Full wwPDB EM Validation Report (i)

Mar 20, 2024 – 06:01 AM JST

PDB ID	:	7BST
EMDB ID	:	EMD-30166
Title	:	EcoR124I-Ocr in the Intermediate State
Authors	:	Gao, Y.; Gao, P.
Deposited on	:	2020-03-31
Resolution	:	4.37 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

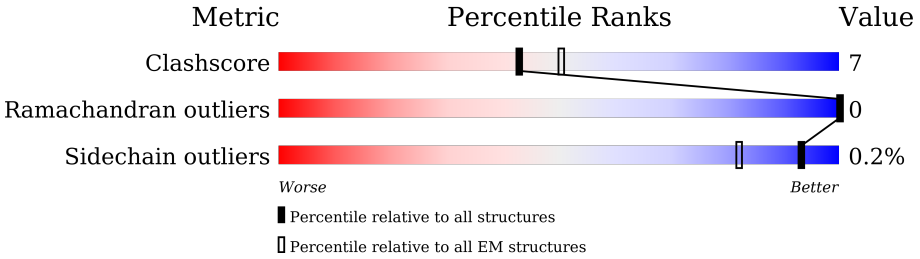
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.37 Å.

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



Metric	Whole archive (#Entries)	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	B	1038	78% 16% 6%
1	C	1038	78% 17% •
2	D	520	72% 18% 9%
2	E	520	68% 22% • 9%
3	F	117	76% 15% 9%
3	G	117	75% 15% 9%
4	A	404	48% 75% 19% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28266 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 Type I restriction enzyme R Protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	975	7906	5022	1343	1524	17	0	0
1	C	992	8042	5108	1363	1554	17	0	0

- Molecule 2 is a protein called Type I restriction enzyme EcoR124II M protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	472	3732	2390	623	713	6	0	0
2	E	473	3735	2391	623	715	6	0	0

- Molecule 3 is a protein called Overcome classical restriction gp0.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	106	876	550	136	185	5	0	0
3	G	106	876	550	136	185	5	0	0

- Molecule 4 is a protein called Type-1 restriction enzyme EcoR124II specificity protein.

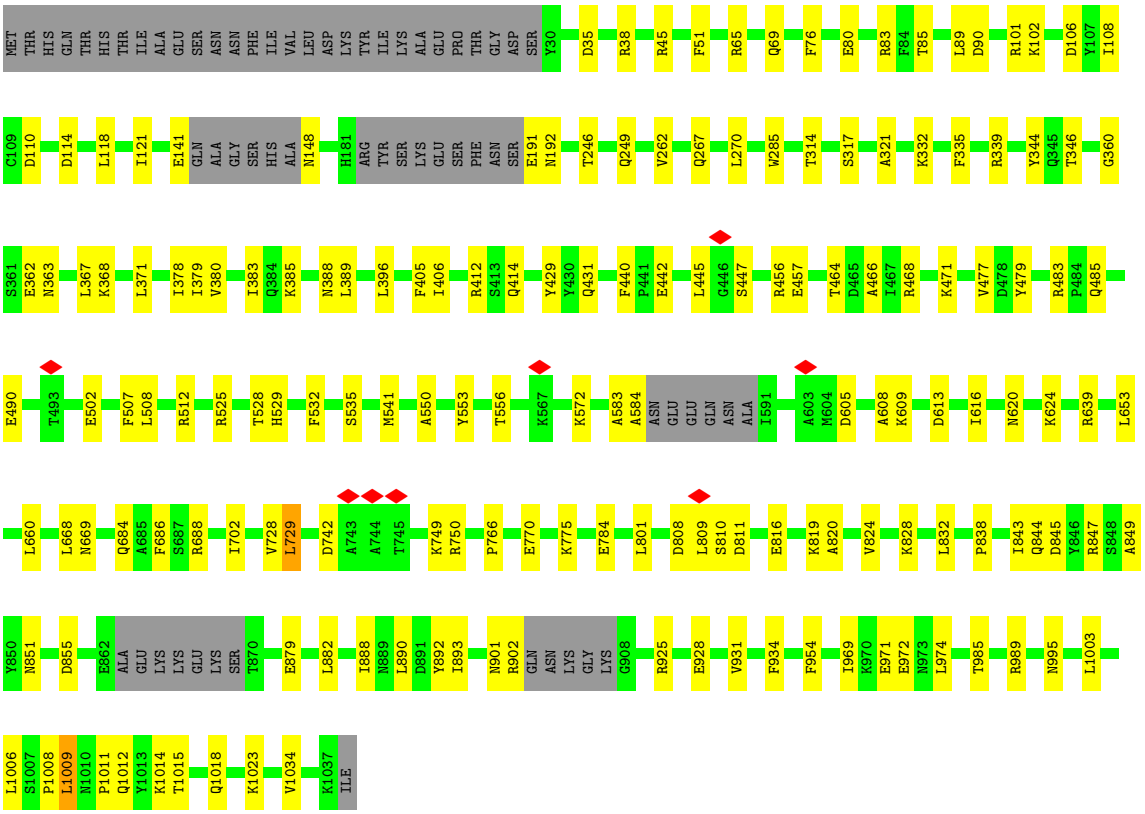
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	384	3099	2001	505	585	8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

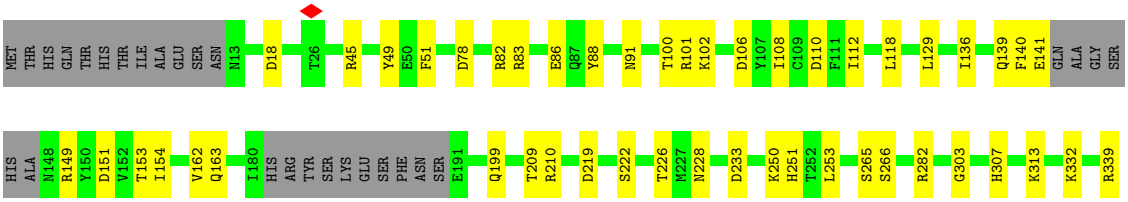
• Molecule 1: Type I restriction enzyme R Protein

Chain B:



• Molecule 1: Type I restriction enzyme R Protein

Chain C:



K340 D341 L342 T346 M347 K348 Q351 S354 S357 E362 L367 L371 N376 I379 V380 L389 M390 L396 V403 V404 K425 Y430 F454 D465 R468 L473 K476 V477 D478 R483 F486 L489 E490 T491 E492 L498

Q504 F507 L508 R512 I516 R525 R530 G537 L542 A543 A550 K551 A552 Y553 Y554 K572 I579 F580 S581 F582 A583 T598 A608 F611 S628 I629 D630 Y638 R639 A642 K646 N647 Q648 I654 L660 T667 L668 N669 V673

N676 L677 R678 L682 F686 S687 R688 T689 N690 K697 I702 V703 T704 F705 R706 I713 I716 T724 K725 T734 M737 F740 K749 L786 R787 L809 S810 D811 P812 V815 E816 K819 D826 R841 Q844 R847 E860 K861 GLU

ALA GLU LYS LYS GLU LYS SER THR THR D872 E879 L882 L890 I893 N901 R902 GLN ASN LYS GLY LYS G908 R916 I917 I918 E928 Q958 I969 K970 E971 E972 N973 L974 N975 A979 R989 E990 Y991 A992 T993 E994 E998 L999 N1000 E1001 T1002 L1009

N1010 P1011 Q1012 Y1013 K1014 K1017 K1023 I1024 V1025 G1035 GLY LYS ILE

- Molecule 2: Type I restriction enzyme EcoR124II M protein

Chain D:

MET LYS MET THR SER ILE GLN GLN ARG A10 H13 W17 R43 E54 A55 GLY ASP ASP SER ILE CYS TYR ALA LYS LEU ASP ASP SER VAL ILE THR D72 D73 I86 S89 Q90 N102 D103 R104 L105 N106 I112 F113 E117 A120 I129 K130 G131

F136 R142 L143 G144 V147 K150 R153 V161 E162 G167 ASP PHE ASN GLU HIS GLN I174 A190 ASN ALA GLY LYS SER GLY GLY E198 T201 V220 N221 Y224 D225 S230 G231 L234 F241 H244 Q253 M265 N266 D275 T286 E287

P288 R291 D292 I299 N302 D313 T316 L317 I318 N319 D320 G327 L341 A353 F362 K370 I371 R372 Q373 D377 N378 N379 T383 V384 A388 P389 N390 T395 L402 V403 L404 K408 T411 N412 V413 Q414 S419 E420 L421 F422 K423 K424

E425 V449 L452 V456 N467 L468 S471 S472 Y473 V474 R480 E481 I485 A486 N489 T494 K498 I506 V510 ALA GLU ILE GLU GLY CYS GLU VAL GLN LYS

- Molecule 2: Type I restriction enzyme EcoR124II M protein

Chain E:

MET LYS MET THR SER ILE GLN GLN ARG A10 H13 I16 W17 N21 G29 K33 R43 E54 A55 GLY ASP ASP SER ILE CYS TYR ALA LYS LEU ASP ASP SER VAL ILE T71 D72 K80 P88 S89 Q90 L91 A96 N100 T101 N102 D108 S111

I112 F113 V114 A115 I116 E117 S118 S119 A120 Y123 P124 S125 E126 I129 K130 G131 L132 F136 D149 R153 L154 V161 L164 G167 ASP PHE ASN GLU HIS GLN I174 G178 D179 A180 Y181 E182 F183 L184 I185 A190 ASN ALA GLY LYS SER GLY GLY E198 Q217

V220 N221 K222 I223 Y224 A227 S230 F250 F251 L262 M265 N266 Y274 D275 K276 F277 T284 K294 D297 A298 I299 I310 G311 S312 D313 L317 D320 K332 S333 K334 A349 K350 G351 R352 A353 V356 C357 F358 I361 F362 Y363 R364

