Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 05:29 PM EST

PDB ID	:	7MOB
EMDB ID	:	EMD-23923
Title	:	Cryo-EM structure of 2:2 c-MET/NK1 complex
Authors	:	Uchikawa, E.; Chen, Z.M.; Xiao, G.Y.; Zhang, X.W.; Bai, X.C.
Deposited on	:	2021-05-01
Resolution	:	5.00 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 ⓘ 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 ⓘ) were used in the production of this report:

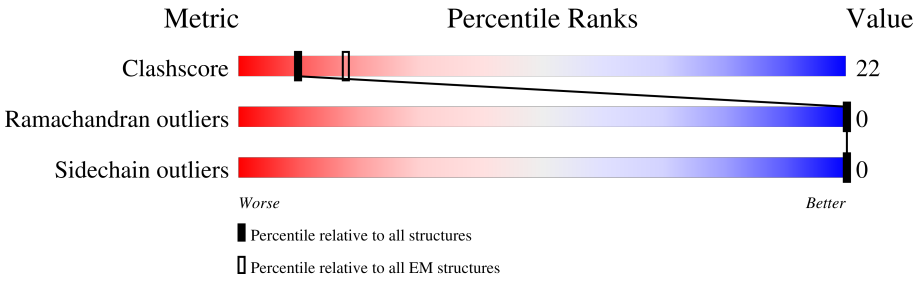
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 5.00 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	A	210	10% 45% 37% 18%
1	B	210	10% 45% 37% 18%
2	C	1390	6% 21% 15% 65%
2	D	1390	6% 20% 15% 65%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10476 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 Hepatocyte growth factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	172	Total	C	N	O	S	0	0
			1377	870	242	253	12		
1	B	172	Total	C	N	O	S	0	0
			1377	870	242	253	12		

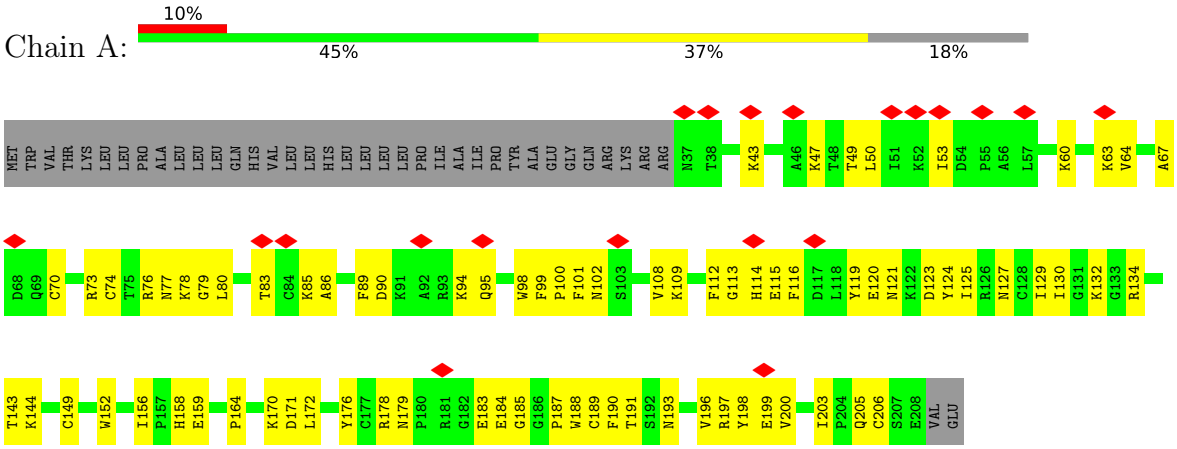
- Molecule 2 is a protein called Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	489	Total	C	N	O	S	0	0
			3861	2447	658	726	30		
2	D	489	Total	C	N	O	S	0	0
			3861	2447	658	726	30		

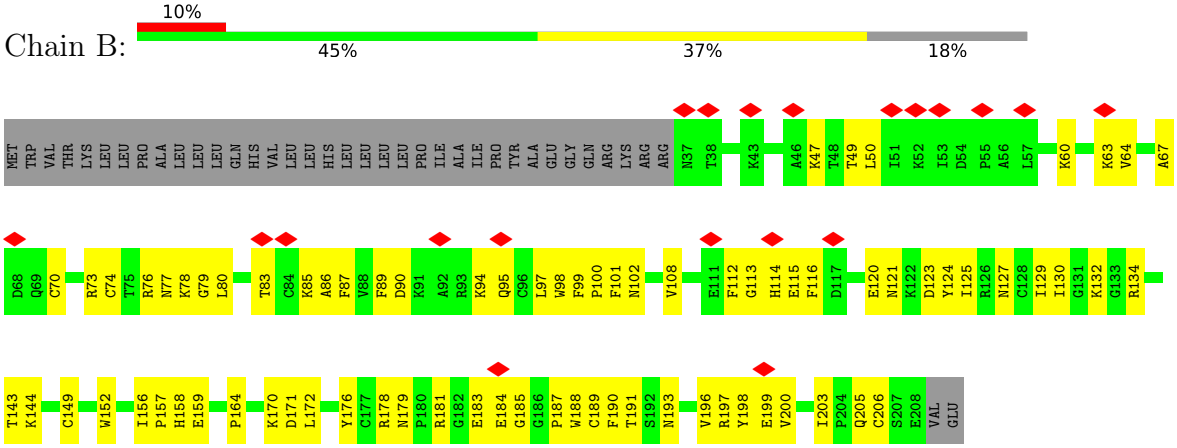
3 Residue-property plots (i)

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.

