WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Feb 22, 2023 – 04:23 PM JST

PDB ID	:	7Y0D
EMDB ID	:	EMD-33540
Title	:	Cryo-EM structure of the Mycobacterium smegmatis DNA integrity scanning protein (MsDisA).
Authors	:	Gautam, S.; Vinothkumar, K.R.; Chatterji, D.
Deposited on	:	2022-06-04
Resolution	:	3.10 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.

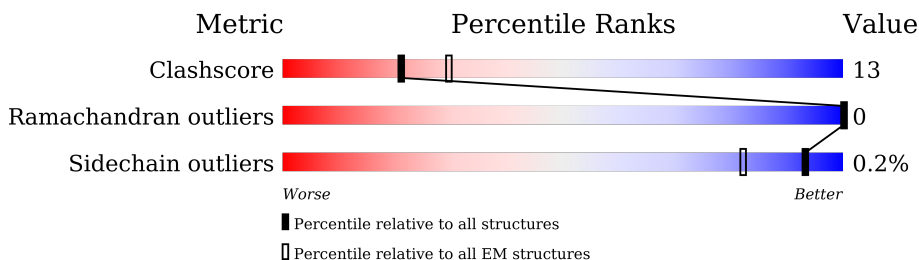The following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		13
Ramachandran outliers		0
Sidechain outliers		0.2%

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

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	383	8% / 67% 23% 10%
1	B	383	16% / 61% 29% 10%
1	C	383	19% / 64% 26% 10%
1	D	383	14% / 58% 33% 10%
1	E	383	37% / 64% 26% 10%
1	F	383	13% / 64% 26% 10%
1	G	383	15% / 59% 31% 10%
1	H	383	7% / 65% 26% 10%

2 Entity composition (i)

There is only 1 type of molecule in this entry. The entry contains 21224 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 DNA integrity scanning protein DisA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	346	Total	C	N	O	S	0	0
			2653	1642	478	525	8		
1	B	346	Total	C	N	O	S	0	0
			2653	1642	478	525	8		
1	C	346	Total	C	N	O	S	0	0
			2653	1642	478	525	8		
1	D	346	Total	C	N	O	S	0	0
			2653	1642	478	525	8		
1	E	346	Total	C	N	O	S	0	0
			2653	1642	478	525	8		
1	F	346	Total	C	N	O	S	0	0
			2653	1642	478	525	8		
1	G	346	Total	C	N	O	S	0	0
			2653	1642	478	525	8		
1	H	346	Total	C	N	O	S	0	0
			2653	1642	478	525	8		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	ALA	-	expression tag	UNP A0R564
A	374	ALA	-	expression tag	UNP A0R564
A	375	ALA	-	expression tag	UNP A0R564
A	376	LEU	-	expression tag	UNP A0R564
A	377	GLU	-	expression tag	UNP A0R564
A	378	HIS	-	expression tag	UNP A0R564
A	379	HIS	-	expression tag	UNP A0R564
A	380	HIS	-	expression tag	UNP A0R564
A	381	HIS	-	expression tag	UNP A0R564
A	382	HIS	-	expression tag	UNP A0R564
A	383	HIS	-	expression tag	UNP A0R564
B	373	ALA	-	expression tag	UNP A0R564
B	374	ALA	-	expression tag	UNP A0R564
B	375	ALA	-	expression tag	UNP A0R564

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Chain	Residue	Modelled	Actual	Comment	Reference
B	376	LEU	-	expression tag	UNP A0R564
B	377	GLU	-	expression tag	UNP A0R564
B	378	HIS	-	expression tag	UNP A0R564
B	379	HIS	-	expression tag	UNP A0R564
B	380	HIS	-	expression tag	UNP A0R564
B	381	HIS	-	expression tag	UNP A0R564
B	382	HIS	-	expression tag	UNP A0R564
B	383	HIS	-	expression tag	UNP A0R564
C	373	ALA	-	expression tag	UNP A0R564
C	374	ALA	-	expression tag	UNP A0R564
C	375	ALA	-	expression tag	UNP A0R564
C	376	LEU	-	expression tag	UNP A0R564
C	377	GLU	-	expression tag	UNP A0R564
C	378	HIS	-	expression tag	UNP A0R564
C	379	HIS	-	expression tag	UNP A0R564
C	380	HIS	-	expression tag	UNP A0R564
C	381	HIS	-	expression tag	UNP A0R564
C	382	HIS	-	expression tag	UNP A0R564
C	383	HIS	-	expression tag	UNP A0R564
D	373	ALA	-	expression tag	UNP A0R564
D	374	ALA	-	expression tag	UNP A0R564
D	375	ALA	-	expression tag	UNP A0R564
D	376	LEU	-	expression tag	UNP A0R564
D	377	GLU	-	expression tag	UNP A0R564
D	378	HIS	-	expression tag	UNP A0R564
D	379	HIS	-	expression tag	UNP A0R564
D	380	HIS	-	expression tag	UNP A0R564
D	381	HIS	-	expression tag	UNP A0R564
D	382	HIS	-	expression tag	UNP A0R564
D	383	HIS	-	expression tag	UNP A0R564
E	373	ALA	-	expression tag	UNP A0R564
E	374	ALA	-	expression tag	UNP A0R564
E	375	ALA	-	expression tag	UNP A0R564
E	376	LEU	-	expression tag	UNP A0R564
E	377	GLU	-	expression tag	UNP A0R564
E	378	HIS	-	expression tag	UNP A0R564
E	379	HIS	-	expression tag	UNP A0R564
E	380	HIS	-	expression tag	UNP A0R564
E	381	HIS	-	expression tag	UNP A0R564
E	382	HIS	-	expression tag	UNP A0R564
E	383	HIS	-	expression tag	UNP A0R564
F	373	ALA	-	expression tag	UNP A0R564

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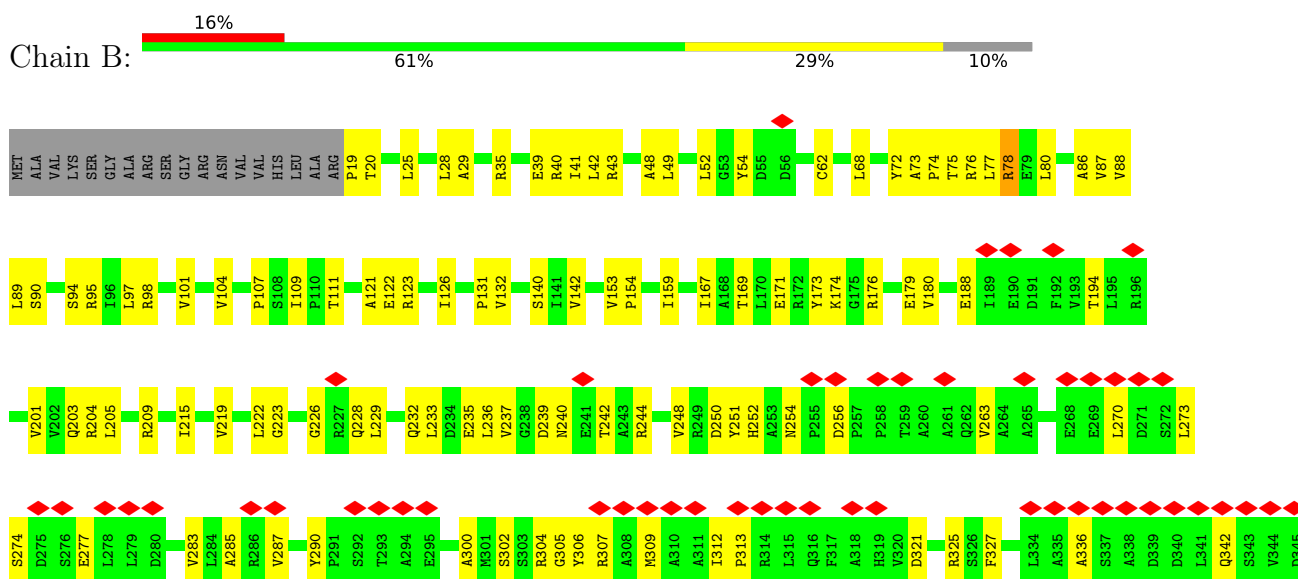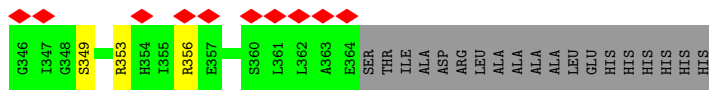| Chain	Residue	Modelled	Actual	Comment	Reference
F	374	ALA	-	expression tag	UNP A0R564
F	375	ALA	-	expression tag	UNP A0R564
F	376	LEU	-	expression tag	UNP A0R564
F	377	GLU	-	expression tag	UNP A0R564
F	378	HIS	-	expression tag	UNP A0R564
F	379	HIS	-	expression tag	UNP A0R564
F	380	HIS	-	expression tag	UNP A0R564
F	381	HIS	-	expression tag	UNP A0R564
F	382	HIS	-	expression tag	UNP A0R564
F	383	HIS	-	expression tag	UNP A0R564
G	373	ALA	-	expression tag	UNP A0R564
G	374	ALA	-	expression tag	UNP A0R564
G	375	ALA	-	expression tag	UNP A0R564
G	376	LEU	-	expression tag	UNP A0R564
G	377	GLU	-	expression tag	UNP A0R564
G	378	HIS	-	expression tag	UNP A0R564
G	379	HIS	-	expression tag	UNP A0R564
G	380	HIS	-	expression tag	UNP A0R564
G	381	HIS	-	expression tag	UNP A0R564
G	382	HIS	-	expression tag	UNP A0R564
G	383	HIS	-	expression tag	UNP A0R564
H	373	ALA	-	expression tag	UNP A0R564
H	374	ALA	-	expression tag	UNP A0R564
H	375	ALA	-	expression tag	UNP A0R564
H	376	LEU	-	expression tag	UNP A0R564
H	377	GLU	-	expression tag	UNP A0R564
H	378	HIS	-	expression tag	UNP A0R564
H	379	HIS	-	expression tag	UNP A0R564
H	380	HIS	-	expression tag	UNP A0R564
H	381	HIS	-	expression tag	UNP A0R564
H	382	HIS	-	expression tag	UNP A0R564
H	383	HIS	-	expression tag	UNP A0R564

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: DNA integrity scanning protein DisA
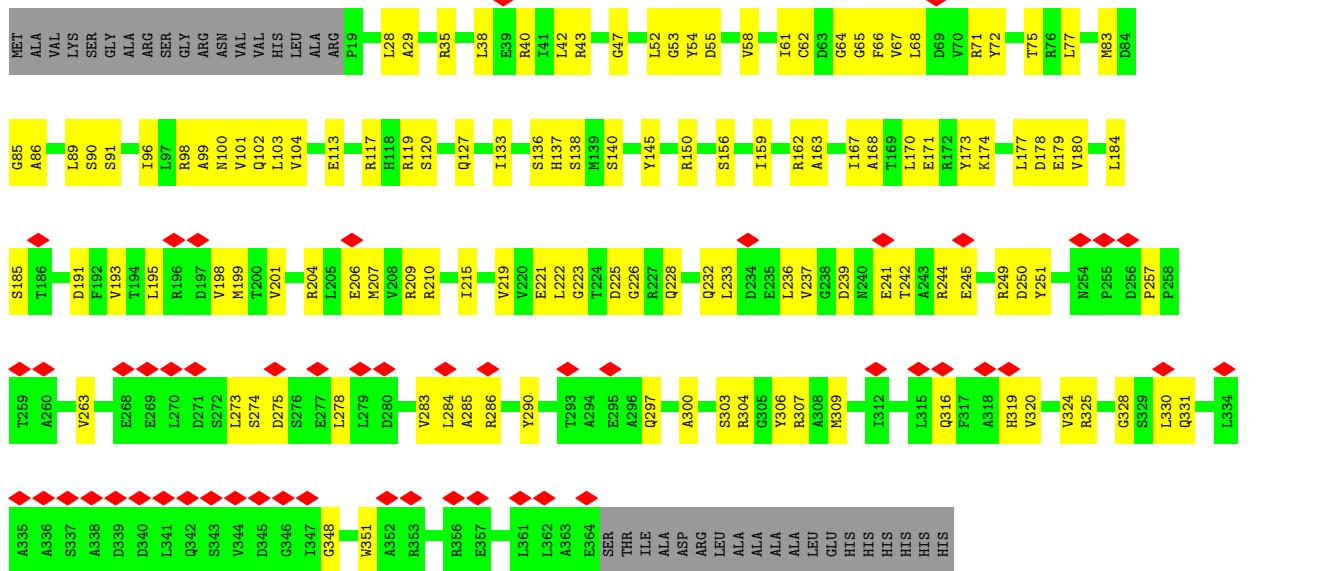

• Molecule 1: DNA integrity scanning protein DisA

G346 I347 G348 S349 R353 H354 I355 R356 E357 S360 L361 L362 A363 E364 SER THR ILE ALA ASP ARG LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: DNA integrity scanning protein DisA

Chain C:

19%

64%   26%   10%

MET ALA VAL LYS SER GLY ALA ARG SER GLY ARG ASN VAL VAL HIS LEU ALA ARG P19 T20 L21 R27 L34 R35 D36 E39 R40 I41 L49 Y54 D55 D56 S57 V58 I61 C62 D63 G64 G65 Y72 A73 P74 T75 R76 L77 D84 V88 L89 S90 S91 D92

