Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 12:04 PM EDT

PDB ID	:	3QYM
Title	:	Structure of p63 DNA Binding Domain in Complex with a 10 Base Pair A/T Rich Response Element Half Site
Authors	:	Herzberg, O.; Chen, C.
Deposited on	:	2011-03-03
Resolution	:	3.20 Å(reported)

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

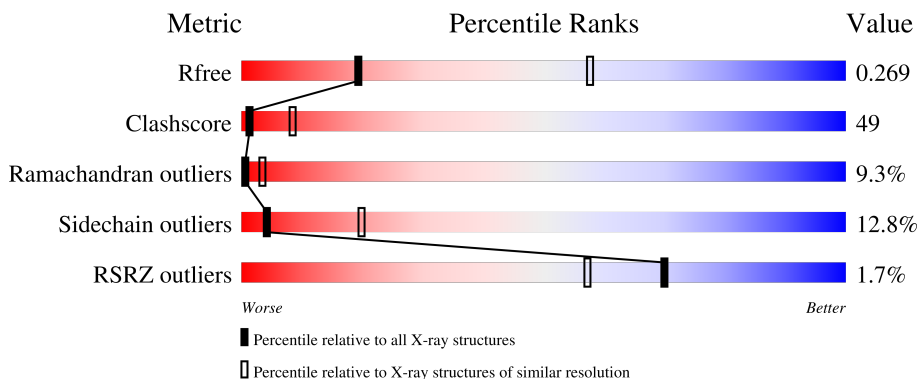|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	Percentile Ranks	Value
Rfree		0.269
Clashscore		49
Ramachandran outliers		9.3%
Sidechain outliers		12.8%
RSRZ outliers		1.7%

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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	203	3% 35% 45% 13% • 5%
1	B	203	3% 34% 45% 14% • 6%
1	C	203	33% 49% 14% • •
1	D	203	% 33% 49% 14% • •
1	E	203	% 34% 46% 16% • •

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Mol	Chain	Length	Quality of chain
1	F	203	.% 34%　　　47%　　　14%　··
1	G	203	2% 33%　　　46%　　　13%　·　6%
1	H	203	.% 31%　　　47%　　　14%　·　7%
2	I	10	100%
2	J	10	100%
2	K	10	10%　　　90%
2	L	10	10%　　　90%
2	M	10	10%　　　90%
2	N	10	10%　　　90%
2	O	10	10%　　　90%
2	P	10	10%　　　90%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13681 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 Tumor protein 63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1497	937	266	282	12			
1	B	191	Total	C	N	O	S	0	0	0
			1496	936	266	282	12			
1	C	195	Total	C	N	O	S	0	0	0
			1518	948	270	288	12			
1	D	196	Total	C	N	O	S	0	0	0
			1523	951	271	289	12			
1	E	197	Total	C	N	O	S	0	0	0
			1534	957	275	290	12			
1	F	195	Total	C	N	O	S	0	0	0
			1518	948	270	288	12			
1	G	190	Total	C	N	O	S	0	0	0
			1487	930	265	280	12			
1	H	189	Total	C	N	O	S	0	0	0
			1484	930	264	278	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	GLY	-	expression tag	UNP Q9H3D4
A	122	SER	-	expression tag	UNP Q9H3D4
A	123	HIS	-	expression tag	UNP Q9H3D4
A	124	MET	-	expression tag	UNP Q9H3D4
A	125	ALA	-	expression tag	UNP Q9H3D4
A	126	SER	-	expression tag	UNP Q9H3D4
B	121	GLY	-	expression tag	UNP Q9H3D4
B	122	SER	-	expression tag	UNP Q9H3D4
B	123	HIS	-	expression tag	UNP Q9H3D4
B	124	MET	-	expression tag	UNP Q9H3D4
B	125	ALA	-	expression tag	UNP Q9H3D4
B	126	SER	-	expression tag	UNP Q9H3D4
C	121	GLY	-	expression tag	UNP Q9H3D4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	122	SER	-	expression tag	UNP Q9H3D4
C	123	HIS	-	expression tag	UNP Q9H3D4
C	124	MET	-	expression tag	UNP Q9H3D4
C	125	ALA	-	expression tag	UNP Q9H3D4
C	126	SER	-	expression tag	UNP Q9H3D4
D	121	GLY	-	expression tag	UNP Q9H3D4
D	122	SER	-	expression tag	UNP Q9H3D4
D	123	HIS	-	expression tag	UNP Q9H3D4
D	124	MET	-	expression tag	UNP Q9H3D4
D	125	ALA	-	expression tag	UNP Q9H3D4
D	126	SER	-	expression tag	UNP Q9H3D4
E	121	GLY	-	expression tag	UNP Q9H3D4
E	122	SER	-	expression tag	UNP Q9H3D4
E	123	HIS	-	expression tag	UNP Q9H3D4
E	124	MET	-	expression tag	UNP Q9H3D4
E	125	ALA	-	expression tag	UNP Q9H3D4
E	126	SER	-	expression tag	UNP Q9H3D4
F	121	GLY	-	expression tag	UNP Q9H3D4
F	122	SER	-	expression tag	UNP Q9H3D4
F	123	HIS	-	expression tag	UNP Q9H3D4
F	124	MET	-	expression tag	UNP Q9H3D4
F	125	ALA	-	expression tag	UNP Q9H3D4
F	126	SER	-	expression tag	UNP Q9H3D4
G	121	GLY	-	expression tag	UNP Q9H3D4
G	122	SER	-	expression tag	UNP Q9H3D4
G	123	HIS	-	expression tag	UNP Q9H3D4
G	124	MET	-	expression tag	UNP Q9H3D4
G	125	ALA	-	expression tag	UNP Q9H3D4
G	126	SER	-	expression tag	UNP Q9H3D4
H	121	GLY	-	expression tag	UNP Q9H3D4
H	122	SER	-	expression tag	UNP Q9H3D4
H	123	HIS	-	expression tag	UNP Q9H3D4
H	124	MET	-	expression tag	UNP Q9H3D4
H	125	ALA	-	expression tag	UNP Q9H3D4
H	126	SER	-	expression tag	UNP Q9H3D4

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	10	Total 202	C 99	N 36	O 58	P 9	0	0	0
2	J	10	Total 202	C 99	N 36	O 58	P 9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	10	Total	C	N	O	P	0	0	0
			202	99	36	58	9			
2	L	10	Total	C	N	O	P	0	0	0
			202	99	36	58	9			
2	M	10	Total	C	N	O	P	0	0	0
			202	99	36	58	9			
2	N	10	Total	C	N	O	P	0	0	0
			202	99	36	58	9			
2	O	10	Total	C	N	O	P	0	0	0
			202	99	36	58	9			
2	P	10	Total	C	N	O	P	0	0	0
			202	99	36	58	9			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

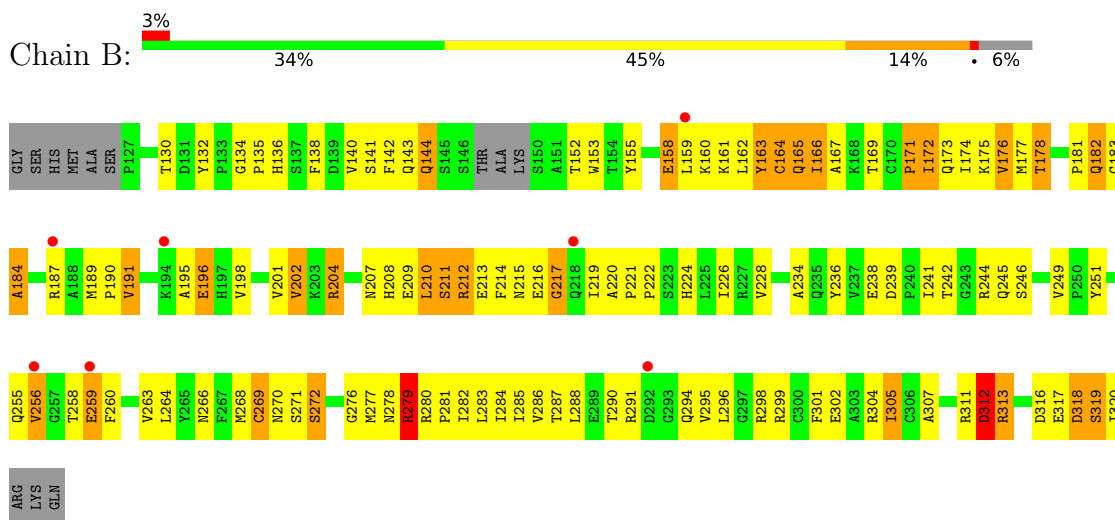| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		

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.
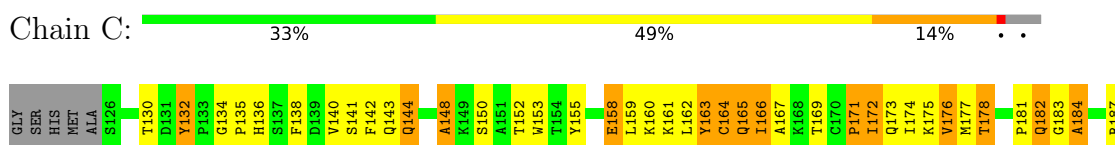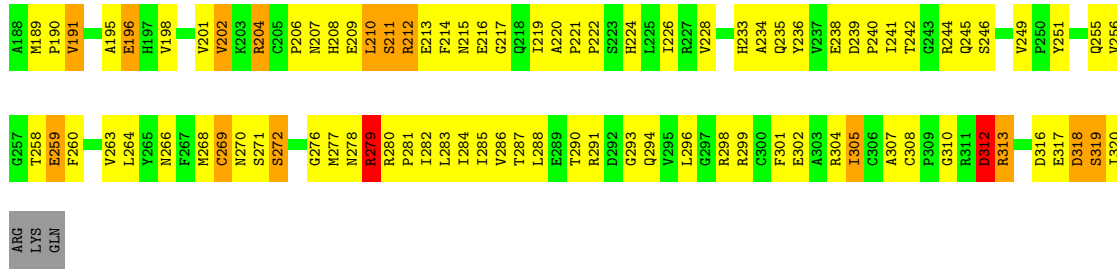
• Molecule 1: Tumor protein 63
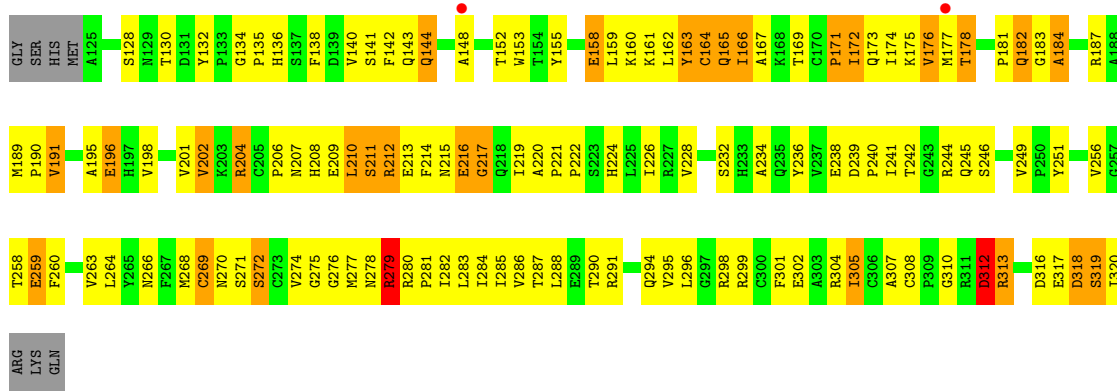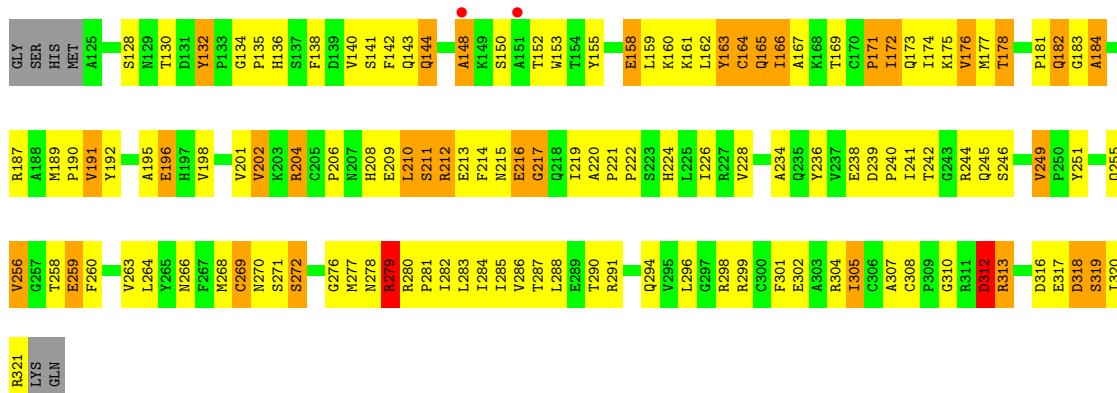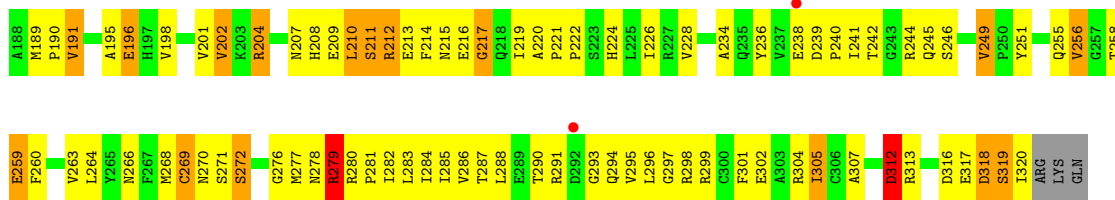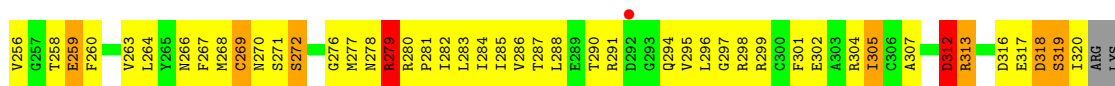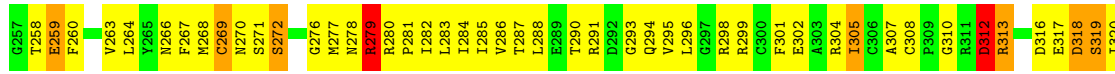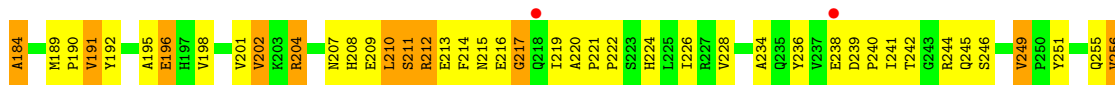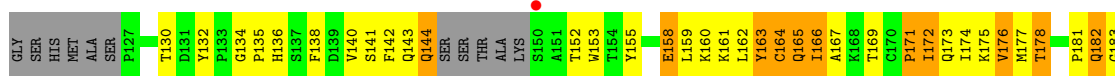
Chain A:

• Molecule 1: Tumor protein 63

Chain B:

• Molecule 1: Tumor protein 63

Chain C:

A188 M189 P190 V191 A195 E196 H197 V198 V201 V202 K203 R204 C205 P206 N207 H208 E209 L210 S211 R212 E213 F214 N215 E216 G217 Q218 I219 A220 P221 P222 S223 H224 L225 I226 R227 V228 H233 A234 Q235 Y236 V237 E238 D239 P240 I241 T242 G243 R244 Q245 S246 V249 P250 Y251 Q255 V256

G257 T258 E259 F260 V263 L264 Y265 N266 F267 M268 C269 N270 S271 S272 G276 M277 N278 R279 R280 P281 I282 L283 I284 I285 V286 T287 L288 E289 T290 D292 G293 Q294 L296 G297 R298 R299 C300 F301 E302 A303 R304 I305 C306 A307 C308 P309 G310 R311 D312 R313 D316 E317 D318 S319 I320

ARG LYS GLN

• Molecule 1: Tumor protein 63

%

Chain D:
33%   49%   14%

GLY SER HIS MET A125 S128 N129 T130 D131 Y132 P133 G134 P135 H136 S137 F138 D139 V140 S141 F142 Q143 Q144 A148 T152 W153 T154 Y155 E158 L159 K160 K161 L162 Y163 C164 Q165 I166 A167 K168 T169 C170 P171 I172 Q173 I174 K175 V176 M177 T178 P181 Q182 G183 A184 R187 A188

M189 P190 V191 A195 E196 H197 V198 V201 V202 K203 R204 C205 P206 N207 H208 E209 L210 S211 R212 F214 N215 E216 G217 Q218 I219 A220 P221 P222 S223 H224 L225 I226 R227 V228 S232 H233 A234 Q235 Y236 V237 E238 D239 P240 I241 T242 G243 Q245 S246 V249 P250 Y251 V256 G257

T258 E259 F260 V263 L264 Y265 N266 F267 M268 C269 N270 S271 S272 C273 V274 G275 Q276 M277 N278 R279 R280 P281 I282 L283 I284 I285 V286 T287 L288 E289 T290 R291 Q294 V295 L296 G297 R298 R299 C300 F301 E302 A303 R304 I305 C306 A307 C308 P309 G310 R311 D312 R313 D316 E317 D318 S319 I320

ARG LYS GLN

• Molecule 1: Tumor protein 63

%

Chain E:
34%   46%   16%

GLY SER HIS MET A125 S128 N129 T130 D131 Y132 P133 G134 P135 H136 S137 F138 D139 V140 S141 F142 Q143 Q144 A148 K149 S150 A151 T152 W153 T154 Y155 E158 L159 K160 K161 L162 Y163 C164 Q165 I166 A167 K168 T169 C170 P171 I172 Q173 I174 K175 V176 M177 T178 P181 Q182 G183 A184

R187 A188 M189 P190 V191 Y192 A195 E196 H197 V198 V201 V202 K203 R204 C205 P206 N207 H208 E209 L210 S211 R212 E213 F214 N215 E216 G217 Q218 I219 A220 P221 P222 S223 H224 L225 I226 R227 V228 A234 Q235 Y236 V237 E238 D239 P240 I241 T242 G243 R244 Q245 S246 V249 P250 Y251 Q255

