 1: 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'

Chain K: 

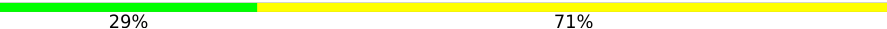


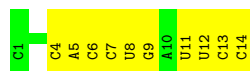
- Molecule 1: 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'

Chain O: 



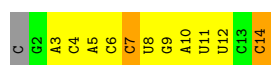
- Molecule 1: 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'

Chain T: 



- Molecule 1: 5'-R(*CP*GP*AP*CP*AP*CP*CP*UP*GP*AP*UP*UP*CP*C)-3'

Chain X: 



- Molecule 2: 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'



- Molecule 2: 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'



- Molecule 2: 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'



- Molecule 2: 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'



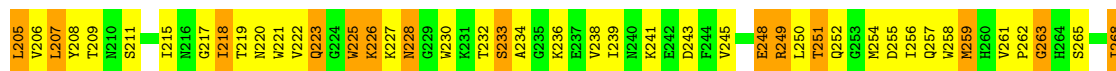
- Molecule 2: 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'



- Molecule 2: 5'-D(*GP*GP*AP*AP*TP*CP*AP*GP*GP*TP*GP*TP*CP*G)-3'



- Molecule 3: Ribonuclease H1



G269
N270
E271
E272
A273
D274
R275
L276
A277
R278
E279
G280
A281
K282
Q283
S284
E285
D286

• Molecule 3: Ribonuclease H1

Chain B: 22% 52% 19% 5%

GLY S134 H135 M136 K137 D138 Q139 F140 V141 V142 D145 G146 C147 C148 S149 S150 R153 R154 R155 R156 P157 R157 A158 G159 T219 T218 T217 T216 T215 T214 T213 T212 T211 T210 T209 T208 T207 T206 T205 T204 T203 T202 T201 N200 D206 G266 F267 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255

I256 Q257 W258 M259 H260 V261 P262 G263 H264 S265 G266 F267 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255

I256 Q257 W258 M259 H260 V261 P262 G263 H264 S265 G266 F267 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255

• Molecule 3: Ribonuclease H1

Chain E: 25% 53% 18%

GLY SER H135 M136 K137 D138 Q139 F140 V141 V142 D145 G146 C147 C148 S149 S150 R153 R154 R155 R156 P157 R157 A158 G159 T219 T218 T217 T216 T215 T214 T213 T212 T211 T210 T209 T208 T207 T206 T205 T204 T203 T202 T201 N200 D206 G266 F267 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255

I194 E195 A196 Q197 M198 H199 V200 P201 G202 H203 S204 G205 F206 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255

Q257 W258 M259 H260 V261 P262 G263 H264 S265 G266 F267 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255

• Molecule 3: Ribonuclease H1

Chain F: 23% 55% 20%

G133 S134 H135 M136 K137 D138 Q139 F140 V141 V142 D145 G146 C147 C148 S149 S150 R153 R154 R155 R156 P157 R157 A158 G159 T219 T218 T217 T216 T215 T214 T213 T212 T211 T210 T209 T208 T207 T206 T205 T204 T203 T202 T201 N200 D206 G266 F267 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255

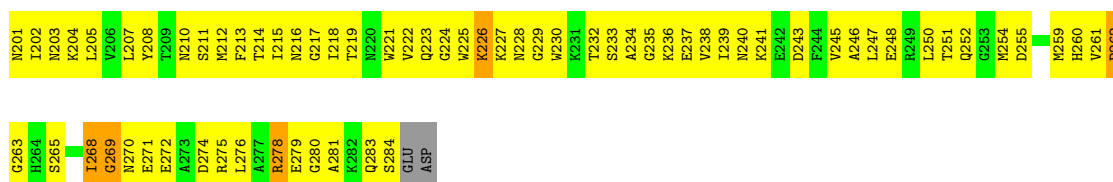
I194 E195 A196 Q197 M198 H199 V200 P201 G202 H203 S204 G205 F206 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255

Q257 W258 M259 H260 V261 P262 G263 H264 S265 G266 F267 T144 T145 T146 T147 T148 T149 T150 T151 T152 T153 T154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164 T165 T166 T167 T168 T169 T170 T171 T172 T173 T174 T175 T176 T177 T178 T179 T180 T181 T182 T183 T184 T185 T186 T187 T188 T189 T190 T191 T192 T193 T194 T244 T245 T246 T247 T248 T249 T250 T251 T252 T253 T254 T255

