W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report (i)

Mar 30, 2025 – 12:40 AM JST

PDB ID	:	8ZIR
EMDB ID	:	EMD-60127
Title	:	DUF4297-HerA complex
Authors	:	Yu, Y.; Chen, Q.
Deposited on	:	2024-05-14
Resolution	:	3.08 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:

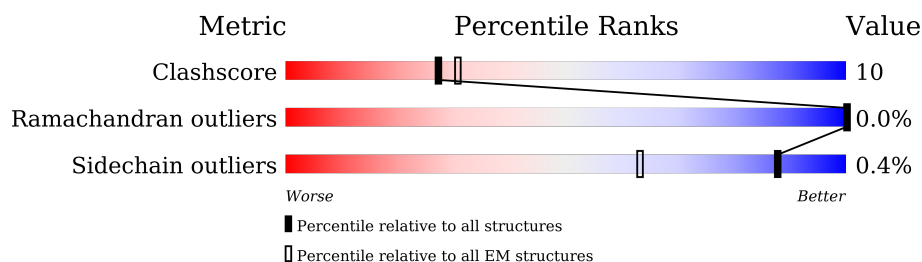|		
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 3.08 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		10
Ramachandran outliers		0.0%
Sidechain outliers		0.4%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	397	11% / 76% / 22% / •
1	B	397	• / 39% / • / 58%
1	C	397	12% / 71% / 25% / ••
1	D	397	• / 39% / • / 57%
1	E	397	13% / 73% / 24% / ••
1	F	397	• / 38% / • / 58%
1	G	397	12% / 73% / 22% / ••
1	H	397	39% / • / 58%

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Mol	Chain	Length	Quality of chain
1	I	397	11% / 71% / 25%
1	J	397	37% / 5% / 57%
1	K	397	14% / 70% / 27%
1	L	397	36% / 7% / 58%
2	M	617	11% / 69% / 19% / 12%
2	N	617	17% / 69% / 17% / 14%
2	O	617	11% / 65% / 22% / 12%
2	P	617	22% / 71% / 19% / 10%
2	Q	617	11% / 68% / 21% / 12%
2	R	617	19% / 70% / 18% / 12%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 102988 atoms, of which 50586 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 DUF4297.

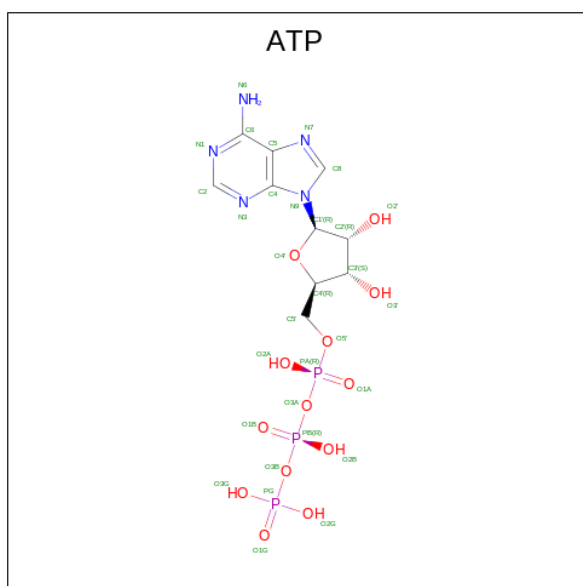| Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	0
			5985	2005	2851	545	576	8		
1	B	167	Total	C	H	N	O	S	0	0
			2789	889	1400	251	245	4		
1	C	386	Total	C	H	N	O	S	0	0
			6002	1990	2890	541	573	8		
1	D	169	Total	C	H	N	O	S	0	0
			2827	902	1418	253	250	4		
1	E	387	Total	C	H	N	O	S	0	0
			5977	1993	2859	544	573	8		
1	F	167	Total	C	H	N	O	S	0	0
			2794	889	1405	251	245	4		
1	G	380	Total	C	H	N	O	S	0	0
			5931	1965	2856	537	565	8		
1	H	168	Total	C	H	N	O	S	0	0
			2806	893	1409	252	248	4		
1	I	385	Total	C	H	N	O	S	0	0
			5959	1988	2851	542	570	8		
1	J	169	Total	C	H	N	O	S	0	0
			2827	902	1418	253	250	4		
1	K	384	Total	C	H	N	O	S	0	0
			5948	1985	2846	541	568	8		
1	L	168	Total	C	H	N	O	S	0	0
			2806	893	1409	252	248	4		

- Molecule 2 is a protein called HerA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	546	Total	C	H	N	O	S	0	0
			8430	2709	4189	713	806	13		
2	N	531	Total	C	H	N	O	S	0	0
			8172	2619	4065	694	781	13		
2	O	543	Total	C	H	N	O	S	0	0
			8390	2697	4168	710	802	13		

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

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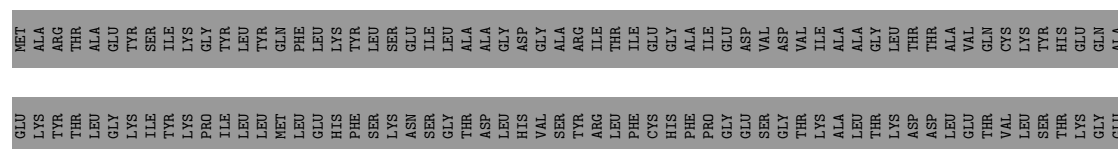| Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	553	Total	C	H	N	O	S	0	0
			8479	2719	4211	724	812	13		
2	Q	546	Total	C	H	N	O	S	0	0
			8401	2703	4168	708	809	13		
2	R	543	Total	C	H	N	O	S	0	0
			8333	2675	4137	707	801	13		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
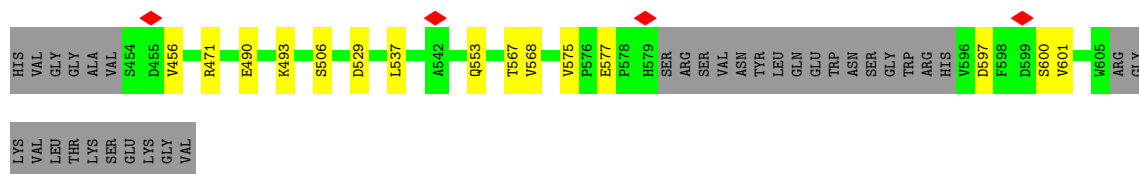

ATP

Mol	Chain	Residues	Atoms						AltConf
3	M	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	O	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	Q	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

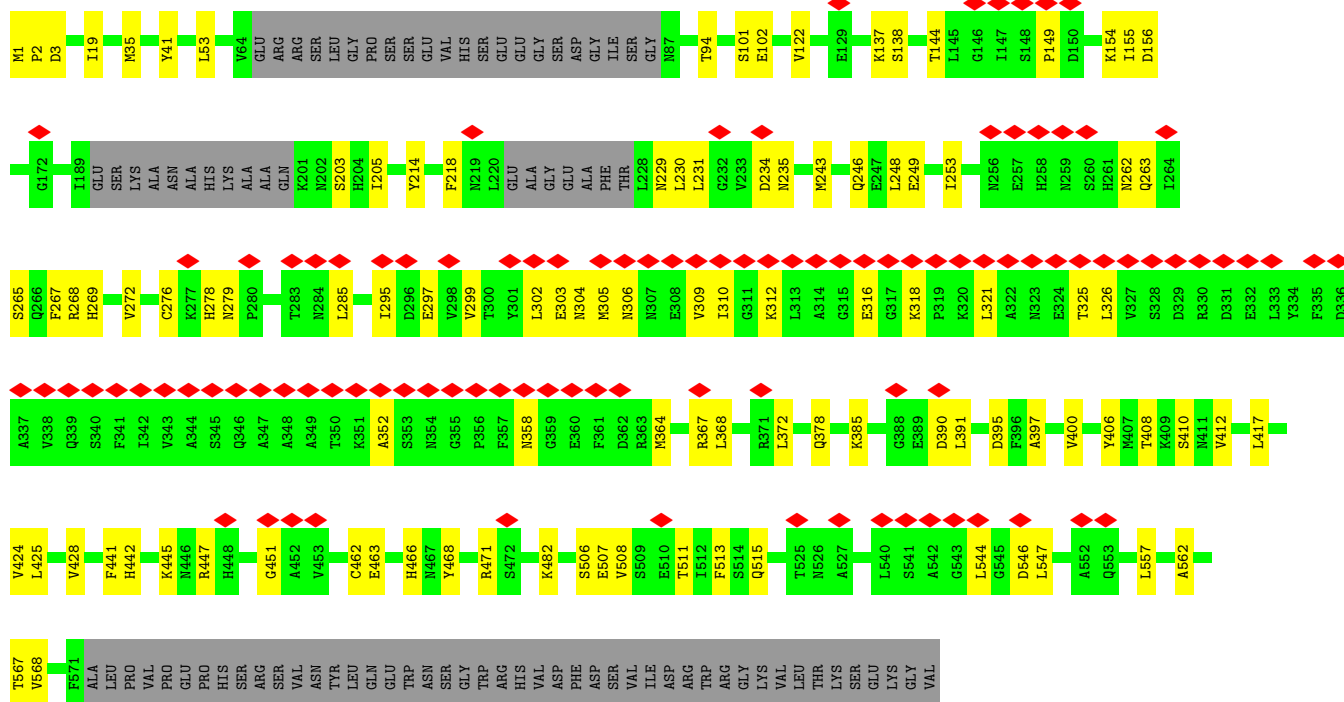- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

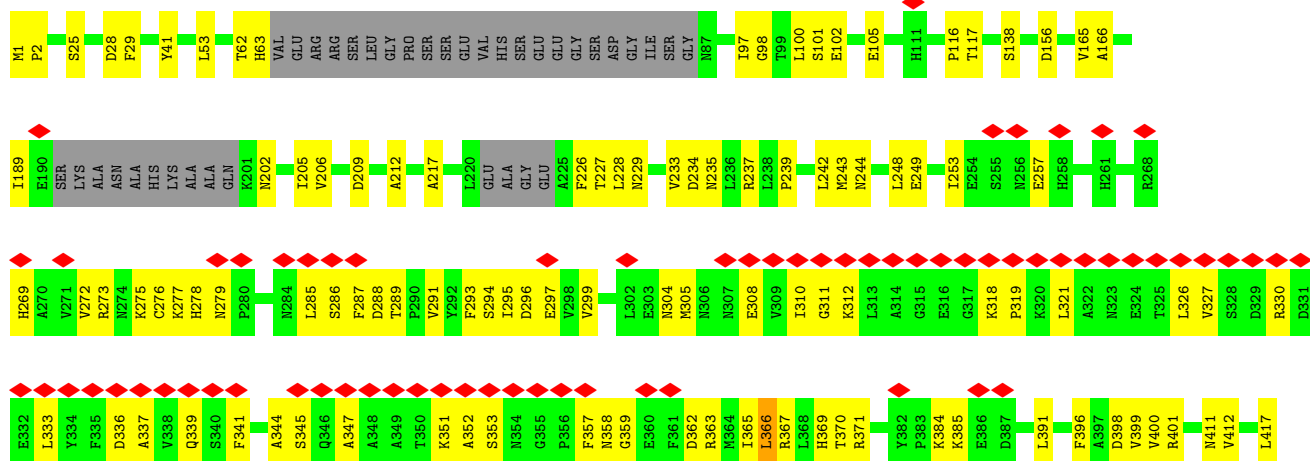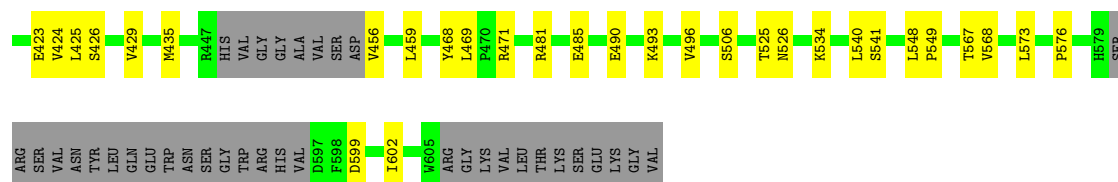| Mol	Chain	Residues	Atoms		AltConf
4	M	1	Total	Mg	0
			1	1	
4	O	1	Total	Mg	0
			1	1	
4	Q	1	Total	Mg	0
			1	1	

3 Residue-property plots ⓘ
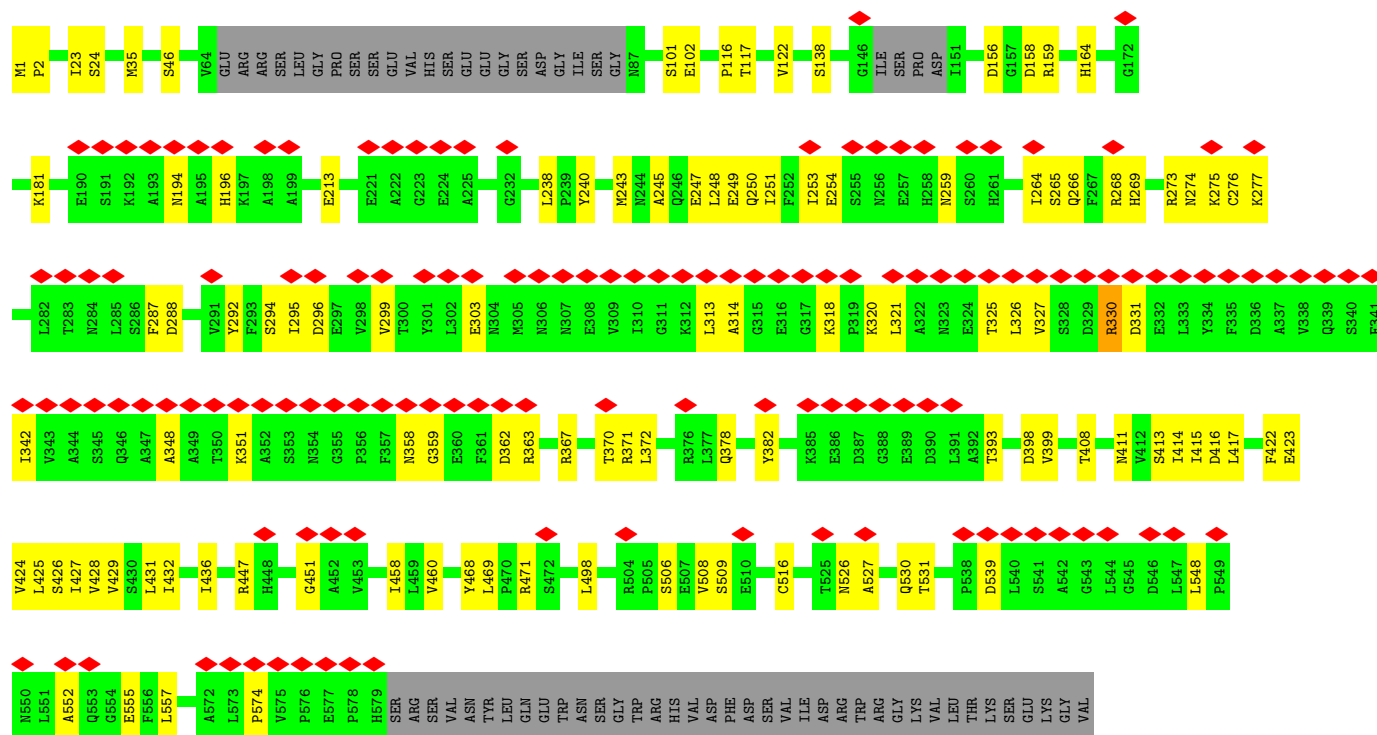
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DUF4297

Chain A:

• Molecule 1: DUF4297

Chain B:

• Molecule 1: DUF4297

Chain C:

12%

71% 25%

Chain D:

39% 57%

• Molecule 1: DUF4297

• Molecule 1: DUF4297

Chain E:

13%

73% 24%

C307 E308 T309 T315 D316 R324 I327 R340 K343 Q352 P355 D366 E367 V373 S384 D385 L386 R393 A397

• Molecule 1: DUF4297

Chain F:

38% • 58%

MET ALA ARG THR ALA GLU TYR SER ILE LYS GLY TYR LEU TYR GLN LEU PHE LEU LYS LEU SER GLU ILE LEU ALA ALA GLY ASP GLY ALA ARG ILE THR ILE GLU GLY ALA ILE GLU ASP VAL VAL ILE ALA ALA GLY LEU THR THR ALA VAL GLN CYS TYR HIS GLN ALA

GLU LYS TYR THR LEU GLY LYS ILE TYR LYS PRO ILE LEU LEU MET LEU GLU HIS PHE SER LYS ASN SER GLY THR ASP LEU HIS VAL SER THR TYR ARG LEU PHE CYS HIS PHE PRO GLY GLU SER GLY THR LYS ALA LEU LEU THR LYS ASP ASP LEU GLU THR VAL LEU SER THR LYS GLY GLU

VAL LEU ARG ALA ILE VAL ALA ARG ILE ASP THR SER VAL ASP TYR GLU ALA PHE LEU ASP ARG PHE ALA ILE GLU PHE GLY PRO SER ALA GLU ASP LEU GLN VAL ALA VAL LEU ALA SER LEU LYS ASP LYS GLY PHE ASP PRO ASP ASP ILE ALA ASP VAL ILE PHE PRO ASN ALA ILE

GLN ARG ILE VAL ASP LEU ALA THR ARG ASP SER ASP VAL ASN ASP ARG THR VAL GLU THR PRO LYS THR PHE LEU ALA GLY LEU ARG GLU GLU VAL ARG ARG VAL THR PHE THR ARG TRP THR ARG GLU LEU ALA THR LYS GLY ARG MET F228 K233 R236 R244 W245 V249 E256

L284 F285 M286 L296 L300 T309 T315 D316 I327 R340 P355 D356 E357 L360 R382 S394 ASP TYR ALA

• Molecule 1: DUF4297

Chain G:

12% 73% 22% • •

MET ALA ARG THR ALA GLU TYR S8 I9 Y12 L13 Y14 Q15 F16 L17 K18 Y19 L20 S21 E22 I23 L24 A25 A26 G27 D28 R31 I32 T33 I34 E35 I38 E39 D40 VAL ASP VAL ILE ALA ALA GLY LEU THR THR A51 V52 E58 Q59 A60 G66 K67 I68 Y69 K70 P71

I72 L73 L74 M75 L76 E77 H78 F79 S80 K81 N82 S83 V89 R92 L93 H96 F97 E100 S101 G102 T103 K104 A105 L106 T107 K108 D109 D110 L111 E112 L115 K118 G119 E120 V121 L122 R123 A124 I125 V126 A127 R128 I129 D130 T131 S132 V133 E136 L139 E145 F146

G147 P148 S149 A150 E151 A159 K162 D163 K164 D167 P168 D169 D170 I171 D172 A173 V174 I175 I180 Q181 T188 R189 S190 D191 V192 R195 T196 K200 T201 F202 L203 A204 G205 L206 V209 R210 R211 V212 T213 F214 T215 T218 R219 E220 L221 A222 T223 R232 R324

I327 L328 I329 R340 P355 V373 S384 Y388 R393 A397

• Molecule 1: DUF4297

Chain H:

39% • 58%

MET ALA ARG THR ALA GLU TYR SER ILE LYS GLY TYR LEU TYR GLN LEU PHE LEU LYS LEU SER GLU ILE LEU ALA ALA GLY ASP GLY ALA ARG ILE THR ILE GLU GLY ALA ILE GLU ASP VAL VAL ILE ALA ALA GLY LEU THR THR ALA VAL GLN CYS TYR HIS GLN ALA

GLU LYS TYR THR LEU GLY LYS ILE TYR LYS PRO ILE LEU LEU MET LEU GLU HIS PHE SER LYS ASN SER GLY THR ASP LEU HIS VAL SER THR TYR ARG LEU PHE CYS HIS PHE PRO GLY GLU SER GLY THR LYS ALA LEU LEU THR LYS ASP ASP LEU GLU THR VAL LEU SER THR LYS GLY GLU

• Molecule 1: DUF4297

Chain I:

11%

71%　25%

• Molecule 1: DUF4297

Chain J:

37%　5%　57%

• Molecule 1: DUF4297

Chain K:

14%

70%　27%

• Molecule 1: DUF4297

Chain L:

• Molecule 2: HerA

Chain M:

• Molecule 2: HerA

Chain N:

• Molecule 2: HerA

Chain O:

E423 V424 L425 S426 V429 M435 R447 HIS VAL GLY GLY ALA VAL SER ASP V456 L459 Y468 L469 P470 R471 R481 E485 E490 K493 V496 S506 T525 N526 K534 L540 S541 L548 P549 T567 V568 L573 P576 H579 SER

ARG SER VAL ASN TYR LEU GLN GLU TRP ASN SER GLY TRP ARG HIS VAL D597 F598 D599 I602 W605 ARG GLY LYS VAL LEU THR LYS SER GLU LYS GLY VAL

• Molecule 2: HerA

Chain P:

22%

71%   19%   10%

M1 P2 I23 S24 M35 S46 V64 GLU ARG ARG SER LEU GLY PRO SER SER GLU VAL HIS SER GLU GLU GLY SER ASP GLY ILE SER GLY N87 S101 E102 P116 T117 V122 S138 G146 ILE SER PRO ASP I151 D156 G157 D158 R159 H164 G172

K181 E190 S191 K192 A193 N194 A195 H196 K197 A198 A199 E213 E221 A222 G223 E224 A225 G232 L238 P239 Y240 M243 N244 A245 Q246 E247 L248 E249 Q250 I251 F252 I253 E254 S255 N256 E257 H258 N259 S260 H261 I264 S265 Q266 F267 R268 H269 R273 N274 K275 C276 K277