Q369 Q373 D377 V381 E382 T383 P389 N390 T395 N400 I401 L404 S405 K406 T411 N412 V413 S419 E420 K446 H451 V456 E459 V462 L468 S469 V470 S471 S472 Y473 V474 E475 A476 K477 D478 N479 R480 E481 I485 N489 T494

K498 R503 I506 I509 V510 ALA GLU ILE GLU GLY CYS GLU VAL GLN LYS

- Molecule 3: Overcome classical restriction gp0.3

Chain F: 76% 15% 9%

MET ALA MET SER ASN M5 T6 Y7 L18 R28 I37 M71 T74 K75 D76 I80 I91 D92 L93 W94 A97 L100 E103 Y104 L105 E106 E107 E110 TYR GLU GLU ASP GLU GLU

- Molecule 3: Overcome classical restriction gp0.3

Chain G: 75% 15% 9%

MET ALA MET SER ASN M5 T6 Y7 L18 R28 L33 I37 S68 M71 T74 K75 D76 I80 I91 D92 L93 W94 A97 L100 E103 Y104 L105 E106 E109 E110 TYR GLU GLU ASP GLU GLU

- Molecule 4: Type-1 restriction enzyme EcoR124II specificity protein

Chain A: 48% 75% 19% 5%

MET SER GLU MET SER TYR LEU GLU LYS LEU LEU ASP G13 V14 E15 V16 E17 W18 L19 P20 L21 G22 E23 P30 T31 K32 Y33 L34 V35 K36 A37 K38 D39 Y40 H41 D42 T43 Y44 T45 I46 P47 V48 L49 T50 A51 G52 K53 T54 F55 I56 L57 G58 Y59 T60 N61 E62 T63 H64 G65

I66 Y67 Q68 A69 A72 P73 V74 I75 I76 F77 D78 D79 F80 T81 T82 A83 N84 K85 W86 V87 D88 F89 D90 F91 K92 A93 K94 S95 S96 A97 M98 K99 M100 V101 D106 N107 K108 T109 L110 V114 Y115 Y116 W117 L118 N119 T120 L121 P122 S123 E124 F125 A126 E127 G128 D129 H130 K131

R132 Q133 W134 N137 Q140 K141 K142 I143 P144 I145 P146 C147 P148 D149 N150 P151 E152 K153 A156 R163 I164 L165 D166 K167 F168 L171 L179 Y188 D191 Q192 L193 L194 S195 F196 K197 E198 G199 E200 V201 E202 W203 L206 G207 E208 I209 G210 K211 W212 Y213 G216

T217 P218 S219 K220 N221 K222 I223 E224 F225 W226 E227 N228 G229 S230 I231 P232 W233 T234 S235 P236 K237 D238 N239 G240 R241 T242 L243 V244 D245 S246 S247 E248 D249 Y250 I251 T252 E253 E254 A255 V256 L257 H258 S259 S260 T261 K262 L263 I264 P265 A266 N267 S268 I269 I277 L278 D279 K280 V281 L282

P283 S284 A285 L286 I287 T292 L293 D296 A299 V300 I301 P302 H303 E304 N305 I306 L307 Y310 R318 G319 S320 D321 I322 L323 R324 A325 A326 K327 K328 T329 G330 G331 S335 I336 D337 S338 K339 K340 L341 F342 S343 F344 K345 I351 N352 Q355 V358 D362 K363

T366 S370 I371 T372 L375 P376 R377 K384 Y388 Y389 R390 S395 F396 PRO LYS PRO GLU THR VAL SER ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64585	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 ($e^-/Å^2$)	60, 60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.241	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	367.2, 367.2, 367.2	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	B	0.29	0/8050	0.55	5/10852 (0.0%)
1	C	0.29	0/8189	0.52	0/11043
2	D	0.33	0/3809	0.67	0/5158
2	E	0.30	0/3812	0.65	2/5164 (0.0%)
3	F	0.26	0/893	0.47	0/1213
3	G	0.26	0/893	0.47	0/1213
4	A	0.30	0/3173	0.67	4/4301 (0.1%)
All	All	0.30	0/28819	0.58	11/38944 (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	C	0	1
2	D	0	3
2	E	0	3
4	A	0	5
All	All	0	12

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1009	LEU	CA-CB-CG	8.21	134.19	115.30
4	A	171	LEU	CA-CB-CG	7.01	131.42	115.30
4	A	194	LEU	CA-CB-CG	6.36	129.94	115.30
1	B	1003	LEU	C-N-CD	-5.79	107.87	120.60
1	B	729	LEU	CA-CB-CG	5.64	128.28	115.30
1	B	845	ASP	CB-CG-OD1	5.56	123.31	118.30
2	E	357	CYS	C-N-CA	5.54	135.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1008	PRO	C-N-CA	5.19	134.68	121.70
2	E	91	LEU	CA-CB-CG	5.08	126.99	115.30
4	A	278	LEU	CA-CB-CG	5.06	126.94	115.30
4	A	282	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	191	ASP	Peptide
4	A	303	HIS	Peptide
4	A	366	THR	Peptide
4	A	72	ALA	Peptide
4	A	94	LYS	Peptide
1	C	678	ARG	Peptide
2	D	131	GLY	Peptide
2	D	313	ASP	Peptide
2	D	474	VAL	Peptide
2	E	274	TYR	Peptide
2	E	294	LYS	Peptide
2	E	474	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7906	0	7718	97	0
1	C	8042	0	7846	110	0
2	D	3732	0	3652	62	0
2	E	3735	0	3648	75	0
3	F	876	0	800	9	0
3	G	876	0	800	10	0
4	A	3099	0	3118	46	0
All	All	28266	0	27582	395	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 7.

