WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Feb 26, 2024 – 03:26 PM EST

PDB ID	:	8G9S
EMDB ID	:	EMD-29877
Title	:	Exploiting Activation and Inactivation Mechanisms in Type I-C CRISPR-Cas3 for Genome Editing Applications
Authors	:	Hu, C.; Nam, K.H.; Ke, A.
Deposited on	:	2023-02-22
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

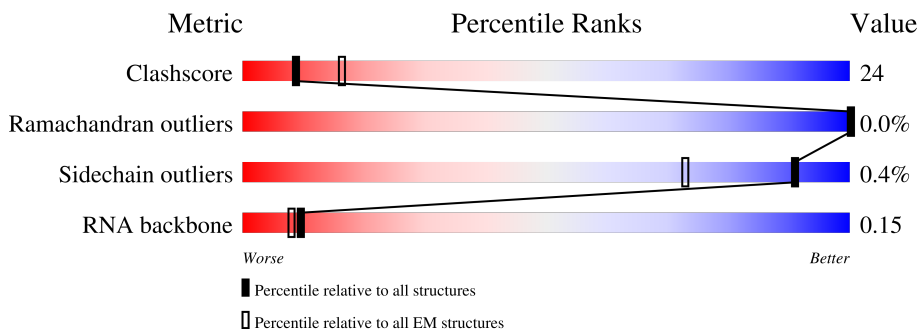|		
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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
Clashscore		24
Ramachandran outliers		0.0%
Sidechain outliers		0.4%
RNA backbone		0.15

Worse   *Better*

▌ Percentile relative to all structures
▯ Percentile relative to all EM structures
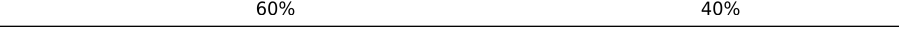
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	283	55% 45%
1	C	283	58% 42% •
1	D	283	60% 40%
1	E	283	53% 47%
1	F	283	46% 47% 6%
1	G	283	47% 49% •
1	M	283	53% 40% 7%

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Mol	Chain	Length	Quality of chain
2	H	124	49% 50%
2	I	124	52% 47%
2	J	124	52% 48%
2	L	124	19% 60% 31% 8%
3	N	205	49% 51%
4	O	42	7% 40% 52%
5	K	409	60% 40%
6	A	70	50% 49%

2   Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 25758 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Cas7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
1	C	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
1	D	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
1	E	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
1	F	265	Total	C	N	O	S	0	0
			2124	1331	379	404	10		
1	G	271	Total	C	N	O	S	0	0
			2173	1360	391	411	11		
1	M	264	Total	C	N	O	S	0	0
			2110	1318	379	402	11		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	284	GLY	-	expression tag	UNP A0A378VEU0
C	284	GLY	-	expression tag	UNP A0A378VEU0
D	284	GLY	-	expression tag	UNP A0A378VEU0
E	284	GLY	-	expression tag	UNP A0A378VEU0
F	284	GLY	-	expression tag	UNP A0A378VEU0
G	284	GLY	-	expression tag	UNP A0A378VEU0
M	284	GLY	-	expression tag	UNP A0A378VEU0

- Molecule 2 is a protein called Cas11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		
2	I	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		
2	L	114	Total	C	N	O	S	0	0
			917	588	163	165	1		

- Molecule 3 is a protein called Cas5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	205	Total	C	N	O	S	0	0
			1673	1067	289	305	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	32	ALA	SER	conflict	UNP D0W8X4

- Molecule 4 is a RNA chain called RNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	42	Total	C	N	O	P	0	0
			895	399	158	296	42		

- Molecule 5 is a protein called Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	409	Total	C	N	O	S	0	0
			3223	2056	569	586	12		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	MET	-	initiating methionine	UNP A0A378VF47
K	2	ILE	-	expression tag	UNP A0A378VF47
K	3	LEU	-	expression tag	UNP A0A378VF47
K	4	HIS	-	expression tag	UNP A0A378VF47
K	5	ALA	-	expression tag	UNP A0A378VF47
K	6	LEU	VAL	conflict	UNP A0A378VF47
K	7	THR	SER	conflict	UNP A0A378VF47
K	9	TYR	ALA	conflict	UNP A0A378VF47
K	10	TYR	ASN	conflict	UNP A0A378VF47
K	12	ARG	THR	conflict	UNP A0A378VF47

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Chain	Residue	Modelled	Actual	Comment	Reference
K	13	LYS	GLN	conflict	UNP A0A378VF47
K	14	ALA	SER	conflict	UNP A0A378VF47
K	15	GLU	ASP	conflict	UNP A0A378VF47
K	16	SER	ASN	conflict	UNP A0A378VF47
K	190	ALA	VAL	conflict	UNP A0A378VF47
K	239	ALA	ILE	conflict	UNP A0A378VF47
K	242	ILE	VAL	conflict	UNP A0A378VF47
K	260	GLY	SER	conflict	UNP A0A378VF47
K	271	THR	ALA	conflict	UNP A0A378VF47

- Molecule 6 is a protein called AcrIC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	70	578	367	102	108	1	0	0

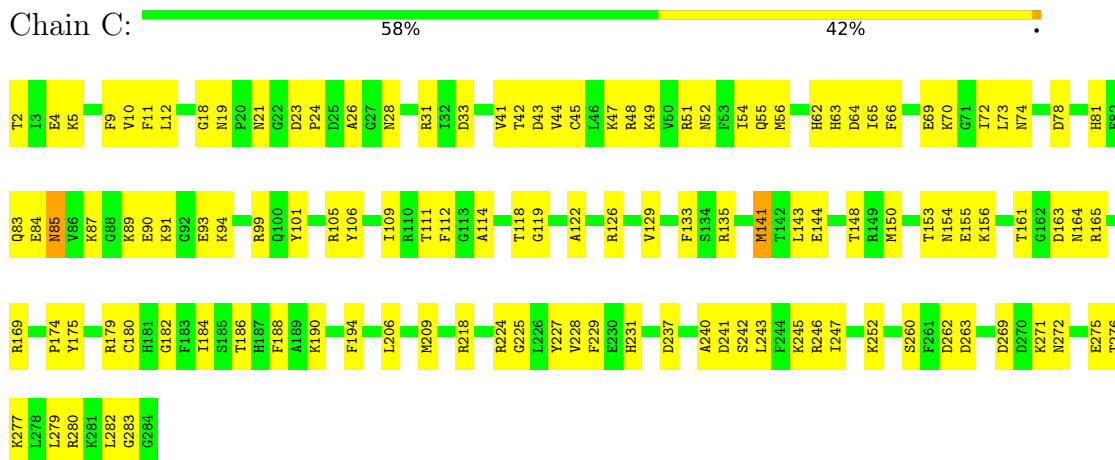# 3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.
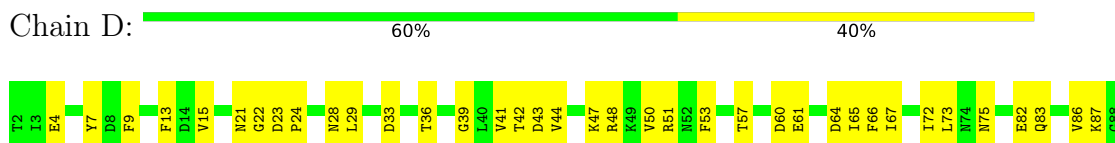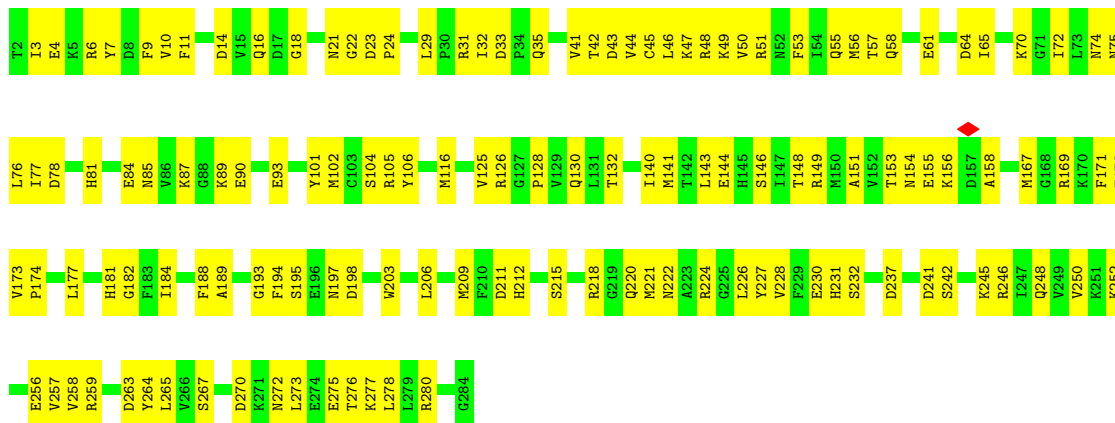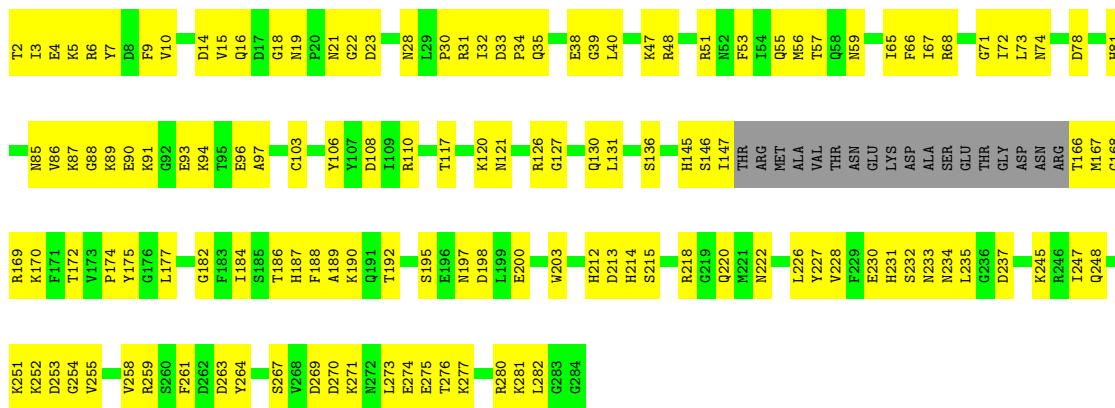
- Molecule 1: Cas7

Chain B:

- Molecule 1: Cas7

Chain C:

- Molecule 1: Cas7

Chain D:

K89 E90 K91 G92 E93 K94 R99 Q100 Y101 S104 R105 Y106 Y107 D108 I109 R110 T111 M116 N121 A122 V129 T132 F133 S136 M141 S146 R149 M150 T153 N154 E155 K156 D157 A158 T161 G162 R165 Y175 G176 H181 G182 F183 I184 H187

F194 L206 M209 H212 S215 R218 M221 N222 A223 R224 V228 F229 E230 H231 S232 D237 S242 L243 R246 V249 K252 D253 G254 V255 E256 V257 V258 R259 D263 V266 D269 D270 K271 N272 L273 E274 E275 T276 K277 L278 L279 R280 K281 L282

G283 G284

• Molecule 1: Cas7

Chain E: 53% 47%

T2 I3 E4 K5 R6 Y7 D8 F9 V10 F11 D14 V15 Q16 D17 G18 N21 G22 D23 P24 L29 P30 R31 I32 D33 P34 Q35 V41 T42 D43 V44 C45 L46 K47 R48 K49 V50 R51 N52 F53 I54 Q55 M56 T57 Q58 E61 D64 I65 K70 G71 I72 L73 N74 N75

L76 I77 D78 H81 E84 N85 V86 K87 G88 K89 E90 E93 Y101 M102 C103 S104 R105 Y106 M116 V125 R126 G127 P128 V129 Q130 L131 T132 I140 M141 T142 L143 E144 H145 S146 I147 T148 R149 M150 A151 V152 T153 N154 E155 K156 D157 A158 M167 G168 R169 K170 F171 T172 ◆

V173 P174 L177 H181 G182 F183 I184 F188 A189 G193 F194 S195 E196 N197 D198 W203 L206 M209 F210 D211 H212 S215 R218 G219 Q220 M221 N222 A223 R224 G225 L226 Y227 V228 F229 E230 H231 S232 D237 D241 S242 K245 R246 I247 Q248 V249 V250 K251 K252

E256 V257 V258 R259 D263 Y264 L265 V266 S267 D270 K271 N272 L273 E274 E275 T276 K277 L278 L279 R280 G284

• Molecule 1: Cas7

Chain F: 46% 47% 6%

T2 I3 E4 K5 R6 Y7 D8 F9 V10 D14 V15 Q16 D17 G18 N19 P20 N21 G22 D23 N28 L29 P30 R31 I32 D33 P34 Q35 E38 G39 L40 K47 R48 R51 N52 F53 I54 Q55 M56 T57 Q58 N59 I65 F66 I67 R68 G71 I72 L73 N74 D78 H81

N85 V86 K87 G88 K89 E90 K91 G92 E93 K94 T95 E96 A97 C103 Y106 Y107 D108 I109 R110 T117 K120 N121 R126 G127 Q130 L131 S136 H145 S146 I147 THR ARG MET ALA VAL THR ASN GLU LYS ASP ALA SER GLU THR GLY ASP ASN ARG T166 M167 G168

R169 K170 F171 T172 V173 P174 Y175 G176 L177 G182 F183 I184 S185 T186 H187 F188 A189 K190 Q191 T192 S195 E196 N197 D198 L199 E200 W203 H212 D213 H214 S215 R218 G219 Q220 M221 N222 L226 Y227 V228 F229 E230 H231 S232 N233 N234 L235 G236 D237 K245 R246 I247 Q248

K251 K252 D253 G254 V255 V258 R259 S260 F261 D262 D263 Y264 S267 V268 D269 D270 K271 N272 L273 E274 E275 T276 K277 R280 K281 L282 G283 G284

• Molecule 1: Cas7

Chain G: 47% 49% •

T2 I3 E4 K5 R6 Y7 D8 F9 V10 F11 L12 F13 Q16 D17 N21 P24 G27 N28 L29 P30 R31 I32 D33 T36 G37 E38 G39 L40 V41 T42 D43 V44 C45 L46 K47 R48 R51 Q55 N59 D60 E61 H62 H63 D64 I65 F66 I67 R68 E69 K70 N74

• Molecule 1: Cas7

Chain M: 53%   40%   7%

• Molecule 2: Cas11

Chain H: 49%   50%

• Molecule 2: Cas11

Chain I: 52%   47%

• Molecule 2: Cas11

Chain J: 52%   48%

G2 L3 D4 R5 N6 R7 I10 G11 Y12 V13 L14 L17 F18 A19 V20 L21 E22 K23 I24 Q25 A26 E27 A28 N29 L32 N33 A34 A37 F41 A50 V51 F52 G53 T54 L55 M56 R57 L58 L59 P60 H61 H62 L63 N64 K65 E69 Q74 W77 E78 I79 R80

Q81 I82 L83 E84 H85 C86 Q87 P90 L93 E96 Q97 Q98 Q99 L100 I103 G104 Y105 Y106 H107 Q110 F111 L112 F113 T114 L121 F122 A125

• Molecule 2: Cas11

Chain L:

19%
60% 31% • 8%

G2 L3 D4 R7 Q8 D9 I10 G11 Y12 V13 L14 G15 R16 L17 F18 A19 V20 L21 E22 K23 I24 Q25 A26 E27 A28 N29 P30 G31 L32 N33 A34 T35 I36 A37 D38 R39 Y40 F41 A44 I49 A50 V51 F52 L55 M56 L59 P60 L66 GLU PHE E69 G70 R71 A72

V73 Q74 W77 E78 I79 H85 CYS GLN ARG PHE PRO ASN HIS LEU N94 L95 E96 F101 A102 I103 Y106 H107 E108 T109 Q110 F111 L112 F113 T114 K115 L118 K119 N120 L121 F122 N123 E124 A125

• Molecule 3: Cas5

Chain N:

49% 51%

R2 F3 I4 L5 E6 D10 F14 T15 R16 S17 E18 L19 K20 V21 E22 R23 V24 S25 Y26 I29 T30 P31 A32 A33 A34 R35 N36 I37 L38 M39 A40 I41 L42 W43 K44 W49 K50 V51 L52 K53 I54 E55 I56 L57 N64 I65 R66 R67 N68 E69 V70 K73 M74

S80 L81 E84 D85 N86 R87 Q88 Q89 R90 A91 S92 M93 D97 V98 A99 Y100 R101 I102 H103 N117 K120 F121 A122 E123 M124 F125 K126 R127 R128 Q133 Y134 F135 H136 Q137 P138 Y139 R143 E144 F145 P146 F149 R150 E153 P160 L161 E162 D163 I164 T165 Q166 D167

L172 Y173 D174 M175 D176 F177 S178 K179 S180 D181 P182 R183 D184 S185 N186 N187 A188 E189 P190 M191 F192 Y193 Q194 C195 K196 N199 G200 V201 I202 T203 P206

• Molecule 4: RNA (42-MER)

Chain O:

7% 40% 52%

A1 U2 U3 G4 A5 A6 A7 C8 A9 G10 G11 G12 U13 C14 A15 G16 C17 U18 U19 G20 C21 C22 G23 U24 A25 C26 G27 U28 C31 A32 U33 C34 G35 C36 C37 C38 U39 C40 G41 U42

• Molecule 5: Cas8

Chain K:

60% 40%

M1 T7 Q8 Y9 Y10 Q11 R12 K13 I194 C195 R206 N209 A210 V211 K212 G213 V214 P218 A219 P220 V224 N225 L226 S227 A228 F229 E230 S231 Y232 Q236 F240 G243 A246 M247 F248 E249 Y250 T251 L257 L258 E261 N262 R263 F264 R265 I266 T270

C273 R278 T279 E282 L285 A286 S287 M288 I289 G292 G293 K294 D295 K296 P297 D302 A303 V304 K305 T306 L307 S310 N313 G314 Q315 Y316 Q317 K318 G321 K324 F325 Y326 L327 P332 N333 V338 F341 W342 H343 E344 T345 T346 V347 A348 A349 L350 S351

E352 S353 I354 W357 L361 G362 M363 V364 R365 G366 E367 E373 N383 L384 V385 L386 K389 M390 L393 D396 L397 Q400 D403 A404 A405 L406 N407 N408 R409 L416 Q417 A418 R421 R422 N423 K424 A425 E426 Q427 R433 Y440 R443 A444 I445 R446

L450 R464 Q465 D466 Y469 L478 I481 Q482 A483 N486 P487 G488 L489 R496 Y497 S500 S503 I506 A507 V508 T511 L512 L516 P517 H518 H519 L520 N521 K522 L523 E524 F525 A529 Q533 W534 E535 I536 R537 Q538 I539 H542 C543 Q544 R545 F546 P547

N551 L552 E553 Q554 H564 L569 F570 N577 L578 E581 A582

• Molecule 6: AcrIC8

Chain A:

50%　　　　　　　　　　　49%　　　　•

S5 M6 Y7 A8 I9 R10 K11 I12 F15 Y16 G17 P18 T19 D20 S23 Y24 E27 E28 A29 G30 G31 R32 L35 A42 R45 I46 E47 D48 L49 E50 E51 G52 V53 N59 E60 S61 G62 R63 P64 D65 Y66 K67 W70 V71 R72 G73 E74

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	67000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.085	Depositor
Minimum map value	-0.631	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.118	Depositor
Map size (Å)	353.1, 353.1, 353.1	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4124, 1.4124, 1.4124	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	B	0.49	0/2303	0.53	0/3101
1	C	0.52	0/2303	0.54	0/3101
1	D	0.48	0/2303	0.55	0/3101
1	E	0.44	0/2303	0.52	0/3101
1	F	0.36	0/2165	0.49	0/2914
1	G	0.29	0/2214	0.48	0/2979
1	M	0.43	0/2150	0.54	0/2896
2	H	0.34	0/1030	0.52	0/1392
2	I	0.37	0/1030	0.47	0/1392
2	J	0.36	0/1030	0.50	0/1392
2	L	0.29	0/934	0.46	0/1259
3	N	0.39	0/1711	0.52	0/2306
4	O	0.98	0/999	1.08	0/1555
5	K	0.38	0/3290	0.51	0/4450
6	A	0.35	0/591	0.52	0/792
All	All	0.45	0/26356	0.55	0/35731