R95 V101 P105 D106 P107 S108 I109 D112 R117 A121 S136 M139 V142 V146 R150 H151 V152 V153 N164 I167 A168 T169 R172 R176 L177 D178 E179 L184 E188 I189 E190 D191 L195 R196 D197 V198 V201 L205 E206 M207

V208 R209 R210 L213 V219 L229 Q232 L233 D234 E235 D239 T242 A243 R244 I247 V248 R249 D250 Y251 H252 A253 N254 P255 D256 P257 P258 T259 A260 A261 L270 D271 S272 L273 S274 D275 S276 E277 L278 L279 D280 F281 T282 V283 R286 V287 F288 P291 S292 T293 A294

E295 A296 Q297 G305 Y306 M309 A310 A311 I312 P313 R314 L315 Q316 F317 A318 H319 V320 D321 L322 L323 V324 R325 S326 F327 L330 Q331 N332 A335 A336 S337 A338 D339 D340 L341 Q342 S343 V344 D345 G346 I347 G348 S349 M350 W351 A352 R353 H354 I355 R356 S360 L361 L362 A363 E364 SER

THR ILE ALA ASP ARG LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: DNA integrity scanning protein DisA

Chain D:

14%

58%   33%   10%

MET ALA VAL LYS SER GLY ALA ARG SER GLY ARG ASN VAL VAL HIS LEU ALA ARG P19 L28 A29 R35 L38 E39 R40 I41 L42 R43 G47 L52 G53 Y54 D55 V58 I61 C62 D63 G64 G65 F66 V67 L68 D69 V70 R71 Y72 T75 R76 L77 M83 D84

G85 A86 L89 S90 S91 I96 L97 R98 A99 N100 V101 Q102 L103 V104 E113 R117 H118 R119 S120 Q127 I133 S136 H137 S138 M139 S140 Y145 R150 S156 I159 R162 A163 I167 A168 T169 L170 E171 R172 Y173 K174 L177 D178 E179 V180 L184

S185 T186 D191 F192 V193 T194 L195 R196 D197 V198 M199 T200 V201 R204 L205 E206 M207 V208 R209 R210 I215 V219 V220 E221 L222 G223 T224 D225 G226 R227 Q228 Q232 L233 D234 E235 L236 V237 G238 D239 N240 E241 T242 A243 R244 E245 R249 D250 Y251 N254 P255 D256 P257 P258

T259 A260 V263 E268 E269 L270 D271 S272 L273 S274 D275 S276 E277 L278 L279 D280 V283 L284 A285 R286 Y290 T293 A294 E295 A296 Q297 A300 S303 R304 G305 Y306 R307 A308 M309 I312 L315 Q316 F317 A318 H319 V320 V324 R325 G328 S329 L330 Q331 L334

A335 A336 S337 A338 D339 D340 L341 Q342 S343 V344 D345 G346 I347 G348 W351 A352 R353 R356 E357 L361 L362 A363 E364 SER THR ILE ALA ASP ARG LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: DNA integrity scanning protein DisA

Chain E:

37%

64%   26%   10%

MET ALA VAL LYS SER GLY ALA ARG SER GLY ARG ASN VAL VAL HIS LEU ALA ARG P19 R22 L25 P30 P33 L34 R35 R40 R45 L49 I50 V51 L52 G53 Y54 D55 D56 S57 V58 E59 D63 F66 D69 Y72 L77 R78 M83 V88

L89 S90 S91 D92 G93 R98 A99 N100 V101 Q102 L103 D106 P107 S108 I109 P110 T111 D112 E113 S114 R117 R123 T124 P131 V132 S138 V142 V146 H151 V152 V153 S156 A157 R162 A163 I167 A168 E171 R172 Y173 K174 G175 R176 L177 D178 E179 V180

S181 R182 Q183 L184 S185 T186 A187 E188 I189 E190 D191 F192 V193 T194 L195 R196 D197 V198 M199 T200 V201 V202 Q203 R204 L205 V208 R209 R210 I211 E214 I215 D216 L222 G223 T224 D225 G226 R227 K230 L231 Q232 L233 V237 G238 D239 N240 E241 T242 A243 R244 E245 L246 I247 V248 R249

D250 Y251 H252 A253 N254 P255 D256 P257 P258 T259 A260 A261 Q262 V263 A264 A265 T266 L267 E268 E269 L270 D271 S272 L273 S274 D275 S276 E277 L278 L279 D280 F281 T282 R286 P291 S292 T293 A294 E295 A296 Q297 D298 S299 A300 M301 S302 S303 R304 G305 Y306 R307 A308 M309 A310 A311 I312 P313 R314

L315 Q316 F317 A318 H319 V320 D321 L322 L323 V324 R325 S326 F327 G328 S329 L330 Q331 N332 L333 L334 A335 A336 S337 A338 D339 D340 L341 Q342 S343 V344 D345 G346 I347 G348 S349 R353 H354 I355 R356 E357 G358 L359 S360 L361 L362 A363 E364 SER THR ILE ALA ASP ARG LEU ALA ALA ALA LEU

GLU HIS HIS HIS HIS HIS

• Molecule 1: DNA integrity scanning protein DisA

Chain F:
13%
64% 26% 10%

MET ALA VAL LYS SER GLY ALA ARG SER GLY ARG ASN VAL VAL HIS LEU ALA ARG P19 T24 L25 L28 P33 R40 R45 G53 V58 I61 D69 Y72 A73 P74 K82 V88 S91 L97 R98 V101 Q102 L103 V104 P105 T111 D112

E113 S114 R117 H118 R119 T128 P131 V132 I133 S134 V135 S136 H137 S138 M139 S140 I141 V142 D155 S156 I159 R162 A163 N164 Q165 T166 I167 A168 T169 L170 E171 R172 Y173 K174 G175 R176 L177 D178 S181 L184 S185 E188 I189 F192 R196 D197 V198 M199

Q203 E206 R210 I211 I215 L222 D225 G226 R227 Q228 L233 D234 E235 L236 V237 R244 D250 Y251 N254 P255 D256 P257 P258 T259 V263 L267 L270 D271 S274 D275 S276 E277 L278 L279 D280 F281 T282 A285 R286 V287 Y290 P291 S292 T293 A294

E295 A296 M301 S302 S303 R304 G305 Y306 R307 A308 M309 I312 P313 R314 L315 Q316 F317 A318 H319 V320 D321 L322 L323 V324 R325 S326 S329 A335 A336 S337 A338 D339 D340 L341 Q342 S343 V344 D345 G346 I347 M350 W351 A352 R353 R356 L361 L362 A363 E364 SER THR ILE ALA

ASP ARG LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS

• Molecule 1: DNA integrity scanning protein DisA

Chain G:
15%
59% 31% 10%

MET ALA VAL LYS SER GLY ALA ARG SER GLY ARG ASN VAL VAL HIS LEU ALA ARG P19 R22 E23 T24 R27 P33 L34 R35 D36 G37 L38 E39 R40 I41 L42 R45 A48 L49 I50 V51 L52 G53 D56 S57 V58 F66 D69 Y72 T75 R76 L77

• Molecule 1: DNA integrity scanning protein DisA

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	204932	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	27.75	Depositor
Minimum defocus (nm)	2100	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	130841	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	8.804	Depositor
Minimum map value	-5.670	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.124	Depositor
Recommended contour level	1.4	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	A	0.27	0/2688	0.55	0/3649
1	B	0.27	0/2688	0.55	0/3649
1	C	0.25	0/2688	0.53	0/3649
1	D	0.27	0/2688	0.58	0/3649
1	E	0.25	0/2688	0.54	0/3649
1	F	0.26	0/2688	0.55	0/3649
1	G	0.27	0/2688	0.56	0/3649
1	H	0.27	0/2688	0.54	0/3649
All	All	0.26	0/21504	0.55	0/29192

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2　Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2653	0	2665	67	0
1	B	2653	0	2665	80	0
1	C	2653	0	2665	64	0
1	D	2653	0	2665	88	0
1	E	2653	0	2665	61	0
1	F	2653	0	2665	70	0
1	G	2653	0	2665	86	0
1	H	2653	0	2665	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21224	0	21320	560	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 13.