All (395) 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:C:682:LEU:CD1	1:C:686:PHE:CE2	2.34	1.09
1:C:682:LEU:HD12	1:C:686:PHE:CE2	1.99	0.98
1:C:682:LEU:CD1	1:C:686:PHE:CZ	2.57	0.88
2:E:13:HIS:O	2:E:17:TRP:HB2	1.77	0.84
2:D:13:HIS:O	2:D:17:TRP:HB2	1.87	0.75
2:D:373:GLN:O	2:D:377:ASP:HB2	1.87	0.74
1:C:971:GLU:HG3	1:C:972:GLU:HG2	1.72	0.71
2:E:29:GLY:O	2:E:33:LYS:HB2	1.91	0.70
1:C:682:LEU:HD13	1:C:686:PHE:CZ	2.27	0.69
1:C:504:GLN:HA	1:C:508:LEU:HB2	1.75	0.69
4:A:69:ALA:HB3	4:A:92:LYS:H	1.58	0.69
2:E:334:LYS:HB3	2:E:364:ARG:HH21	1.58	0.68
2:D:224:TYR:HB3	2:D:299:ILE:HG22	1.77	0.67
1:B:108:ILE:HA	1:B:121:ILE:O	1.96	0.66
1:C:682:LEU:HD11	1:C:686:PHE:CZ	2.30	0.64
2:E:227:ALA:H	2:E:284:THR:HG21	1.62	0.64
1:B:405:PHE:HB2	1:B:431:GLN:HA	1.79	0.64
1:B:985:THR:O	1:B:989:ARG:HB2	1.98	0.63
2:E:178:GLY:O	2:E:181:TYR:HB3	1.99	0.63
2:D:136:PHE:HZ	2:D:265:MET:HB3	1.65	0.62
4:A:372:THR:HA	4:A:377:ARG:HD3	1.81	0.62
2:D:129:ILE:HG23	2:D:130:LYS:HG3	1.80	0.62
1:B:766:PRO:HB3	1:B:849:ALA:HB2	1.82	0.62
1:C:1012:GLN:HG3	1:C:1014:LYS:H	1.64	0.62
2:E:185:ILE:HD11	2:E:262:LEU:HD13	1.81	0.62
1:C:129:LEU:HD11	1:C:251:HIS:HA	1.82	0.61
1:C:110:ASP:HB3	1:C:118:LEU:HD11	1.83	0.60
1:C:45:ARG:HH11	1:C:51:PHE:HB3	1.65	0.60
4:A:82:THR:HG21	4:A:134:TRP:HB2	1.83	0.60
1:B:335:PHE:HB2	1:B:378:ILE:HD11	1.82	0.60
1:B:246:THR:O	1:B:249:GLN:NE2	2.35	0.60
2:E:481:GLU:HG2	4:A:384:LYS:HB3	1.82	0.60
1:B:1012:GLN:HE22	1:B:1015:THR:H	1.50	0.60
1:B:995:ASN:ND2	2:D:90:GLN:O	2.35	0.59
4:A:168:PHE:HA	4:A:171:LEU:HG	1.84	0.59
4:A:145:ILE:HG22	4:A:147:CYS:H	1.67	0.59
2:E:481:GLU:HB2	4:A:388:TYR:HB2	1.85	0.59
1:B:477:VAL:HG22	1:B:702:ILE:HB	1.85	0.58
1:C:786:LEU:HB3	1:C:882:LEU:HD11	1.85	0.58
1:B:855:ASP:OD2	1:B:925:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.36	0.58
1:C:473:LEU:H	1:C:690:ASN:HB2	1.69	0.58
4:A:77:PHE:HB2	4:A:84:ASN:HB3	1.85	0.58
4:A:119:ASN:HB3	4:A:390:ARG:HH22	1.68	0.58
1:C:209:THR:O	1:C:228:ASN:ND2	2.36	0.58
1:B:971:GLU:HG3	1:B:972:GLU:HG2	1.86	0.57
1:C:233:ASP:O	1:C:468:ARG:NH2	2.37	0.57
1:C:819:LYS:NZ	1:C:826:ASP:OD1	2.35	0.57
3:G:68:SER:H	4:A:237:LYS:HD3	1.69	0.57
1:B:851:ASN:HB3	1:B:925:ARG:HH22	1.70	0.57
1:C:815:VAL:HG12	1:C:819:LYS:HE2	1.86	0.57
2:E:217:GLN:O	2:E:222:LYS:NZ	2.37	0.57
2:E:136:PHE:HZ	2:E:265:MET:HB3	1.69	0.57
4:A:85:LYS:HD2	4:A:118:LEU:HD12	1.85	0.57
1:B:101:ARG:HB2	1:B:267:GLN:HE22	1.70	0.56
2:E:224:TYR:HB3	2:E:299:ILE:HG22	1.86	0.56
2:E:356:VAL:HG12	2:E:401:ILE:HG12	1.88	0.56
1:B:35:ASP:OD1	1:B:38:ARG:NH1	2.37	0.56
1:C:639:ARG:NH2	2:E:320:ASP:O	2.37	0.56
2:E:88:PRO:HA	2:E:91:LEU:HB3	1.86	0.56
4:A:370:SER:HB2	4:A:371:ILE:HG13	1.87	0.56
1:C:676:ASN:OD1	1:C:706:ARG:NH1	2.39	0.56
2:E:349:ALA:HA	2:E:406:LYS:HB2	1.88	0.56
1:C:787:ARG:NH2	1:C:879:GLU:OE2	2.39	0.55
1:C:542:LEU:HD23	1:C:654:ILE:HG12	1.87	0.55
1:C:673:VAL:HB	1:C:704:THR:HG22	1.88	0.55
1:C:465:ASP:OD1	1:C:468:ARG:NH2	2.40	0.55
2:E:43:ARG:NH1	2:E:161:VAL:O	2.40	0.55
1:B:879:GLU:HB3	1:B:882:LEU:HB2	1.89	0.55
1:B:888:ILE:HG23	1:B:892:TYR:HB3	1.89	0.55
1:B:750:ARG:NH2	1:B:784:GLU:OE1	2.40	0.55
2:E:13:HIS:O	2:E:17:TRP:CB	2.52	0.55
4:A:75:ILE:HD11	4:A:86:TRP:HB2	1.89	0.55
1:C:682:LEU:HD11	1:C:686:PHE:CE2	2.34	0.54
1:C:83:ARG:NH2	1:C:112:ILE:O	2.41	0.54
2:E:179:ASP:O	2:E:182:GLU:HB3	2.08	0.54
4:A:234:ILE:HB	4:A:293:LEU:HB3	1.90	0.54
1:C:108:ILE:HB	2:D:147:VAL:HG11	1.89	0.54
1:C:530:ARG:HE	1:C:537:GLY:HA3	1.71	0.54
2:E:382:GLU:HG2	2:E:383:THR:HG23	1.90	0.54
1:B:363:ASN:O	1:B:385:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:18:LEU:HD22	3:F:93:LEU:HD22	1.90	0.53
1:B:925:ARG:O	1:B:928:GLU:HB3	2.09	0.53
1:B:931:VAL:O	1:B:934:PHE:HB3	2.08	0.53
1:C:1014:LYS:HB3	1:C:1017:LYS:HE2	1.89	0.53
1:C:543:ALA:HB3	1:C:673:VAL:HA	1.91	0.53
4:A:67:TYR:H	4:A:94:LYS:HD3	1.73	0.53
1:B:528:THR:HA	1:B:669:ASN:HD21	1.74	0.53
1:B:770:GLU:O	1:B:775:LYS:NZ	2.41	0.53
1:C:716:ILE:HD13	1:C:725:LYS:HB3	1.89	0.53
2:E:381:VAL:HA	2:E:404:LEU:HG	1.90	0.53
4:A:79:ASP:OD1	4:A:133:GLN:NE2	2.42	0.53
1:B:80:GLU:HG2	1:B:83:ARG:HH21	1.74	0.52
3:G:18:LEU:HD22	3:G:93:LEU:HD22	1.90	0.52
1:B:89:LEU:O	1:B:102:LYS:NZ	2.42	0.52
2:D:383:THR:HG22	2:D:413:VAL:HG23	1.92	0.52
1:B:742:ASP:H	1:B:749:LYS:HG3	1.73	0.52
2:E:117:GLU:HA	2:E:120:ALA:HB3	1.92	0.52
4:A:358:VAL:O	4:A:362:ASP:HB2	2.10	0.52
1:C:101:ARG:NH1	1:C:106:ASP:OD2	2.42	0.52
1:C:992:ALA:HB3	1:C:1025:VAL:HG12	1.91	0.52
1:C:581:SER:OG	1:C:598:THR:O	2.28	0.51
2:E:411:THR:OG1	2:E:456:VAL:O	2.28	0.51
1:B:620:ASN:HA	1:B:624:LYS:H	1.75	0.51
2:D:54:GLU:OE2	2:D:72:ASP:N	2.44	0.51
2:D:372:ARG:HH12	2:D:468:LEU:HB2	1.74	0.51
2:E:43:ARG:HH12	2:E:164:LEU:HB2	1.74	0.51
1:C:139:GLN:NE2	1:C:149:ARG:O	2.43	0.51
1:C:153:THR:OG1	1:C:163:GLN:NE2	2.43	0.51
1:C:219:ASP:HA	1:C:222:SER:HB3	1.93	0.51
1:C:713:ILE:HA	1:C:716:ILE:HD12	1.93	0.51
1:B:483:ARG:HD3	1:B:485:GLN:HB3	1.92	0.51
1:B:335:PHE:HB3	1:B:380:VAL:HA	1.93	0.51
2:D:43:ARG:NH1	2:D:161:VAL:O	2.43	0.51
1:B:525:ARG:HH22	1:B:572:LYS:H	1.58	0.51
1:B:45:ARG:HH11	1:B:51:PHE:HB3	1.76	0.51
1:C:210:ARG:NH1	1:C:226:THR:O	2.43	0.50
1:C:812:PRO:O	1:C:816:GLU:HB2	2.11	0.50
2:E:131:GLY:O	2:E:274:TYR:OH	2.23	0.50
1:C:682:LEU:HD13	1:C:686:PHE:CE2	2.34	0.50
1:B:69:GLN:HE21	1:B:76:PHE:HD2	1.57	0.50
4:A:265:PRO:HD2	4:A:301:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:HD3	1:B:360:GLY:HA3	1.92	0.50
2:E:485:ILE:O	2:E:489:ASN:ND2	2.45	0.50
1:B:550:ALA:HA	1:B:553:TYR:HD2	1.77	0.50
2:D:411:THR:HG23	2:D:413:VAL:HG13	1.93	0.50
4:A:269:ILE:HG13	4:A:300:VAL:HB	1.94	0.50
1:B:529:HIS:ND1	1:B:820:ALA:O	2.35	0.50
1:B:819:LYS:HA	1:B:824:VAL:HB	1.94	0.49
1:C:507:PHE:O	1:C:512:ARG:NH1	2.44	0.49
1:C:404:VAL:HG22	1:C:430:TYR:HB2	1.92	0.49
4:A:30:PRO:HD3	4:A:99:LYS:HA	1.94	0.49
1:B:660:LEU:O	1:B:688:ARG:NH1	2.46	0.49
1:C:139:GLN:HB3	1:C:151:ASP:HB2	1.94	0.49
2:E:390:ASN:OD1	2:E:395:THR:OG1	2.30	0.49
1:C:958:GLN:HE21	1:C:1035:GLY:HA2	1.77	0.49
1:C:136:ILE:HG22	1:C:154:ILE:HG12	1.93	0.49
1:C:648:GLN:HE21	1:C:667:THR:HB	1.78	0.49
1:C:972:GLU:OE2	1:C:1023:LYS:NZ	2.46	0.49
2:E:54:GLU:OE1	2:E:72:ASP:N	2.45	0.49
2:E:353:ALA:HB3	2:E:404:LEU:HB2	1.94	0.49
1:C:390:MET:O	1:C:425:LYS:NZ	2.34	0.49