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2261	0	2193	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2261	0	2193	103	0
1	D	2261	0	2193	116	0
1	E	2261	0	2193	122	0
1	F	2124	0	2064	116	0
1	G	2173	0	2120	131	0
1	M	2110	0	2050	110	0
2	H	1007	0	992	59	0
2	I	1007	0	992	50	0
2	J	1007	0	992	51	0
2	L	917	0	909	35	0
3	N	1673	0	1663	110	0
4	O	895	0	453	76	0
5	K	3223	0	3241	126	0
6	A	578	0	557	36	0
All	All	25758	0	24805	1189	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1189) 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)
6:A:11:LYS:HB3	6:A:23:SER:O	1.42	1.16
2:H:16:ARG:HG3	2:H:108:GLU:HG3	1.45	0.96
2:H:95:LEU:HD21	2:I:53:GLY:HA3	1.50	0.93
1:M:165:ARG:HD3	6:A:53:VAL:HG22	1.51	0.92
1:M:56:MET:SD	1:M:212:HIS:ND1	2.45	0.89
1:B:44:VAL:HG21	1:M:147:ILE:HD11	1.54	0.89
3:N:167:ASP:HA	3:N:196:LYS:HB3	1.56	0.88
1:D:141:MET:SD	1:E:35:GLN:NE2	2.48	0.86
1:B:51:ARG:NH2	4:O:13:U:OP1	2.09	0.86
1:M:45:CYS:SG	1:M:49:LYS:NZ	2.49	0.85
1:E:51:ARG:NH2	4:O:31:C:OP1	2.09	0.84
2:L:71:ARG:HA	2:L:74:GLN:HE21	1.42	0.83
5:K:424:LYS:O	5:K:427:GLN:NE2	2.12	0.83
1:E:56:MET:SD	1:E:212:HIS:ND1	2.52	0.81
1:E:222:ASN:HB2	1:E:224:ARG:HH22	1.45	0.81
1:F:55:GLN:HB2	1:F:65:ILE:HG13	1.64	0.80
1:G:5:LYS:HG2	1:G:232:SER:HA	1.63	0.80
1:D:22:GLY:HA3	4:O:27:G:H3'	1.61	0.80
1:M:48:ARG:NH2	4:O:8:C:OP2	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PHE:HB3	1:C:180:CYS:HB3	1.63	0.79
1:F:56:MET:SD	1:G:187:HIS:ND1	2.56	0.79
1:G:48:ARG:HH21	1:G:69:GLU:HB3	1.46	0.78
1:M:6:ARG:HH11	1:M:231:HIS:HE1	1.30	0.78
2:H:80:ARG:NH2	2:L:106:TYR:HB3	1.99	0.78
1:B:110:ARG:NH2	1:B:198:ASP:OD2	2.15	0.78
1:M:230:GLU:HB2	1:M:280:ARG:HH12	1.45	0.78
3:N:87:ARG:NH2	4:O:8:C:N3	2.30	0.78
5:K:324:LYS:HA	5:K:346:THR:HA	1.64	0.77
1:M:226:LEU:H	1:M:283:GLY:HA3	1.49	0.77
1:D:161:THR:HA	1:E:70:LYS:HE2	1.66	0.77
1:C:126:ARG:HG2	4:O:17:C:H4'	1.66	0.76
1:M:195:SER:OG	1:M:197:ASN:OD1	2.04	0.76
1:D:224:ARG:NH2	1:E:241:ASP:OD2	2.19	0.76
1:D:259:ARG:NH1	1:E:33:ASP:OD2	2.18	0.76
1:E:258:VAL:HG23	1:E:263:ASP:HB2	1.67	0.76
1:E:89:LYS:HD3	1:E:90:GLU:H	1.49	0.75
1:D:156:LYS:HG3	1:D:158:ALA:H	1.51	0.75
1:C:275:GLU:HG2	1:C:276:THR:HG23	1.69	0.75
5:K:288:MET:HA	5:K:292:GLY:HA3	1.66	0.75
1:B:241:ASP:HB2	1:M:222:ASN:HD21	1.52	0.75
1:F:227:TYR:HD2	1:F:247:ILE:HD13	1.49	0.75
1:G:90:GLU:O	1:G:94:LYS:N	2.20	0.75
1:M:246:ARG:HH12	1:M:273:LEU:H	1.35	0.75
1:G:96:GLU:O	1:G:100:GLN:NE2	2.20	0.75
1:E:75:ASN:OD1	1:E:76:LEU:N	2.21	0.74
1:D:146:SER:O	1:E:31:ARG:NH2	2.19	0.74
2:H:80:ARG:HH22	2:H:83:LEU:HD12	1.52	0.74
2:I:2:GLY:N	2:J:84:GLU:OE2	2.20	0.74
6:A:6:MET:HB3	6:A:35:LEU:HD22	1.68	0.74
1:F:213:ASP:HB3	1:F:218:ARG:HH22	1.52	0.74
1:M:6:ARG:HH11	1:M:231:HIS:CE1	2.05	0.74
1:G:146:SER:HB2	1:G:169:ARG:HG3	1.69	0.73
1:G:33:ASP:HB3	1:G:37:GLY:H	1.53	0.73
1:M:213:ASP:HB3	1:M:218:ARG:HH12	1.51	0.73
1:G:21:ASN:HA	1:G:218:ARG:HH21	1.53	0.73
1:F:255:VAL:HG21	1:F:263:ASP:HB3	1.71	0.73
1:M:163:ASP:OD1	1:M:165:ARG:NH2	2.22	0.72
3:N:34:ALA:HA	3:N:37:ILE:HD12	1.71	0.72
1:B:218:ARG:NH2	4:O:16:G:OP1	2.21	0.72
1:M:230:GLU:HB3	1:M:280:ARG:HH22	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:ASN:HB2	1:D:41:VAL:HG23	1.70	0.72
5:K:263:ARG:HH21	5:K:265:ARG:HG3	1.54	0.71
1:M:64:ASP:HB3	1:M:106:TYR:HD1	1.54	0.71
1:D:21:ASN:OD1	1:D:22:GLY:N	2.23	0.71
6:A:11:LYS:CB	6:A:23:SER:O	2.33	0.71
1:F:89:LYS:HZ2	1:F:96:GLU:HB3	1.54	0.71
2:H:29:ASN:HB3	2:H:32:LEU:HB2	1.71	0.71
1:F:91:LYS:HA	1:F:94:LYS:HB3	1.72	0.71
3:N:18:GLU:HA	5:K:240:PHE:HD1	1.54	0.71
1:G:67:ILE:HD12	1:G:70:LYS:HB2	1.72	0.71
1:C:45:CYS:SG	1:C:49:LYS:NZ	2.64	0.70
1:E:189:ALA:O	1:E:193:GLY:N	2.24	0.70
1:B:237:ASP:OD1	1:B:276:THR:OG1	2.09	0.70
5:K:464:ARG:NH1	5:K:466:ASP:OD2	2.24	0.70
3:N:149:PHE:O	3:N:150:ARG:NH2	2.22	0.70
1:M:249:VAL:HG22	1:M:266:VAL:HG12	1.73	0.70
3:N:139:TYR:CZ	3:N:143:ARG:HG2	2.26	0.70
5:K:365:ARG:HH21	5:K:373:GLU:HB3	1.56	0.70
1:D:242:SER:O	1:D:246:ARG:NH2	2.24	0.70
1:F:146:SER:OG	1:F:169:ARG:NH2	2.24	0.70
3:N:20:LYS:NZ	4:O:3:U:O2'	2.24	0.70
2:J:32:LEU:HG	2:J:34:ALA:H	1.57	0.70
2:H:80:ARG:HA	2:H:80:ARG:CZ	2.22	0.70
3:N:36:ASN:ND2	4:O:2:U:OP2	2.23	0.69
1:C:161:THR:OG1	1:C:163:ASP:OD1	2.10	0.69
1:M:237:ASP:OD2	1:M:276:THR:OG1	2.10	0.69
3:N:162:GLU:HG3	3:N:199:ASN:HD22	1.57	0.69
3:N:173:TYR:HB2	3:N:192:PHE:HD1	1.57	0.69
5:K:265:ARG:NH2	6:A:29:ALA:O	2.24	0.69
2:H:94:ASN:H	2:H:97:GLN:NE2	1.90	0.69
1:C:85:ASN:O	1:C:94:LYS:NZ	2.22	0.69
2:J:110:GLN:HA	5:K:537:ARG:HH21	1.58	0.69
2:I:12:TYR:OH	2:I:107:HIS:ND1	2.16	0.69
1:M:4:GLU:O	1:M:234:ASN:ND2	2.26	0.69
6:A:45:ARG:HD3	6:A:49:LEU:HD23	1.75	0.69
1:G:36:THR:HG22	1:G:139:PRO:HG3	1.75	0.69
3:N:5:LEU:HD11	3:N:149:PHE:HB2	1.75	0.69
1:B:146:SER:O	1:C:31:ARG:NH2	2.26	0.68
2:H:93:LEU:O	2:H:98:GLN:NE2	2.25	0.68
1:F:51:ARG:NH2	4:O:37:C:OP1	2.22	0.68
2:I:60:PRO:O	2:I:64:ASN:ND2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ARG:HH11	1:D:282:LEU:HD21	1.59	0.68
1:F:38:GLU:OE1	1:F:136:SER:OG	2.11	0.68
1:G:128:PRO:HD3	1:G:192:THR:HG21	1.76	0.68
1:G:108:ASP:O	1:G:112:PHE:N	2.20	0.68
1:E:22:GLY:N	4:O:34:C:OP2	2.27	0.67
5:K:206:ARG:NH1	5:K:236:GLN:OE1	2.27	0.67
1:D:33:ASP:OD2	1:D:36:THR:N	2.21	0.67
1:F:195:SER:OG	1:F:197:ASN:OD1	2.11	0.67
1:B:246:ARG:HB3	1:B:269:ASP:HB3	1.76	0.67
1:C:144:GLU:OE2	1:C:169:ARG:NH2	2.26	0.67
5:K:445:ILE:HG22	5:K:450:LEU:HB3	1.77	0.67
1:D:89:LYS:HE2	1:D:93:GLU:HB3	1.77	0.67
1:D:90:GLU:H	1:D:93:GLU:HB2	1.60	0.67
1:F:230:GLU:O	1:F:277:LYS:HA	1.93	0.67
1:D:86:VAL:O	1:D:94:LYS:NZ	2.25	0.67
3:N:124:MET:HA	3:N:127:ARG:HE	1.61	0.66
1:C:74:ASN:ND2	1:C:118:THR:OG1	2.29	0.66
1:F:220:GLN:NE2	1:F:222:ASN:OD1	2.27	0.66
1:B:101:TYR:O	1:B:104:SER:OG	2.11	0.66
1:B:149:ARG:HG2	1:B:151:ALA:H	1.61	0.66
1:C:10:VAL:HG11	1:C:247:ILE:HD13	1.78	0.66
1:F:147:ILE:HG21	1:G:42:THR:HG21	1.78	0.66
5:K:486:ASN:ND2	5:K:488:GLY:O	2.29	0.66
5:K:553:GLU:OE1	5:K:553:GLU:N	2.27	0.66
1:B:48:ARG:HH21	1:M:150:MET:HG3	1.60	0.66
1:B:84:GLU:OE2	1:B:84:GLU:N	2.28	0.66
1:C:161:THR:H	1:C:164:ASN:HB2	1.61	0.66
1:E:14:ASP:HB3	1:E:177:LEU:HD23	1.76	0.66
6:A:72:ARG:NH1	6:A:73:GLY:O	2.29	0.66
1:C:5:LYS:O	1:C:186:THR:OG1	2.13	0.66
1:E:232:SER:H	1:E:277:LYS:HZ3	1.43	0.66
1:E:89:LYS:HD3	1:E:90:GLU:N	2.10	0.65
1:E:74:ASN:HA	1:E:77:ILE:HG12	1.79	0.65
1:C:246:ARG:HH22	1:C:271:LYS:HG2	1.61	0.65
1:F:89:LYS:HB3	1:F:93:GLU:HB2	1.77	0.65
1:D:230:GLU:HG2	1:D:278:LEU:HB2	1.77	0.65
1:B:33:ASP:OD1	1:B:36:THR:N	2.30	0.65
1:C:62:HIS:O	1:C:63:HIS:ND1	2.30	0.65
1:M:124:GLN:OE1	4:O:4:G:N2	2.30	0.65
1:C:23:ASP:OD2	1:C:26:ALA:N	2.27	0.65
1:G:252:LYS:HA	1:G:265:LEU:HD22	1.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:NH1	1:B:52:ASN:OD1	2.31	0.64
1:G:82:GLU:HA	1:G:86:VAL:HG22	1.78	0.64
2:I:93:LEU:HD12	2:I:97:GLN:HB3	1.79	0.64
1:B:51:ARG:NE	1:B:108:ASP:OD1	2.30	0.64
1:D:232:SER:HB3	1:D:276:THR:HB	1.79	0.64
1:F:237:ASP:HB2	1:F:277:LYS:HZ3	1.62	0.64
1:F:227:TYR:HE1	1:F:281:LYS:HE2	1.62	0.64
6:A:6:MET:O	6:A:71:VAL:N	2.29	0.64
1:F:89:LYS:NZ	1:F:96:GLU:OE1	2.30	0.64
1:G:6:ARG:HG2	1:G:186:THR:H	1.62	0.64
1:B:229:PHE:HE1	1:B:279:LEU:HD12	1.61	0.64
5:K:390:MET:SD	5:K:390:MET:N	2.70	0.64
1:M:51:ARG:NE	1:M:108:ASP:OD1	2.31	0.63
5:K:302:ASP:OD1	5:K:305:LYS:NZ	2.30	0.63
1:E:156:LYS:HG3	1:E:158:ALA:H	1.64	0.63
1:M:106:TYR:HB2	1:M:109:ILE:HG22	1.81	0.63
1:G:9:PHE:HB3	1:G:228:VAL:HG12	1.79	0.63
3:N:20:LYS:HE2	5:K:231:SER:HB2	1.79	0.63
1:D:106:TYR:O	1:D:110:ARG:NH2	2.32	0.63
1:C:21:ASN:OD1	1:C:31:ARG:NH1	2.31	0.63
1:D:60:ASP:OD1	1:D:61:GLU:N	2.32	0.63
1:E:49:LYS:HB3	1:E:209:MET:HE2	1.80	0.63
1:G:200:GLU:O	1:G:204:GLN:NE2	2.31	0.63
3:N:68:ASN:HB3	3:N:87:ARG:HD2	1.81	0.63
1:D:23:ASP:HB3	1:D:28:ASN:HA	1.81	0.63
1:F:166:THR:HA	1:F:169:ARG:HH12	1.63	0.63
1:G:102:MET:HB3	1:G:109:ILE:HG21	1.81	0.63
5:K:325:PHE:N	5:K:345:THR:O	2.30	0.63
1:E:230:GLU:HB3	1:E:278:LEU:HB2	1.80	0.63
2:I:57:ARG:HA	2:I:57:ARG:CZ	2.28	0.63
2:L:23:LYS:HZ2	2:L:112:LEU:HD13	1.64	0.63
1:F:3:ILE:HG22	1:F:5:LYS:H	1.64	0.62
1:C:165:ARG:NH2	4:O:26:G:N7	2.46	0.62
2:J:56:MET:HA	2:J:59:LEU:HD23	1.81	0.62
2:H:79:ILE:O	2:H:83:LEU:HG	1.99	0.62
1:C:48:ARG:O	1:C:52:ASN:ND2	2.32	0.62
2:I:7:ARG:HH12	2:J:87:GLN:HB3	1.64	0.62
1:M:142:THR:OG1	5:K:421:ARG:NH2	2.32	0.62
1:E:43:ASP:OD1	1:E:44:VAL:N	2.33	0.62
3:N:162:GLU:HA	3:N:199:ASN:HB2	1.82	0.62
5:K:310:SER:O	5:K:318:LYS:NZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:ASN:O	1:G:94:LYS:NZ	2.33	0.62
2:H:105:TYR:O	2:H:109:THR:HG23	1.98	0.61
1:E:81:HIS:O	1:E:85:ASN:N	2.32	0.61
3:N:177:PHE:CZ	4:O:1:A:H8	2.18	0.61
5:K:517:PRO:HA	5:K:520:LEU:HD12	1.82	0.61
1:D:162:GLY:O	1:D:165:ARG:NH2	2.33	0.61
1:M:48:ARG:HH21	4:O:8:C:P	2.22	0.61
1:G:4:GLU:HG2	1:G:5:LYS:HG3	1.81	0.61
5:K:341:PHE:HB2	5:K:343:HIS:HE1	1.65	0.61
1:F:32:ILE:HA	1:F:39:GLY:HA2	1.83	0.61
1:F:33:ASP:N	1:F:38:GLU:O	2.27	0.61
2:I:61:HIS:HA	2:I:64:ASN:HD21	1.65	0.61
2:J:79:ILE:HA	2:J:82:ILE:HG22	1.83	0.61
1:C:9:PHE:CZ	1:C:182:GLY:HA3	2.36	0.60
1:G:55:GLN:HB2	1:G:65:ILE:HG21	1.84	0.60
1:M:64:ASP:OD1	1:M:65:ILE:N	2.31	0.60
2:L:74:GLN:HA	2:L:77:TRP:HE3	1.64	0.60
1:M:154:ASN:HB2	1:M:156:LYS:HG2	1.82	0.60
3:N:86:ASN:O	3:N:88:GLN:NE2	2.30	0.60
5:K:273:CYS:HB2	5:K:325:PHE:HE2	1.64	0.60
1:C:99:ARG:HG3	1:C:122:ALA:O	2.02	0.60
1:D:259:ARG:N	1:D:263:ASP:OD2	2.22	0.60
1:E:146:SER:O	1:F:31:ARG:NH2	2.35	0.60
1:M:253:ASP:OD1	1:M:254:GLY:N	2.35	0.60
1:D:43:ASP:OD1	1:D:44:VAL:N	2.34	0.60
2:J:20:VAL:HG22	2:J:112:LEU:HD11	1.83	0.60
1:F:231:HIS:CD2	1:F:277:LYS:HE3	2.37	0.60
2:I:48:PRO:O	2:I:52:PHE:HB2	2.02	0.60
1:M:51:ARG:NH1	4:O:7:A:OP1	2.30	0.60
2:I:42:GLY:O	2:J:57:ARG:NH2	2.34	0.60
5:K:224:VAL:HG13	5:K:229:PHE:HB2	1.83	0.60
1:C:83:GLN:HG3	1:C:84:GLU:H	1.66	0.59
1:C:154:ASN:HD22	1:C:156:LYS:HE2	1.66	0.59
1:D:253:ASP:OD1	1:D:254:GLY:N	2.33	0.59
4:O:14:C:H5	4:O:16:G:HO2'	1.49	0.59
2:I:110:GLN:HA	2:J:80:ARG:NH2	2.16	0.59
1:B:280:ARG:CZ	1:B:282:LEU:HD11	2.33	0.59
1:F:5:LYS:O	1:F:186:THR:OG1	2.20	0.59
1:F:245:LYS:O	1:F:248:GLN:NE2	2.35	0.59
2:I:24:ILE:HG12	2:I:75:LEU:HD13	1.83	0.59
1:M:130:GLN:NE2	3:N:143:ARG:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:176:ASP:O	3:N:187:ASN:ND2	2.24	0.59
1:C:85:ASN:C	1:C:85:ASN:HD22	2.04	0.59
2:I:77:TRP:O	2:I:81:GLN:HG2	2.03	0.59
1:M:33:ASP:OD2	1:M:135:ARG:NH1	2.35	0.59
4:O:36:C:O2'	4:O:37:C:O5'	2.19	0.59
1:G:16:GLN:NE2	1:G:174:PRO:O	2.35	0.59
1:M:183:PHE:HE2	3:N:137:GLN:HG2	1.67	0.59
1:B:147:ILE:N	1:B:168:GLY:O	2.28	0.58
1:F:55:GLN:OE1	1:F:68:ARG:NH1	2.36	0.58
2:H:23:LYS:HD2	2:H:112:LEU:HB3	1.85	0.58
3:N:68:ASN:HB3	3:N:87:ARG:HH11	1.68	0.58
1:D:154:ASN:OD1	1:D:155:GLU:N	2.37	0.58
1:E:155:GLU:HB3	1:F:72:ILE:HG21	1.86	0.58
1:G:252:LYS:HD3	1:G:255:VAL:HG23	1.85	0.58
2:H:10:ILE:HD12	2:H:10:ILE:H	1.67	0.58
1:M:55:GLN:HB2	1:M:65:ILE:HG13	1.84	0.58
1:E:3:ILE:HD11	1:E:194:PHE:HD2	1.69	0.58
1:E:148:THR:N	4:O:39:U:OP2	2.35	0.58
3:N:18:GLU:HA	5:K:240:PHE:CD1	2.35	0.58
1:C:64:ASP:OD1	1:C:65:ILE:N	2.37	0.58
1:G:107:TYR:HE1	1:G:198:ASP:HB3	1.69	0.58
1:G:275:GLU:N	1:G:275:GLU:OE1	2.36	0.58
1:B:229:PHE:CE1	1:B:279:LEU:HD12	2.39	0.58
1:C:260:SER:OG	1:C:262:ASP:OD1	2.15	0.58
1:D:237:ASP:HB2	1:D:277:LYS:HD2	1.85	0.58
1:E:9:PHE:CZ	1:E:182:GLY:HA3	2.38	0.58
1:G:41:VAL:HB	1:G:134:SER:HB3	1.85	0.58
5:K:483:ALA:HA	5:K:489:LEU:HD11	1.86	0.58
1:D:90:GLU:O	1:D:94:LYS:N	2.26	0.58
3:N:20:LYS:O	3:N:90:ARG:NH2	2.37	0.58
1:G:174:PRO:HB2	1:G:259:ARG:HH22	1.68	0.58
1:G:4:GLU:OE2	1:G:5:LYS:NZ	2.35	0.58
3:N:16:ARG:HG2	3:N:26:TYR:CE1	2.39	0.58
2:L:9:ASP:HB2	2:L:12:TYR:HB2	1.85	0.58
2:J:14:LEU:HD22	2:J:52:PHE:HE1	1.69	0.58
2:J:86:CYS:SG	2:J:87:GLN:N	2.76	0.57
5:K:423:ASN:N	5:K:433:ARG:HH12	2.02	0.57
5:K:518:HIS:HA	5:K:521:ASN:ND2	2.19	0.57
1:G:39:GLY:N	1:G:136:SER:OG	2.30	0.57
1:G:230:GLU:O	1:G:277:LYS:HA	2.04	0.57
2:I:95:LEU:HD21	2:J:50:ALA:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:ARG:HH11	1:E:270:ASP:HA	1.67	0.57
1:M:163:ASP:HB3	6:A:63:ARG:HH12	1.69	0.57
5:K:422:ARG:NH2	5:K:426:GLU:OE2	2.37	0.57
1:F:280:ARG:NH1	1:F:282:LEU:HD21	2.20	0.57
1:G:47:LYS:HE3	1:G:112:PHE:CG	2.39	0.57
5:K:195:CYS:SG	5:K:243:GLY:N	2.77	0.57
1:E:32:ILE:HD12	1:E:140:ILE:HD11	1.85	0.57
1:E:246:ARG:HH21	1:E:273:LEU:HD12	1.69	0.57
4:O:24:U:O2'	4:O:25:A:O5'	2.18	0.57
5:K:226:LEU:HG	5:K:227:SER:H	1.69	0.57
1:F:81:HIS:CE1	1:F:120:LYS:HB2	2.40	0.57
1:D:82:GLU:HA	1:D:87:LYS:NZ	2.20	0.57
1:M:252:LYS:HZ2	1:M:265:LEU:HB2	1.70	0.57
1:B:86:VAL:O	1:B:94:LYS:NZ	2.37	0.57
1:G:48:ARG:NH2	1:G:69:GLU:OE1	2.38	0.57
1:M:26:ALA:HB1	5:K:393:LEU:HB3	1.87	0.57
5:K:212:LYS:HG3	5:K:218:PRO:HG3	1.87	0.57
1:B:129:VAL:HG22	1:B:184:ILE:HG12	1.86	0.57
1:D:7:TYR:HB2	1:D:184:ILE:HB	1.87	0.57
1:D:206:LEU:HA	1:D:209:MET:HE3	1.86	0.57
1:C:150:MET:SD	1:D:48:ARG:NH2	2.77	0.56
5:K:10:TYR:CG	5:K:249:GLU:HB2	2.40	0.56