All (560) 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:D:170:LEU:HG	1:D:174:LYS:HZ3	1.30	0.96
1:D:199:MET:HB3	1:D:284:LEU:HD23	1.60	0.83
1:B:62:CYS:HB2	1:B:101:VAL:HG21	1.63	0.81
1:G:97:LEU:HD12	1:G:98:ARG:HG2	1.63	0.81
1:F:61:ILE:HD12	1:F:105:PRO:HA	1.67	0.76
1:F:40:ARG:HH11	1:F:74:PRO:HB2	1.50	0.76
1:G:119:ARG:HD2	1:H:102:GLN:HG3	1.66	0.75
1:B:353:ARG:HA	1:B:356:ARG:HE	1.53	0.74
1:E:224:THR:HA	1:E:227:ARG:HD2	1.70	0.74
1:B:285:ALA:HB1	1:B:290:TYR:HB2	1.72	0.72
1:E:184:LEU:HD22	1:E:201:VAL:HG21	1.71	0.72
1:D:285:ALA:HB1	1:D:290:TYR:HB2	1.73	0.71
1:F:45:ARG:HE	1:F:138:SER:HA	1.55	0.71
1:B:252:HIS:ND1	1:B:254:ASN:OD1	2.23	0.71
1:D:210:ARG:NH2	1:D:273:LEU:O	2.24	0.71
1:E:162:ARG:NH2	1:E:214:GLU:OE2	2.25	0.70
1:A:277:GLU:HB2	1:A:283:VAL:HG11	1.74	0.70
1:D:304:ARG:HE	1:D:306:TYR:HE2	1.39	0.69
1:B:39:GLU:HB2	1:B:43:ARG:HH12	1.57	0.69
1:B:228:GLN:HB3	1:B:232:GLN:HE22	1.56	0.69
1:D:75:THR:HG21	1:H:113:GLU:HA	1.72	0.69
1:B:277:GLU:HB3	1:B:283:VAL:HG11	1.75	0.69
1:G:353:ARG:HA	1:G:356:ARG:HG2	1.74	0.69
1:C:312:ILE:HB	1:C:315:LEU:HD22	1.75	0.69
1:B:49:LEU:HD23	1:B:86:ALA:HB2	1.75	0.68
1:D:257:PRO:HB3	1:D:304:ARG:HH22	1.58	0.68
1:B:29:ALA:HB1	1:B:223:GLY:HA3	1.75	0.67
1:D:38:LEU:HD21	1:D:133:ILE:HG21	1.75	0.67
1:D:170:LEU:HG	1:D:174:LYS:NZ	2.08	0.67
1:F:113:GLU:OE2	1:G:40:ARG:NH2	2.28	0.67
1:A:353:ARG:HA	1:A:356:ARG:HE	1.58	0.67
1:D:29:ALA:HB1	1:D:223:GLY:HA3	1.76	0.67
1:G:199:MET:HG3	1:G:284:LEU:HD22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLN:O	1:B:232:GLN:NE2	2.27	0.67
1:A:278:LEU:HD12	1:A:284:LEU:HD21	1.78	0.66
1:C:282:THR:HB	1:C:286:ARG:HH12	1.60	0.66
1:H:316:GLN:HB2	1:H:319:HIS:HB2	1.78	0.66
1:D:171:GLU:HA	1:D:174:LYS:HE2	1.76	0.66
1:A:61:ILE:HD12	1:A:105:PRO:HA	1.78	0.65
1:D:113:GLU:O	1:D:119:ARG:NH1	2.28	0.65
1:G:247:ILE:HD11	1:G:307:ARG:HH11	1.59	0.65
1:G:323:LEU:HD21	1:G:333:LEU:HD21	1.77	0.65
1:F:181:SER:OG	1:F:307:ARG:NH2	2.28	0.65
1:B:174:LYS:NZ	1:B:236:LEU:O	2.28	0.65
1:C:189:ILE:HD11	1:C:363:ALA:HA	1.79	0.64
1:B:40:ARG:NH1	1:B:75:THR:OG1	2.30	0.64
1:F:254:ASN:HD21	1:F:258:PRO:HD3	1.62	0.64
1:E:49:LEU:HD21	1:E:117:ARG:HB2	1.80	0.64
1:C:188:GLU:OE2	1:C:251:TYR:OH	2.16	0.64
1:F:291:PRO:HG2	1:F:296:ALA:HB2	1.79	0.64
1:B:90:SER:HG	1:B:94:SER:H	1.44	0.64
1:F:58:VAL:HG22	1:F:128:THR:HG21	1.79	0.64
1:D:222:LEU:HD21	1:D:226:GLY:HA3	1.79	0.63
1:G:116:THR:HG22	1:H:102:GLN:HG2	1.80	0.63
1:G:274:SER:N	1:G:277:GLU:OE2	2.29	0.63
1:G:41:ILE:HG21	1:G:48:ALA:HB2	1.81	0.63
1:B:188:GLU:OE1	1:B:307:ARG:NH1	2.32	0.63
1:C:254:ASN:HD21	1:C:258:PRO:HD3	1.62	0.63
1:F:114:SER:HA	1:F:119:ARG:HH21	1.63	0.62
1:B:88:VAL:HB	1:B:98:ARG:HB3	1.80	0.62
1:E:45:ARG:NH1	1:E:138:SER:O	2.33	0.62
1:G:24:THR:HG22	1:G:27:ARG:HH21	1.62	0.62
1:H:184:LEU:HD22	1:H:201:VAL:HG21	1.82	0.62
1:F:53:GLY:HA2	1:F:91:SER:HA	1.81	0.62
1:E:83:MET:HB3	1:E:100:ASN:HB2	1.82	0.62
1:A:40:ARG:HH11	1:A:74:PRO:HB2	1.65	0.62
1:D:40:ARG:HG2	1:D:43:ARG:HH22	1.65	0.62
1:B:194:THR:HA	1:B:300:ALA:HA	1.82	0.61
1:F:211:ILE:O	1:F:215:ILE:HG12	1.99	0.61
1:G:206:GLU:OE1	1:G:244:ARG:NH1	2.27	0.61
1:H:33:PRO:HB2	1:H:72:TYR:HE2	1.65	0.61
1:D:64:GLY:HA3	1:F:119:ARG:HH12	1.66	0.60
1:H:181:SER:OG	1:H:307:ARG:NH2	2.27	0.60
1:F:203:GLN:NE2	1:F:278:LEU:O	2.24	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:GLU:OE2	1:E:251:TYR:OH	2.19	0.60
1:G:154:PRO:HG2	1:G:159:ILE:HD11	1.84	0.60
1:H:117:ARG:HH12	1:H:137:HIS:H	1.48	0.60
1:A:244:ARG:HH21	1:A:267:LEU:HD22	1.67	0.60
1:B:270:LEU:HD23	1:B:273:LEU:HD21	1.84	0.60
1:F:98:ARG:HD3	1:F:101:VAL:HG11	1.84	0.59
1:A:113:GLU:OE2	1:E:40:ARG:NH2	2.35	0.59
1:F:250:ASP:OD2	1:F:306:TYR:N	2.35	0.59
1:H:278:LEU:HD23	1:H:284:LEU:HD21	1.84	0.59
1:E:227:ARG:HB3	1:E:230:LYS:HZ3	1.67	0.59
1:B:40:ARG:HB3	1:B:78:ARG:HG3	1.82	0.59
1:B:219:VAL:HG22	1:B:229:LEU:HB3	1.82	0.59
1:B:111:THR:OG1	1:B:122:GLU:OE1	2.21	0.59
1:C:61:ILE:HD12	1:C:105:PRO:HA	1.84	0.59
1:G:38:LEU:HD21	1:G:133:ILE:HG21	1.83	0.59
1:G:195:LEU:HD22	1:G:297:GLN:HA	1.83	0.59
1:F:24:THR:HG21	1:F:131:PRO:HG3	1.85	0.58
1:H:245:GLU:OE2	1:H:249:ARG:NE	2.35	0.58
1:D:185:SER:OG	1:D:307:ARG:NH2	2.35	0.58
1:A:290:TYR:OH	1:A:301:MET:SD	2.60	0.58
1:C:40:ARG:HH11	1:C:74:PRO:HB2	1.67	0.58
1:C:309:MET:HE2	1:C:315:LEU:HD21	1.83	0.58
1:C:347:ILE:HG23	1:C:351:TRP:HD1	1.69	0.58
1:D:174:LYS:HE3	1:D:236:LEU:HB3	1.85	0.58
1:G:222:LEU:HD13	1:G:226:GLY:HA3	1.85	0.58
1:D:52:LEU:HD23	1:D:89:LEU:HB2	1.86	0.58
1:E:63:ASP:O	1:E:102:GLN:N	2.34	0.58
1:A:206:GLU:OE2	1:A:210:ARG:NH2	2.37	0.58
1:G:321:ASP:OD1	1:G:325:ARG:NH1	2.37	0.58
1:E:321:ASP:OD1	1:E:325:ARG:NH1	2.37	0.57
1:G:53:GLY:N	1:G:89:LEU:O	2.30	0.57
1:G:303:SER:H	1:G:330:LEU:HD22	1.69	0.57
1:H:53:GLY:HA2	1:H:91:SER:HA	1.86	0.57
1:D:68:LEU:HD22	1:G:66:PHE:HD2	1.69	0.57
1:B:250:ASP:HB2	1:B:306:TYR:HB2	1.86	0.57
1:F:33:PRO:HB2	1:F:72:TYR:HE2	1.69	0.57
1:G:239:ASP:HB2	1:G:242:THR:HB	1.86	0.57
1:G:350:MET:O	1:G:354:HIS:ND1	2.36	0.57
1:A:196:ARG:NH2	1:A:298:ASP:OD1	2.38	0.57
1:A:209:ARG:HG2	1:A:244:ARG:HH12	1.70	0.57
1:D:210:ARG:NH1	1:D:275:ASP:OD1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:MET:HE3	1:D:320:VAL:HG13	1.87	0.57
1:B:250:ASP:OD2	1:B:306:TYR:N	2.38	0.57
1:E:89:LEU:HB3	1:E:93:GLY:HA2	1.87	0.57
1:C:342:GLN:HB2	1:C:353:ARG:HH22	1.70	0.57
1:H:246:LEU:HD12	1:H:306:TYR:HB3	1.87	0.57
1:C:353:ARG:HD3	1:C:356:ARG:HH21	1.70	0.56
1:E:59:GLU:OE1	1:E:98:ARG:NH2	2.31	0.56
1:H:249:ARG:HG2	1:H:263:VAL:HG21	1.86	0.56
1:C:65:GLY:HA3	1:C:101:VAL:HG22	1.86	0.56
1:A:286:ARG:NH2	1:A:291:PRO:O	2.38	0.56
1:C:210:ARG:HE	1:C:213:LEU:HD21	1.69	0.56
1:E:195:LEU:HD22	1:E:297:GLN:HA	1.87	0.56
1:G:245:GLU:OE2	1:G:249:ARG:NE	2.37	0.56
1:D:195:LEU:HA	1:D:198:VAL:HG12	1.87	0.56
1:B:54:TYR:CG	1:B:97:LEU:HD11	2.40	0.56
1:G:117:ARG:NH1	1:G:135:VAL:O	2.39	0.56
1:F:174:LYS:NZ	1:F:236:LEU:O	2.34	0.56
1:G:338:ALA:O	1:G:356:ARG:NH2	2.39	0.56
1:D:178:ASP:OD1	1:D:179:GLU:N	2.39	0.56
1:G:109:ILE:HG21	1:G:126:ILE:HG21	1.86	0.56
1:G:277:GLU:HB2	1:G:283:VAL:HG11	1.87	0.56
1:B:188:GLU:OE2	1:B:251:TYR:OH	2.23	0.56
1:C:252:HIS:NE2	1:C:288:PHE:O	2.39	0.56
1:D:195:LEU:HB3	1:D:297:GLN:HA	1.86	0.56
1:A:98:ARG:HE	1:A:101:VAL:HG11	1.72	0.55
1:D:233:LEU:O	1:D:237:VAL:HG12	2.06	0.55
1:E:33:PRO:HB2	1:E:72:TYR:HE2	1.70	0.55
1:H:324:VAL:O	1:H:328:GLY:N	2.37	0.55
1:C:338:ALA:O	1:C:353:ARG:NH2	2.39	0.55
1:D:159:ILE:HG12	1:D:162:ARG:HH21	1.71	0.55
1:F:135:VAL:HG22	1:F:142:VAL:HG13	1.88	0.55
1:E:178:ASP:OD1	1:E:179:GLU:N	2.40	0.55
1:B:39:GLU:HG3	1:B:43:ARG:HH22	1.72	0.55
1:B:215:ILE:HG21	1:B:233:LEU:HD21	1.89	0.55
1:B:305:GLY:O	1:B:309:MET:HG3	2.06	0.55
1:A:199:MET:HA	1:A:202:VAL:HG22	1.89	0.54
1:B:222:LEU:HD13	1:B:226:GLY:HA3	1.89	0.54
1:B:68:LEU:HD13	1:E:66:PHE:CE2	2.41	0.54
1:C:184:LEU:HD22	1:C:201:VAL:HG21	1.89	0.54
1:D:204:ARG:NH1	1:D:207:MET:SD	2.79	0.54
1:E:250:ASP:HB2	1:E:306:TYR:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG22	1:A:142:VAL:HG22	1.88	0.54
1:A:184:LEU:HD22	1:A:201:VAL:HG21	1.88	0.54
1:B:173:TYR:OH	1:H:228:GLN:OE1	2.25	0.54
1:D:85:GLY:HA3	1:D:100:ASN:HA	1.89	0.54
1:G:351:TRP:HA	1:G:354:HIS:HD1	1.73	0.54
1:F:312:ILE:HB	1:F:315:LEU:HD11	1.90	0.54
1:G:49:LEU:HB3	1:G:86:ALA:HA	1.89	0.54
1:G:34:LEU:HD22	1:G:52:LEU:HD11	1.89	0.53
1:E:180:VAL:O	1:E:183:GLN:HG3	2.09	0.53
1:H:135:VAL:HG22	1:H:142:VAL:HG22	1.90	0.53
1:B:77:LEU:HD11	1:B:87:VAL:HG11	1.90	0.53
1:B:154:PRO:HG2	1:B:159:ILE:HD11	1.90	0.53
1:B:205:LEU:HG	1:B:244:ARG:NH2	2.23	0.53
1:D:28:LEU:HD21	1:D:133:ILE:HD11	1.91	0.53
1:H:305:GLY:O	1:H:309:MET:HG3	2.08	0.53
1:A:176:ARG:HG2	1:A:204:ARG:HH21	1.74	0.53
1:B:62:CYS:SG	1:B:98:ARG:NH1	2.82	0.53
1:F:274:SER:OG	1:F:277:GLU:OE1	2.24	0.53
1:B:90:SER:HB3	1:B:95:ARG:HB2	1.92	0.52
1:B:327:PHE:HE2	1:B:336:ALA:HB2	1.75	0.52
1:F:168:ALA:O	1:F:171:GLU:HG3	2.09	0.52
1:E:142:VAL:HG21	1:E:153:VAL:HB	1.90	0.52
1:C:280:ASP:OD2	1:C:282:THR:OG1	2.24	0.52
1:E:40:ARG:HB3	1:E:78:ARG:HG3	1.90	0.52
1:D:117:ARG:HH11	1:D:136:SER:HA	1.74	0.52
1:G:250:ASP:OD1	1:G:303:SER:OG	2.22	0.52
1:G:306:TYR:OH	1:G:321:ASP:OD1	2.28	0.52
1:C:286:ARG:HD2	1:C:292:SER:HB2	1.90	0.52
1:E:51:VAL:HG23	1:E:132:VAL:HG22	1.91	0.52
1:B:321:ASP:OD1	1:B:325:ARG:NH1	2.43	0.52
1:E:222:LEU:HD13	1:E:226:GLY:HA3	1.91	0.51
1:B:42:LEU:HD22	1:B:140:SER:HA	1.93	0.51
1:D:232:GLN:HE22	1:H:173:TYR:HE1	1.57	0.51
1:E:174:LYS:HE2	1:E:237:VAL:HA	1.92	0.51
1:B:176:ARG:O	1:B:179:GLU:HG3	2.10	0.51
1:C:72:TYR:HE1	1:C:77:LEU:HD22	1.75	0.51
1:F:88:VAL:HB	1:F:98:ARG:HB2	1.93	0.51
1:H:168:ALA:O	1:H:171:GLU:HG3	2.10	0.51
1:G:305:GLY:O	1:G:309:MET:HG3	2.09	0.51
1:H:273:LEU:HG	1:H:277:GLU:HG3	1.92	0.51
1:A:349:SER:O	1:A:353:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:GLU:O	1:B:126:ILE:HG12	2.11	0.51
1:B:342:GLN:HE21	1:B:349:SER:HA	1.76	0.51
1:D:250:ASP:HB2	1:D:306:TYR:HB2	1.91	0.51
1:E:254:ASN:HD21	1:E:258:PRO:HD3	1.75	0.51
1:F:172:ARG:HH21	1:G:232:GLN:HG2	1.76	0.51
1:F:345:ASP:N	1:F:345:ASP:OD1	2.44	0.51
1:H:24:THR:HG21	1:H:131:PRO:HG3	1.93	0.51
1:A:45:ARG:NH2	1:A:139:MET:O	2.39	0.51
1:C:206:GLU:O	1:C:210:ARG:HG2	2.10	0.51
1:D:162:ARG:NH2	1:D:221:GLU:OE2	2.44	0.51
1:D:168:ALA:O	1:D:171:GLU:HG3	2.10	0.51
1:F:113:GLU:HA	1:G:75:THR:HG21	1.93	0.51
1:G:184:LEU:HD13	1:G:201:VAL:HG21	1.92	0.51
1:G:202:VAL:HG22	1:G:247:ILE:HG21	1.93	0.51
1:H:195:LEU:HD23	1:H:297:GLN:HA	1.93	0.51
1:C:63:ASP:N	1:C:63:ASP:OD1	2.43	0.50
1:C:195:LEU:HB3	1:C:297:GLN:HA	1.93	0.50
1:E:245:GLU:OE2	1:E:249:ARG:NE	2.42	0.50
1:G:286:ARG:HD3	1:G:292:SER:HB2	1.92	0.50
1:H:254:ASN:ND2	1:H:256:ASP:O	2.44	0.50
1:A:180:VAL:HG12	1:A:201:VAL:HG22	1.93	0.50
1:E:176:ARG:O	1:E:179:GLU:HG3	2.11	0.50
1:H:306:TYR:O	1:H:310:ALA:HB2	2.11	0.50
1:A:305:GLY:HA2	1:A:330:LEU:HG	1.92	0.50
1:B:203:GLN:HE22	1:B:204:ARG:NH1	2.08	0.50
1:G:90:SER:OG	1:G:92:ASP:OD1	2.27	0.50
1:H:22:ARG:NH2	1:H:216:ASP:OD1	2.45	0.50
1:C:250:ASP:OD2	1:C:306:TYR:N	2.38	0.50
1:D:156:SER:OG	1:D:225:ASP:OD1	2.18	0.50
1:G:215:ILE:HD11	1:G:229:LEU:HD21	1.92	0.50
1:C:73:ALA:HB3	1:C:76:ARG:HG3	1.94	0.50
1:F:184:LEU:O	1:F:188:GLU:HB2	2.12	0.50
1:G:306:TYR:O	1:G:310:ALA:HB2	2.12	0.50
1:A:107:PRO:O	1:A:123:ARG:NH2	2.44	0.50
1:G:66:PHE:HB2	1:G:99:ALA:HB3	1.93	0.50
1:H:22:ARG:HE	1:H:217:ALA:HA	1.77	0.50
1:H:327:PHE:HE2	1:H:336:ALA:HB2	1.76	0.50
1:A:267:LEU:HD23	1:A:270:LEU:HD21	1.93	0.50
1:C:21:LEU:HA	1:C:146:VAL:HG11	1.94	0.50
1:D:193:VAL:HB	1:D:300:ALA:HA	1.93	0.50
1:D:206:GLU:O	1:D:210:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:MET:HB2	1:G:83:MET:HE3	1.94	0.49
1:F:162:ARG:O	1:F:166:THR:HG22	2.12	0.49
1:F:198:VAL:HG13	1:F:251:TYR:CD2	2.47	0.49
1:C:54:TYR:HD1	1:C:88:VAL:HG11	1.76	0.49
1:A:111:THR:HG21	1:A:119:ARG:HG3	1.93	0.49
1:B:283:VAL:O	1:B:287:VAL:HG23	2.13	0.49
1:B:302:SER:O	1:B:304:ARG:NH1	2.45	0.49
1:F:167:ILE:HD12	1:F:170:LEU:HD23	1.93	0.49
1:B:240:ASN:OD1	1:B:244:ARG:NH2	2.45	0.49
1:C:84:ASP:OD2	1:F:82:LYS:NZ	2.45	0.49
1:E:215:ILE:HG21	1:E:233:LEU:HD21	1.95	0.49
1:D:304:ARG:NH2	1:D:325:ARG:HH12	2.11	0.49
1:F:102:GLN:HG2	1:F:104:VAL:HG13	1.95	0.49
1:G:52:LEU:HD23	1:G:89:LEU:HB2	1.94	0.49
1:B:169:THR:HG22	1:B:173:TYR:CZ	2.48	0.49
1:G:51:VAL:HG13	1:G:88:VAL:HG13	1.95	0.49
1:A:248:VAL:HG11	1:A:263:VAL:HG13	1.93	0.49
1:E:305:GLY:O	1:E:309:MET:HG3	2.12	0.49
1:F:210:ARG:HH12	1:F:271:ASP:HA	1.78	0.49
1:A:45:ARG:HH21	1:A:137:HIS:HA	1.77	0.49
1:A:176:ARG:HG2	1:A:204:ARG:NH2	2.28	0.49
1:A:189:ILE:HD11	1:A:362:LEU:HB3	1.95	0.49
1:D:274:SER:O	1:D:278:LEU:N	2.45	0.49
1:E:250:ASP:OD2	1:E:303:SER:OG	2.31	0.49
1:A:219:VAL:HG11	1:A:230:LYS:HD2	1.93	0.49
1:D:184:LEU:HD22	1:D:201:VAL:HG11	1.95	0.49
1:E:25:LEU:HD11	1:E:151:HIS:CE1	2.48	0.49
1:G:250:ASP:HB2	1:G:306:TYR:HB2	1.95	0.49
1:A:167:ILE:HD13	1:A:215:ILE:HD13	1.93	0.48
1:A:197:ASP:HA	1:A:200:THR:HG22	1.93	0.48
1:G:123:ARG:O	1:G:126:ILE:HG22	2.13	0.48
1:D:316:GLN:HG2	1:D:319:HIS:H	1.79	0.48
1:F:69:ASP:H	1:F:97:LEU:HA	1.78	0.48
1:F:233:LEU:O	1:F:237:VAL:HG12	2.13	0.48
1:B:171:GLU:HB3	1:B:236:LEU:HD11	1.96	0.48
1:C:55:ASP:OD1	1:C:56:ASP:N	2.40	0.48
1:F:156:SER:HA	1:F:159:ILE:HD12	1.95	0.48
1:F:185:SER:OG	1:F:307:ARG:NH1	2.43	0.48
1:A:106:ASP:OD2	1:A:108:SER:OG	2.29	0.48
1:D:225:ASP:OD2	1:D:225:ASP:N	2.46	0.48
1:H:103:LEU:O	1:H:105:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ASP:HB2	1:C:242:THR:OG1	2.14	0.48
1:E:263:VAL:O	1:E:267:LEU:HG	2.14	0.48
1:H:180:VAL:HG12	1:H:201:VAL:HG22	1.95	0.48
1:D:283:VAL:HA	1:D:286:ARG:HG2	1.96	0.48
1:E:222:LEU:HD22	1:E:225:ASP:HB3	1.96	0.48
1:A:342:GLN:HB2	1:A:353:ARG:HH12	1.79	0.47
1:B:229:LEU:O	1:B:233:LEU:HD23	2.14	0.47
1:G:172:ARG:HH21	1:G:176:ARG:HH21	1.60	0.47
1:C:112:ASP:OD1	1:C:112:ASP:N	2.47	0.47
1:D:250:ASP:OD2	1:D:307:ARG:N	2.34	0.47
1:H:98:ARG:HE	1:H:101:VAL:HG11	1.79	0.47
1:H:176:ARG:HD3	1:H:204:ARG:HE	1.79	0.47
1:C:249:ARG:HA	1:C:258:PRO:HG2	1.96	0.47
1:E:250:ASP:OD1	1:E:305:GLY:N	2.47	0.47
1:E:257:PRO:O	1:E:325:ARG:NH2	2.47	0.47
1:C:306:TYR:O	1:C:310:ALA:HB2	2.15	0.47