L282 T283 N284 L285 S286 F287 D288 V291 Y292 F293 S294 I295 D296 E297 V298 V299 T300 Y301 L302 E303 N304 M305 N306 N307 E308 V309 I310 G311 K312 L313 A314 G315 E316 G317 K318 P319 K320 L321 A322 N323 E324 T325 L326 V327 S328 D329 R330 D331 E332 L333 Y334 F335 D336 A337 V338 Q339 S340 F341

I342 V343 A344 S345 Q346 A347 A348 A349 T350 K351 A352 S353 N354 G355 P356 F357 N358 G359 E360 F361 D362 R363 R367 T370 R371 L372 R376 L377 Q378 Y382 K385 E386 D387 G388 E389 D390 L391 A392 T393 D398 V399 T408 N411 V412 S413 I414 I415 D416 L417 F422 E423

V424 L425 S426 I427 V428 V429 S430 L431 I432 I436 R447 H448 G451 A452 V453 I458 L459 V460 Y468 L469 P470 R471 S472 L498 R504 P505 S506 E507 V508 S509 E510 C516 T525 N526 A527 Q530 T531 P538 D539 L540 S541 A542 G543 L544 G545 D546 I547 L548 P549

N550 L551 A552 Q553 G554 E555 F556 L557 A572 L573 P574 V575 P576 E577 P578 H579 SER ARG SER VAL ASN TYR LEU GLN GLU TRP ASN SER GLY TRP ARG HIS VAL ASP PHE ASP SER VAL ILE ASP ARG TRP ARG GLY LYS VAL LEU THR LYS SER GLU LYS GLY VAL

• Molecule 2: HerA

Chain Q:

11%

68%   21%   12%

M1 P2 L43 Y51 A54 T57 V64 GLU ARG ARG SER LEU GLY PRO SER SER GLU VAL HIS SER GLU GLU GLY SER ASP GLY ILE SER GLY N87 T94 S101 E102 P116 T117 K137 S138 L142 D150 I151 D156 G157 D158 R159 V165 A166

S170 T171 I189 GLU SER LYS ALA ASN ALA HIS LYS ALA ALA GLN LYS N202 D209 A212 N219 L220 V233 D234 N235 L236 R237 N244 A245 Q246 E247 E264 S255 N256 E257 H258 N259 N262 Q263 I264 S265 Q266 F267 R268 H269 A270 V271 V272 R273 N274 K275 C276 N279

T283 N284 L285 S286 F287 V291 Y292 F293 S294 I295 D296 E297 V298 V299 L302 E303 N304 N307 E308 V309 I310 G311 K312 L313 A314 G315 E316 G317 K318 P319 K320 L321 A322 N323 E324 T325 L326 V327 S328 D329 R330 D331 E332 L333 Y334 F335 D336 A337 V338 Q339 S340 F341 I342 V343 A344 S345

Q346 A347 A348 A349 T350 K351 A352 S353 N354 G355 P356 G359 E360 F361 D362 I365 L366 R367 R371 Y382 P383 K384 K385 E386 D387 G388 E389 D390 L391 A397 V400 R401 M407 N411 V412 E423 Y443 S444 K445 ASN ARG HIS VAL GLY GLY ALA VAL S454 D465 V456

P457 I458 L459 V460 Y468 L469 P470 R471 A488 V496 T497 L498 Q503 S506 F519 L524 D529 L537 P538 D539 L540 S541 A542 G543 L544 L548 P549 I558 V559 T567 V568 H579 SER ARG SER VAL ASN TYR LEU GLU GLN GLU TRP ASN SER GLY TRP ARG

HIS VAL D597 W605 ARG GLY LYS VAL VAL LEU THR LYS SER GLU LYS GLY VAL

- Molecule 2: HerA

Chain R:

M1 P2 T12 D13 S14 E22 I23 S24 V64 GLU ARG ARG SER LEU GLY PRO SER SER GLU VAL HIS SER GLU GLU GLY SER ASP GLY ILE SER GLY N87 P116 T117 P124 V127 L128 E129 K137 G146 ILE SER PRO D150 H164 G172 V179 L183

V187 G188 I189 E190 SER LYS ALA ASN ALA HIS LYS ALA ALA GLN LYS N202 S203 H204 I205 V206 I210 F218 E221 A222 G223 E224 A225 F226 T227 L231 G232 V233 D234 N235 L236 R237 L238 W241 L242 M243 L248 I251 F252 I253 E254 S255 N256 E257 H258 N259 S260 H261

N262 Q263 I264 R268 V271 K277 H278 N279 P280 L285 V291 V292 F293 S294 I295 D296 E297 V298 V299 T300 Y301 L302 E303 N304 M305 R306 N307 E308 V309 I310 G311 K312 L313 A314 G315 E316 G317 K318 P319 K320 L321 A322 N323 E324 T325 L326 V327 S328 D329 R330 D331 E332 L333 Y334 F335

D336 A337 V338 Q339 S340 F341 I342 V343 A344 S345 Q346 A347 A348 A349 T350 K351 A352 S353 N354 G355 P356 F357 N358 G359 E360 F361 D362 R363 M364 I365 L366 R367 L372 P375 R376 L377 Q378 Y382 K385 E386 D390 L391 D395 V399 Q402 Y406 M407 T408 K409 S410 N411

V412 I415 H448 G451 A452 V453 V460 E464 A465 H466 L469 S472 D478 R481 K482 E485 V496 V501 E507 V508 S509 E510 S514 Q515 C516 F519 I520 S521 T525 N526 A527 V528 D529 Q530 T531 Y532 L536 L537 P538 D539 L540 S541 A542

D546 L547 L548 P549 N550 L551 A552 F556 L557 A572 L573 P574 V575 P576 E577 P578 H579 SER ARG SER VAL ASN TYR LEU GLN GLU TRP ASN SER GLY TRP ARG HIS VAL ASP PHE ASP SER VAL ILE ASP ARG TRP ARG GLY LYS VAL LEU THR LYS SER GLU LYS GLY VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	158570	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	65.58	Depositor
Minimum defocus (nm)	328	Depositor
Maximum defocus (nm)	5899	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.780	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	484.0, 484.0, 484.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.51	0/3196	0.52	0/4316
1	B	0.65	0/1419	0.52	0/1912
1	C	0.52	0/3172	0.56	2/4280 (0.0%)
1	D	0.65	0/1440	0.55	0/1941
1	E	0.52	0/3179	0.51	0/4292
1	F	0.66	0/1419	0.53	0/1912
1	G	0.52	0/3136	0.58	3/4232 (0.1%)
1	H	0.65	0/1427	0.54	0/1923
1	I	0.52	0/3169	0.53	0/4279
1	J	0.65	0/1440	0.54	1/1941 (0.1%)
1	K	0.52	0/3163	0.54	0/4272
1	L	0.67	0/1427	0.54	0/1923
2	M	0.50	0/4331	0.51	1/5875 (0.0%)
2	N	0.46	0/4192	0.52	0/5684
2	O	0.49	0/4312	0.51	0/5848
2	P	0.44	0/4359	0.53	2/5913 (0.0%)
2	Q	0.49	0/4324	0.50	0/5868
2	R	0.45	0/4285	0.54	2/5814 (0.0%)
All	All	0.52	0/53390	0.53	11/72225 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	I	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	330	ARG	NE-CZ-NH2	-8.52	116.04	120.30
2	R	293	PHE	CB-CG-CD1	-6.50	116.25	120.80
2	P	330	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	G	79	PHE	CB-CG-CD2	-6.26	116.42	120.80
2	R	293	PHE	CB-CG-CD2	5.93	124.95	120.80
1	J	328	LEU	CB-CG-CD2	5.84	120.94	111.00
1	C	291	TYR	CB-CG-CD1	5.79	124.48	121.00
1	C	291	TYR	CB-CG-CD2	-5.69	117.58	121.00
1	G	106	LEU	CB-CG-CD2	5.67	120.64	111.00
1	G	79	PHE	CB-CG-CD1	5.61	124.72	120.80
2	M	537	LEU	CB-CG-CD2	5.14	119.73	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	113	THR	Peptide
1	I	47	GLY	Peptide

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	3134	2851	3150	66	0
1	B	1389	1400	1404	8	0
1	C	3112	2890	3128	76	0
1	D	1409	1418	1417	10	0
1	E	3118	2859	3138	82	0
1	F	1389	1405	1404	11	0
1	G	3075	2856	3089	63	0
1	H	1397	1409	1408	8	0
1	I	3108	2851	3130	80	0
1	J	1409	1418	1417	14	0
1	K	3102	2846	3125	81	0
1	L	1397	1409	1408	18	0
2	M	4241	4189	4201	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	4107	4065	4082	73	0
2	O	4222	4168	4181	94	0
2	P	4268	4211	4234	77	0
2	Q	4233	4168	4181	88	0
2	R	4196	4137	4152	82	0
3	M	31	12	12	2	0
3	O	31	12	12	1	0
3	Q	31	12	12	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
All	All	52402	50586	52285	1007	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 10.