5:K:418:ALA:HA	5:K:421:ARG:HD2	1.86	0.56
1:E:55:GLN:HB2	1:E:65:ILE:HG13	1.86	0.56
1:G:228:VAL:O	1:G:279:LEU:HA	2.05	0.56
1:B:2:THR:HG21	1:B:190:LYS:HA	1.87	0.56
1:D:13:PHE:HZ	1:D:41:VAL:HG11	1.69	0.56
1:E:48:ARG:HB2	4:O:32:A:OP2	2.05	0.56
5:K:307:LEU:O	5:K:310:SER:OG	2.17	0.56
2:L:12:TYR:O	2:L:16:ARG:HG3	2.05	0.56
6:A:7:TYR:HA	6:A:70:TRP:HA	1.88	0.56
1:D:9:PHE:CZ	1:D:182:GLY:HA3	2.40	0.56
1:G:205:ALA:O	1:G:209:MET:HG3	2.05	0.56
1:B:135:ARG:O	1:B:178:TYR:HA	2.05	0.56
1:E:53:PHE:HB2	1:E:209:MET:SD	2.46	0.56
1:F:127:GLY:O	1:F:130:GLN:NE2	2.35	0.56
1:G:10:VAL:HG22	1:G:181:HIS:CD2	2.40	0.56
1:G:230:GLU:HB2	1:G:278:LEU:HB2	1.87	0.56
3:N:31:PRO:HG2	3:N:192:PHE:CE1	2.41	0.56
1:D:89:LYS:HB3	1:D:93:GLU:HB2	1.88	0.56
2:H:107:HIS:CD2	2:I:84:GLU:HA	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:341:PHE:HB2	5:K:343:HIS:CE1	2.40	0.56
1:B:150:MET:SD	1:C:48:ARG:NH2	2.75	0.56
1:F:166:THR:OG1	1:F:167:MET:N	2.38	0.56
2:J:100:LEU:HD23	2:J:103:ILE:HD13	1.88	0.56
5:K:407:ASN:O	5:K:409:ARG:NH2	2.38	0.56
1:C:4:GLU:N	1:C:4:GLU:OE1	2.39	0.56
1:E:89:LYS:HD2	1:E:93:GLU:HG2	1.88	0.56
1:G:175:TYR:H	1:G:259:ARG:HH12	1.52	0.56
1:G:197:ASN:OD1	1:G:198:ASP:N	2.39	0.56
1:B:138:ASP:OD2	1:B:264:TYR:OH	2.16	0.56
1:D:228:VAL:HB	1:D:280:ARG:HG3	1.88	0.56
1:F:280:ARG:HH22	1:F:282:LEU:HD11	1.70	0.56
2:H:16:ARG:HH21	2:H:82:ILE:HG23	1.71	0.56
2:J:12:TYR:OH	2:J:107:HIS:ND1	2.29	0.56
5:K:469:TYR:HH	5:K:564:HIS:HD1	1.50	0.56
1:D:22:GLY:HA3	4:O:27:G:C3'	2.36	0.55
1:G:12:LEU:HD22	1:G:249:VAL:HG11	1.88	0.55
1:C:18:GLY:HA3	1:C:218:ARG:O	2.06	0.55
1:C:93:GLU:N	1:C:93:GLU:OE1	2.39	0.55
1:M:9:PHE:CZ	1:M:182:GLY:HA3	2.42	0.55
1:C:271:LYS:HG3	1:C:272:ASN:N	2.21	0.55
1:F:14:ASP:OD1	1:F:15:VAL:N	2.39	0.55
3:N:53:LYS:HE2	3:N:103:HIS:CG	2.42	0.55
5:K:389:LYS:NZ	6:A:29:ALA:HB2	2.21	0.55
1:F:55:GLN:O	1:F:59:ASN:ND2	2.39	0.55
1:F:7:TYR:HB2	1:F:184:ILE:HG13	1.87	0.55
1:M:64:ASP:HB3	1:M:106:TYR:CD1	2.39	0.55
1:B:39:GLY:N	1:B:136:SER:OG	2.35	0.55
1:E:177:LEU:HD12	1:E:264:TYR:HD2	1.71	0.55
1:F:197:ASN:OD1	1:F:198:ASP:N	2.39	0.55
1:F:258:VAL:HG21	1:F:264:TYR:HE1	1.71	0.55
2:L:18:PHE:CZ	2:L:44:ALA:HB1	2.42	0.55
1:C:237:ASP:HB3	1:C:277:LYS:HD3	1.87	0.55
1:D:15:VAL:HA	1:D:221:MET:HG2	1.88	0.55
1:F:35:GLN:OE1	2:H:91:ASN:ND2	2.40	0.55
1:F:81:HIS:CE1	1:F:120:LYS:HE2	2.41	0.55
2:J:28:ALA:O	2:J:65:LYS:NZ	2.39	0.55
1:M:15:VAL:HG12	1:M:221:MET:HG3	1.87	0.55
4:O:15:A:C8	4:O:16:G:C4	2.95	0.55
5:K:264:PHE:HE2	5:K:266:ILE:HD11	1.72	0.55
1:C:4:GLU:CD	1:C:4:GLU:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:GLU:HG2	1:E:276:THR:HG23	1.88	0.55
2:I:4:ASP:OD1	2:I:5:ARG:N	2.40	0.55
2:L:10:ILE:O	2:L:14:LEU:HG	2.07	0.55
1:B:11:PHE:HB3	1:B:180:CYS:SG	2.47	0.55
1:C:129:VAL:HG22	1:C:184:ILE:HG12	1.89	0.55
1:F:215:SER:OG	4:O:41:G:OP2	2.25	0.55
3:N:128:ARG:HG2	3:N:133:GLN:OE1	2.07	0.55
5:K:313:ASN:O	5:K:315:GLN:N	2.40	0.55
5:K:357:TRP:CE2	5:K:361:LEU:HD11	2.43	0.54
1:E:237:ASP:OD2	1:E:277:LYS:NZ	2.33	0.54
2:H:78:GLU:O	2:H:82:ILE:HD12	2.07	0.54
1:C:55:GLN:HG3	1:C:65:ILE:HD12	1.88	0.54
1:E:144:GLU:HG2	1:E:171:PHE:CE1	2.42	0.54
1:M:184:ILE:HG22	1:M:185:SER:H	1.72	0.54
1:C:126:ARG:HD3	1:C:188:PHE:CE1	2.43	0.54
3:N:80:SER:OG	3:N:81:LEU:N	2.40	0.54
1:F:103:CYS:O	1:F:110:ARG:NE	2.40	0.54
1:G:31:ARG:NH2	1:G:42:THR:OG1	2.40	0.54
1:B:130:GLN:HG3	1:M:214:HIS:O	2.08	0.54
1:C:19:ASN:ND2	1:C:28:ASN:O	2.41	0.54
1:C:51:ARG:NH2	4:O:19:U:OP1	2.41	0.54
1:C:148:THR:HB	4:O:26:G:O2'	2.07	0.54
1:F:258:VAL:HG21	1:F:264:TYR:CE1	2.42	0.54
5:K:9:TYR:HA	5:K:12:ARG:HG2	1.88	0.54
5:K:367:GLU:OE2	5:K:570:PHE:HB3	2.08	0.54
3:N:43:TRP:H	3:N:135:PHE:HE2	1.54	0.54
5:K:303:ALA:O	5:K:306:THR:OG1	2.19	0.54
1:B:218:ARG:NH2	4:O:16:G:H5'	2.22	0.54
1:E:215:SER:OG	4:O:36:C:OP2	2.24	0.54
5:K:316:TYR:CZ	5:K:318:LYS:HB2	2.42	0.54
6:A:6:MET:HG2	6:A:73:GLY:HA2	1.89	0.54
1:D:21:ASN:ND2	1:D:42:THR:H	2.06	0.54
1:F:212:HIS:CE1	1:G:187:HIS:HD1	2.25	0.54
1:M:149:ARG:NH2	1:M:153:THR:OG1	2.41	0.53
1:F:4:GLU:N	1:F:4:GLU:OE1	2.37	0.53
2:H:16:ARG:HG3	2:H:108:GLU:CG	2.31	0.53
2:H:24:ILE:HG12	2:H:75:LEU:HD13	1.90	0.53
2:J:17:LEU:O	2:J:21:LEU:HG	2.08	0.53
1:M:271:LYS:HD2	1:M:272:ASN:HB2	1.91	0.53
3:N:54:ILE:HB	3:N:201:VAL:CG2	2.39	0.53
5:K:213:GLY:HA3	5:K:258:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:TYR:O	1:D:104:SER:OG	2.16	0.53
2:H:29:ASN:HB2	2:H:65:LYS:NZ	2.23	0.53
1:C:246:ARG:HB3	1:C:269:ASP:HB3	1.91	0.53
1:G:51:ARG:HH22	1:G:68:ARG:HA	1.74	0.53
1:G:64:ASP:OD2	1:G:105:ARG:NH1	2.37	0.53
2:J:51:VAL:HG13	2:J:52:PHE:HD2	1.73	0.53
1:D:129:VAL:HG22	1:D:184:ILE:HD12	1.89	0.53
1:E:177:LEU:HD12	1:E:264:TYR:CD2	2.44	0.53
2:J:99:GLY:O	2:J:103:ILE:HD12	2.08	0.53
1:D:47:LYS:NZ	4:O:24:U:O3'	2.37	0.53
1:E:61:GLU:OE1	1:E:105:ARG:NH2	2.42	0.53
5:K:7:THR:HG22	5:K:11:GLN:HE22	1.74	0.53
1:B:246:ARG:NH1	1:B:272:ASN:OD1	2.41	0.53
1:G:129:VAL:HG13	1:G:184:ILE:HG12	1.91	0.53
5:K:543:CYS:SG	5:K:544:GLN:N	2.82	0.53
1:B:55:GLN:HG2	1:B:65:ILE:HD13	1.90	0.53
1:E:230:GLU:HG2	1:E:278:LEU:HD13	1.91	0.53
1:G:107:TYR:HA	1:G:110:ARG:CZ	2.39	0.53
1:G:149:ARG:O	1:G:165:ARG:HD2	2.09	0.53
1:G:210:PHE:HB3	1:G:221:MET:HG3	1.89	0.53
1:G:252:LYS:HD2	1:G:262:ASP:O	2.09	0.53
2:I:6:ASN:OD1	2:I:85:HIS:NE2	2.42	0.53
1:F:19:ASN:ND2	1:F:28:ASN:O	2.42	0.53
1:G:274:GLU:HA	1:G:277:LYS:O	2.09	0.53
1:M:21:ASN:ND2	1:M:41:VAL:HG13	2.23	0.53
1:D:218:ARG:HH12	4:O:28:U:P	2.32	0.53
1:B:14:ASP:HB3	1:B:177:LEU:HD23	1.91	0.52
1:F:21:ASN:HA	4:O:40:C:OP1	2.09	0.52
2:H:116:ASP:HA	2:H:119:LYS:NZ	2.24	0.52
1:M:156:LYS:C	1:M:158:ALA:H	2.12	0.52
1:G:24:PRO:HG2	1:G:28:ASN:HA	1.90	0.52
1:B:249:VAL:HG12	1:B:266:VAL:HG22	1.90	0.52
1:C:85:ASN:O	1:C:85:ASN:ND2	2.33	0.52
1:D:87:LYS:O	1:D:94:LYS:NZ	2.41	0.52
1:G:170:LYS:HD3	1:G:171:PHE:H	1.74	0.52
1:B:248:GLN:OE1	1:B:248:GLN:N	2.42	0.52
2:I:28:ALA:HA	2:I:66:LEU:HD13	1.92	0.52
2:J:25:GLN:HG2	2:J:62:HIS:CE1	2.44	0.52
2:L:20:VAL:HG21	2:L:79:ILE:HG12	1.91	0.52
1:E:231:HIS:HA	1:E:277:LYS:HZ3	1.74	0.52
1:F:200:GLU:HA	1:F:203:TRP:HD1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:55:GLU:HB2	3:N:101:ARG:HB3	1.92	0.52
5:K:465:GLN:OE1	5:K:542:HIS:ND1	2.43	0.52
2:L:23:LYS:HD2	2:L:112:LEU:HD22	1.91	0.52
1:C:154:ASN:ND2	1:C:156:LYS:HB2	2.24	0.52
1:F:89:LYS:HE2	1:F:97:ALA:HB2	1.92	0.52
2:I:57:ARG:HA	2:I:57:ARG:NE	2.25	0.52
1:B:226:LEU:HD23	1:B:282:LEU:HB2	1.91	0.52
1:D:64:ASP:OD1	1:D:65:ILE:N	2.38	0.52
2:H:57:ARG:HA	2:L:41:PHE:HE2	1.75	0.52
3:N:160:PRO:HB2	3:N:199:ASN:HD21	1.74	0.52
3:N:122:ALA:O	3:N:126:LYS:HG2	2.09	0.52
2:L:95:LEU:HD12	2:L:96:GLU:N	2.24	0.52
1:G:129:VAL:HG22	1:G:184:ILE:HG23	1.92	0.52
2:H:8:GLN:OE1	2:H:85:HIS:ND1	2.43	0.52
5:K:210:ALA:HA	5:K:220:PRO:HA	1.91	0.52
1:C:150:MET:SD	1:D:48:ARG:NE	2.78	0.52
2:H:47:THR:OG1	2:H:91:ASN:O	2.20	0.52
2:J:93:LEU:O	2:J:98:GLN:NE2	2.41	0.52
1:F:18:GLY:H	1:F:172:THR:HG23	1.75	0.51
1:F:175:TYR:OH	1:F:261:PHE:HA	2.09	0.51
1:D:61:GLU:OE2	1:D:105:ARG:HB2	2.10	0.51
1:G:51:ARG:NH1	1:G:66:PHE:O	2.43	0.51
1:M:14:ASP:HB3	1:M:177:LEU:HD12	1.93	0.51
6:A:32:ARG:HH22	6:A:35:LEU:HD12	1.75	0.51
1:D:156:LYS:HG3	1:D:158:ALA:N	2.22	0.51
1:E:195:SER:OG	1:E:197:ASN:OD1	2.18	0.51
1:C:12:LEU:HD21	1:C:179:ARG:HG3	1.93	0.51
1:E:11:PHE:CD1	1:E:226:LEU:HD12	2.46	0.51
1:B:169:ARG:HH11	1:B:171:PHE:HZ	1.58	0.51
1:C:109:ILE:HG23	1:C:114:ALA:HB3	1.91	0.51
1:D:212:HIS:CD2	1:E:6:ARG:HH12	2.29	0.51
1:D:222:ASN:HD21	1:D:224:ARG:NH1	2.08	0.51
1:E:18:GLY:HA3	1:E:218:ARG:O	2.10	0.51
1:F:56:MET:SD	1:F:212:HIS:CE1	3.04	0.51
1:G:117:THR:OG1	1:G:123:GLY:N	2.43	0.51
5:K:285:LEU:HD12	5:K:288:MET:HB2	1.91	0.51
2:L:16:ARG:HA	2:L:108:GLU:HG3	1.92	0.51
1:C:229:PHE:CE1	1:C:279:LEU:HD13	2.45	0.51
1:F:258:VAL:HG13	1:F:263:ASP:HB2	1.92	0.51
1:M:241:ASP:HB2	3:N:150:ARG:NH1	2.26	0.51
1:M:240:ALA:HA	1:M:243:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ILE:HD13	1:B:199:LEU:HD11	1.93	0.51
1:D:4:GLU:OE1	1:D:4:GLU:N	2.44	0.51
1:M:49:LYS:HE3	1:M:218:ARG:HH11	1.76	0.51
1:M:144:GLU:OE2	5:K:421:ARG:HD3	2.11	0.51
1:D:272:ASN:O	1:D:274:GLU:N	2.44	0.51
1:M:229:PHE:CE1	1:M:279:LEU:HD13	2.46	0.51
1:M:235:LEU:HB3	3:N:133:GLN:HB3	1.93	0.51
5:K:246:ALA:O	5:K:249:GLU:HG3	2.10	0.51
1:E:23:ASP:HB2	1:E:31:ARG:HG2	1.93	0.51
2:J:25:GLN:HG2	2:J:62:HIS:HE1	1.76	0.51
1:C:42:THR:HG22	1:C:133:PHE:CE2	2.45	0.50
1:C:242:SER:O	1:C:246:ARG:NE	2.44	0.50
1:D:24:PRO:HD3	1:D:29:LEU:O	2.11	0.50
1:M:33:ASP:HB3	1:M:36:THR:HG22	1.93	0.50
1:B:179:ARG:HH11	1:B:181:HIS:HE1	1.60	0.50
1:F:117:THR:HA	1:F:121:ASN:HB2	1.94	0.50
1:D:270:ASP:HA	1:D:273:LEU:HD23	1.93	0.50
1:E:84:GLU:OE2	1:E:87:LYS:HB2	2.11	0.50
2:H:11:GLY:O	2:H:101:PHE:HA	2.11	0.50
3:N:4:ILE:HD12	3:N:153:GLU:O	2.11	0.50
3:N:66:ARG:NH2	3:N:89:GLN:OE1	2.44	0.50
3:N:117:ASN:HB3	3:N:120:LYS:HG2	1.94	0.50
5:K:500:SER:O	5:K:503:SER:OG	2.22	0.50
1:B:68:ARG:HH11	1:B:76:LEU:HD11	1.76	0.50
1:G:233:ASN:HB3	1:G:237:ASP:OD2	2.12	0.50
1:D:53:PHE:O	1:D:57:THR:OG1	2.20	0.50
1:F:10:VAL:HG21	1:F:247:ILE:HD12	1.94	0.50
1:F:174:PRO:HB2	1:F:259:ARG:NE	2.26	0.50
1:G:27:GLY:HA3	2:L:40:TYR:HE1	1.77	0.50
3:N:87:ARG:NH1	4:O:8:C:O2	2.44	0.50
1:B:237:ASP:HB3	1:B:277:LYS:NZ	2.27	0.50
1:D:218:ARG:HH22	4:O:28:U:P	2.35	0.50
1:E:248:GLN:HB2	1:E:267:SER:OG	2.11	0.50
2:H:43:SER:O	2:H:46:SER:OG	2.24	0.50
5:K:578:LEU:HD13	5:K:581:GLU:OE1	2.11	0.50
1:F:200:GLU:HA	1:F:203:TRP:CD1	2.46	0.50
1:M:18:GLY:HA3	1:M:218:ARG:O	2.11	0.50
5:K:321:GLY:HA2	5:K:347:VAL:HB	1.93	0.50
1:B:9:PHE:CZ	1:B:182:GLY:HA3	2.47	0.50
1:B:187:HIS:HE1	1:M:72:ILE:HG23	1.76	0.50
1:F:9:PHE:CZ	1:F:182:GLY:HA3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:ASN:OD1	1:F:234:ASN:N	2.44	0.50
1:G:227:TYR:HD2	1:G:247:ILE:HG23	1.76	0.50
2:L:37:ALA:O	2:L:41:PHE:HD1	1.95	0.50
1:E:21:ASN:HD22	1:E:42:THR:H	1.60	0.50
1:F:251:LYS:HA	1:F:264:TYR:CD1	2.47	0.50
1:G:124:GLN:NE2	4:O:41:G:N3	2.59	0.50
1:G:252:LYS:N	1:G:263:ASP:O	2.30	0.50
6:A:9:ILE:HD11	6:A:42:ALA:HB1	1.93	0.50
1:E:45:CYS:SG	1:E:49:LYS:HE2	2.52	0.49
1:F:145:HIS:O	1:F:170:LYS:N	2.45	0.49
1:C:262:ASP:OD1	1:C:262:ASP:N	2.42	0.49
1:F:252:LYS:HB3	1:F:255:VAL:HG22	1.94	0.49
3:N:5:LEU:HD12	3:N:6:GLU:H	1.77	0.49
1:B:116:MET:HG3	1:B:122:ALA:HB3	1.95	0.49
1:C:56:MET:SD	1:D:187:HIS:ND1	2.80	0.49
1:F:48:ARG:HD3	4:O:38:C:OP2	2.11	0.49
1:G:44:VAL:HG12	1:G:48:ARG:HD2	1.93	0.49
1:G:224:ARG:HG3	1:G:261:PHE:CE1	2.48	0.49
1:M:4:GLU:N	1:M:4:GLU:OE1	2.45	0.49
6:A:42:ALA:O	6:A:46:ILE:HG12	2.11	0.49
1:D:155:GLU:HB3	1:E:72:ILE:HD12	1.93	0.49
1:D:276:THR:C	1:D:277:LYS:HD3	2.32	0.49
5:K:363:MET:HG2	5:K:364:VAL:H	1.77	0.49
1:C:33:ASP:OD2	1:C:135:ARG:NH1	2.46	0.49
1:F:232:SER:N	1:F:276:THR:O	2.45	0.49
1:D:155:GLU:CD	1:E:72:ILE:HD12	2.33	0.49
1:E:7:TYR:HB2	1:E:184:ILE:HB	1.93	0.49
1:F:168:GLY:O	1:F:169:ARG:NH2	2.35	0.49
2:H:54:THR:HA	2:H:57:ARG:NH1	2.28	0.49
2:I:12:TYR:O	2:I:16:ARG:HG3	2.12	0.49
5:K:296:LYS:CG	5:K:297:PRO:HD3	2.43	0.49
2:L:73:VAL:HG22	2:L:77:TRP:CZ3	2.48	0.49
1:E:42:THR:HG22	1:E:44:VAL:HG12	1.94	0.49
1:G:174:PRO:HG2	1:G:259:ARG:NH1	2.27	0.49
1:M:31:ARG:NH2	3:N:66:ARG:O	2.43	0.49
1:M:187:HIS:CE1	3:N:135:PHE:HA	2.47	0.49
1:B:49:LYS:HB3	1:B:209:MET:SD	2.53	0.49
1:E:197:ASN:OD1	1:E:198:ASP:N	2.44	0.49
3:N:120:LYS:HE3	3:N:121:PHE:CE2	2.48	0.49
4:O:17:C:H2'	4:O:18:U:H5"	1.95	0.49
5:K:214:VAL:HG12	5:K:332:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ARG:HG3	1:D:269:ASP:HB2	1.95	0.49
2:H:62:HIS:HA	2:H:65:LYS:HE3	1.94	0.48
2:I:11:GLY:O	2:I:101:PHE:HA	2.13	0.48
2:J:4:ASP:OD1	2:J:6:ASN:N	2.45	0.48
1:D:47:LYS:O	1:D:50:VAL:HG12	2.13	0.48
1:E:14:ASP:OD2	1:E:224:ARG:NH1	2.46	0.48
1:E:252:LYS:NZ	1:E:264:TYR:O	2.40	0.48
1:F:66:PHE:HB2	1:F:106:TYR:CD1	2.48	0.48
1:G:258:VAL:O	1:G:259:ARG:NE	2.46	0.48
2:J:77:TRP:O	2:J:81:GLN:HG2	2.13	0.48
1:M:66:PHE:HZ	3:N:74:MET:HB2	1.78	0.48
6:A:47:GLU:O	6:A:51:GLU:HG3	2.12	0.48
6:A:48:ASP:HA	6:A:51:GLU:HG3	1.95	0.48
1:B:141:MET:N	1:B:141:MET:SD	2.86	0.48
1:F:248:GLN:HB2	1:F:267:SER:OG	2.13	0.48
1:G:134:SER:OG	1:G:178:TYR:HB3	2.13	0.48
3:N:18:GLU:OE1	3:N:18:GLU:N	2.30	0.48
1:D:150:MET:HG2	1:E:48:ARG:NH2	2.28	0.48
1:E:21:ASN:ND2	1:E:41:VAL:HG13	2.29	0.48
1:E:101:TYR:O	1:E:104:SER:OG	2.24	0.48
1:G:48:ARG:HB3	1:G:68:ARG:HG3	1.96	0.48
1:G:237:ASP:HB2	1:G:277:LYS:HD2	1.96	0.48
1:M:106:TYR:HB2	1:M:109:ILE:CG2	2.43	0.48
4:O:39:U:O2'	4:O:40:C:O5'	2.31	0.48
1:G:5:LYS:HD2	1:G:230:GLU:HB3	1.95	0.48
1:G:39:GLY:O	1:G:135:ARG:HA	2.13	0.48
1:G:65:ILE:HD12	1:G:108:ASP:HB3	1.96	0.48
1:G:136:SER:HB3	1:G:178:TYR:CE1	2.48	0.48
1:M:197:ASN:OD1	1:M:198:ASP:N	2.46	0.48
5:K:403:ASP:OD1	5:K:407:ASN:ND2	2.45	0.48
1:B:81:HIS:ND1	1:B:120:LYS:HD2	2.27	0.48
1:C:153:THR:HA	1:D:73:LEU:HB2	1.96	0.48
1:C:206:LEU:HD23	1:C:206:LEU:HA	1.70	0.48
1:C:252:LYS:HB2	1:C:263:ASP:O	2.13	0.48
1:D:39:GLY:N	1:D:136:SER:OG	2.27	0.48
1:G:62:HIS:O	1:G:62:HIS:ND1	2.47	0.48