1:G:42:LEU:HD22	1:G:140:SER:HA	1.96	0.47
1:H:280:ASP:HB3	1:H:283:VAL:HG22	1.97	0.47
1:C:205:LEU:HB3	1:C:244:ARG:HD3	1.96	0.47
1:F:164:ASN:HA	1:F:167:ILE:HG22	1.97	0.47
1:H:162:ARG:NH2	1:H:218:ASP:OD1	2.48	0.47
1:H:195:LEU:O	1:H:199:MET:HG2	2.15	0.47
1:H:205:LEU:HD21	1:H:244:ARG:HA	1.96	0.47
1:A:195:LEU:HD11	1:A:199:MET:HE3	1.97	0.47
1:B:40:ARG:CZ	1:B:74:PRO:HB2	2.45	0.47
1:D:228:GLN:O	1:D:232:GLN:HG2	2.14	0.47
1:E:323:LEU:HD23	1:E:344:VAL:HG11	1.97	0.47
1:F:309:MET:HE1	1:F:315:LEU:HD13	1.96	0.47
1:G:117:ARG:HH11	1:G:136:SER:HA	1.78	0.47
1:A:342:GLN:OE1	1:A:353:ARG:NH2	2.41	0.47
1:E:92:ASP:N	1:E:92:ASP:OD1	2.47	0.47
1:E:131:PRO:HB3	1:E:146:VAL:HG12	1.96	0.47
1:A:252:HIS:HB3	1:A:304:ARG:HH12	1.80	0.47
1:C:282:THR:HB	1:C:286:ARG:NH1	2.27	0.47
1:D:47:GLY:HA3	1:D:117:ARG:HH22	1.80	0.47
1:D:191:ASP:OD1	1:D:331:GLN:NE2	2.48	0.47
1:D:145:TYR:CD2	1:D:150:ARG:HB3	2.49	0.47
1:C:150:ARG:HH22	1:C:152:VAL:HG23	1.80	0.46
1:F:164:ASN:O	1:F:167:ILE:HG22	2.15	0.46
1:G:163:ALA:O	1:G:167:ILE:HG12	2.15	0.46
1:D:72:TYR:OH	1:D:77:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HG2	1:A:159:ILE:HD11	1.96	0.46
1:C:316:GLN:HB2	1:C:319:HIS:ND1	2.30	0.46
1:D:55:ASP:OD1	1:D:58:VAL:N	2.33	0.46
1:E:275:ASP:HA	1:E:278:LEU:HB3	1.97	0.46
1:F:170:LEU:HD13	1:F:211:ILE:HG23	1.97	0.46
1:G:33:PRO:HB2	1:G:72:TYR:HE2	1.79	0.46
1:H:254:ASN:HD21	1:H:258:PRO:HD3	1.81	0.46
1:D:137:HIS:O	1:D:138:SER:OG	2.30	0.46
1:F:305:GLY:O	1:F:309:MET:HG3	2.14	0.46
1:G:252:HIS:O	1:G:304:ARG:NH2	2.48	0.46
1:H:113:GLU:OE2	1:H:150:ARG:NH1	2.48	0.46
1:H:196:ARG:NH1	1:H:298:ASP:HA	2.31	0.46
1:A:211:ILE:O	1:A:215:ILE:HG13	2.16	0.46
1:E:209:ARG:HG2	1:E:244:ARG:HH12	1.80	0.46
1:F:263:VAL:O	1:F:267:LEU:HG	2.15	0.46
1:H:145:TYR:CE1	1:H:150:ARG:HG3	2.51	0.46
1:A:104:VAL:O	1:A:104:VAL:HG13	2.15	0.46
1:A:280:ASP:OD2	1:A:282:THR:OG1	2.33	0.46
1:B:72:TYR:N	1:B:94:SER:O	2.36	0.46
1:B:205:LEU:HG	1:B:244:ARG:HH21	1.80	0.46
1:C:232:GLN:O	1:C:235:GLU:HG2	2.16	0.46
1:D:113:GLU:OE1	1:D:150:ARG:NH1	2.48	0.46
1:D:215:ILE:O	1:D:219:VAL:HG13	2.16	0.46
1:A:286:ARG:NH1	1:A:292:SER:HA	2.31	0.46
1:C:92:ASP:OD1	1:C:92:ASP:N	2.47	0.46
1:H:30:PRO:HA	1:H:35:ARG:HG2	1.98	0.46
1:A:282:THR:O	1:A:286:ARG:HG2	2.16	0.45
1:B:239:ASP:OD1	1:B:239:ASP:N	2.48	0.45
1:C:191:ASP:OD1	1:C:191:ASP:N	2.49	0.45
1:F:282:THR:O	1:F:286:ARG:HG2	2.16	0.45
1:G:264:ALA:O	1:G:267:LEU:HB2	2.16	0.45
1:A:69:ASP:H	1:A:97:LEU:HA	1.81	0.45
1:A:176:ARG:O	1:A:179:GLU:HG3	2.16	0.45
1:B:72:TYR:HE1	1:B:89:LEU:HD21	1.81	0.45
1:C:142:VAL:HG13	1:C:153:VAL:HB	1.98	0.45
1:E:208:VAL:HA	1:E:211:ILE:HG22	1.99	0.45
1:D:42:LEU:HD22	1:D:140:SER:HA	1.99	0.45
1:D:324:VAL:O	1:D:328:GLY:N	2.48	0.45
1:F:227:ARG:HD2	1:F:227:ARG:HA	1.79	0.45
1:H:348:GLY:H	1:H:351:TRP:HE3	1.63	0.45
1:A:33:PRO:HB2	1:A:72:TYR:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HD2	1:B:101:VAL:HB	1.98	0.45
1:C:164:ASN:O	1:C:167:ILE:HG22	2.17	0.45
1:D:209:ARG:NH1	1:D:244:ARG:HH11	2.14	0.45
1:B:77:LEU:CD1	1:B:87:VAL:HG11	2.47	0.45
1:C:305:GLY:O	1:C:309:MET:HG3	2.16	0.45
1:D:54:TYR:HD2	1:D:90:SER:HA	1.82	0.45
1:D:102:GLN:OE1	1:F:119:ARG:HD2	2.16	0.45
1:H:356:ARG:HA	1:H:359:LEU:HD12	1.97	0.45
1:C:49:LEU:HD11	1:C:121:ALA:HB2	1.99	0.45
1:H:196:ARG:HD2	1:H:297:GLN:HG3	1.99	0.45
1:B:73:ALA:HB3	1:B:76:ARG:HG3	1.99	0.45
1:G:264:ALA:O	1:G:268:GLU:OE1	2.35	0.45
1:B:256:ASP:OD1	1:B:256:ASP:N	2.50	0.45
1:E:186:THR:O	1:E:189:ILE:HG22	2.17	0.45
1:F:250:ASP:HB2	1:F:306:TYR:HB2	1.99	0.45
1:G:199:MET:CE	1:G:281:PHE:HB3	2.47	0.45
1:D:303:SER:O	1:D:330:LEU:N	2.50	0.44
1:F:169:THR:HG23	1:F:211:ILE:HD11	1.98	0.44
1:F:286:ARG:NH2	1:F:291:PRO:O	2.50	0.44
1:G:97:LEU:CD1	1:G:98:ARG:HG2	2.43	0.44
1:G:176:ARG:O	1:G:180:VAL:HG23	2.17	0.44
1:B:19:PRO:HB2	1:B:20:THR:H	1.59	0.44
1:D:61:ILE:HD11	1:D:127:GLN:HE22	1.83	0.44
1:D:173:TYR:O	1:D:177:LEU:HD23	2.16	0.44
1:D:180:VAL:HG12	1:D:201:VAL:HG12	1.98	0.44
1:D:250:ASP:OD1	1:D:304:ARG:N	2.50	0.44
1:F:270:LEU:HD23	1:F:287:VAL:HG11	2.00	0.44
1:B:121:ALA:HA	1:B:132:VAL:HG11	1.99	0.44
1:B:237:VAL:HG12	1:B:240:ASN:HB2	2.00	0.44
1:C:41:ILE:HD11	1:C:77:LEU:HG	1.99	0.44
1:C:195:LEU:HA	1:C:198:VAL:HG12	1.98	0.44
1:C:210:ARG:O	1:C:213:LEU:HG	2.17	0.44
1:H:85:GLY:HA3	1:H:100:ASN:HA	1.99	0.44
1:A:244:ARG:HE	1:A:267:LEU:HD22	1.83	0.44
1:F:210:ARG:NH1	1:F:271:ASP:OD1	2.51	0.44
1:G:181:SER:OG	1:G:307:ARG:NH2	2.38	0.44
1:G:252:HIS:HA	1:G:288:PHE:CZ	2.52	0.44
1:G:252:HIS:HA	1:G:288:PHE:HZ	1.82	0.44
1:A:88:VAL:HB	1:A:98:ARG:HB2	2.00	0.44
1:A:286:ARG:NE	1:A:290:TYR:O	2.51	0.44
1:D:38:LEU:HD11	1:D:133:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PRO:HD2	1:A:222:LEU:O	2.17	0.44
1:E:264:ALA:O	1:E:268:GLU:OE1	2.36	0.44
1:G:24:THR:HG22	1:G:27:ARG:NH2	2.29	0.44
1:G:303:SER:O	1:G:330:LEU:N	2.51	0.44
1:G:348:GLY:H	1:G:351:TRP:HE3	1.66	0.44
1:A:332:ASN:OD1	1:A:333:LEU:N	2.51	0.44
1:B:180:VAL:HG12	1:B:201:VAL:HG22	1.99	0.44
1:B:248:VAL:HG12	1:B:263:VAL:HG22	2.01	0.43
1:D:117:ARG:NH1	1:D:136:SER:HA	2.33	0.43
1:F:176:ARG:NH1	1:G:235:GLU:OE2	2.51	0.43
1:G:252:HIS:NE2	1:G:258:PRO:HB3	2.33	0.43
1:D:89:LEU:CD2	1:D:96:ILE:HG22	2.48	0.43
1:D:163:ALA:O	1:D:167:ILE:HG12	2.18	0.43
1:E:30:PRO:HA	1:E:35:ARG:HG2	2.00	0.43
1:F:117:ARG:NH1	1:F:136:SER:HA	2.32	0.43
1:F:139:MET:HB3	1:F:141:ILE:HG12	2.00	0.43
1:A:119:ARG:HD3	1:A:123:ARG:NH1	2.33	0.43
1:C:349:SER:O	1:C:353:ARG:HG2	2.18	0.43
1:F:227:ARG:O	1:F:228:GLN:NE2	2.50	0.43
1:G:50:ILE:HD13	1:G:77:LEU:HD13	2.00	0.43
1:G:215:ILE:HG21	1:G:233:LEU:HD11	2.00	0.43
1:B:39:GLU:HB2	1:B:43:ARG:NH1	2.29	0.43
1:B:239:ASP:HB2	1:B:242:THR:OG1	2.18	0.43
1:D:104:VAL:O	1:D:104:VAL:HG13	2.18	0.43
1:E:124:THR:HG23	1:E:132:VAL:HG21	2.00	0.43
1:E:237:VAL:HG22	1:E:240:ASN:HB2	2.01	0.43
1:E:293:THR:HG23	1:E:296:ALA:H	1.84	0.43
1:F:225:ASP:OD1	1:F:225:ASP:N	2.51	0.43
1:C:176:ARG:O	1:C:179:GLU:HG3	2.19	0.43
1:D:249:ARG:HG2	1:D:263:VAL:HG21	2.00	0.43
1:H:246:LEU:HD11	1:H:317:PHE:HE1	1.83	0.43
1:B:109:ILE:HB	1:B:123:ARG:HG2	2.00	0.43
1:B:232:GLN:HA	1:B:235:GLU:HG2	2.00	0.43
1:D:65:GLY:HA3	1:D:99:ALA:O	2.19	0.43
1:G:208:VAL:O	1:G:211:ILE:HG22	2.19	0.43
1:A:285:ALA:O	1:A:289:GLY:N	2.46	0.43
1:A:342:GLN:HG3	1:A:349:SER:HA	2.00	0.43
1:B:97:LEU:H	1:B:97:LEU:HD23	1.84	0.43
1:C:283:VAL:O	1:C:287:VAL:HG23	2.19	0.43
1:F:199:MET:HE1	1:F:285:ALA:HB2	2.01	0.43
1:G:42:LEU:HD23	1:G:42:LEU:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:THR:HG21	1:H:119:ARG:HG3	2.01	0.43
1:H:154:PRO:HG2	1:H:159:ILE:HD11	2.00	0.43
1:A:163:ALA:O	1:A:167:ILE:HG12	2.19	0.43
1:A:200:THR:O	1:A:204:ARG:HG2	2.19	0.43
1:E:50:ILE:HD13	1:E:77:LEU:HD23	2.01	0.43
1:G:249:ARG:HG2	1:G:263:VAL:HG21	2.00	0.43
1:A:24:THR:HG21	1:A:131:PRO:HG3	2.00	0.42
1:A:222:LEU:HD13	1:A:226:GLY:HA3	2.00	0.42
1:B:35:ARG:HH11	1:B:35:ARG:HG3	1.83	0.42
1:D:42:LEU:HD23	1:D:42:LEU:HA	1.86	0.42
1:E:109:ILE:O	1:E:123:ARG:NE	2.52	0.42
1:F:256:ASP:OD1	1:F:256:ASP:N	2.51	0.42
1:H:29:ALA:HB1	1:H:223:GLY:HA3	2.01	0.42
1:H:249:ARG:HB3	1:H:306:TYR:CE2	2.55	0.42
1:B:41:ILE:HG21	1:B:48:ALA:HB2	2.01	0.42
1:B:274:SER:OG	1:B:277:GLU:OE1	2.29	0.42
1:D:103:LEU:O	1:D:120:SER:OG	2.31	0.42
1:E:51:VAL:HG13	1:E:88:VAL:HA	2.00	0.42
1:B:25:LEU:HA	1:B:28:LEU:HB2	2.00	0.42
1:C:35:ARG:HD2	1:C:35:ARG:HA	1.85	0.42
1:D:251:TYR:HE1	1:D:303:SER:HA	1.84	0.42
1:F:206:GLU:HA	1:F:244:ARG:NH2	2.35	0.42
1:G:45:ARG:NH1	1:G:138:SER:O	2.51	0.42
1:G:51:VAL:HG23	1:G:132:VAL:HG22	2.01	0.42
1:B:104:VAL:O	1:B:104:VAL:HG13	2.19	0.42
1:B:142:VAL:HB	1:B:153:VAL:HB	2.01	0.42
1:C:36:ASP:O	1:C:39:GLU:HG2	2.19	0.42
1:C:169:THR:HG22	1:C:172:ARG:HH12	1.84	0.42
1:C:196:ARG:NE	1:C:297:GLN:OE1	2.51	0.42
1:C:205:LEU:HA	1:C:208:VAL:HG12	2.01	0.42
1:D:71:ARG:NH2	1:H:112:ASP:OD1	2.52	0.42
1:F:199:MET:HE3	1:F:281:PHE:HD2	1.84	0.42
1:G:342:GLN:HG2	1:G:349:SER:HA	2.01	0.42
1:H:164:ASN:O	1:H:167:ILE:HG22	2.20	0.42
1:A:275:ASP:OD1	1:A:279:LEU:HD23	2.19	0.42
1:D:245:GLU:OE2	1:D:249:ARG:NH2	2.47	0.42
1:D:348:GLY:HA3	1:D:351:TRP:HE3	1.85	0.42
1:H:253:ALA:HB3	1:H:289:GLY:O	2.20	0.42
1:H:264:ALA:O	1:H:268:GLU:OE1	2.38	0.42
1:C:136:SER:OG	1:C:139:MET:HB2	2.19	0.42
1:F:222:LEU:HD23	1:F:222:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:PRO:HB2	1:C:325:ARG:CZ	2.50	0.42
1:G:58:VAL:HG23	1:G:128:THR:HG21	2.01	0.42
1:D:67:VAL:HG23	1:D:98:ARG:HH11	1.83	0.42
1:E:107:PRO:HA	1:E:123:ARG:NH1	2.35	0.42
1:E:239:ASP:HB2	1:E:242:THR:HG22	2.02	0.42
1:H:71:ARG:HH21	1:H:95:ARG:HD3	1.85	0.42
1:C:244:ARG:O	1:C:247:ILE:HG22	2.20	0.41
1:E:266:THR:HA	1:E:269:GLU:HG3	2.01	0.41
1:A:210:ARG:NH2	1:A:273:LEU:O	2.52	0.41
1:B:209:ARG:HB2	1:B:244:ARG:NH2	2.35	0.41
1:C:55:ASP:H	1:C:58:VAL:HB	1.85	0.41
1:G:303:SER:HB3	1:G:330:LEU:HD22	2.01	0.41
1:B:68:LEU:HD11	1:B:80:LEU:HD11	2.03	0.41
1:C:219:VAL:HG22	1:C:229:LEU:HB3	2.02	0.41
1:C:270:LEU:O	1:C:273:LEU:HG	2.19	0.41
1:D:53:GLY:HA2	1:D:91:SER:HA	2.02	0.41
1:D:257:PRO:HB3	1:D:304:ARG:NH2	2.32	0.41
1:F:111:THR:HG21	1:F:119:ARG:HG3	2.02	0.41
1:G:301:MET:SD	1:G:301:MET:N	2.90	0.41
1:H:62:CYS:HB2	1:H:101:VAL:HB	2.03	0.41
1:B:312:ILE:HA	1:B:313:PRO:HD3	1.92	0.41
1:D:86:ALA:HB3	1:D:101:VAL:HG23	2.01	0.41
1:D:239:ASP:HB2	1:D:242:THR:OG1	2.20	0.41
1:F:28:LEU:HD11	1:F:133:ILE:HD11	2.02	0.41
1:A:104:VAL:HG21	1:B:107:PRO:HB3	2.03	0.41
1:D:159:ILE:HG21	1:D:222:LEU:HD13	2.02	0.41
1:G:340:ASP:OD1	1:G:341:LEU:N	2.52	0.41
1:A:195:LEU:HD23	1:A:297:GLN:HA	2.02	0.41
1:E:53:GLY:O	1:E:58:VAL:HG21	2.20	0.41
1:G:66:PHE:HE1	1:G:100:ASN:HD22	1.68	0.41
1:F:235:GLU:HG3	1:F:236:LEU:HD22	2.02	0.41
1:F:341:LEU:HB2	1:F:352:ALA:HB1	2.02	0.41
1:G:36:ASP:O	1:G:40:ARG:HG3	2.21	0.41
1:G:228:GLN:O	1:G:231:LEU:HG	2.19	0.41
1:H:42:LEU:HD22	1:H:140:SER:HA	2.03	0.41
1:H:61:ILE:HG23	1:H:104:VAL:O	2.20	0.41
1:A:159:ILE:HG21	1:A:222:LEU:HG	2.03	0.41
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.89	0.41
1:B:52:LEU:HD12	1:B:131:PRO:HG2	2.03	0.41
1:D:177:LEU:HD22	1:D:204:ARG:HB3	2.03	0.41
1:E:230:LYS:HG2	1:E:231:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:VAL:O	1:E:266:THR:OG1	2.36	0.41
1:F:97:LEU:HD23	1:F:97:LEU:H	1.84	0.41
1:B:167:ILE:O	1:B:171:GLU:OE1	2.38	0.41
1:E:227:ARG:HB3	1:E:230:LYS:NZ	2.35	0.41
1:H:206:GLU:HG3	1:H:210:ARG:HH21	1.86	0.41
1:C:27:ARG:HG2	1:C:34:LEU:HD22	2.03	0.40
1:E:53:GLY:N	1:E:90:SER:O	2.54	0.40
1:F:303:SER:O	1:F:329:SER:HA	2.21	0.40
1:G:312:ILE:HB	1:G:315:LEU:HD22	2.04	0.40
1:G:324:VAL:O	1:G:328:GLY:N	2.54	0.40
1:A:273:LEU:HD12	1:A:277:GLU:HG2	2.02	0.40
1:B:28:LEU:O	1:B:35:ARG:HD3	2.21	0.40
1:D:35:ARG:HA	1:D:35:ARG:HD2	1.79	0.40
1:F:290:TYR:OH	1:F:301:MET:SD	2.57	0.40
1:G:312:ILE:HA	1:G:313:PRO:HD3	1.95	0.40
1:C:184:LEU:O	1:C:188:GLU:HG3	2.21	0.40
1:E:163:ALA:O	1:E:167:ILE:HG12	2.22	0.40
1:E:168:ALA:O	1:E:171:GLU:HG2	2.22	0.40
1:E:315:LEU:HD12	1:E:315:LEU:HA	1.90	0.40
1:F:25:LEU:HD23	1:F:25:LEU:HA	1.87	0.40
1:G:267:LEU:HD23	1:G:267:LEU:HA	1.89	0.40
1:H:80:LEU:HD13	1:H:96:ILE:HG21	2.03	0.40
1:H:206:GLU:HA	1:H:206:GLU:OE2	2.22	0.40
1:D:66:PHE:O	1:D:98:ARG:NH1	2.53	0.40
1:D:241:GLU:HG2	1:D:242:THR:N	2.36	0.40
1:H:61:ILE:HD13	1:H:61:ILE:HA	1.96	0.40
1:H:71:ARG:HE	1:H:95:ARG:HG2	1.87	0.40
1:A:197:ASP:O	1:A:201:VAL:HG23	2.21	0.40
1:A:222:LEU:HD22	1:A:225:ASP:HB3	2.03	0.40
1:A:342:GLN:HB2	1:A:353:ARG:NH1	2.37	0.40
1:C:90:SER:HB2	1:C:95:ARG:HB2	2.04	0.40
1:C:306:TYR:CZ	1:C:324:VAL:HG21	2.57	0.40
1:D:62:CYS:HB2	1:D:101:VAL:HB	2.04	0.40
1:F:40:ARG:NH1	1:F:74:PRO:HB2	2.27	0.40
1:G:257:PRO:HG2	1:G:325:ARG:HD3	2.03	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	344/383 (90%)	324 (94%)	20 (6%)	0	100	100
1	B	344/383 (90%)	330 (96%)	14 (4%)	0	100	100
1	C	344/383 (90%)	332 (96%)	12 (4%)	0	100	100
1	D	344/383 (90%)	325 (94%)	19 (6%)	0	100	100
1	E	344/383 (90%)	326 (95%)	18 (5%)	0	100	100
1	F	344/383 (90%)	329 (96%)	15 (4%)	0	100	100
1	G	344/383 (90%)	325 (94%)	19 (6%)	0	100	100
1	H	344/383 (90%)	322 (94%)	22 (6%)	0	100	100
All	All	2752/3064 (90%)	2613 (95%)	139 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	290/317 (92%)	290 (100%)	0	100	100
1	B	290/317 (92%)	289 (100%)	1 (0%)	92	96
1	C	290/317 (92%)	290 (100%)	0	100	100
1	D	290/317 (92%)	290 (100%)	0	100	100
1	E	290/317 (92%)	289 (100%)	1 (0%)	92	96
1	F	290/317 (92%)	290 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	290/317 (92%)	289 (100%)	1 (0%)	92	96
1	H	290/317 (92%)	289 (100%)	1 (0%)	92	96
All	All	2320/2536 (92%)	2316 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	78	ARG
1	E	162	ARG
1	G	353	ARG
1	H	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	228	GLN
1	B	232	GLN
1	D	331	GLN
1	H	232	GLN
1	H	252	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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-33540. 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 ⓘ
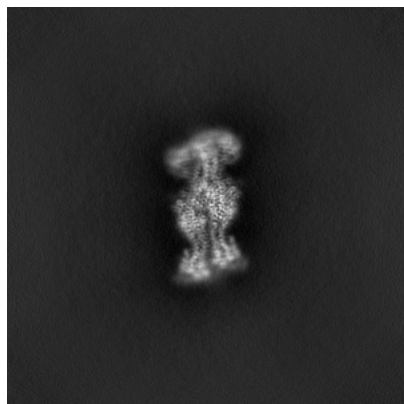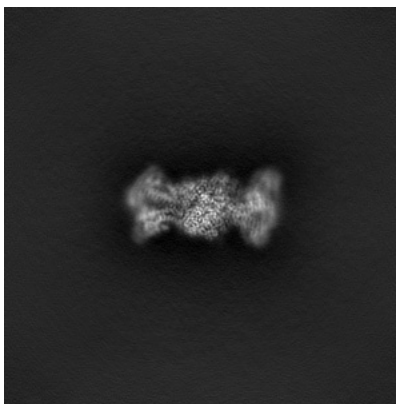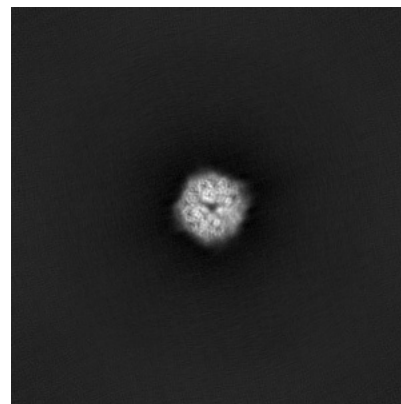
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