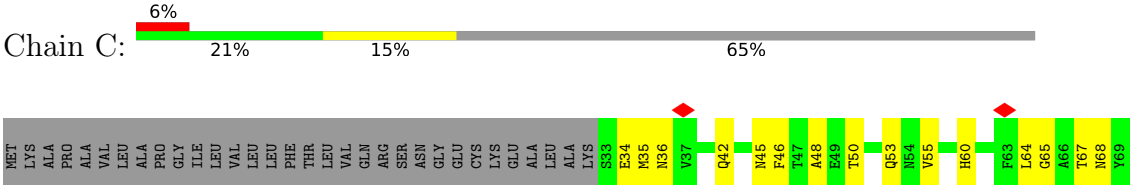
• Molecule 1: Hepatocyte growth factor

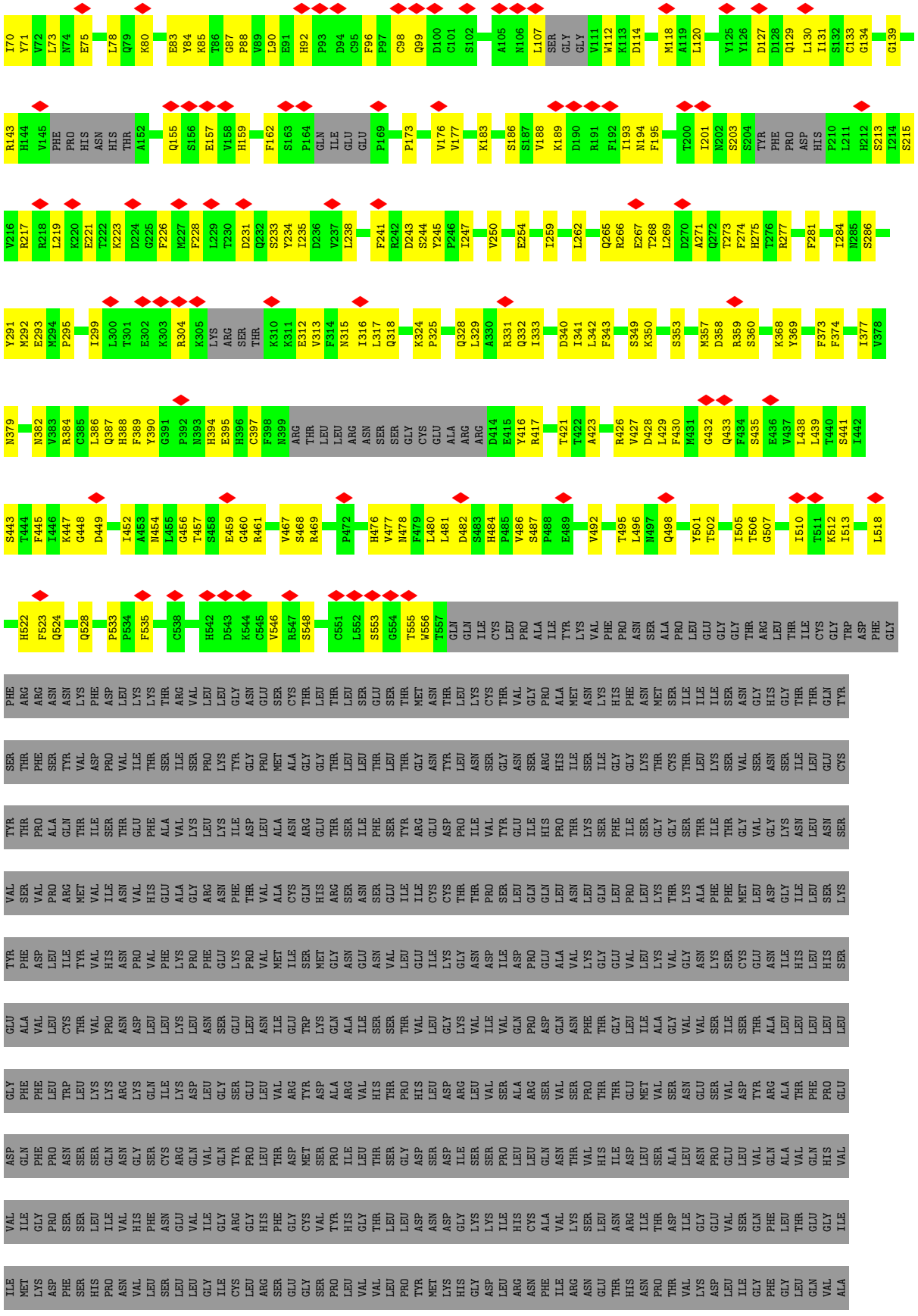


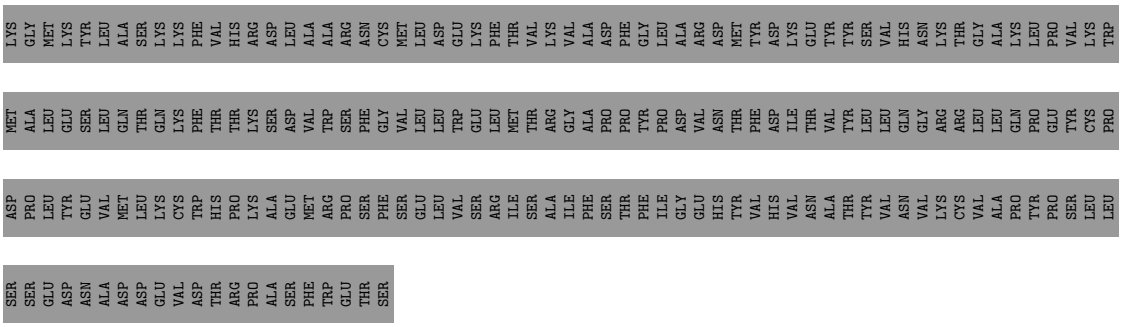
• Molecule 1: Hepatocyte growth factor



• Molecule 2: Hepatocyte growth factor receptor

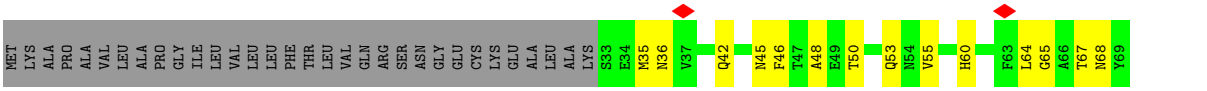


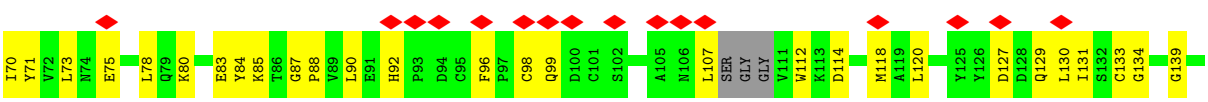

I70 Y71 V72 L73 N74 E75 L78 Q79 K80 E83 Y84 K85 T86 G87 P88 V89 L90 E91 H92 P93 D94 C95 F96 P97 C98 Q99 D100 C101 S102 A105 N106 L107 SER GLY GLY V111 W112 K113 D114 M118 A119 L120 Y125 Y126 D127 D128 Q129 L130 I131 S132 C133 G134 G139
R143 H144 V145 PHE PRO HIS ASN HIS THR A152 Q155 S156 E157 V158 H159 F162 S163 P164 GLN ILE GLU GLU P169 P173 V176 V177 K183 S186 S187 V188 K189 D190 R191 F192 I193 N194 F195 T200 I201 N202 S203 S204 TYR PHE PRO ASP HIS P210 L211 H212 S213 I214 S215
V216 R217 R218 L219 K220 E221 T222 K223 D224 G225 F226 M227 F228 L229 T230 D231 Q232 S233 Y234 I235 D236 V237 L238 F241 R242 D243 S244 Y245 P246 I247 V250 E254 I259 L262 Q265 R266 E267 T268 L269 D270 A271 Q272 T273 F274 H275 T276 R277 F281 I284 N285 S286
Y291 M292 E293 M294 P295 I299 L300 T301 E302 K303 R304 K305 LYS ARG SER THR K310 K311 E312 V313 F314 N315 I316 L317 Q318 K324 P325 Q328 L329 A330 R331 Q332 I333 D340 I341 L342 F343 S349 K350 S353 M357 D358 R359 S360 K368 Y369 F373 F374 I377 V378
N379 N382 V383 R384 C385 L386 Q387 H388 F389 Y390 G391 P392 N393 H394 E395 H396 C397 F398 N399 ARG THR LEU LEU ARG ASN SER SER GLY CYS GLU ALA ARG ARG D414 E415 Y416 R417 T421 T422 A423 R426 V427 D428 L429 F430 M431 G432 Q433 F434 S435 E436 V437 L438 L439 T440 S441 I442
S443 T444 F445 I446 K447 G448 D449 I452 A453 N454 L455 G456 T457 S458 E459 G460 R461 V467 S468 R469 P472 H476 V477 N478 F479 L480 L481 D482 S483 H484 P485 V486 S487 P488 E489 V492 T495 L496 N497 Q498 Y501 T502 I505 T506 G507 I510 T511 K512 I513 L518
H522 F523 Q524 Q528 P533 P534 F535 C538 H542 D543 K544 C545 V546 R547 S548 C551 L552 S553 G554 T555 W556 T557 GLN GLN ILE CYS LEU PRO ALA ILE TYR LYS VAL PHE PRO ASN SER ALA PRO LEU GLU GLU GLY GLY THR ARG LEU THR ILE CYS GLY TRP ASP PHE GLY
PHE ARG ARG ASN ASN LYS PHE ASP LEU LYS LYS THR ARG VAL LEU LEU GLY ASN GLU SER CYS THR LEU LEU THR LEU SER GLU SER THR MET ASN THR LEU LYS CYS THR VAL GLY PRO ALA MET ASN LYS HIS PHE ASN MET SER ILE ILE ILE SER ASN GLY HIS GLY THR THR GLN TYR