1:G:77:ILE:HG22	1:G:81:HIS:CE1	2.48	0.48
1:G:144:GLU:HG2	1:G:171:PHE:HB3	1.95	0.48
2:I:77:TRP:HD1	2:I:80:ARG:NH2	2.11	0.48
6:A:20:ASP:OD1	6:A:20:ASP:N	2.47	0.48
1:C:2:THR:HG21	1:C:190:LYS:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:TYR:HE1	1:E:230:GLU:HB2	1.79	0.48
1:E:258:VAL:HG21	1:E:264:TYR:CZ	2.48	0.48
2:H:100:LEU:HD23	2:H:103:ILE:HD12	1.96	0.48
3:N:172:LEU:HA	3:N:191:MET:SD	2.54	0.48
4:O:4:G:C5	4:O:5:A:C2	3.02	0.48
2:I:120:ASN:O	2:I:123:ASN:N	2.46	0.48
2:J:32:LEU:HD21	2:J:34:ALA:HB3	1.95	0.48
3:N:194:GLN:HE22	3:N:196:LYS:HA	1.79	0.48
5:K:224:VAL:HG23	5:K:240:PHE:CZ	2.49	0.48
1:B:41:VAL:HB	1:B:134:SER:OG	2.13	0.48
1:B:54:ILE:HG22	1:B:65:ILE:HD11	1.95	0.48
1:B:116:MET:HG2	1:B:123:GLY:O	2.13	0.48
1:C:24:PRO:HA	4:O:21:C:C6	2.49	0.48
1:D:51:ARG:NH1	4:O:25:A:OP2	2.42	0.48
1:E:206:LEU:HD23	1:E:206:LEU:HA	1.75	0.48
5:K:247:MET:HA	5:K:250:TYR:CE1	2.47	0.48
5:K:478:LEU:HD21	5:K:512:LEU:HB3	1.96	0.48
5:K:534:TRP:HH2	5:K:578:LEU:HB3	1.79	0.48
1:B:60:ASP:OD1	1:B:61:GLU:N	2.46	0.48
1:B:66:PHE:HB2	1:B:109:ILE:HD11	1.95	0.48
1:D:21:ASN:HD22	1:D:41:VAL:HG23	1.79	0.48
1:G:16:GLN:CG	1:G:220:GLN:HB3	2.44	0.48
2:J:7:ARG:HH12	5:K:544:GLN:HB3	1.78	0.48
1:M:184:ILE:HG22	1:M:185:SER:N	2.29	0.48
3:N:16:ARG:HG2	3:N:26:TYR:CD1	2.49	0.48
4:O:24:U:HO2'	4:O:25:A:P	2.37	0.48
1:C:126:ARG:HA	4:O:17:C:O3'	2.14	0.47
1:D:149:ARG:NH1	1:D:153:THR:OG1	2.47	0.47
1:D:252:LYS:HB2	1:D:263:ASP:O	2.12	0.47
1:F:214:HIS:C	1:G:126:ARG:HH21	2.17	0.47
2:J:60:PRO:HA	2:J:63:LEU:HD12	1.95	0.47
1:M:235:LEU:HD12	3:N:133:GLN:HB3	1.96	0.47
3:N:67:ARG:HG3	3:N:69:GLU:OE2	2.14	0.47
5:K:296:LYS:HG3	5:K:297:PRO:HD3	1.96	0.47
5:K:383:ASN:HB3	5:K:433:ARG:HG2	1.95	0.47
5:K:545:ARG:HH21	5:K:547:PRO:HA	1.79	0.47
1:G:106:TYR:HB2	1:G:109:ILE:HG12	1.96	0.47
3:N:16:ARG:HG3	3:N:24:VAL:O	2.14	0.47
1:B:106:TYR:HB2	1:B:109:ILE:HD12	1.94	0.47
1:D:212:HIS:O	1:D:212:HIS:ND1	2.47	0.47
1:D:256:GLU:HG2	1:D:257:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:551:ASN:OD1	5:K:554:GLN:HG2	2.14	0.47
1:B:55:GLN:NE2	1:B:68:ARG:HG2	2.30	0.47
1:B:81:HIS:CD2	1:B:120:LYS:HB3	2.49	0.47
1:C:21:ASN:ND2	1:C:41:VAL:HA	2.29	0.47
1:G:210:PHE:CE2	1:G:223:ALA:HB2	2.49	0.47
3:N:43:TRP:HB3	3:N:135:PHE:CE2	2.49	0.47
5:K:285:LEU:O	5:K:288:MET:N	2.46	0.47
5:K:534:TRP:CH2	5:K:578:LEU:HB3	2.50	0.47
5:K:577:ASN:O	5:K:581:GLU:HG3	2.15	0.47
1:B:65:ILE:HG22	1:B:67:ILE:H	1.79	0.47
1:G:3:ILE:HD12	1:G:7:TYR:CE2	2.50	0.47
1:G:9:PHE:CE2	1:G:182:GLY:HA3	2.48	0.47
2:H:74:GLN:HE22	2:H:119:LYS:HA	1.79	0.47
6:A:32:ARG:HH12	6:A:35:LEU:HG	1.80	0.47
1:B:121:ASN:OD1	1:B:122:ALA:N	2.48	0.47
1:D:232:SER:HB3	1:D:276:THR:O	2.15	0.47
1:D:280:ARG:NH1	1:D:282:LEU:HD11	2.29	0.47
1:F:48:ARG:HB2	4:O:38:C:H5'	1.96	0.47
1:M:49:LYS:HE3	1:M:218:ARG:NH1	2.29	0.47
1:B:7:TYR:HE1	1:B:230:GLU:HG3	1.78	0.47
1:B:247:ILE:HG22	1:B:268:VAL:HG23	1.96	0.47
1:F:269:ASP:OD2	1:F:271:LYS:NZ	2.46	0.47
2:J:23:LYS:HG3	2:J:27:GLU:OE1	2.15	0.47
1:M:38:GLU:OE2	1:M:135:ARG:NE	2.42	0.47
3:N:6:GLU:O	3:N:149:PHE:HA	2.15	0.47
3:N:30:THR:HG22	3:N:32:ALA:H	1.79	0.47
1:D:9:PHE:CE1	1:D:182:GLY:HA3	2.50	0.47
1:E:218:ARG:NH2	4:O:34:C:O5'	2.48	0.47
3:N:54:ILE:HB	3:N:201:VAL:HG23	1.97	0.47
3:N:84:GLU:OE2	3:N:84:GLU:N	2.45	0.47
5:K:404:ALA:HA	5:K:409:ARG:HB2	1.96	0.47
6:A:7:TYR:CE2	6:A:70:TRP:HB3	2.50	0.47
1:F:93:GLU:O	1:F:96:GLU:N	2.42	0.47
1:M:32:ILE:HA	1:M:39:GLY:HA2	1.97	0.47
3:N:163:ASP:OD1	3:N:163:ASP:N	2.48	0.47
5:K:393:LEU:HB2	5:K:397:LEU:HD23	1.97	0.47
1:D:132:THR:HG22	1:D:181:HIS:O	2.15	0.47
1:E:228:VAL:HB	1:E:280:ARG:HG2	1.97	0.47
1:F:89:LYS:O	1:F:90:GLU:HG3	2.14	0.47
3:N:178:SER:OG	3:N:179:LYS:N	2.47	0.47
5:K:285:LEU:HG	5:K:289:ILE:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:HH22	1:B:273:LEU:HA	1.79	0.46
1:C:87:LYS:NZ	1:C:90:GLU:HA	2.30	0.46
1:D:121:ASN:OD1	1:D:122:ALA:N	2.48	0.46
1:G:251:LYS:HZ3	1:G:258:VAL:HA	1.80	0.46
1:M:179:ARG:HH11	1:M:181:HIS:CE1	2.33	0.46
1:M:196:GLU:OE1	1:M:196:GLU:N	2.36	0.46
1:M:230:GLU:O	1:M:277:LYS:HA	2.15	0.46
3:N:124:MET:HB2	3:N:127:ARG:HH21	1.80	0.46
4:O:2:U:OP1	4:O:4:G:N2	2.38	0.46
2:L:118:LEU:HD12	2:L:121:LEU:HD11	1.95	0.46
1:B:113:GLY:HA3	4:O:12:G:H5'	1.97	0.46
1:E:4:GLU:N	1:E:4:GLU:OE1	2.47	0.46
1:E:144:GLU:OE2	1:E:169:ARG:HG2	2.15	0.46
1:E:172:THR:OG1	1:E:173:VAL:N	2.47	0.46
2:J:74:GLN:HA	2:J:122:PHE:CD1	2.50	0.46
3:N:16:ARG:HH22	5:K:1:MET:N	2.12	0.46
3:N:21:VAL:C	3:N:90:ARG:HH21	2.17	0.46
4:O:4:G:C6	5:K:232:TYR:CZ	3.03	0.46
6:A:16:TYR:HB2	6:A:59:ASN:OD1	2.15	0.46
1:B:10:VAL:HG22	1:B:181:HIS:ND1	2.30	0.46
1:D:149:ARG:HG3	4:O:31:C:O2'	2.14	0.46
1:F:273:LEU:HD23	1:F:273:LEU:H	1.79	0.46
2:H:36:ILE:HD12	2:H:36:ILE:H	1.81	0.46
1:M:188:PHE:HZ	3:N:136:HIS:HD2	1.62	0.46
3:N:14:PHE:CE2	3:N:29:ILE:HA	2.51	0.46
3:N:23:ARG:HD2	3:N:92:SER:OG	2.15	0.46
5:K:261:GLU:OE1	5:K:261:GLU:N	2.43	0.46
1:B:81:HIS:CE1	1:B:120:LYS:HD2	2.51	0.46
1:D:66:PHE:CD2	1:D:109:ILE:HD11	2.50	0.46
1:E:203:TRP:CD2	1:E:280:ARG:NH1	2.83	0.46
1:G:175:TYR:HB3	1:G:259:ARG:CZ	2.46	0.46
2:H:12:TYR:HE2	2:H:103:ILE:HG22	1.80	0.46
2:J:21:LEU:HD22	2:J:59:LEU:HD21	1.96	0.46
1:M:13:PHE:O	1:M:178:TYR:HB2	2.16	0.46
5:K:282:GLU:HB3	5:K:286:ALA:HB2	1.98	0.46
1:G:45:CYS:SG	1:G:218:ARG:NH2	2.89	0.46
3:N:39:MET:HG2	3:N:49:TRP:CD1	2.50	0.46
3:N:44:LYS:HG3	3:N:121:PHE:HE1	1.78	0.46
4:O:38:C:H2'	4:O:39:U:H4'	1.98	0.46
2:L:11:GLY:O	2:L:101:PHE:HA	2.16	0.46
2:H:71:ARG:HA	2:H:71:ARG:NE	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:46:SER:HB3	2:J:57:ARG:NH2	2.31	0.46
1:B:150:MET:SD	1:C:48:ARG:NE	2.85	0.46
1:C:154:ASN:ND2	1:C:156:LYS:HE2	2.29	0.46
1:D:132:THR:OG1	1:D:133:PHE:N	2.49	0.46
1:D:243:LEU:HA	1:D:246:ARG:HH21	1.80	0.46
1:E:252:LYS:HZ2	1:E:265:LEU:HB2	1.80	0.46
2:J:29:ASN:ND2	2:J:32:LEU:HD22	2.30	0.46
1:B:187:HIS:ND1	1:M:56:MET:HG3	2.31	0.46
1:D:44:VAL:HG11	4:O:25:A:O2'	2.15	0.46
1:D:72:ILE:O	1:D:75:ASN:ND2	2.48	0.46
1:D:175:TYR:CG	1:D:176:GLY:N	2.84	0.46
1:G:3:ILE:HD12	1:G:7:TYR:HE2	1.80	0.46
2:I:16:ARG:HA	2:I:108:GLU:HG3	1.97	0.46
1:M:137:ILE:HG22	1:M:138:ASP:OD1	2.15	0.46
1:M:183:PHE:CE2	3:N:137:GLN:HG2	2.50	0.46
5:K:265:ARG:HG2	5:K:270:THR:HG22	1.97	0.46
1:C:271:LYS:HG3	1:C:272:ASN:H	1.80	0.46
1:F:30:PRO:O	1:F:32:ILE:HG23	2.16	0.46
1:G:62:HIS:HA	1:G:104:SER:O	2.16	0.46
1:G:103:CYS:O	1:G:110:ARG:NH2	2.39	0.46
2:H:18:PHE:HZ	2:H:40:TYR:HB2	1.81	0.46
2:H:19:ALA:HB2	2:H:105:TYR:CD1	2.51	0.46
2:H:91:ASN:OD1	2:H:92:HIS:N	2.45	0.46
1:D:153:THR:HB	1:D:156:LYS:NZ	2.31	0.46
1:E:10:VAL:HG12	1:E:227:TYR:HB2	1.97	0.46
1:F:233:ASN:CG	1:F:235:LEU:H	2.19	0.46
1:F:274:GLU:HA	1:F:277:LYS:O	2.16	0.46
1:G:111:THR:HG22	1:G:112:PHE:HD1	1.80	0.46
2:J:110:GLN:HA	5:K:537:ARG:NH2	2.27	0.46
1:M:188:PHE:HA	1:M:191:GLN:NE2	2.31	0.46
2:L:7:ARG:HG3	2:L:12:TYR:CE2	2.51	0.46
1:E:171:PHE:N	1:E:171:PHE:CD1	2.84	0.45
1:E:222:ASN:HB2	1:E:224:ARG:NH2	2.22	0.45
2:I:77:TRP:HH2	2:I:121:LEU:HB3	1.81	0.45
2:J:10:ILE:HG21	2:J:90:PRO:HG3	1.98	0.45
1:M:226:LEU:N	1:M:283:GLY:HA3	2.25	0.45
1:M:241:ASP:HB2	3:N:150:ARG:HH11	1.79	0.45
3:N:68:ASN:CB	3:N:87:ARG:HH11	2.27	0.45
5:K:294:LYS:NZ	6:A:31:GLY:HA2	2.31	0.45
1:D:141:MET:CE	1:E:35:GLN:HE22	2.29	0.45
1:G:4:GLU:OE1	1:G:4:GLU:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:TYR:N	1:G:259:ARG:HH12	2.15	0.45
2:I:67:GLU:H	2:I:67:GLU:CD	2.19	0.45
2:J:53:GLY:O	2:J:57:ARG:HG3	2.17	0.45
1:M:26:ALA:HB1	5:K:393:LEU:HD22	1.98	0.45
1:M:70:LYS:N	3:N:84:GLU:OE1	2.42	0.45
3:N:41:ILE:HD13	3:N:134:TYR:HB3	1.98	0.45
3:N:167:ASP:CB	3:N:196:LYS:HD2	2.46	0.45
2:L:14:LEU:HD22	2:L:52:PHE:CZ	2.51	0.45
1:B:24:PRO:HA	4:O:15:A:C2	2.52	0.45
1:C:228:VAL:HB	1:C:280:ARG:HG3	1.97	0.45
1:E:126:ARG:HG2	1:E:188:PHE:CE1	2.52	0.45
1:E:256:GLU:HG2	1:E:257:VAL:HG13	1.98	0.45
2:H:96:GLU:O	2:H:100:LEU:HG	2.17	0.45
2:J:14:LEU:HD22	2:J:52:PHE:CE1	2.49	0.45
1:B:42:THR:HG22	1:B:133:PHE:CE1	2.52	0.45
1:D:149:ARG:NE	4:O:31:C:O2	2.49	0.45
1:E:102:MET:HG3	1:E:116:MET:SD	2.56	0.45
1:E:242:SER:O	1:E:246:ARG:HG3	2.17	0.45
1:M:109:ILE:HG13	1:M:114:ALA:HB2	1.97	0.45
3:N:73:LYS:HG3	5:K:228:ALA:HA	1.98	0.45
5:K:354:ILE:HD11	5:K:406:LEU:HD23	1.97	0.45
1:B:17:ASP:O	1:B:219:GLY:HA3	2.16	0.45
1:C:106:TYR:HB2	1:C:109:ILE:HD12	1.99	0.45
1:C:47:LYS:HD3	1:C:112:PHE:CG	2.52	0.45
1:C:243:LEU:HD21	1:C:277:LYS:HE2	1.98	0.45
1:G:51:ARG:HG2	1:G:65:ILE:HD11	1.99	0.45
1:G:98:ALA:O	1:G:102:MET:HG2	2.17	0.45
1:M:163:ASP:HB3	6:A:63:ARG:NH1	2.30	0.45
1:M:187:HIS:ND1	3:N:135:PHE:HA	2.31	0.45
3:N:53:LYS:HE2	3:N:103:HIS:CD2	2.52	0.45
1:B:54:ILE:HD13	1:B:54:ILE:HA	1.84	0.45
1:D:90:GLU:HG3	1:D:91:LYS:H	1.81	0.45
2:H:71:ARG:O	2:H:75:LEU:HG	2.17	0.45
1:B:74:ASN:HB2	1:M:154:ASN:OD1	2.16	0.45
1:C:280:ARG:NH1	1:C:282:LEU:HD11	2.31	0.45
1:E:24:PRO:O	2:I:39:ARG:NH2	2.46	0.45
1:F:252:LYS:HB2	1:F:263:ASP:O	2.17	0.45
1:G:13:PHE:O	1:G:177:LEU:HD12	2.17	0.45
1:G:16:GLN:HB2	1:G:220:GLN:HB3	1.97	0.45
1:G:29:LEU:HA	1:G:171:PHE:HE2	1.82	0.45
1:G:90:GLU:OE1	1:G:93:GLU:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:7:ARG:NH2	2:J:87:GLN:O	2.48	0.45
1:D:23:ASP:HA	1:D:29:LEU:O	2.17	0.45
1:F:189:ALA:HA	1:F:192:THR:HG22	1.98	0.45
1:G:80:ALA:HA	1:G:83:GLN:HG2	1.99	0.45
1:G:81:HIS:O	1:G:86:VAL:HA	2.16	0.45
2:J:7:ARG:NH1	5:K:544:GLN:HB3	2.32	0.45
3:N:43:TRP:O	3:N:44:LYS:HE2	2.17	0.45
2:L:103:ILE:HG12	2:L:107:HIS:CD2	2.52	0.45
1:B:130:GLN:OE1	1:M:216:ALA:N	2.49	0.45
1:D:51:ARG:NE	1:D:67:ILE:HD11	2.32	0.45
1:E:228:VAL:HB	1:E:280:ARG:CG	2.47	0.45
1:G:115:VAL:HG23	4:O:42:U:C2	2.52	0.45
2:L:59:LEU:HB3	2:L:60:PRO:HD3	1.99	0.45
1:B:273:LEU:O	1:B:275:GLU:N	2.50	0.44
1:C:21:ASN:HD21	1:C:41:VAL:HA	1.82	0.44
1:C:141:MET:SD	1:C:141:MET:N	2.90	0.44
1:D:89:LYS:HB2	1:D:94:LYS:HE2	1.99	0.44
3:N:98:VAL:HB	3:N:100:TYR:HE2	1.82	0.44
5:K:257:LEU:HD23	5:K:257:LEU:HA	1.79	0.44
1:B:222:ASN:ND2	1:C:241:ASP:OD2	2.50	0.44
1:D:87:LYS:HE2	1:D:87:LYS:HA	1.98	0.44
1:F:275:GLU:OE1	1:F:275:GLU:N	2.45	0.44
1:G:210:PHE:HE2	1:G:223:ALA:HB2	1.82	0.44
1:G:224:ARG:HA	1:G:224:ARG:HD3	1.82	0.44
2:I:17:LEU:HD23	2:I:52:PHE:HE2	1.82	0.44
2:I:88:ARG:HD2	2:I:89:PHE:O	2.17	0.44
3:N:180:SER:HB2	3:N:185:SER:N	2.33	0.44
6:A:9:ILE:HD12	6:A:46:ILE:HD11	1.99	0.44
6:A:10:ARG:HH21	6:A:24:TYR:N	2.15	0.44
1:C:245:LYS:HD2	1:C:245:LYS:N	2.32	0.44
1:F:167:MET:CE	1:G:69:GLU:HB2	2.47	0.44
2:H:22:GLU:O	2:H:25:GLN:HG2	2.18	0.44
2:H:66:LEU:HD12	2:H:67:GLU:H	1.82	0.44
1:M:213:ASP:HB3	1:M:218:ARG:NH1	2.25	0.44
1:M:224:ARG:HD3	1:M:224:ARG:HA	1.63	0.44
3:N:160:PRO:HG2	3:N:162:GLU:OE2	2.17	0.44
5:K:333:ASN:HB2	5:K:338:VAL:HG23	1.98	0.44
1:C:101:TYR:OH	1:C:105:ARG:NH1	2.50	0.44
1:E:242:SER:HA	1:E:245:LYS:HE3	2.00	0.44
1:F:86:VAL:O	1:F:87:LYS:HE2	2.17	0.44
1:G:74:ASN:OD1	1:G:75:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:TYR:CD1	1:G:281:LYS:HG3	2.52	0.44
2:J:51:VAL:O	2:J:55:LEU:HG	2.18	0.44
1:M:106:TYR:O	1:M:109:ILE:HG22	2.18	0.44
5:K:212:LYS:HA	5:K:218:PRO:HA	1.99	0.44
1:C:206:LEU:HD23	1:C:209:MET:HE3	1.99	0.44
1:M:20:PRO:HB3	1:M:221:MET:HE2	1.99	0.44
1:M:149:ARG:HD3	4:O:13:U:O2	2.18	0.44
1:M:249:VAL:HA	1:M:265:LEU:O	2.18	0.44
3:N:174:ASP:O	3:N:190:PRO:HD2	2.18	0.44
2:L:17:LEU:O	2:L:20:VAL:HG22	2.17	0.44
1:B:118:THR:OG1	1:B:119:GLY:N	2.51	0.44
1:C:66:PHE:CZ	1:C:73:LEU:HD12	2.52	0.44
1:D:282:LEU:HD23	1:D:282:LEU:HA	1.77	0.44
1:F:237:ASP:CB	1:F:277:LYS:HZ3	2.30	0.44
2:H:66:LEU:HD23	2:H:72:ALA:HB2	2.00	0.44
5:K:508:VAL:O	5:K:511:THR:OG1	2.29	0.44
2:L:51:VAL:HG12	2:L:55:LEU:HG	2.00	0.44
6:A:10:ARG:CB	6:A:67:LYS:HE3	2.47	0.44
1:B:61:GLU:O	1:B:62:HIS:HB2	2.17	0.44
1:B:148:THR:HA	1:B:166:THR:O	2.17	0.44
1:C:70:LYS:HD2	1:C:70:LYS:HA	1.72	0.44
1:C:90:GLU:O	1:C:91:LYS:HG2	2.18	0.44
1:C:218:ARG:NH1	4:O:23:G:OP1	2.51	0.44
1:F:51:ARG:NE	1:F:67:ILE:HD13	2.33	0.44
1:D:116:MET:HB3	1:D:122:ALA:HB3	2.00	0.44
1:D:230:GLU:CG	1:D:278:LEU:HB2	2.44	0.44
1:E:47:LYS:O	1:E:51:ARG:HG3	2.18	0.44
1:E:250:VAL:HG23	1:E:265:LEU:HB3	1.98	0.44
1:G:7:TYR:HB2	1:G:184:ILE:HD12	1.99	0.44
2:I:12:TYR:HE1	2:I:103:ILE:HG22	1.82	0.44
2:J:111:PHE:O	2:J:114:THR:OG1	2.20	0.44
5:K:533:GLN:O	5:K:536:ILE:HG22	2.18	0.44
1:C:179:ARG:NH1	1:C:247:ILE:O	2.50	0.44
1:D:246:ARG:HG2	1:D:273:LEU:HD21	2.00	0.44
1:E:212:HIS:CD2	1:F:6:ARG:HH22	2.36	0.44
1:F:275:GLU:HG2	1:F:276:THR:HG23	1.99	0.44
2:H:18:PHE:O	2:H:22:GLU:HG3	2.17	0.44
2:I:71:ARG:HA	2:I:71:ARG:NE	2.33	0.44
1:M:107:TYR:CE2	1:M:201:LEU:HD23	2.53	0.44
3:N:51:VAL:O	3:N:203:THR:OG1	2.26	0.44
5:K:316:TYR:CE2	5:K:318:LYS:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:524:GLU:HG2	5:K:525:PHE:N	2.33	0.44
2:L:10:ILE:H	2:L:10:ILE:HD12	1.83	0.44
6:A:15:PHE:HD1	6:A:60:GLU:HA	1.83	0.44
1:E:14:ASP:HB3	1:E:177:LEU:CD2	2.45	0.43
1:F:85:ASN:O	1:F:94:LYS:NZ	2.33	0.43
3:N:167:ASP:HB2	3:N:196:LYS:HD2	2.00	0.43
1:B:81:HIS:CE1	1:B:94:LYS:HD3	2.53	0.43
1:B:90:GLU:O	1:B:94:LYS:HB2	2.17	0.43