All (1007) 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:G:107:THR:OG1	1:G:109:ASP:OD2	1.80	0.97
1:K:38:ILE:HB	1:K:51:ALA:HB1	1.44	0.96
1:A:14:TYR:OH	1:A:148:PRO:O	1.84	0.95
1:B:322:LEU:O	1:B:340:ARG:NH1	2.00	0.95
1:I:117:THR:O	1:I:123:ARG:NH1	2.00	0.94
2:O:138:SER:OG	2:O:156:ASP:OD1	1.88	0.91
2:P:251:ILE:O	2:P:371:ARG:NH2	2.05	0.90
2:O:294:SER:OG	2:O:296:ASP:OD1	1.91	0.87
1:C:212:VAL:HG11	1:C:231:LEU:HD11	1.56	0.86
1:I:120:GLU:OE2	1:I:123:ARG:NH2	2.08	0.86
1:C:113:THR:O	1:C:116:SER:OG	1.95	0.85
1:E:324:ARG:O	1:E:340:ARG:NH2	2.09	0.85
2:R:407:MET:SD	2:R:408:THR:OG1	2.35	0.85
1:D:387:GLU:N	1:D:387:GLU:OE1	2.09	0.84
2:M:304:ASN:ND2	2:M:339:GLN:OE1	2.10	0.84
2:O:534:LYS:NZ	2:O:540:LEU:O	2.09	0.84
1:I:212:VAL:HG11	1:I:231:LEU:HD11	1.60	0.83
2:M:597:ASP:O	2:M:600:SER:OG	1.95	0.83
2:N:138:SER:OG	2:N:156:ASP:OD2	1.94	0.83
2:O:28:ASP:OD1	2:O:29:PHE:N	2.12	0.83
2:N:214:TYR:OH	2:N:463:GLU:OE2	1.97	0.81
1:I:393:ARG:NH1	1:I:395:ASP:O	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:272:ARG:NH1	1:J:391:GLN:O	2.15	0.80
1:K:387:GLU:OE1	1:K:393:ARG:NH2	2.15	0.80
2:Q:309:VAL:O	2:Q:320:LYS:N	2.13	0.80
1:I:185:ASP:OD1	1:I:186:LEU:N	2.15	0.79
2:R:514:SER:OG	2:R:515:GLN:OE1	1.99	0.79
2:Q:138:SER:OG	2:Q:156:ASP:OD2	2.00	0.78
2:M:225:ALA:O	2:M:409:LYS:NZ	2.17	0.78
2:Q:275:LYS:O	2:Q:285:LEU:HD12	1.84	0.78
2:R:372:LEU:O	2:R:378:GLN:NE2	2.16	0.77
2:R:116:PRO:O	2:R:117:THR:OG1	2.02	0.77
1:E:120:GLU:OE1	1:E:123:ARG:NE	2.17	0.76
2:O:278:HIS:NE2	2:O:297:GLU:OE1	2.18	0.76
1:G:131:THR:O	1:G:133:VAL:HG13	1.87	0.75
1:A:212:VAL:HG11	1:A:231:LEU:HD11	1.67	0.75
2:M:490:GLU:OE1	2:M:493:LYS:NZ	2.19	0.75
2:M:262:ASN:O	2:M:265:SER:OG	2.03	0.75
2:O:344:ALA:HB2	2:O:352:ALA:HB3	1.69	0.75
1:G:324:ARG:O	1:G:340:ARG:NH2	2.20	0.75
1:K:324:ARG:O	1:K:340:ARG:NH2	2.20	0.75
2:M:254:GLU:OE2	2:M:367:ARG:NH1	2.19	0.74
2:R:306:ASN:ND2	2:R:358:ASN:OD1	2.19	0.74
2:O:363:ARG:O	2:O:366:LEU:HD23	1.87	0.74
2:M:275:LYS:NZ	2:M:291:VAL:O	2.20	0.74
2:O:275:LYS:NZ	2:O:289:THR:O	2.21	0.73
2:O:1:MET:HB3	2:O:2:PRO:HD3	1.70	0.73
2:P:411:ASN:OD1	2:P:413:SER:OG	2.07	0.73
2:Q:1:MET:HB3	2:Q:2:PRO:HD3	1.70	0.73
2:Q:344:ALA:HA	2:Q:352:ALA:HB3	1.70	0.72
1:I:219:ARG:O	1:I:224:LYS:HG2	1.88	0.72
1:I:186:LEU:O	1:I:195:ARG:NH1	2.23	0.72
1:K:215:THR:HA	1:K:381:GLU:OE2	1.90	0.71
2:O:116:PRO:O	2:O:117:THR:OG1	2.09	0.71
2:P:358:ASN:OD1	2:P:359:GLY:N	2.23	0.71
1:B:384:SER:O	1:B:393:ARG:NH2	2.24	0.70
1:C:14:TYR:OH	1:C:148:PRO:O	2.08	0.70
2:Q:219:ASN:OD1	2:Q:220:LEU:N	2.23	0.70
2:M:1:MET:HB3	2:M:2:PRO:HD3	1.73	0.70
2:N:385:LYS:NZ	2:N:395:ASP:OD1	2.17	0.70
1:C:385:ASP:OD2	1:C:386:LEU:N	2.24	0.70
1:A:214:PHE:HB2	1:A:380:ILE:HD13	1.73	0.70
1:C:220:GLU:O	1:C:221:LEU:HD12	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:PRO:O	1:E:373:VAL:HG22	1.92	0.70
2:Q:116:PRO:O	2:Q:117:THR:OG1	2.10	0.70
1:G:80:SER:O	1:G:83:SER:OG	2.10	0.69
1:G:18:LYS:O	1:G:21:SER:OG	2.08	0.69
2:P:138:SER:OG	2:P:156:ASP:OD1	2.10	0.69
1:E:35:GLU:HB3	1:E:50:THR:O	1.91	0.69
2:O:367:ARG:O	2:O:370:THR:OG1	2.09	0.69
2:O:275:LYS:O	2:O:279:ASN:N	2.25	0.69
1:C:300:LEU:HD22	1:C:305:LEU:HD12	1.75	0.69
2:N:321:LEU:HD13	2:N:325:THR:O	1.93	0.68
1:E:115:LEU:HD21	1:E:135:TYR:CE1	2.29	0.68
1:E:153:LEU:O	1:E:157:VAL:HG23	1.93	0.68
1:E:219:ARG:O	1:E:224:LYS:HG2	1.94	0.68
1:I:42:ASP:OD2	1:I:44:ILE:N	2.27	0.68
1:A:153:LEU:O	1:A:157:VAL:HG23	1.94	0.68
1:G:174:VAL:HG12	1:G:212:VAL:HG22	1.76	0.67
2:O:471:ARG:NH2	2:O:506:SER:O	2.28	0.67
2:O:25:SER:OG	2:O:28:ASP:OD2	2.11	0.67
2:R:202:ASN:OD1	2:R:410:SER:OG	2.12	0.67
1:K:215:THR:HG22	1:K:218:THR:HG23	1.77	0.67
2:O:365:ILE:O	2:O:369:HIS:ND1	2.27	0.67
2:P:548:LEU:HD21	2:P:557:LEU:HD21	1.76	0.67
2:Q:279:ASN:HB2	2:Q:285:LEU:HD11	1.75	0.67
2:N:397:ALA:O	2:N:400:VAL:HG12	1.95	0.67
1:C:215:THR:HG22	1:C:218:THR:HG23	1.76	0.67
1:K:205:GLY:O	1:K:209:VAL:HG13	1.96	0.66
2:P:1:MET:HB3	2:P:2:PRO:HD3	1.77	0.66
1:I:163:ASP:OD2	1:I:164:LYS:N	2.29	0.66
1:C:39:GLU:OE2	1:C:39:GLU:N	2.28	0.66
2:O:233:VAL:HG13	2:O:234:ASP:H	1.61	0.66
1:G:136:GLU:N	1:G:136:GLU:OE1	2.29	0.66
2:O:358:ASN:OD1	2:O:359:GLY:N	2.29	0.65
1:E:385:ASP:OD2	1:E:386:LEU:N	2.29	0.65
1:L:344:ARG:NH2	1:L:366:ASP:OD1	2.28	0.65
2:O:233:VAL:HG13	2:O:234:ASP:N	2.10	0.65
2:Q:171:THR:OG1	2:Q:503:GLN:NE2	2.28	0.65
2:O:228:LEU:O	2:O:228:LEU:HD23	1.97	0.65
1:I:221:LEU:HD12	1:I:222:ALA:H	1.60	0.65
2:M:239:PRO:HD2	2:M:242:LEU:HD12	1.79	0.64
2:Q:292:TYR:OH	2:Q:390:ASP:OD2	2.09	0.64
1:D:261:ASP:HB3	1:D:383:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:LEU:HB2	1:E:139:LEU:HD21	1.80	0.64
1:C:218:THR:O	1:C:221:LEU:HD13	1.97	0.64
2:N:471:ARG:NH1	2:N:507:GLU:O	2.30	0.64
1:C:384:SER:OG	1:C:393:ARG:NH1	2.31	0.64
2:N:203:SER:N	2:N:410:SER:OG	2.31	0.64
2:N:278:HIS:NE2	2:N:297:GLU:OE1	2.31	0.64
1:C:109:ASP:O	1:C:113:THR:HG23	1.97	0.64
1:G:109:ASP:OD2	1:G:110:ASP:N	2.30	0.64
2:N:309:VAL:CG2	2:N:352:ALA:HB1	2.28	0.64
1:E:176:PHE:HE2	1:E:221:LEU:HD11	1.63	0.64
1:E:352:GLN:OE1	1:E:352:GLN:N	2.31	0.63
1:G:215:THR:O	1:G:219:ARG:HG3	1.98	0.63
2:M:233:VAL:HG13	2:M:234:ASP:N	2.13	0.63
2:N:1:MET:HB2	2:N:2:PRO:HD3	1.80	0.63
1:A:80:SER:OG	1:A:128:ARG:NH1	2.31	0.63
1:K:72:ILE:O	1:K:76:LEU:N	2.27	0.63
2:P:247:GLU:OE1	2:P:427:ILE:HG23	1.96	0.63
1:K:64:THR:HG22	1:K:67:LYS:HZ3	1.63	0.63
2:P:259:ASN:ND2	2:Q:284:ASN:OD1	2.32	0.63
2:R:507:GLU:N	2:R:507:GLU:OE1	2.32	0.63
2:R:1:MET:HB3	2:R:2:PRO:HD3	1.81	0.63
1:C:38:ILE:HG13	1:C:52:VAL:O	1.99	0.63
2:P:275:LYS:NZ	2:P:287:PHE:O	2.32	0.62
2:M:101:SER:OG	2:M:102:GLU:N	2.33	0.62
2:N:144:THR:OG1	2:N:149:PRO:O	2.16	0.62
2:M:597:ASP:O	2:M:600:SER:N	2.33	0.62
1:C:31:ARG:NH2	1:C:198:GLU:OE1	2.32	0.62
2:M:577:GLU:N	2:M:577:GLU:OE1	2.31	0.62
1:I:35:GLU:HB2	1:I:50:THR:OG1	2.00	0.61
2:P:378:GLN:O	2:P:382:TYR:N	2.25	0.61
1:C:38:ILE:HG12	1:C:51:ALA:HB1	1.82	0.61
1:F:256:GLU:OE2	1:F:382:ARG:NE	2.32	0.61
1:A:369:LYS:NZ	1:A:375:VAL:HG11	2.16	0.61
1:G:31:ARG:NH2	1:G:196:THR:OG1	2.32	0.61
1:G:163:ASP:OD1	1:G:164:LYS:N	2.34	0.61
2:P:251:ILE:HD11	2:P:427:ILE:HD13	1.82	0.61
1:A:219:ARG:HB3	1:A:224:LYS:HE2	1.81	0.61
2:M:303:GLU:O	2:M:307:ASN:ND2	2.33	0.61
1:D:282:PRO:O	1:D:340:ARG:NH1	2.34	0.61
2:Q:443:TYR:OH	2:Q:455:ASP:OD1	2.12	0.61
1:E:384:SER:OG	1:E:393:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:362:ASP:HA	2:R:365:ILE:HD12	1.83	0.61
2:Q:455:ASP:OD2	2:Q:456:VAL:N	2.34	0.60
2:R:1:MET:HB3	2:R:2:PRO:CD	2.31	0.60
2:O:344:ALA:CB	2:O:352:ALA:HB3	2.31	0.60
2:P:348:ALA:O	2:P:351:LYS:HE3	2.01	0.60
1:C:322:LEU:O	1:C:340:ARG:NE	2.34	0.60
1:I:116:SER:OG	1:I:118:LYS:NZ	2.35	0.60
2:Q:299:VAL:HA	2:Q:302:LEU:HD12	1.83	0.60
1:I:31:ARG:O	1:I:32:ILE:HD13	2.01	0.60
2:Q:537:LEU:HD23	2:Q:559:VAL:CG2	2.30	0.60
1:K:232:ARG:NH1	1:K:388:TYR:O	2.34	0.60
1:G:33:THR:HG23	1:G:195:ARG:O	2.01	0.59
1:K:211:ARG:HH22	1:K:379:LYS:HD2	1.67	0.59
1:I:41:VAL:O	1:I:41:VAL:HG13	2.02	0.59
1:K:44:ILE:HG13	1:K:45:ALA:N	2.17	0.59
2:N:205:ILE:HB	2:N:412:VAL:HG13	1.85	0.59
1:C:38:ILE:HD12	1:C:53:GLN:HB2	1.84	0.59
2:N:390:ASP:OD1	2:N:391:LEU:N	2.36	0.59
1:C:216:ARG:O	1:C:216:ARG:HD3	2.02	0.59
2:O:234:ASP:O	2:O:237:ARG:NH1	2.36	0.58
2:N:424:VAL:HG22	2:N:424:VAL:O	2.04	0.58
1:C:12:TYR:O	1:C:15:GLN:HG3	2.03	0.58
1:C:35:GLU:HB2	1:C:50:THR:O	2.03	0.58
1:K:41:VAL:HG23	1:K:41:VAL:O	2.03	0.58
1:K:199:PRO:O	1:K:203:LEU:HD13	2.04	0.58
2:P:35:MET:SD	2:P:122:VAL:HG11	2.43	0.58
1:E:43:VAL:HG22	1:E:43:VAL:O	2.02	0.58
1:E:366:ASP:OD1	1:E:367:GLU:N	2.37	0.58
1:K:60:ALA:HB3	1:K:97:PHE:CE1	2.39	0.58
2:M:350:THR:HG22	2:M:350:THR:O	2.02	0.58
1:E:206:LEU:HA	1:E:209:VAL:HG12	1.85	0.58
1:I:164:LYS:HE3	1:I:203:LEU:HD12	1.86	0.58
1:C:157:VAL:O	1:C:160:SER:OG	2.19	0.57
2:R:395:ASP:O	2:R:399:VAL:HG23	2.03	0.57
1:K:44:ILE:HG13	1:K:45:ALA:H	1.69	0.57
2:P:527:ALA:O	2:P:530:GLN:HG2	2.04	0.57
1:C:324:ARG:O	1:C:340:ARG:NH2	2.38	0.57
2:Q:150:ASP:OD2	2:Q:151:ILE:N	2.37	0.57
2:N:243:MET:HB2	2:N:248:LEU:HB2	1.87	0.57
2:Q:411:ASN:OD1	2:Q:412:VAL:N	2.37	0.57
2:M:138:SER:OG	2:M:156:ASP:OD1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:209:ASP:OD1	2:Q:212:ALA:N	2.38	0.57
1:I:218:THR:O	1:I:221:LEU:HB3	2.05	0.57
2:R:243:MET:SD	2:R:251:ILE:HD12	2.45	0.57
1:A:6:GLU:HA	1:A:6:GLU:OE1	2.05	0.57
2:N:302:LEU:HD22	2:N:364:MET:HE1	1.86	0.57
1:I:117:THR:HG21	1:I:126:VAL:HG21	1.87	0.56
1:C:107:THR:OG1	1:C:110:ASP:OD2	2.23	0.56
1:A:324:ARG:O	1:A:340:ARG:NH2	2.37	0.56
1:K:327:ILE:HG21	1:L:327:ILE:HG21	1.86	0.56
2:N:155:ILE:HG22	2:N:156:ASP:H	1.69	0.56
2:N:462:CYS:SG	2:N:468:TYR:OH	2.63	0.56
2:P:238:LEU:HD12	2:P:238:LEU:O	2.05	0.56
2:R:363:ARG:HA	2:R:366:LEU:HG	1.86	0.56
1:C:24:LEU:HD13	1:C:160:SER:HB2	1.86	0.56
2:M:204:HIS:NE2	2:M:456:VAL:HG11	2.20	0.56
2:M:297:GLU:O	2:M:300:THR:HG22	2.05	0.56
1:I:38:ILE:HG13	1:I:51:ALA:HB1	1.88	0.56
2:Q:274:ASN:HD22	2:Q:298:VAL:HG23	1.71	0.56
1:E:212:VAL:HG11	1:E:231:LEU:HD11	1.86	0.56
1:K:24:LEU:HD13	1:K:160:SER:HB2	1.86	0.56
2:P:436:ILE:HD11	2:P:458:ILE:HG21	1.87	0.56
2:Q:57:THR:O	2:Q:57:THR:HG22	2.06	0.56
1:G:175:ILE:HG23	1:G:206:LEU:HD21	1.88	0.55
1:K:214:PHE:HD2	1:K:385:ASP:OD2	1.89	0.55
2:N:364:MET:O	2:N:368:LEU:HD13	2.04	0.55
2:Q:268:ARG:O	2:Q:272:VAL:HG23	2.05	0.55
1:A:272:ARG:NH1	1:A:391:GLN:O	2.39	0.55
1:A:219:ARG:CB	1:A:224:LYS:HE2	2.37	0.55
1:C:154:GLN:O	1:C:158:LEU:HD23	2.06	0.55
1:C:355:PRO:O	1:C:373:VAL:HG22	2.07	0.55
1:I:307:CYS:SG	1:I:308:GLU:N	2.79	0.55
1:C:215:THR:CG2	1:C:218:THR:HG23	2.36	0.55
2:R:206:VAL:CG2	2:R:460:VAL:HG22	2.36	0.55
1:E:297:GLN:NE2	1:E:307:CYS:SG	2.80	0.55
2:M:142:LEU:HD22	2:M:155:ILE:HD13	1.88	0.55
2:N:316:GLU:OE2	2:N:326:LEU:HD11	2.07	0.55
2:N:466:HIS:HA	2:N:508:VAL:HG22	1.88	0.55
1:B:312:VAL:HG12	1:B:312:VAL:O	2.07	0.55
1:A:315:THR:HG23	1:A:316:ASP:OD1	2.07	0.55
1:C:212:VAL:HG21	1:C:231:LEU:HD21	1.88	0.55
2:M:233:VAL:HG13	2:M:234:ASP:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:362:ASP:OD1	2:O:363:ARG:N	2.39	0.55
1:C:109:ASP:OD1	1:C:110:ASP:N	2.40	0.55
1:H:282:PRO:O	1:H:340:ARG:NH1	2.40	0.55
1:I:19:TYR:CE2	1:I:23:ILE:HD11	2.42	0.55
1:E:115:LEU:HD21	1:E:135:TYR:HE1	1.71	0.54
1:I:100:GLU:OE2	1:I:100:GLU:N	2.40	0.54
1:I:132:SER:O	1:I:132:SER:OG	2.23	0.54
2:O:417:LEU:HD13	2:O:425:LEU:HD11	1.89	0.54
2:P:320:LYS:HE3	2:P:342:ILE:HD11	1.89	0.54
2:P:552:ALA:HB3	2:P:555:GLU:OE1	2.08	0.54
1:C:65:LEU:HD23	1:C:65:LEU:O	2.07	0.54
1:F:296:LEU:O	1:F:300:LEU:HD13	2.06	0.54
2:O:286:SER:OG	2:O:288:ASP:OD2	2.24	0.54
1:A:232:ARG:NH1	1:A:388:TYR:O	2.41	0.54
1:K:19:TYR:CD1	1:K:34:ILE:HD12	2.42	0.54
1:A:219:ARG:O	1:A:224:LYS:HE3	2.07	0.54
1:C:35:GLU:HG3	1:C:52:VAL:HB	1.89	0.54
1:I:35:GLU:O	1:I:35:GLU:HG2	2.07	0.54
1:K:38:ILE:HG22	1:K:52:VAL:O	2.08	0.54
2:O:227:THR:HB	2:O:411:ASN:HB3	1.89	0.54
1:I:108:LYS:HZ2	1:I:135:TYR:HB3	1.72	0.54
1:J:261:ASP:OD1	1:J:264:ARG:NH2	2.40	0.54
1:K:200:LYS:H	1:K:200:LYS:HD2	1.72	0.54
1:A:327:ILE:HG21	1:B:327:ILE:HG21	1.90	0.54
2:Q:158:ASP:OD1	2:Q:159:ARG:N	2.39	0.54
1:E:211:ARG:HG3	1:E:211:ARG:HH11	1.72	0.54
1:E:227:MET:HG3	1:E:228:PHE:HD1	1.73	0.54
1:I:9:ILE:HD11	1:I:217:TRP:NE1	2.22	0.54
2:M:396:PHE:O	2:M:399:VAL:HG22	2.07	0.54
1:G:38:ILE:HB	1:G:52:VAL:HG12	1.89	0.54
1:A:54:CYS:SG	1:A:55:LYS:N	2.81	0.54
2:O:363:ARG:HA	2:O:366:LEU:CD2	2.38	0.54
2:Q:262:ASN:OD1	2:Q:263:GLN:N	2.41	0.54
1:I:153:LEU:O	1:I:157:VAL:HG23	2.08	0.53
1:K:76:LEU:HD23	1:K:129:ILE:HD11	1.91	0.53
2:P:116:PRO:O	2:P:117:THR:OG1	2.20	0.53
2:Q:519:PHE:CB	2:Q:537:LEU:HD21	2.37	0.53
1:A:224:LYS:HD3	1:A:228:PHE:CE2	2.43	0.53
1:L:228:PHE:HA	1:L:231:LEU:HD13	1.90	0.53
2:M:304:ASN:O	2:M:307:ASN:N	2.42	0.53
2:M:321:LEU:HD22	2:M:325:THR:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:264:ILE:HG23	2:Q:265:SER:N	2.23	0.53
1:C:215:THR:O	1:C:219:ARG:HG3	2.09	0.53
1:K:355:PRO:O	1:K:373:VAL:HG22	2.08	0.53
2:O:336:ASP:OD1	2:O:337:ALA:N	2.41	0.53
2:Q:275:LYS:HE3	2:Q:291:VAL:HG23	1.90	0.53
2:Q:233:VAL:HG13	2:Q:234:ASP:N	2.24	0.53
1:A:219:ARG:HA	1:A:224:LYS:HG3	1.90	0.53
2:Q:458:ILE:HD11	2:Q:496:VAL:HG12	1.91	0.53
1:G:205:GLY:O	1:G:209:VAL:HG23	2.09	0.53
2:N:309:VAL:HG21	2:N:352:ALA:HB1	1.90	0.53
2:P:238:LEU:HD13	2:P:431:LEU:HD23	1.90	0.53
1:G:215:THR:CG2	1:G:218:THR:HG23	2.39	0.53
1:I:185:ASP:O	1:I:189:ARG:N	2.41	0.53
1:I:261:ASP:OD2	1:I:262:ILE:N	2.42	0.53
2:N:303:GLU:OE2	2:N:303:GLU:N	2.41	0.53
1:G:20:LEU:HD22	1:G:180:ILE:HD13	1.90	0.53
2:O:347:ALA:O	2:O:351:LYS:N	2.42	0.53
1:K:215:THR:O	1:K:219:ARG:HG3	2.10	0.52
1:C:220:GLU:C	1:C:221:LEU:HD12	2.29	0.52
1:C:153:LEU:O	1:C:157:VAL:HG23	2.09	0.52
2:M:237:ARG:NH1	2:M:384:LYS:O	2.41	0.52
1:C:192:VAL:O	1:C:193:ASN:ND2	2.43	0.52
1:D:284:LEU:HD12	1:D:340:ARG:HB2	1.90	0.52
2:M:273:ARG:O	2:M:277:LYS:NZ	2.42	0.52
1:C:35:GLU:HG3	1:C:52:VAL:CG1	2.40	0.52
1:E:215:THR:HG23	1:E:218:THR:H	1.75	0.52
1:G:202:PHE:CD2	1:G:203:LEU:HD23	2.45	0.52
1:G:355:PRO:O	1:G:373:VAL:HG22	2.09	0.52
2:O:310:ILE:O	2:O:352:ALA:HB1	2.09	0.52
2:P:447:ARG:O	2:P:451:GLY:N	2.43	0.52
2:Q:519:PHE:HB2	2:Q:537:LEU:HD21	1.90	0.52
2:R:469:LEU:HD23	2:R:481:ARG:HB2	1.90	0.52
1:A:37:ALA:HB1	1:A:39:GLU:OE1	2.10	0.52
1:C:192:VAL:O	1:C:192:VAL:HG23	2.09	0.52
2:O:272:VAL:HG22	2:O:287:PHE:N	2.24	0.52
2:O:327:VAL:HG21	2:O:333:LEU:HD22	1.90	0.52
1:E:174:VAL:HG11	1:E:210:ARG:HH12	1.75	0.52
1:K:64:THR:HG22	1:K:67:LYS:NZ	2.24	0.52
2:P:508:VAL:HG12	2:P:509:SER:N	2.25	0.52
2:Q:236:LEU:HD12	2:Q:237:ARG:H	1.74	0.52
1:A:66:GLY:HA2	1:A:69:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:GLY:O	1:E:207:ARG:NH1	2.42	0.52
1:I:54:CYS:SG	1:I:55:LYS:N	2.83	0.52
2:M:268:ARG:O	2:M:272:VAL:HG23	2.09	0.52
2:P:294:SER:OG	2:P:296:ASP:OD1	2.20	0.52
1:A:369:LYS:HZ3	1:A:375:VAL:HG11	1.74	0.52
1:E:327:ILE:HG21	1:F:327:ILE:HG21	1.92	0.52
2:R:385:LYS:HG2	2:R:386:GLU:N	2.25	0.52
1:I:38:ILE:CG1	1:I:51:ALA:HB1	2.40	0.52
1:K:14:TYR:O	1:K:18:LYS:NZ	2.33	0.52
1:K:73:LEU:O	1:K:76:LEU:HB3	2.09	0.52
2:N:41:TYR:CD1	2:N:53:LEU:HD21	2.45	0.52
2:N:154:LYS:O	2:N:155:ILE:HD13	2.09	0.51
2:N:544:LEU:HD21	2:N:557:LEU:HD11	1.91	0.51
2:O:244:ASN:O	2:O:248:LEU:HD23	2.09	0.51
2:N:372:LEU:O	2:N:378:GLN:NE2	2.42	0.51
1:A:38:ILE:HD12	1:A:38:ILE:H	1.74	0.51
1:I:214:PHE:HE1	1:I:228:PHE:CE1	2.28	0.51
1:K:66:GLY:HA2	1:K:69:TYR:CE2	2.46	0.51
1:L:293:LEU:HD11	1:L:343:LYS:HG3	1.93	0.51
2:M:57:THR:HG23	2:M:57:THR:O	2.09	0.51
2:O:53:LEU:HD22	2:O:97:ILE:HD11	1.91	0.51
2:O:396:PHE:O	2:O:399:VAL:HG22	2.10	0.51
2:R:254:GLU:N	2:R:254:GLU:OE1	2.43	0.51
2:R:309:VAL:HG22	2:R:354:ASN:OD1	2.11	0.51
1:A:41:VAL:HG23	1:A:41:VAL:O	2.09	0.51
1:E:221:LEU:HD12	1:E:222:ALA:H	1.76	0.51
2:M:275:LYS:O	2:M:285:LEU:HD12	2.10	0.51
2:M:471:ARG:NH2	2:M:506:SER:O	2.40	0.51
2:N:155:ILE:HG21	2:N:562:ALA:HB1	1.92	0.51
2:N:218:PHE:HE1	2:N:412:VAL:HG21	1.76	0.51
2:O:205:ILE:HG12	2:O:459:LEU:HD21	1.92	0.51
2:O:534:LYS:NZ	2:O:541:SER:O	2.39	0.51
1:I:64:THR:OG1	1:I:67:LYS:HE2	2.10	0.51
1:K:38:ILE:CB	1:K:51:ALA:HB1	2.29	0.51
2:Q:367:ARG:O	2:Q:371:ARG:HG2	2.11	0.51
1:I:49:THR:HG1	1:I:88:HIS:N	2.09	0.51
1:I:391:GLN:C	1:I:392:LEU:HD12	2.30	0.51
1:L:231:LEU:HD12	1:L:231:LEU:H	1.76	0.51
2:M:137:LYS:H	2:M:137:LYS:HD2	1.76	0.51
2:P:398:ASP:OD2	2:P:399:VAL:N	2.44	0.51
2:Q:397:ALA:O	2:Q:401:ARG:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:ARG:NE	1:F:357:GLU:OE1	2.43	0.51
1:G:9:ILE:O	1:G:13:LEU:HD23	2.10	0.51
2:P:416:ASP:OD1	2:P:417:LEU:N	2.44	0.51
1:L:284:LEU:HD12	1:L:340:ARG:HB2	1.93	0.51
2:N:155:ILE:HG22	2:N:156:ASP:N	2.26	0.51
1:I:102:GLY:H	1:I:146:PHE:HB2	1.76	0.51
1:F:249:VAL:HB	1:F:360:LEU:HD23	1.93	0.50
2:O:239:PRO:HD2	2:O:242:LEU:HD12	1.93	0.50
2:O:426:SER:O	2:O:429:VAL:HG22	2.12	0.50
1:G:126:VAL:HA	1:G:129:ILE:HD12	1.92	0.50
2:O:189:ILE:HD11	2:O:226:PHE:CZ	2.47	0.50
1:C:54:CYS:SG	1:C:55:LYS:N	2.85	0.50
2:Q:275:LYS:CE	2:Q:291:VAL:HG23	2.41	0.50
1:E:31:ARG:NH2	1:E:198:GLU:OE2	2.44	0.50
1:I:38:ILE:HD11	1:I:89:VAL:HG13	1.94	0.50
1:K:322:LEU:O	1:K:340:ARG:NE	2.44	0.50
2:P:253:ILE:HG21	2:P:264:ILE:CG1	2.42	0.50
2:R:210:ILE:HD12	2:R:464:GLU:HB2	1.93	0.50
1:E:208:GLU:O	1:E:210:ARG:HG2	2.11	0.50
1:G:188:THR:HG23	1:G:188:THR:O	2.11	0.50
1:G:60:ALA:HB3	1:G:97:PHE:CE1	2.47	0.50
2:N:262:ASN:OD1	2:N:265:SER:OG	2.29	0.50
2:O:272:VAL:HG22	2:O:286:SER:C	2.31	0.50
2:Q:54:ALA:HB1	2:Q:94:THR:HB	1.94	0.50
2:N:137:LYS:N	2:N:137:LYS:HD2	2.26	0.50
2:O:101:SER:OG	2:O:102:GLU:N	2.45	0.50
1:L:319:ILE:HD11	1:L:347:VAL:HG13	1.94	0.50
2:N:406:TYR:HB3	2:N:408:THR:O	2.11	0.50
2:N:447:ARG:O	2:N:451:GLY:N	2.44	0.50
2:N:471:ARG:NH2	2:N:506:SER:O	2.40	0.50
1:A:151:GLU:O	1:A:155:VAL:HG23	2.12	0.49
1:E:215:THR:H	1:E:218:THR:CG2	2.24	0.49
1:E:315:THR:HG23	1:E:316:ASP:N	2.27	0.49
1:I:174:VAL:HG12	1:I:174:VAL:O	2.11	0.49
1:G:89:VAL:HG13	1:G:89:VAL:O	2.12	0.49
2:O:318:LYS:HD2	2:O:326:LEU:HB3	1.93	0.49
1:G:115:LEU:HD23	1:G:115:LEU:O	2.12	0.49
1:E:16:PHE:CE2	1:E:184:VAL:HG22	2.47	0.49
1:I:182:ARG:O	1:I:185:ASP:OD1	2.30	0.49
2:O:234:ASP:OD1	2:O:235:ASN:N	2.44	0.49
2:O:100:LEU:HD12	2:O:105:GLU:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:158:ASP:OD1	2:P:159:ARG:N	2.46	0.49
2:Q:275:LYS:HD2	2:Q:293:PHE:HB2	1.95	0.49
2:R:187:VAL:HG12	2:R:187:VAL:O	2.12	0.49
1:C:186:LEU:HD11	1:C:197:VAL:HG11	1.93	0.49
1:I:212:VAL:HG21	1:I:231:LEU:HD21	1.94	0.49
2:M:299:VAL:O	2:M:302:LEU:HG	2.13	0.49
2:M:325:THR:O	2:M:326:LEU:HD23	2.13	0.49
2:Q:423:GLU:OE1	2:Q:423:GLU:N	2.43	0.49
2:R:466:HIS:HA	2:R:508:VAL:HG22	1.94	0.49
1:B:244:ARG:NE	1:B:357:GLU:OE1	2.44	0.49
1:G:122:LEU:HD23	1:G:125:ILE:HD12	1.95	0.49
1:K:89:VAL:HG13	1:K:89:VAL:O	2.11	0.49
2:M:411:ASN:OD1	2:M:412:VAL:N	2.46	0.49
2:O:243:MET:HB2	2:O:248:LEU:HD22	1.95	0.49
2:P:423:GLU:HG3	2:P:424:VAL:HG13	1.94	0.49
1:E:309:THR:HG22	1:E:309:THR:O	2.11	0.49
1:G:34:ILE:HG22	1:G:35:GLU:N	2.28	0.49
1:G:221:LEU:HB3	1:G:223:THR:HG22	1.95	0.49
2:N:229:ASN:OD1	2:N:230:LEU:N	2.46	0.49
1:G:112:GLU:HA	1:G:115:LEU:HB3	1.95	0.49
2:M:399:VAL:O	2:M:402:GLN:HG2	2.13	0.49
2:Q:318:LYS:HE3	2:Q:328:SER:HA	1.94	0.49
1:A:309:THR:HG22	1:A:309:THR:O	2.13	0.48
1:E:194:ASP:OD2	1:E:196:THR:HG22	2.13	0.48
1:K:365:ASP:OD1	1:K:366:ASP:N	2.46	0.48
2:M:175:LYS:NZ	3:M:1501:ATP:O2B	2.40	0.48
2:M:283:THR:OG1	2:M:284:ASN:N	2.46	0.48
2:R:124:PRO:HG2	2:R:127:VAL:HG23	1.95	0.48
2:R:313:LEU:HD23	2:R:314:ALA:N	2.28	0.48
1:G:384:SER:OG	1:G:393:ARG:NH2	2.46	0.48
1:K:193:ASN:O	1:K:195:ARG:NH1	2.46	0.48
2:M:251:ILE:HG12	2:M:427:ILE:HD13	1.94	0.48
2:O:296:ASP:OD1	2:O:296:ASP:N	2.46	0.48
2:O:310:ILE:HG22	2:O:311:GLY:N	2.27	0.48
2:Q:101:SER:OG	2:Q:102:GLU:N	2.45	0.48
2:Q:468:TYR:O	2:Q:469:LEU:HG	2.14	0.48
2:R:529:ASP:OD2	2:R:530:GLN:N	2.45	0.48
2:M:325:THR:HG22	2:M:326:LEU:H	1.77	0.48
2:N:230:LEU:O	2:N:231:LEU:HD12	2.13	0.48
2:P:265:SER:O	2:P:269:HIS:ND1	2.36	0.48
1:A:106:LEU:O	1:A:139:LEU:HD22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LYS:HD3	1:A:162:LYS:O	2.13	0.48
2:M:236:LEU:HD12	2:M:237:ARG:H	1.78	0.48
1:I:184:VAL:HG21	1:I:217:TRP:CD2	2.48	0.48
1:K:215:THR:HG23	1:K:217:TRP:H	1.79	0.48
2:N:299:VAL:O	2:N:303:GLU:OE2	2.31	0.48
2:N:310:ILE:HG22	2:N:312:LYS:CE	2.43	0.48
2:P:213:GLU:N	2:P:213:GLU:OE2	2.46	0.48
2:R:243:MET:CE	2:R:251:ILE:HD12	2.43	0.48
1:G:82:ASN:OD1	1:G:82:ASN:N	2.45	0.48
2:M:283:THR:HG22	2:R:360:GLU:HG3	1.96	0.48
2:M:318:LYS:HB2	2:M:326:LEU:HD22	1.94	0.48
2:N:511:THR:O	2:N:515:GLN:NE2	2.43	0.48
2:Q:254:GLU:OE2	2:Q:254:GLU:HA	2.14	0.48
2:M:279:ASN:ND2	2:M:292:TYR:O	2.47	0.48
2:M:417:LEU:HD23	2:M:425:LEU:HD11	1.96	0.48
1:A:70:LYS:N	1:A:71:PRO:CD	2.77	0.48
1:E:174:VAL:HG12	1:E:174:VAL:O	2.13	0.48
1:E:215:THR:H	1:E:218:THR:HG22	1.78	0.48
1:G:329:ILE:HD11	1:H:327:ILE:HG23	1.94	0.48
2:M:116:PRO:O	2:M:117:THR:OG1	2.21	0.48
2:P:320:LYS:CE	2:P:342:ILE:HD11	2.43	0.48
2:Q:471:ARG:NH2	2:Q:506:SER:O	2.43	0.48
1:A:35:GLU:HB2	1:A:50:THR:O	2.14	0.48
1:K:13:LEU:O	1:K:17:LEU:HG	2.14	0.48
1:K:172:ASP:CG	1:K:226:ARG:HH21	2.18	0.48
1:K:226:ARG:HG3	1:K:226:ARG:HH11	1.79	0.48
2:M:302:LEU:O	2:M:305:MET:HG2	2.13	0.48
1:I:206:LEU:O	1:I:209:VAL:HG12	2.14	0.47
1:I:365:ASP:OD2	1:I:365:ASP:N	2.47	0.47
1:K:42:ASP:HB2	1:K:44:ILE:HG12	1.96	0.47
1:C:244:ARG:HD2	1:C:356:ASP:HB2	1.95	0.47
1:L:345:ASP:OD1	1:L:346:GLU:N	2.47	0.47
2:R:295:ILE:O	2:R:298:VAL:N	2.45	0.47
1:C:258:PHE:HA	1:C:261:ASP:OD2	2.14	0.47
1:I:28:ASP:OD1	1:I:29:GLY:N	2.48	0.47
1:I:215:THR:HA	1:I:381:GLU:CG	2.44	0.47
2:M:64:VAL:O	2:M:87:ASN:N	2.47	0.47
2:M:204:HIS:CD2	2:M:456:VAL:HG11	2.49	0.47
2:N:295:ILE:O	2:N:299:VAL:HG13	2.14	0.47
2:P:181:LYS:HE2	2:P:574:PRO:HB3	1.95	0.47
1:G:66:GLY:O	1:G:69:TYR:CG	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:337:ALA:O	2:M:339:GLN:NE2	2.43	0.47
2:N:101:SER:OG	2:N:102:GLU:N	2.47	0.47
2:O:249:GLU:O	2:O:253:ILE:HB	2.14	0.47
2:O:273:ARG:HA	2:O:276:CYS:SG	2.54	0.47
2:P:253:ILE:HG21	2:P:264:ILE:HG12	1.95	0.47
1:C:107:THR:OG1	1:C:109:ASP:OD1	2.07	0.47
1:D:348:ILE:O	1:D:348:ILE:HG13	2.15	0.47
1:E:108:LYS:HE2	1:E:135:TYR:HB3	1.96	0.47
1:E:211:ARG:HH12	1:E:213:THR:HG22	1.77	0.47
1:I:96:HIS:ND1	1:I:147:GLY:O	2.42	0.47
2:R:243:MET:HE1	2:R:251:ILE:HD12	1.96	0.47
2:R:313:LEU:HD23	2:R:314:ALA:O	2.15	0.47
1:E:176:PHE:CE2	1:E:221:LEU:HD11	2.45	0.47
2:P:245:ALA:HB2	2:P:288:ASP:HB3	1.96	0.47
1:A:215:THR:H	1:A:218:THR:CG2	2.28	0.47
1:E:33:THR:HG23	1:E:195:ARG:HB3	1.97	0.47
2:O:400:VAL:HG22	2:O:435:MET:HE2	1.97	0.47
2:P:243:MET:HG3	2:P:247:GLU:HB3	1.95	0.47
2:Q:267:PHE:O	2:Q:271:VAL:HG23	2.15	0.47
2:Q:274:ASN:HD21	2:Q:297:GLU:CG	2.27	0.47
1:G:32:ILE:HG22	1:G:33:THR:N	2.30	0.47
2:N:557:LEU:HD13	2:N:568:VAL:HG12	1.97	0.47
2:R:378:GLN:O	2:R:382:TYR:N	2.46	0.47
2:R:548:LEU:HD21	2:R:557:LEU:HD21	1.97	0.47
1:C:315:THR:HG23	1:C:316:ASP:N	2.30	0.47
1:I:19:TYR:HE2	1:I:23:ILE:HD11	1.80	0.47
1:I:204:ALA:O	1:I:208:GLU:OE1	2.33	0.47
1:J:348:ILE:O	1:J:348:ILE:HG13	2.15	0.47
1:K:16:PHE:O	1:K:20:LEU:HD23	2.14	0.47
2:P:299:VAL:HG12	2:P:303:GLU:OE2	2.14	0.47
1:E:76:LEU:HD12	1:E:76:LEU:H	1.80	0.46
2:M:356:PRO:O	2:M:360:GLU:OE2	2.33	0.46
2:N:316:GLU:CD	2:N:326:LEU:HD11	2.34	0.46
2:O:41:TYR:CD1	2:O:53:LEU:HD21	2.50	0.46
2:O:385:LYS:HZ1	2:O:391:LEU:HA	1.80	0.46
1:G:327:ILE:HG23	1:H:329:ILE:HD11	1.97	0.46
1:H:284:LEU:HD13	1:H:340:ARG:HB2	1.97	0.46
1:I:35:GLU:HG3	1:I:52:VAL:HG23	1.97	0.46
1:I:221:LEU:HD12	1:I:222:ALA:N	2.28	0.46
1:I:245:TRP:HE3	1:I:281:ASN:HD21	1.64	0.46
1:K:173:ALA:HB2	1:K:227:MET:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:THR:OG1	1:G:110:ASP:OD2	2.33	0.46
1:K:106:LEU:HD23	1:K:107:THR:O	2.15	0.46
1:L:274:SER:O	1:L:274:SER:OG	2.28	0.46
1:A:117:THR:CG2	1:A:123:ARG:HB3	2.46	0.46
1:E:171:ILE:HD13	1:E:175:ILE:HD11	1.96	0.46
1:J:249:VAL:HB	1:J:360:LEU:HD23	1.96	0.46
2:N:269:HIS:HA	2:N:272:VAL:HG12	1.96	0.46
1:A:96:HIS:HB2	1:A:147:GLY:O	2.16	0.46
1:C:7:TYR:CD1	1:C:39:GLU:HG2	2.50	0.46