SER THR PHE SER TYR VAL ASP PRO VAL ILE THR SER ILE SER PRO LYS TYR GLY PRO MET ALA GLY GLY THR LEU LEU THR LEU THR GLY ASN TYR LEU ASN SER GLY ASN SER ARG HIS ILE SER ILE GLY GLY LYS THR CYS THR LEU LYS SER VAL SER ASN SER ILE LEU LEU GLU CYS
TYR THR PRO ALA GLN THR ILE SER THR GLU PHE ALA VAL LYS LEU LYS ILE ASP LEU ALA ASN ARG GLU THR SER ILE PHE SER TYR ARG GLU ASP PRO ILE VAL VAL TYR GLU ILE HIS PRO THR LYS SER PHE ILE SER GLY GLY SER THR ILE THR GLY VAL GLY LYS ASN LEU ASN SER
VAL SER VAL PRO ARG MET VAL ILE ASN VAL HIS GLU ALA GLY ARG ASN PHE THR VAL ALA CYS GLN HIS ARG SER ASN SER GLU ILE ILE CYS CYS THR THR PRO SER LEU GLN GLN LEU ASN LEU GLN LEU PRO LEU LYS THR LYS ALA PHE PHE MET LEU ASP GLY ILE LEU SER SER LYS
TYR PHE ASP LEU ILE TYR VAL HIS ASN PRO VAL PHE LYS PRO PHE GLU LYS PRO VAL MET ILE SER MET GLY ASN GLU ASN VAL LEU LEU GLU ILE LYS GLY ASN ASP ILE ASP PRO GLU ALA VAL LYS GLY GLU VAL LEU LYS VAL GLY ASN LYS SER CYS GLU ASN ILE HIS LEU LEU HIS SER
GLU ALA VAL LEU CYS THR VAL PRO ASN ASP LEU LEU LYS LEU ASN SER GLU LEU ASN ILE GLU TRP LYS GLN ALA ILE SER SER THR VAL LEU GLU ILE GLY GLY LYS VAL ILE VAL GLN PRO ASP GLN ASN PHE THR GLY LEU ILE ALA GLY VAL VAL SER ILE SER SER THR ALA LEU LEU LEU LEU
GLY PHE PHE LEU TRP LEU LYS LYS ARG LYS GLN ILE LYS ASP LEU GLY SER GLU LEU VAL ARG TYR ASP ALA ARG VAL HIS THR PRO HIS LEU ASP ARG LEU VAL VAL SER ALA ARG SER VAL PRO THR THR GLU MET VAL SER ASN GLU SER ILE SER VAL ASP TYR ARG ALA THR PHE PRO GLU
ASP GLN PHE PRO ASN SER SER GLN CYS ARG GLN VAL GLN TYR PRO LEU THR ASP MET SER PRO ILE LEU THR SER GLY ASP SER ASP ILE SER SER PRO LEU LEU GLN ASN THR VAL HIS ILE ASP LEU SER ALA LEU ASN PRO GLU LEU VAL ASP GLN ALA VAL THR PHE PRO GLU HIS VAL
VAL ILE GLY PRO SER SER LEU ILE VAL HIS PHE ASN GLU VAL ILE GLY ARG GLY HIS PHE GLY CYS VAL TYR HIS GLY THR LEU LEU PRO TYR MET LYS HIS GLY LYS ASP LEU ILE ASP GLY LYS LYS ILE HIS CYS ALA VAL LYS SER LEU ASN ASN ARG ILE THR ASP ILE GLY GLY GLU VAL SER GLN PHE LEU THR GLU GLY VAL
ILE MET LYS ASP PHE SER HIS PRO ASN VAL LEU LEU SER HIS PRO LEU VAL VAL LEU PRO TYR MET LYS HIS GLY LYS LEU ARG SER GLU GLY SER VAL PRO LEU VAL VAL LEU ARG ASN PHE ILE ARG ASN GLU THR HIS ASN PRO THR VAL LYS ASP LEU ILE LEU GLY PHE GLY LEU GLN VAL ALA