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.82	0.43
1:C:118:THR:OG1	1:C:119:GLY:N	2.51	0.43
1:F:14:ASP:OD2	1:F:16:GLN:NE2	2.51	0.43
1:G:55:GLN:O	1:G:59:ASN:HB3	2.19	0.43
1:G:249:VAL:HG13	1:G:266:VAL:HG22	2.00	0.43
2:J:110:GLN:O	2:J:114:THR:HG23	2.17	0.43
1:M:124:GLN:HG3	4:O:5:A:O2'	2.18	0.43
4:O:10:G:C6	4:O:11:G:N1	2.86	0.43
5:K:209:ASN:HB3	5:K:251:THR:HG21	2.00	0.43
2:L:23:LYS:NZ	2:L:112:LEU:HB2	2.33	0.43
1:E:141:MET:O	1:E:174:PRO:HD2	2.17	0.43
1:E:149:ARG:HG3	4:O:37:C:O2	2.18	0.43
1:E:151:ALA:HB1	1:F:71:GLY:O	2.18	0.43
2:I:110:GLN:NE2	2:I:110:GLN:O	2.51	0.43
1:M:124:GLN:NE2	1:M:126:ARG:HH11	2.16	0.43
3:N:177:PHE:CZ	4:O:1:A:C8	3.02	0.43
4:O:4:G:C6	4:O:5:A:H2	2.35	0.43
4:O:14:C:H5	4:O:16:G:O2'	2.01	0.43
6:A:7:TYR:CZ	6:A:70:TRP:HB3	2.53	0.43
1:B:21:ASN:O	1:B:30:PRO:HA	2.18	0.43
1:B:157:ASP:OD1	1:B:157:ASP:N	2.52	0.43
1:E:212:HIS:HE1	1:F:187:HIS:NE2	2.17	0.43
1:F:66:PHE:CZ	1:F:73:LEU:HD22	2.53	0.43
1:G:17:ASP:CG	1:G:174:PRO:HA	2.38	0.43
1:G:249:VAL:HG22	1:G:266:VAL:HG13	2.00	0.43
2:H:73:VAL:HA	2:H:76:GLN:OE1	2.17	0.43
6:A:12:ILE:HG22	6:A:65:ASP:O	2.17	0.43
1:B:66:PHE:CZ	1:B:73:LEU:HD22	2.53	0.43
1:B:148:THR:O	4:O:19:U:O2'	2.36	0.43
1:D:243:LEU:O	1:D:246:ARG:HB2	2.19	0.43
1:E:246:ARG:NH2	1:E:273:LEU:HD12	2.34	0.43
1:F:81:HIS:O	1:F:94:LYS:NZ	2.50	0.43
2:H:48:PRO:HA	2:H:51:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:LEU:HA	2:H:98:GLN:OE1	2.18	0.43
2:H:116:ASP:HA	2:H:119:LYS:HZ1	1.83	0.43
1:M:54:ILE:HG22	1:M:65:ILE:HD11	1.99	0.43
3:N:6:GLU:HG2	3:N:101:ARG:HA	2.01	0.43
5:K:481:ILE:HD13	5:K:516:LEU:HD11	2.00	0.43
1:D:256:GLU:OE1	1:D:256:GLU:N	2.48	0.43
1:E:258:VAL:O	1:E:259:ARG:NE	2.52	0.43
1:F:253:ASP:OD1	1:F:254:GLY:N	2.51	0.43
1:G:21:ASN:HD21	1:G:48:ARG:HH12	1.65	0.43
3:N:34:ALA:HB3	3:N:51:VAL:HG21	1.99	0.43
4:O:22:C:N4	4:O:23:G:O6	2.52	0.43
5:K:9:TYR:CZ	5:K:257:LEU:HD21	2.53	0.43
5:K:279:THR:O	5:K:279:THR:HG23	2.19	0.43
1:B:6:ARG:NH2	1:M:211:ASP:O	2.48	0.43
1:E:3:ILE:HG22	1:E:4:GLU:H	1.83	0.43
1:F:226:LEU:HD21	1:F:228:VAL:HG23	2.00	0.43
1:F:231:HIS:HA	1:F:277:LYS:HD2	2.00	0.43
1:G:36:THR:HB	1:G:38:GLU:OE1	2.18	0.43
1:G:248:GLN:HB3	1:G:267:SER:OG	2.19	0.43
2:H:94:ASN:HB2	2:H:97:GLN:HE22	1.83	0.43
3:N:181:ASP:HB2	3:N:182:PRO:HD2	1.99	0.43
5:K:353:SER:OG	5:K:408:ASN:N	2.52	0.43
1:C:175:TYR:CZ	1:C:260:SER:HA	2.54	0.43
1:C:231:HIS:CG	1:C:277:LYS:NZ	2.87	0.43
1:D:149:ARG:HA	4:O:31:C:O2'	2.19	0.43
1:D:155:GLU:OE1	1:E:74:ASN:HB2	2.19	0.43
1:E:246:ARG:HD2	1:E:273:LEU:HD12	2.00	0.43
1:E:252:LYS:HZ3	1:E:264:TYR:C	2.17	0.43
1:F:53:PHE:CE1	1:F:57:THR:HG21	2.53	0.43
2:H:80:ARG:HA	2:H:80:ARG:NE	2.34	0.43
1:M:246:ARG:HE	1:M:269:ASP:HB2	1.84	0.43
2:L:35:THR:O	2:L:39:ARG:HG2	2.18	0.43
6:A:24:TYR:HB2	6:A:27:GLU:OE2	2.17	0.43
1:B:21:ASN:ND2	1:B:31:ARG:HE	2.17	0.43
1:B:228:VAL:HB	1:B:280:ARG:HG3	2.01	0.43
1:B:242:SER:O	1:B:246:ARG:HG3	2.19	0.43
1:F:23:ASP:N	1:F:23:ASP:OD1	2.51	0.43
2:H:54:THR:HG22	2:H:57:ARG:HH12	1.84	0.43
2:I:77:TRP:CH2	2:I:121:LEU:HB3	2.54	0.43
5:K:443:ARG:HG2	5:K:446:ARG:HH22	1.84	0.43
5:K:569:LEU:HD23	5:K:569:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLY:HA2	1:B:172:THR:HA	2.00	0.43
1:C:85:ASN:HB2	1:C:89:LYS:HD3	2.00	0.43
1:E:64:ASP:HB3	1:E:106:TYR:HD1	1.84	0.43
1:G:126:ARG:HD3	1:G:188:PHE:CE1	2.53	0.43
1:G:175:TYR:HB3	1:G:259:ARG:NH1	2.33	0.43
2:I:103:ILE:HD13	2:J:83:LEU:HD21	2.01	0.43
2:I:110:GLN:HA	2:J:80:ARG:HH21	1.84	0.43
1:M:275:GLU:HG3	1:M:276:THR:H	1.84	0.43
3:N:34:ALA:O	3:N:38:LEU:HD23	2.19	0.43
5:K:496:ARG:HB2	5:K:497:TYR:HD1	1.84	0.43
1:D:111:THR:OG1	1:D:194:PHE:HE1	2.01	0.42
1:G:79:GLU:O	1:G:83:GLN:HG2	2.18	0.42
4:O:14:C:H2'	4:O:15:A:H4'	1.99	0.42
1:B:222:ASN:OD1	1:B:222:ASN:N	2.52	0.42
1:C:24:PRO:HA	4:O:21:C:C5	2.54	0.42
1:D:28:ASN:C	1:D:29:LEU:HD12	2.40	0.42
1:D:215:SER:HA	1:E:130:GLN:HE21	1.84	0.42
1:E:153:THR:HG23	1:E:156:LYS:HZ1	1.85	0.42
1:E:211:ASP:O	1:F:6:ARG:NH1	2.52	0.42
2:H:52:PHE:O	2:H:56:MET:HG2	2.19	0.42
2:I:78:GLU:O	2:I:82:ILE:HG12	2.19	0.42
3:N:39:MET:HG2	3:N:49:TRP:HD1	1.84	0.42
5:K:389:LYS:HZ3	6:A:29:ALA:HB2	1.84	0.42
6:A:10:ARG:HH21	6:A:23:SER:C	2.22	0.42
1:B:155:GLU:HG2	1:C:72:ILE:HG13	2.01	0.42
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.85	0.42
1:C:247:ILE:O	1:C:247:ILE:HG23	2.20	0.42
1:D:66:PHE:O	1:D:66:PHE:CG	2.72	0.42
1:D:83:GLN:O	1:D:87:LYS:HG2	2.19	0.42
1:D:154:ASN:HB3	1:D:156:LYS:NZ	2.34	0.42
1:G:46:LEU:HD23	1:G:46:LEU:HA	1.87	0.42
1:G:51:ARG:HH12	1:G:67:ILE:C	2.23	0.42
1:M:61:GLU:CD	1:M:62:HIS:H	2.22	0.42
1:M:130:GLN:HE21	3:N:143:ARG:HB3	1.84	0.42
1:M:242:SER:O	1:M:246:ARG:HG2	2.19	0.42
1:C:155:GLU:OE1	1:D:72:ILE:HG13	2.19	0.42
1:E:72:ILE:O	1:E:72:ILE:HG13	2.18	0.42
1:F:22:GLY:O	4:O:39:U:H3'	2.19	0.42
1:G:5:LYS:HB2	1:G:7:TYR:CZ	2.54	0.42
1:G:38:GLU:OE1	1:G:38:GLU:N	2.53	0.42
1:G:61:GLU:HG2	1:G:105:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:PHE:HB3	1:G:221:MET:O	2.20	0.42
2:H:57:ARG:HA	2:L:41:PHE:CE2	2.53	0.42
2:I:14:LEU:HD23	2:I:14:LEU:HA	1.81	0.42
2:I:91:ASN:OD1	2:I:92:HIS:N	2.53	0.42
5:K:416:LEU:HD22	5:K:440:TYR:HE2	1.84	0.42
1:C:69:GLU:OE1	1:C:69:GLU:N	2.39	0.42
1:D:99:ARG:HG3	1:D:122:ALA:O	2.20	0.42
2:I:16:ARG:NH2	2:I:108:GLU:OE2	2.52	0.42
3:N:4:ILE:HD13	3:N:103:HIS:CE1	2.54	0.42
3:N:182:PRO:HB3	3:N:183:ARG:NH1	2.35	0.42
5:K:325:PHE:HD2	5:K:327:LEU:HD22	1.84	0.42
5:K:350:LEU:O	5:K:354:ILE:HG12	2.19	0.42
6:A:16:TYR:CZ	6:A:61:SER:HA	2.55	0.42
1:C:240:ALA:O	1:C:243:LEU:HB2	2.19	0.42
1:C:252:LYS:HB2	1:C:252:LYS:HE3	1.82	0.42
1:E:77:ILE:HG13	1:E:78:ASP:N	2.34	0.42
1:E:257:VAL:HB	1:E:259:ARG:NH2	2.35	0.42
1:F:280:ARG:NH2	1:F:282:LEU:HD11	2.35	0.42
1:M:54:ILE:HD13	1:M:54:ILE:HA	1.82	0.42
1:M:142:THR:HG22	1:M:173:VAL:HG12	2.00	0.42
3:N:56:ILE:C	3:N:57:LEU:HD22	2.40	0.42
5:K:363:MET:HG2	5:K:364:VAL:N	2.34	0.42
5:K:385:VAL:HG22	5:K:386:LEU:H	1.84	0.42
5:K:408:ASN:HA	5:K:443:ARG:HH22	1.85	0.42
1:B:53:PHE:CZ	1:B:57:THR:HG21	2.55	0.42
1:E:57:THR:OG1	1:E:58:GLN:OE1	2.20	0.42
1:F:3:ILE:HD12	1:F:3:ILE:H	1.85	0.42
1:F:51:ARG:NE	1:F:108:ASP:OD1	2.52	0.42
1:G:7:TYR:CE1	1:G:230:GLU:HG2	2.55	0.42
1:G:103:CYS:O	1:G:110:ARG:HD3	2.19	0.42
5:K:348:ALA:O	5:K:352:GLU:HG2	2.18	0.42
5:K:464:ARG:HH21	5:K:464:ARG:HG3	1.83	0.42
2:L:71:ARG:HA	2:L:74:GLN:NE2	2.21	0.42
1:F:212:HIS:O	1:F:212:HIS:ND1	2.51	0.42
1:M:72:ILE:H	1:M:72:ILE:HD12	1.85	0.42
5:K:545:ARG:NH2	5:K:547:PRO:HA	2.35	0.42
1:B:243:LEU:HD21	1:B:277:LYS:HE2	2.01	0.42
1:D:51:ARG:HE	1:D:108:ASP:CG	2.23	0.42
1:F:66:PHE:O	1:F:66:PHE:CG	2.72	0.42
1:F:270:ASP:OD2	1:F:270:ASP:N	2.51	0.42
2:I:28:ALA:HB1	2:I:65:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:69:GLU:OE1	2:J:69:GLU:N	2.46	0.42
2:J:105:TYR:HD2	2:J:106:TYR:CD1	2.37	0.42
3:N:10:ASP:O	3:N:97:ASP:N	2.37	0.42
3:N:144:GLU:O	3:N:146:PRO:HD3	2.20	0.42
5:K:433:ARG:HE	5:K:433:ARG:HB3	1.69	0.42
1:B:105:ARG:NH2	1:B:106:TYR:OH	2.53	0.42
1:B:280:ARG:NH2	1:B:282:LEU:HD11	2.34	0.42
1:C:229:PHE:HE1	1:C:279:LEU:HD22	1.85	0.42
1:D:44:VAL:HG12	4:O:26:G:H5"	2.00	0.42
1:E:272:ASN:OD1	1:E:273:LEU:N	2.53	0.42
1:F:32:ILE:O	1:F:34:PRO:HD3	2.20	0.42
5:K:524:GLU:OE1	5:K:524:GLU:N	2.51	0.42
1:B:51:ARG:HE	1:B:108:ASP:CG	2.24	0.41
1:D:277:LYS:HD3	1:D:277:LYS:N	2.35	0.41
1:E:132:THR:HG22	1:E:181:HIS:O	2.20	0.41
1:G:251:LYS:NZ	1:G:258:VAL:HA	2.34	0.41
2:I:116:ASP:HA	2:I:119:LYS:HE2	2.01	0.41
1:M:246:ARG:NH1	1:M:272:ASN:H	2.19	0.41
3:N:69:GLU:O	3:N:87:ARG:HA	2.20	0.41
1:B:48:ARG:HD3	4:O:14:C:P	2.60	0.41
1:C:78:ASP:O	1:C:81:HIS:N	2.52	0.41
1:E:29:LEU:HA	1:E:171:PHE:CD2	2.55	0.41
1:E:143:LEU:HD13	1:E:174:PRO:HD3	2.01	0.41
2:J:74:GLN:HA	2:J:122:PHE:CE1	2.56	0.41
3:N:70:VAL:HG23	3:N:86:ASN:HB3	2.02	0.41
5:K:10:TYR:O	5:K:13:LYS:HG3	2.20	0.41
5:K:535:GLU:OE2	5:K:539:ILE:HG12	2.20	0.41
1:B:121:ASN:HB2	6:A:18:PRO:HG3	2.02	0.41
1:D:249:VAL:HG12	1:D:266:VAL:HG22	2.02	0.41
1:D:275:GLU:HB2	1:D:277:LYS:HZ1	1.84	0.41
1:E:16:GLN:HG3	1:E:220:GLN:OE1	2.21	0.41
1:E:125:VAL:HG12	1:E:126:ARG:H	1.85	0.41
3:N:2:ARG:HH11	3:N:103:HIS:HB3	1.84	0.41
3:N:163:ASP:O	3:N:165:THR:HG23	2.20	0.41
1:E:154:ASN:OD1	1:E:155:GLU:N	2.52	0.41
1:E:232:SER:N	1:E:277:LYS:HZ3	2.12	0.41
2:H:75:LEU:O	2:H:79:ILE:HG13	2.19	0.41
2:I:16:ARG:CB	2:I:108:GLU:HG3	2.50	0.41
2:I:105:TYR:O	2:I:109:THR:HG23	2.21	0.41
2:J:51:VAL:HG13	2:J:52:PHE:CD2	2.52	0.41
1:M:95:THR:HG21	1:M:119:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:148:THR:OG1	1:M:149:ARG:N	2.53	0.41
5:K:506:ILE:HG23	5:K:547:PRO:O	2.20	0.41
1:C:43:ASP:OD1	1:C:44:VAL:N	2.53	0.41
1:C:111:THR:OG1	1:C:194:PHE:HE2	2.03	0.41
1:D:48:ARG:HB2	4:O:26:G:H5'	2.02	0.41
1:F:269:ASP:N	1:F:269:ASP:OD1	2.53	0.41
2:H:57:ARG:CA	2:L:41:PHE:HE2	2.33	0.41
2:J:96:GLU:HG2	2:J:97:GLN:N	2.35	0.41
3:N:64:ASN:OD1	3:N:93:MET:HG2	2.20	0.41
2:L:21:LEU:HD13	2:L:55:LEU:HD13	2.03	0.41
1:B:251:LYS:H	1:B:251:LYS:HG3	1.71	0.41
1:C:224:ARG:HD3	1:C:224:ARG:HA	1.77	0.41
1:F:147:ILE:HD13	1:G:31:ARG:HH12	1.86	0.41
1:G:252:LYS:HG3	1:G:255:VAL:H	1.85	0.41
2:I:3:LEU:HD22	2:I:111:PHE:HB2	2.03	0.41
1:M:138:ASP:OD2	1:M:264:TYR:OH	2.18	0.41
3:N:18:GLU:O	3:N:19:LEU:HD22	2.21	0.41
4:O:39:U:O2'	4:O:40:C:O4'	2.39	0.41
5:K:396:ASP:OD1	5:K:400:GLN:HG3	2.21	0.41
1:B:177:LEU:HD11	1:B:261:PHE:HE1	1.84	0.41
1:D:48:ARG:HD3	4:O:26:G:H5'	2.02	0.41
1:D:218:ARG:HD2	1:D:221:MET:HE1	2.02	0.41
1:E:6:ARG:HD3	1:E:184:ILE:O	2.21	0.41
1:E:128:PRO:O	1:E:184:ILE:HA	2.21	0.41
2:H:93:LEU:HD12	2:H:93:LEU:HA	1.93	0.41
2:H:120:ASN:HA	2:H:123:ASN:OD1	2.21	0.41
3:N:57:LEU:HB2	3:N:99:ALA:O	2.21	0.41
5:K:213:GLY:HA3	5:K:258:LEU:CD2	2.49	0.41
5:K:246:ALA:HA	5:K:249:GLU:HG3	2.02	0.41
1:C:143:LEU:HD13	1:C:174:PRO:HD3	2.01	0.41
1:E:246:ARG:HH11	1:E:270:ASP:CA	2.32	0.41
1:F:78:ASP:O	1:F:81:HIS:N	2.54	0.41
2:L:4:ASP:O	2:L:7:ARG:HG2	2.21	0.41
1:B:81:HIS:CG	1:B:120:LYS:HD2	2.56	0.41
1:B:153:THR:O	1:C:73:LEU:HB2	2.20	0.41
1:B:248:GLN:NE2	1:B:267:SER:HB3	2.36	0.41
1:D:183:PHE:O	1:D:184:ILE:HD13	2.20	0.41
1:E:21:ASN:ND2	1:E:42:THR:H	2.17	0.41
1:E:29:LEU:HA	1:E:171:PHE:HD2	1.86	0.41
1:F:47:LYS:HZ3	1:F:131:LEU:HB2	1.86	0.41
1:F:169:ARG:HD3	1:F:169:ARG:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:ASP:OD2	1:G:36:THR:N	2.37	0.41
2:H:68:PHE:HB3	2:H:71:ARG:HG2	2.03	0.41
2:I:7:ARG:HD2	2:I:12:TYR:CG	2.56	0.41
2:J:3:LEU:HD12	2:J:107:HIS:HB3	2.03	0.41
2:J:37:ALA:HB1	2:J:41:PHE:HE2	1.86	0.41
4:O:4:G:C6	4:O:5:A:C2	3.09	0.41
5:K:294:LYS:HZ3	6:A:31:GLY:HA2	1.86	0.41
2:L:4:ASP:HB2	2:L:7:ARG:HD3	2.02	0.41
1:B:84:GLU:HG2	1:B:85:ASN:N	2.36	0.41
1:B:249:VAL:HA	1:B:265:LEU:O	2.21	0.41
1:E:46:LEU:O	1:E:50:VAL:HG23	2.21	0.41
1:G:135:ARG:O	1:G:179:ARG:N	2.50	0.41
1:G:205:ALA:HA	1:G:208:ASN:OD1	2.21	0.41
1:G:233:ASN:OD1	1:G:234:ASN:N	2.55	0.41
2:H:106:TYR:O	2:H:109:THR:OG1	2.30	0.41
1:M:68:ARG:NH1	3:N:80:SER:HB2	2.36	0.41
3:N:180:SER:HB2	3:N:185:SER:H	1.86	0.41
3:N:189:GLU:O	5:K:194:ILE:HD11	2.20	0.41
1:C:87:LYS:HZ3	1:C:90:GLU:HA	1.85	0.40
1:E:146:SER:HB2	1:E:167:MET:HB3	2.04	0.40
1:F:40:LEU:HD23	1:F:40:LEU:HA	1.91	0.40
2:J:77:TRP:CH2	2:J:121:LEU:HB3	2.56	0.40
3:N:29:ILE:HB	3:N:100:TYR:CE1	2.56	0.40
3:N:65:ILE:HG22	3:N:92:SER:HB2	2.03	0.40
5:K:264:PHE:CE2	5:K:266:ILE:HD11	2.52	0.40
5:K:523:LEU:HD23	5:K:529:ALA:HB2	2.03	0.40
2:L:49:ILE:HD12	2:L:49:ILE:H	1.86	0.40
1:C:54:ILE:HA	1:C:54:ILE:HD13	1.86	0.40
1:C:56:MET:HB3	1:D:187:HIS:HD1	1.85	0.40
1:E:218:ARG:HG2	1:E:221:MET:CE	2.51	0.40
1:F:89:LYS:HB2	1:F:94:LYS:N	2.36	0.40
1:F:177:LEU:HD12	1:F:177:LEU:HA	1.86	0.40
1:G:126:ARG:HD3	1:G:188:PHE:CZ	2.56	0.40
2:H:69:GLU:OE1	2:H:69:GLU:N	2.54	0.40
2:J:18:PHE:HA	2:J:21:LEU:HD12	2.03	0.40
1:M:213:ASP:HB3	1:M:218:ARG:HH22	1.86	0.40
3:N:31:PRO:HG2	3:N:192:PHE:CZ	2.56	0.40
1:C:10:VAL:HG12	1:C:227:TYR:HB2	2.04	0.40
1:F:2:THR:HG21	1:F:190:LYS:HG3	2.02	0.40
1:F:85:ASN:HB3	1:F:88:GLY:HA3	2.03	0.40
1:G:9:PHE:HE1	1:G:184:ILE:HG13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:94:ASN:O	2:I:98:GLN:HG3	2.21	0.40
2:I:96:GLU:HG2	2:I:97:GLN:N	2.36	0.40
1:M:189:ALA:O	1:M:193:GLY:N	2.55	0.40
3:N:21:VAL:O	3:N:90:ARG:NH2	2.47	0.40
4:O:27:G:H1'	4:O:28:U:C6	2.56	0.40
4:O:39:U:H1'	4:O:40:C:N3	2.37	0.40
5:K:12:ARG:HH22	5:K:278:ARG:HD3	1.86	0.40
2:L:21:LEU:HD21	2:L:59:LEU:HD12	2.02	0.40
6:A:47:GLU:OE1	6:A:47:GLU:HA	2.22	0.40
1:B:136:SER:HB3	1:B:178:TYR:CE1	2.56	0.40
1:C:48:ARG:HD3	4:O:20:G:OP2	2.22	0.40
1:C:225:GLY:HA2	1:C:283:GLY:HA3	2.03	0.40
1:E:232:SER:H	1:E:277:LYS:NZ	2.14	0.40
1:F:126:ARG:HD3	1:F:188:PHE:CZ	2.57	0.40
2:H:25:GLN:HE22	2:H:36:ILE:HG21	1.86	0.40
2:H:100:LEU:HA	2:H:103:ILE:HD12	2.04	0.40
2:I:20:VAL:O	2:I:24:ILE:HG13	2.22	0.40
1:B:5:LYS:HE2	1:B:231:HIS:O	2.21	0.40
1:C:280:ARG:HH12	1:C:282:LEU:HD11	1.87	0.40
3:N:30:THR:HG22	3:N:32:ALA:N	2.37	0.40
3:N:124:MET:HA	3:N:127:ARG:NE	2.32	0.40
5:K:351:SER:OG	5:K:352:GLU:OE2	2.27	0.40