2:D:241:PHE:HB3	2:D:244:HIS:HB2	1.94	0.49
4:A:229:GLY:HA3	4:A:252:THR:HA	1.95	0.49
1:B:456:ARG:HH12	2:D:319:ASN:HB2	1.78	0.48
1:C:486:PHE:HD1	1:C:489:LEU:HD12	1.78	0.48
2:D:225:ASP:HB2	2:D:234:LEU:HD21	1.94	0.48
2:E:112:ILE:HA	2:E:113:PHE:HA	1.61	0.48
4:A:116:TYR:O	4:A:390:ARG:NH2	2.36	0.48
1:C:969:ILE:HG23	1:C:974:LEU:HB2	1.95	0.48
2:D:320:ASP:OD1	2:D:320:ASP:N	2.47	0.48
2:E:361:ILE:O	4:A:132:ARG:NH1	2.46	0.48
1:B:583:ALA:HA	1:B:584:ALA:HA	1.64	0.48
1:B:684:GLN:O	1:B:688:ARG:NH1	2.47	0.48
2:D:106:ASN:ND2	2:D:162:GLU:OE1	2.47	0.48
2:E:224:TYR:HA	2:E:251:PHE:HB2	1.94	0.48
1:B:141:GLU:OE2	1:B:148:ASN:N	2.47	0.48
1:B:728:VAL:HG12	1:B:729:LEU:HB2	1.96	0.48
1:B:808:ASP:HB3	1:B:811:ASP:HB2	1.96	0.48
2:D:253:GLN:NE2	2:D:287:GLU:O	2.39	0.48
2:E:220:VAL:HG23	2:E:221:ASN:HB3	1.95	0.48
4:A:252:THR:HG22	4:A:254:GLU:H	1.79	0.48
1:B:389:LEU:HD11	1:B:396:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:SER:O	1:C:376:ASN:ND2	2.40	0.48
1:C:994:GLU:HA	1:C:999:LEU:HD23	1.96	0.48
2:D:231:GLY:H	2:D:266:ASN:HD22	1.60	0.48
2:D:384:VAL:HG12	2:D:402:LEU:HG	1.96	0.48
4:A:179:LEU:HD13	4:A:375:LEU:HD22	1.96	0.48
4:A:319:GLY:HA2	4:A:322:ILE:HG12	1.96	0.48
1:C:476:LYS:NZ	1:C:478:ASP:OD1	2.33	0.47
2:E:115:ALA:O	2:E:118:SER:HB3	2.14	0.47
2:D:275:ASP:OD1	2:D:275:ASP:N	2.46	0.47
2:D:286:THR:HG22	2:D:317:LEU:HD11	1.95	0.47
1:B:383:ILE:HG12	1:B:414:GLN:HB3	1.96	0.47
1:B:844:GLN:OE1	1:B:847:ARG:NH1	2.47	0.47
3:F:71:MET:HG3	3:F:80:ILE:HG12	1.97	0.47
1:B:972:GLU:OE2	1:B:1023:LYS:NZ	2.48	0.47
1:C:844:GLN:OE1	1:C:847:ARG:NH1	2.47	0.47
2:E:43:ARG:HB2	2:E:102:ASN:HD22	1.79	0.47
4:A:277:ILE:HG23	4:A:282:LEU:HB3	1.95	0.47
1:B:890:LEU:HD23	1:B:893:ILE:HD12	1.97	0.47
1:B:901:ASN:HA	1:B:902:ARG:HA	1.63	0.47
1:C:554:TYR:HB3	1:C:611:PHE:HZ	1.78	0.47
2:D:390:ASN:OD1	2:D:395:THR:OG1	2.29	0.47
2:E:451:HIS:HE1	2:E:476:ALA:HB2	1.80	0.47
3:F:100:LEU:HA	3:F:103:GLU:HB3	1.97	0.47
1:B:344:TYR:HA	1:B:639:ARG:HH21	1.79	0.47
1:B:362:GLU:O	1:B:388:ASN:ND2	2.48	0.47
2:D:370:LYS:HA	2:D:373:GLN:HB3	1.97	0.47
2:E:29:GLY:O	2:E:33:LYS:CB	2.61	0.47
3:G:71:MET:HG3	3:G:80:ILE:HG12	1.97	0.47
1:B:367:LEU:HD21	1:B:389:LEU:HD22	1.96	0.47
1:B:1014:LYS:O	1:B:1018:GLN:N	2.47	0.47
1:C:86:GLU:O	1:C:91:ASN:ND2	2.48	0.47
1:C:357:SER:HA	1:C:379:ILE:HA	1.95	0.47
2:E:230:SER:OG	2:E:266:ASN:ND2	2.48	0.47
2:E:16:ILE:HG23	2:E:164:LEU:HD22	1.97	0.46
1:B:412:ARG:HH12	1:B:445:LEU:HB2	1.80	0.46
1:C:483:ARG:HH12	1:C:516:ILE:HG13	1.81	0.46
1:C:669:ASN:HB3	1:C:697:LYS:HE3	1.97	0.46
1:B:456:ARG:NH2	2:D:316:THR:OG1	2.47	0.46
2:D:384:VAL:HG23	2:D:414:GLN:HG3	1.96	0.46
2:E:311:GLY:HA2	2:E:313:ASP:HA	1.97	0.46
3:G:100:LEU:HA	3:G:103:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:TRP:HZ3	2:D:327:GLY:H	1.64	0.46
1:C:110:ASP:HB2	2:D:142:ARG:HH21	1.81	0.46
1:B:85:THR:O	1:B:90:ASP:N	2.41	0.46
1:C:367:LEU:HD23	1:C:389:LEU:HD13	1.97	0.46
1:C:734:THR:HA	1:C:737:MET:HB2	1.98	0.46
2:E:451:HIS:CE1	2:E:476:ALA:HB2	2.50	0.46
4:A:19:LEU:HD13	4:A:145:ILE:HB	1.97	0.46
1:B:969:ILE:HD12	1:B:974:LEU:HD22	1.98	0.46
1:C:102:LYS:HA	1:C:106:ASP:HB2	1.97	0.46
3:G:28:ARG:HG2	3:G:105:LEU:HD22	1.98	0.46
3:F:91:ILE:HA	3:F:94:TRP:HD1	1.81	0.46
2:D:419:SER:HA	2:D:420:GLU:HA	1.64	0.46
1:B:405:PHE:HE2	1:B:429:TYR:HB2	1.82	0.45
1:C:140:PHE:HA	1:C:141:GLU:HA	1.74	0.45
1:C:307:HIS:HB2	1:C:313:LYS:HD3	1.98	0.45
1:C:483:ARG:NH2	1:C:490:GLU:OE2	2.48	0.45
1:C:975:ASN:O	1:C:979:ALA:N	2.44	0.45
4:A:233:TRP:HB3	4:A:249:ASP:HB3	1.97	0.45
3:F:28:ARG:HG2	3:F:105:LEU:HD22	1.98	0.45
1:B:529:HIS:O	1:B:535:SER:OG	2.31	0.45
1:C:303:GLY:N	1:C:454:PHE:O	2.49	0.45
2:E:310:ILE:HA	2:E:332:LYS:HG3	1.97	0.45
1:B:541:MET:HG3	1:B:668:LEU:HD11	1.98	0.45
3:G:91:ILE:HA	3:G:94:TRP:HD1	1.81	0.45
4:A:114:VAL:O	4:A:118:LEU:HB2	2.17	0.45
1:C:88:TYR:O	1:C:102:LYS:NZ	2.37	0.45
1:C:357:SER:HB3	1:C:380:VAL:H	1.81	0.45
2:E:129:ILE:HG23	2:E:130:LYS:HG3	1.98	0.45
1:B:532:PHE:HD1	1:B:816:GLU:HG3	1.80	0.45
1:B:824:VAL:HG13	1:B:828:LYS:HB2	1.98	0.45
1:C:18:ASP:OD1	1:C:282:ARG:NH2	2.49	0.45
2:E:116:ILE:O	2:E:120:ALA:N	2.47	0.45
2:E:123:TYR:HA	2:E:126:GLU:HG3	1.99	0.45
1:B:110:ASP:HB2	1:B:118:LEU:HD11	1.98	0.45
1:B:969:ILE:HG23	1:B:974:LEU:HB2	1.98	0.45
2:E:468:LEU:HA	2:E:469:SER:HA	1.64	0.45
3:F:37:ILE:HD11	3:F:97:ALA:HB2	1.99	0.45
4:A:193:LEU:HD23	4:A:194:LEU:HB2	1.99	0.45
2:D:102:ASN:OD1	2:D:106:ASN:ND2	2.50	0.45
2:E:297:ASP:HA	2:E:351:GLY:HA3	1.98	0.45
1:B:368:LYS:HA	1:B:371:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ALA:HB1	1:B:471:LYS:HB2	2.00	0.45
2:D:288:PRO:HG2	2:D:291:ARG:HD2	1.97	0.45
2:E:100:ASN:ND2	2:E:123:TYR:OH	2.50	0.45
4:A:363:LYS:HA	4:A:366:THR:HG22	1.99	0.45
1:C:348:LYS:HA	1:C:351:GLN:HG2	1.97	0.44
1:C:901:ASN:HA	1:C:902:ARG:HA	1.72	0.44
1:C:998:GLU:HA	1:C:1001:GLU:HB2	1.99	0.44
2:D:388:ALA:HB1	2:D:423:LYS:HG2	1.98	0.44
2:D:388:ALA:HB2	2:D:421:LEU:HB3	1.99	0.44
3:G:37:ILE:HD11	3:G:97:ALA:HB2	1.99	0.44
4:A:307:LEU:HD23	4:A:358:VAL:HG11	1.99	0.44
2:D:341:LEU:HD11	2:D:371:ILE:HD12	1.98	0.44
1:C:579:ILE:HD13	1:C:638:TYR:HD1	1.81	0.44
2:D:379:ASN:HD22	2:D:408:LYS:HA	1.83	0.44
2:E:262:LEU:HA	2:E:265:MET:HG2	1.98	0.44
4:A:244:VAL:H	4:A:285:ALA:HB1	1.83	0.44
1:B:314:THR:HG23	1:B:346:THR:HG22	1.98	0.44
1:C:642:ALA:O	1:C:646:LYS:HB2	2.18	0.44
2:D:485:ILE:O	2:D:489:ASN:ND2	2.51	0.44
2:E:54:GLU:O	2:E:71:THR:N	2.49	0.44
2:E:361:ILE:HG13	2:E:364:ARG:HG2	1.99	0.44
1:B:1011:PRO:HA	1:B:1012:GLN:HA	1.75	0.44
2:D:86:ILE:HA	2:D:89:SER:HB3	2.00	0.44
2:D:112:ILE:HA	2:D:113:PHE:HA	1.66	0.44
1:B:332:LYS:HD2	1:B:379:ILE:HD11	1.99	0.44
1:B:686:PHE:HE1	1:B:702:ILE:HG21	1.82	0.44
1:C:809:LEU:HA	1:C:810:SER:HA	1.77	0.44
1:B:925:ARG:O	1:B:928:GLU:CB	2.65	0.44
1:C:339:ARG:HA	1:C:340:LYS:HA	1.73	0.44
1:C:389:LEU:HD11	1:C:396:LEU:HD11	1.99	0.44
4:A:64:HIS:HB2	4:A:66:ILE:HG23	1.98	0.44
1:B:507:PHE:HA	1:B:512:ARG:HH22	1.83	0.44
1:B:954:PHE:HD1	1:B:1034:VAL:HG23	1.82	0.43
2:D:86:ILE:O	2:D:90:GLN:N	2.47	0.43
2:E:317:LEU:HA	2:E:320:ASP:HB3	2.00	0.43
2:E:419:SER:HA	2:E:420:GLU:HA	1.69	0.43
2:D:481:GLU:HB2	4:A:188:TYR:HB2	1.99	0.43
3:F:74:THR:HG23	3:F:76:ASP:H	1.83	0.43
1:C:478:ASP:N	1:C:702:ILE:O	2.45	0.43
2:D:220:VAL:HA	2:D:221:ASN:HA	1.52	0.43