V256 G257 T258 E259 F260 V263 L264 Y265 N266 F267 M268 C269 N270 S271 S272 G276 M277 N278 R279 R280 P281 I282 L283 I284 I285 V286 T287 L288 E289 T290 R291 Q294 V295 L296 G297 R298 R299 C300 F301 E302 A303 R304 I305 C306 A307 C308 P309 G310 R311 D312 R313 D316 E317 D318 S319 I320

R321 LYS GLN

• Molecule 1: Tumor protein 63

%

Chain F:
34%   47%   14%

GLY SER HIS MET ALA S126 T130 D131 Y132 P133 G134 P135 H136 S137 F138 D139 V140 S141 F142 Q143 Q144 A148 K149 S150 A151 T152 W153 T154 Y155 E158 L159 K160 K161 L162 Y163 C164 Q165 I166 A167 K168 T169 C170 P171 I172 Q173 I174 K175 V176 M177 T178 P181 Q182 G183 A184 R187

A188 M189 P190 V191 A195 E196 H197 V198 V201 V202 K203 R204 N207 H208 E209 L210 S211 R212 E213 F214 N215 E216 G217 Q218 I219 A220 P221 P222 S223 H224 L225 I226 R227 V228 A234 Q235 Y236 V237 E238 D239 P240 I241 T242 G243 R244 Q245 S246 V249 P250 Y251 Q255 V256 G257 T258

E259 F260 V263 L264 Y265 N266 F267 M268 C269 N270 S271 S272 G276 M277 N278 R279 R280 P281 I282 L283 I284 I285 V286 T287 L288 E289 T290 R291 D292 G293 Q294 V295 L296 G297 R298 R299 C300 F301 E302 A303 R304 I305 C306 A307 D312 R313 D316 E317 D318 S319 I320 ARG LYS GLN

• Molecule 1: Tumor protein 63

Chain G:

GLY SER HIS MET ALA SER PRO S128 N129 T130 D131 Y132 P133 G134 P135 H136 S137 F138 D139 V140 S141 F142 Q143 Q144 S145 SER THR ALA K149 T152 W153 T154 Y155 E158 L159 K160 K161 L162 Y163 C164 Q165 I166 A167 K168 T169 C170 P171 I172 Q173 I174 K175 V176 M177 T178 P181 Q182 G183

A184 R187 A188 M189 P190 V191 A195 E196 H197 V198 V201 V202 K203 R204 N207 H208 E209 L210 S211 R212 E213 F214 N215 E216 G217 Q218 I219 A220 P221 P222 S223 H224 L225 I226 R227 V228 E229 A234 Q235 Y236 V237 E238 D239 P240 I241 T242 G243 R244 Q245 S246 V249 P250 Y251

V256 G257 T258 E259 F260 V263 L264 Y265 N266 F267 M268 C269 N270 S271 S272 G276 M277 N278 R279 R280 P281 I282 L283 I284 I285 V286 T287 L288 E289 T290 D292 G293 Q294 V295 L296 G297 R298 R299 C300 F301 E302 A303 R304 I305 C306 A307 D312 R313 D316 E317 D318 S319 I320 ARG LYS

GLN

• Molecule 1: Tumor protein 63

Chain H:

GLY SER HIS MET ALA SER P127 T130 D131 Y132 P133 G134 P135 H136 S137 F138 D139 V140 S141 F142 Q143 Q144 SER THR ALA LYS S150 A151 T152 W153 T154 Y155 E158 L159 K160 K161 L162 Y163 C164 Q165 I166 A167 K168 T169 C170 P171 I172 Q173 I174 K175 V176 M177 T178 P181 Q182 G183

A184 M189 P190 V191 Y192 A195 E196 H197 V198 V201 V202 K203 R204 N207 H208 E209 L210 S211 R212 E213 F214 N215 E216 G217 Q218 I219 A220 P221 P222 S223 H224 I226 L225 R227 V228 A234 Q235 Y236 V237 E238 D239 P240 I241 T242 G243 R244 Q245 S246 V249 P250 Y251 Q255 V256

G257 T258 E259 F260 V263 L264 Y265 N266 F267 M268 C269 N270 S271 S272 G276 M277 N278 R279 R280 P281 I282 L283 I284 I285 V286 T287 L288 E289 T290 R291 D292 G293 Q294 V295 L296 G297 R298 R299 C300 F301 E302 A303 R304 I305 C306 A307 C308 P309 G310 R311 D312 R313 D316 E317 D318 S319 I320

ARG LYS GLN

• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'

Chain I: 100%

A1 A2 A3 C4 A5 T6 G7 T8 T9 T10

• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'

Chain J: 100%

A1 A2 A3 C4 A5 T6 G7 T8 T9 T10

• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'

Chain K: 10% 90%

A1 A2 A3 C4 A5 T6 G7 T8 T9 T10

• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'

Chain L: 10% 90%

A1 A2 A3 C4 A5 T6 G7 T8 T9 T10

• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'

Chain M: 10% 90%

A1 A2 A3 C4 A5 T6 G7 T8 T9 T10

• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'

Chain N: 10% 90%

A1 A2 A3 C4 A5 T6 G7 T8 T9 T10

• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'

Chain O: 10% 90%

A1 A2 A3 C4 A5 T6 G7 T8 T9 T10

• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'

Chain P: 10% 90%

A1 A2 A3 C4 A5 T6 G7 T8 T9 T10

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.87Å 180.20Å 104.38Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	19.72 – 3.20 19.72 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.72-3.20) 97.4 (19.72-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.245 , 0.271 0.240 , 0.269	Depositor DCC
R_{free} test set	1917 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	82.2	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 66.7	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.39, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.085 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13681	wwPDB-VP
Average B, all atoms (Å^2)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.38	0/1532	0.66	0/2082
1	B	0.37	0/1531	0.65	1/2079 (0.0%)
1	C	0.43	0/1554	0.66	0/2113
1	D	0.40	0/1559	0.66	1/2120 (0.0%)
1	E	0.43	0/1570	0.67	1/2134 (0.0%)
1	F	0.40	0/1554	0.66	1/2113 (0.0%)
1	G	0.39	0/1521	0.65	0/2065
1	H	0.40	0/1519	0.66	1/2063 (0.0%)
2	I	0.67	0/226	0.79	0/347
2	J	0.74	0/226	0.78	0/347
2	K	0.75	0/226	0.82	0/347
2	L	0.64	0/226	0.83	0/347
2	M	0.57	0/226	0.78	0/347
2	N	0.57	0/226	0.80	0/347
2	O	0.55	0/226	0.78	0/347
2	P	0.55	0/226	0.79	0/347
All	All	0.44	0/14148	0.68	5/19545 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	217	GLY	N-CA-C	-5.11	100.32	113.10
1	H	217	GLY	N-CA-C	-5.10	100.36	113.10
1	B	217	GLY	N-CA-C	-5.07	100.43	113.10
1	E	217	GLY	N-CA-C	-5.07	100.44	113.10
1	D	217	GLY	N-CA-C	-5.05	100.46	113.10