There are no symmetry-related clashes.

5.3　Torsion angles　ⓘ

5.3.1　Protein backbone　ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	B	281/283 (99%)	256 (91%)	25 (9%)	0	100	100
1	C	281/283 (99%)	254 (90%)	27 (10%)	0	100	100
1	D	281/283 (99%)	250 (89%)	31 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	281/283 (99%)	264 (94%)	17 (6%)	0	100	100
1	F	261/283 (92%)	248 (95%)	13 (5%)	0	100	100
1	G	267/283 (94%)	245 (92%)	22 (8%)	0	100	100
1	M	260/283 (92%)	227 (87%)	33 (13%)	0	100	100
2	H	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
2	I	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
2	J	122/124 (98%)	115 (94%)	7 (6%)	0	100	100
2	L	108/124 (87%)	106 (98%)	2 (2%)	0	100	100
3	N	203/205 (99%)	172 (85%)	31 (15%)	0	100	100
5	K	405/409 (99%)	368 (91%)	36 (9%)	1 (0%)	47	78
6	A	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
All	All	3062/3161 (97%)	2800 (91%)	261 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	K	314	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 PDB entries followed by that with respect to all EM entries.

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	B	245/245 (100%)	245 (100%)	0	100	100
1	C	245/245 (100%)	243 (99%)	2 (1%)	81	91
1	D	245/245 (100%)	245 (100%)	0	100	100
1	E	245/245 (100%)	245 (100%)	0	100	100
1	F	230/245 (94%)	229 (100%)	1 (0%)	91	95
1	G	235/245 (96%)	235 (100%)	0	100	100
1	M	229/245 (94%)	228 (100%)	1 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	104/104 (100%)	103 (99%)	1 (1%)	76	88
2	I	104/104 (100%)	103 (99%)	1 (1%)	76	88
2	J	104/104 (100%)	104 (100%)	0	100	100
2	L	94/104 (90%)	93 (99%)	1 (1%)	73	86
3	N	181/181 (100%)	180 (99%)	1 (1%)	86	94
5	K	334/336 (99%)	333 (100%)	1 (0%)	92	97
6	A	57/57 (100%)	56 (98%)	1 (2%)	59	79
All	All	2652/2705 (98%)	2642 (100%)	10 (0%)	91	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	85	ASN
1	C	141	MET
1	F	74	ASN
2	H	65	LYS
2	I	65	LYS
1	M	271	LYS
3	N	120	LYS
5	K	13	LYS
2	L	71	ARG
6	A	67	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	HIS
1	B	187	HIS
1	C	52	ASN
1	C	74	ASN
1	D	75	ASN
1	E	21	ASN
1	G	100	GLN
1	G	204	GLN
1	G	222	ASN
2	I	64	ASN
1	M	21	ASN
1	M	130	GLN

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Mol	Chain	Res	Type
1	M	231	HIS
1	M	234	ASN
3	N	199	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	O	41/42 (97%)	25 (60%)	2 (4%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	O	3	U
4	O	4	G
4	O	6	A
4	O	9	A
4	O	13	U
4	O	15	A
4	O	16	G
4	O	19	U
4	O	20	G
4	O	21	C
4	O	22	C
4	O	23	G
4	O	24	U
4	O	25	A
4	O	27	G
4	O	31	C
4	O	32	A
4	O	33	U
4	O	34	C
4	O	36	C
4	O	37	C
4	O	38	C
4	O	39	U
4	O	40	C
4	O	41	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	O	24	U
4	O	39	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	16:SER	C	190:ALA	N	30.88

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-29877. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ
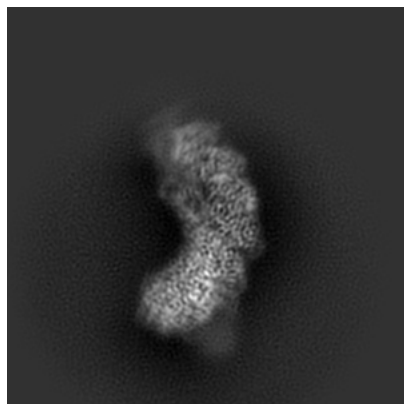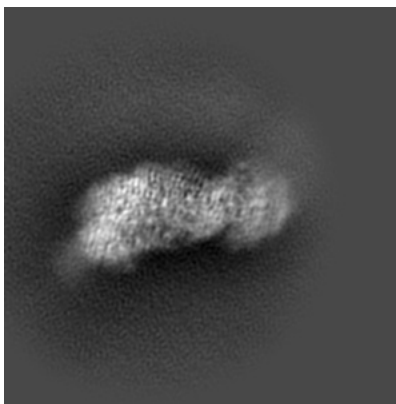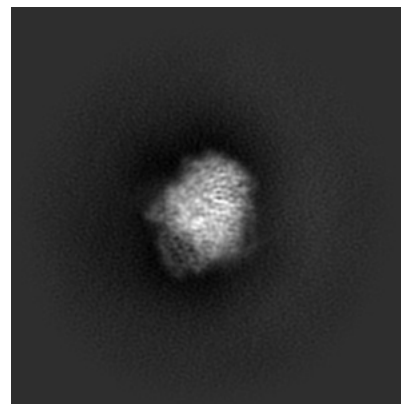
6.1.1 Primary map