1:B:321:ALA:HB1	1:B:378:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:362:PHE:HD2	2:E:363:TYR:HD1	1.66	0.43
1:B:65:ARG:NH2	1:B:76:PHE:O	2.50	0.43
4:A:95:SER:N	4:A:98:MET:SD	2.88	0.43
4:A:194:LEU:HD21	4:A:310:TYR:HE1	1.84	0.43
2:D:486:ALA:HA	2:D:489:ASN:HD22	1.83	0.43
2:E:33:LYS:HE2	2:E:33:LYS:HB3	1.92	0.43
1:C:100:THR:HG23	1:C:199:GLN:HE22	1.84	0.43
1:C:1009:LEU:O	1:C:1014:LYS:NZ	2.46	0.43
4:A:213:TYR:HD2	4:A:264:ILE:HG22	1.84	0.43
1:B:440:PHE:HB3	1:B:442:GLU:H	1.83	0.43
1:B:477:VAL:H	1:B:729:LEU:HD11	1.83	0.43
1:C:78:ASP:O	1:C:82:ARG:HB2	2.18	0.43
1:C:1009:LEU:HD12	1:C:1011:PRO:HG2	1.99	0.43
2:D:372:ARG:NH2	2:D:467:ASN:O	2.51	0.43
1:C:812:PRO:O	1:C:816:GLU:CB	2.67	0.43
2:D:117:GLU:HA	2:D:120:ALA:HB3	2.01	0.43
1:B:479:TYR:OH	1:B:490:GLU:O	2.37	0.42
1:C:362:GLU:N	3:F:107:GLU:OE2	2.41	0.42
2:D:129:ILE:HA	2:D:130:LYS:HA	1.79	0.42
2:E:275:ASP:N	2:E:275:ASP:OD1	2.51	0.42
2:D:13:HIS:O	2:D:17:TRP:CB	2.62	0.42
2:D:471:SER:HA	2:D:472:SER:HA	1.79	0.42
1:B:262:VAL:HB	1:B:270:LEU:HB2	2.01	0.42
2:D:54:GLU:OE2	2:D:73:ASP:N	2.44	0.42
2:E:459:GLU:HA	2:E:462:VAL:HG13	2.00	0.42
3:G:74:THR:HG23	3:G:76:ASP:H	1.83	0.42
2:D:102:ASN:O	2:D:106:ASN:ND2	2.52	0.42
2:D:103:ASP:HB3	2:D:104:ARG:HH21	1.85	0.42
2:D:449:VAL:HB	2:D:452:LEU:HD22	2.00	0.42
1:B:457:GLU:O	2:D:319:ASN:ND2	2.52	0.42
1:B:1006:LEU:HD12	1:B:1009:LEU:HD11	2.01	0.42
2:D:201:THR:OG1	2:D:302:ASN:ND2	2.50	0.42
2:E:21:ASN:HD21	2:E:183:PHE:HE2	1.68	0.42
4:A:233:TRP:O	4:A:247:SER:OG	2.30	0.42
1:B:191:GLU:HA	1:B:192:ASN:HA	1.84	0.42
1:C:162:VAL:HG21	1:C:253:LEU:HD21	2.01	0.42
1:C:332:LYS:O	1:C:403:VAL:HA	2.20	0.42
2:E:222:LYS:HG3	2:E:298:ALA:HB3	2.01	0.42
4:A:94:LYS:O	4:A:96:SER:N	2.46	0.42
4:A:355:GLN:HA	4:A:358:VAL:HG12	2.02	0.42
1:B:541:MET:HG2	1:B:653:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ILE:HB	1:C:162:VAL:HB	2.01	0.42
1:B:412:ARG:HH21	1:B:447:SER:HB2	1.85	0.42
2:D:144:GLY:HA3	2:D:150:LYS:HE2	2.01	0.42
2:E:250:PHE:H	2:E:277:PHE:HD1	1.67	0.42
1:C:740:PHE:H	1:C:749:LYS:HB2	1.85	0.42
1:C:890:LEU:HD23	1:C:893:ILE:HD12	2.02	0.42
1:C:265:SER:HA	1:C:266:SER:HA	1.59	0.41
2:D:411:THR:OG1	2:D:456:VAL:O	2.38	0.41
2:E:363:TYR:HB2	2:E:369:GLN:HB2	2.02	0.41
1:B:317:SER:HB2	1:B:406:ILE:HG21	2.01	0.41
1:C:525:ARG:NH2	1:C:572:LYS:O	2.50	0.41
1:C:841:ARG:HE	1:C:916:ARG:HH21	1.68	0.41
1:B:76:PHE:HD1	1:B:80:GLU:HB3	1.85	0.41
1:B:502:GLU:HG3	1:B:508:LEU:HD11	2.01	0.41
1:B:809:LEU:HA	1:B:810:SER:HA	1.71	0.41
1:C:342:LEU:O	1:C:346:THR:OG1	2.31	0.41
1:C:1009:LEU:HD21	1:C:1012:GLN:HE21	1.84	0.41
2:D:144:GLY:HA2	2:D:153:ARG:HH12	1.84	0.41
2:E:389:PRO:HA	2:E:390:ASN:HA	1.69	0.41
4:A:203:TRP:HB3	4:A:345:LYS:HB3	2.02	0.41
1:B:605:ASP:O	1:B:609:LYS:N	2.41	0.41
1:C:628:SER:OG	1:C:630:ASP:OD1	2.36	0.41
2:D:230:SER:OG	2:D:231:GLY:N	2.54	0.41
2:D:362:PHE:O	2:D:467:ASN:ND2	2.54	0.41
2:E:90:GLN:OE1	2:E:130:LYS:N	2.53	0.41
1:B:838:PRO:HG2	1:B:843:ILE:HD11	2.01	0.41
1:C:550:ALA:HA	1:C:553:TYR:HD2	1.85	0.41
2:E:217:GLN:NE2	2:E:350:LYS:O	2.53	0.41
1:C:677:LEU:HB2	1:C:682:LEU:HD22	2.03	0.41
2:E:469:SER:HB2	2:E:473:TYR:CZ	2.56	0.41
1:B:605:ASP:H	1:B:608:ALA:HB3	1.86	0.41
1:B:801:LEU:HD13	1:B:832:LEU:HD12	2.01	0.41
2:E:358:PHE:O	2:E:400:ASN:ND2	2.53	0.41
1:C:551:LYS:HD3	1:C:608:ALA:HA	2.02	0.41
1:C:918:ILE:HD13	1:C:928:GLU:HA	2.02	0.41
1:C:989:ARG:NE	1:C:991:TYR:O	2.50	0.41
2:E:108:ASP:HB3	2:E:111:SER:HB3	2.03	0.41
1:B:613:ASP:HA	1:B:616:ILE:HD12	2.03	0.41
1:C:332:LYS:HE2	1:C:371:LEU:HD23	2.02	0.41
1:C:660:LEU:O	1:C:688:ARG:NH1	2.44	0.41
2:D:353:ALA:HB3	2:D:404:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:494:THR:O	2:D:498:LYS:HD2	2.21	0.41
2:E:113:PHE:HE2	2:E:115:ALA:HB3	1.86	0.41
2:E:114:VAL:HG23	2:E:154:LEU:HD13	2.03	0.41
2:E:149:ASP:OD2	2:E:153:ARG:NH2	2.52	0.41
2:E:222:LYS:HA	2:E:223:ILE:HA	1.89	0.41
2:E:413:VAL:HG21	2:E:446:LYS:HZ2	1.85	0.41
2:E:494:THR:O	2:E:498:LYS:HD2	2.21	0.41
1:C:49:TYR:HE1	1:C:250:LYS:HB2	1.86	0.41
1:C:492:GLU:HB3	1:C:498:LEU:HD21	2.03	0.41
1:C:716:ILE:HG23	1:C:724:THR:HB	2.03	0.41
4:A:46:ILE:HG22	4:A:59:TYR:H	1.86	0.41
1:B:69:GLN:NE2	1:B:76:PHE:H	2.19	0.40
1:C:860:GLU:HA	1:C:861:LYS:HE2	2.02	0.40
2:E:471:SER:HA	2:E:472:SER:HA	1.73	0.40
3:G:33:LEU:HD23	3:G:33:LEU:HA	1.89	0.40
4:A:74:VAL:HG23	4:A:101:VAL:HB	2.02	0.40
1:B:80:GLU:OE2	1:B:114:ASP:N	2.51	0.40
3:F:7:TYR:OH	3:F:92:ASP:OD2	2.29	0.40
1:C:998:GLU:O	1:C:1002:THR:N	2.54	0.40
2:D:292:ASP:OD1	2:D:292:ASP:N	2.54	0.40
2:E:373:GLN:O	2:E:377:ASP:HB2	2.22	0.40
3:G:7:TYR:OH	3:G:92:ASP:OD2	2.29	0.40
4:A:209:ILE:H	4:A:209:ILE:HG13	1.77	0.40
1:B:464:THR:O	1:B:468:ARG:HB2	2.21	0.40
1:C:582:PHE:CD1	1:C:583:ALA:HB2	2.56	0.40
2:D:422:PHE:HE2	2:D:425:GLU:HG2	1.86	0.40
2:E:96:ALA:HB2	2:E:124:PRO:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	963/1038 (93%)	897 (93%)	66 (7%)	0	100	100
1	C	982/1038 (95%)	898 (91%)	84 (9%)	0	100	100
2	D	464/520 (89%)	385 (83%)	79 (17%)	0	100	100
2	E	465/520 (89%)	389 (84%)	76 (16%)	0	100	100
3	F	104/117 (89%)	102 (98%)	2 (2%)	0	100	100
3	G	104/117 (89%)	102 (98%)	2 (2%)	0	100	100
4	A	382/404 (95%)	333 (87%)	49 (13%)	0	100	100
All	All	3464/3754 (92%)	3106 (90%)	358 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	847/927 (91%)	846 (100%)	1 (0%)	93	97
1	C	862/927 (93%)	861 (100%)	1 (0%)	93	97
2	D	399/439 (91%)	398 (100%)	1 (0%)	92	95
2	E	399/439 (91%)	397 (100%)	2 (0%)	88	93
3	F	95/105 (90%)	95 (100%)	0	100	100
3	G	95/105 (90%)	95 (100%)	0	100	100
4	A	344/364 (94%)	344 (100%)	0	100	100
All	All	3041/3306 (92%)	3036 (100%)	5 (0%)	93	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	556	THR
1	C	682	LEU
2	D	291	ARG
2	E	132	LEU
2	E	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	GLN
1	B	91	ASN
1	B	267	GLN
1	B	370	ASN
1	B	376	ASN
1	B	388	ASN
1	B	622	HIS
1	B	648	GLN
1	B	924	ASN
1	B	1000	ASN
1	C	69	GLN
1	C	91	ASN
1	C	163	GLN
1	C	622	HIS
1	C	635	GLN
1	C	958	GLN
1	C	995	ASN
1	C	1012	GLN
2	D	21	ASN
2	D	106	ASN
2	D	319	ASN
2	D	400	ASN
2	D	489	ASN
2	E	21	ASN
2	E	100	ASN
2	E	102	ASN
2	E	379	ASN
2	E	451	HIS
2	E	467	ASN
2	E	489	ASN
3	F	21	ASN
3	F	43	ASN
3	G	43	ASN
4	A	133	GLN
4	A	313	HIS
4	A	354	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