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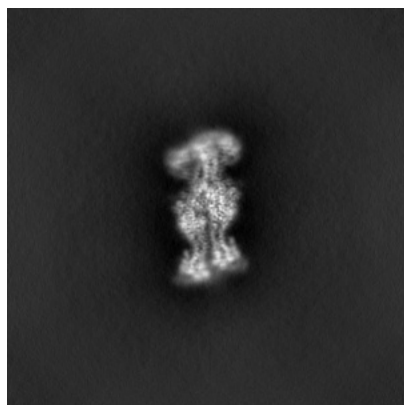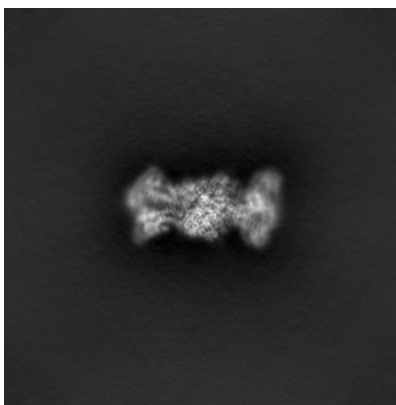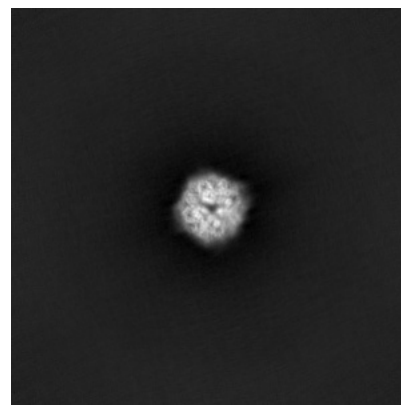
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map
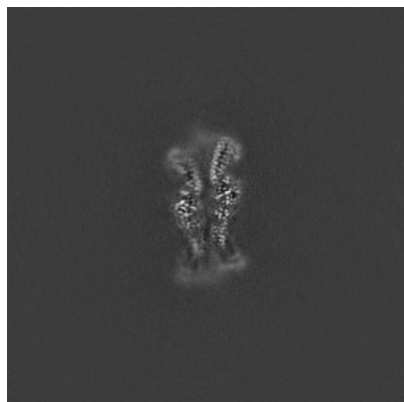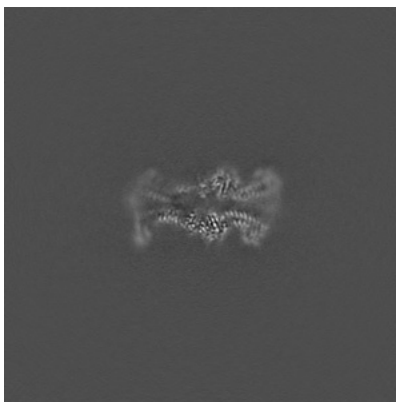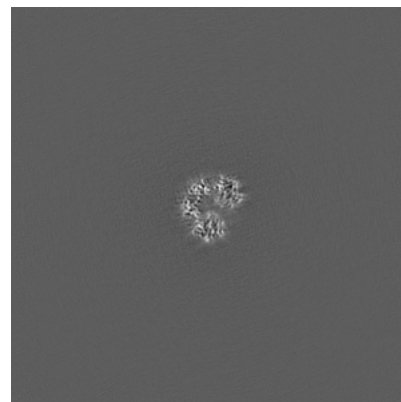
| X Index: 220 | Y Index: 220 | Z Index: 220 |