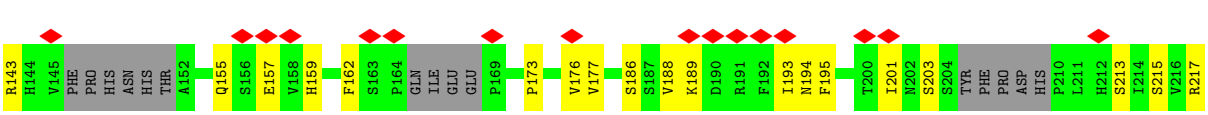


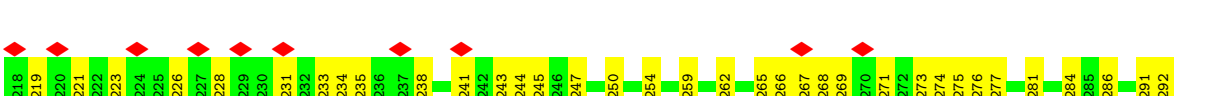
• Molecule 2: Hepatocyte growth factor receptor

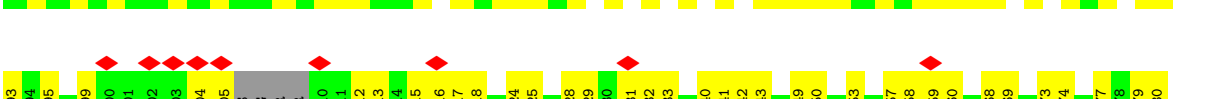
Chain D:

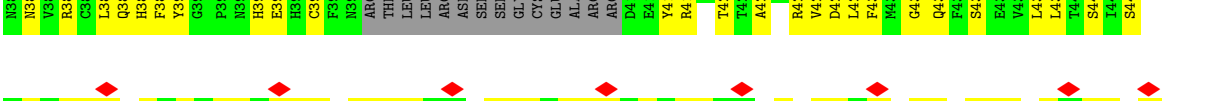


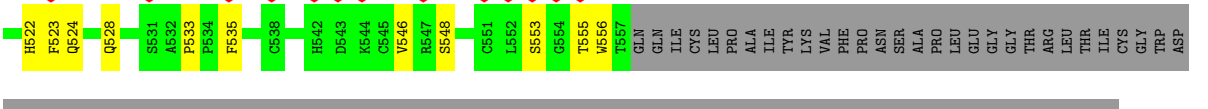


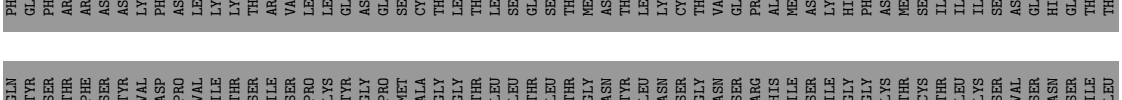


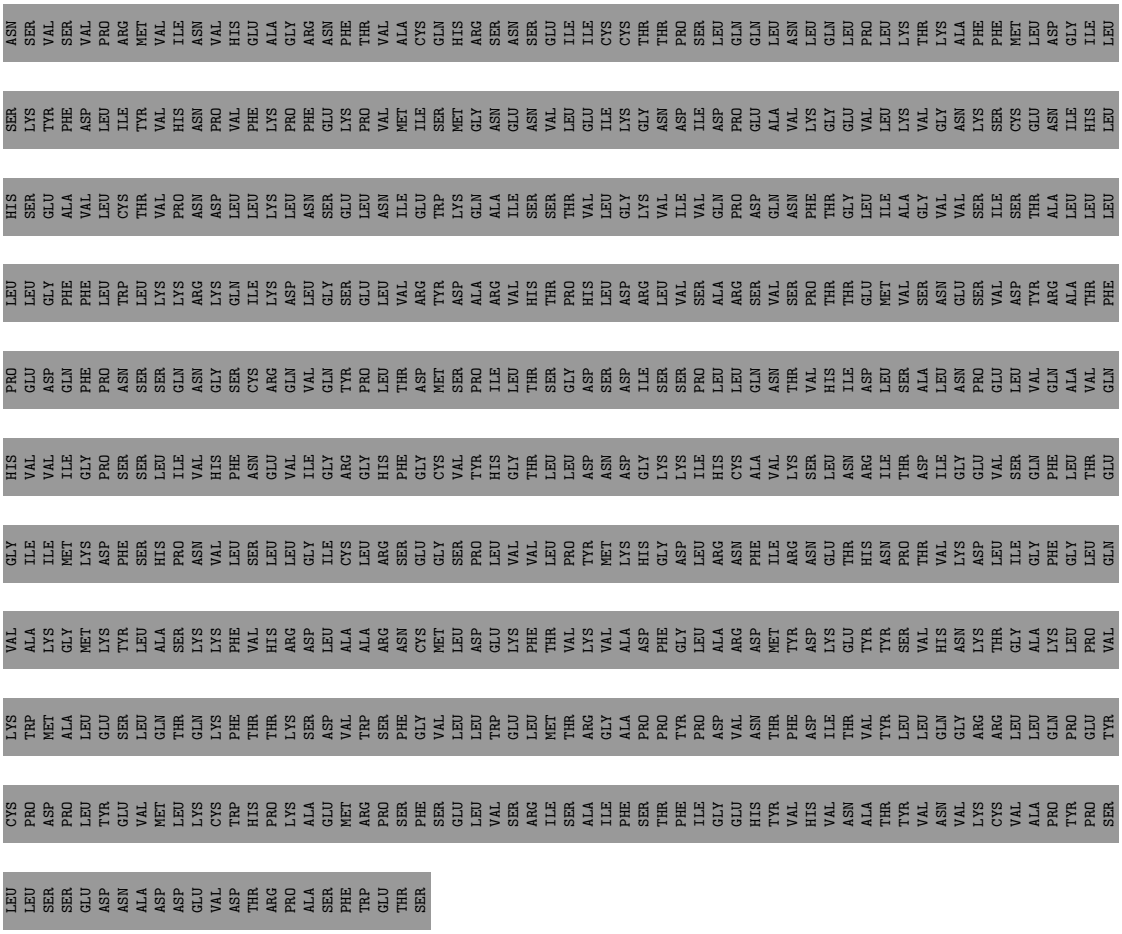








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SER LYS TYR PHE ASP LEU ILE TYR VAL HIS ASN PRO VAL PHE LYS PRO PHE GLU LYS PRO VAL MET ILE GLU SER MET GLY ASN GLU ASN VAL LEU GLU ILE LYS GLY ASN ASP ILE ASP PRO GLU ALA VAL LYS GLY GLU VAL LEU LYS VAL GLY ASN LYS SER CYS GLU ASN ILE HIS LEU
HIS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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11570	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	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	291.6, 291.6, 291.6	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	0.33	0/1412	0.46	0/1899
1	B	0.33	0/1412	0.46	0/1899
2	C	0.32	0/3947	0.50	0/5346
2	D	0.32	0/3947	0.50	0/5346
All	All	0.33	0/10718	0.49	0/14490

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	1377	0	1344	69	0
1	B	1377	0	1344	67	0
2	C	3861	0	3733	164	0
2	D	3861	0	3733	167	0
All	All	10476	0	10154	454	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 22.