X   Y   Z

6.1.2 Raw map

X   Y   Z
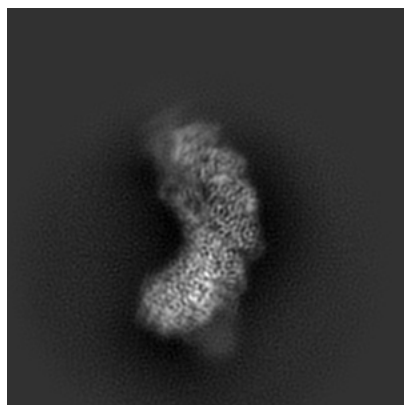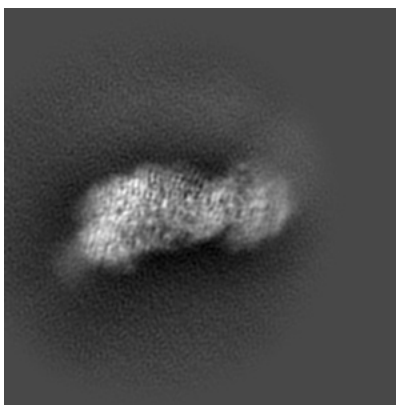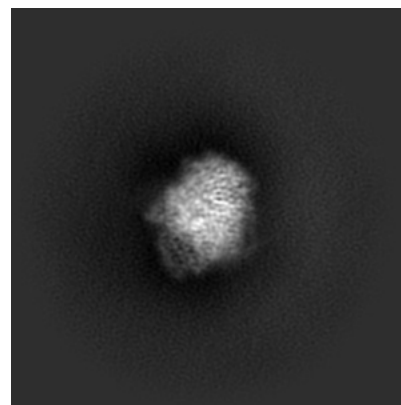
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map
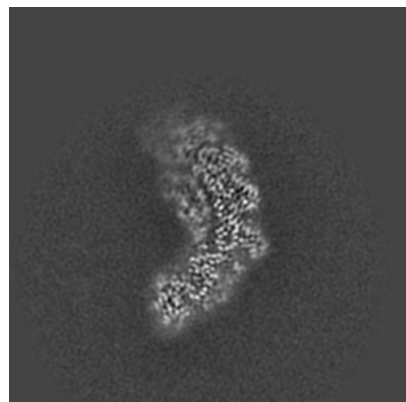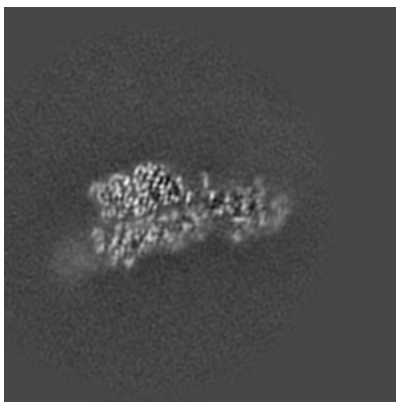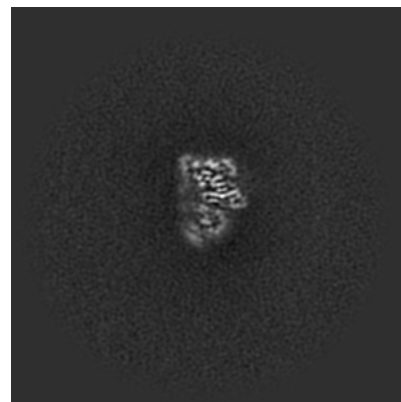
| X Index: 125 | Y Index: 125 | Z Index: 125 |

6.2.2 Raw map
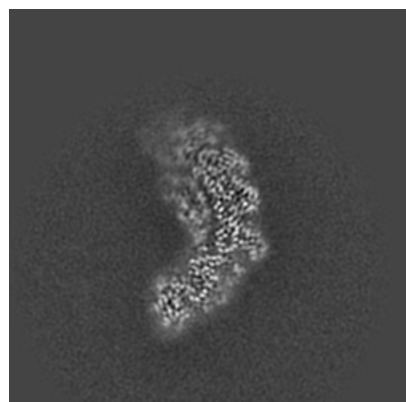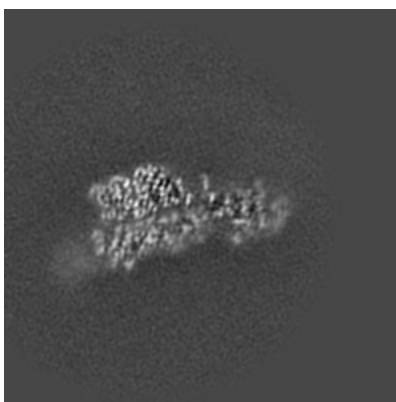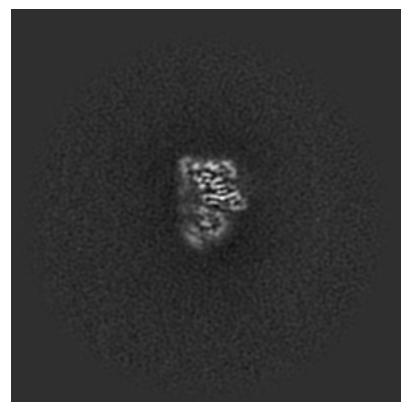
| X Index: 125 | Y Index: 125 | Z Index: 125 |

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map
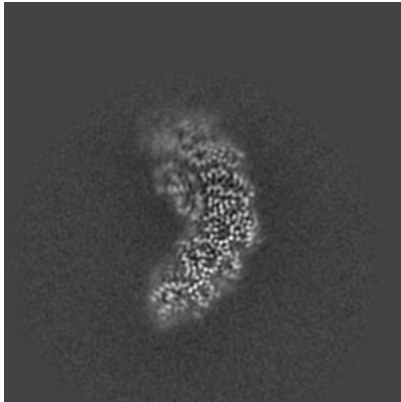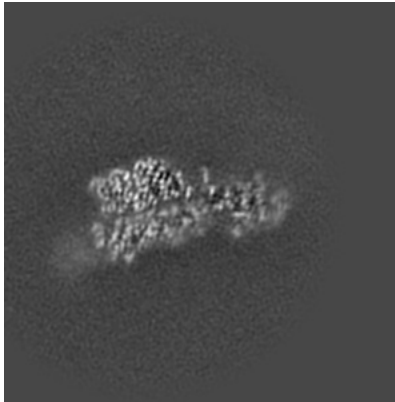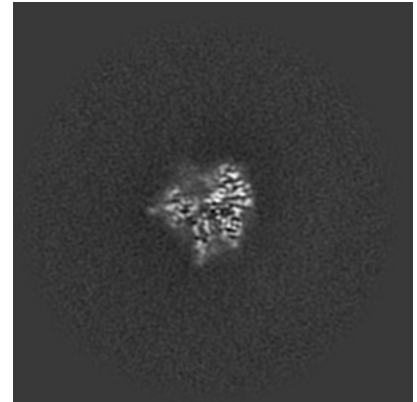
X Index: 128   Y Index: 125   Z Index: 82

6.3.2 Raw map
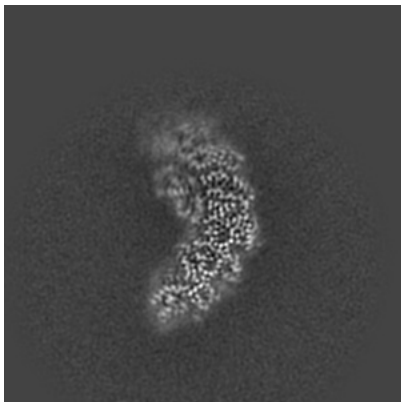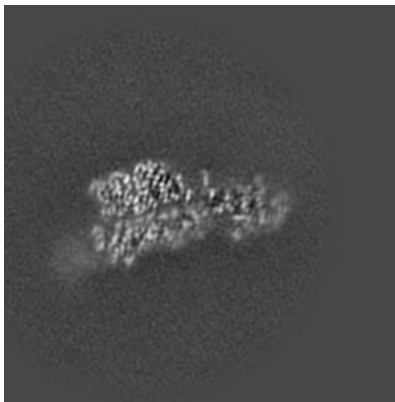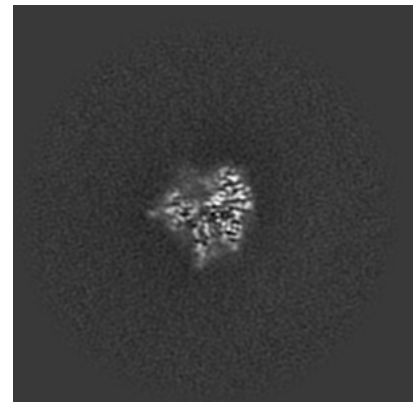
X Index: 128   Y Index: 125   Z Index: 82

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map

X

Y

Z

6.4.2 Raw map

X

Y

Z
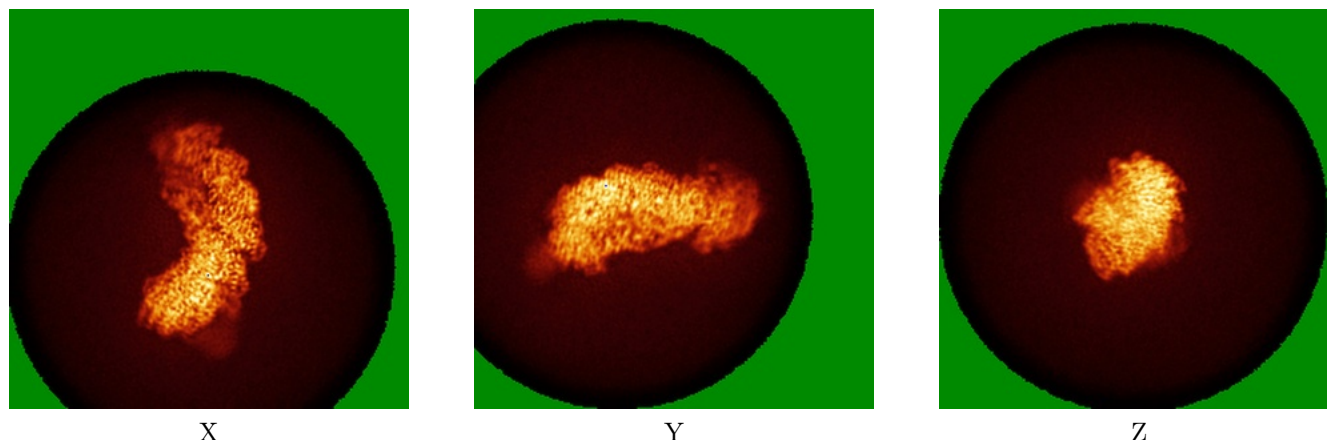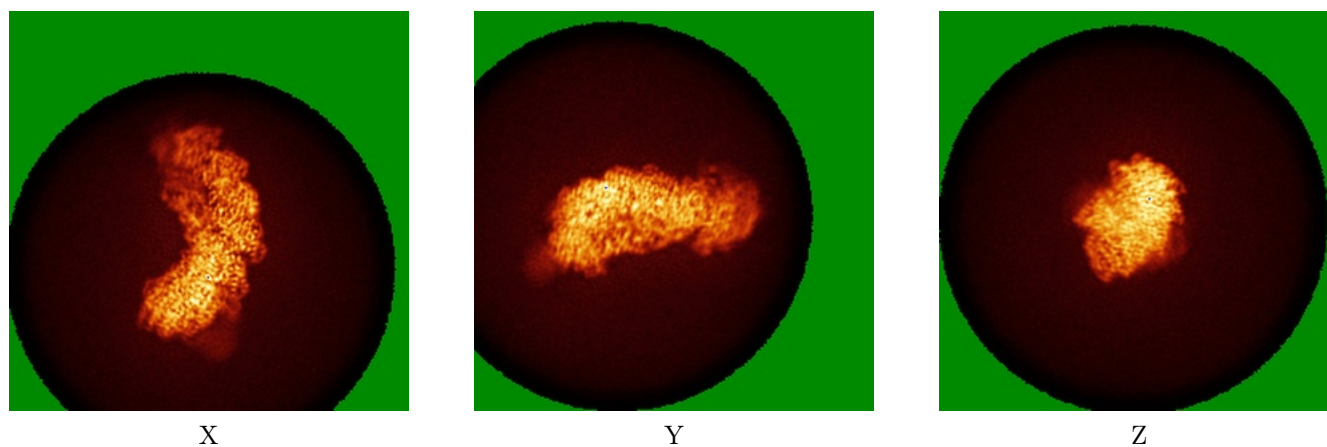
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X	Y	Z
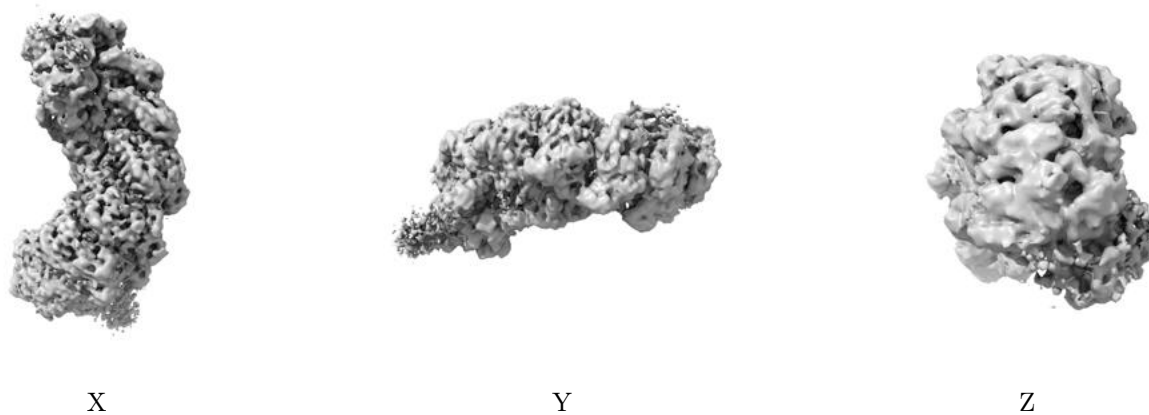
The images above show the 3D surface view of the map at the recommended contour level 0.118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X	Y	Z
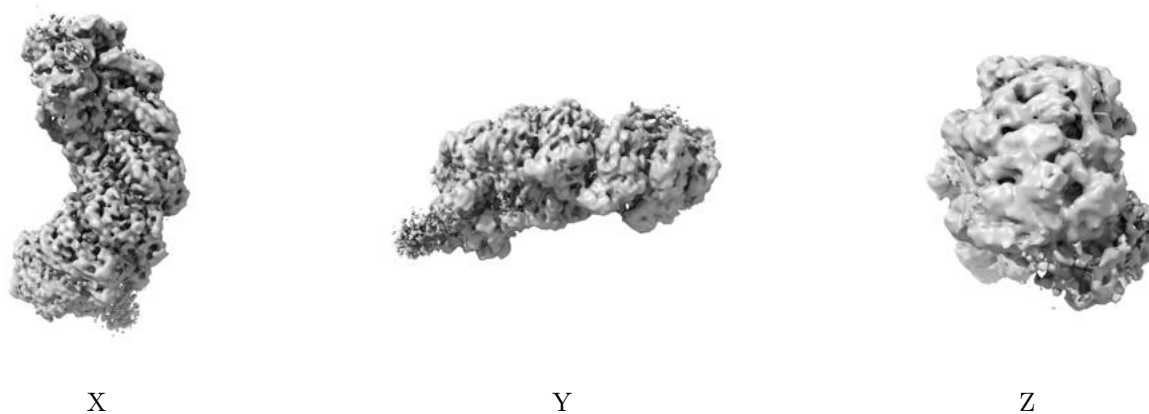
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ
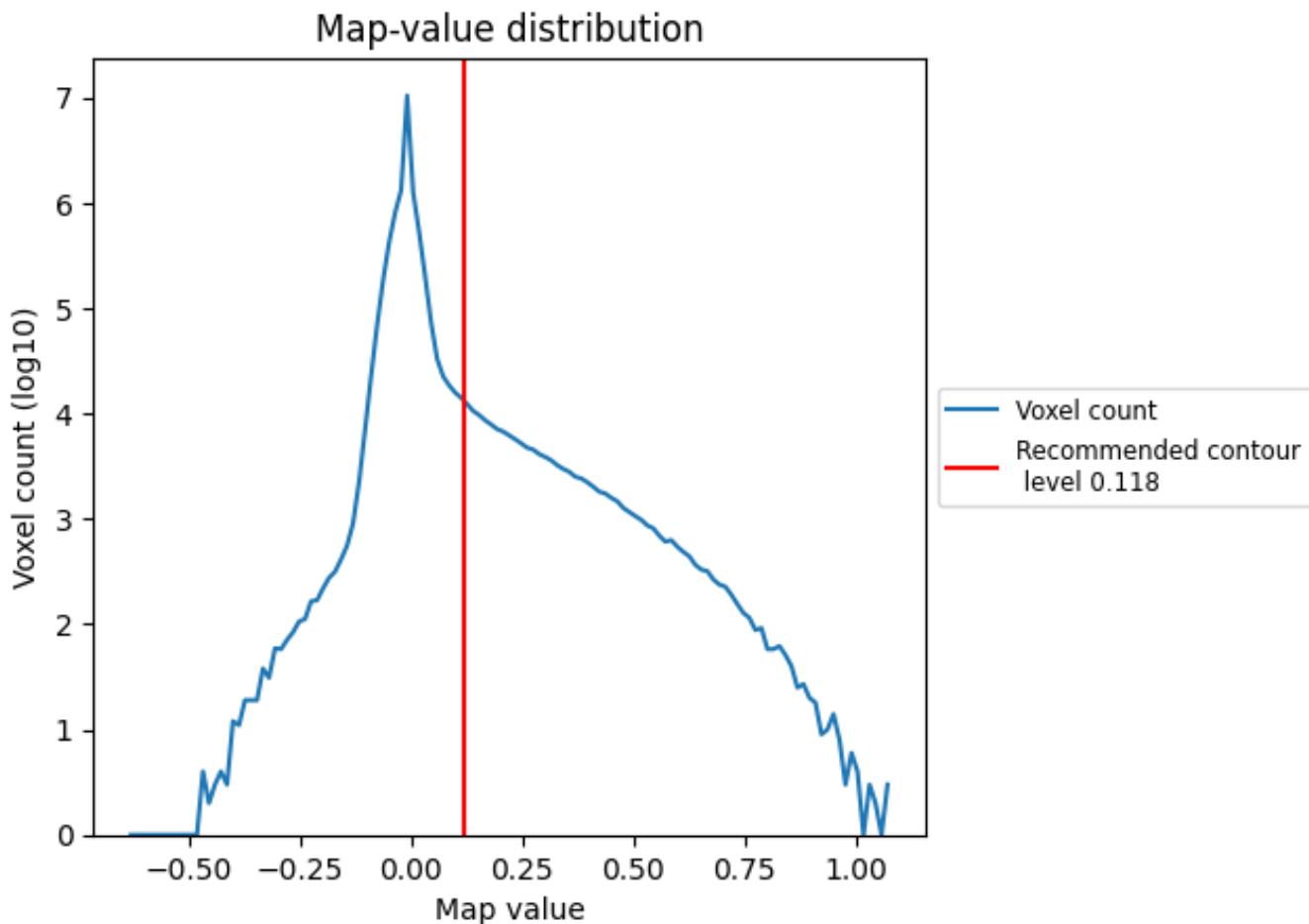
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
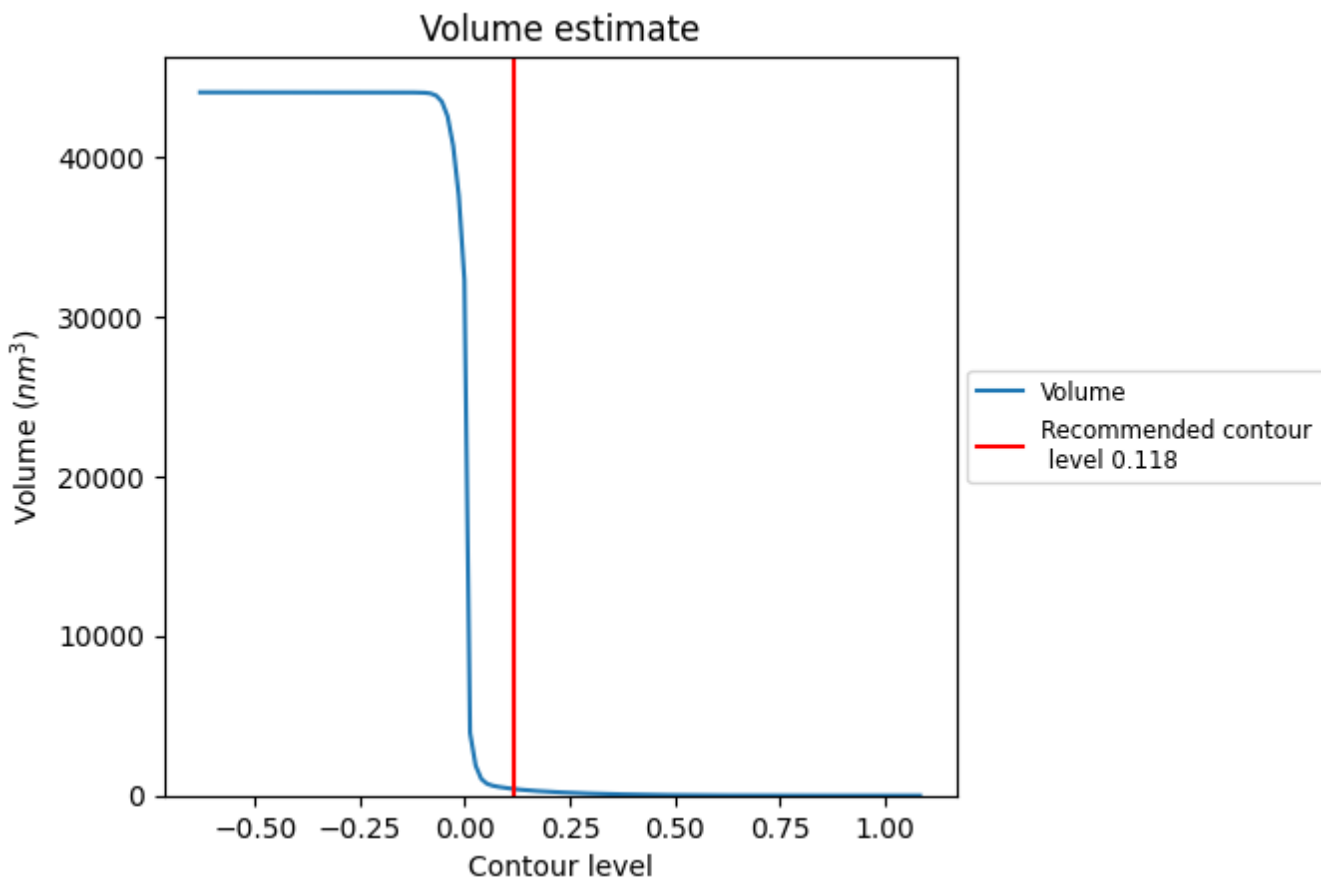
The volume at the recommended contour level is 412 nm^3; this corresponds to an approximate mass of 372 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)
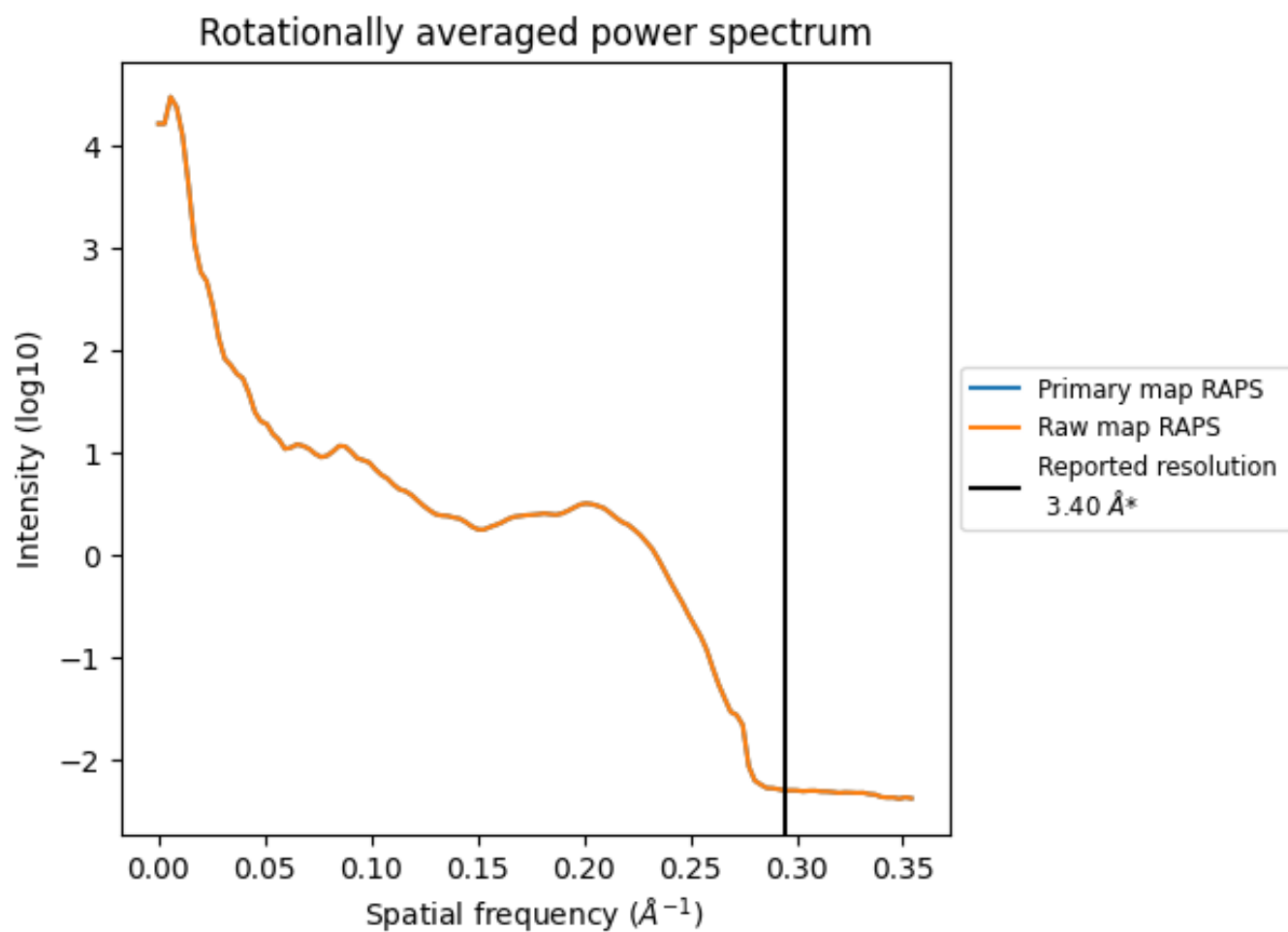
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8　Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1　FSC ⓘ
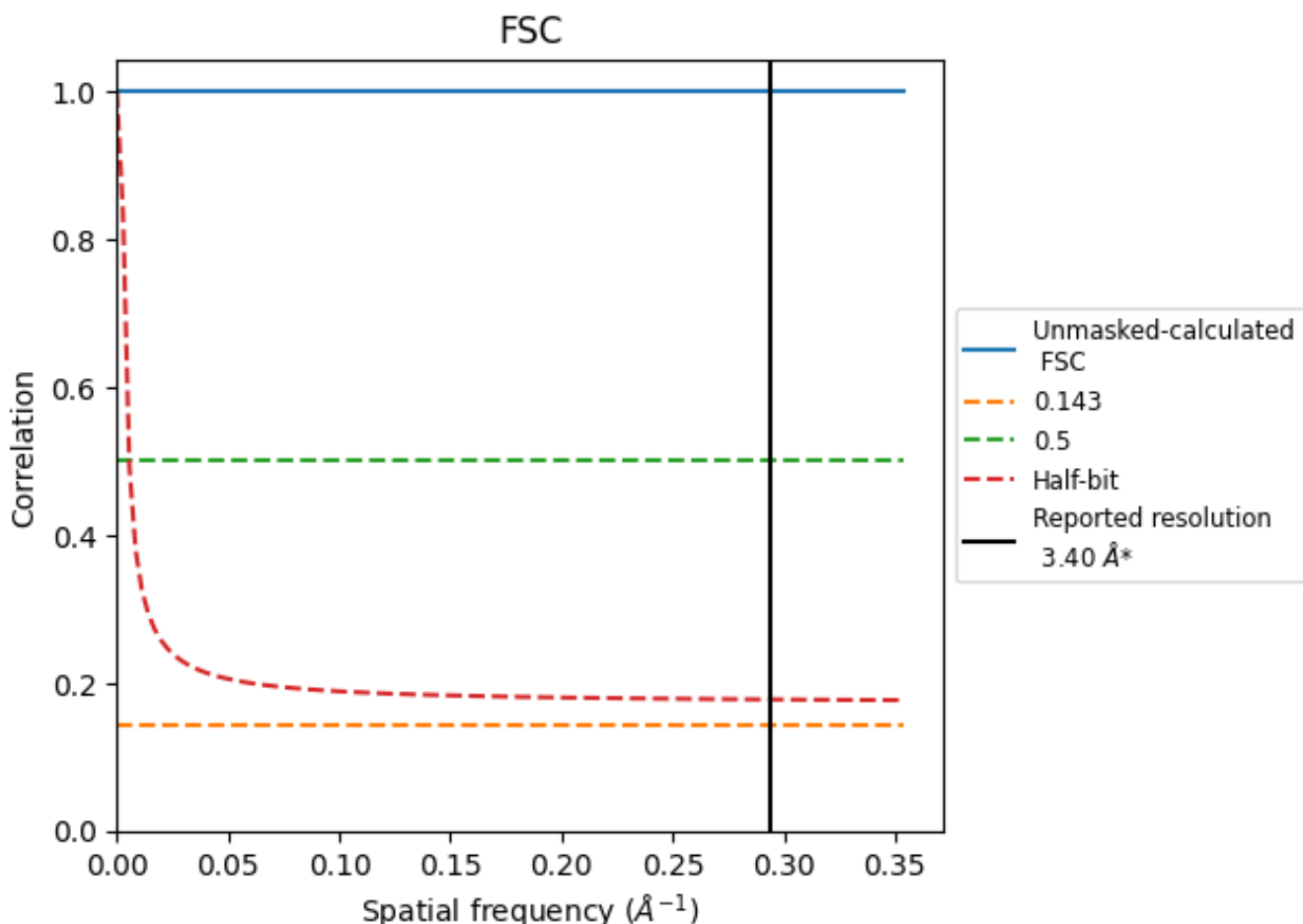
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2   Resolution estimates   ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-29877 and PDB model 8G9S. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ