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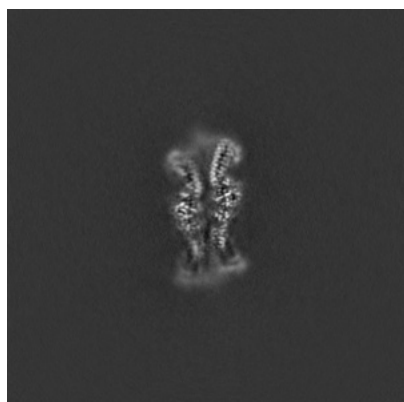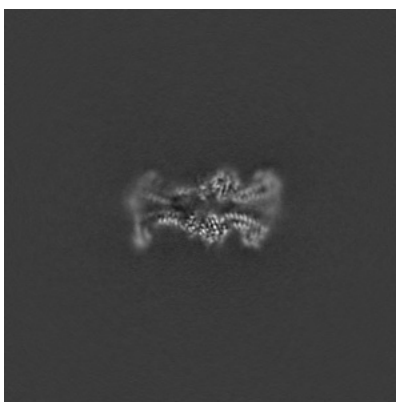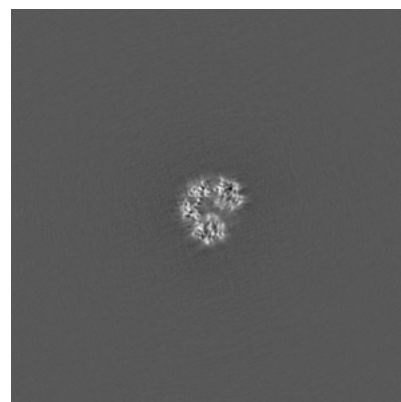
| X Index: 220 | Y Index: 220 | Z Index: 220 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
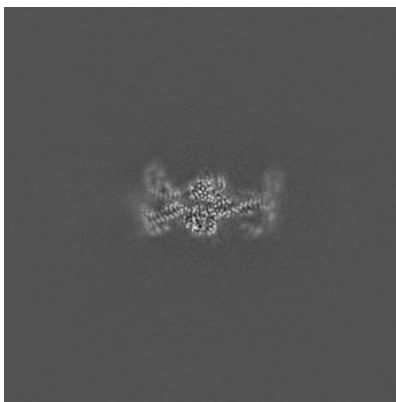
X Index: 207	Y Index: 235	Z Index: 222
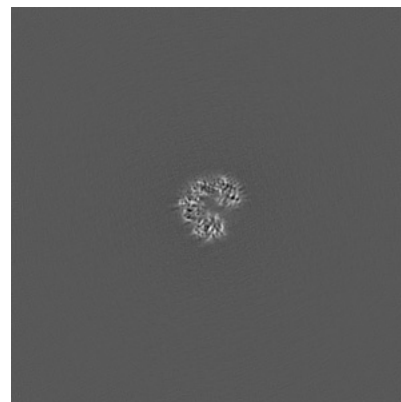
6.3.2 Raw map
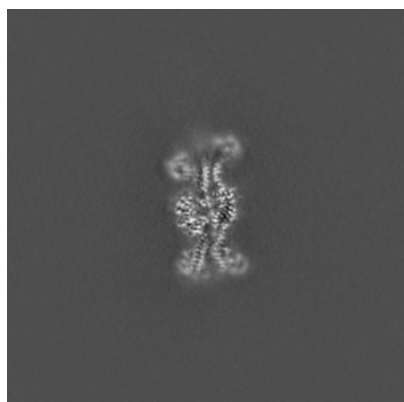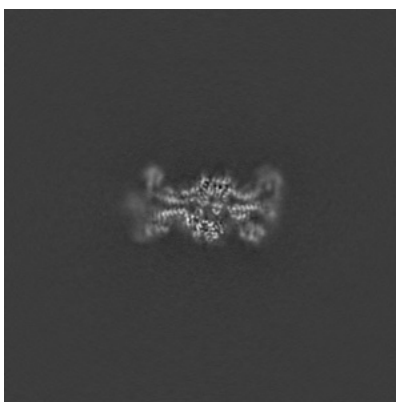
X Index: 211	Y Index: 228	Z Index: 222
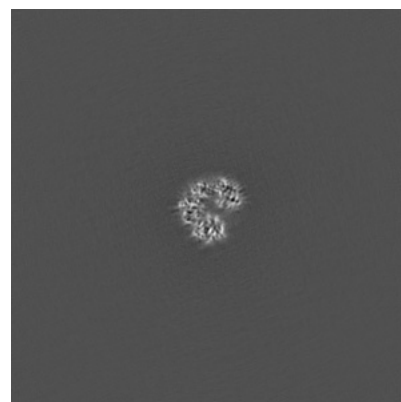
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
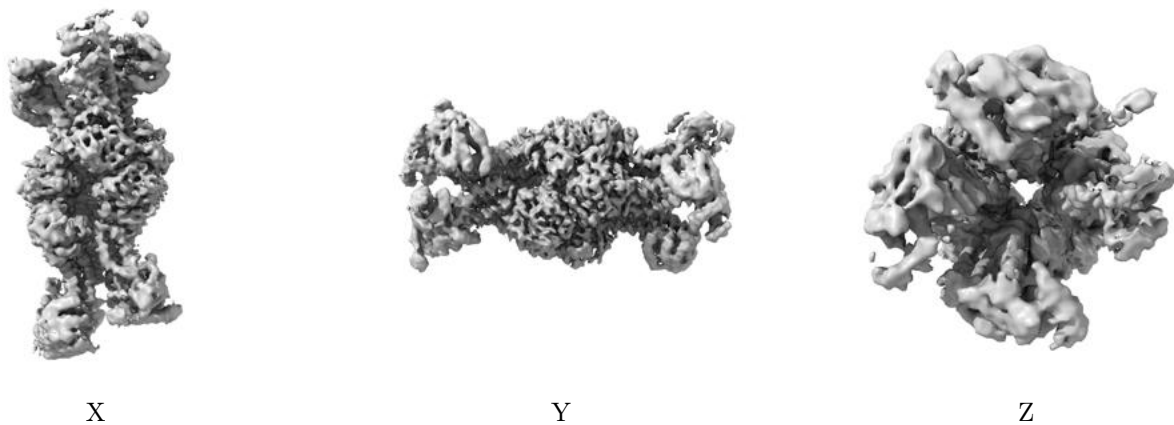
The images above show the 3D surface view of the map at the recommended contour level 1.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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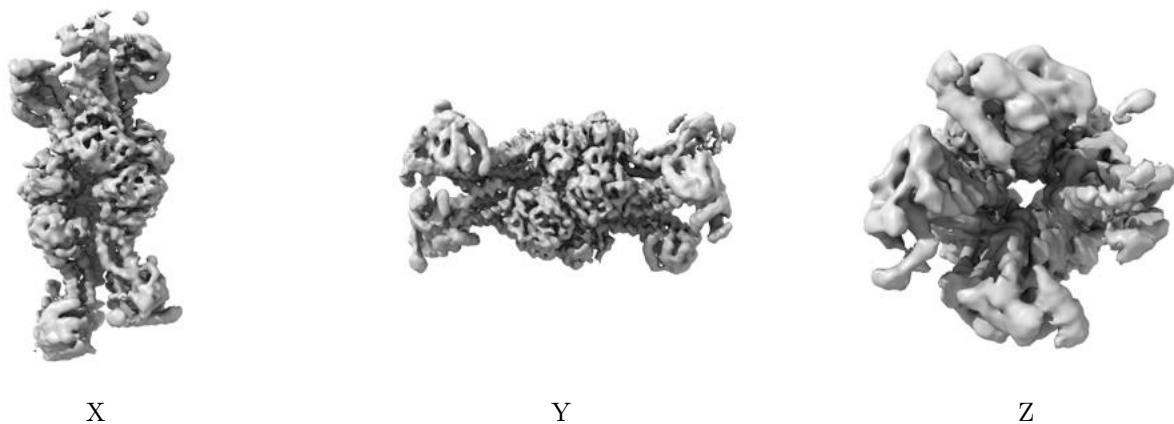
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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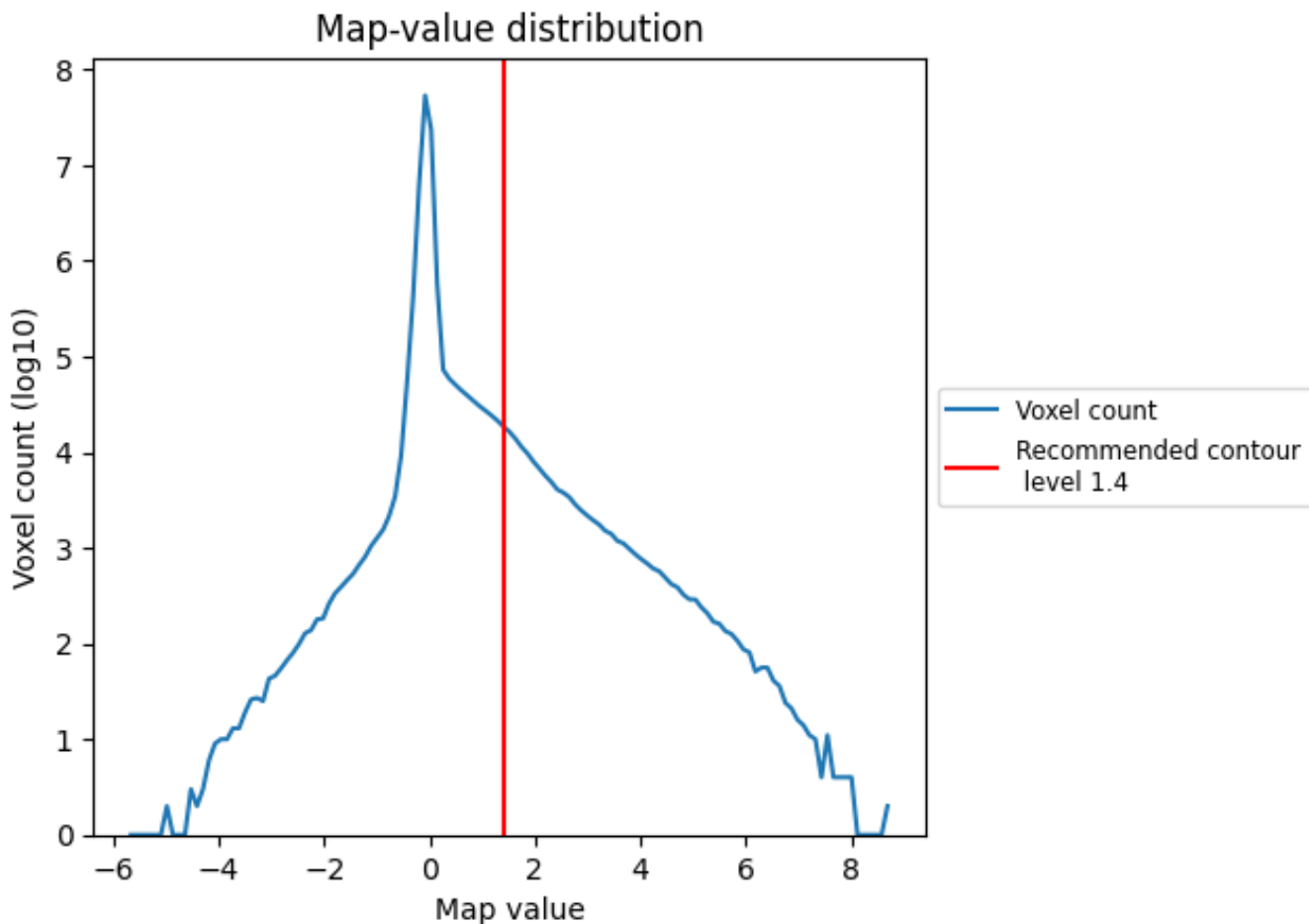
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
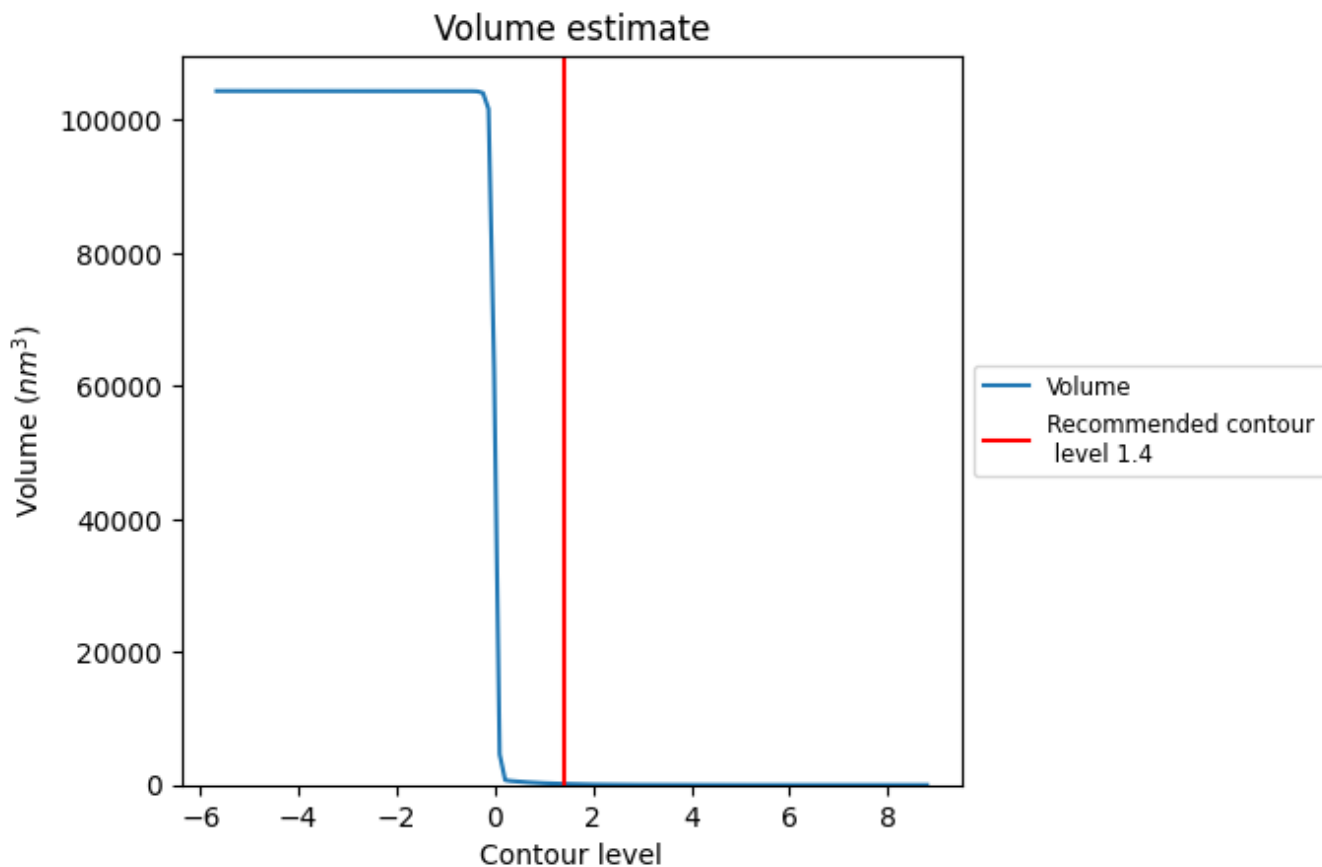
The volume at the recommended contour level is 161 nm^3; this corresponds to an approximate mass of 145 kDa.