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	1497	0	1472	147	0
1	B	1496	0	1473	143	0
1	C	1518	0	1491	163	3
1	D	1523	0	1496	169	0
1	E	1534	0	1509	174	2
1	F	1518	0	1491	154	0
1	G	1487	0	1461	140	0
1	H	1484	0	1463	150	1
2	I	202	0	116	8	0
2	J	202	0	116	20	0
2	K	202	0	116	7	0
2	L	202	0	116	17	0
2	M	202	0	116	22	0
2	N	202	0	116	8	0
2	O	202	0	116	23	0
2	P	202	0	116	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	13681	0	12784	1290	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All (1290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:HD2	1:A:268:MET:HB2	1.34	1.08
1:H:204:ARG:HD2	1:H:268:MET:HB2	1.35	1.07
1:C:204:ARG:HD2	1:C:268:MET:HB2	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ARG:HD2	1:E:268:MET:HB2	1.35	1.06
1:D:204:ARG:HD2	1:D:268:MET:HB2	1.35	1.05
1:F:204:ARG:HD2	1:F:268:MET:HB2	1.34	1.04
1:B:204:ARG:HD2	1:B:268:MET:HB2	1.35	1.04
1:G:204:ARG:HD2	1:G:268:MET:HB2	1.35	1.03
1:C:207:ASN:ND2	1:D:274:VAL:O	1.94	1.00
1:C:169:THR:HG21	1:E:196:GLU:N	1.76	1.00
2:L:8:DT:H2"	2:L:9:DT:H5"	1.43	1.00
1:G:238:GLU:HG2	1:G:245:GLN:HG2	1.45	0.99
1:D:166:ILE:HG13	1:D:167:ALA:H	1.28	0.99
1:H:238:GLU:HG2	1:H:245:GLN:HG2	1.45	0.98
1:B:166:ILE:HG13	1:B:167:ALA:H	1.28	0.98
1:F:238:GLU:HG2	1:F:245:GLN:HG2	1.45	0.98
1:B:238:GLU:HG2	1:B:245:GLN:HG2	1.45	0.97
1:G:166:ILE:HG13	1:G:167:ALA:H	1.27	0.97
1:G:136:HIS:HA	1:G:178:THR:HG23	1.46	0.97
1:A:166:ILE:HG13	1:A:167:ALA:H	1.28	0.97
1:D:238:GLU:HG2	1:D:245:GLN:HG2	1.45	0.97
1:A:136:HIS:HA	1:A:178:THR:HG23	1.47	0.97
1:A:238:GLU:HG2	1:A:245:GLN:HG2	1.46	0.96
1:C:136:HIS:HA	1:C:178:THR:HG23	1.46	0.96
2:O:8:DT:H2"	2:O:9:DT:H5"	1.45	0.96
2:M:8:DT:H2"	2:M:9:DT:H5"	1.46	0.96
2:J:8:DT:H2"	2:J:9:DT:H5"	1.47	0.96
1:C:166:ILE:HG13	1:C:167:ALA:H	1.28	0.95
1:D:136:HIS:HA	1:D:178:THR:HG23	1.48	0.95
1:H:166:ILE:HG13	1:H:167:ALA:H	1.29	0.95
1:F:166:ILE:HG13	1:F:167:ALA:H	1.28	0.95
1:B:136:HIS:HA	1:B:178:THR:HG23	1.47	0.94
1:F:136:HIS:HA	1:F:178:THR:HG23	1.47	0.94
1:E:136:HIS:HA	1:E:178:THR:HG23	1.48	0.94
1:H:136:HIS:HA	1:H:178:THR:HG23	1.47	0.93
2:M:9:DT:H2"	2:M:10:DT:H5'	1.48	0.93
2:O:9:DT:H2"	2:O:10:DT:H5'	1.49	0.93
1:E:238:GLU:HG2	1:E:245:GLN:HG2	1.46	0.93
2:L:9:DT:H2"	2:L:10:DT:H5'	1.48	0.93
1:E:166:ILE:HG13	1:E:167:ALA:H	1.33	0.93
1:C:238:GLU:HG2	1:C:245:GLN:HG2	1.46	0.92
1:D:196:GLU:N	1:F:169:THR:HG21	1.85	0.92
1:E:216:GLU:HG3	1:H:264:LEU:HD11	1.51	0.91
1:C:255:GLN:HE21	1:E:128:SER:N	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:9:DT:H2"	2:J:10:DT:H5'	1.50	0.90
1:A:264:LEU:HD11	1:D:216:GLU:HG3	1.56	0.88
1:D:166:ILE:HG13	1:D:167:ALA:N	1.89	0.88
1:G:166:ILE:HG13	1:G:167:ALA:N	1.89	0.87
1:E:166:ILE:HG13	1:E:167:ALA:N	1.90	0.87
2:O:3:DA:H1'	2:O:4:DC:H5'	1.57	0.87
2:L:3:DA:H1'	2:L:4:DC:H5'	1.55	0.86
1:A:166:ILE:HG13	1:A:167:ALA:N	1.90	0.86
2:J:3:DA:H1'	2:J:4:DC:H5'	1.57	0.86
1:C:166:ILE:HG13	1:C:167:ALA:N	1.90	0.86
2:M:3:DA:H1'	2:M:4:DC:H5'	1.56	0.86
1:F:166:ILE:HG13	1:F:167:ALA:N	1.89	0.86
1:B:166:ILE:HG13	1:B:167:ALA:N	1.91	0.85
1:H:272:SER:HA	1:H:279:ARG:H	1.42	0.85
1:H:166:ILE:HG13	1:H:167:ALA:N	1.90	0.84
1:D:212:ARG:HE	1:D:212:ARG:HA	1.43	0.84
1:C:212:ARG:HE	1:C:212:ARG:HA	1.43	0.83
1:G:290:THR:HB	1:G:296:LEU:HD21	1.59	0.83
1:A:290:THR:HB	1:A:296:LEU:HD21	1.60	0.83
1:G:272:SER:HA	1:G:279:ARG:H	1.43	0.83
1:H:212:ARG:HA	1:H:212:ARG:HE	1.42	0.83
1:F:272:SER:HA	1:F:279:ARG:H	1.43	0.83
1:G:212:ARG:HE	1:G:212:ARG:HA	1.43	0.83
1:A:212:ARG:HE	1:A:212:ARG:HA	1.42	0.83
1:D:290:THR:HB	1:D:296:LEU:HD21	1.61	0.83
1:F:290:THR:HB	1:F:296:LEU:HD21	1.61	0.82
1:E:290:THR:HB	1:E:296:LEU:HD21	1.59	0.82
1:B:212:ARG:HE	1:B:212:ARG:HA	1.42	0.82
1:D:196:GLU:CA	1:F:169:THR:HG21	2.10	0.82
1:C:272:SER:HA	1:C:279:ARG:H	1.42	0.82
1:E:272:SER:HA	1:E:279:ARG:H	1.44	0.82
1:D:272:SER:HA	1:D:279:ARG:H	1.43	0.82
1:B:290:THR:HB	1:B:296:LEU:HD21	1.59	0.81
1:F:212:ARG:HE	1:F:212:ARG:HA	1.43	0.81
1:B:272:SER:HA	1:B:279:ARG:H	1.45	0.81
1:H:290:THR:HB	1:H:296:LEU:HD21	1.60	0.81
1:C:290:THR:HB	1:C:296:LEU:HD21	1.62	0.81
1:B:241:ILE:HG23	1:B:242:THR:HG23	1.63	0.81
1:D:241:ILE:HG23	1:D:242:THR:HG23	1.62	0.81
1:F:241:ILE:HG23	1:F:242:THR:HG23	1.63	0.81
1:A:272:SER:HA	1:A:279:ARG:H	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:241:ILE:HG23	1:H:242:THR:HG23	1.63	0.80
1:E:212:ARG:HE	1:E:212:ARG:HA	1.44	0.80
1:E:269:CYS:C	1:E:305:ILE:HD11	2.02	0.80
1:C:269:CYS:C	1:C:305:ILE:HD11	2.02	0.80
1:G:241:ILE:HG23	1:G:242:THR:HG23	1.63	0.80
1:E:241:ILE:HG23	1:E:242:THR:HG23	1.62	0.80
1:A:241:ILE:HG23	1:A:242:THR:HG23	1.63	0.79
1:C:241:ILE:HG23	1:C:242:THR:HG23	1.62	0.79
1:F:269:CYS:C	1:F:305:ILE:HD11	2.03	0.79
1:C:206:PRO:HB2	1:D:207:ASN:ND2	1.96	0.79
1:A:172:ILE:HG22	1:A:263:VAL:O	1.83	0.79
1:F:172:ILE:HG22	1:F:263:VAL:O	1.83	0.79
1:A:269:CYS:C	1:A:305:ILE:HD11	2.04	0.78
1:E:172:ILE:HG22	1:E:263:VAL:O	1.83	0.78
1:D:172:ILE:HG22	1:D:263:VAL:O	1.84	0.78
1:H:172:ILE:HG22	1:H:263:VAL:O	1.84	0.78
1:H:269:CYS:C	1:H:305:ILE:HD11	2.04	0.78
1:G:269:CYS:C	1:G:305:ILE:HD11	2.03	0.78
1:B:269:CYS:C	1:B:305:ILE:HD11	2.03	0.77
1:B:172:ILE:HG22	1:B:263:VAL:O	1.84	0.77
1:D:269:CYS:C	1:D:305:ILE:HD11	2.05	0.77
1:G:172:ILE:HG22	1:G:263:VAL:O	1.84	0.77
1:F:226:ILE:HD11	1:F:284:ILE:HD12	1.67	0.76
1:A:264:LEU:HD11	1:D:216:GLU:CB	2.15	0.76
1:C:172:ILE:HG22	1:C:263:VAL:O	1.84	0.76
1:D:226:ILE:HD11	1:D:284:ILE:HD12	1.67	0.76
1:E:226:ILE:HD11	1:E:284:ILE:HD12	1.68	0.76
1:D:196:GLU:HB3	1:F:169:THR:HG22	1.66	0.75
1:A:264:LEU:HD11	1:D:216:GLU:CG	2.16	0.75
1:A:207:ASN:OD1	1:B:207:ASN:ND2	2.18	0.75
1:G:204:ARG:HD2	1:G:268:MET:CB	2.16	0.75
2:L:8:DT:H2"	2:L:9:DT:C5'	2.14	0.75
1:H:226:ILE:HD11	1:H:284:ILE:HD12	1.68	0.75
2:L:1:DA:HO5'	2:L:1:DA:H8	1.35	0.75
1:C:255:GLN:NE2	1:E:128:SER:N	2.35	0.74
1:F:204:ARG:HD2	1:F:268:MET:CB	2.16	0.74
1:G:226:ILE:HD11	1:G:284:ILE:HD12	1.68	0.74
2:O:8:DT:H2"	2:O:9:DT:C5'	2.16	0.74
1:A:204:ARG:HD2	1:A:268:MET:CB	2.14	0.74
1:B:226:ILE:HD11	1:B:284:ILE:HD12	1.67	0.74
1:D:204:ARG:HD2	1:D:268:MET:CB	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:ILE:HG13	1:E:321:ARG:N	2.01	0.74
2:M:8:DT:H2"	2:M:9:DT:C5'	2.16	0.74
2:J:8:DT:H2"	2:J:9:DT:C5'	2.16	0.74
1:H:239:ASP:OD1	1:H:241:ILE:HG22	1.88	0.74
1:E:216:GLU:CG	1:H:264:LEU:HD11	2.18	0.73
1:A:226:ILE:HD11	1:A:284:ILE:HD12	1.69	0.73
1:B:204:ARG:HD2	1:B:268:MET:CB	2.16	0.73
1:C:204:ARG:HD2	1:C:268:MET:CB	2.16	0.73
1:E:204:ARG:HD2	1:E:268:MET:CB	2.16	0.73
1:E:317:GLU:O	1:E:320:ILE:HG12	1.87	0.73
1:D:239:ASP:OD1	1:D:241:ILE:HG22	1.89	0.72
1:F:183:GLY:HA2	1:F:291:ARG:HH21	1.54	0.72
2:M:10:DT:H2'	2:O:1:DA:O4'	1.89	0.72
1:A:239:ASP:OD1	1:A:241:ILE:HG22	1.88	0.72
1:B:183:GLY:HA2	1:B:291:ARG:HH21	1.54	0.72
1:F:239:ASP:OD1	1:F:241:ILE:HG22	1.89	0.72
1:D:183:GLY:HA2	1:D:291:ARG:HH21	1.55	0.72
1:B:239:ASP:OD1	1:B:241:ILE:HG22	1.89	0.72
1:C:183:GLY:HA2	1:C:291:ARG:HH21	1.53	0.72
1:A:183:GLY:HA2	1:A:291:ARG:HH21	1.54	0.72
1:H:183:GLY:HA2	1:H:291:ARG:HH21	1.55	0.72
1:C:255:GLN:HB3	1:E:128:SER:HB2	1.70	0.72
1:G:183:GLY:HA2	1:G:291:ARG:HH21	1.55	0.72
1:G:239:ASP:OD1	1:G:241:ILE:HG22	1.89	0.72
1:C:169:THR:HG21	1:E:196:GLU:H	1.52	0.71
1:C:169:THR:CG2	1:E:196:GLU:HB3	2.21	0.71
1:E:183:GLY:HA2	1:E:291:ARG:HH21	1.55	0.71
2:O:8:DT:C2'	2:O:9:DT:H5"	2.21	0.71
2:L:9:DT:C2'	2:L:10:DT:H5'	2.21	0.71
1:C:226:ILE:HD11	1:C:284:ILE:HD12	1.71	0.71
1:E:239:ASP:OD1	1:E:241:ILE:HG22	1.91	0.71
1:D:169:THR:HA	1:D:266:ASN:ND2	2.06	0.70
2:M:1:DA:H8	2:M:1:DA:HO5'	1.39	0.70
1:H:317:GLU:O	1:H:320:ILE:HG12	1.91	0.70
1:C:239:ASP:OD1	1:C:241:ILE:HG22	1.90	0.70
1:C:258:THR:HG22	1:C:259:GLU:H	1.57	0.70
1:C:317:GLU:O	1:C:320:ILE:HG12	1.91	0.70
1:H:204:ARG:HD2	1:H:268:MET:CB	2.16	0.70
1:C:169:THR:HG21	1:E:196:GLU:CA	2.22	0.70
1:E:234:ALA:HB2	1:E:249:VAL:HG12	1.74	0.70
2:L:8:DT:C2'	2:L:9:DT:H5"	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:5:DA:H2"	2:N:6:DT:H5'	1.73	0.70
1:A:290:THR:HG22	1:A:294:GLN:O	1.92	0.70
2:K:5:DA:H2"	2:K:6:DT:H5'	1.74	0.70
2:J:8:DT:C2'	2:J:9:DT:H5"	2.22	0.69
2:P:5:DA:H2"	2:P:6:DT:H5'	1.74	0.69
1:G:169:THR:HA	1:G:266:ASN:ND2	2.07	0.69
1:G:207:ASN:ND2	1:H:207:ASN:OD1	2.25	0.69
1:G:290:THR:HG22	1:G:294:GLN:O	1.92	0.69
1:H:169:THR:HA	1:H:266:ASN:ND2	2.07	0.69
2:I:5:DA:H2"	2:I:6:DT:H5'	1.74	0.69
1:C:169:THR:HA	1:C:266:ASN:ND2	2.07	0.69
1:F:290:THR:HG22	1:F:294:GLN:O	1.92	0.69
1:F:158:GLU:CD	1:F:159:LEU:H	1.96	0.69
1:E:169:THR:HA	1:E:266:ASN:ND2	2.07	0.69
1:H:290:THR:HG22	1:H:294:GLN:O	1.92	0.69
2:M:9:DT:C2'	2:M:10:DT:H5'	2.21	0.69
2:O:9:DT:C2'	2:O:10:DT:H5'	2.22	0.69
1:A:169:THR:HA	1:A:266:ASN:ND2	2.08	0.69
1:B:234:ALA:HB2	1:B:249:VAL:HG12	1.75	0.69
1:D:290:THR:HG22	1:D:294:GLN:O	1.93	0.68
1:G:234:ALA:HB2	1:G:249:VAL:HG12	1.75	0.68
1:G:258:THR:HG22	1:G:259:GLU:H	1.58	0.68
1:B:290:THR:HG22	1:B:294:GLN:O	1.93	0.68
1:F:317:GLU:O	1:F:320:ILE:HG12	1.93	0.68
1:A:158:GLU:CD	1:A:159:LEU:H	1.96	0.68
1:D:317:GLU:O	1:D:320:ILE:HG12	1.94	0.68
1:C:290:THR:HG22	1:C:294:GLN:O	1.92	0.68
1:F:258:THR:HG22	1:F:259:GLU:H	1.57	0.68
1:G:158:GLU:CD	1:G:159:LEU:H	1.97	0.68
1:A:190:PRO:HG2	1:A:202:VAL:CG2	2.24	0.68
1:D:234:ALA:HB2	1:D:249:VAL:HG12	1.75	0.68
1:F:169:THR:HA	1:F:266:ASN:ND2	2.08	0.68
1:F:234:ALA:HB2	1:F:249:VAL:HG12	1.75	0.68
2:M:5:DA:H2"	2:M:6:DT:H5'	1.74	0.68
1:B:169:THR:HA	1:B:266:ASN:ND2	2.08	0.68
2:O:5:DA:H2"	2:O:6:DT:H5'	1.75	0.68
1:A:153:TRP:HB3	1:A:164:CYS:HB2	1.76	0.68
1:E:190:PRO:HG2	1:E:202:VAL:CG2	2.24	0.68
1:A:317:GLU:O	1:A:320:ILE:HG12	1.94	0.68
1:E:258:THR:HG22	1:E:259:GLU:H	1.59	0.68
1:E:290:THR:HG22	1:E:294:GLN:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ALA:HB2	1:C:249:VAL:HG12	1.76	0.68
2:L:5:DA:H2"	2:L:6:DT:H5'	1.75	0.68
1:D:196:GLU:HA	1:F:169:THR:HG21	1.75	0.67
2:M:8:DT:C2'	2:M:9:DT:H5"	2.22	0.67
1:A:258:THR:HG22	1:A:259:GLU:H	1.59	0.67
1:H:158:GLU:CD	1:H:159:LEU:H	1.97	0.67
2:J:5:DA:H2"	2:J:6:DT:H5'	1.75	0.67
1:B:258:THR:HG22	1:B:259:GLU:H	1.59	0.67
1:D:190:PRO:HG2	1:D:202:VAL:CG2	2.24	0.67
2:J:9:DT:C2'	2:J:10:DT:H5'	2.22	0.67
1:H:258:THR:HG22	1:H:259:GLU:H	1.58	0.67
1:C:158:GLU:CD	1:C:159:LEU:H	1.98	0.66
1:D:158:GLU:CD	1:D:159:LEU:H	1.98	0.66
1:F:190:PRO:HG2	1:F:202:VAL:CG2	2.25	0.66
1:H:234:ALA:HB2	1:H:249:VAL:HG12	1.75	0.66
1:E:158:GLU:CD	1:E:159:LEU:H	1.97	0.66
1:A:234:ALA:HB2	1:A:249:VAL:HG12	1.76	0.66
1:C:190:PRO:HG2	1:C:202:VAL:CG2	2.26	0.66
1:A:204:ARG:NH1	1:A:208:HIS:HB3	2.11	0.66
1:G:317:GLU:O	1:G:320:ILE:HG12	1.95	0.66
1:H:190:PRO:HG2	1:H:202:VAL:CG2	2.26	0.66
1:B:190:PRO:HG2	1:B:202:VAL:CG2	2.26	0.66
1:B:158:GLU:CD	1:B:159:LEU:H	1.99	0.66
1:H:204:ARG:NH1	1:H:208:HIS:HB3	2.11	0.66
1:B:317:GLU:O	1:B:320:ILE:HG12	1.96	0.66
1:D:204:ARG:NH1	1:D:208:HIS:HB3	2.11	0.66
1:G:140:VAL:HG11	1:G:286:VAL:HG21	1.78	0.66
1:C:204:ARG:NH1	1:C:208:HIS:HB3	2.11	0.65
1:D:171:PRO:O	1:D:172:ILE:HB	1.96	0.65
1:E:216:GLU:CB	1:H:264:LEU:HD11	2.27	0.65
1:A:171:PRO:O	1:A:172:ILE:HB	1.97	0.65
1:F:171:PRO:O	1:F:172:ILE:HB	1.94	0.65
1:G:204:ARG:NH1	1:G:208:HIS:HB3	2.11	0.65
1:B:153:TRP:HB3	1:B:164:CYS:HB2	1.79	0.65
1:B:204:ARG:NH1	1:B:208:HIS:HB3	2.12	0.65
1:D:258:THR:HG22	1:D:259:GLU:H	1.60	0.65
1:H:140:VAL:HG11	1:H:286:VAL:HG21	1.78	0.65
1:E:171:PRO:O	1:E:172:ILE:HB	1.97	0.65
1:G:153:TRP:HB3	1:G:164:CYS:HB2	1.77	0.65
1:H:153:TRP:HB3	1:H:164:CYS:HB2	1.77	0.65
1:C:140:VAL:HG11	1:C:286:VAL:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:TRP:HB3	1:C:164:CYS:HB2	1.78	0.64
1:F:204:ARG:NH1	1:F:208:HIS:HB3	2.12	0.64
1:D:169:THR:HA	1:D:266:ASN:HD21	1.61	0.64
1:E:153:TRP:HB3	1:E:164:CYS:HB2	1.80	0.64
1:G:169:THR:HA	1:G:266:ASN:HD21	1.62	0.64
1:H:171:PRO:O	1:H:172:ILE:HB	1.96	0.64
1:F:140:VAL:HG11	1:F:286:VAL:HG21	1.78	0.64
1:G:190:PRO:HG2	1:G:202:VAL:CG2	2.27	0.64
1:B:171:PRO:O	1:B:172:ILE:HB	1.97	0.64
1:G:171:PRO:O	1:G:172:ILE:HB	1.97	0.64
1:D:140:VAL:HG11	1:D:286:VAL:HG21	1.79	0.64
1:E:169:THR:HA	1:E:266:ASN:HD21	1.63	0.64
1:D:153:TRP:HB3	1:D:164:CYS:HB2	1.80	0.63
1:F:153:TRP:HB3	1:F:164:CYS:HB2	1.79	0.63
1:B:140:VAL:HG11	1:B:286:VAL:HG21	1.78	0.63
1:C:171:PRO:O	1:C:172:ILE:HB	1.97	0.63
1:D:152:THR:HG23	1:D:153:TRP:HD1	1.64	0.63
1:D:166:ILE:CG1	1:D:167:ALA:N	2.60	0.63
1:F:169:THR:HA	1:F:266:ASN:HD21	1.64	0.63
1:E:140:VAL:HG11	1:E:286:VAL:HG21	1.80	0.63
1:E:152:THR:HG23	1:E:153:TRP:HD1	1.63	0.63
1:E:204:ARG:NH1	1:E:208:HIS:HB3	2.12	0.63
1:A:264:LEU:CD1	1:D:216:GLU:HB2	2.29	0.63
1:A:140:VAL:HG11	1:A:286:VAL:HG21	1.79	0.63
1:B:169:THR:HA	1:B:266:ASN:HD21	1.64	0.63
1:B:209:GLU:O	1:B:209:GLU:HG3	1.99	0.63
1:D:190:PRO:HG2	1:D:202:VAL:HG21	1.80	0.63
1:F:290:THR:HG21	1:F:294:GLN:HG2	1.81	0.63
1:A:204:ARG:HD3	1:A:224:HIS:O	1.99	0.62
1:C:169:THR:HA	1:C:266:ASN:HD21	1.62	0.62
1:G:204:ARG:HD3	1:G:224:HIS:O	2.00	0.62
1:F:204:ARG:HD3	1:F:224:HIS:O	1.99	0.62
1:H:169:THR:HA	1:H:266:ASN:HD21	1.63	0.62
1:A:190:PRO:HG2	1:A:202:VAL:HG21	1.81	0.62
1:D:204:ARG:HD3	1:D:224:HIS:O	1.99	0.62
1:E:152:THR:HG23	1:E:153:TRP:CD1	2.35	0.62
1:B:290:THR:HG21	1:B:294:GLN:HG2	1.82	0.62
1:A:290:THR:HG21	1:A:294:GLN:HG2	1.82	0.62
1:B:204:ARG:HD3	1:B:224:HIS:O	2.00	0.62
1:E:209:GLU:HG3	1:E:209:GLU:O	1.99	0.62
1:G:290:THR:HG21	1:G:294:GLN:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ILE:HG23	1:C:172:ILE:O	1.99	0.62
1:D:209:GLU:O	1:D:209:GLU:HG3	1.99	0.62
1:A:166:ILE:CG1	1:A:167:ALA:H	2.01	0.62
1:H:290:THR:HG21	1:H:294:GLN:HG2	1.82	0.62
1:D:152:THR:HG23	1:D:153:TRP:CD1	2.35	0.61
1:C:204:ARG:HD3	1:C:224:HIS:O	1.99	0.61
1:F:190:PRO:HG2	1:F:202:VAL:HG21	1.82	0.61
1:G:132:TYR:CE2	1:G:134:GLY:HA2	2.35	0.61
1:C:152:THR:HG23	1:C:153:TRP:HD1	1.66	0.61
1:C:204:ARG:HH21	1:C:215:ASN:HD21	1.48	0.61
1:E:290:THR:HG21	1:E:294:GLN:HG2	1.82	0.61
2:O:1:DA:H8	2:O:1:DA:HO5'	1.48	0.61
1:A:172:ILE:HG23	1:A:172:ILE:O	2.00	0.61
1:B:172:ILE:HG23	1:B:172:ILE:O	2.00	0.61
1:C:255:GLN:HB3	1:E:128:SER:CB	2.31	0.61
1:G:172:ILE:HG23	1:G:172:ILE:O	1.99	0.61
1:B:132:TYR:CE2	1:B:134:GLY:HA2	2.36	0.61
1:F:132:TYR:CE2	1:F:134:GLY:HA2	2.35	0.61
1:H:204:ARG:HD3	1:H:224:HIS:O	2.00	0.61
1:D:172:ILE:O	1:D:172:ILE:HG23	2.01	0.61
1:G:209:GLU:HG3	1:G:209:GLU:O	2.00	0.61
1:H:209:GLU:O	1:H:209:GLU:HG3	2.00	0.61
1:B:152:THR:HG23	1:B:153:TRP:HD1	1.65	0.61
1:C:290:THR:HG21	1:C:294:GLN:HG2	1.82	0.61
1:E:320:ILE:HD11	1:E:321:ARG:NH1	2.16	0.61
1:G:204:ARG:HH21	1:G:215:ASN:HD21	1.49	0.61
1:H:132:TYR:CE2	1:H:134:GLY:HA2	2.35	0.61
1:A:132:TYR:CE2	1:A:134:GLY:HA2	2.36	0.60
1:A:169:THR:HA	1:A:266:ASN:HD21	1.64	0.60
1:E:204:ARG:HD3	1:E:224:HIS:O	2.00	0.60
1:B:152:THR:HG23	1:B:153:TRP:CD1	2.36	0.60
1:D:132:TYR:CE2	1:D:134:GLY:HA2	2.36	0.60
1:H:190:PRO:HG2	1:H:202:VAL:HG21	1.83	0.60
1:E:132:TYR:CE2	1:E:134:GLY:HA2	2.36	0.60
1:F:152:THR:HG23	1:F:153:TRP:HD1	1.66	0.60
1:A:204:ARG:HH21	1:A:215:ASN:HD21	1.49	0.60
1:C:152:THR:HG23	1:C:153:TRP:CD1	2.37	0.60
1:D:290:THR:HG21	1:D:294:GLN:HG2	1.82	0.60
1:C:132:TYR:CE2	1:C:134:GLY:HA2	2.36	0.60
1:D:196:GLU:CA	1:F:169:THR:CG2	2.79	0.60
1:B:190:PRO:HG2	1:B:202:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:PRO:HG2	1:C:202:VAL:HG21	1.82	0.60
1:C:209:GLU:O	1:C:209:GLU:HG3	2.00	0.60
1:E:166:ILE:HG23	1:E:167:ALA:N	2.15	0.60
1:F:172:ILE:HG23	1:F:172:ILE:O	2.01	0.60
1:F:258:THR:HG22	1:F:259:GLU:N	2.17	0.60
1:H:173:GLN:HB3	1:H:260:PHE:CG	2.37	0.60
1:B:173:GLN:HB3	1:B:260:PHE:CG	2.37	0.60
1:F:209:GLU:O	1:F:209:GLU:HG3	2.01	0.60
1:A:152:THR:HG23	1:A:153:TRP:HD1	1.67	0.60
1:C:278:ASN:N	1:C:278:ASN:HD22	2.00	0.60
1:E:190:PRO:HG2	1:E:202:VAL:HG21	1.82	0.60
1:F:173:GLN:HB3	1:F:260:PHE:CG	2.37	0.60
1:H:166:ILE:CG1	1:H:167:ALA:N	2.61	0.60
1:H:172:ILE:HG23	1:H:172:ILE:O	2.01	0.59
1:E:172:ILE:HG23	1:E:172:ILE:O	2.01	0.59
1:F:204:ARG:HH21	1:F:215:ASN:HD21	1.49	0.59
1:H:152:THR:HG23	1:H:153:TRP:CD1	2.37	0.59
1:C:312:ASP:O	1:C:316:ASP:HB2	2.02	0.59
1:F:152:THR:HG23	1:F:153:TRP:CD1	2.38	0.59
1:A:173:GLN:HB3	1:A:260:PHE:CG	2.37	0.59
1:D:173:GLN:HB3	1:D:260:PHE:CG	2.37	0.59
1:E:204:ARG:HH21	1:E:215:ASN:HD21	1.48	0.59
1:G:173:GLN:HB3	1:G:260:PHE:CG	2.37	0.59
1:H:204:ARG:HH21	1:H:215:ASN:HD21	1.49	0.59
1:C:173:GLN:HB3	1:C:260:PHE:CG	2.37	0.59
1:C:258:THR:HG22	1:C:259:GLU:N	2.16	0.59
1:H:152:THR:HG23	1:H:153:TRP:HD1	1.67	0.59
1:A:209:GLU:O	1:A:209:GLU:HG3	2.00	0.59
1:C:169:THR:HG22	1:E:196:GLU:CD	2.23	0.59
1:E:173:GLN:HB3	1:E:260:PHE:CG	2.37	0.59
1:F:312:ASP:O	1:F:316:ASP:HB2	2.02	0.59
2:J:1:DA:HO5'	2:J:1:DA:H8	1.51	0.59
1:G:152:THR:HG23	1:G:153:TRP:HD1	1.66	0.59
1:A:258:THR:HG22	1:A:259:GLU:N	2.18	0.59
1:E:189:MET:HE3	1:E:246:SER:HB2	1.85	0.59
1:A:152:THR:HG23	1:A:153:TRP:CD1	2.37	0.58
1:B:312:ASP:O	1:B:316:ASP:HB2	2.02	0.58
1:F:166:ILE:HG23	1:F:167:ALA:N	2.18	0.58
1:G:166:ILE:HG23	1:G:167:ALA:N	2.18	0.58
1:B:204:ARG:HH21	1:B:215:ASN:HD21	1.50	0.58
1:C:169:THR:HG22	1:E:196:GLU:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:THR:HA	1:C:165:GLN:OE1	2.03	0.58
1:C:278:ASN:HD22	1:C:278:ASN:H	1.51	0.58
1:D:196:GLU:HB3	1:F:169:THR:CG2	2.34	0.58
1:G:152:THR:HG23	1:G:153:TRP:CD1	2.37	0.58
1:H:130:THR:O	1:H:298:ARG:NH1	2.36	0.58
1:C:130:THR:O	1:C:298:ARG:NH1	2.36	0.58
1:C:166:ILE:HG23	1:C:167:ALA:N	2.18	0.58
1:H:258:THR:HG22	1:H:259:GLU:N	2.18	0.58
1:E:130:THR:O	1:E:298:ARG:NH1	2.37	0.58
1:E:163:TYR:O	1:E:164:CYS:HB3	2.03	0.58
1:H:312:ASP:O	1:H:316:ASP:HB2	2.04	0.58
1:E:312:ASP:O	1:E:316:ASP:HB2	2.03	0.57
1:D:204:ARG:HH21	1:D:215:ASN:HD21	1.50	0.57
1:E:269:CYS:O	1:E:305:ILE:HD11	2.05	0.57
1:F:163:TYR:N	1:F:163:TYR:CD1	2.72	0.57
1:G:312:ASP:O	1:G:316:ASP:HB2	2.04	0.57
1:C:169:THR:HG22	1:E:196:GLU:OE1	2.04	0.57
1:B:130:THR:O	1:B:298:ARG:NH1	2.38	0.57
1:D:166:ILE:HG23	1:D:167:ALA:N	2.20	0.57
1:G:258:THR:HG22	1:G:259:GLU:N	2.18	0.57
1:B:166:ILE:CG1	1:B:167:ALA:N	2.61	0.57
1:B:166:ILE:HG23	1:B:167:ALA:N	2.20	0.57
1:G:190:PRO:HG2	1:G:202:VAL:HG21	1.84	0.57
1:G:209:GLU:O	1:G:210:LEU:HG	2.04	0.57
1:G:269:CYS:O	1:G:305:ILE:HD11	2.04	0.57
1:E:278:ASN:HD22	1:E:278:ASN:H	1.51	0.57
1:G:163:TYR:CD1	1:G:163:TYR:N	2.73	0.57
1:H:163:TYR:O	1:H:164:CYS:HB3	2.04	0.57
1:C:269:CYS:O	1:C:305:ILE:HD11	2.05	0.57
1:E:258:THR:HG22	1:E:259:GLU:N	2.19	0.57
1:G:152:THR:HA	1:G:165:GLN:OE1	2.05	0.57
1:H:166:ILE:HG23	1:H:167:ALA:N	2.19	0.57
2:L:3:DA:H1'	2:L:4:DC:C5'	2.33	0.57
1:A:163:TYR:N	1:A:163:TYR:CD1	2.73	0.57
1:H:278:ASN:N	1:H:278:ASN:HD22	2.03	0.57
1:A:312:ASP:O	1:A:316:ASP:HB2	2.04	0.57
1:D:204:ARG:NH2	1:D:208:HIS:O	2.38	0.57
1:D:312:ASP:O	1:D:316:ASP:HB2	2.04	0.57
1:H:204:ARG:NH2	1:H:208:HIS:O	2.38	0.57
1:A:130:THR:O	1:A:298:ARG:NH1	2.38	0.57
1:D:258:THR:HG22	1:D:259:GLU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:ASN:HD22	1:E:278:ASN:N	2.01	0.57
1:B:258:THR:HG22	1:B:259:GLU:N	2.18	0.56
1:C:163:TYR:N	1:C:163:TYR:CD1	2.72	0.56