1:I:35:GLU:N	1:I:35:GLU:OE1	2.48	0.46
1:I:58:GLU:HG2	1:I:59:GLN:H	1.79	0.46
1:I:261:ASP:CG	1:I:383:LEU:HD12	2.36	0.46
2:O:367:ARG:O	2:O:371:ARG:HG2	2.15	0.46
2:P:318:LYS:HE2	2:P:326:LEU:HB3	1.98	0.46
1:E:175:ILE:HG13	1:E:176:PHE:N	2.31	0.46
1:E:211:ARG:HH12	1:E:213:THR:CG2	2.29	0.46
1:G:8:SER:O	1:G:12:TYR:HD2	1.98	0.46
1:G:71:PRO:O	1:G:74:LEU:HD23	2.15	0.46
2:M:54:ALA:HB1	2:M:94:THR:HB	1.97	0.46
2:P:530:GLN:CG	2:P:531:THR:N	2.78	0.46
2:R:385:LYS:HG2	2:R:386:GLU:H	1.80	0.46
1:C:9:ILE:HG21	1:C:216:ARG:CZ	2.46	0.46
1:I:38:ILE:HG22	1:I:38:ILE:O	2.16	0.46
2:M:367:ARG:O	2:M:371:ARG:HG2	2.15	0.46
2:Q:362:ASP:OD1	2:Q:362:ASP:N	2.48	0.46
2:Q:524:LEU:HD21	2:Q:529:ASP:HB2	1.97	0.46
2:R:137:LYS:HD2	2:R:137:LYS:N	2.31	0.46
1:A:9:ILE:HG23	1:A:10:LYS:N	2.31	0.46
1:A:212:VAL:HG21	1:A:231:LEU:HD21	1.98	0.46
1:C:75:MET:O	1:C:78:HIS:HB3	2.15	0.46
1:E:108:LYS:HA	1:E:139:LEU:HD11	1.98	0.46
1:E:140:ASP:OD2	1:E:141:ARG:N	2.49	0.46
1:H:261:ASP:HB2	1:H:383:LEU:HD12	1.97	0.46
1:I:169:ASP:OD2	1:I:170:ASP:N	2.49	0.46
2:M:165:VAL:HG12	2:M:166:ALA:N	2.31	0.46
2:M:234:ASP:OD2	2:M:235:ASN:N	2.48	0.46
2:Q:170:SER:OG	2:Q:171:THR:N	2.49	0.46
2:R:279:ASN:ND2	2:R:291:VAL:HG21	2.30	0.46
2:R:330:ARG:HD2	2:R:330:ARG:N	2.31	0.46
2:R:406:TYR:CD2	2:R:408:THR:O	2.69	0.46
1:A:60:ALA:HB3	1:A:97:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:GLN:O	1:I:18:LYS:HG3	2.15	0.46
1:K:327:ILE:HD12	1:K:336:GLU:OE2	2.16	0.46
2:N:253:ILE:HG12	2:N:267:PHE:CE2	2.51	0.46
1:E:38:ILE:HG12	1:E:78:HIS:NE2	2.31	0.46
1:I:104:LYS:O	1:I:144:ILE:HG22	2.16	0.46
1:J:262:ILE:HG23	1:J:263:VAL:N	2.31	0.46
1:A:39:GLU:OE1	1:A:39:GLU:N	2.29	0.45
2:P:240:TYR:O	2:P:243:MET:HB3	2.16	0.45
2:R:238:LEU:HG	2:R:238:LEU:O	2.17	0.45
2:O:400:VAL:HG22	2:O:435:MET:CE	2.46	0.45
2:O:423:GLU:HG2	2:O:424:VAL:HG13	1.99	0.45
1:E:54:CYS:HG	1:E:94:PHE:HE1	1.64	0.45
1:G:15:GLN:O	1:G:19:TYR:CD2	2.70	0.45
1:I:48:LEU:HD12	1:I:50:THR:HG23	1.98	0.45
1:K:227:MET:HG3	1:K:228:PHE:N	2.30	0.45
2:O:481:ARG:O	2:O:485:GLU:HG2	2.17	0.45
2:P:417:LEU:HB3	2:P:425:LEU:HD11	1.98	0.45
2:R:243:MET:HB2	2:R:248:LEU:HD12	1.97	0.45
1:E:174:VAL:HG11	1:E:210:ARG:NH1	2.32	0.45
2:O:345:SER:O	2:O:351:LYS:HA	2.17	0.45
2:M:310:ILE:HA	2:M:319:PRO:HA	1.98	0.45
2:R:260:SER:HA	2:R:263:GLN:HB2	1.97	0.45
1:E:176:PHE:CD2	1:E:221:LEU:HD21	2.51	0.45
1:F:284:LEU:HD12	1:F:340:ARG:HB2	1.98	0.45
1:G:14:TYR:OH	1:G:148:PRO:O	2.34	0.45
1:I:315:THR:HG23	1:I:316:ASP:N	2.32	0.45
2:M:43:LEU:HG	2:M:123:THR:HG22	1.99	0.45
2:M:423:GLU:OE1	2:M:423:GLU:N	2.43	0.45
2:N:35:MET:SD	2:N:122:VAL:HG11	2.56	0.45
2:N:218:PHE:CE1	2:N:412:VAL:HG21	2.52	0.45
2:P:46:SER:O	2:P:46:SER:OG	2.30	0.45
2:Q:283:THR:OG1	2:Q:284:ASN:N	2.50	0.45
2:R:13:ASP:OD1	2:R:14:SER:N	2.49	0.45
2:R:330:ARG:HD2	2:R:330:ARG:H	1.81	0.45
1:C:44:ILE:HG23	1:C:45:ALA:N	2.31	0.45
1:C:64:THR:HG22	1:C:67:LYS:HE2	1.98	0.45
1:C:72:ILE:HG22	1:C:76:LEU:HD13	1.98	0.45
1:C:203:LEU:HA	1:C:206:LEU:HG	1.99	0.45
1:E:39:GLU:OE2	1:E:39:GLU:N	2.49	0.45
1:E:169:ASP:OD1	1:E:169:ASP:N	2.50	0.45
1:E:212:VAL:HG21	1:E:231:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:211:ARG:NH2	1:K:379:LYS:HB2	2.31	0.45
2:Q:541:SER:OG	2:Q:542:ALA:N	2.50	0.45
2:R:237:ARG:NH1	2:R:402:GLN:OE1	2.50	0.45
2:R:258:HIS:O	2:R:258:HIS:ND1	2.50	0.45
1:A:34:ILE:HG22	1:A:35:GLU:N	2.32	0.45
1:E:106:LEU:N	1:E:106:LEU:HD12	2.31	0.45
1:K:73:LEU:O	1:K:76:LEU:CB	2.65	0.45
2:O:273:ARG:O	2:O:277:LYS:HG2	2.16	0.45
2:P:101:SER:OG	2:P:102:GLU:N	2.50	0.45
2:M:204:HIS:CE1	2:M:410:SER:HA	2.52	0.45
2:N:249:GLU:O	2:N:253:ILE:HB	2.17	0.45
2:N:310:ILE:HG22	2:N:312:LYS:HE3	1.99	0.45
2:N:316:GLU:HG3	2:N:316:GLU:O	2.17	0.45
2:O:308:GLU:OE2	2:O:330:ARG:NH2	2.50	0.45
2:P:539:ASP:O	2:P:539:ASP:OD2	2.35	0.45
2:R:232:GLY:O	2:R:236:LEU:HG	2.17	0.45
1:I:68:ILE:O	1:I:68:ILE:HG22	2.17	0.45
2:P:253:ILE:HG22	2:P:254:GLU:N	2.31	0.45
2:P:362:ASP:OD1	2:P:363:ARG:N	2.50	0.45
2:R:241:TRP:CB	2:R:293:PHE:HE1	2.29	0.45
2:R:482:LYS:O	2:R:485:GLU:HG3	2.17	0.45
2:R:496:VAL:O	2:R:496:VAL:HG13	2.17	0.45
1:A:125:ILE:O	1:A:128:ARG:N	2.43	0.44
1:B:262:ILE:HG23	1:B:263:VAL:N	2.32	0.44
1:E:215:THR:O	1:E:218:THR:HG22	2.17	0.44
1:G:215:THR:HG22	1:G:218:THR:HG23	1.98	0.44
2:R:227:THR:OG1	2:R:411:ASN:ND2	2.46	0.44
1:E:38:ILE:O	1:E:38:ILE:HG13	2.16	0.44
1:K:131:THR:O	1:K:133:VAL:HG13	2.18	0.44
1:K:280:SER:O	1:K:325:ARG:NH2	2.50	0.44
1:A:133:VAL:HG13	1:A:133:VAL:O	2.17	0.44
1:A:152:ASP:N	1:A:152:ASP:OD1	2.49	0.44
1:C:245:TRP:HE3	1:C:281:ASN:HD21	1.63	0.44
1:E:212:VAL:HG12	1:E:213:THR:N	2.32	0.44
1:I:67:LYS:HD3	1:I:67:LYS:N	2.32	0.44
1:K:297:GLN:NE2	1:K:307:CYS:SG	2.90	0.44
2:Q:320:LYS:HG3	2:Q:324:GLU:OE1	2.17	0.44
1:C:125:ILE:HD12	1:C:125:ILE:H	1.81	0.44
1:E:206:LEU:O	1:E:209:VAL:HG12	2.18	0.44
1:K:329:ILE:HD11	1:L:327:ILE:HG23	1.98	0.44
2:N:3:ASP:OD2	2:N:3:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:321:LEU:HD13	2:P:325:THR:O	2.18	0.44
2:Q:412:VAL:HG13	2:Q:412:VAL:O	2.18	0.44
2:R:204:HIS:CE1	2:R:410:SER:OG	2.71	0.44
1:A:111:LEU:HB2	1:A:139:LEU:HD11	2.00	0.44
1:C:185:ASP:O	1:C:189:ARG:HD2	2.17	0.44
1:I:10:LYS:O	1:I:13:LEU:HG	2.17	0.44
1:J:353:ARG:HG3	1:J:353:ARG:HH11	1.82	0.44
2:M:202:ASN:HB2	2:M:456:VAL:HG22	1.98	0.44
2:R:23:ILE:HG22	2:R:24:SER:N	2.33	0.44
1:G:108:LYS:O	1:G:111:LEU:HB3	2.17	0.44
1:G:211:ARG:HG3	1:G:211:ARG:O	2.18	0.44
1:H:262:ILE:HG23	1:H:263:VAL:N	2.33	0.44
1:J:284:LEU:HD12	1:J:340:ARG:HB2	1.99	0.44
1:J:329:ILE:O	1:J:333:PHE:HA	2.18	0.44
2:M:362:ASP:OD1	2:M:362:ASP:N	2.51	0.44
2:N:306:ASN:OD1	2:N:358:ASN:OD1	2.35	0.44
2:P:164:HIS:HB2	2:P:516:CYS:HA	2.00	0.44
2:P:194:ASN:OD1	2:P:196:HIS:N	2.50	0.44
2:P:372:LEU:O	2:P:378:GLN:NE2	2.51	0.44
2:Q:245:ALA:HA	2:Q:287:PHE:CE2	2.53	0.44
2:R:302:LEU:HD22	2:R:365:ILE:HD11	1.99	0.44
1:C:61:GLU:O	1:C:98:PRO:HG2	2.18	0.44
1:E:200:LYS:O	1:E:200:LYS:HD3	2.18	0.44
2:P:468:TYR:O	2:P:469:LEU:HG	2.17	0.44
2:Q:296:ASP:HB3	2:Q:382:TYR:OH	2.18	0.44
1:F:245:TRP:HD1	1:F:355:PRO:HA	1.82	0.44
1:G:73:LEU:O	1:G:76:LEU:HB2	2.18	0.44
1:J:292:ASP:OD1	1:J:292:ASP:N	2.47	0.44
1:K:69:TYR:O	1:K:73:LEU:HD13	2.18	0.44
2:N:321:LEU:HD22	2:N:325:THR:HB	1.98	0.44
2:R:304:ASN:OD1	2:R:338:VAL:HG23	2.18	0.44
1:C:24:LEU:HD12	1:C:25:ALA:N	2.33	0.44
1:C:60:ALA:CB	1:C:67:LYS:HE3	2.48	0.44
1:E:109:ASP:OD1	1:E:110:ASP:N	2.50	0.44
1:K:66:GLY:O	1:K:69:TYR:CD2	2.71	0.44
2:M:529:ASP:OD1	2:M:529:ASP:N	2.51	0.44
2:O:321:LEU:HD13	2:O:341:PHE:HE1	1.83	0.44
2:O:321:LEU:HD13	2:O:341:PHE:CE1	2.53	0.44
1:A:215:THR:H	1:A:218:THR:HG22	1.82	0.43
1:E:16:PHE:CD2	1:E:184:VAL:HG22	2.52	0.43
1:E:44:ILE:HG23	1:E:45:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:198:GLU:N	1:K:198:GLU:OE2	2.51	0.43
2:M:423:GLU:HG2	2:M:424:VAL:HG13	1.99	0.43
2:O:573:LEU:HD21	3:O:1501:ATP:C2	2.53	0.43
2:P:460:VAL:HG23	2:P:460:VAL:O	2.18	0.43
2:R:323:ASN:O	2:R:323:ASN:ND2	2.51	0.43
1:G:181:GLN:NE2	1:G:215:THR:HG21	2.33	0.43
2:M:233:VAL:CG1	2:M:234:ASP:N	2.80	0.43
2:M:297:GLU:OE2	2:M:297:GLU:N	2.40	0.43
2:N:19:ILE:HB	2:N:94:THR:OG1	2.18	0.43
2:O:567:THR:HG22	2:O:568:VAL:N	2.33	0.43
2:P:295:ILE:HG13	2:P:296:ASP:N	2.34	0.43
2:Q:263:GLN:HA	2:Q:266:GLN:HB2	2.01	0.43
2:Q:304:ASN:O	2:Q:307:ASN:N	2.51	0.43
2:Q:359:GLY:O	2:R:261:HIS:HD2	2.01	0.43
2:R:234:ASP:OD1	2:R:235:ASN:N	2.51	0.43
1:A:206:LEU:O	1:A:209:VAL:HG12	2.19	0.43
1:C:181:GLN:HA	1:C:184:VAL:HG12	2.01	0.43
1:E:40:ASP:OD2	1:E:42:ASP:N	2.51	0.43
1:E:120:GLU:O	1:E:123:ARG:HG3	2.17	0.43
1:F:284:LEU:CD2	1:F:286:MET:SD	3.07	0.43
1:G:35:GLU:OE1	1:G:51:ALA:O	2.36	0.43
1:H:361:ILE:O	1:H:362:ASN:HB2	2.18	0.43
1:I:126:VAL:O	1:I:129:ILE:HG12	2.18	0.43
2:M:363:ARG:O	2:M:366:LEU:HG	2.18	0.43
2:O:362:ASP:O	2:O:365:ILE:HG12	2.18	0.43
2:O:363:ARG:HA	2:O:366:LEU:HD22	1.99	0.43
2:Q:264:ILE:HG23	2:Q:265:SER:H	1.83	0.43
2:Q:331:ASP:N	2:Q:331:ASP:OD1	2.52	0.43
2:R:377:LEU:N	2:R:377:LEU:HD12	2.32	0.43
2:R:521:SER:O	2:R:556:PHE:HA	2.19	0.43
1:C:216:ARG:HD3	1:C:216:ARG:C	2.38	0.43
1:C:308:GLU:OE2	1:C:324:ARG:NH2	2.51	0.43
1:D:383:LEU:O	1:D:387:GLU:OE1	2.36	0.43
1:K:138:PHE:O	1:K:141:ARG:N	2.52	0.43
1:L:387:GLU:HG3	1:L:392:LEU:HD12	2.01	0.43
2:M:285:LEU:HD13	2:M:291:VAL:CG2	2.48	0.43
2:Q:165:VAL:HG12	2:Q:166:ALA:N	2.33	0.43
2:Q:456:VAL:O	2:Q:456:VAL:HG23	2.18	0.43
2:Q:540:LEU:HB2	2:Q:544:LEU:HD23	1.99	0.43
2:R:532:TYR:CE2	2:R:536:LEU:HD11	2.53	0.43
1:A:18:LYS:O	1:A:18:LYS:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:CYS:SG	1:B:339:LEU:HD21	2.57	0.43
1:C:32:ILE:HG22	1:C:33:THR:N	2.33	0.43
1:G:15:GLN:NE2	1:G:16:PHE:CE1	2.86	0.43
1:K:38:ILE:HG13	1:K:38:ILE:O	2.18	0.43
2:N:441:PHE:O	2:N:445:LYS:HG2	2.18	0.43
2:O:269:HIS:O	2:O:273:ARG:HG2	2.19	0.43
2:O:496:VAL:HG13	2:O:496:VAL:O	2.18	0.43
2:R:12:THR:HG21	2:R:22:GLU:OE1	2.18	0.43
1:A:224:LYS:HD3	1:A:228:PHE:HE2	1.83	0.43
1:A:366:ASP:OD1	1:A:367:GLU:N	2.47	0.43
1:C:65:LEU:HG	1:C:68:ILE:HD11	1.99	0.43
1:E:258:PHE:HA	1:E:261:ASP:OD1	2.18	0.43
1:I:215:THR:HA	1:I:381:GLU:HG2	2.01	0.43
1:I:247:VAL:HB	1:I:358:LEU:HD12	1.99	0.43
2:M:338:VAL:HG12	2:M:339:GLN:N	2.32	0.43
2:N:318:LYS:HD2	2:N:326:LEU:HD13	1.99	0.43
2:N:417:LEU:HD13	2:N:425:LEU:HD11	2.01	0.43
2:Q:259:ASN:O	2:Q:263:GLN:HG2	2.18	0.43
1:D:262:ILE:HG23	1:D:263:VAL:N	2.33	0.43
1:I:212:VAL:HB	1:I:378:PHE:HD1	1.84	0.43
1:K:92:ARG:HA	1:K:92:ARG:HH11	1.83	0.43
2:O:398:ASP:HA	2:O:401:ARG:HG2	2.00	0.43
2:P:526:ASN:OD1	2:P:527:ALA:N	2.52	0.43
1:A:5:ALA:HA	1:A:7:TYR:CE1	2.53	0.43
1:A:73:LEU:O	1:A:76:LEU:HD12	2.19	0.43
1:C:106:LEU:HG	1:C:107:THR:N	2.34	0.43
1:C:168:PRO:HA	1:C:171:ILE:HD12	2.01	0.43
1:E:286:MET:O	1:E:287:LEU:HD23	2.18	0.43
1:I:117:THR:OG1	1:I:123:ARG:HB2	2.19	0.43
1:J:328:LEU:CD2	1:J:335:MET:HG2	2.49	0.43
2:O:490:GLU:HG3	2:O:493:LYS:HE3	2.01	0.43
2:P:269:HIS:O	2:P:273:ARG:HG2	2.19	0.43
2:P:422:PHE:N	2:P:422:PHE:CD1	2.84	0.43
2:R:526:ASN:O	2:R:530:GLN:HB2	2.19	0.43
1:A:164:LYS:C	1:A:164:LYS:HD3	2.39	0.43
1:J:353:ARG:HG3	1:J:353:ARG:NH1	2.34	0.43
2:M:300:THR:OG1	2:M:338:VAL:HG22	2.19	0.43
2:M:342:ILE:HG22	2:M:343:VAL:N	2.34	0.43
2:O:233:VAL:CG1	2:O:234:ASP:N	2.78	0.43
2:P:243:MET:HG3	2:P:247:GLU:CB	2.49	0.43
2:P:264:ILE:O	2:P:268:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:18:LYS:HZ2	1:K:153:LEU:HD21	1.83	0.43
1:L:231:LEU:H	1:L:231:LEU:CD1	2.31	0.43
2:M:553:GLN:HG2	3:M:1501:ATP:C2	2.53	0.43
2:N:424:VAL:O	2:N:428:VAL:HG23	2.19	0.43
2:O:165:VAL:HG12	2:O:166:ALA:N	2.34	0.43
2:O:295:ILE:O	2:O:299:VAL:HG23	2.18	0.43
2:O:305:MET:HB3	2:O:357:PHE:HB3	2.01	0.43
2:R:375:PRO:HA	2:R:378:GLN:CG	2.49	0.43
1:C:300:LEU:CD2	1:C:305:LEU:HD12	2.45	0.42
2:N:234:ASP:OD1	2:N:235:ASN:N	2.52	0.42
2:N:546:ASP:OD1	2:N:547:LEU:N	2.52	0.42
2:O:202:ASN:HB3	2:O:456:VAL:HG13	2.01	0.42
2:P:265:SER:OG	2:P:266:GLN:N	2.52	0.42
2:Q:142:LEU:HG	2:Q:142:LEU:O	2.19	0.42
1:A:164:LYS:HE2	1:A:203:LEU:HD11	2.01	0.42
1:E:293:LEU:HD11	1:E:343:LYS:HG3	2.01	0.42
1:G:38:ILE:HB	1:G:52:VAL:CG1	2.49	0.42
2:M:287:PHE:CD1	2:M:288:ASP:N	2.87	0.42
2:M:292:TYR:HB2	2:M:393:THR:OG1	2.19	0.42
2:O:62:THR:HG22	2:O:63:HIS:N	2.34	0.42
2:O:243:MET:CB	2:O:248:LEU:HD22	2.48	0.42
2:O:304:ASN:ND2	2:O:339:GLN:OE1	2.52	0.42
2:P:471:ARG:NH1	2:P:506:SER:O	2.52	0.42
2:Q:268:ARG:HG3	2:Q:287:PHE:CD1	2.54	0.42
1:B:249:VAL:HB	1:B:360:LEU:HD23	2.00	0.42
1:C:57:HIS:CE1	1:C:59:GLN:OE1	2.72	0.42
1:E:66:GLY:O	1:E:69:TYR:HB2	2.19	0.42
1:E:110:ASP:O	1:E:113:THR:HB	2.18	0.42
1:J:328:LEU:HD23	1:J:335:MET:HG2	2.01	0.42
2:N:395:ASP:OD2	2:N:395:ASP:N	2.51	0.42
2:O:209:ASP:OD1	2:O:212:ALA:N	2.51	0.42
2:P:331:ASP:OD2	2:P:331:ASP:N	2.51	0.42
2:Q:276:CYS:SG	2:Q:285:LEU:O	2.77	0.42
2:Q:303:GLU:OE1	2:Q:365:ILE:HD12	2.18	0.42
2:Q:321:LEU:HD13	2:Q:325:THR:O	2.20	0.42
2:R:526:ASN:OD1	2:R:527:ALA:N	2.52	0.42
1:C:385:ASP:O	1:C:389:ILE:HG13	2.20	0.42
1:K:8:SER:CB	1:K:54:CYS:O	2.67	0.42
1:K:62:LYS:O	1:K:67:LYS:NZ	2.52	0.42
1:K:109:ASP:N	1:K:109:ASP:OD1	2.50	0.42
1:L:348:ILE:O	1:L:348:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:333:LEU:O	2:O:339:GLN:NE2	2.52	0.42
2:R:179:VAL:HG21	2:R:501:VAL:HG21	2.01	0.42
2:R:271:VAL:HG13	2:R:293:PHE:CE2	2.54	0.42
2:R:478:ASP:HA	2:R:481:ARG:HG3	2.02	0.42
2:R:519:PHE:CD1	2:R:537:LEU:HD11	2.54	0.42
1:E:211:ARG:HG3	1:E:211:ARG:O	2.19	0.42
1:K:21:SER:O	1:K:24:LEU:HG	2.19	0.42
2:M:262:ASN:OD1	2:M:263:GLN:N	2.53	0.42
2:N:276:CYS:HA	2:N:285:LEU:HD22	2.00	0.42
2:N:304:ASN:OD1	2:N:305:MET:N	2.52	0.42
2:R:231:LEU:O	2:R:231:LEU:HD12	2.19	0.42
1:A:290:ASP:N	1:A:290:ASP:OD1	2.46	0.42
1:K:153:LEU:O	1:K:157:VAL:HG23	2.19	0.42
1:K:255:ILE:HG22	1:K:256:GLU:N	2.35	0.42
2:O:257:GLU:N	2:O:363:ARG:NH2	2.68	0.42
2:Q:320:LYS:NZ	2:Q:351:LYS:O	2.48	0.42
2:Q:460:VAL:CG1	2:Q:498:LEU:HD23	2.49	0.42
2:R:218:PHE:CE2	2:R:412:VAL:HG11	2.55	0.42
1:C:10:LYS:O	1:C:13:LEU:HG	2.20	0.42
1:I:213:THR:HG23	1:I:213:THR:O	2.20	0.42
1:I:224:LYS:HD2	1:I:224:LYS:O	2.20	0.42
2:P:327:VAL:HB	2:P:330:ARG:HH21	1.85	0.42
2:P:428:VAL:O	2:P:432:ILE:HG13	2.20	0.42
2:Q:537:LEU:HD12	2:Q:537:LEU:N	2.35	0.42
2:R:189:ILE:HD12	2:R:189:ILE:H	1.84	0.42
2:R:231:LEU:HD11	2:R:415:ILE:HG12	2.01	0.42
1:A:210:ARG:NE	1:A:210:ARG:HA	2.35	0.42
1:C:134:ASP:OD1	1:C:137:ALA:HB3	2.20	0.42
1:E:197:VAL:HG13	1:E:202:PHE:CE1	2.55	0.42
1:E:211:ARG:HG3	1:E:211:ARG:NH1	2.35	0.42
1:F:309:THR:O	1:F:309:THR:HG22	2.19	0.42
1:G:9:ILE:HA	1:G:12:TYR:HD2	1.85	0.42
1:G:9:ILE:HA	1:G:12:TYR:CD2	2.54	0.42
1:G:58:GLU:HG3	1:G:96:HIS:O	2.20	0.42
1:J:366:ASP:OD1	1:J:367:GLU:N	2.48	0.42
1:K:367:GLU:HG3	1:K:367:GLU:O	2.20	0.42
2:M:342:ILE:CG2	2:M:343:VAL:N	2.83	0.42
2:O:206:VAL:HG23	2:O:206:VAL:O	2.19	0.42
2:O:312:LYS:HE3	2:O:353:SER:HB3	2.01	0.42
2:P:548:LEU:CD2	2:P:557:LEU:HD21	2.46	0.42
2:Q:342:ILE:HG22	2:Q:343:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:183:LEU:HD22	2:R:205:ILE:HD13	2.02	0.42
1:A:109:ASP:OD1	1:A:110:ASP:OD1	2.38	0.42
1:D:385:ASP:O	1:D:389:ILE:HG13	2.20	0.42
1:G:32:ILE:CG2	1:G:33:THR:N	2.83	0.42
1:I:49:THR:O	1:I:88:HIS:HB3	2.19	0.42
1:I:58:GLU:O	1:I:59:GLN:HB2	2.19	0.42
1:K:110:ASP:O	1:K:114:VAL:HG23	2.19	0.42
1:K:182:ARG:O	1:K:186:LEU:HD23	2.20	0.42
1:L:319:ILE:HG23	1:L:323:PHE:CE2	2.54	0.42
2:M:575:VAL:O	2:M:575:VAL:HG13	2.19	0.42
2:N:246:GLN:O	2:N:249:GLU:HB3	2.20	0.42
2:P:23:ILE:HG22	2:P:24:SER:N	2.34	0.42
2:P:243:MET:SD	2:P:248:LEU:HA	2.60	0.42
2:Q:279:ASN:OD1	2:Q:279:ASN:N	2.51	0.42
2:R:375:PRO:HA	2:R:378:GLN:HG2	2.02	0.42
1:A:60:ALA:HB3	1:A:97:PHE:CE1	2.55	0.42
1:A:297:GLN:NE2	1:A:307:CYS:SG	2.93	0.42
1:C:73:LEU:HD23	1:C:125:ILE:HD13	2.01	0.42
1:E:73:LEU:HB3	1:E:125:ILE:HG21	2.02	0.42
1:G:102:GLY:O	1:G:146:PHE:HB2	2.20	0.42
2:M:304:ASN:HB3	2:M:334:TYR:CD1	2.55	0.42
2:P:251:ILE:CD1	2:P:427:ILE:HD13	2.49	0.42
2:Q:233:VAL:HG13	2:Q:234:ASP:H	1.83	0.42
2:Q:234:ASP:OD1	2:Q:235:ASN:N	2.53	0.42
2:R:206:VAL:O	2:R:206:VAL:HG23	2.20	0.42
1:A:60:ALA:O	1:A:97:PHE:CD1	2.73	0.41
1:E:212:VAL:HG12	1:E:213:THR:H	1.85	0.41
1:G:159:ALA:O	1:G:162:LYS:HB3	2.20	0.41
1:L:229:SER:O	1:L:233:LYS:NZ	2.53	0.41
1:L:241:HIS:CG	1:L:244:ARG:HH21	2.38	0.41
1:L:261:ASP:HB2	1:L:383:LEU:HD12	2.02	0.41
2:M:23:ILE:HG22	2:M:24:SER:N	2.35	0.41
2:R:231:LEU:HD13	2:R:236:LEU:CD2	2.50	0.41
1:A:117:THR:O	1:A:117:THR:HG23	2.20	0.41
1:E:117:THR:OG1	1:E:122:LEU:HB3	2.19	0.41
1:G:31:ARG:HH21	1:G:196:THR:HG1	1.62	0.41
1:K:19:TYR:OH	1:K:35:GLU:HB3	2.20	0.41
2:O:279:ASN:HB2	2:O:285:LEU:HD21	2.03	0.41
2:O:293:PHE:CD2	2:O:294:SER:N	2.88	0.41
2:P:414:ILE:HG22	2:P:415:ILE:N	2.36	0.41
2:R:248:LEU:HD21	2:R:252:PHE:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:MET:O	1:A:287:LEU:HD23	2.20	0.41
1:A:355:PRO:O	1:A:373:VAL:HG22	2.20	0.41
1:C:35:GLU:HG3	1:C:52:VAL:CB	2.50	0.41
1:D:319:ILE:HG23	1:D:323:PHE:CE2	2.55	0.41
1:G:139:LEU:O	1:G:139:LEU:HD23	2.21	0.41
1:K:54:CYS:SG	1:K:55:LYS:N	2.93	0.41
2:O:525:THR:HG23	2:O:526:ASN:N	2.35	0.41
1:C:65:LEU:HD21	1:C:114:VAL:HG21	2.03	0.41
1:C:108:LYS:O	1:C:111:LEU:HB3	2.20	0.41
1:E:171:ILE:HA	1:E:175:ILE:HD11	2.02	0.41
1:K:35:GLU:HG2	1:K:36:GLY:N	2.35	0.41
1:K:110:ASP:O	1:K:113:THR:OG1	2.28	0.41
2:N:263:GLN:NE2	2:N:364:MET:SD	2.94	0.41
2:N:265:SER:HA	2:N:268:ARG:HB3	2.02	0.41
1:A:211:ARG:HG3	1:A:212:VAL:H	1.86	0.41
1:E:171:ILE:CD1	1:E:175:ILE:HD11	2.49	0.41
1:I:45:ALA:O	1:I:47:GLY:N	2.53	0.41
1:I:212:VAL:HB	1:I:378:PHE:CD1	2.55	0.41
2:M:345:SER:O	2:M:351:LYS:HA	2.21	0.41
2:N:267:PHE:O	2:N:268:ARG:C	2.58	0.41
2:N:367:ARG:HA	2:N:367:ARG:NE	2.34	0.41
2:O:275:LYS:HZ3	2:O:291:VAL:H	1.69	0.41
2:O:468:TYR:O	2:O:469:LEU:HG	2.19	0.41
2:P:292:TYR:HB2	2:P:393:THR:HG23	2.03	0.41
2:R:164:HIS:HB2	2:R:516:CYS:HA	2.01	0.41
1:A:245:TRP:HD1	1:A:355:PRO:HA	1.85	0.41
1:A:315:THR:HG23	1:A:316:ASP:N	2.36	0.41
1:C:92:ARG:HH22	1:C:145:GLU:HB3	1.86	0.41
1:D:361:ILE:O	1:D:362:ASN:HB2	2.20	0.41
1:F:315:THR:HG23	1:F:316:ASP:N	2.36	0.41
1:G:108:LYS:O	1:G:112:GLU:OE2	2.39	0.41
1:K:34:ILE:HG22	1:K:35:GLU:N	2.35	0.41
2:M:170:SER:OG	2:M:171:THR:N	2.52	0.41
2:M:243:MET:HB3	2:M:248:LEU:HB2	2.02	0.41
2:M:282:LEU:HD11	2:M:285:LEU:HG	2.03	0.41
2:M:283:THR:HG22	2:R:360:GLU:CG	2.50	0.41
2:P:274:ASN:O	2:P:277:LYS:HB3	2.21	0.41
2:P:426:SER:O	2:P:429:VAL:HG12	2.21	0.41
2:R:548:LEU:HD23	2:R:551:LEU:HD11	2.01	0.41
1:C:35:GLU:HG3	1:C:52:VAL:HG11	2.03	0.41
1:G:212:VAL:HG12	1:G:213:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:ARG:NH1	1:G:388:TYR:O	2.53	0.41
1:K:101:SER:O	1:K:101:SER:OG	2.38	0.41
1:K:245:TRP:HD1	1:K:355:PRO:HA	1.84	0.41
2:N:557:LEU:HD12	2:N:567:THR:O	2.21	0.41
2:Q:269:HIS:CE1	2:Q:273:ARG:HG3	2.56	0.41
2:Q:397:ALA:HA	2:Q:400:VAL:HG12	2.01	0.41
1:A:96:HIS:O	1:A:97:PHE:CD1	2.73	0.41
1:G:73:LEU:HG	1:G:122:LEU:HD22	2.02	0.41
2:O:548:LEU:HB2	2:O:549:PRO:HD3	2.03	0.41
1:G:23:ILE:O	1:G:26:ALA:HB3	2.21	0.41
1:G:33:THR:CG2	1:G:195:ARG:HB3	2.51	0.41
1:H:316:ASP:OD2	1:H:316:ASP:N	2.52	0.41
1:I:17:LEU:HD21	1:I:154:GLN:HB3	2.02	0.41
1:J:244:ARG:NH2	1:J:357:GLU:OE2	2.52	0.41
1:K:22:GLU:O	1:K:26:ALA:N	2.54	0.41
1:K:174:VAL:O	1:K:174:VAL:HG12	2.20	0.41
1:L:280:SER:O	1:L:282:PRO:HD3	2.21	0.41
2:M:318:LYS:CE	2:M:327:VAL:O	2.69	0.41
2:M:409:LYS:HA	2:M:409:LYS:HD2	1.84	0.41
2:M:601:VAL:HG13	2:N:442:HIS:HB3	2.02	0.41
2:P:327:VAL:O	2:P:330:ARG:NH2	2.44	0.41
2:P:460:VAL:CG2	2:P:498:LEU:HD23	2.49	0.41
2:Q:244:ASN:OD1	2:Q:247:GLU:HG2	2.20	0.41
2:Q:294:SER:OG	2:Q:296:ASP:OD1	2.39	0.41
2:Q:356:PRO:O	2:Q:360:GLU:OE2	2.38	0.41
2:Q:407:MET:O	2:Q:407:MET:HG2	2.21	0.41
2:Q:558:ILE:O	2:Q:558:ILE:HG23	2.20	0.41
2:R:299:VAL:HG13	2:R:300:THR:N	2.36	0.41
2:R:309:VAL:HG12	2:R:310:ILE:N	2.36	0.41
1:K:203:LEU:CD1	1:K:203:LEU:N	2.84	0.41
2:M:244:ASN:OD1	2:M:245:ALA:N	2.54	0.41
1:A:11:GLY:O	1:A:15:GLN:OE1	2.38	0.40
1:A:158:LEU:HD11	1:A:171:ILE:HD12	2.03	0.40
1:E:176:PHE:CE2	1:E:221:LEU:HD21	2.56	0.40
1:E:203:LEU:HD23	1:E:203:LEU:O	2.21	0.40
1:E:286:MET:C	1:E:287:LEU:HD23	2.42	0.40
1:F:245:TRP:CH2	1:F:340:ARG:NH2	2.89	0.40
2:O:97:ILE:HG13	2:O:98:GLY:N	2.36	0.40
2:O:217:ALA:HA	2:O:576:PRO:HG2	2.04	0.40
2:O:229:ASN:OD1	2:O:412:VAL:O	2.39	0.40
2:O:233:VAL:CG1	2:O:234:ASP:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:599:ASP:HA	2:O:602:ILE:HG12	2.04	0.40
2:R:238:LEU:HD23	2:R:238:LEU:H	1.86	0.40
1:C:239:LEU:HD11	1:C:390:LEU:HD23	2.02	0.40
1:E:64:THR:OG1	1:E:67:LYS:HE2	2.21	0.40
1:E:221:LEU:HD12	1:E:222:ALA:N	2.36	0.40
1:I:8:SER:O	1:I:12:TYR:HD2	2.04	0.40
1:I:108:LYS:NZ	1:I:135:TYR:HB3	2.35	0.40
1:I:192:VAL:HG23	1:I:192:VAL:O	2.22	0.40
1:K:189:ARG:HD3	1:K:190:SER:N	2.36	0.40
2:N:508:VAL:HB	2:N:513:PHE:CE2	2.56	0.40
2:O:310:ILE:HD13	2:O:319:PRO:HA	2.03	0.40
2:P:367:ARG:HA	2:P:370:THR:OG1	2.22	0.40
2:P:408:THR:O	2:P:408:THR:HG22	2.20	0.40
2:Q:258:HIS:O	2:Q:258:HIS:CG	2.74	0.40
2:Q:383:PRO:HG2	2:Q:391:LEU:HD22	2.02	0.40
1:C:190:SER:O	1:C:190:SER:OG	2.33	0.40
1:E:19:TYR:O	1:E:23:ILE:HG13	2.21	0.40
1:I:12:TYR:O	1:I:15:GLN:HG3	2.21	0.40
1:I:214:PHE:HE1	1:I:228:PHE:HE1	1.70	0.40
1:K:16:PHE:HA	1:K:19:TYR:HD2	1.87	0.40
1:K:152:ASP:HA	1:K:155:VAL:HG12	2.03	0.40
2:Q:43:LEU:HD22	2:Q:51:TYR:HB3	2.03	0.40
2:Q:385:LYS:HG3	2:Q:391:LEU:HD12	2.03	0.40
1:G:35:GLU:CD	1:G:92:ARG:HH12	2.24	0.40
1:I:58:GLU:CG	1:I:59:GLN:H	2.33	0.40
1:K:111:LEU:CD2	1:K:135:TYR:HB3	2.52	0.40
2:M:302:LEU:HD13	2:M:365:ILE:CD1	2.52	0.40
2:P:273:ARG:HA	2:P:276:CYS:SG	2.62	0.40
2:Q:137:LYS:H	2:Q:137:LYS:HD2	1.87	0.40
2:Q:236:LEU:HD12	2:Q:237:ARG:N	2.36	0.40
2:Q:548:LEU:HB2	2:Q:549:PRO:HD3	2.03	0.40
2:Q:567:THR:HG22	2:Q:568:VAL:N	2.35	0.40
2:R:366:LEU:HD12	2:R:367:ARG:NE	2.37	0.40
1:A:34:ILE:O	1:A:195:ARG:HG2	2.21	0.40
1:C:162:LYS:HD3	1:C:162:LYS:C	2.41	0.40
1:E:214:PHE:HE2	1:E:228:PHE:CE1	2.39	0.40
1:K:75:MET:O	1:K:78:HIS:HB3	2.22	0.40
1:K:142:PHE:CD1	1:K:143:ALA:N	2.89	0.40
2:M:567:THR:HG22	2:M:568:VAL:N	2.37	0.40
2:N:279:ASN:HB2	2:N:285:LEU:HD21	2.04	0.40
2:P:249:GLU:OE1	2:P:250:GLN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:313:LEU:HD23	2:P:314:ALA:O	2.22	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	A	384/397 (97%)	364 (95%)	20 (5%)	0	100	100
1	B	165/397 (42%)	161 (98%)	4 (2%)	0	100	100
1	C	380/397 (96%)	358 (94%)	22 (6%)	0	100	100
1	D	167/397 (42%)	160 (96%)	7 (4%)	0	100	100
1	E	383/397 (96%)	372 (97%)	10 (3%)	1 (0%)	37	66
1	F	165/397 (42%)	158 (96%)	7 (4%)	0	100	100
1	G	376/397 (95%)	360 (96%)	16 (4%)	0	100	100
1	H	166/397 (42%)	157 (95%)	9 (5%)	0	100	100
1	I	381/397 (96%)	363 (95%)	17 (4%)	1 (0%)	37	66
1	J	167/397 (42%)	160 (96%)	7 (4%)	0	100	100
1	K	380/397 (96%)	365 (96%)	15 (4%)	0	100	100
1	L	166/397 (42%)	161 (97%)	5 (3%)	0	100	100
2	M	534/617 (86%)	506 (95%)	28 (5%)	0	100	100
2	N	523/617 (85%)	500 (96%)	23 (4%)	0	100	100
2	O	531/617 (86%)	505 (95%)	26 (5%)	0	100	100
2	P	547/617 (89%)	518 (95%)	29 (5%)	0	100	100
2	Q	536/617 (87%)	508 (95%)	28 (5%)	0	100	100
2	R	535/617 (87%)	512 (96%)	22 (4%)	1 (0%)	44	72
All	All	6486/8466 (77%)	6188 (95%)	295 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	46	ALA
1	E	114	VAL
2	R	356	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	337/346 (97%)	337 (100%)	0	100	100
1	B	154/346 (44%)	154 (100%)	0	100	100
1	C	334/346 (96%)	330 (99%)	4 (1%)	67	82
1	D	156/346 (45%)	156 (100%)	0	100	100
1	E	336/346 (97%)	335 (100%)	1 (0%)	91	94
1	F	154/346 (44%)	154 (100%)	0	100	100
1	G	332/346 (96%)	329 (99%)	3 (1%)	75	86
1	H	155/346 (45%)	155 (100%)	0	100	100
1	I	335/346 (97%)	332 (99%)	3 (1%)	75	86
1	J	156/346 (45%)	156 (100%)	0	100	100
1	K	335/346 (97%)	335 (100%)	0	100	100
1	L	155/346 (45%)	153 (99%)	2 (1%)	65	80
2	M	470/525 (90%)	469 (100%)	1 (0%)	92	96
2	N	454/525 (86%)	453 (100%)	1 (0%)	92	96
2	O	467/525 (89%)	465 (100%)	2 (0%)	89	93
2	P	468/525 (89%)	468 (100%)	0	100	100
2	Q	468/525 (89%)	466 (100%)	2 (0%)	89	93
2	R	462/525 (88%)	460 (100%)	2 (0%)	89	93
All	All	5728/7302 (78%)	5707 (100%)	21 (0%)	88	93