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 ⓘ
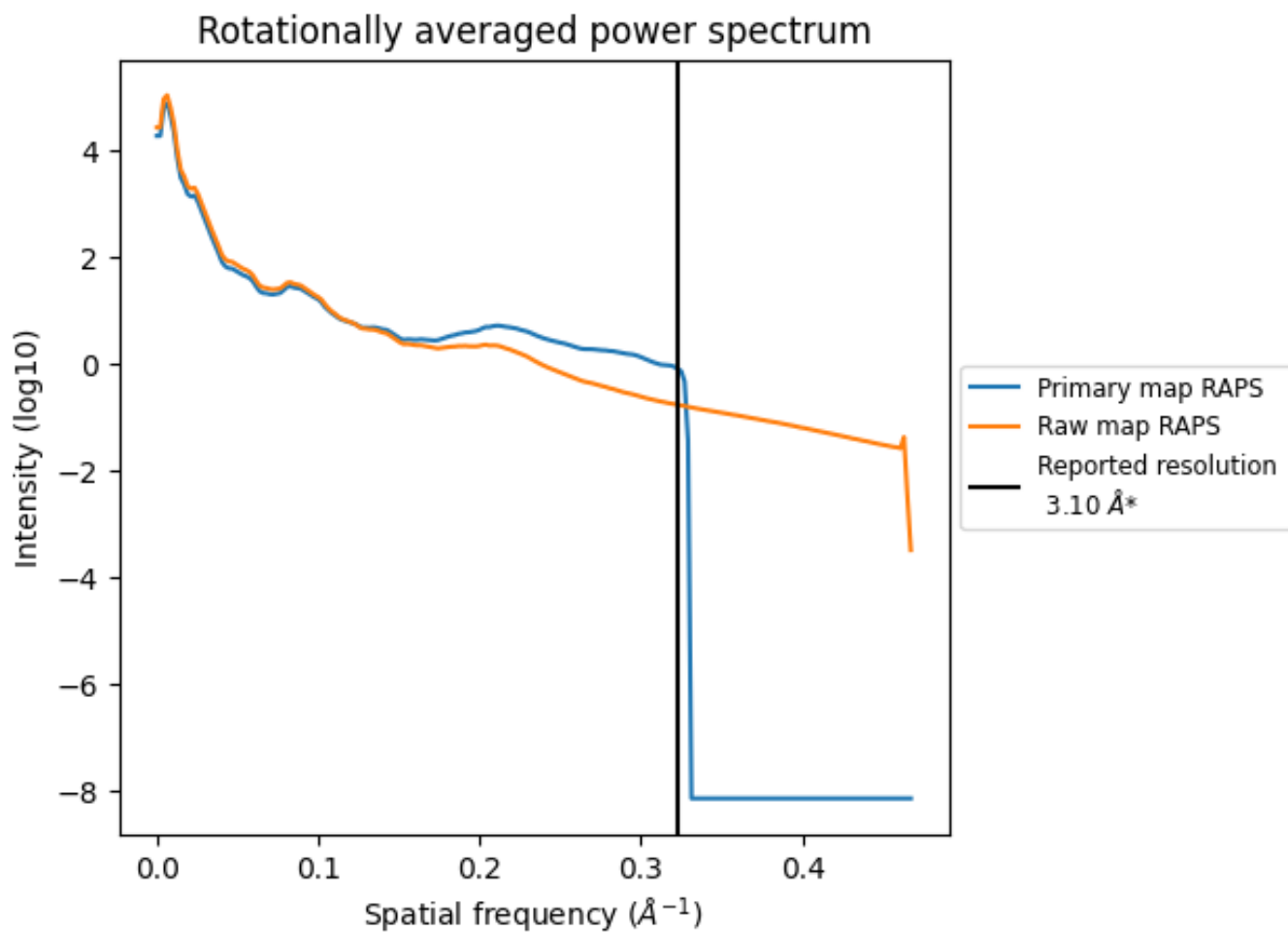
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 ⓘ
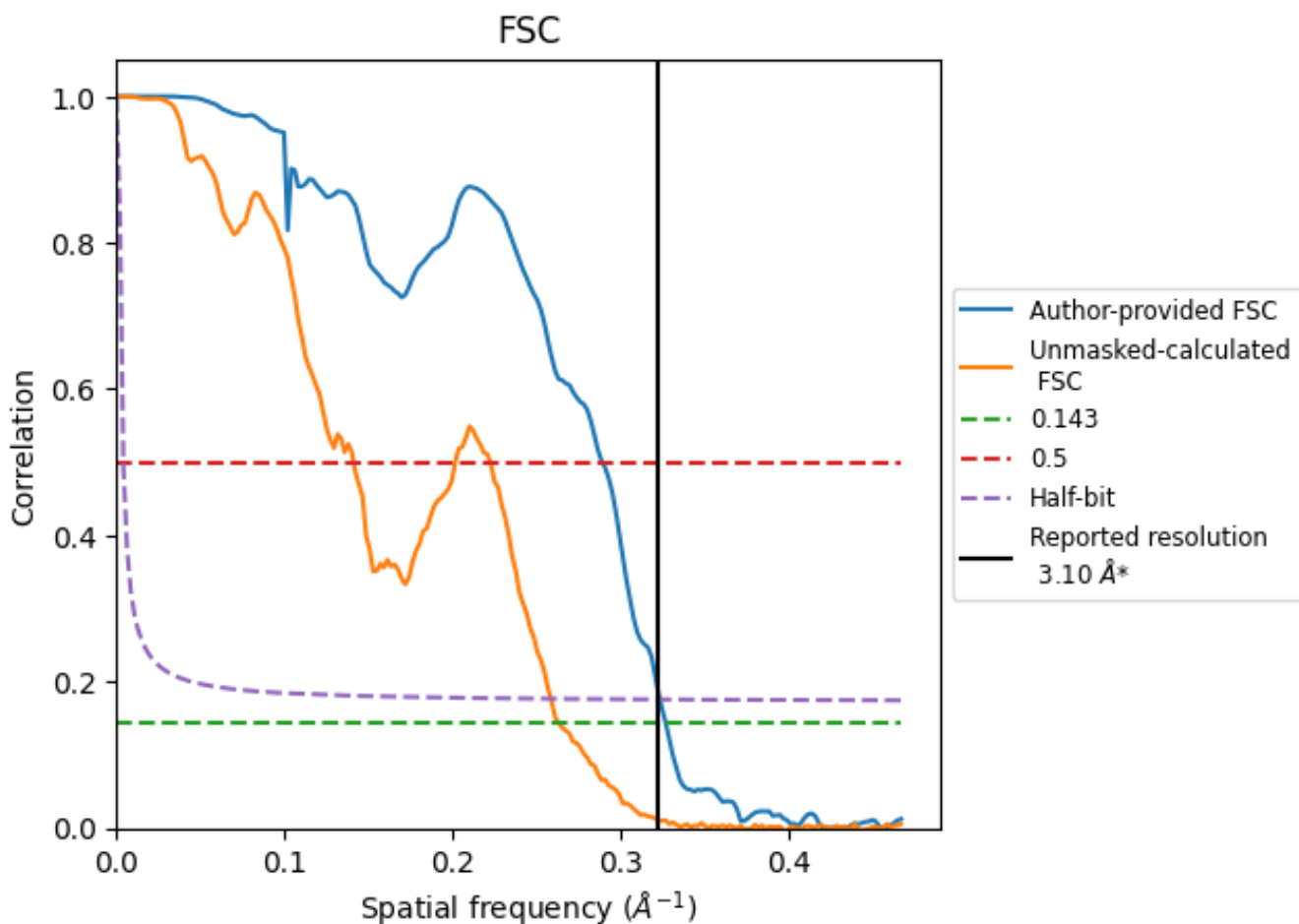
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.46	3.09
Unmasked-calculated*	3.79	7.08	3.86