1:G:130:THR:O	1:G:298:ARG:NH1	2.38	0.56
1:C:255:GLN:NE2	1:E:128:SER:H	2.02	0.56
1:E:163:TYR:CD1	1:E:163:TYR:N	2.72	0.56
1:A:153:TRP:CB	1:A:164:CYS:HB2	2.35	0.56
1:A:270:ASN:O	1:A:272:SER:N	2.37	0.56
1:B:278:ASN:HD22	1:B:278:ASN:H	1.53	0.56
1:C:209:GLU:O	1:C:210:LEU:HG	2.05	0.56
1:D:189:MET:HE3	1:D:246:SER:HB2	1.87	0.56
1:E:166:ILE:HG23	1:E:167:ALA:H	1.70	0.56
1:E:209:GLU:O	1:E:210:LEU:HG	2.05	0.56
1:F:278:ASN:H	1:F:278:ASN:HD22	1.54	0.56
1:B:204:ARG:NH2	1:B:208:HIS:O	2.38	0.56
1:D:163:TYR:CD1	1:D:163:TYR:N	2.73	0.56
1:F:152:THR:HA	1:F:165:GLN:OE1	2.06	0.56
1:B:152:THR:HA	1:B:165:GLN:OE1	2.06	0.56
1:B:270:ASN:O	1:B:272:SER:N	2.37	0.56
1:B:278:ASN:HD22	1:B:278:ASN:N	2.03	0.56
1:D:270:ASN:O	1:D:272:SER:N	2.38	0.56
1:H:163:TYR:CD1	1:H:163:TYR:N	2.72	0.56
2:O:3:DA:H1'	2:O:4:DC:C5'	2.34	0.56
1:A:166:ILE:HG23	1:A:167:ALA:N	2.20	0.56
1:C:182:GLN:OE1	1:C:182:GLN:HA	2.06	0.56
1:G:270:ASN:O	1:G:272:SER:N	2.38	0.56
1:G:278:ASN:HD22	1:G:278:ASN:N	2.04	0.56
1:F:204:ARG:NH2	1:F:215:ASN:HD21	2.04	0.56
1:A:264:LEU:HD11	1:D:216:GLU:HB2	1.85	0.56
1:B:204:ARG:NH2	1:B:215:ASN:HD21	2.04	0.56
1:B:269:CYS:O	1:B:305:ILE:HD11	2.05	0.56
1:G:204:ARG:NH2	1:G:215:ASN:HD21	2.04	0.56
1:H:278:ASN:HD22	1:H:278:ASN:H	1.53	0.56
1:A:204:ARG:NH2	1:A:208:HIS:O	2.39	0.56
1:C:204:ARG:NH2	1:C:215:ASN:HD21	2.03	0.56
1:E:204:ARG:NH2	1:E:215:ASN:HD21	2.03	0.56
1:A:278:ASN:H	1:A:278:ASN:HD22	1.54	0.55
1:B:163:TYR:O	1:B:164:CYS:HB3	2.06	0.55
1:H:152:THR:HA	1:H:165:GLN:OE1	2.06	0.55
1:G:204:ARG:NH2	1:G:208:HIS:O	2.38	0.55
1:C:286:VAL:HG23	1:C:286:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ARG:NH2	1:E:208:HIS:O	2.38	0.55
1:H:210:LEU:O	1:H:212:ARG:N	2.40	0.55
1:B:163:TYR:N	1:B:163:TYR:CD1	2.73	0.55
1:D:182:GLN:HA	1:D:182:GLN:OE1	2.07	0.55
1:F:209:GLU:O	1:F:210:LEU:HG	2.06	0.55
1:D:278:ASN:N	1:D:278:ASN:HD22	2.03	0.55
1:F:130:THR:O	1:F:298:ARG:NH1	2.39	0.55
1:A:210:LEU:O	1:A:212:ARG:N	2.40	0.55
1:B:209:GLU:O	1:B:210:LEU:HG	2.06	0.55
1:D:163:TYR:O	1:D:164:CYS:HB3	2.05	0.55
1:E:152:THR:HA	1:E:165:GLN:OE1	2.06	0.55
1:G:163:TYR:O	1:G:164:CYS:HB3	2.05	0.55
1:A:163:TYR:O	1:A:164:CYS:HB3	2.06	0.55
1:D:204:ARG:NH2	1:D:215:ASN:HD21	2.05	0.55
1:F:269:CYS:O	1:F:305:ILE:HD11	2.06	0.55
1:G:153:TRP:CB	1:G:164:CYS:HB2	2.37	0.55
1:A:209:GLU:O	1:A:210:LEU:HG	2.07	0.55
1:A:286:VAL:HG23	1:A:286:VAL:O	2.07	0.55
1:F:182:GLN:HA	1:F:182:GLN:OE1	2.07	0.55
1:H:153:TRP:CB	1:H:164:CYS:HB2	2.37	0.55
1:A:278:ASN:HD22	1:A:278:ASN:N	2.03	0.55
1:B:238:GLU:CG	1:B:245:GLN:HG2	2.31	0.55
1:C:169:THR:CG2	1:E:196:GLU:CB	2.85	0.55
1:D:130:THR:O	1:D:298:ARG:NH1	2.39	0.55
1:E:270:ASN:O	1:E:272:SER:N	2.37	0.55
1:F:258:THR:HG22	1:F:260:PHE:H	1.72	0.55
1:B:214:PHE:C	1:B:215:ASN:HD22	2.11	0.54
1:D:214:PHE:C	1:D:215:ASN:HD22	2.10	0.54
1:E:182:GLN:OE1	1:E:182:GLN:HA	2.07	0.54
1:F:204:ARG:NH2	1:F:208:HIS:O	2.40	0.54
1:H:182:GLN:OE1	1:H:182:GLN:HA	2.07	0.54
1:C:183:GLY:HA2	1:C:291:ARG:NH2	2.22	0.54
1:F:278:ASN:HD22	1:F:278:ASN:N	2.03	0.54
1:A:183:GLY:O	1:A:184:ALA:C	2.46	0.54
1:B:155:TYR:OH	1:B:160:LYS:HD3	2.08	0.54
1:C:204:ARG:NH2	1:C:208:HIS:O	2.40	0.54
1:G:278:ASN:HD22	1:G:278:ASN:H	1.55	0.54
1:A:258:THR:HG22	1:A:260:PHE:H	1.73	0.54
1:D:209:GLU:O	1:D:210:LEU:HG	2.08	0.54
1:F:286:VAL:HG23	1:F:286:VAL:O	2.07	0.54
1:C:183:GLY:O	1:C:184:ALA:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:GLN:OE1	1:G:182:GLN:HA	2.08	0.54
1:H:270:ASN:O	1:H:272:SER:N	2.40	0.54
1:H:286:VAL:HG23	1:H:286:VAL:O	2.08	0.54
1:C:214:PHE:C	1:C:215:ASN:HD22	2.11	0.54
1:G:304:ARG:HG2	1:G:304:ARG:O	2.07	0.54
1:H:204:ARG:NH2	1:H:215:ASN:HD21	2.04	0.54
1:H:269:CYS:O	1:H:305:ILE:HD11	2.07	0.54
1:B:210:LEU:O	1:B:212:ARG:N	2.41	0.54
1:B:286:VAL:HG23	1:B:286:VAL:O	2.07	0.54
2:J:3:DA:H1'	2:J:4:DC:C5'	2.34	0.54
1:B:182:GLN:OE1	1:B:182:GLN:HA	2.07	0.54
1:C:153:TRP:CB	1:C:164:CYS:HB2	2.38	0.54
1:D:152:THR:HA	1:D:165:GLN:OE1	2.07	0.54
1:D:278:ASN:HD22	1:D:278:ASN:H	1.55	0.54
1:F:210:LEU:O	1:F:212:ARG:N	2.41	0.54
1:G:210:LEU:O	1:G:212:ARG:N	2.41	0.54
2:J:2:DA:H2''	2:J:3:DA:OP2	2.06	0.54
2:L:2:DA:H2''	2:L:3:DA:OP2	2.08	0.54
1:A:204:ARG:NH2	1:A:215:ASN:HD21	2.04	0.54
1:D:183:GLY:O	1:D:184:ALA:C	2.46	0.54
1:B:183:GLY:O	1:B:184:ALA:C	2.47	0.53
1:C:258:THR:HG22	1:C:260:PHE:H	1.73	0.53
1:F:183:GLY:O	1:F:184:ALA:C	2.46	0.53
1:G:258:THR:HG22	1:G:260:PHE:H	1.72	0.53
1:A:278:ASN:O	1:A:279:ARG:HG2	2.09	0.53
1:E:286:VAL:O	1:E:286:VAL:HG23	2.07	0.53
1:F:155:TYR:OH	1:F:160:LYS:HD3	2.08	0.53
1:A:269:CYS:O	1:A:305:ILE:HD11	2.07	0.53
1:C:255:GLN:CB	1:E:128:SER:HB2	2.39	0.53
1:E:278:ASN:O	1:E:279:ARG:HG2	2.08	0.53
1:F:163:TYR:O	1:F:164:CYS:HB3	2.08	0.53
1:H:304:ARG:O	1:H:304:ARG:HG2	2.08	0.53
1:A:152:THR:HA	1:A:165:GLN:OE1	2.08	0.53
1:C:238:GLU:CG	1:C:245:GLN:HG2	2.31	0.53
1:E:258:THR:HG22	1:E:260:PHE:H	1.74	0.53
1:F:160:LYS:O	1:F:301:PHE:HB2	2.08	0.53
1:F:304:ARG:O	1:F:304:ARG:HG2	2.09	0.53
1:G:286:VAL:HG23	1:G:286:VAL:O	2.07	0.53
1:A:162:LEU:HD23	1:A:163:TYR:N	2.24	0.53
1:B:153:TRP:CB	1:B:164:CYS:HB2	2.39	0.53
1:C:163:TYR:O	1:C:164:CYS:HB3	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:HD23	1:D:163:TYR:N	2.23	0.53
1:E:214:PHE:C	1:E:215:ASN:HD22	2.12	0.53
1:G:214:PHE:C	1:G:215:ASN:HD22	2.12	0.53
2:O:2:DA:H2"	2:O:3:DA:OP2	2.07	0.53
1:A:182:GLN:HA	1:A:182:GLN:OE1	2.07	0.53
1:B:278:ASN:O	1:B:279:ARG:HG2	2.09	0.53
1:C:270:ASN:O	1:C:272:SER:N	2.41	0.53
1:E:318:ASP:O	1:E:320:ILE:N	2.41	0.53
1:H:209:GLU:O	1:H:210:LEU:HG	2.07	0.53
2:M:2:DA:H2"	2:M:3:DA:OP2	2.06	0.53
1:E:183:GLY:O	1:E:184:ALA:C	2.46	0.53
1:E:190:PRO:HG2	1:E:202:VAL:HG23	1.91	0.53
1:A:166:ILE:CG1	1:A:167:ALA:N	2.60	0.53
1:B:258:THR:HG22	1:B:260:PHE:H	1.74	0.53
1:E:210:LEU:O	1:E:212:ARG:N	2.42	0.53
1:H:155:TYR:OH	1:H:160:LYS:HD3	2.09	0.53
2:N:9:DT:H1'	2:N:10:DT:H5'	1.91	0.53
1:C:207:ASN:HD22	1:D:275:GLY:HA3	1.74	0.53
1:D:155:TYR:OH	1:D:160:LYS:HD3	2.08	0.53
1:E:162:LEU:HD23	1:E:163:TYR:N	2.24	0.53
1:F:278:ASN:O	1:F:279:ARG:HG2	2.09	0.53
1:H:258:THR:HG22	1:H:260:PHE:H	1.73	0.53
1:F:171:PRO:O	1:F:172:ILE:CB	2.57	0.53
1:H:214:PHE:C	1:H:215:ASN:HD22	2.12	0.53
1:B:278:ASN:C	1:B:279:ARG:HG2	2.30	0.52
1:D:258:THR:HG22	1:D:260:PHE:H	1.74	0.52
1:E:155:TYR:OH	1:E:160:LYS:HD3	2.09	0.52
1:G:183:GLY:HA2	1:G:291:ARG:NH2	2.24	0.52
1:H:162:LEU:HD23	1:H:163:TYR:N	2.24	0.52
1:D:160:LYS:O	1:D:301:PHE:HB2	2.09	0.52
1:D:278:ASN:O	1:D:279:ARG:HG2	2.09	0.52
1:B:183:GLY:HA2	1:B:291:ARG:NH2	2.23	0.52
1:C:155:TYR:OH	1:C:160:LYS:HD3	2.09	0.52
1:D:153:TRP:CB	1:D:164:CYS:HB2	2.39	0.52
1:D:171:PRO:O	1:D:172:ILE:CB	2.58	0.52
1:G:155:TYR:OH	1:G:160:LYS:HD3	2.09	0.52
1:H:278:ASN:O	1:H:279:ARG:HG2	2.09	0.52
1:A:155:TYR:OH	1:A:160:LYS:HD3	2.09	0.52
1:A:214:PHE:C	1:A:215:ASN:HD22	2.12	0.52
1:D:286:VAL:HG23	1:D:286:VAL:O	2.08	0.52
1:G:278:ASN:O	1:G:279:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:GLY:O	1:H:184:ALA:C	2.47	0.52
2:M:10:DT:H2"	2:O:1:DA:H1'	1.90	0.52
1:A:190:PRO:HG2	1:A:202:VAL:HG23	1.91	0.52
1:D:210:LEU:O	1:D:212:ARG:N	2.43	0.52
1:E:153:TRP:CB	1:E:164:CYS:HB2	2.39	0.52
1:C:162:LEU:HD23	1:C:163:TYR:N	2.24	0.52
1:E:278:ASN:C	1:E:279:ARG:HG2	2.30	0.52
1:B:162:LEU:HD23	1:B:163:TYR:N	2.25	0.52
1:C:210:LEU:O	1:C:212:ARG:N	2.43	0.52
1:D:269:CYS:O	1:D:305:ILE:HD11	2.09	0.52
1:F:270:ASN:O	1:F:272:SER:N	2.40	0.52
1:F:278:ASN:C	1:F:279:ARG:HG2	2.30	0.52
1:H:173:GLN:OE1	1:H:173:GLN:N	2.43	0.52
1:C:173:GLN:OE1	1:C:173:GLN:N	2.43	0.52
1:G:160:LYS:O	1:G:301:PHE:HB2	2.10	0.52
1:G:162:LEU:HD23	1:G:163:TYR:N	2.24	0.52
1:B:304:ARG:HG2	1:B:304:ARG:O	2.10	0.52
1:F:214:PHE:C	1:F:215:ASN:HD22	2.12	0.52
1:H:160:LYS:O	1:H:301:PHE:HB2	2.10	0.52
1:F:153:TRP:CB	1:F:164:CYS:HB2	2.39	0.51
1:G:183:GLY:O	1:G:184:ALA:C	2.47	0.51
1:A:160:LYS:O	1:A:301:PHE:HB2	2.10	0.51
1:A:278:ASN:C	1:A:279:ARG:HG2	2.30	0.51
1:G:207:ASN:HD21	1:H:207:ASN:H	1.58	0.51
2:M:10:DT:C2'	2:O:1:DA:O4'	2.57	0.51
1:A:173:GLN:OE1	1:A:173:GLN:N	2.44	0.51
1:B:160:LYS:O	1:B:301:PHE:HB2	2.11	0.51
1:C:160:LYS:O	1:C:301:PHE:HB2	2.10	0.51
1:E:183:GLY:HA2	1:E:291:ARG:NH2	2.24	0.51
1:F:162:LEU:HD23	1:F:163:TYR:N	2.24	0.51
1:H:190:PRO:HG2	1:H:202:VAL:HG23	1.92	0.51
1:A:189:MET:HE3	1:A:246:SER:HB2	1.93	0.51
1:A:304:ARG:O	1:A:304:ARG:HG2	2.10	0.51
1:E:189:MET:CE	1:E:246:SER:HB2	2.40	0.51
1:H:213:GLU:O	1:H:214:PHE:HB2	2.11	0.51
1:C:318:ASP:O	1:C:320:ILE:N	2.44	0.51
1:D:173:GLN:N	1:D:173:GLN:OE1	2.44	0.51
1:D:278:ASN:C	1:D:279:ARG:HG2	2.30	0.51
1:E:171:PRO:O	1:E:172:ILE:CB	2.59	0.51
1:G:278:ASN:C	1:G:279:ARG:HG2	2.31	0.51
1:C:210:LEU:HD12	1:D:206:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:9:DT:H1'	2:I:10:DT:H5'	1.92	0.51
1:B:196:GLU:CD	1:B:196:GLU:H	2.14	0.51
1:E:173:GLN:N	1:E:173:GLN:OE1	2.44	0.51
2:M:3:DA:H1'	2:M:4:DC:C5'	2.33	0.51
1:D:213:GLU:O	1:D:214:PHE:HB2	2.11	0.51
1:E:160:LYS:O	1:E:301:PHE:HB2	2.10	0.51
1:F:173:GLN:OE1	1:F:173:GLN:N	2.43	0.51
1:B:173:GLN:N	1:B:173:GLN:OE1	2.44	0.51
1:C:278:ASN:O	1:C:279:ARG:HG2	2.11	0.51
1:F:213:GLU:O	1:F:214:PHE:HB2	2.11	0.51
2:M:5:DA:C2'	2:M:6:DT:H5'	2.41	0.51
1:A:189:MET:CE	1:A:246:SER:HB2	2.42	0.50
1:D:189:MET:CE	1:D:246:SER:HB2	2.41	0.50
1:D:190:PRO:HG2	1:D:202:VAL:HG23	1.92	0.50
1:B:171:PRO:O	1:B:172:ILE:CB	2.59	0.50
1:C:278:ASN:C	1:C:279:ARG:HG2	2.32	0.50
1:E:269:CYS:O	1:E:305:ILE:CD1	2.59	0.50
1:E:304:ARG:O	1:E:304:ARG:HG2	2.10	0.50
1:G:189:MET:HE3	1:G:246:SER:HB2	1.93	0.50
1:H:318:ASP:O	1:H:320:ILE:N	2.44	0.50
1:A:211:SER:HB3	1:A:213:GLU:HG2	1.94	0.50
1:C:211:SER:HB3	1:C:213:GLU:HG2	1.94	0.50
1:C:269:CYS:O	1:C:305:ILE:CD1	2.59	0.50
1:B:213:GLU:O	1:B:214:PHE:HB2	2.12	0.50
1:E:213:GLU:O	1:E:214:PHE:HB2	2.12	0.50
1:G:165:GLN:O	1:G:166:ILE:O	2.30	0.50
1:G:269:CYS:O	1:G:305:ILE:CD1	2.60	0.50
2:P:9:DT:H1'	2:P:10:DT:H5'	1.93	0.50
1:B:190:PRO:HG2	1:B:202:VAL:HG23	1.93	0.50
1:E:211:SER:HB3	1:E:213:GLU:HG2	1.94	0.50
1:E:228:VAL:HG11	1:E:234:ALA:CB	2.42	0.50
1:C:189:MET:HE3	1:C:246:SER:HB2	1.94	0.50
1:C:190:PRO:HG2	1:C:202:VAL:HG23	1.94	0.50
1:D:166:ILE:CG1	1:D:167:ALA:H	2.01	0.50
1:G:171:PRO:O	1:G:172:ILE:CB	2.59	0.50
2:O:5:DA:C2'	2:O:6:DT:H5'	2.42	0.50
1:A:171:PRO:O	1:A:172:ILE:CB	2.59	0.50
1:B:165:GLN:O	1:B:166:ILE:O	2.30	0.50
1:E:196:GLU:H	1:E:196:GLU:CD	2.15	0.50
1:F:173:GLN:HB3	1:F:260:PHE:HB3	1.94	0.50
1:H:143:GLN:HG2	1:H:144:GLN:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:GLN:HG2	1:F:144:GLN:N	2.26	0.50
1:F:189:MET:CE	1:F:246:SER:HB2	2.42	0.50
1:H:171:PRO:O	1:H:172:ILE:CB	2.59	0.50
1:H:278:ASN:C	1:H:279:ARG:HG2	2.30	0.50
1:E:238:GLU:CG	1:E:245:GLN:HG2	2.31	0.49
1:F:190:PRO:HG2	1:F:202:VAL:HG23	1.93	0.49
1:G:161:LYS:HA	1:G:302:GLU:O	2.12	0.49
1:H:165:GLN:O	1:H:166:ILE:O	2.30	0.49
1:A:318:ASP:O	1:A:320:ILE:N	2.44	0.49
1:C:228:VAL:HG11	1:C:234:ALA:CB	2.43	0.49
1:E:318:ASP:O	1:E:319:SER:C	2.49	0.49
1:F:165:GLN:O	1:F:166:ILE:O	2.30	0.49
1:G:173:GLN:N	1:G:173:GLN:OE1	2.45	0.49
1:H:228:VAL:HA	1:H:264:LEU:O	2.12	0.49
1:B:228:VAL:HA	1:B:264:LEU:O	2.13	0.49
1:C:143:GLN:HG2	1:C:144:GLN:N	2.27	0.49
1:D:196:GLU:N	1:F:169:THR:CG2	2.66	0.49
1:F:269:CYS:O	1:F:305:ILE:CD1	2.60	0.49
1:H:162:LEU:HD23	1:H:162:LEU:C	2.33	0.49
1:A:196:GLU:CD	1:A:196:GLU:H	2.16	0.49
1:A:212:ARG:HA	1:A:212:ARG:NE	2.21	0.49
1:D:304:ARG:O	1:D:304:ARG:HG2	2.12	0.49
1:E:161:LYS:HA	1:E:302:GLU:O	2.13	0.49
1:H:183:GLY:HA2	1:H:291:ARG:NH2	2.24	0.49
2:K:9:DT:H1'	2:K:10:DT:H5'	1.93	0.49
1:C:165:GLN:O	1:C:166:ILE:O	2.30	0.49
1:D:211:SER:HB3	1:D:213:GLU:HG2	1.95	0.49
1:D:228:VAL:HG11	1:D:234:ALA:CB	2.42	0.49
1:E:165:GLN:O	1:E:166:ILE:O	2.30	0.49
1:F:318:ASP:O	1:F:320:ILE:N	2.46	0.49
1:A:238:GLU:CG	1:A:245:GLN:HG2	2.31	0.49
1:B:269:CYS:O	1:B:305:ILE:CD1	2.60	0.49
1:C:255:GLN:CG	1:E:128:SER:HB2	2.42	0.49
1:H:196:GLU:CD	1:H:196:GLU:H	2.16	0.49
1:H:211:SER:HB3	1:H:213:GLU:HG2	1.93	0.49
1:B:135:PRO:HD2	1:B:296:LEU:O	2.12	0.49
1:D:318:ASP:O	1:D:320:ILE:N	2.45	0.49
1:E:220:ALA:HB2	1:E:236:TYR:CE1	2.48	0.49
1:F:183:GLY:HA2	1:F:291:ARG:NH2	2.24	0.49
1:G:189:MET:CE	1:G:246:SER:HB2	2.43	0.49
2:N:2:DA:H2"	2:N:3:DA:OP2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HD23	1:A:162:LEU:C	2.33	0.49
1:B:173:GLN:HB3	1:B:260:PHE:HB3	1.95	0.49
1:C:140:VAL:HG12	1:C:174:ILE:CD1	2.43	0.49
1:C:162:LEU:HD23	1:C:162:LEU:C	2.33	0.49
1:D:162:LEU:HD23	1:D:162:LEU:C	2.33	0.49
1:D:165:GLN:O	1:D:166:ILE:O	2.30	0.49
1:D:183:GLY:HA2	1:D:291:ARG:NH2	2.24	0.49
1:E:162:LEU:HD23	1:E:162:LEU:C	2.33	0.49
1:F:228:VAL:HG11	1:F:234:ALA:CB	2.43	0.49
2:J:5:DA:C2'	2:J:6:DT:H5'	2.43	0.49
1:A:135:PRO:HD2	1:A:296:LEU:O	2.13	0.49
1:A:173:GLN:HB3	1:A:260:PHE:HB3	1.95	0.49
1:B:162:LEU:HD23	1:B:162:LEU:C	2.34	0.49
1:F:162:LEU:HD23	1:F:162:LEU:C	2.33	0.49
1:H:161:LYS:HA	1:H:302:GLU:O	2.12	0.49
2:K:2:DA:H2''	2:K:3:DA:OP2	2.12	0.49
1:A:140:VAL:HG12	1:A:174:ILE:CD1	2.43	0.49
1:A:213:GLU:O	1:A:214:PHE:HB2	2.13	0.49
1:C:171:PRO:O	1:C:172:ILE:CB	2.59	0.49
1:G:143:GLN:HG2	1:G:144:GLN:N	2.28	0.49
1:G:162:LEU:HD23	1:G:162:LEU:C	2.33	0.49
1:G:166:ILE:CG1	1:G:167:ALA:N	2.60	0.49
1:A:161:LYS:HA	1:A:302:GLU:O	2.12	0.48
1:B:189:MET:CE	1:B:246:SER:HB2	2.42	0.48
1:C:212:ARG:HA	1:C:212:ARG:NE	2.21	0.48
1:A:165:GLN:O	1:A:166:ILE:O	2.30	0.48
1:A:318:ASP:O	1:A:319:SER:C	2.51	0.48
1:B:143:GLN:HG2	1:B:144:GLN:N	2.28	0.48
1:B:211:SER:HB3	1:B:213:GLU:HG2	1.94	0.48
1:D:173:GLN:HB3	1:D:260:PHE:HB3	1.94	0.48
1:B:159:LEU:C	1:B:161:LYS:N	2.66	0.48
1:C:189:MET:CE	1:C:246:SER:HB2	2.43	0.48
1:D:228:VAL:HA	1:D:264:LEU:O	2.13	0.48
1:F:142:PHE:CZ	1:F:162:LEU:HD12	2.48	0.48
1:F:161:LYS:HA	1:F:302:GLU:O	2.14	0.48
1:F:211:SER:HB3	1:F:213:GLU:HG2	1.94	0.48
1:G:220:ALA:HB2	1:G:236:TYR:CE1	2.48	0.48
1:G:318:ASP:O	1:G:320:ILE:N	2.47	0.48
1:H:166:ILE:HG23	1:H:167:ALA:H	1.79	0.48
1:H:318:ASP:O	1:H:319:SER:C	2.51	0.48
1:A:183:GLY:HA2	1:A:291:ARG:NH2	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:VAL:HA	1:C:264:LEU:O	2.13	0.48
1:E:140:VAL:HG12	1:E:174:ILE:CD1	2.43	0.48
1:G:135:PRO:HD2	1:G:296:LEU:O	2.13	0.48
1:G:278:ASN:O	1:G:280:ARG:N	2.47	0.48
1:H:173:GLN:HB3	1:H:260:PHE:HB3	1.94	0.48
1:H:189:MET:CE	1:H:246:SER:HB2	2.43	0.48
1:A:244:ARG:HH11	1:A:244:ARG:HG2	1.79	0.48
1:F:196:GLU:CD	1:F:196:GLU:H	2.15	0.48
1:G:195:ALA:O	1:G:198:VAL:HG22	2.14	0.48
1:H:189:MET:HE3	1:H:246:SER:HB2	1.94	0.48
1:A:228:VAL:HG11	1:A:234:ALA:CB	2.44	0.48
1:C:213:GLU:O	1:C:214:PHE:HB2	2.13	0.48
1:E:143:GLN:HG2	1:E:144:GLN:N	2.28	0.48
1:F:189:MET:HE3	1:F:246:SER:HB2	1.96	0.48
1:G:213:GLU:O	1:G:214:PHE:HB2	2.13	0.48
1:H:228:VAL:HG11	1:H:234:ALA:CB	2.43	0.48
2:P:1:DA:H2"	2:P:2:DA:O5'	2.13	0.48
1:A:204:ARG:HH12	1:A:208:HIS:HB3	1.79	0.48
1:B:161:LYS:HA	1:B:302:GLU:O	2.14	0.48
1:C:318:ASP:O	1:C:319:SER:C	2.51	0.48
1:D:135:PRO:HD2	1:D:296:LEU:O	2.14	0.48
1:E:142:PHE:CZ	1:E:162:LEU:HD12	2.49	0.48
1:F:228:VAL:HA	1:F:264:LEU:O	2.13	0.48
1:G:211:SER:HB3	1:G:213:GLU:HG2	1.95	0.48
1:G:280:ARG:O	1:G:281:PRO:C	2.52	0.48
1:H:135:PRO:HD2	1:H:296:LEU:O	2.13	0.48
2:L:4:DC:H2"	2:L:5:DA:OP2	2.13	0.48
1:A:228:VAL:HA	1:A:264:LEU:O	2.14	0.48
1:D:140:VAL:HG12	1:D:174:ILE:CD1	2.44	0.48
1:F:135:PRO:HD2	1:F:296:LEU:O	2.14	0.48
1:G:140:VAL:HG12	1:G:174:ILE:CD1	2.44	0.48
1:G:173:GLN:HB3	1:G:260:PHE:HB3	1.94	0.48
1:G:228:VAL:HA	1:G:264:LEU:O	2.14	0.48
1:H:220:ALA:HA	1:H:236:TYR:CD1	2.49	0.48
1:A:269:CYS:O	1:A:305:ILE:CD1	2.61	0.48
1:B:220:ALA:HB2	1:B:236:TYR:CE1	2.49	0.48
1:B:271:SER:O	1:B:272:SER:HB3	2.14	0.48
1:E:228:VAL:HA	1:E:264:LEU:O	2.14	0.48
1:G:228:VAL:HG11	1:G:234:ALA:CB	2.44	0.48
2:L:3:DA:C1'	2:L:4:DC:H5'	2.38	0.48
2:L:5:DA:C2'	2:L:6:DT:H5'	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:PRO:HD2	1:C:296:LEU:O	2.14	0.47
1:D:161:LYS:HA	1:D:302:GLU:O	2.14	0.47
1:D:212:ARG:HA	1:D:212:ARG:NE	2.21	0.47
1:H:142:PHE:CZ	1:H:162:LEU:HD12	2.49	0.47
1:A:195:ALA:O	1:A:198:VAL:HG22	2.14	0.47
1:A:220:ALA:HB2	1:A:236:TYR:CE1	2.49	0.47
1:C:158:GLU:CD	1:C:158:GLU:H	2.18	0.47
1:D:196:GLU:CD	1:D:196:GLU:H	2.16	0.47
1:E:173:GLN:HB3	1:E:260:PHE:HB3	1.95	0.47
1:C:173:GLN:HB3	1:C:260:PHE:HB3	1.95	0.47
1:C:244:ARG:HH11	1:C:244:ARG:HG2	1.79	0.47
1:E:244:ARG:HG2	1:E:244:ARG:HH11	1.79	0.47
1:F:318:ASP:O	1:F:319:SER:C	2.53	0.47
1:G:196:GLU:CD	1:G:196:GLU:H	2.16	0.47
2:I:2:DA:H2"	2:I:3:DA:OP2	2.13	0.47
1:A:142:PHE:CZ	1:A:162:LEU:HD12	2.49	0.47
1:B:228:VAL:HG11	1:B:234:ALA:CB	2.43	0.47
1:B:290:THR:HB	1:B:296:LEU:CD2	2.39	0.47
1:D:166:ILE:HG23	1:D:167:ALA:H	1.79	0.47
1:D:204:ARG:HH12	1:D:208:HIS:HB3	1.80	0.47
1:F:220:ALA:HB2	1:F:236:TYR:CE1	2.49	0.47
1:H:278:ASN:O	1:H:280:ARG:N	2.47	0.47
1:C:166:ILE:HG23	1:C:167:ALA:H	1.78	0.47
1:D:195:ALA:O	1:D:198:VAL:HG22	2.15	0.47
1:D:220:ALA:HB2	1:D:236:TYR:CE1	2.50	0.47
1:F:166:ILE:HG23	1:F:167:ALA:H	1.79	0.47
1:G:212:ARG:HA	1:G:212:ARG:NE	2.21	0.47
1:H:140:VAL:HG12	1:H:174:ILE:CD1	2.45	0.47
1:H:220:ALA:HB2	1:H:236:TYR:CE1	2.48	0.47
1:B:212:ARG:HA	1:B:212:ARG:NE	2.21	0.47
1:C:161:LYS:HA	1:C:302:GLU:O	2.14	0.47
1:C:220:ALA:HB2	1:C:236:TYR:CE1	2.49	0.47
1:F:158:GLU:CD	1:F:158:GLU:H	2.18	0.47
1:H:159:LEU:C	1:H:161:LYS:N	2.66	0.47
1:H:204:ARG:HH12	1:H:208:HIS:HB3	1.79	0.47
1:B:142:PHE:CZ	1:B:162:LEU:HD12	2.50	0.47
1:C:195:ALA:O	1:C:198:VAL:HG22	2.14	0.47
1:C:204:ARG:HH12	1:C:208:HIS:HB3	1.79	0.47
1:D:196:GLU:CB	1:F:169:THR:HG22	2.40	0.47
1:D:269:CYS:O	1:D:305:ILE:CD1	2.63	0.47
1:E:166:ILE:CG1	1:E:167:ALA:N	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:ILE:CG1	1:H:167:ALA:H	2.02	0.47
1:H:176:VAL:HG21	1:H:251:TYR:OH	2.15	0.47
2:M:4:DC:H2"	2:M:5:DA:OP2	2.15	0.47
1:A:166:ILE:HG23	1:A:167:ALA:H	1.80	0.47
1:A:210:LEU:C	1:A:212:ARG:H	2.18	0.47
1:D:318:ASP:O	1:D:319:SER:C	2.52	0.47
1:G:166:ILE:HG23	1:G:167:ALA:H	1.78	0.47
2:P:2:DA:H2"	2:P:3:DA:OP2	2.14	0.47
1:A:210:LEU:C	1:A:212:ARG:N	2.68	0.47
1:B:140:VAL:HG12	1:B:174:ILE:CD1	2.44	0.47
1:D:220:ALA:HA	1:D:236:TYR:CD1	2.50	0.47
1:E:195:ALA:O	1:E:198:VAL:HG22	2.15	0.47
1:E:271:SER:O	1:E:272:SER:HB3	2.15	0.47
1:G:318:ASP:O	1:G:319:SER:C	2.53	0.47
1:C:280:ARG:O	1:C:281:PRO:C	2.54	0.46
1:E:158:GLU:CD	1:E:158:GLU:H	2.18	0.46
1:E:165:GLN:HG2	1:E:307:ALA:O	2.16	0.46
1:E:216:GLU:HB2	1:H:264:LEU:CD1	2.45	0.46
1:E:320:ILE:CG1	1:E:321:ARG:N	2.75	0.46
1:F:140:VAL:HG12	1:F:174:ILE:CD1	2.45	0.46
1:F:159:LEU:C	1:F:161:LYS:N	2.67	0.46
1:G:271:SER:O	1:G:272:SER:HB3	2.15	0.46
1:H:195:ALA:O	1:H:198:VAL:HG22	2.15	0.46
1:H:238:GLU:CG	1:H:245:GLN:HG2	2.30	0.46
1:H:269:CYS:O	1:H:305:ILE:CD1	2.62	0.46
2:J:4:DC:H2"	2:J:5:DA:OP2	2.15	0.46
1:B:305:ILE:O	1:B:305:ILE:CG1	2.63	0.46
1:F:210:LEU:C	1:F:212:ARG:H	2.19	0.46
1:F:210:LEU:C	1:F:212:ARG:N	2.69	0.46
1:G:210:LEU:C	1:G:212:ARG:N	2.69	0.46
1:H:210:LEU:C	1:H:212:ARG:N	2.68	0.46
1:B:195:ALA:O	1:B:198:VAL:HG22	2.15	0.46
1:C:159:LEU:C	1:C:161:LYS:N	2.68	0.46