All (21) residues with a non-rotameric sidechain are listed below:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type
1	C	108	LYS
1	C	158	LEU
1	C	189	ARG
1	C	216	ARG
1	E	224	LYS
1	G	15	GLN
1	G	82	ASN
1	G	108	LYS
1	I	18	LYS
1	I	210	ARG
1	I	224	LYS
1	L	231	LEU
1	L	393	ARG
2	M	384	LYS
2	N	482	LYS
2	O	366	LEU
2	O	384	LYS
2	Q	279	ASN
2	Q	313	LEU
2	R	293	PHE
2	R	367	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	82	ASN
1	A	297	GLN
1	C	96	HIS
1	C	193	ASN
1	C	281	ASN
1	E	154	GLN
1	E	297	GLN
1	E	331	ASN
1	G	181	GLN
1	I	57	HIS
1	I	178	ASN
1	I	279	HIS
1	I	281	ASN
1	I	331	ASN
1	J	391	GLN
1	K	178	ASN
1	K	297	GLN

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Mol	Chain	Res	Type
2	M	63	HIS
2	M	235	ASN
2	M	304	ASN
2	M	307	ASN
2	M	354	ASN
2	M	466	HIS
2	M	530	GLN
2	M	579	HIS
2	N	48	ASN
2	N	134	HIS
2	N	258	HIS
2	N	259	ASN
2	N	263	GLN
2	N	269	HIS
2	N	279	ASN
2	N	284	ASN
2	N	307	ASN
2	N	354	ASN
2	N	442	HIS
2	N	530	GLN
2	N	550	ASN
2	N	570	HIS
2	O	48	ASN
2	O	95	GLN
2	O	202	ASN
2	O	307	ASN
2	O	354	ASN
2	O	466	HIS
2	O	518	ASN
2	O	570	HIS
2	O	579	HIS
2	P	48	ASN
2	P	63	HIS
2	P	258	HIS
2	P	266	GLN
2	P	278	HIS
2	P	307	ASN
2	P	339	GLN
2	P	354	ASN
2	P	442	HIS
2	P	550	ASN
2	P	570	HIS