*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 3.79 differs from the reported value 3.1 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-33540 and PDB model 7Y0D. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)

X	Y	Z
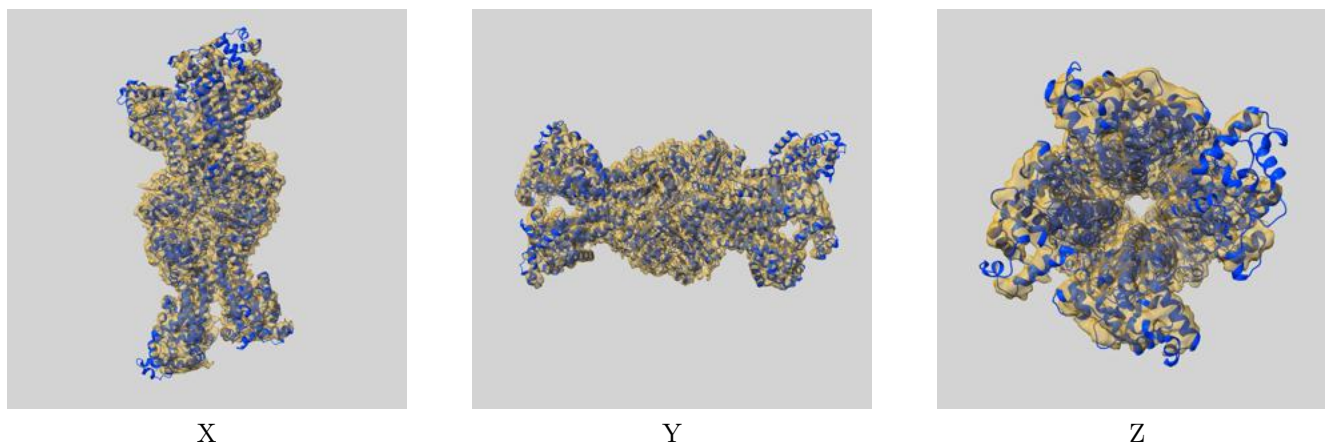
The images above show the 3D surface view of the map at the recommended contour level 1.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ
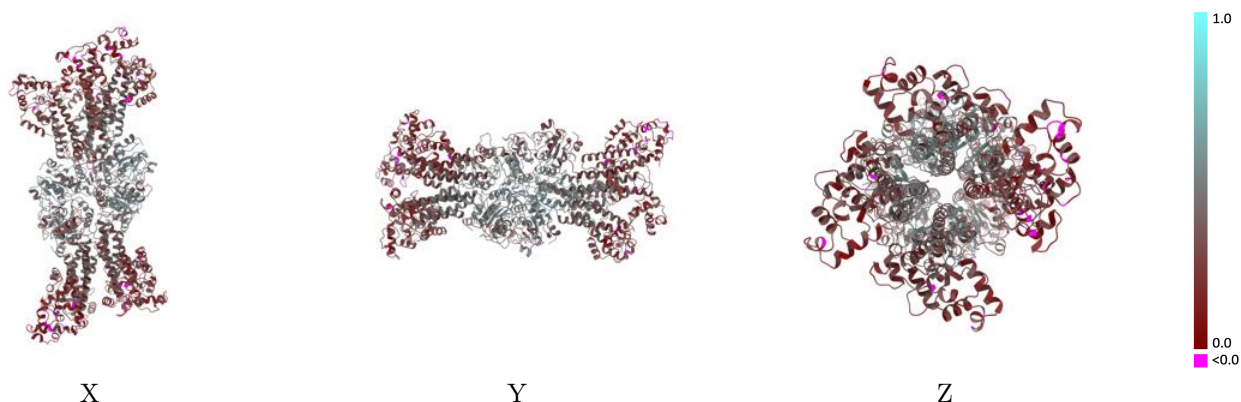
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
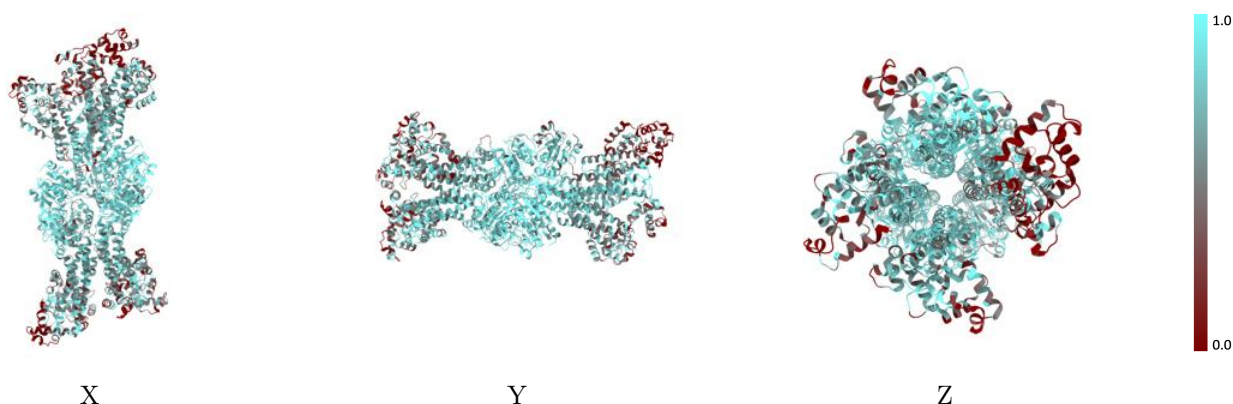
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.4).

9.4　Atom inclusion ⓘ
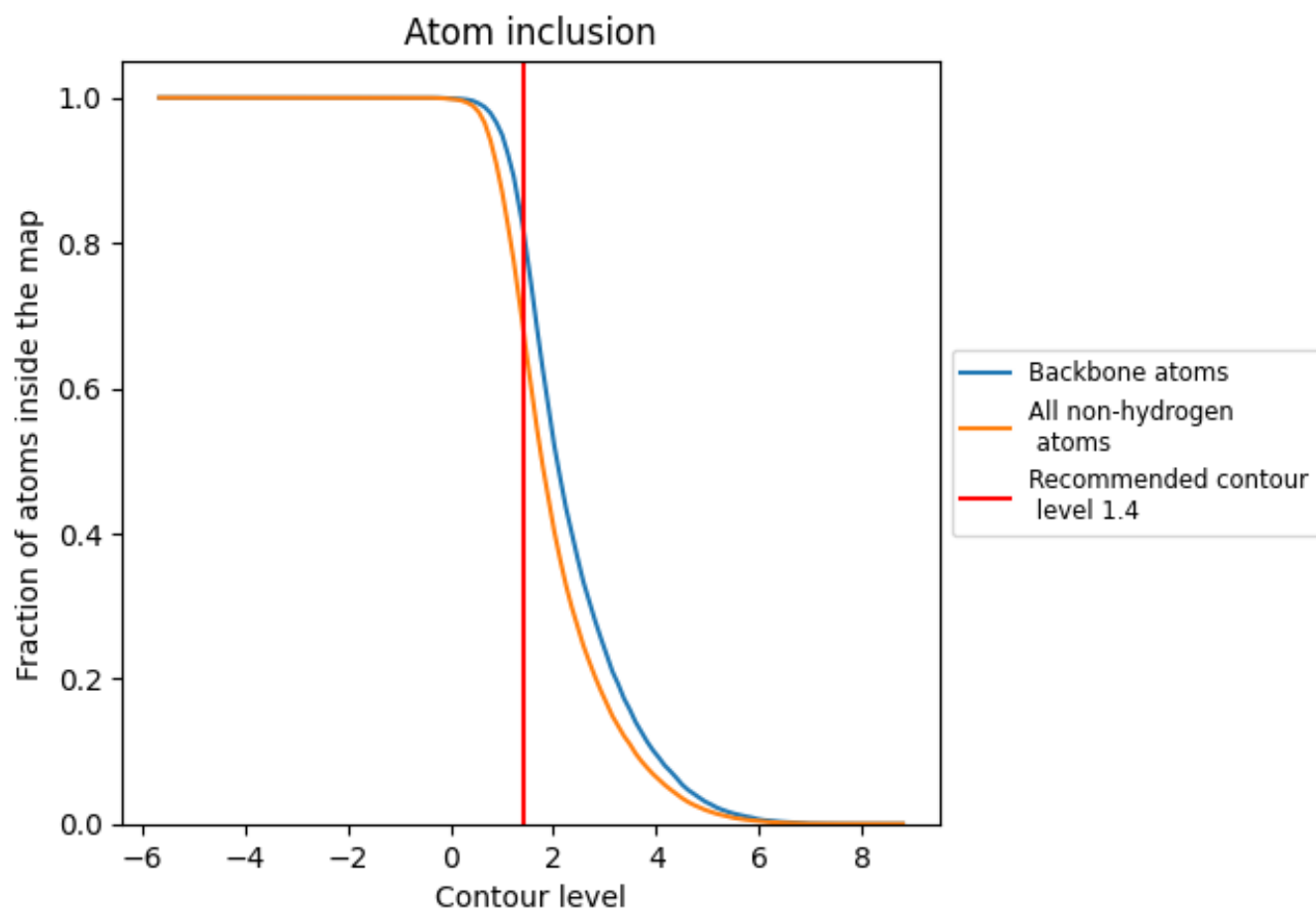
At the recommended contour level, 83% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6890	0.3470
A	0.7851	0.4020
B	0.6652	0.3280
C	0.6427	0.3040
D	0.7219	0.3510
E	0.4868	0.2720
F	0.7258	0.3650
G	0.7021	0.3580
H	0.7820	0.3940

1.0

0.0
<0.0