| X | Y | Z |
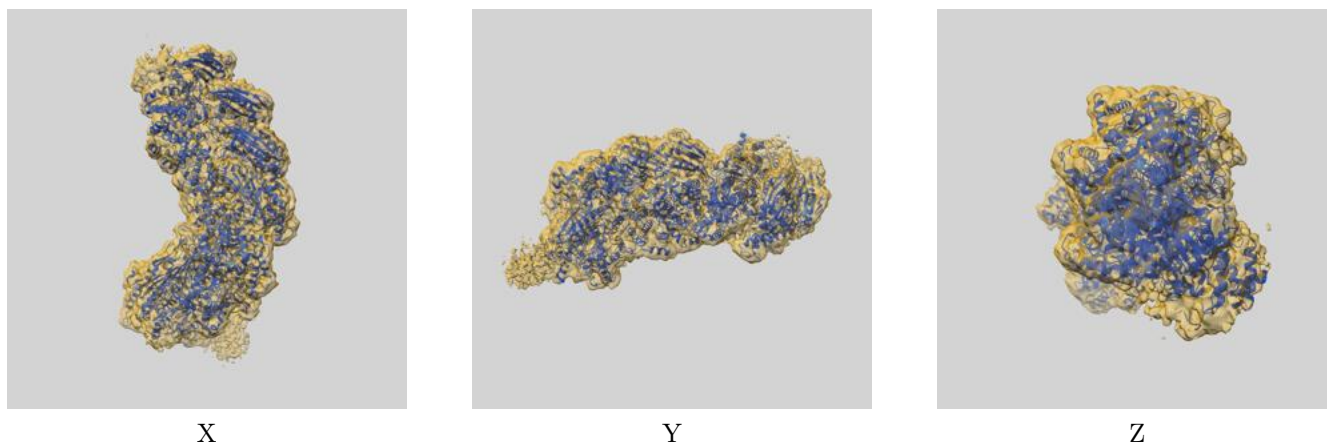
The images above show the 3D surface view of the map at the recommended contour level 0.118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z
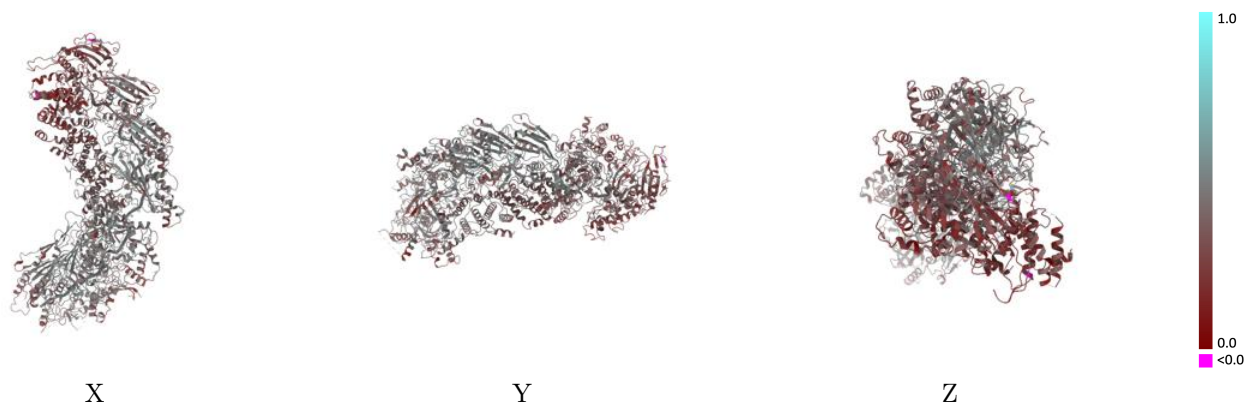
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3　Atom inclusion mapped to coordinate model ⓘ

X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z
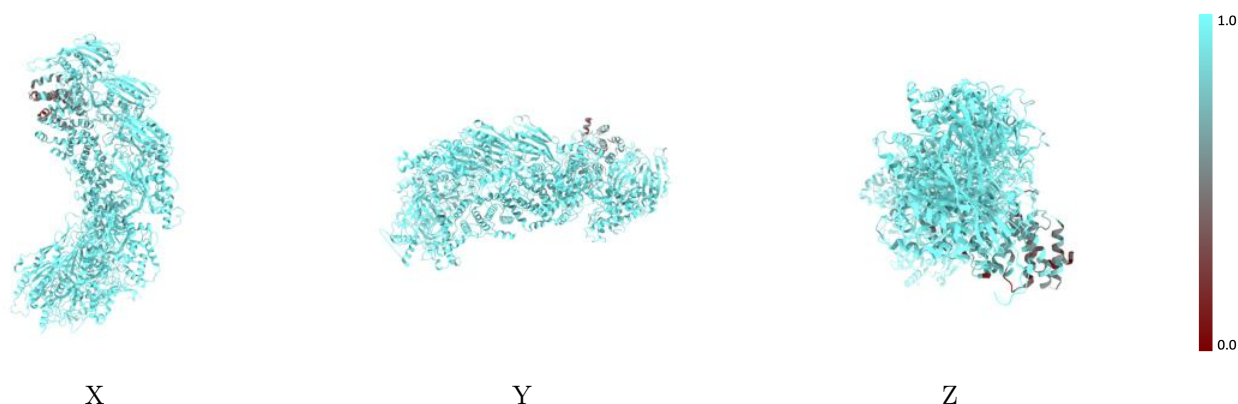
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.118).

9.4 Atom inclusion ⓘ
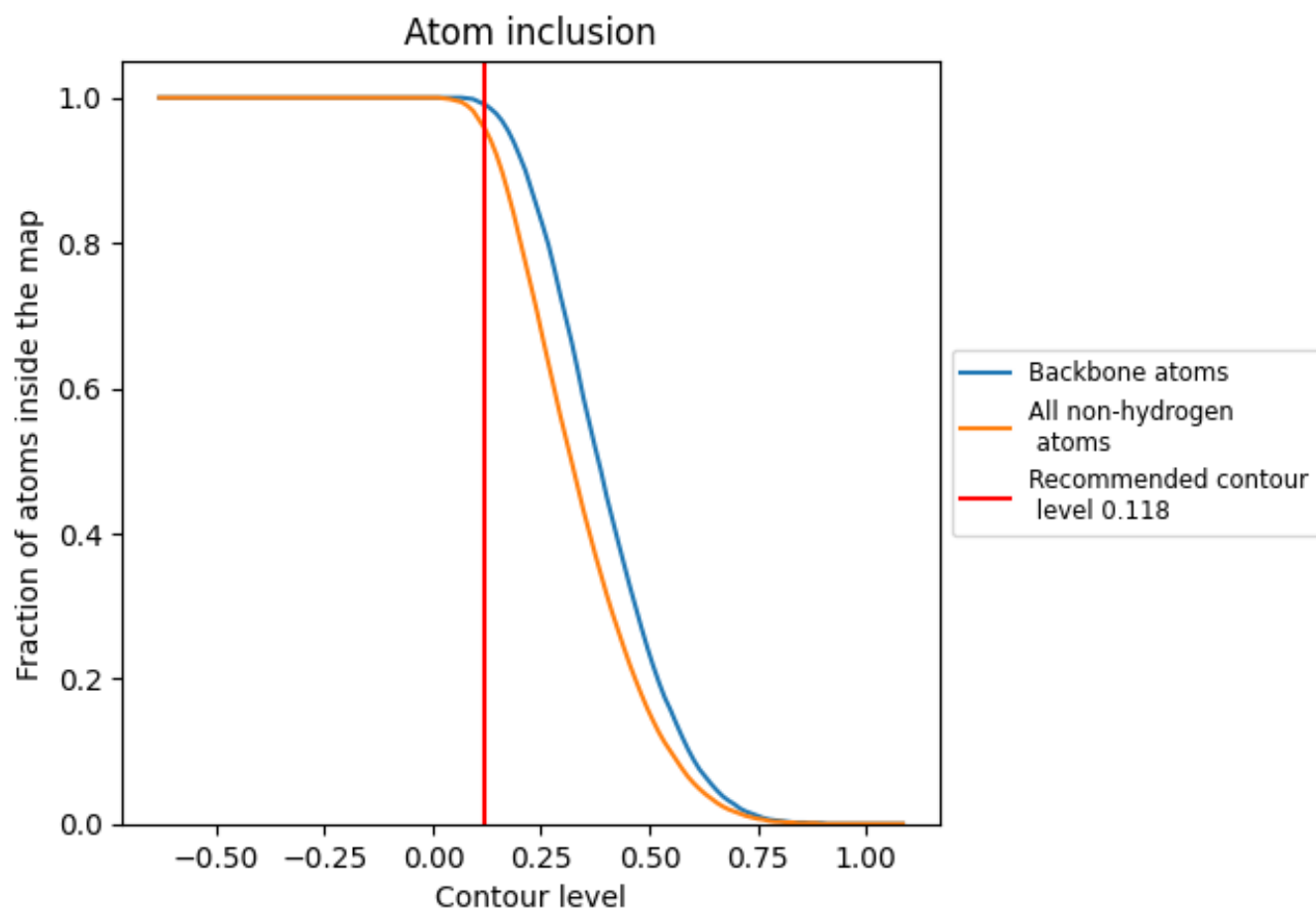
At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9590	0.4010
A	0.9790	0.3730
B	0.9930	0.4580
C	0.9840	0.4570
D	0.9790	0.4550
E	0.9630	0.4190
F	0.9660	0.3680
G	0.9400	0.2840
H	0.8500	0.3180
I	0.9480	0.3630
J	0.9860	0.3680
K	0.9850	0.4050
L	0.6140	0.2610
M	0.9950	0.4460
N	0.9880	0.4170
O	0.9970	0.4780

1.0

0.0
<0.0