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Mol	Chain	Res	Type
2	Q	48	ASN
2	Q	111	HIS
2	Q	274	ASN
2	Q	278	HIS
2	Q	369	HIS
2	Q	503	GLN
2	Q	550	ASN
2	Q	570	HIS
2	R	202	ASN
2	R	204	HIS
2	R	258	HIS
2	R	262	ASN
2	R	274	ASN
2	R	278	HIS
2	R	279	ASN
2	R	284	ASN
2	R	323	ASN
2	R	369	HIS
2	R	550	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	ATP	O	1501	4	26,33,33	0.98	2 (7%)	31,52,52	1.51	4 (12%)
3	ATP	Q	1501	4	26,33,33	0.95	2 (7%)	31,52,52	1.54	5 (16%)
3	ATP	M	1501	-	26,33,33	0.96	2 (7%)	31,52,52	1.66	6 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	O	1501	4	-	3/18/38/38	0/3/3/3
3	ATP	Q	1501	4	-	5/18/38/38	0/3/3/3
3	ATP	M	1501	-	-	7/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1501	ATP	C5-C4	2.33	1.47	1.40
3	Q	1501	ATP	C5-C4	2.32	1.47	1.40
3	O	1501	ATP	C5-C4	2.29	1.47	1.40
3	O	1501	ATP	O4'-C1'	2.22	1.44	1.41
3	M	1501	ATP	O4'-C1'	2.04	1.43	1.41
3	Q	1501	ATP	O4'-C1'	2.03	1.43	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1501	ATP	PB-O3B-PG	-4.17	118.50	132.83
3	O	1501	ATP	PB-O3B-PG	-3.89	119.46	132.83
3	Q	1501	ATP	PB-O3B-PG	-3.64	120.34	132.83
3	O	1501	ATP	N3-C2-N1	-3.63	123.00	128.68
3	Q	1501	ATP	PA-O3A-PB	-3.61	120.43	132.83
3	Q	1501	ATP	N3-C2-N1	-3.60	123.05	128.68
3	O	1501	ATP	PA-O3A-PB	-3.59	120.50	132.83
3	M	1501	ATP	O4'-C1'-C2'	-3.49	101.82	106.93
3	M	1501	ATP	N3-C2-N1	-3.30	123.53	128.68
3	M	1501	ATP	PA-O3A-PB	-3.13	122.08	132.83
3	M	1501	ATP	C4-C5-N7	-2.66	106.63	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	1501	ATP	C3'-C2'-C1'	2.62	104.92	100.98
3	Q	1501	ATP	C4-C5-N7	-2.61	106.68	109.40
3	O	1501	ATP	C4-C5-N7	-2.54	106.75	109.40
3	Q	1501	ATP	C3'-C2'-C1'	2.51	104.76	100.98

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	1501	ATP	C5'-O5'-PA-O3A
3	M	1501	ATP	C4'-C5'-O5'-PA
3	O	1501	ATP	C5'-O5'-PA-O2A
3	O	1501	ATP	C5'-O5'-PA-O3A
3	Q	1501	ATP	C5'-O5'-PA-O3A
3	Q	1501	ATP	C3'-C4'-C5'-O5'
3	M	1501	ATP	O4'-C4'-C5'-O5'
3	M	1501	ATP	C3'-C4'-C5'-O5'
3	Q	1501	ATP	O4'-C4'-C5'-O5'
3	M	1501	ATP	PB-O3B-PG-O1G
3	M	1501	ATP	PB-O3B-PG-O2G
3	M	1501	ATP	C5'-O5'-PA-O1A
3	Q	1501	ATP	C5'-O5'-PA-O1A
3	O	1501	ATP	PG-O3B-PB-O2B
3	Q	1501	ATP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1501	ATP	1	0
3	M	1501	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP O 1501

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP Q 1501

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP M 1501

Bond lengths

Bond angles

Torsions

Rings
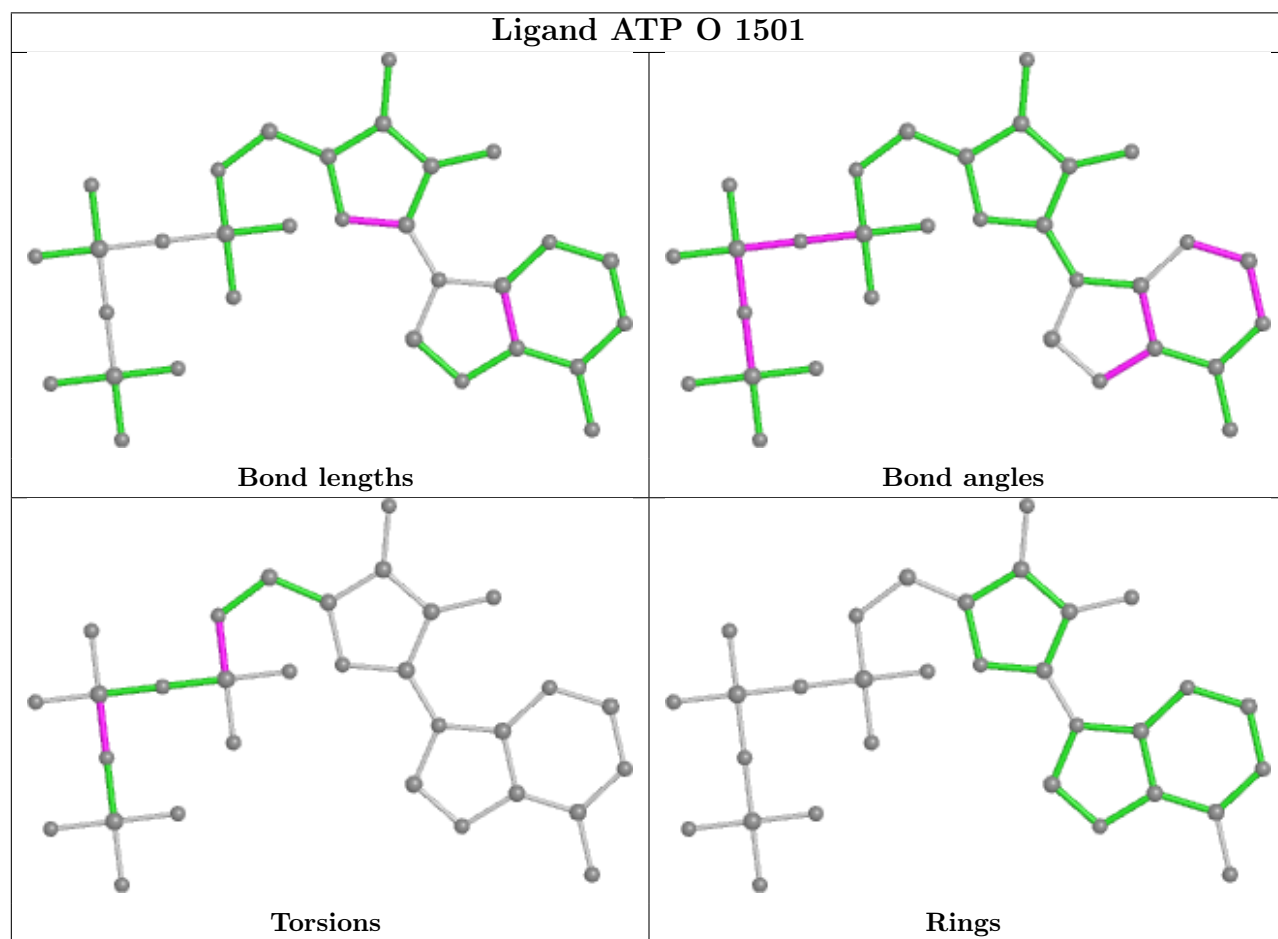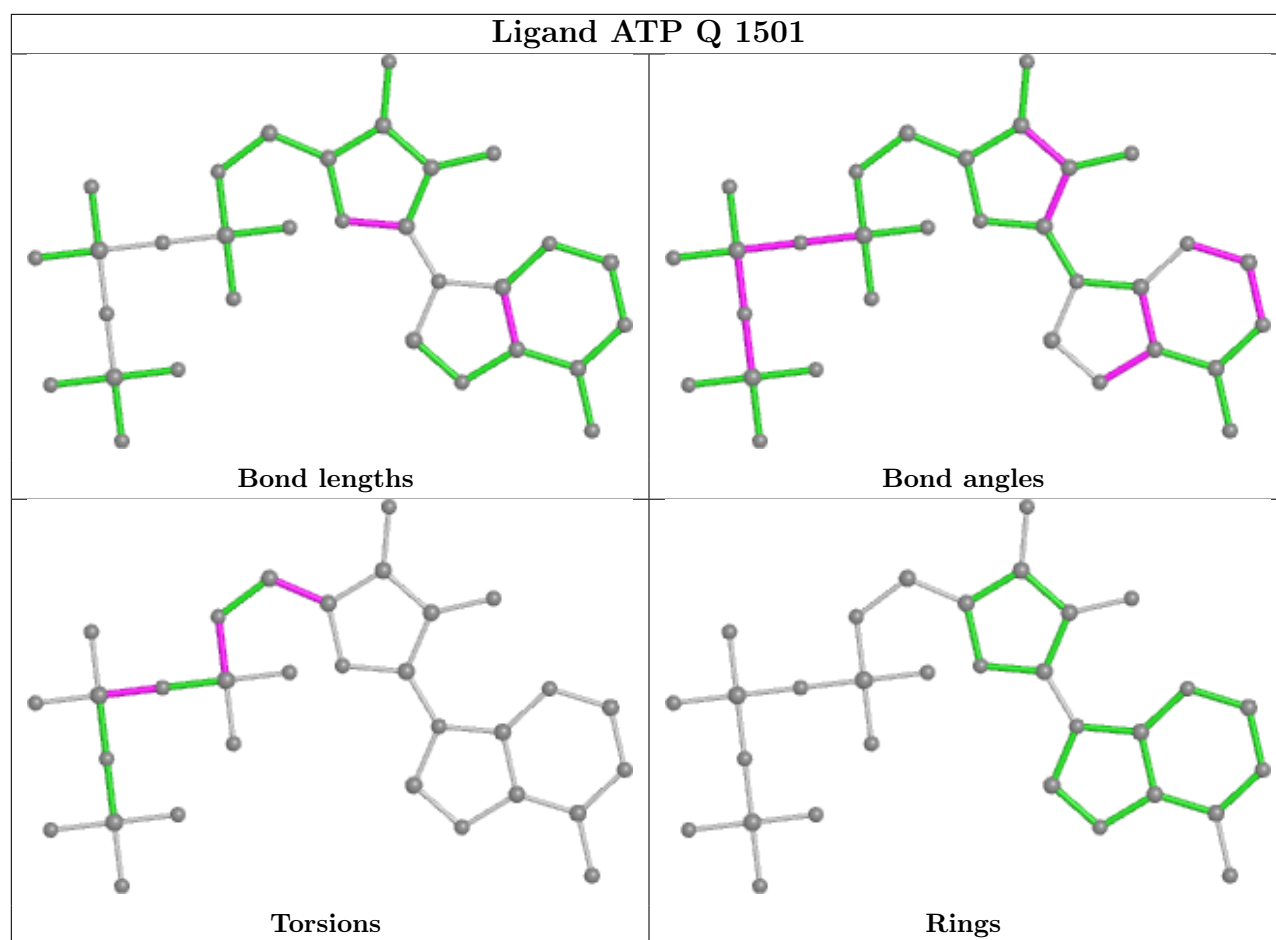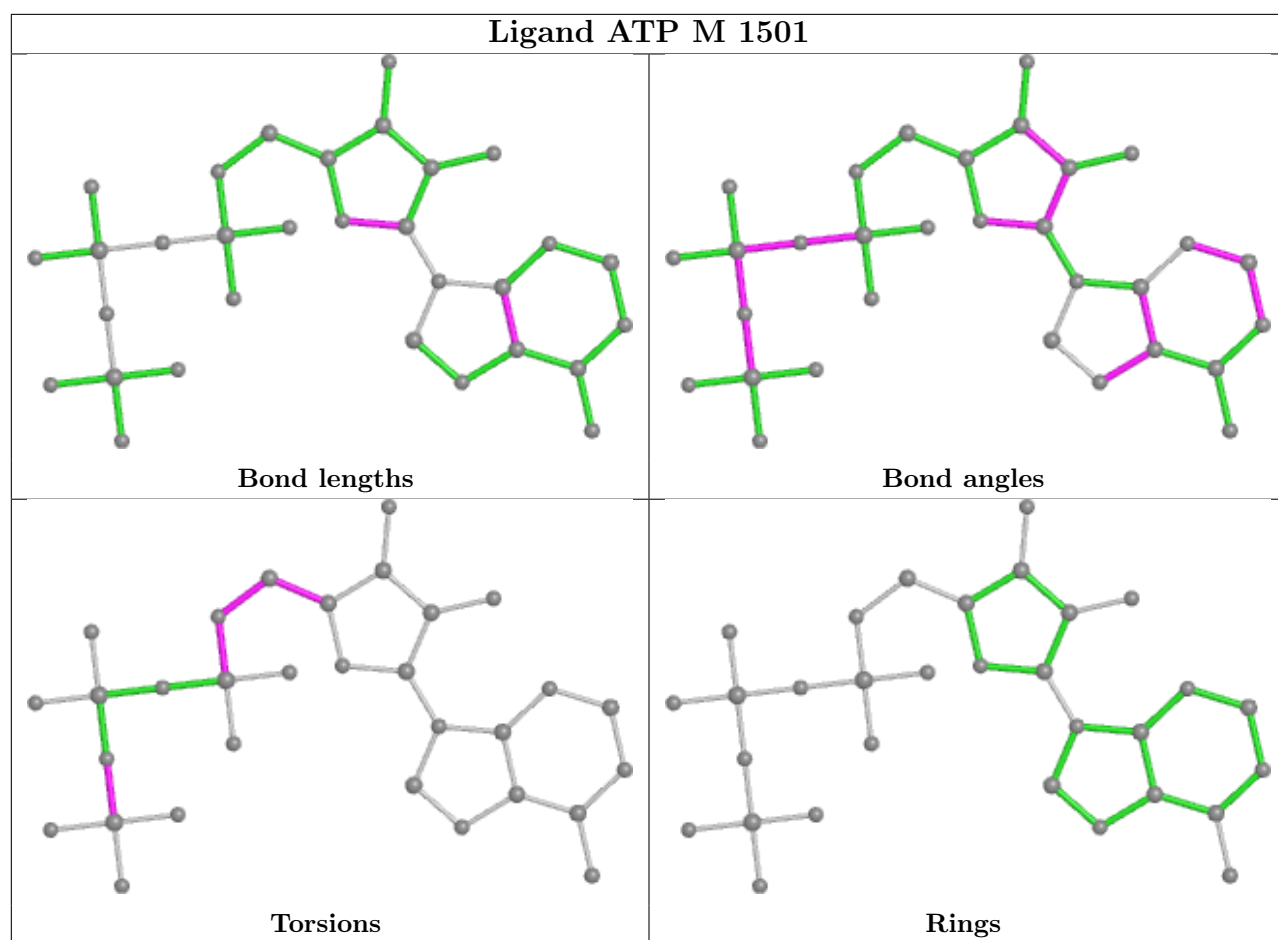
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-60127. 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 ⓘ
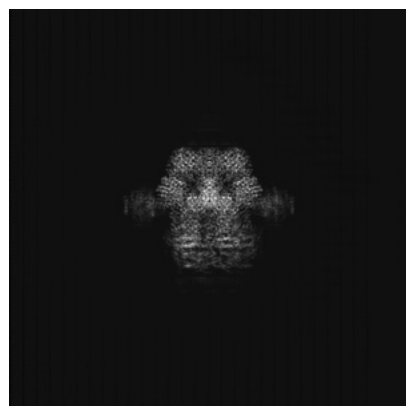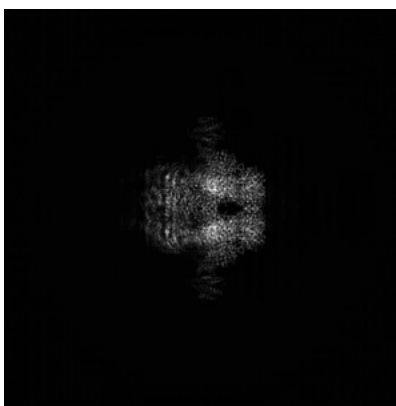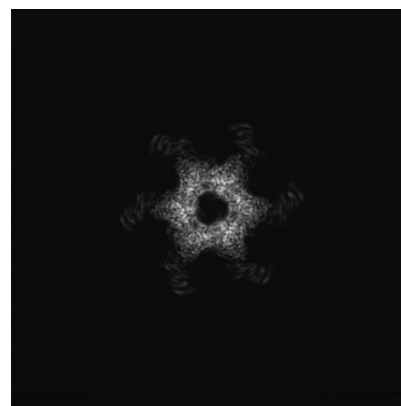
6.1.1 Primary map