All (454) 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)
2:D:265:GLN:HE22	2:D:277:ARG:HE	1.25	0.84
2:C:265:GLN:HE22	2:C:277:ARG:HE	1.26	0.84
2:C:250:VAL:HG21	2:C:317:LEU:HD22	1.66	0.77
2:D:250:VAL:HG21	2:D:317:LEU:HD22	1.66	0.76
2:C:394:HIS:HB3	2:C:397:CYS:HB2	1.66	0.76
2:D:394:HIS:HB3	2:D:397:CYS:HB2	1.66	0.76
1:A:179:ASN:ND2	1:A:183:GLU:O	2.18	0.75
2:D:268:THR:HG22	2:D:269:LEU:HD23	1.69	0.74
2:C:268:THR:HG22	2:C:269:LEU:HD23	1.69	0.74
1:B:179:ASN:ND2	1:B:183:GLU:O	2.18	0.73
1:B:171:ASP:O	1:B:178:ARG:NH2	2.24	0.71
1:A:134:ARG:O	1:A:170:LYS:NZ	2.22	0.71
1:A:171:ASP:O	1:A:178:ARG:NH2	2.24	0.70
1:B:134:ARG:O	1:B:170:LYS:NZ	2.22	0.70
2:C:461:ARG:NH2	2:C:478:ASN:OD1	2.25	0.70
1:B:191:THR:OG1	1:B:196:VAL:O	2.10	0.69
2:C:447:LYS:HE3	2:C:498:GLN:HB3	1.74	0.69
1:A:129:ILE:O	1:A:205:GLN:NE2	2.25	0.69
1:A:191:THR:OG1	1:A:196:VAL:O	2.10	0.69
1:B:129:ILE:HG13	1:B:205:GLN:HG2	1.74	0.68
2:D:291:TYR:HB3	2:D:417:ARG:HD3	1.75	0.68
2:C:267:GLU:HA	2:C:275:HIS:HB2	1.74	0.68
2:C:291:TYR:HB3	2:C:417:ARG:HD3	1.75	0.68
2:D:267:GLU:HA	2:D:275:HIS:HB2	1.74	0.68
2:D:447:LYS:HE3	2:D:498:GLN:HB3	1.74	0.68
1:B:129:ILE:O	1:B:205:GLN:NE2	2.25	0.68
2:D:461:ARG:NH2	2:D:478:ASN:OD1	2.25	0.68
1:A:129:ILE:HG13	1:A:205:GLN:HG2	1.74	0.68
1:A:73:ARG:HG3	1:A:78:LYS:HB2	1.75	0.67
1:B:73:ARG:HG3	1:B:78:LYS:HB2	1.75	0.66
1:A:86:ALA:HB2	1:A:102:ASN:HB3	1.78	0.66
1:B:74:CYS:HB2	1:B:98:TRP:CD1	2.31	0.66
2:C:299:ILE:HD12	2:C:313:VAL:HG22	1.78	0.66
2:D:50:THR:HB	2:D:67:THR:HB	1.78	0.65
1:A:74:CYS:HB2	1:A:98:TRP:CD1	2.31	0.65
2:C:50:THR:HB	2:C:67:THR:HB	1.78	0.65
1:A:60:LYS:NZ	1:A:79:GLY:O	2.30	0.65
1:A:193:ASN:OD1	1:A:196:VAL:N	2.28	0.65
2:D:428:ASP:OD2	2:D:432:GLY:N	2.23	0.65
1:B:60:LYS:NZ	1:B:79:GLY:O	2.30	0.64
2:D:201:ILE:HG12	2:D:203:SER:H	1.63	0.64
1:B:86:ALA:HB2	1:B:102:ASN:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:GLU:HB2	2:D:259:ILE:HD13	1.80	0.64
2:D:299:ILE:HD12	2:D:313:VAL:HG22	1.78	0.64
2:D:98:CYS:SG	2:D:162:PHE:HB2	2.38	0.63
1:B:70:CYS:HA	1:B:98:TRP:HZ2	1.63	0.63
2:C:98:CYS:SG	2:C:162:PHE:HB2	2.38	0.63
2:D:73:LEU:HG	2:D:80:LYS:HA	1.80	0.63
2:D:217:ARG:HB2	2:D:226:PHE:HB3	1.80	0.63
2:C:201:ILE:HG12	2:C:203:SER:H	1.62	0.63
1:B:193:ASN:OD1	1:B:196:VAL:N	2.28	0.63
2:C:217:ARG:HB2	2:C:226:PHE:HB3	1.80	0.62
1:B:158:HIS:CD2	1:B:197:ARG:HG3	2.35	0.62
2:D:461:ARG:NH1	2:D:480:LEU:HB2	2.14	0.62
2:C:254:GLU:HB2	2:C:259:ILE:HD13	1.80	0.62
2:D:349:SER:OG	2:D:353:SER:O	2.15	0.62
1:A:70:CYS:HA	1:A:98:TRP:HZ2	1.63	0.62
1:A:158:HIS:CD2	1:A:197:ARG:HG3	2.34	0.62
2:C:73:LEU:HG	2:C:80:LYS:HA	1.80	0.62
2:C:329:LEU:HD12	2:C:468:SER:HA	1.82	0.62
2:C:461:ARG:NH1	2:C:480:LEU:HB2	2.14	0.61
1:A:123:ASP:O	1:B:127:ASN:ND2	2.32	0.61
2:C:68:ASN:ND2	2:C:114:ASP:OD1	2.33	0.61
1:A:49:THR:HB	1:A:116:PHE:HB3	1.81	0.61
1:A:121:ASN:HB3	1:A:124:TYR:HB2	1.82	0.61
1:B:76:ARG:HG3	1:B:78:LYS:HG2	1.83	0.61
2:D:68:ASN:ND2	2:D:114:ASP:OD1	2.33	0.61
1:A:158:HIS:CG	1:A:197:ARG:HG3	2.35	0.61
1:B:121:ASN:HB3	1:B:124:TYR:HB2	1.82	0.61
1:B:158:HIS:CG	1:B:197:ARG:HG3	2.35	0.60
2:D:329:LEU:HD12	2:D:468:SER:HA	1.82	0.60
1:B:49:THR:HB	1:B:116:PHE:HB3	1.81	0.60
2:C:501:TYR:HA	2:C:513:ILE:O	2.02	0.60
2:C:46:PHE:HB3	2:C:510:ILE:HG22	1.84	0.60
1:B:47:LYS:HG2	1:B:114:HIS:HA	1.84	0.60