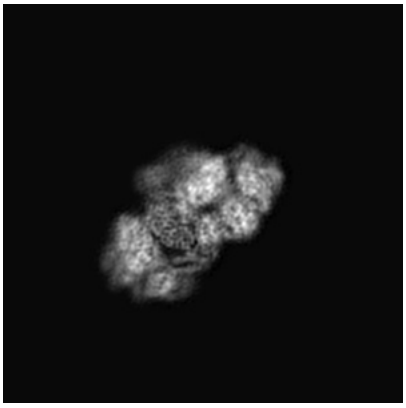
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30166. These allow visual inspection of the internal detail of the map and identification of artifacts.

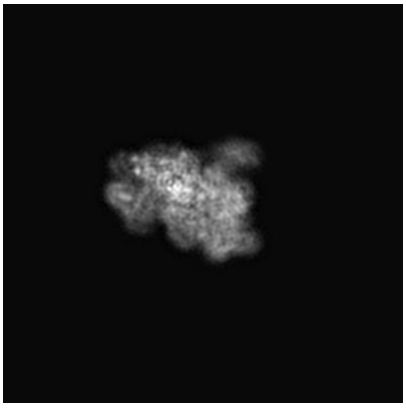
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

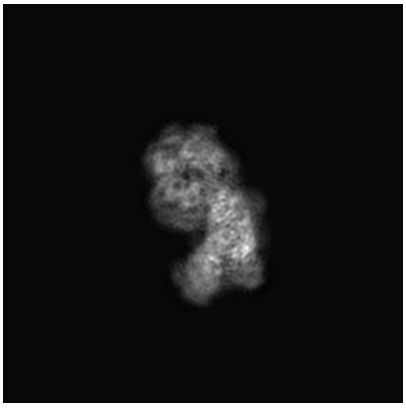
6.1.1 Primary map



X



Y

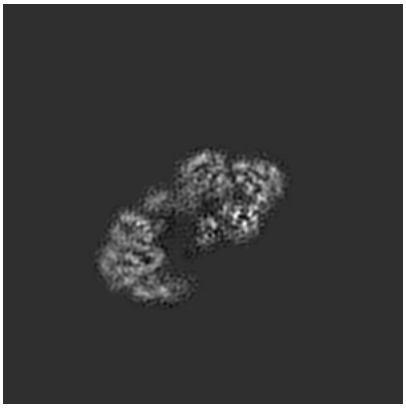


Z

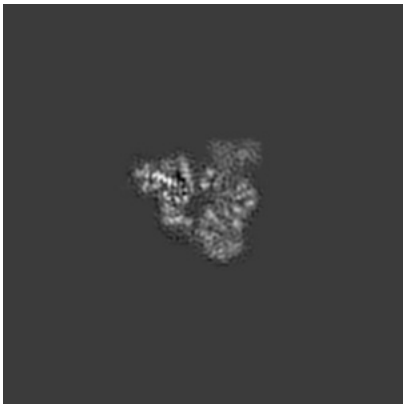
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 136



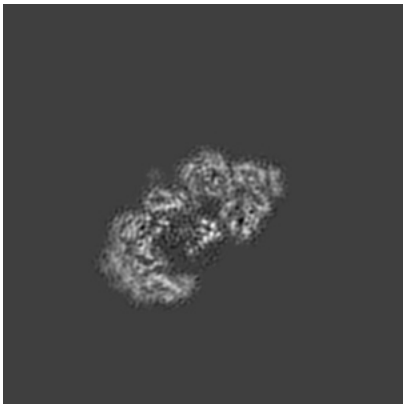
Y Index: 136

Z Index: 136

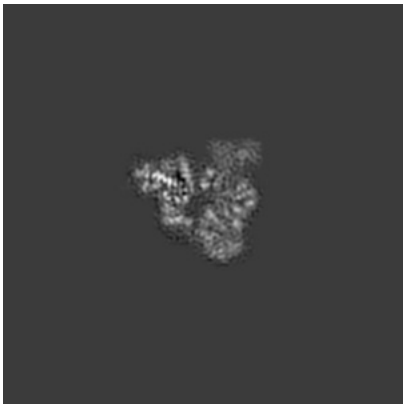
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

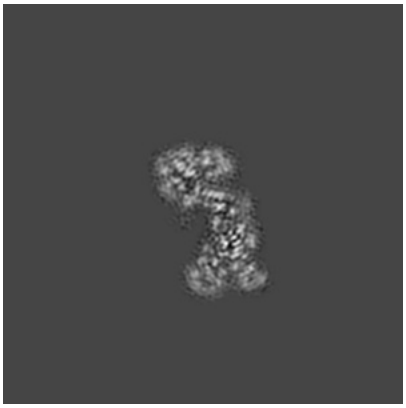
6.3.1 Primary map



X Index: 140



Y Index: 136

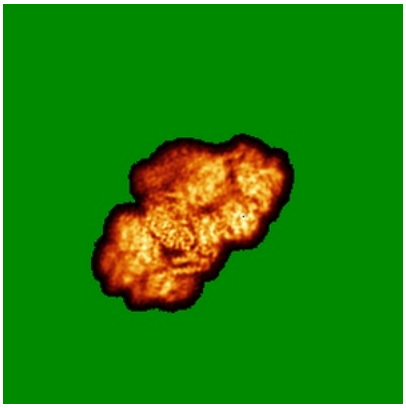


Z Index: 120

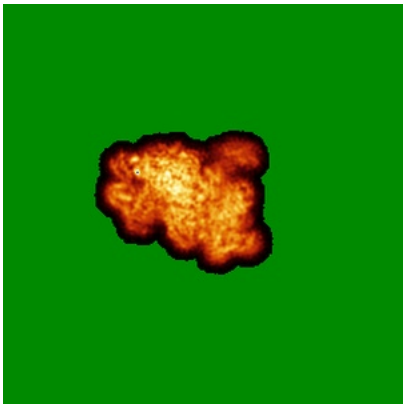
The images above show the largest variance slices of the map in three orthogonal directions.

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

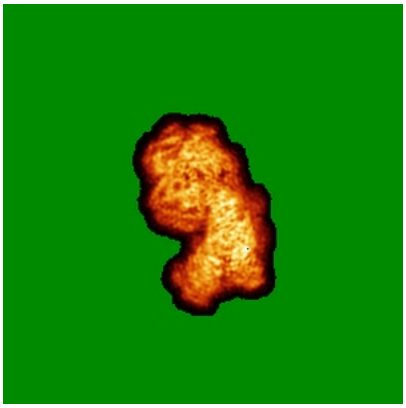
6.4.1 Primary map



X



Y

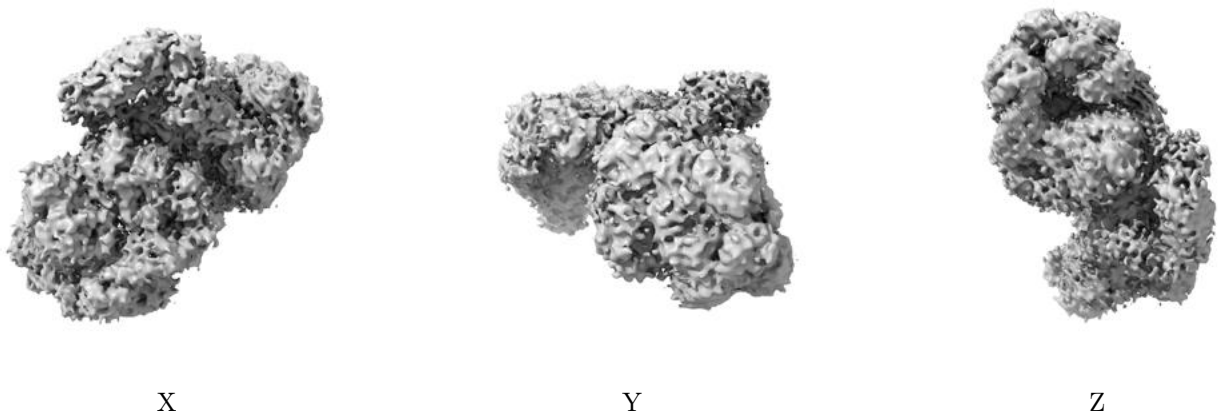


Z

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 (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