X   Y   Z

6.1.2 Raw map

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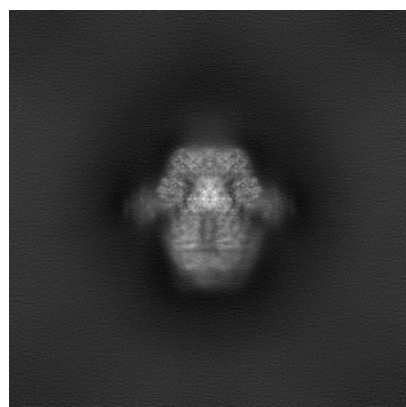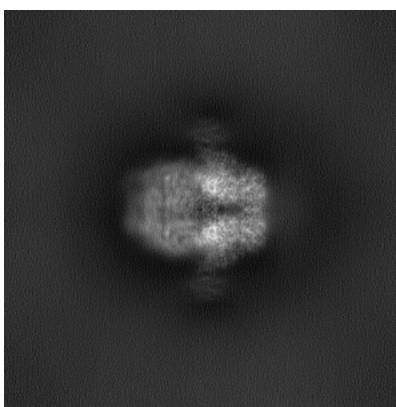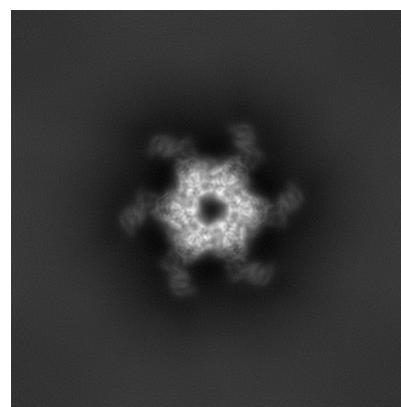
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
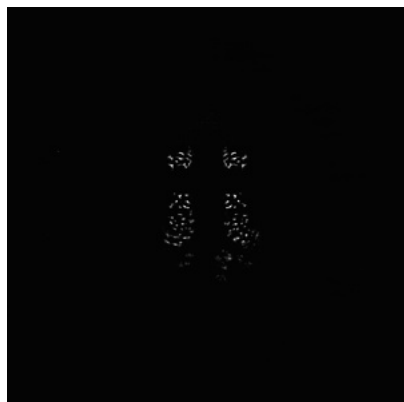
6.2.1 Primary map
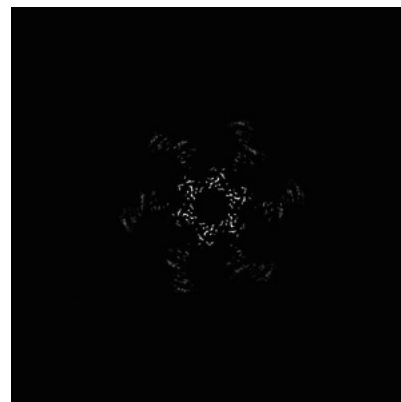
| X Index: 220 | Y Index: 220 | Z Index: 220 |

6.2.2 Raw map
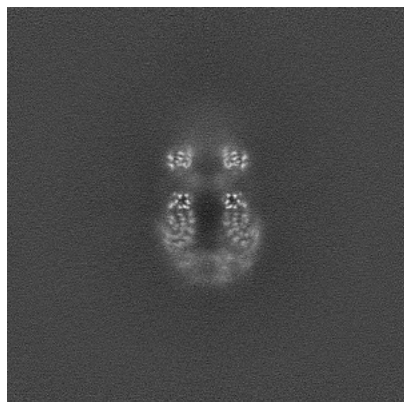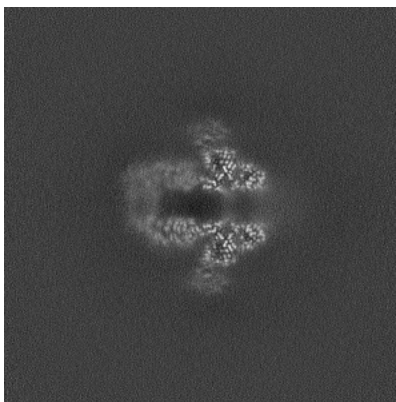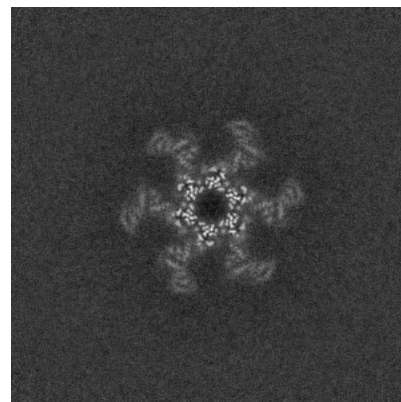
| X Index: 220 | Y Index: 220 | Z Index: 220 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
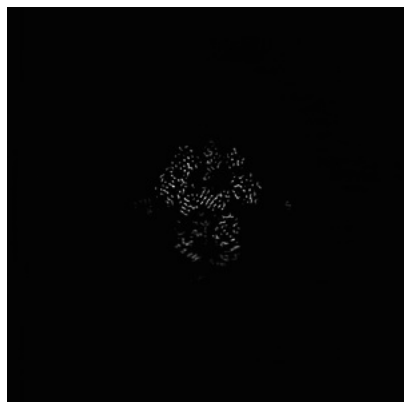
X Index: 241	Y Index: 250	Z Index: 231
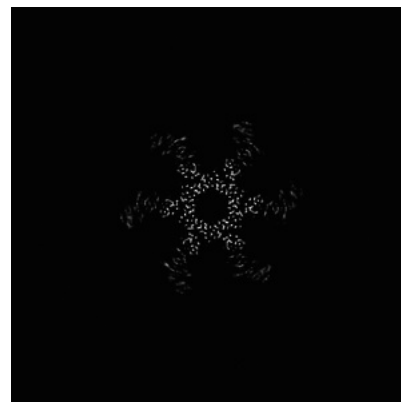
6.3.2 Raw map
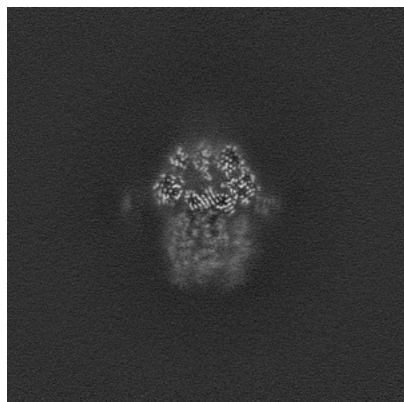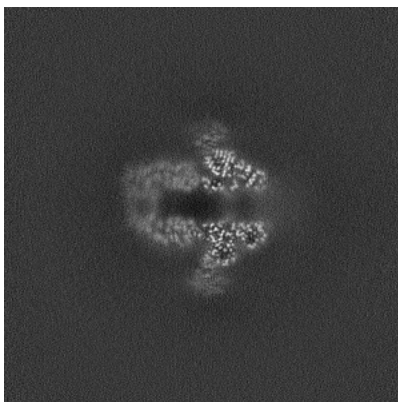
X Index: 199	Y Index: 218	Z Index: 232
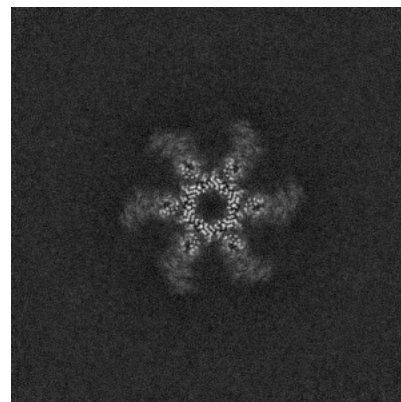
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
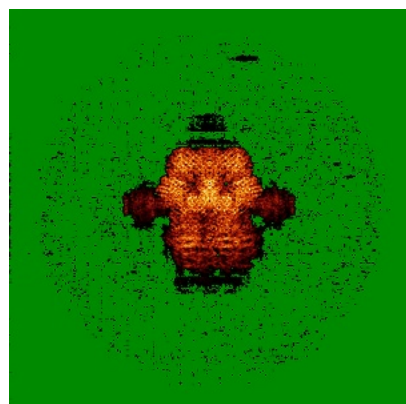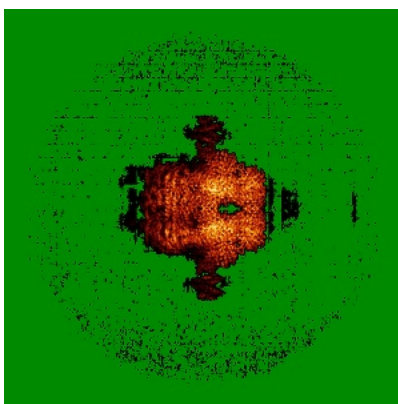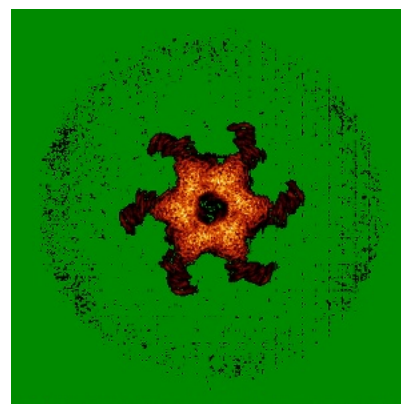
X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z

6.4.2 Raw map

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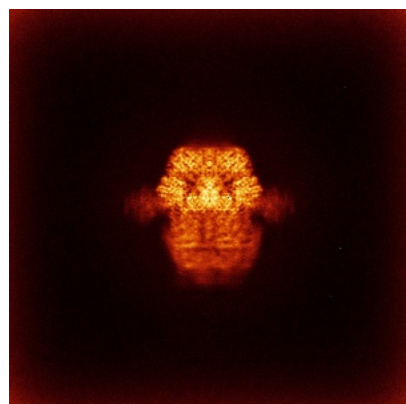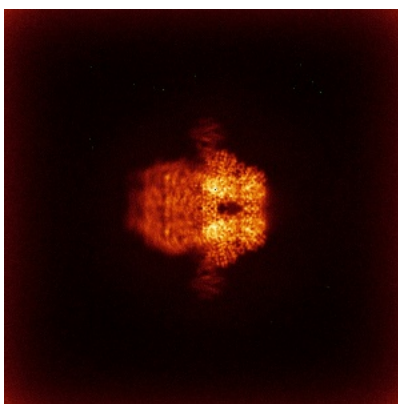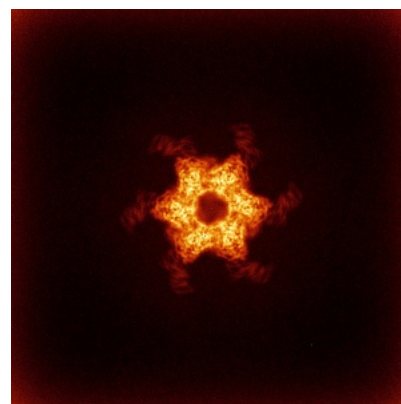
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
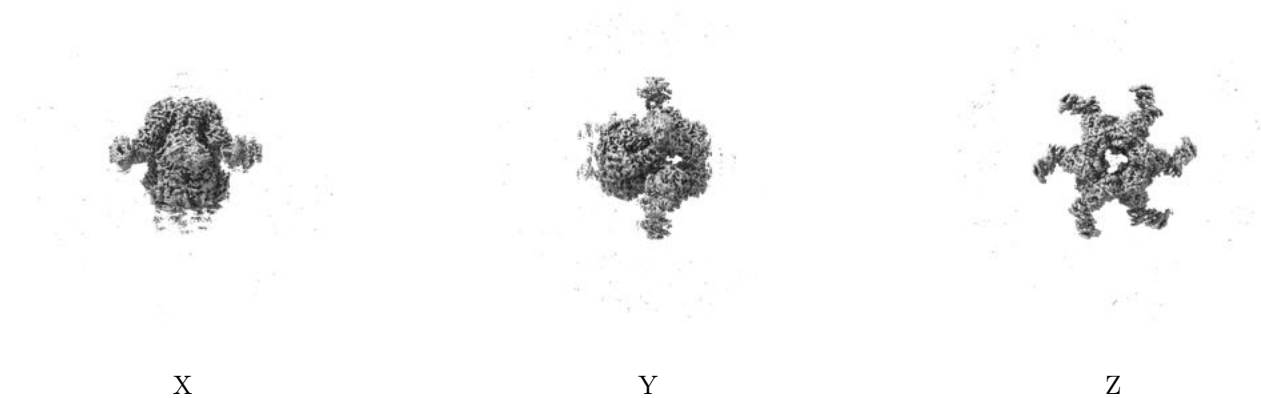
The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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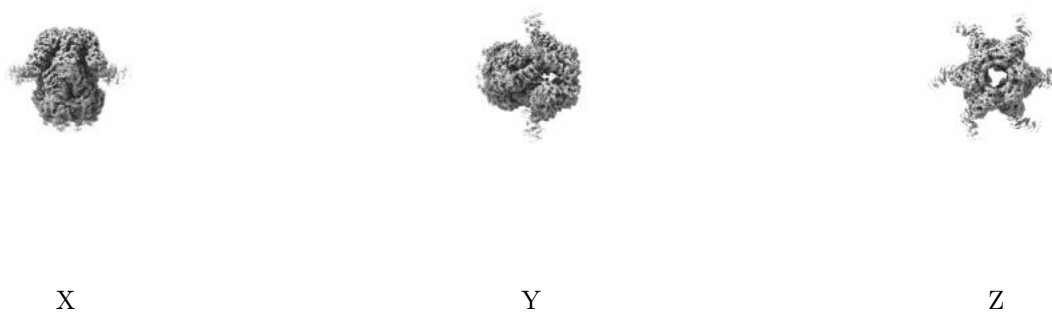
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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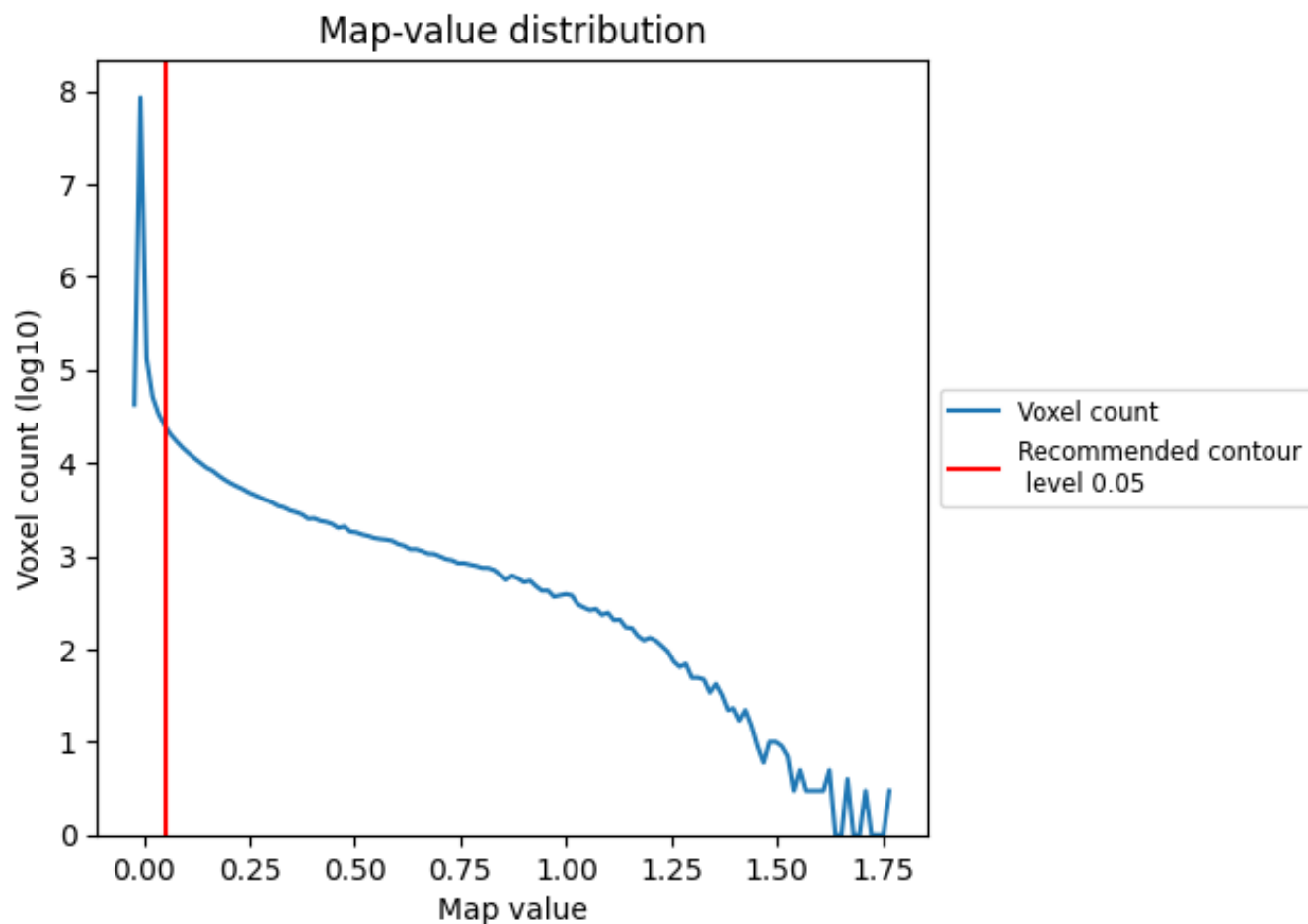
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
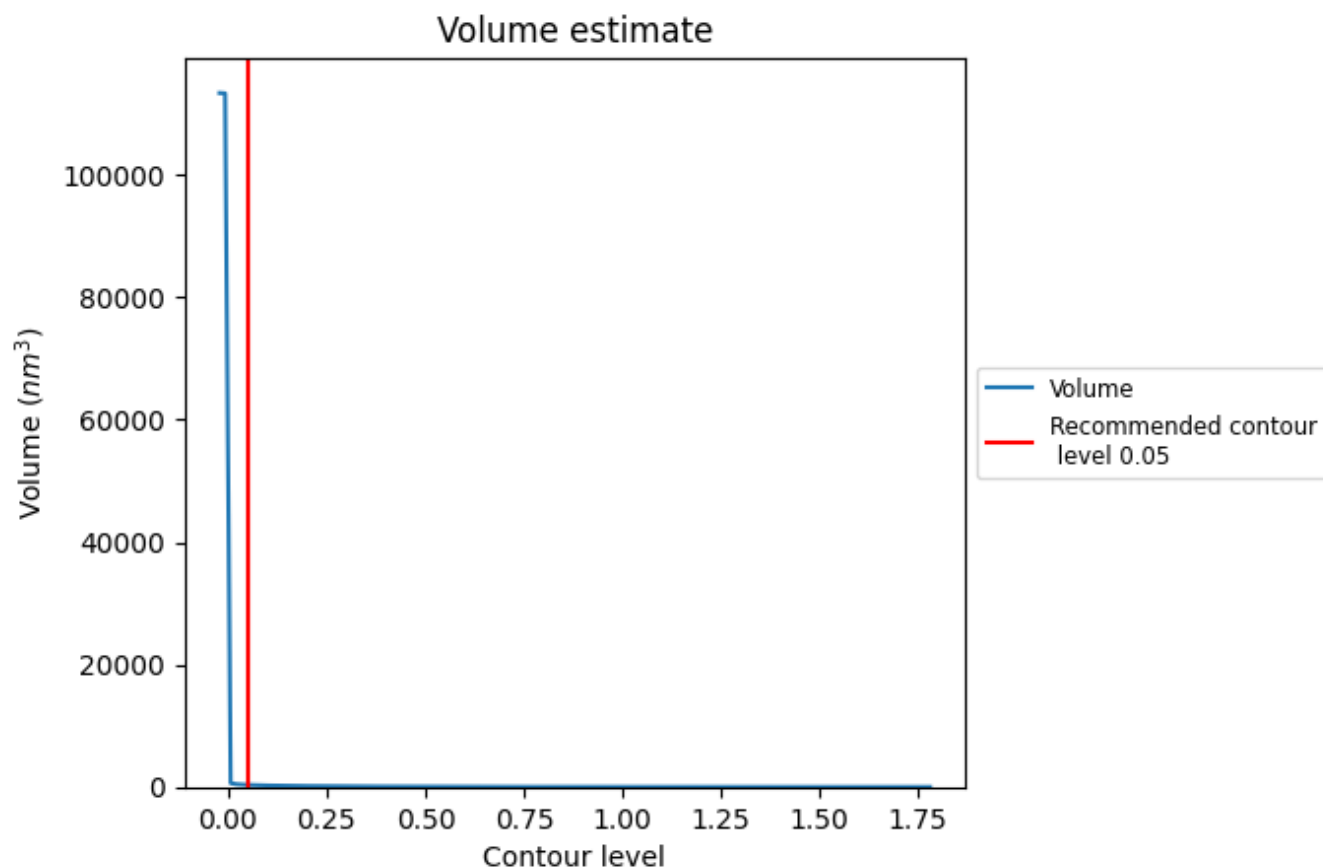
The volume at the recommended contour level is 332 nm^3; this corresponds to an approximate mass of 300 kDa.