1:E:166:ILE:CG1	1:E:167:ALA:H	2.03	0.46
2:N:1:DA:H2"	2:N:2:DA:O5'	2.15	0.46
1:C:221:PRO:HB2	1:C:224:HIS:CD2	2.51	0.46
1:D:142:PHE:CZ	1:D:162:LEU:HD12	2.49	0.46
1:E:220:ALA:HA	1:E:236:TYR:CD1	2.50	0.46
1:G:158:GLU:CD	1:G:158:GLU:H	2.18	0.46
1:H:138:PHE:O	1:H:299:ARG:HD3	2.16	0.46
1:H:210:LEU:C	1:H:212:ARG:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:212:ARG:HA	1:H:212:ARG:NE	2.21	0.46
1:A:278:ASN:O	1:A:280:ARG:N	2.49	0.46
1:B:220:ALA:HA	1:B:236:TYR:CD1	2.51	0.46
1:D:158:GLU:CD	1:D:158:GLU:H	2.18	0.46
1:D:159:LEU:C	1:D:161:LYS:N	2.67	0.46
1:F:195:ALA:O	1:F:198:VAL:HG22	2.14	0.46
1:G:210:LEU:C	1:G:212:ARG:H	2.19	0.46
2:I:1:DA:H2"	2:I:2:DA:O5'	2.15	0.46
1:B:166:ILE:HG23	1:B:167:ALA:H	1.80	0.46
1:B:210:LEU:C	1:B:212:ARG:N	2.69	0.46
1:C:196:GLU:CD	1:C:196:GLU:H	2.17	0.46
1:D:271:SER:O	1:D:272:SER:HB3	2.16	0.46
1:E:135:PRO:HD2	1:E:296:LEU:O	2.16	0.46
1:E:241:ILE:HG23	1:E:242:THR:N	2.31	0.46
1:E:277:MET:O	1:E:278:ASN:C	2.54	0.46
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.31	0.46
1:C:220:ALA:HA	1:C:236:TYR:CD1	2.50	0.46
1:E:201:VAL:HG12	1:E:244:ARG:HG2	1.98	0.46
1:F:220:ALA:HA	1:F:236:TYR:CD1	2.51	0.46
1:F:277:MET:O	1:F:278:ASN:C	2.54	0.46
1:G:220:ALA:HA	1:G:236:TYR:CD1	2.51	0.46
2:K:1:DA:H2"	2:K:2:DA:O5'	2.16	0.46
2:M:3:DA:C1'	2:M:4:DC:H5'	2.39	0.46
1:D:143:GLN:HG2	1:D:144:GLN:N	2.29	0.46
1:E:204:ARG:HH12	1:E:208:HIS:HB3	1.81	0.46
1:F:183:GLY:HA2	1:F:291:ARG:HE	1.81	0.46
1:F:244:ARG:HG2	1:F:244:ARG:HH11	1.80	0.46
1:G:142:PHE:CZ	1:G:162:LEU:HD12	2.50	0.46
1:A:159:LEU:C	1:A:161:LYS:N	2.67	0.46
1:C:142:PHE:CZ	1:C:162:LEU:HD12	2.50	0.46
1:C:244:ARG:HG2	1:C:244:ARG:NH1	2.31	0.46
1:D:280:ARG:O	1:D:281:PRO:C	2.54	0.46
1:E:305:ILE:O	1:E:305:ILE:CG1	2.64	0.46
1:H:290:THR:HB	1:H:296:LEU:CD2	2.41	0.46
1:A:264:LEU:CD1	1:D:216:GLU:CB	2.86	0.46
1:E:220:ALA:HB2	1:E:236:TYR:HE1	1.81	0.46
1:F:241:ILE:HG23	1:F:242:THR:N	2.31	0.46
1:F:278:ASN:O	1:F:280:ARG:N	2.49	0.46
1:A:220:ALA:HA	1:A:236:TYR:CD1	2.51	0.45
1:A:241:ILE:HG23	1:A:242:THR:N	2.31	0.45
1:C:176:VAL:HG21	1:C:251:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:GLU:CG	1:F:245:GLN:HG2	2.30	0.45
1:H:158:GLU:CD	1:H:158:GLU:H	2.19	0.45
1:H:241:ILE:HG23	1:H:242:THR:N	2.32	0.45
1:A:138:PHE:O	1:A:299:ARG:HD3	2.16	0.45
1:A:165:GLN:HG2	1:A:307:ALA:O	2.16	0.45
1:B:189:MET:HE3	1:B:246:SER:HB2	1.98	0.45
1:D:183:GLY:HA2	1:D:291:ARG:HE	1.81	0.45
1:D:278:ASN:O	1:D:280:ARG:N	2.49	0.45
1:D:305:ILE:O	1:D:305:ILE:CG1	2.64	0.45
1:H:290:THR:OG1	1:H:291:ARG:N	2.50	0.45
2:O:4:DC:H2"	2:O:5:DA:OP2	2.17	0.45
1:B:278:ASN:O	1:B:280:ARG:N	2.48	0.45
1:D:140:VAL:O	1:D:141:SER:HB3	2.16	0.45
1:E:176:VAL:HG21	1:E:251:TYR:OH	2.16	0.45
1:G:190:PRO:HG2	1:G:202:VAL:HG23	1.94	0.45
1:A:224:HIS:HA	1:A:245:GLN:NE2	2.32	0.45
1:C:210:LEU:C	1:C:212:ARG:H	2.20	0.45
1:C:305:ILE:O	1:C:305:ILE:CG1	2.64	0.45
1:F:175:LYS:HG2	1:F:176:VAL:N	2.31	0.45
1:G:238:GLU:CG	1:G:245:GLN:HG2	2.30	0.45
1:H:244:ARG:HH11	1:H:244:ARG:HG2	1.81	0.45
1:H:271:SER:O	1:H:272:SER:HB3	2.15	0.45
1:H:280:ARG:O	1:H:281:PRO:C	2.55	0.45
1:A:183:GLY:HA2	1:A:291:ARG:HE	1.81	0.45
1:B:176:VAL:HG21	1:B:251:TYR:OH	2.16	0.45
1:B:241:ILE:HG23	1:B:242:THR:N	2.32	0.45
1:B:318:ASP:O	1:B:320:ILE:N	2.50	0.45
1:C:210:LEU:C	1:C:212:ARG:N	2.70	0.45
1:D:210:LEU:C	1:D:212:ARG:H	2.20	0.45
1:E:241:ILE:HG23	1:E:242:THR:CG2	2.41	0.45
1:E:244:ARG:HG2	1:E:244:ARG:NH1	2.31	0.45
1:F:165:GLN:HG2	1:F:307:ALA:O	2.16	0.45
1:G:305:ILE:O	1:G:305:ILE:CG1	2.64	0.45
2:L:9:DT:H6	2:L:9:DT:H5'	1.81	0.45
1:A:280:ARG:O	1:A:281:PRO:C	2.54	0.45
1:B:165:GLN:HG2	1:B:307:ALA:O	2.16	0.45
1:C:220:ALA:HB2	1:C:236:TYR:HE1	1.82	0.45
1:C:278:ASN:O	1:C:280:ARG:N	2.49	0.45
1:C:304:ARG:O	1:C:304:ARG:HG2	2.15	0.45
1:D:128:SER:HB2	1:F:255:GLN:HB3	1.98	0.45
1:D:165:GLN:HG2	1:D:307:ALA:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ALA:CB	1:E:236:TYR:CE1	3.00	0.45
1:F:244:ARG:HG2	1:F:244:ARG:NH1	2.32	0.45
1:F:280:ARG:O	1:F:281:PRO:C	2.54	0.45
1:F:305:ILE:O	1:F:305:ILE:CG1	2.64	0.45
1:A:176:VAL:HG21	1:A:251:TYR:OH	2.17	0.45
1:A:305:ILE:O	1:A:305:ILE:CG1	2.65	0.45
1:C:138:PHE:O	1:C:299:ARG:HD3	2.17	0.45
1:D:196:GLU:HA	1:F:169:THR:CG2	2.45	0.45
1:G:138:PHE:O	1:G:299:ARG:HD3	2.17	0.45
1:G:159:LEU:C	1:G:161:LYS:N	2.66	0.45
1:G:165:GLN:HG2	1:G:307:ALA:O	2.17	0.45
1:G:183:GLY:HA2	1:G:291:ARG:HE	1.81	0.45
2:M:10:DT:H2"	2:O:2:DA:H5'	1.97	0.45
1:B:244:ARG:HG2	1:B:244:ARG:HH11	1.81	0.45
1:C:313:ARG:HG3	1:C:313:ARG:HH11	1.82	0.45
1:D:238:GLU:CG	1:D:245:GLN:HG2	2.30	0.45
1:E:210:LEU:C	1:E:212:ARG:N	2.70	0.45
1:G:176:VAL:HG21	1:G:251:TYR:OH	2.17	0.45
1:C:207:ASN:ND2	1:D:274:VAL:C	2.67	0.45
1:D:241:ILE:HG23	1:D:242:THR:N	2.32	0.45
1:E:221:PRO:HB2	1:E:224:HIS:CD2	2.52	0.45
1:E:290:THR:HB	1:E:296:LEU:CD2	2.40	0.45
1:A:232:SER:HB2	1:D:232:SER:CB	2.47	0.44
1:B:183:GLY:HA2	1:B:291:ARG:HE	1.81	0.44
1:B:210:LEU:C	1:B:212:ARG:H	2.19	0.44
1:C:241:ILE:HG23	1:C:242:THR:N	2.32	0.44
1:D:184:ALA:HB1	1:D:251:TYR:HB3	1.99	0.44
1:E:206:PRO:HD2	1:F:207:ASN:ND2	2.32	0.44
1:F:220:ALA:HB2	1:F:236:TYR:HE1	1.82	0.44
2:J:1:DA:H2"	2:J:2:DA:O5'	2.17	0.44
1:B:313:ARG:HG3	1:B:313:ARG:HH11	1.83	0.44
1:E:217:GLY:C	1:E:219:ILE:H	2.21	0.44
1:G:220:ALA:HB2	1:G:236:TYR:HE1	1.82	0.44
1:G:244:ARG:HG2	1:G:244:ARG:HH11	1.81	0.44
1:H:165:GLN:HG2	1:H:307:ALA:O	2.17	0.44
1:B:140:VAL:O	1:B:141:SER:HB3	2.17	0.44
1:E:138:PHE:O	1:E:299:ARG:HD3	2.18	0.44
1:E:210:LEU:C	1:E:212:ARG:H	2.20	0.44
1:G:277:MET:O	1:G:278:ASN:C	2.55	0.44
1:H:175:LYS:HG2	1:H:176:VAL:N	2.33	0.44
1:H:183:GLY:HA2	1:H:291:ARG:HE	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:264:LEU:CD1	1:H:264:LEU:N	2.80	0.44
2:M:9:DT:H6	2:M:9:DT:H5'	1.82	0.44
1:B:244:ARG:HG2	1:B:244:ARG:NH1	2.33	0.44
1:E:183:GLY:HA2	1:E:291:ARG:HE	1.81	0.44
1:F:201:VAL:HG12	1:F:244:ARG:HG2	2.00	0.44
1:F:271:SER:O	1:F:272:SER:HB3	2.17	0.44
1:G:204:ARG:HH12	1:G:208:HIS:HB3	1.80	0.44
1:G:224:HIS:HA	1:G:245:GLN:NE2	2.32	0.44
2:M:5:DA:H1'	2:M:6:DT:H5'	1.99	0.44
1:A:158:GLU:CD	1:A:158:GLU:H	2.19	0.44
1:A:191:VAL:HG11	1:A:285:ILE:HD11	1.99	0.44
1:A:271:SER:O	1:A:272:SER:HB3	2.17	0.44
1:B:221:PRO:HB2	1:B:224:HIS:CD2	2.52	0.44
1:C:183:GLY:HA2	1:C:291:ARG:HE	1.82	0.44
1:D:138:PHE:O	1:D:299:ARG:HD3	2.18	0.44
1:F:204:ARG:HH12	1:F:208:HIS:HB3	1.82	0.44
1:F:221:PRO:HB2	1:F:224:HIS:CD2	2.52	0.44
1:G:220:ALA:CB	1:G:236:TYR:CE1	3.01	0.44
2:M:10:DT:H2"	2:O:1:DA:C1'	2.48	0.44
2:N:6:DT:H1'	2:N:7:DG:C8	2.53	0.44
1:B:158:GLU:CD	1:B:158:GLU:H	2.19	0.44
1:C:271:SER:O	1:C:272:SER:HB3	2.17	0.44
1:C:277:MET:O	1:C:278:ASN:C	2.55	0.44
1:D:277:MET:O	1:D:278:ASN:C	2.55	0.44
1:E:140:VAL:O	1:E:141:SER:HB3	2.18	0.44
1:E:184:ALA:HB1	1:E:251:TYR:HB3	2.00	0.44
2:L:5:DA:H1'	2:L:6:DT:H5'	2.00	0.44
1:B:277:MET:O	1:B:278:ASN:C	2.55	0.44
1:D:176:VAL:HG21	1:D:251:TYR:OH	2.17	0.44
1:D:196:GLU:OE1	1:F:152:THR:HG21	2.17	0.44
1:D:210:LEU:C	1:D:212:ARG:N	2.70	0.44
1:G:140:VAL:O	1:G:141:SER:HB3	2.18	0.44
1:G:241:ILE:HG23	1:G:242:THR:N	2.32	0.44
1:H:184:ALA:HB1	1:H:251:TYR:HB3	2.00	0.44
1:H:220:ALA:HB2	1:H:236:TYR:HE1	1.82	0.44
1:H:313:ARG:HG3	1:H:313:ARG:HH11	1.83	0.44
1:A:201:VAL:HG12	1:A:244:ARG:HG2	1.99	0.44
1:A:277:MET:O	1:A:278:ASN:C	2.55	0.44
1:C:255:GLN:CD	1:E:128:SER:HB2	2.37	0.44
1:D:244:ARG:HG2	1:D:244:ARG:HH11	1.81	0.44
1:F:290:THR:HB	1:F:296:LEU:CD2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:LEU:O	1:G:296:LEU:HB2	2.18	0.44
1:H:140:VAL:O	1:H:141:SER:HB3	2.17	0.44
1:H:305:ILE:O	1:H:305:ILE:CG1	2.65	0.44
2:L:1:DA:H2"	2:L:2:DA:O5'	2.18	0.44
1:B:201:VAL:HG12	1:B:244:ARG:HG2	1.99	0.44
1:C:290:THR:OG1	1:C:291:ARG:N	2.51	0.44
1:D:196:GLU:CB	1:F:169:THR:CG2	2.95	0.44
1:E:209:GLU:HB2	1:E:222:PRO:O	2.18	0.44
1:F:140:VAL:O	1:F:141:SER:HB3	2.18	0.44
1:G:175:LYS:HG2	1:G:176:VAL:N	2.33	0.44
1:H:201:VAL:HG12	1:H:244:ARG:HG2	2.00	0.44
1:H:209:GLU:HB2	1:H:222:PRO:O	2.18	0.44
1:A:184:ALA:HB1	1:A:251:TYR:HB3	2.00	0.43
1:B:138:PHE:O	1:B:299:ARG:HD3	2.18	0.43
1:C:217:GLY:C	1:C:219:ILE:H	2.21	0.43
1:D:220:ALA:HB2	1:D:236:TYR:HE1	1.83	0.43
1:G:244:ARG:HG2	1:G:244:ARG:NH1	2.33	0.43
1:G:313:ARG:HG3	1:G:313:ARG:HH11	1.82	0.43
2:O:9:DT:H6	2:O:9:DT:H5'	1.83	0.43
1:A:221:PRO:HB2	1:A:224:HIS:CD2	2.52	0.43
1:A:290:THR:OG1	1:A:291:ARG:N	2.51	0.43
1:B:280:ARG:O	1:B:281:PRO:C	2.55	0.43
1:E:159:LEU:C	1:E:161:LYS:N	2.67	0.43
1:E:313:ARG:HH11	1:E:313:ARG:HG3	1.83	0.43
1:G:290:THR:HB	1:G:296:LEU:CD2	2.40	0.43
1:H:221:PRO:HB2	1:H:224:HIS:CD2	2.53	0.43
1:H:224:HIS:HA	1:H:245:GLN:NE2	2.33	0.43
1:A:313:ARG:HG3	1:A:313:ARG:HH11	1.83	0.43
1:B:209:GLU:HB2	1:B:222:PRO:O	2.18	0.43
1:D:220:ALA:CB	1:D:236:TYR:CE1	3.02	0.43
1:D:290:THR:HB	1:D:296:LEU:CD2	2.41	0.43
2:J:3:DA:C1'	2:J:4:DC:H5'	2.40	0.43
2:N:5:DA:H1'	2:N:6:DT:H5"	2.00	0.43
1:F:158:GLU:CD	1:F:159:LEU:N	2.69	0.43
1:F:212:ARG:HA	1:F:212:ARG:NE	2.21	0.43
1:F:290:THR:OG1	1:F:291:ARG:N	2.52	0.43
1:A:220:ALA:CB	1:A:236:TYR:CE1	3.01	0.43
1:B:184:ALA:HB1	1:B:251:TYR:HB3	2.00	0.43
1:B:217:GLY:C	1:B:219:ILE:H	2.21	0.43
1:C:148:ALA:O	1:C:150:SER:N	2.46	0.43
1:C:165:GLN:HG2	1:C:307:ALA:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:VAL:HG12	1:C:244:ARG:HG2	1.99	0.43
1:C:220:ALA:CB	1:C:236:TYR:CE1	3.01	0.43
1:D:221:PRO:HB2	1:D:224:HIS:CD2	2.54	0.43
1:D:290:THR:OG1	1:D:291:ARG:N	2.52	0.43
1:E:175:LYS:HG2	1:E:176:VAL:N	2.33	0.43
1:G:217:GLY:C	1:G:219:ILE:H	2.20	0.43
1:G:221:PRO:HB2	1:G:224:HIS:CD2	2.53	0.43
2:J:5:DA:H1'	2:J:6:DT:H5'	2.01	0.43
1:A:220:ALA:HB2	1:A:236:TYR:HE1	1.83	0.43
1:C:175:LYS:HG2	1:C:176:VAL:N	2.33	0.43
1:C:184:ALA:HB1	1:C:251:TYR:HB3	2.00	0.43
1:H:191:VAL:HG11	1:H:285:ILE:HD11	2.00	0.43
1:A:140:VAL:O	1:A:141:SER:HB3	2.19	0.43
1:B:224:HIS:HA	1:B:245:GLN:NE2	2.33	0.43
1:C:239:ASP:OD1	1:C:240:PRO:HD2	2.19	0.43
1:D:224:HIS:HA	1:D:245:GLN:NE2	2.33	0.43
1:D:244:ARG:HG2	1:D:244:ARG:NH1	2.33	0.43
1:E:224:HIS:HA	1:E:245:GLN:NE2	2.34	0.43
1:F:209:GLU:HB2	1:F:222:PRO:O	2.18	0.43
1:G:295:VAL:HG22	1:G:296:LEU:N	2.34	0.43
1:H:220:ALA:CB	1:H:236:TYR:CE1	3.00	0.43
1:H:244:ARG:HG2	1:H:244:ARG:NH1	2.33	0.43
1:A:209:GLU:HB2	1:A:222:PRO:O	2.19	0.43
1:F:220:ALA:CB	1:F:236:TYR:CE1	3.02	0.43
1:G:201:VAL:HG12	1:G:244:ARG:HG2	1.99	0.43
2:J:9:DT:H1'	2:J:10:DT:C5'	2.49	0.43
1:A:175:LYS:HG2	1:A:176:VAL:N	2.33	0.43
1:D:313:ARG:HG3	1:D:313:ARG:HH11	1.84	0.43
1:E:239:ASP:OD1	1:E:240:PRO:HD2	2.19	0.43
1:F:217:GLY:C	1:F:219:ILE:H	2.22	0.43
1:F:224:HIS:HA	1:F:245:GLN:NE2	2.33	0.43
1:B:220:ALA:CB	1:B:236:TYR:CE1	3.02	0.43
1:D:201:VAL:HG12	1:D:244:ARG:HG2	1.99	0.43
1:F:176:VAL:HG21	1:F:251:TYR:OH	2.18	0.43
1:G:209:GLU:HB2	1:G:222:PRO:O	2.19	0.43
2:I:5:DA:H1'	2:I:6:DT:H5"	2.01	0.43
2:I:5:DA:C2'	2:I:6:DT:H5'	2.48	0.43
1:C:169:THR:CG2	1:E:196:GLU:CD	2.87	0.42
1:D:175:LYS:HG2	1:D:176:VAL:N	2.33	0.42
1:D:217:GLY:C	1:D:219:ILE:H	2.22	0.42
1:E:278:ASN:O	1:E:280:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:PHE:O	1:F:299:ARG:HD3	2.18	0.42
1:H:278:ASN:HA	1:H:279:ARG:HH12	1.84	0.42
1:A:217:GLY:C	1:A:219:ILE:H	2.20	0.42
1:B:220:ALA:HB2	1:B:236:TYR:HE1	1.83	0.42
1:C:158:GLU:CD	1:C:159:LEU:N	2.71	0.42
1:C:158:GLU:CD	1:C:158:GLU:N	2.73	0.42
1:H:217:GLY:C	1:H:219:ILE:H	2.22	0.42
2:O:5:DA:H1'	2:O:6:DT:H5'	2.01	0.42
1:B:191:VAL:HG11	1:B:285:ILE:HD11	2.00	0.42
1:B:278:ASN:HA	1:B:279:ARG:HH12	1.84	0.42
1:B:311:ARG:NH2	2:J:7:DG:N7	2.45	0.42
1:E:212:ARG:HA	1:E:212:ARG:NE	2.22	0.42
1:F:184:ALA:HB1	1:F:251:TYR:HB3	2.00	0.42
1:G:184:ALA:HB1	1:G:251:TYR:HB3	2.01	0.42
1:A:201:VAL:HA	1:A:244:ARG:HH12	1.85	0.42
1:B:175:LYS:HG2	1:B:176:VAL:N	2.33	0.42
1:D:209:GLU:HB2	1:D:222:PRO:O	2.18	0.42
1:F:288:LEU:O	1:F:296:LEU:HB2	2.19	0.42
1:G:158:GLU:CD	1:G:158:GLU:N	2.73	0.42
2:J:9:DT:H6	2:J:9:DT:H5'	1.84	0.42
1:B:290:THR:OG1	1:B:291:ARG:N	2.53	0.42
1:C:140:VAL:O	1:C:141:SER:HB3	2.19	0.42
1:F:136:HIS:HB3	1:F:178:THR:O	2.20	0.42
1:G:191:VAL:HG11	1:G:285:ILE:HD11	2.01	0.42
1:G:279:ARG:CB	2:O:6:DT:OP1	2.67	0.42
1:G:290:THR:OG1	1:G:291:ARG:N	2.53	0.42
1:B:288:LEU:O	1:B:296:LEU:HB2	2.19	0.42
1:E:280:ARG:O	1:E:281:PRO:C	2.56	0.42
1:F:166:ILE:CG1	1:F:167:ALA:N	2.60	0.42
1:G:159:LEU:O	1:G:160:LYS:C	2.58	0.42
1:G:264:LEU:CD1	1:G:264:LEU:N	2.82	0.42
1:H:239:ASP:OD1	1:H:240:PRO:HD2	2.19	0.42
1:H:288:LEU:O	1:H:296:LEU:HB2	2.19	0.42
1:A:136:HIS:HB3	1:A:178:THR:O	2.20	0.42
1:C:169:THR:CB	1:E:196:GLU:HB3	2.49	0.42
1:C:290:THR:HG23	1:C:293:GLY:H	1.85	0.42
1:F:213:GLU:O	1:F:214:PHE:CB	2.67	0.42
1:F:239:ASP:OD1	1:F:240:PRO:HD2	2.20	0.42
1:G:136:HIS:HB3	1:G:178:THR:O	2.19	0.42
1:H:277:MET:O	1:H:278:ASN:C	2.56	0.42
1:H:295:VAL:HG22	1:H:296:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:9:DT:H1'	2:L:10:DT:C5'	2.50	0.42
2:M:1:DA:H2"	2:M:2:DA:O5'	2.19	0.42
1:C:136:HIS:HB3	1:C:178:THR:O	2.19	0.42
1:C:304:ARG:HH11	1:C:304:ARG:HG3	1.84	0.42
1:E:288:LEU:O	1:E:296:LEU:HB2	2.19	0.42
1:F:158:GLU:OE2	1:F:159:LEU:HG	2.20	0.42
1:H:213:GLU:O	1:H:214:PHE:CB	2.68	0.42
1:H:241:ILE:HG23	1:H:242:THR:CG2	2.43	0.42
1:A:158:GLU:OE2	1:A:159:LEU:HG	2.20	0.42
1:A:187:ARG:HG3	1:A:246:SER:OG	2.20	0.42
1:A:264:LEU:CD1	1:A:264:LEU:N	2.83	0.42
1:B:204:ARG:HH12	1:B:208:HIS:HB3	1.81	0.42
2:I:3:DA:H1'	2:I:4:DC:H5'	2.01	0.42
1:B:215:ASN:HD22	1:B:215:ASN:N	2.18	0.42
1:C:213:GLU:O	1:C:214:PHE:CB	2.68	0.42
1:D:158:GLU:CD	1:D:158:GLU:N	2.73	0.42
1:D:239:ASP:OD1	1:D:240:PRO:HD2	2.20	0.42
1:E:158:GLU:CD	1:E:158:GLU:N	2.73	0.42
1:F:158:GLU:CD	1:F:158:GLU:N	2.73	0.42
2:O:1:DA:H2"	2:O:2:DA:O5'	2.19	0.42
2:P:5:DA:C2'	2:P:6:DT:H5'	2.48	0.42
2:P:6:DT:H1'	2:P:7:DG:C8	2.55	0.42
1:D:213:GLU:O	1:D:214:PHE:CB	2.66	0.41
1:E:308:CYS:O	1:E:310:GLY:N	2.53	0.41
1:F:264:LEU:N	1:F:264:LEU:CD1	2.83	0.41
2:P:5:DA:H1'	2:P:6:DT:H5"	2.01	0.41
1:A:148:ALA:O	1:A:150:SER:N	2.48	0.41
1:B:136:HIS:HB3	1:B:178:THR:O	2.20	0.41
1:B:213:GLU:O	1:B:214:PHE:CB	2.68	0.41
1:C:221:PRO:HB2	1:C:224:HIS:HD2	1.84	0.41
1:D:304:ARG:HH11	1:D:304:ARG:HG3	1.85	0.41
1:F:304:ARG:HG3	1:F:304:ARG:HH11	1.85	0.41
2:I:7:DG:H1'	2:I:8:DT:H5'	2.02	0.41
1:B:187:ARG:HG3	1:B:246:SER:OG	2.20	0.41
1:B:201:VAL:HA	1:B:244:ARG:HH12	1.85	0.41
1:B:221:PRO:HB2	1:B:224:HIS:HD2	1.85	0.41
1:C:169:THR:HB	1:E:196:GLU:HB3	2.01	0.41
1:D:278:ASN:HA	1:D:279:ARG:HH12	1.85	0.41
1:E:278:ASN:HA	1:E:279:ARG:HH12	1.84	0.41
1:E:290:THR:OG1	1:E:291:ARG:N	2.53	0.41
1:H:201:VAL:HA	1:H:244:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:5:DA:H1'	2:K:6:DT:H5"	2.00	0.41
2:P:7:DG:H1'	2:P:8:DT:H5'	2.02	0.41
1:A:290:THR:HB	1:A:296:LEU:CD2	2.41	0.41
1:B:158:GLU:CD	1:B:159:LEU:N	2.72	0.41
1:E:148:ALA:O	1:E:150:SER:N	2.46	0.41
1:E:213:GLU:O	1:E:214:PHE:CB	2.68	0.41
1:E:320:ILE:HG13	1:E:321:ARG:H	1.81	0.41
1:F:148:ALA:O	1:F:150:SER:N	2.47	0.41
1:F:295:VAL:HG22	1:F:297:GLY:H	1.84	0.41
2:M:9:DT:H1'	2:M:10:DT:C5'	2.51	0.41
1:B:158:GLU:CD	1:B:158:GLU:N	2.74	0.41
1:B:318:ASP:O	1:B:319:SER:C	2.59	0.41
1:C:255:GLN:NE2	1:E:128:SER:HB2	2.36	0.41
1:C:308:CYS:O	1:C:310:GLY:N	2.54	0.41
1:D:241:ILE:HG23	1:D:242:THR:CG2	2.43	0.41
1:D:264:LEU:CD1	1:D:264:LEU:N	2.83	0.41
1:D:295:VAL:HG22	1:D:296:LEU:N	2.35	0.41
1:D:308:CYS:O	1:D:310:GLY:N	2.53	0.41
1:G:187:ARG:HG3	1:G:246:SER:OG	2.21	0.41
1:H:158:GLU:OE2	1:H:159:LEU:HG	2.19	0.41
2:O:3:DA:C1'	2:O:4:DC:H5'	2.39	0.41
1:A:158:GLU:CD	1:A:159:LEU:N	2.69	0.41
1:A:215:ASN:HD22	1:A:215:ASN:N	2.18	0.41
1:B:159:LEU:O	1:B:160:LYS:C	2.58	0.41
1:C:209:GLU:HB2	1:C:222:PRO:O	2.20	0.41
1:D:215:ASN:HD22	1:D:215:ASN:N	2.16	0.41
1:E:318:ASP:O	1:E:321:ARG:N	2.53	0.41
1:F:295:VAL:HG22	1:F:296:LEU:N	2.36	0.41
1:G:213:GLU:O	1:G:214:PHE:CB	2.68	0.41
1:A:221:PRO:HB2	1:A:224:HIS:HD2	1.86	0.41
1:B:279:ARG:HB2	2:J:6:DT:OP1	2.21	0.41
1:C:187:ARG:HG3	1:C:246:SER:OG	2.21	0.41
1:C:191:VAL:HG11	1:C:285:ILE:HD11	2.01	0.41
1:C:224:HIS:HA	1:C:245:GLN:NE2	2.36	0.41
1:C:288:LEU:O	1:C:296:LEU:HB2	2.21	0.41
1:D:136:HIS:HB3	1:D:178:THR:O	2.20	0.41
1:D:187:ARG:HG3	1:D:246:SER:OG	2.21	0.41
1:E:201:VAL:HA	1:E:244:ARG:HH12	1.85	0.41
1:A:278:ASN:HA	1:A:279:ARG:HH12	1.86	0.41
1:C:210:LEU:CD1	1:D:206:PRO:HB3	2.51	0.41
1:E:215:ASN:HD22	1:E:215:ASN:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:PRO:HB2	1:E:224:HIS:HD2	1.86	0.41
1:E:304:ARG:HH11	1:E:304:ARG:HG3	1.85	0.41
1:A:290:THR:HG23	1:A:293:GLY:H	1.86	0.41
1:C:201:VAL:HA	1:C:244:ARG:HH12	1.86	0.41
1:D:191:VAL:HG11	1:D:285:ILE:HD11	2.01	0.41
1:E:187:ARG:HG3	1:E:246:SER:OG	2.20	0.41
1:F:255:GLN:O	1:F:256:VAL:C	2.59	0.41
1:G:226:ILE:HG12	1:G:267:PHE:CE2	2.56	0.41
1:G:295:VAL:HG22	1:G:297:GLY:H	1.86	0.41
1:H:158:GLU:CD	1:H:159:LEU:N	2.70	0.41
1:H:158:GLU:CD	1:H:158:GLU:N	2.74	0.41
2:K:3:DA:H1'	2:K:4:DC:H5'	2.02	0.41
2:K:6:DT:H1'	2:K:7:DG:C8	2.56	0.41
1:D:158:GLU:OE2	1:D:159:LEU:HG	2.21	0.41
1:D:163:TYR:N	1:D:163:TYR:HD1	2.19	0.41
1:H:215:ASN:HD22	1:H:215:ASN:N	2.19	0.41
1:H:255:GLN:O	1:H:256:VAL:C	2.60	0.41
2:N:3:DA:H1'	2:N:4:DC:H5'	2.03	0.41
1:A:239:ASP:OD1	1:A:240:PRO:HD2	2.21	0.40
1:A:304:ARG:HH11	1:A:304:ARG:HG3	1.87	0.40
1:B:255:GLN:O	1:B:256:VAL:C	2.59	0.40
1:B:295:VAL:HG22	1:B:296:LEU:N	2.36	0.40
1:B:304:ARG:HG3	1:B:304:ARG:HH11	1.86	0.40
1:C:166:ILE:CG2	1:C:167:ALA:H	2.34	0.40
1:D:288:LEU:O	1:D:296:LEU:HB2	2.20	0.40
1:E:264:LEU:N	1:E:264:LEU:CD1	2.83	0.40
1:F:187:ARG:HG3	1:F:246:SER:OG	2.20	0.40
1:G:163:TYR:N	1:G:163:TYR:HD1	2.19	0.40
1:G:183:GLY:HA3	1:G:291:ARG:HB2	2.03	0.40
2:N:6:DT:H2"	2:N:7:DG:C8	2.56	0.40
1:A:232:SER:HB2	1:D:232:SER:HB3	2.01	0.40
1:D:221:PRO:HB2	1:D:224:HIS:HD2	1.87	0.40
1:E:189:MET:HG3	1:E:190:PRO:HD2	2.02	0.40
1:F:278:ASN:HA	1:F:279:ARG:HH12	1.86	0.40
1:H:136:HIS:HB3	1:H:178:THR:O	2.21	0.40
1:H:226:ILE:HG12	1:H:267:PHE:CE2	2.56	0.40
1:B:279:ARG:CB	2:J:6:DT:OP1	2.69	0.40
1:D:166:ILE:CG2	1:D:167:ALA:H	2.35	0.40
1:E:192:TYR:OH	1:E:280:ARG:NH2	2.54	0.40
1:F:166:ILE:CG2	1:F:167:ALA:H	2.34	0.40
1:F:191:VAL:HG11	1:F:285:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:O	1:A:214:PHE:CB	2.69	0.40
1:B:264:LEU:N	1:B:264:LEU:CD1	2.83	0.40
1:C:290:THR:HB	1:C:296:LEU:CD2	2.42	0.40
1:E:159:LEU:O	1:E:160:LYS:C	2.59	0.40
1:E:255:GLN:O	1:E:256:VAL:C	2.60	0.40
1:H:308:CYS:O	1:H:310:GLY:N	2.54	0.40
1:D:159:LEU:O	1:D:160:LYS:C	2.59	0.40
1:E:158:GLU:OE2	1:E:159:LEU:HG	2.21	0.40
1:E:191:VAL:HG11	1:E:285:ILE:HD11	2.03	0.40
1:F:159:LEU:O	1:F:160:LYS:C	2.59	0.40
1:F:290:THR:HG23	1:F:293:GLY:H	1.87	0.40
1:G:158:GLU:CD	1:G:159:LEU:N	2.70	0.40
1:H:159:LEU:O	1:H:160:LYS:C	2.58	0.40
1:H:192:TYR:OH	1:H:280:ARG:NH2	2.55	0.40
1:H:290:THR:HG23	1:H:293:GLY:H	1.87	0.40
2:O:9:DT:H1'	2:O:10:DT:C5'	2.51	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ARG:NH1	1:E:239:ASP:OD1[2_555]	1.98	0.22
1:C:233:HIS:CE1	1:C:233:HIS:CE1[2_555]	2.02	0.18
1:H:132:TYR:OH	1:H:132:TYR:OH[2_455]	2.05	0.15
1:C:235:GLN:OE1	1:E:240:PRO:O[2_555]	2.07	0.13