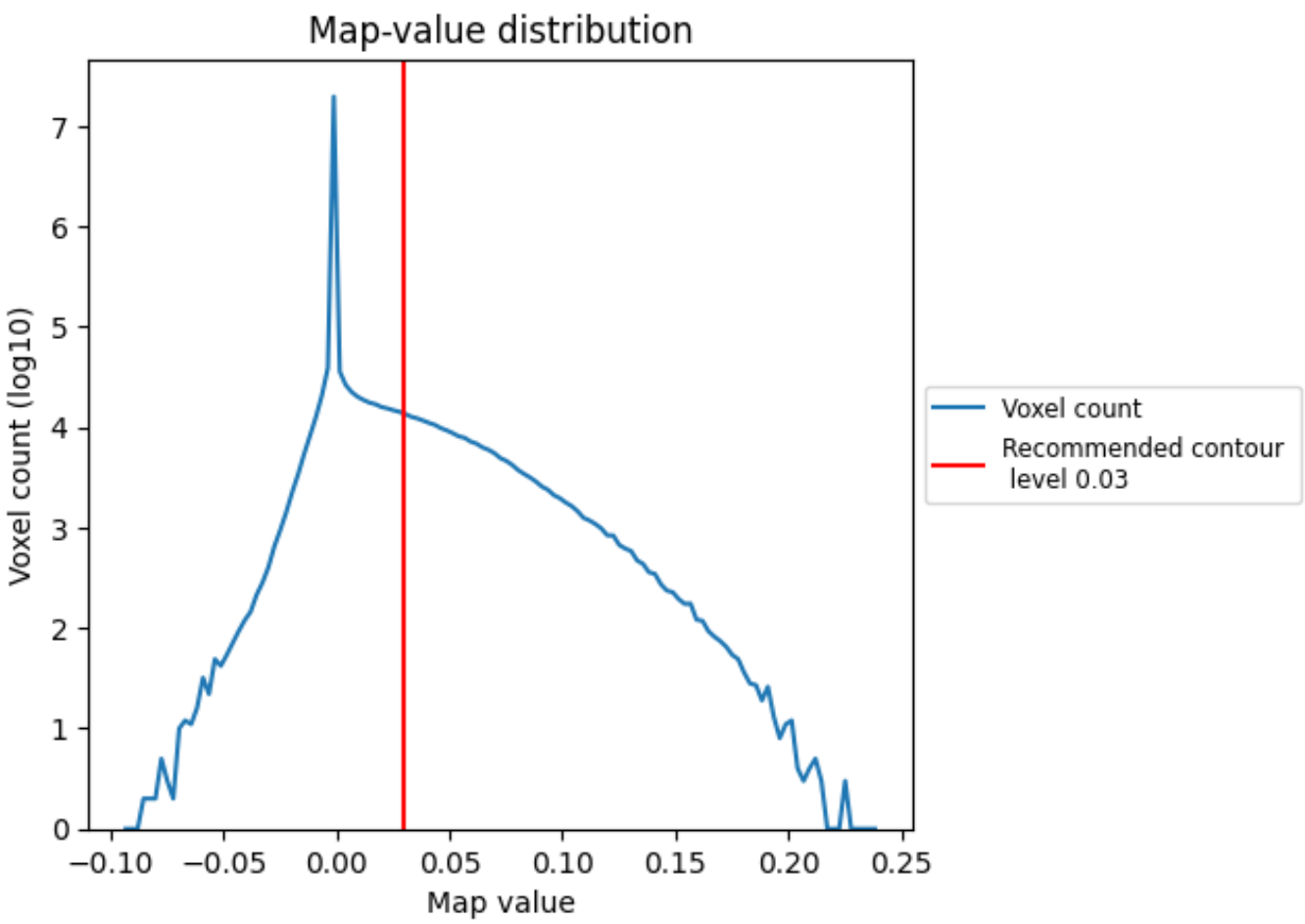
6.6 Mask visualisation (i)

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

7 Map analysis (i)

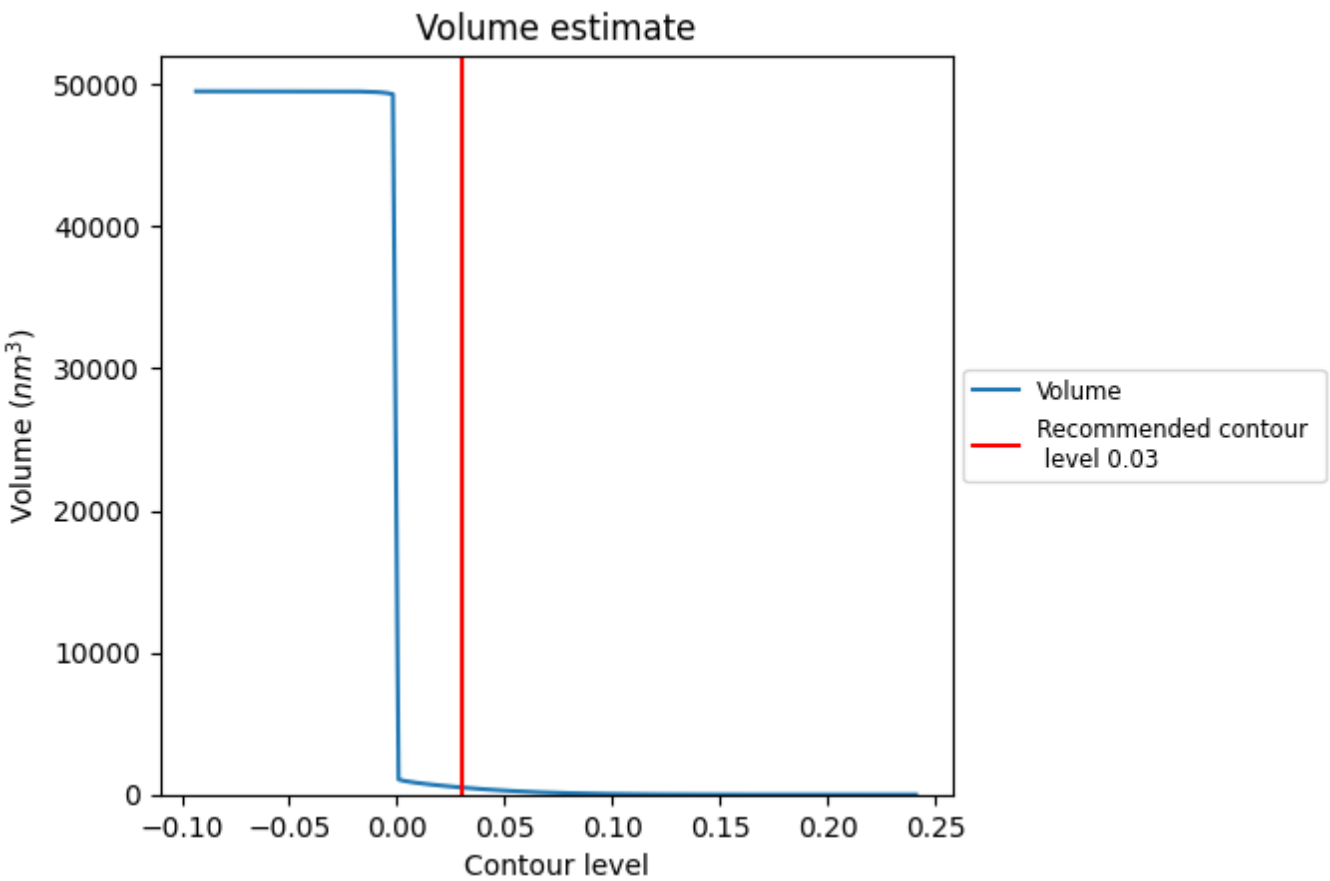
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