• Molecule 3: Ribonuclease H1

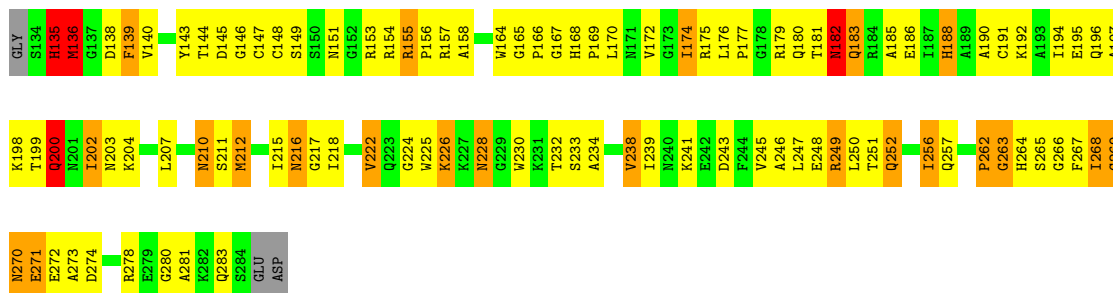
Chain I: 25% 60% 10%

GLY SER HIS M136 F139 V142 Y143 C148 S149 S150 N151 N152 N153 N154 N155 N156 N157 N158 N159 N160 N161 N162 N163 N164 H168 P169 L170 N171 V172 G173 I174 L175 L176 L177 G178 R179 Q180 T181 N182 N183 Q184 A185 E186 I187 H188 A189 A190 C191 K192 L250 T251 C191 Q252 Q253 Q254 Q255 Q256 Q257 Q258 Q259



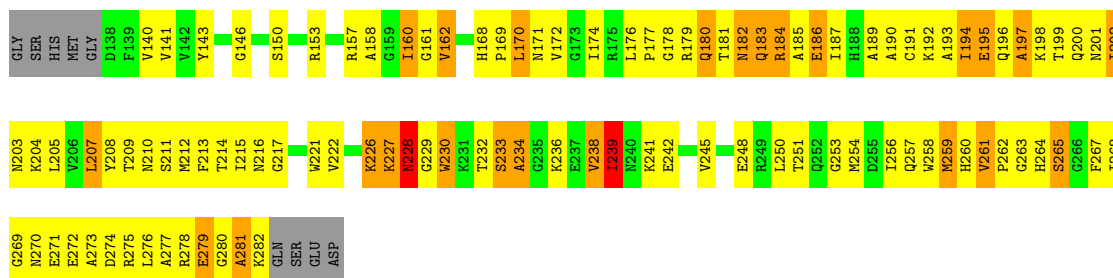
• Molecule 3: Ribonuclease H1

Chain J: 33% 48% 14% . .



• Molecule 3: Ribonuclease H1

Chain M: 27% 51% 16% . 6%



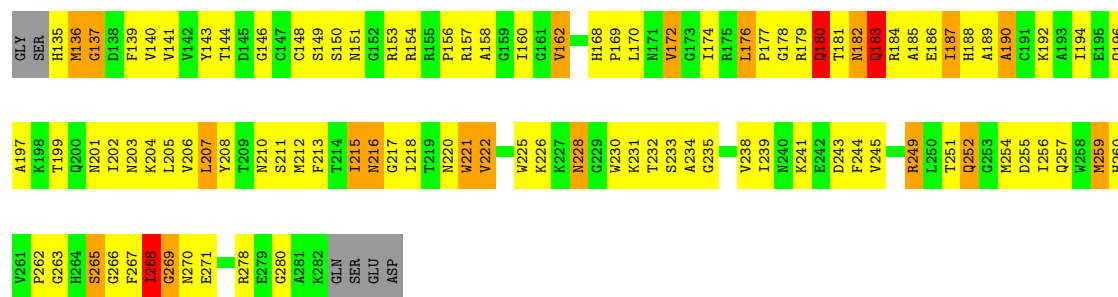
• Molecule 3: Ribonuclease H1

Chain N: 25% 47% 21% . 5%



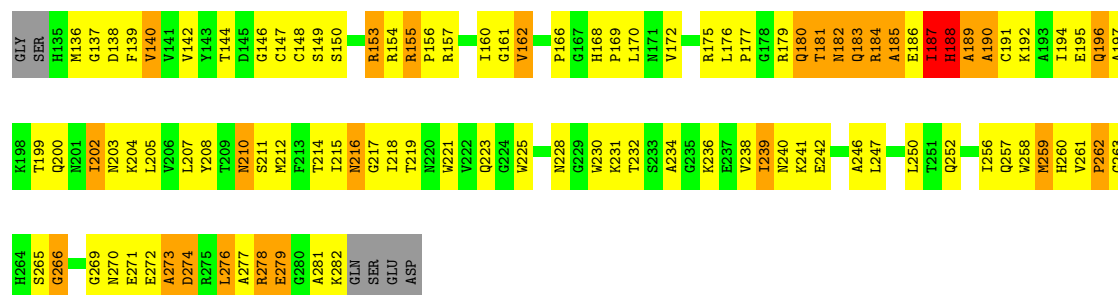
• Molecule 3: Ribonuclease H1

Chain R: 32% 50% 12% . .