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	188/203 (93%)	131 (70%)	39 (21%)	18 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	B	187/203 (92%)	131 (70%)	39 (21%)	17 (9%)	1	3	
1	C	193/203 (95%)	132 (68%)	43 (22%)	18 (9%)	0	3	
1	D	194/203 (96%)	134 (69%)	42 (22%)	18 (9%)	0	3	
1	E	195/203 (96%)	135 (69%)	42 (22%)	18 (9%)	1	3	
1	F	193/203 (95%)	133 (69%)	42 (22%)	18 (9%)	0	3	
1	G	186/203 (92%)	129 (69%)	40 (22%)	17 (9%)	1	3	
1	H	185/203 (91%)	130 (70%)	38 (20%)	17 (9%)	1	3	
All	All	1521/1624 (94%)	1055 (69%)	325 (21%)	141 (9%)	0	3	

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	A	166	ILE
1	A	172	ILE
1	A	256	VAL
1	A	272	SER
1	A	279	ARG
1	A	319	SER
1	B	166	ILE
1	B	172	ILE
1	B	181	PRO
1	B	256	VAL
1	B	272	SER
1	B	279	ARG
1	B	319	SER
1	C	148	ALA
1	C	166	ILE
1	C	172	ILE
1	C	256	VAL
1	C	272	SER
1	C	279	ARG
1	C	319	SER
1	D	148	ALA
1	D	166	ILE
1	D	172	ILE
1	D	256	VAL
1	D	272	SER
1	D	279	ARG
1	D	319	SER