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 ⓘ
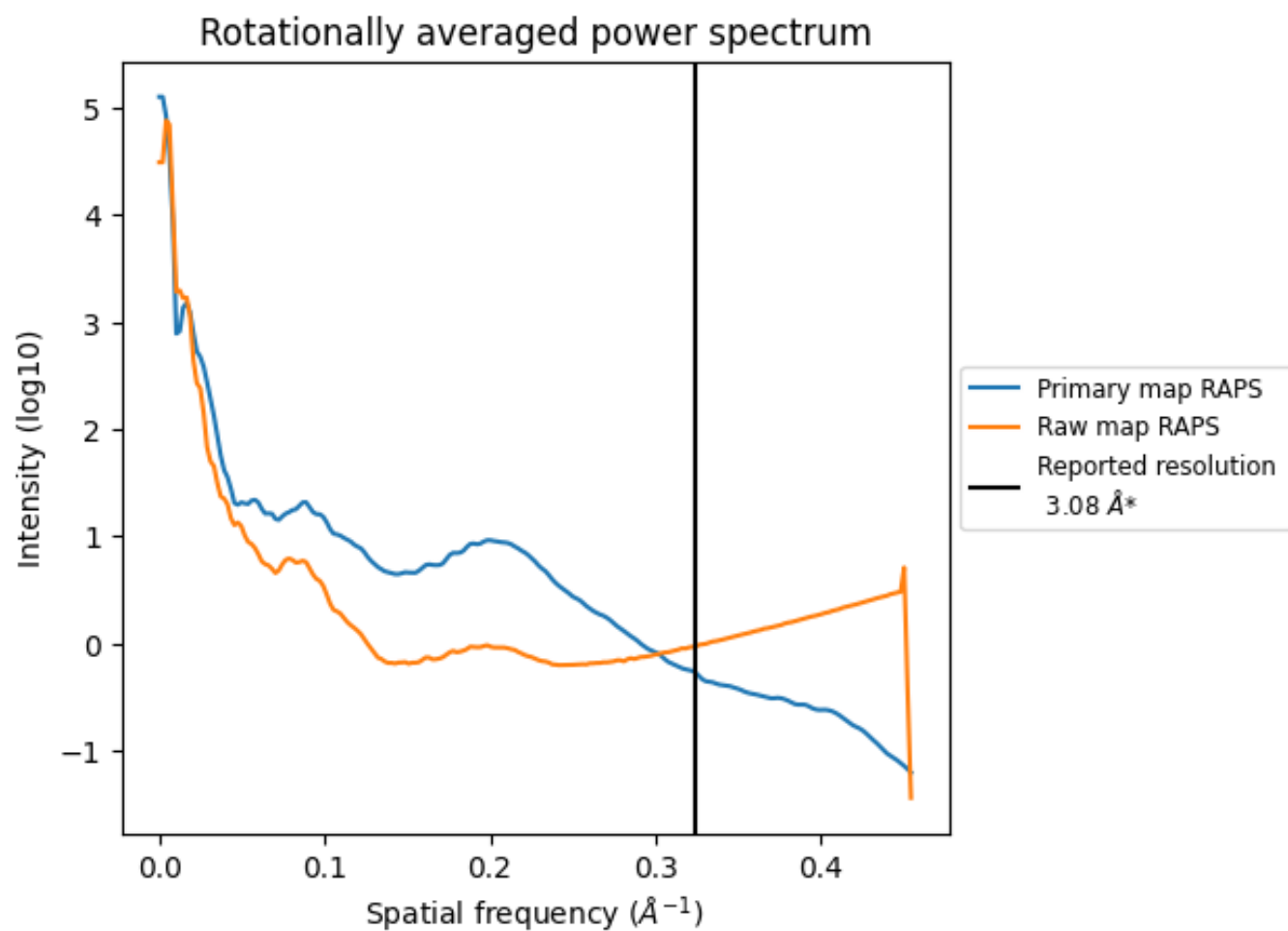
*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

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 ⓘ
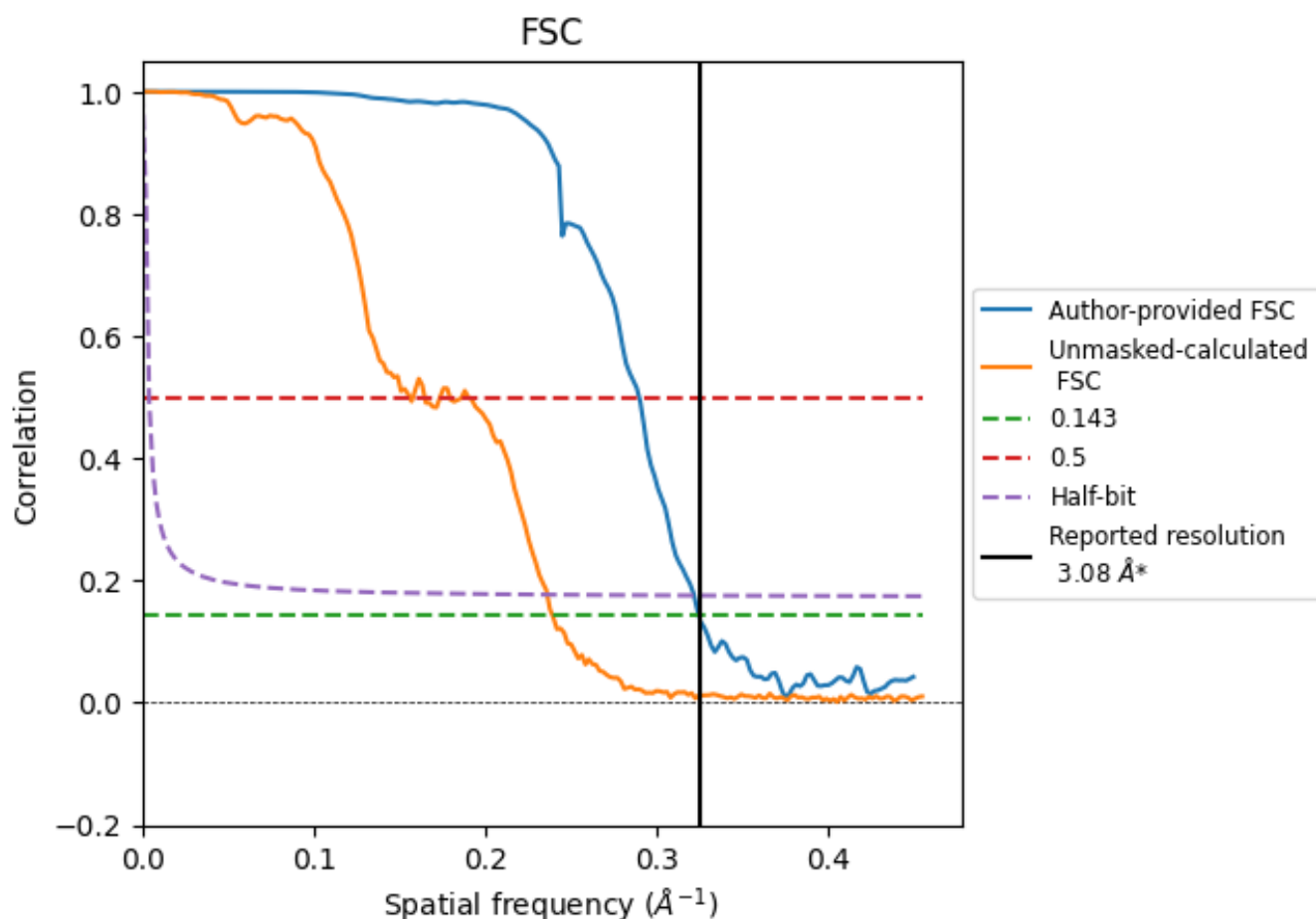
*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.45	3.11
Unmasked-calculated*	4.18	6.42	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.08 by more than 10 %

9　Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-60127 and PDB model 8ZIR. Per-residue inclusion information can be found in section 3 on page 6.

9.1　Map-model overlay ⓘ

X　　　　　　　　　　　Y　　　　　　　　　　　Z
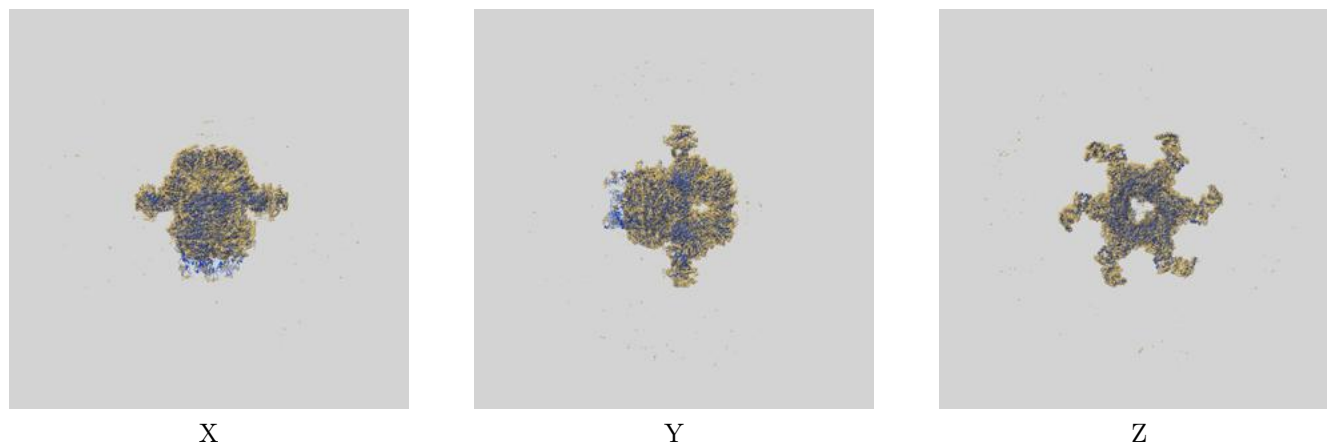
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ
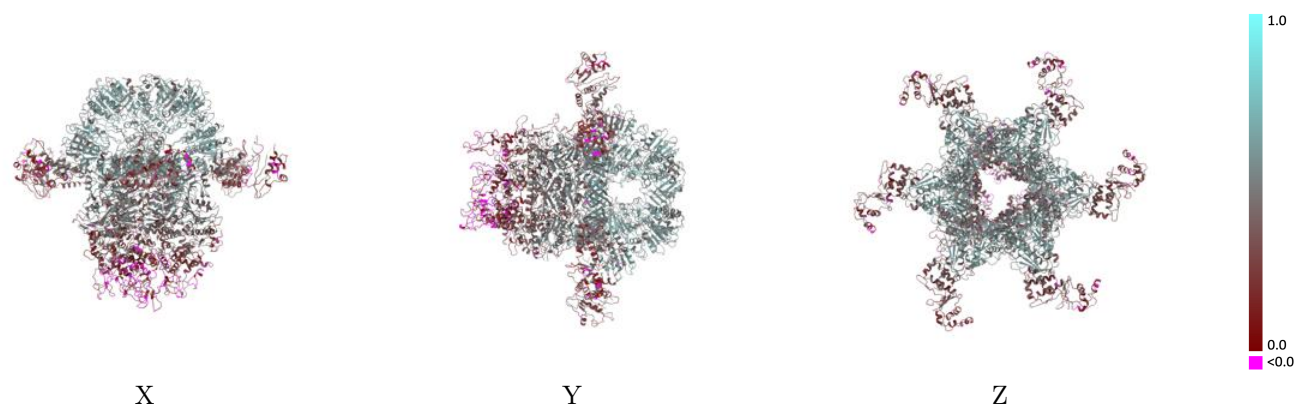
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
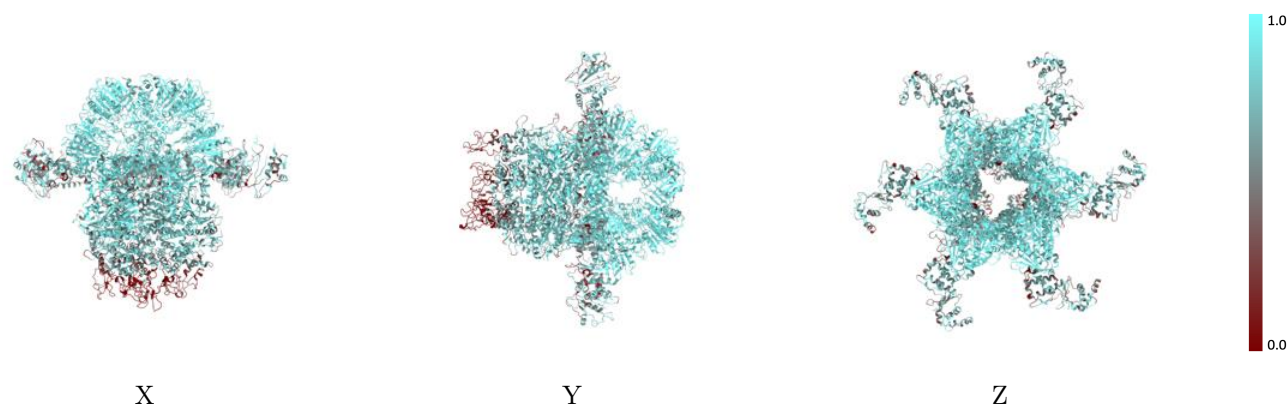
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion ⓘ
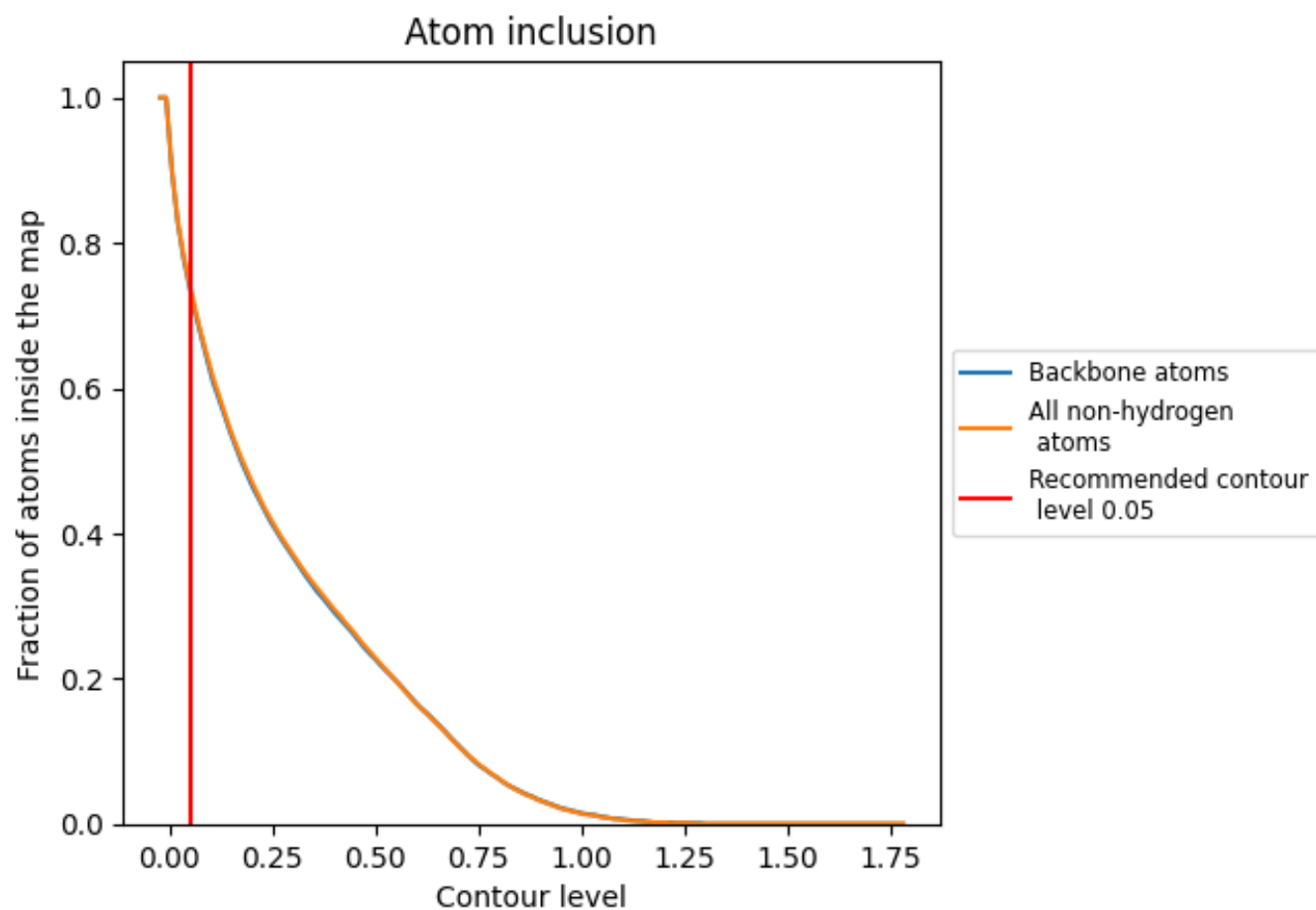
At the recommended contour level, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7410	0.4110
A	0.7450	0.4090
B	0.8950	0.5380
C	0.7570	0.4100
D	0.8940	0.5360
E	0.7430	0.4090
F	0.8890	0.5340
G	0.7530	0.4150
H	0.9010	0.5390
I	0.7450	0.4040
J	0.8850	0.5250
K	0.7340	0.4060
L	0.8920	0.5290
M	0.7590	0.3960
N	0.6770	0.3560
O	0.7590	0.3930
P	0.6490	0.3480
Q	0.7470	0.3850
R	0.6710	0.3530

1.0

0.0
<0.0