2:C:360:SER:HB2	2:C:439:LEU:HD13	1.84	0.59
2:C:428:ASP:OD2	2:C:432:GLY:N	2.23	0.59
2:D:501:TYR:HA	2:D:513:ILE:O	2.02	0.59
2:D:46:PHE:HB3	2:D:510:ILE:HG22	1.84	0.59
1:A:76:ARG:HG3	1:A:78:LYS:HG2	1.83	0.59
1:B:159:GLU:HG2	2:C:426:ARG:HH11	1.67	0.59
2:C:238:LEU:HB2	2:C:241:PHE:HD2	1.67	0.59
2:D:360:SER:HB2	2:D:439:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:OD1	1:A:123:ASP:N	2.36	0.58
2:C:55:VAL:HG22	2:C:64:LEU:HG	1.84	0.58
2:D:513:ILE:HG23	2:D:518:LEU:HD21	1.85	0.58
1:A:47:LYS:HG2	1:A:114:HIS:HA	1.84	0.58
2:C:315:ASN:HD21	2:C:349:SER:HB3	1.68	0.58
2:C:46:PHE:CD1	2:C:73:LEU:HD21	2.39	0.58
2:D:281:PHE:HB3	2:D:291:TYR:HA	1.85	0.58
2:C:96:PHE:H	2:C:99:GLN:HE22	1.51	0.58
2:D:315:ASN:HD21	2:D:349:SER:HB3	1.68	0.58
2:D:502:THR:O	2:D:512:LYS:HA	2.04	0.58
2:C:281:PHE:HB3	2:C:291:TYR:HA	1.85	0.58
2:C:513:ILE:HG23	2:C:518:LEU:HD21	1.85	0.58
2:D:46:PHE:CD1	2:D:73:LEU:HD21	2.39	0.58
2:D:120:LEU:HG	2:D:130:LEU:HD11	1.86	0.58
1:B:121:ASN:OD1	1:B:123:ASP:N	2.36	0.58
2:C:120:LEU:HG	2:C:130:LEU:HD11	1.86	0.58
2:C:390:TYR:HB3	2:C:394:HIS:CG	2.39	0.58
2:C:267:GLU:O	2:C:277:ARG:NH2	2.37	0.57
2:C:428:ASP:OD1	2:C:430:PHE:N	2.27	0.57
2:D:238:LEU:HB2	2:D:241:PHE:HD2	1.67	0.57
2:C:219:LEU:HD11	2:C:223:LYS:HA	1.85	0.57
2:C:502:THR:O	2:C:512:LYS:HA	2.04	0.57
2:D:96:PHE:H	2:D:99:GLN:HE22	1.51	0.57
2:D:219:LEU:HD11	2:D:223:LYS:HA	1.85	0.57
2:D:358:ASP:HA	2:D:438:LEU:HB2	1.86	0.57
2:D:84:TYR:HB2	2:D:155:GLN:HB3	1.87	0.57
2:D:390:TYR:HB3	2:D:394:HIS:CG	2.39	0.57
2:D:395:GLU:OE2	2:D:395:GLU:N	2.34	0.57
2:C:358:ASP:HA	2:C:438:LEU:HB2	1.86	0.57
2:D:457:THR:HG22	2:D:459:GLU:H	1.69	0.57
2:C:84:TYR:HB2	2:C:155:GLN:HB3	1.87	0.56
2:C:268:THR:HB	2:C:271:ALA:HB2	1.87	0.56
2:C:457:THR:HG22	2:C:459:GLU:H	1.69	0.56
2:D:35:MET:HA	2:D:524:GLN:HG3	1.88	0.56
2:D:55:VAL:HG22	2:D:64:LEU:HG	1.85	0.56
2:D:267:GLU:O	2:D:277:ARG:NH2	2.37	0.56
2:D:533:PRO:HB2	2:D:535:PHE:CD2	2.40	0.56
2:C:35:MET:HA	2:C:524:GLN:HG3	1.87	0.56
2:C:533:PRO:HB2	2:C:535:PHE:CD2	2.40	0.56
1:B:132:LYS:HD3	1:B:184:GLU:HA	1.88	0.56
2:C:243:ASP:OD1	2:C:244:SER:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ILE:O	1:B:205:GLN:NE2	2.39	0.56
2:C:36:ASN:HD21	2:C:522:HIS:HA	1.71	0.55
2:D:36:ASN:HD21	2:D:522:HIS:HA	1.71	0.55
2:C:332:GLN:NE2	2:C:468:SER:OG	2.32	0.55
1:A:130:ILE:O	1:A:205:GLN:NE2	2.39	0.55
1:A:132:LYS:HD3	1:A:184:GLU:HA	1.88	0.55
2:C:324:LYS:NZ	2:C:340:ASP:OD1	2.27	0.55
2:D:118:MET:H	2:D:134:GLY:HA2	1.72	0.55
1:A:190:PHE:CD1	1:A:198:TYR:HB3	2.42	0.55
1:B:190:PHE:CD1	1:B:198:TYR:HB3	2.42	0.55
2:D:332:GLN:NE2	2:D:468:SER:OG	2.32	0.55
2:D:441:SER:O	2:D:456:GLY:N	2.40	0.55
2:D:533:PRO:HB2	2:D:535:PHE:HD2	1.72	0.55
2:C:384:ARG:HD2	2:C:421:THR:HG22	1.88	0.55
2:C:533:PRO:HB2	2:C:535:PHE:HD2	1.72	0.55
2:D:384:ARG:HD2	2:D:421:THR:HG22	1.88	0.55
1:A:159:GLU:HG2	2:D:426:ARG:HH11	1.71	0.54
2:C:492:VAL:HG22	2:C:502:THR:HG22	1.89	0.54
2:D:92:HIS:HD2	2:D:107:LEU:HA	1.72	0.54
2:D:268:THR:HB	2:D:271:ALA:HB2	1.87	0.54
2:C:416:TYR:O	2:C:417:ARG:NE	2.40	0.54
2:C:457:THR:HG22	2:C:459:GLU:N	2.23	0.54
1:A:77:ASN:HA	1:A:80:LEU:HD12	1.90	0.54
1:A:127:ASN:ND2	1:B:123:ASP:O	2.41	0.54
2:D:428:ASP:OD1	2:D:429:LEU:N	2.41	0.54
2:D:481:LEU:HG	2:D:482:ASP:H	1.72	0.54