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Mol	Chain	Res	Type
1	E	148	ALA
1	E	166	ILE
1	E	172	ILE
1	E	181	PRO
1	E	256	VAL
1	E	272	SER
1	E	279	ARG
1	E	319	SER
1	F	148	ALA
1	F	166	ILE
1	F	172	ILE
1	F	256	VAL
1	F	272	SER
1	F	279	ARG
1	F	319	SER
1	G	166	ILE
1	G	172	ILE
1	G	181	PRO
1	G	256	VAL
1	G	272	SER
1	G	279	ARG
1	G	319	SER
1	H	165	GLN
1	H	166	ILE
1	H	172	ILE
1	H	256	VAL
1	H	272	SER
1	H	279	ARG
1	H	319	SER
1	A	165	GLN
1	A	181	PRO
1	A	184	ALA
1	A	191	VAL
1	A	196	GLU
1	A	211	SER
1	B	165	GLN
1	B	184	ALA
1	B	191	VAL
1	B	196	GLU
1	B	211	SER
1	C	165	GLN
1	C	181	PRO

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Mol	Chain	Res	Type
1	C	184	ALA
1	C	196	GLU
1	C	211	SER
1	D	165	GLN
1	D	181	PRO
1	D	184	ALA
1	D	196	GLU
1	D	211	SER
1	E	165	GLN
1	E	184	ALA
1	E	191	VAL
1	E	196	GLU
1	E	211	SER
1	F	165	GLN
1	F	181	PRO
1	F	184	ALA
1	F	191	VAL
1	F	196	GLU
1	F	211	SER
1	G	165	GLN
1	G	184	ALA
1	G	191	VAL
1	G	196	GLU
1	G	211	SER
1	H	181	PRO
1	H	184	ALA
1	H	191	VAL
1	H	196	GLU
1	H	211	SER
1	A	210	LEU
1	A	318	ASP
1	B	210	LEU
1	B	318	ASP
1	C	191	VAL
1	C	210	LEU
1	C	318	ASP
1	D	191	VAL
1	D	210	LEU
1	E	210	LEU
1	E	318	ASP
1	F	210	LEU
1	G	210	LEU