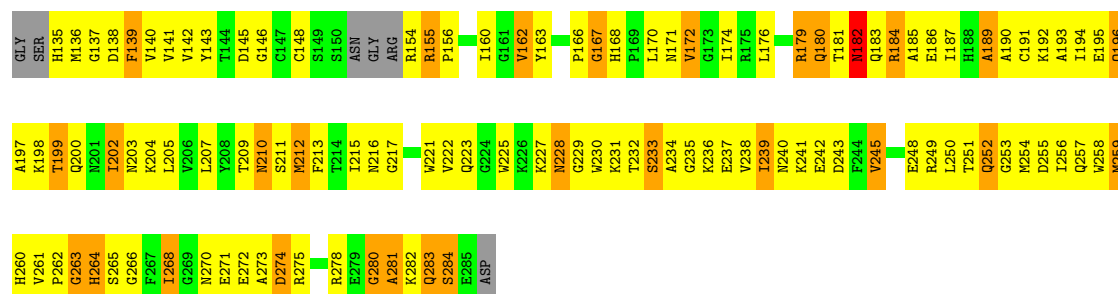
• Molecule 3: Ribonuclease H1

Chain S: 29% 49% 16% . .



• Molecule 3: Ribonuclease H1

Chain W: 22% 55% 18% . .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.06Å 176.20Å 125.84Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-3.20) 91.8 (30.00-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.269 0.212 , 0.258	Depositor DCC
R_{free} test set	1752 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.816	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.177 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16231	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CA, MES, TRS

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	C	0.46	0/321	0.84	0/497
1	G	0.45	0/321	0.88	0/497
1	K	0.35	0/321	0.69	0/497
1	O	0.33	0/321	0.66	0/497
1	T	0.36	0/321	0.68	0/497
1	X	0.32	0/299	0.64	0/463
2	D	0.40	0/326	1.20	4/503 (0.8%)
2	H	0.41	0/326	0.93	3/503 (0.6%)
2	L	0.32	0/326	1.15	3/503 (0.6%)
2	P	0.36	0/326	1.24	4/503 (0.8%)
2	U	0.31	0/326	1.22	2/503 (0.4%)
2	Z	0.29	0/258	1.25	4/398 (1.0%)
3	A	0.61	0/1212	1.12	3/1637 (0.2%)
3	B	0.56	1/1201 (0.1%)	1.45	17/1622 (1.0%)
3	E	0.56	0/1172	1.08	12/1586 (0.8%)
3	F	0.59	0/1200	1.09	6/1620 (0.4%)
3	I	0.43	0/1158	0.98	3/1571 (0.2%)
3	J	0.49	0/1192	1.08	10/1611 (0.6%)
3	M	0.48	0/1142	1.09	11/1546 (0.7%)
3	N	0.55	0/1145	1.16	16/1550 (1.0%)
3	R	0.50	0/1170	1.06	6/1583 (0.4%)
3	S	0.47	0/1151	1.04	11/1560 (0.7%)
3	W	0.42	0/1166	1.02	10/1576 (0.6%)
All	All	0.49	1/16701 (0.0%)	1.08	125/23323 (0.5%)

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
2	D	0	6
2	H	0	4
2	L	0	6
2	P	0	6
2	U	0	5
2	Z	0	6
All	All	0	33

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	212	MET	SD-CE	6.03	1.94	1.79

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	155	ARG	CA-C-N	23.37	149.06	119.84
3	B	155	ARG	C-N-CA	23.37	149.06	119.84
3	I	152	GLY	N-CA-C	-13.69	99.08	111.67
3	S	279	GLU	N-CA-C	-9.90	100.96	113.43
3	B	155	ARG	C-N-CD	-9.81	84.79	125.00

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	15	DG	Sidechain
2	D	18	DA	Sidechain
2	D	19	DT	Sidechain
2	D	20	DC	Sidechain
2	D	22	DG	Sidechain