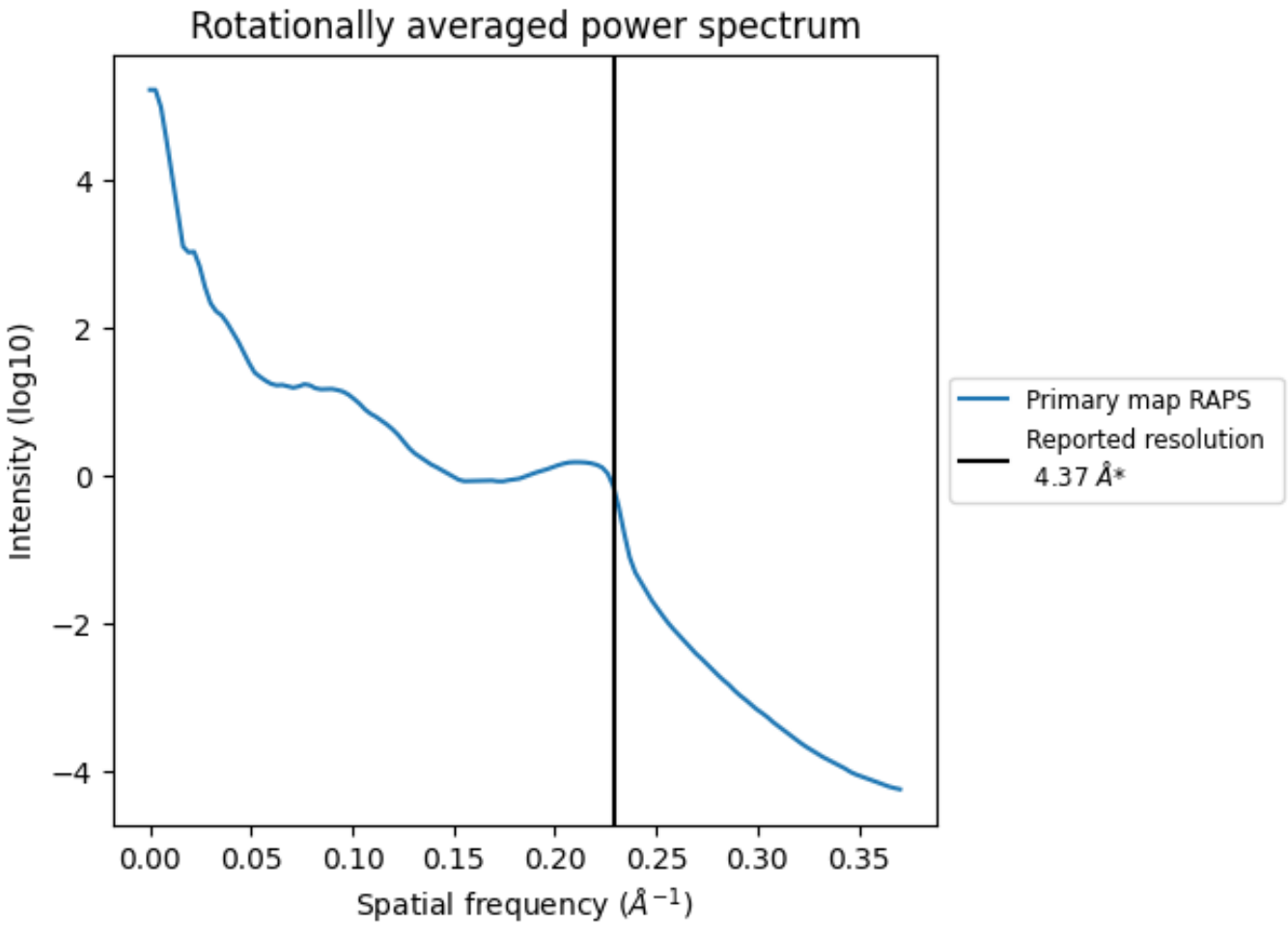
7.2 Volume estimate (i)



The volume at the recommended contour level is 497 nm^3; this corresponds to an approximate mass of 449 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.229 Å^{-1}

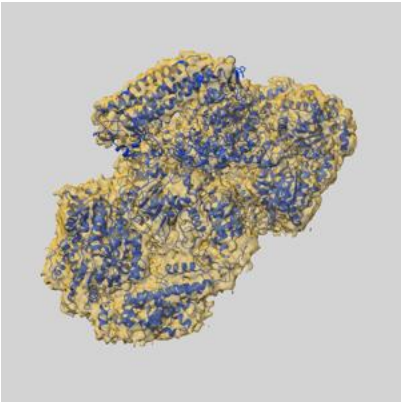
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

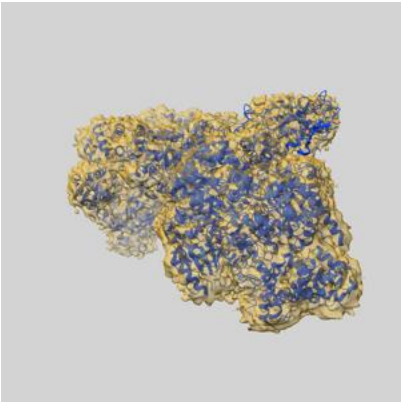
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30166 and PDB model 7BST. Per-residue inclusion information can be found in section 3 on page 4.

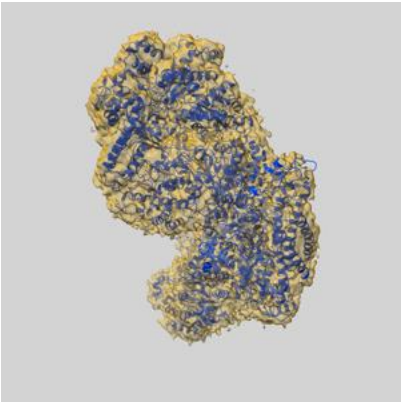
9.1 Map-model overlay (i)



X



Y



Z

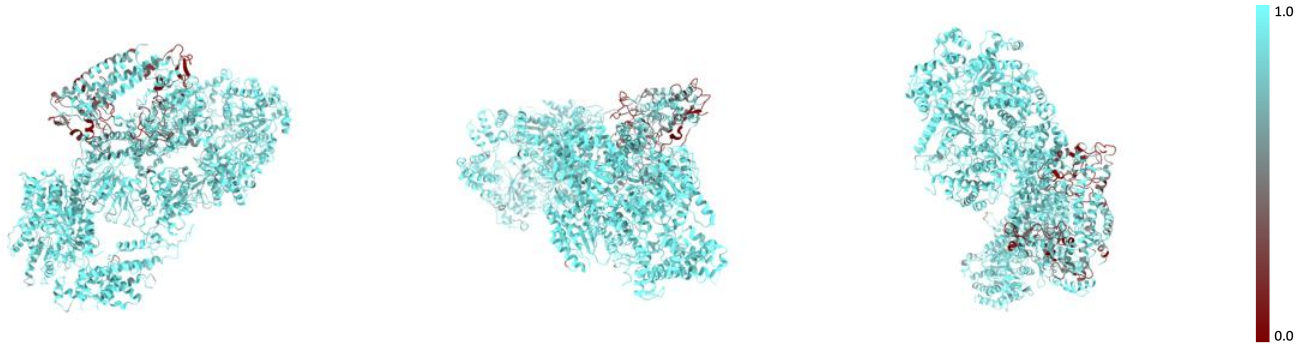
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

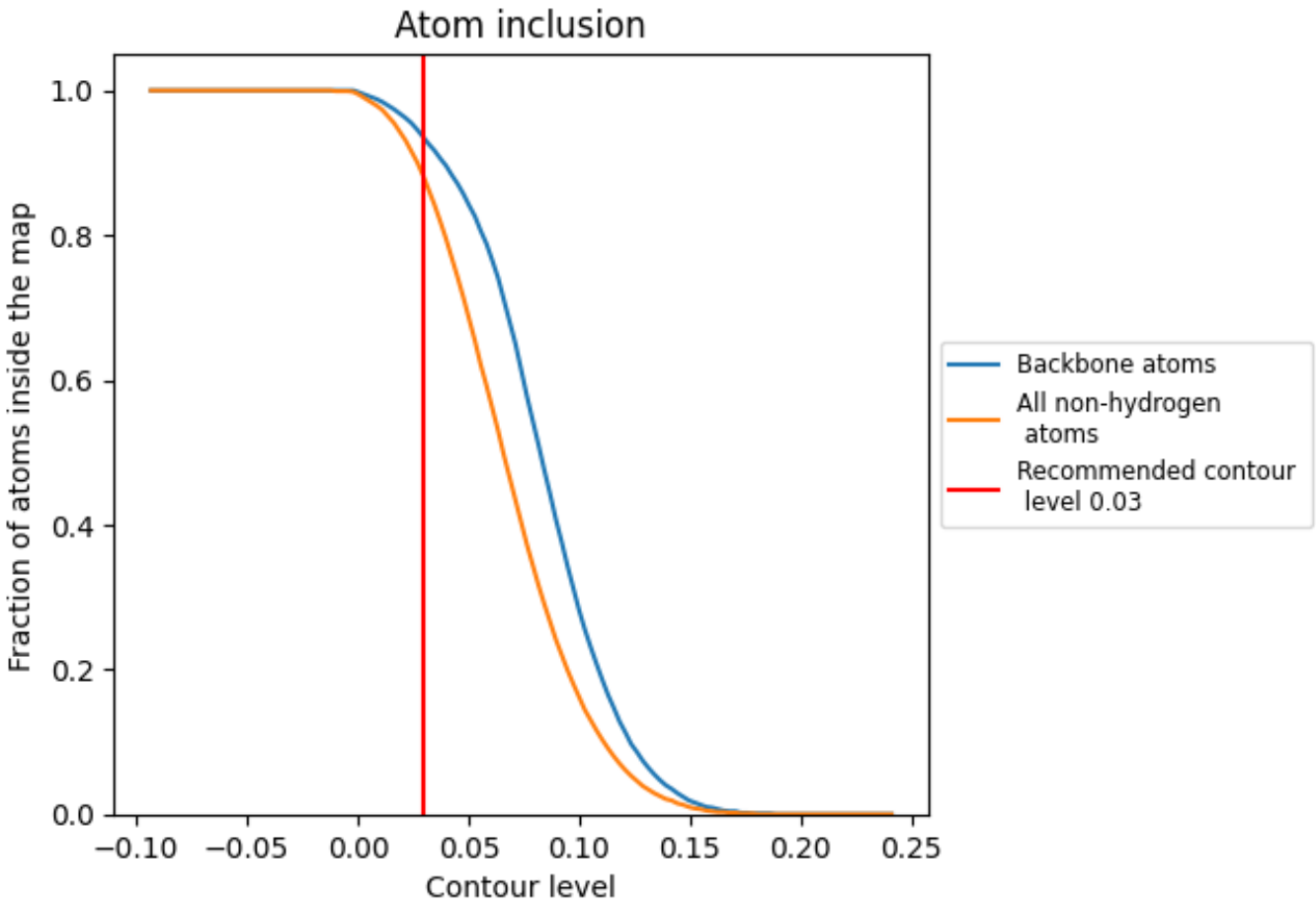
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.2450
A	0.4510	0.0720
B	0.9420	0.2710
C	0.9490	0.2750
D	0.9100	0.3010
E	0.9160	0.2220
F	0.8960	0.2210
G	0.8620	0.2260