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Mol	Chain	Res	Type
1	H	210	LEU
1	D	318	ASP
1	F	312	ASP
1	F	318	ASP
1	G	318	ASP
1	H	318	ASP
1	A	312	ASP
1	B	312	ASP
1	C	312	ASP
1	D	312	ASP
1	E	312	ASP
1	G	312	ASP
1	H	312	ASP
1	B	171	PRO
1	C	171	PRO
1	D	171	PRO
1	D	276	GLY
1	F	171	PRO
1	H	171	PRO
1	A	171	PRO
1	A	276	GLY
1	B	276	GLY
1	C	276	GLY
1	E	171	PRO
1	E	276	GLY
1	F	276	GLY
1	G	171	PRO
1	G	276	GLY
1	H	276	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	169/179 (94%)	148 (88%)	21 (12%)	4	21
1	B	170/179 (95%)	149 (88%)	21 (12%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	C	172/179 (96%)	150 (87%)	22 (13%)	4	20	
1	D	172/179 (96%)	151 (88%)	21 (12%)	5	22	
1	E	173/179 (97%)	150 (87%)	23 (13%)	4	18	
1	F	172/179 (96%)	150 (87%)	22 (13%)	4	20	
1	G	168/179 (94%)	146 (87%)	22 (13%)	4	19	
1	H	168/179 (94%)	146 (87%)	22 (13%)	4	19	
All	All	1364/1432 (95%)	1190 (87%)	174 (13%)	4	20	

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	GLU
1	A	163	TYR
1	A	164	CYS
1	A	176	VAL
1	A	177	MET
1	A	178	THR
1	A	182	GLN
1	A	202	VAL
1	A	204	ARG
1	A	212	ARG
1	A	216	GLU
1	A	249	VAL
1	A	259	GLU
1	A	269	CYS
1	A	279	ARG
1	A	282	ILE
1	A	283	LEU
1	A	287	THR
1	A	305	ILE
1	A	312	ASP
1	A	313	ARG
1	B	144	GLN
1	B	158	GLU
1	B	163	TYR
1	B	164	CYS
1	B	176	VAL
1	B	177	MET
1	B	178	THR
1	B	182	GLN

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Mol	Chain	Res	Type
1	B	202	VAL
1	B	204	ARG
1	B	212	ARG
1	B	216	GLU
1	B	259	GLU
1	B	269	CYS
1	B	279	ARG
1	B	282	ILE
1	B	283	LEU
1	B	287	THR
1	B	305	ILE
1	B	312	ASP
1	B	313	ARG
1	C	132	TYR
1	C	144	GLN
1	C	158	GLU
1	C	163	TYR
1	C	164	CYS
1	C	176	VAL
1	C	177	MET
1	C	178	THR
1	C	182	GLN
1	C	202	VAL
1	C	204	ARG
1	C	212	ARG
1	C	216	GLU
1	C	259	GLU
1	C	269	CYS
1	C	279	ARG
1	C	282	ILE
1	C	283	LEU
1	C	287	THR
1	C	305	ILE
1	C	312	ASP
1	C	313	ARG
1	D	144	GLN
1	D	158	GLU
1	D	163	TYR
1	D	164	CYS
1	D	176	VAL
1	D	177	MET
1	D	178	THR

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Mol	Chain	Res	Type
1	D	182	GLN
1	D	202	VAL
1	D	204	ARG
1	D	212	ARG
1	D	216	GLU
1	D	259	GLU
1	D	269	CYS
1	D	279	ARG
1	D	282	ILE
1	D	283	LEU
1	D	287	THR
1	D	305	ILE
1	D	312	ASP
1	D	313	ARG
1	E	132	TYR
1	E	144	GLN
1	E	158	GLU
1	E	163	TYR
1	E	164	CYS
1	E	176	VAL
1	E	177	MET
1	E	178	THR
1	E	182	GLN
1	E	202	VAL
1	E	204	ARG
1	E	212	ARG
1	E	216	GLU
1	E	249	VAL
1	E	259	GLU
1	E	269	CYS
1	E	279	ARG
1	E	282	ILE
1	E	283	LEU
1	E	287	THR
1	E	305	ILE
1	E	312	ASP
1	E	313	ARG
1	F	144	GLN
1	F	158	GLU
1	F	163	TYR
1	F	164	CYS
1	F	176	VAL

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Mol	Chain	Res	Type
1	F	177	MET
1	F	178	THR
1	F	182	GLN
1	F	202	VAL
1	F	204	ARG
1	F	212	ARG
1	F	216	GLU
1	F	249	VAL
1	F	259	GLU
1	F	269	CYS
1	F	279	ARG
1	F	282	ILE
1	F	283	LEU
1	F	287	THR
1	F	305	ILE
1	F	312	ASP
1	F	313	ARG
1	G	144	GLN
1	G	158	GLU
1	G	163	TYR
1	G	164	CYS
1	G	176	VAL
1	G	177	MET
1	G	178	THR
1	G	182	GLN
1	G	202	VAL
1	G	204	ARG
1	G	212	ARG
1	G	216	GLU
1	G	249	VAL
1	G	259	GLU
1	G	269	CYS
1	G	279	ARG
1	G	282	ILE
1	G	283	LEU
1	G	287	THR
1	G	305	ILE
1	G	312	ASP
1	G	313	ARG
1	H	144	GLN
1	H	158	GLU
1	H	163	TYR

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Mol	Chain	Res	Type
1	H	164	CYS
1	H	176	VAL
1	H	177	MET
1	H	178	THR
1	H	182	GLN
1	H	202	VAL
1	H	204	ARG
1	H	212	ARG
1	H	216	GLU
1	H	249	VAL
1	H	259	GLU
1	H	269	CYS
1	H	279	ARG
1	H	282	ILE
1	H	283	LEU
1	H	287	THR
1	H	305	ILE
1	H	312	ASP
1	H	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	215	ASN
1	A	218	GLN
1	A	224	HIS
1	A	266	ASN
1	A	278	ASN
1	B	207	ASN
1	B	215	ASN
1	B	218	GLN
1	B	224	HIS
1	B	266	ASN
1	B	278	ASN
1	C	207	ASN
1	C	215	ASN
1	C	218	GLN
1	C	224	HIS
1	C	255	GLN
1	C	266	ASN
1	C	278	ASN

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Mol	Chain	Res	Type
1	D	207	ASN
1	D	215	ASN
1	D	218	GLN
1	D	224	HIS
1	D	266	ASN
1	D	278	ASN
1	E	215	ASN
1	E	218	GLN
1	E	224	HIS
1	E	266	ASN
1	E	278	ASN
1	F	215	ASN
1	F	218	GLN
1	F	224	HIS
1	F	266	ASN
1	F	278	ASN
1	G	207	ASN
1	G	215	ASN
1	G	218	GLN
1	G	224	HIS
1	G	266	ASN
1	G	278	ASN
1	H	207	ASN
1	H	215	ASN
1	H	218	GLN
1	H	224	HIS
1	H	266	ASN
1	H	278	ASN

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 ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	192/203 (94%)	-0.01	7 (3%)	42	27	99, 154, 212, 235	0
1	B	191/203 (94%)	-0.04	7 (3%)	41	26	104, 156, 215, 247	0
1	C	195/203 (96%)	-0.19	0	100	100	66, 118, 175, 218	0
1	D	196/203 (96%)	-0.17	2 (1%)	82	72	83, 137, 204, 237	0
1	E	197/203 (97%)	-0.18	2 (1%)	82	72	76, 123, 197, 244	0
1	F	195/203 (96%)	-0.17	3 (1%)	73	61	81, 130, 193, 218	0
1	G	190/203 (93%)	-0.06	4 (2%)	63	49	90, 140, 202, 227	0
1	H	189/203 (93%)	-0.09	3 (1%)	72	59	81, 141, 196, 233	0
2	I	10/10 (100%)	-0.69	0	100	100	93, 112, 127, 128	0
2	J	10/10 (100%)	-0.63	0	100	100	97, 110, 118, 118	0
2	K	10/10 (100%)	-0.64	0	100	100	75, 100, 119, 120	0
2	L	10/10 (100%)	-0.52	0	100	100	89, 98, 114, 117	0
2	M	10/10 (100%)	-0.66	0	100	100	82, 94, 101, 111	0
2	N	10/10 (100%)	-0.60	0	100	100	79, 98, 120, 120	0
2	O	10/10 (100%)	-0.55	0	100	100	93, 104, 110, 115	0
2	P	10/10 (100%)	-0.57	0	100	100	79, 95, 112, 114	0
All	All	1625/1704 (95%)	-0.14	28 (1%)	70	57	66, 137, 205, 247	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	144	GLN	5.6
1	A	239	ASP	4.1
1	G	182	GLN	3.2
1	D	177	MET	3.0
1	A	240	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	292	ASP	2.8
1	A	147	THR	2.7
1	H	150	SER	2.7
1	F	238	GLU	2.7
1	A	238	GLU	2.7
1	H	238	GLU	2.7
1	F	292	ASP	2.7
1	G	292	ASP	2.6
1	D	148	ALA	2.5
1	H	218	GLN	2.5
1	F	138	PHE	2.5
1	A	218	GLN	2.4
1	G	229	GLU	2.4
1	A	243	GLY	2.3
1	E	148	ALA	2.2
1	B	159	LEU	2.2
1	B	218	GLN	2.2
1	E	151	ALA	2.2
1	A	150	SER	2.2
1	B	259	GLU	2.1
1	B	187	ARG	2.1
1	B	194	LYS	2.0
1	B	256	VAL	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 monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	901	1/1	0.92	0.22	116,116,116,116	0
3	ZN	B	901	1/1	0.96	0.17	132,132,132,132	0
3	ZN	E	901	1/1	0.97	0.20	126,126,126,126	0
3	ZN	G	901	1/1	0.97	0.19	140,140,140,140	0
3	ZN	F	901	1/1	0.98	0.17	112,112,112,112	0
3	ZN	A	901	1/1	0.98	0.15	155,155,155,155	0
3	ZN	H	901	1/1	0.99	0.20	140,140,140,140	0
3	ZN	C	901	1/1	1.00	0.15	99,99,99,99	0

6.5 Other polymers ⓘ

There are no such residues in this entry.