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	C	289	0	153	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	289	0	153	13	0
1	K	289	0	153	17	0
1	O	289	0	153	14	0
1	T	289	0	153	13	0
1	X	269	0	142	9	0
2	D	290	0	159	27	0
2	H	290	0	159	33	1
2	L	290	0	159	47	0
2	P	290	0	159	35	0
2	U	290	0	159	41	0
2	Z	229	0	125	36	0
3	A	1186	0	1137	124	0
3	B	1175	0	1144	128	0
3	E	1147	0	1105	130	0
3	F	1175	0	1135	164	0
3	I	1133	0	1074	140	0
3	J	1166	0	1130	118	0
3	M	1117	0	1083	121	0
3	N	1121	0	1075	132	0
3	R	1144	0	1104	120	0
3	S	1126	0	1077	145	0
3	W	1141	0	1101	152	0
4	D	8	0	12	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	M	2	0	0	0	0
5	N	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	W	1	0	0	0	0
6	A	12	0	13	1	0
7	B	1	0	0	0	0
8	A	16	0	0	1	0
8	B	15	0	0	4	0
8	C	2	0	0	0	0
8	D	5	0	0	1	0
8	E	16	0	0	4	0
8	F	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	8	0	0	0	0
8	H	9	0	0	0	0
8	I	3	0	0	1	0
8	J	12	0	0	5	0
8	K	4	0	0	1	0
8	L	4	0	0	2	0
8	M	6	0	0	1	0
8	N	7	0	0	0	0
8	O	4	0	0	0	0
8	P	6	0	0	3	0
8	R	7	0	0	2	0
8	S	11	0	0	2	0
8	T	3	0	0	0	0
8	U	3	0	0	0	0
8	W	10	0	0	2	0
8	X	5	0	0	1	0
8	Z	3	0	0	0	0
All	All	16231	0	14017	1668	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 56.

The worst 5 of 1668 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:L:15:DG:H4'	2:L:16:DG:H5'	1.16	1.15
2:L:15:DG:H4'	2:L:16:DG:C5'	1.77	1.14
3:W:199:THR:HG23	3:W:200:GLN:HE21	1.12	1.14
3:A:183:GLN:HE21	3:A:183:GLN:HA	1.10	1.11
3:R:187:ILE:HD11	3:R:243:ASP:HB3	1.37	1.07

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)
2:H:15:DG:C5'	2:H:15:DG:C5'[2_455]	1.91	0.29

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	
3	A	152/154 (99%)	112 (74%)	34 (22%)	6 (4%)	2	18
3	B	149/154 (97%)	106 (71%)	28 (19%)	15 (10%)	0	2
3	E	147/154 (96%)	111 (76%)	29 (20%)	7 (5%)	2	14
3	F	148/154 (96%)	112 (76%)	23 (16%)	13 (9%)	0	3
3	I	147/154 (96%)	104 (71%)	30 (20%)	13 (9%)	0	3
3	J	149/154 (97%)	111 (74%)	29 (20%)	9 (6%)	1	10
3	M	143/154 (93%)	103 (72%)	34 (24%)	6 (4%)	2	16
3	N	142/154 (92%)	98 (69%)	31 (22%)	13 (9%)	0	3
3	R	146/154 (95%)	107 (73%)	30 (20%)	9 (6%)	1	9
3	S	146/154 (95%)	98 (67%)	38 (26%)	10 (7%)	1	7
3	W	144/154 (94%)	101 (70%)	29 (20%)	14 (10%)	0	3
All	All	1613/1694 (95%)	1163 (72%)	335 (21%)	115 (7%)	1	6

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	228	ASN
3	B	135	HIS
3	B	150	SER
3	B	155	ARG
3	B	156	PRO

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	
3	A	120/124 (97%)	99 (82%)	21 (18%)	2	10
3	B	121/124 (98%)	97 (80%)	24 (20%)	1	8
3	E	115/124 (93%)	98 (85%)	17 (15%)	3	15
3	F	120/124 (97%)	98 (82%)	22 (18%)	2	9
3	I	112/124 (90%)	102 (91%)	10 (9%)	9	34
3	J	119/124 (96%)	102 (86%)	17 (14%)	3	16
3	M	113/124 (91%)	95 (84%)	18 (16%)	2	13
3	N	113/124 (91%)	97 (86%)	16 (14%)	3	17
3	R	116/124 (94%)	101 (87%)	15 (13%)	4	20
3	S	112/124 (90%)	98 (88%)	14 (12%)	4	21
3	W	115/124 (93%)	102 (89%)	13 (11%)	5	24
All	All	1276/1364 (94%)	1089 (85%)	187 (15%)	3	16

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	184	ARG
3	N	265	SER
3	M	202	ILE
3	N	170	LEU
3	R	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
3	R	257	GLN
3	W	216	ASN
3	R	270	ASN
3	S	228	ASN
3	I	171	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	13/14 (92%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	13/14 (92%)	1 (7%)	0
1	K	13/14 (92%)	2 (15%)	0
1	O	13/14 (92%)	1 (7%)	0
1	T	13/14 (92%)	0	0
1	X	12/14 (85%)	2 (16%)	0
All	All	77/84 (91%)	6 (7%)	0

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	G	7	C
1	K	7	C
1	K	14	C
1	O	7	C
1	X	7	C

There are no RNA pucker outliers to report.

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](#)

Of 17 ligands modelled in this entry, 15 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	TRS	D	2003	-	7,7,7	0.88	0	9,9,9	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MES	A	2002	-	12,12,12	1.08	1 (8%)	15,16,16	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	D	2003	-	-	0/9/9/9	-
6	MES	A	2002	-	-	0/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2002	MES	C8-S	2.57	1.81	1.77

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2002	MES	1	0

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	C	14/14 (100%)	-1.64	0 100 100	17, 24, 34, 40	0
1	G	14/14 (100%)	-1.65	0 100 100	24, 31, 38, 41	0
1	K	14/14 (100%)	-1.63	0 100 100	56, 62, 72, 75	0
1	O	14/14 (100%)	-1.76	0 100 100	44, 52, 74, 76	0
1	T	14/14 (100%)	-1.61	0 100 100	44, 57, 76, 85	0
1	X	13/14 (92%)	-1.07	0 100 100	68, 89, 144, 152	0
2	D	14/14 (100%)	-1.30	0 100 100	22, 32, 43, 50	0
2	H	14/14 (100%)	-1.22	0 100 100	28, 36, 43, 48	0
2	L	14/14 (100%)	-1.15	0 100 100	55, 74, 92, 123	0
2	P	14/14 (100%)	-1.27	0 100 100	42, 56, 81, 103	0
2	U	14/14 (100%)	-1.16	0 100 100	54, 69, 83, 91	0
2	Z	11/14 (78%)	-0.84	0 100 100	82, 88, 117, 131	0
3	A	154/154 (100%)	-1.20	0 100 100	18, 36, 73, 96	0
3	B	151/154 (98%)	-1.17	0 100 100	30, 51, 82, 108	1 (0%)
3	E	149/154 (96%)	-1.07	0 100 100	32, 51, 77, 93	0
3	F	152/154 (98%)	-1.16	0 100 100	30, 50, 83, 101	1 (0%)
3	I	149/154 (96%)	-0.94	0 100 100	44, 92, 117, 129	1 (0%)
3	J	151/154 (98%)	-1.05	0 100 100	35, 64, 87, 96	2 (1%)
3	M	145/154 (94%)	-1.19	0 100 100	35, 59, 80, 102	1 (0%)
3	N	146/154 (94%)	-1.07	0 100 100	46, 68, 87, 96	1 (0%)
3	R	148/154 (96%)	-1.22	0 100 100	34, 56, 80, 87	1 (0%)
3	S	148/154 (96%)	-1.07	0 100 100	29, 70, 98, 109	3 (2%)
3	W	148/154 (96%)	-1.06	0 100 100	45, 75, 96, 102	3 (2%)
All	All	1805/1862 (96%)	-1.13	0 100 100	17, 63, 98, 152	14 (0%)

There are no RSRZ outliers to report.

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TRS	D	2003	8/8	0.92	0.10	94,96,97,97	0
5	CA	E	1004	1/1	0.96	0.04	68,68,68,68	0
7	CL	B	2001	1/1	0.97	0.09	49,49,49,49	0
6	MES	A	2002	12/12	0.98	0.08	136,136,138,138	0
5	CA	A	1001	1/1	0.99	0.03	44,44,44,44	0
5	CA	I	1006	1/1	0.99	0.04	78,78,78,78	0
5	CA	M	1014	1/1	0.99	0.03	106,106,106,106	0
5	CA	R	1011	1/1	0.99	0.03	64,64,64,64	0
5	CA	A	1002	1/1	0.99	0.02	23,23,23,23	0
5	CA	E	1003	1/1	0.99	0.03	44,44,44,44	0
5	CA	F	1013	1/1	1.00	0.03	32,32,32,32	0
5	CA	N	1005	1/1	1.00	0.02	56,56,56,56	0
5	CA	B	1009	1/1	1.00	0.02	38,38,38,38	0
5	CA	S	1007	1/1	1.00	0.02	77,77,77,77	0
5	CA	W	1012	1/1	1.00	0.03	81,81,81,81	0
5	CA	J	1008	1/1	1.00	0.03	53,53,53,53	0
5	CA	M	1010	1/1	1.00	0.01	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.