1:B:77:ASN:HA	1:B:80:LEU:HD12	1.90	0.54
2:C:395:GLU:OE2	2:C:395:GLU:N	2.34	0.54
2:D:233:SER:OG	2:D:286:SER:O	2.26	0.54
2:D:324:LYS:NZ	2:D:340:ASP:OD1	2.27	0.54
1:B:188:TRP:HB3	1:B:200:VAL:HA	1.89	0.54
2:C:428:ASP:OD1	2:C:429:LEU:N	2.41	0.54
2:C:429:LEU:HD21	2:C:467:VAL:HG13	1.88	0.54
2:C:481:LEU:HG	2:C:482:ASP:H	1.73	0.54
2:D:429:LEU:HD21	2:D:467:VAL:HG13	1.88	0.54
2:C:213:SER:OG	2:C:235:ILE:O	2.17	0.54
2:C:441:SER:O	2:C:456:GLY:N	2.40	0.54
2:D:243:ASP:OD1	2:D:244:SER:N	2.39	0.54
1:B:113:GLY:HA3	1:B:116:PHE:HD2	1.73	0.54
2:C:262:LEU:HD23	2:C:317:LEU:HD11	1.89	0.54
2:C:349:SER:OG	2:C:353:SER:O	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:457:THR:HG22	2:D:459:GLU:N	2.22	0.54
2:D:492:VAL:HG22	2:D:502:THR:HG22	1.89	0.54
2:D:416:TYR:O	2:D:417:ARG:NE	2.40	0.53
2:C:118:MET:H	2:C:134:GLY:HA2	1.71	0.53
1:A:121:ASN:O	1:A:125:ILE:HG13	2.09	0.53
2:D:262:LEU:HD23	2:D:317:LEU:HD11	1.89	0.53
2:D:299:ILE:HG13	2:D:312:GLU:O	2.08	0.53
1:B:121:ASN:O	1:B:125:ILE:HG13	2.08	0.53
2:C:92:HIS:HD2	2:C:107:LEU:HA	1.72	0.53
2:D:487:SER:HB2	2:D:505:ILE:HB	1.90	0.53
2:C:215:SER:HB3	2:C:234:TYR:HB3	1.91	0.53
2:C:299:ILE:HG13	2:C:312:GLU:O	2.08	0.53
2:C:127:ASP:OD1	2:C:129:GLN:NE2	2.42	0.53
2:C:233:SER:OG	2:C:286:SER:O	2.26	0.53
1:A:113:GLY:HA3	1:A:116:PHE:HD2	1.73	0.53
1:A:188:TRP:HB3	1:A:200:VAL:HA	1.89	0.53
2:C:284:ILE:HG22	2:C:286:SER:H	1.74	0.53
2:C:487:SER:HB2	2:C:505:ILE:HB	1.90	0.53
2:D:215:SER:HB3	2:D:234:TYR:HB3	1.91	0.53
2:D:269:LEU:HD22	2:D:387:GLN:HB3	1.91	0.53
1:B:143:THR:HB	1:B:199:GLU:HG2	1.91	0.52
1:A:143:THR:HB	1:A:199:GLU:HG2	1.91	0.52
2:C:350:LYS:HG2	2:C:357:MET:HG3	1.92	0.52
2:D:244:SER:HB2	2:D:266:ARG:HH12	1.74	0.52
2:D:284:ILE:HG22	2:D:286:SER:H	1.74	0.52
1:B:70:CYS:HA	1:B:98:TRP:CZ2	2.45	0.52
2:C:269:LEU:HD22	2:C:387:GLN:HB3	1.92	0.52
2:D:127:ASP:OD1	2:D:129:GLN:NE2	2.42	0.52
2:D:188:VAL:O	2:D:189:LYS:NZ	2.41	0.52
1:A:67:ALA:HB2	1:A:89:PHE:CG	2.45	0.52
1:B:152:TRP:CH2	1:B:189:CYS:HA	2.45	0.52
2:D:46:PHE:HE1	2:D:80:LYS:HB2	1.75	0.52
2:C:266:ARG:HA	2:C:274:PHE:HA	1.92	0.51
2:D:85:LYS:NZ	2:D:87:GLY:H	2.09	0.51
1:B:64:VAL:O	1:B:94:LYS:HB3	2.11	0.51
2:C:244:SER:HB2	2:C:266:ARG:HH12	1.74	0.51
2:D:299:ILE:O	2:D:427:VAL:HA	2.10	0.51
2:C:85:LYS:NZ	2:C:87:GLY:H	2.09	0.51
2:D:42:GLN:HE22	2:D:45:ASN:HD21	1.58	0.51
2:C:46:PHE:HE1	2:C:80:LYS:HB2	1.75	0.51
2:C:173:PRO:HB2	2:C:226:PHE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:266:ARG:HA	2:D:274:PHE:HA	1.92	0.51
2:D:143:ARG:HG3	2:D:159:HIS:ND1	2.26	0.51
2:D:173:PRO:HB2	2:D:226:PHE:O	2.10	0.51
2:D:350:LYS:HG2	2:D:357:MET:HG3	1.92	0.51
1:A:64:VAL:O	1:A:94:LYS:HB3	2.10	0.51
2:C:143:ARG:HG3	2:C:159:HIS:ND1	2.26	0.51
2:D:53:GLN:N	2:D:53:GLN:OE1	2.44	0.51
1:A:70:CYS:HA	1:A:98:TRP:CZ2	2.44	0.50
2:C:299:ILE:O	2:C:427:VAL:HA	2.10	0.50
2:C:328:GLN:N	2:C:449:ASP:OD1	2.43	0.50
1:A:152:TRP:CH2	1:A:189:CYS:HA	2.45	0.50
2:C:247:ILE:HA	2:C:265:GLN:HB3	1.93	0.50
2:C:53:GLN:N	2:C:53:GLN:OE1	2.44	0.50
2:D:328:GLN:N	2:D:449:ASP:OD1	2.43	0.50
2:C:42:GLN:HE22	2:C:45:ASN:HD21	1.58	0.50
2:D:265:GLN:NE2	2:D:277:ARG:HE	2.03	0.50
1:A:67:ALA:HA	1:A:70:CYS:SG	2.52	0.50
1:B:67:ALA:HB2	1:B:89:PHE:CG	2.45	0.50
1:A:49:THR:HB	1:A:116:PHE:CB	2.42	0.49
1:B:67:ALA:HA	1:B:70:CYS:SG	2.52	0.49
2:C:430:PHE:HB3	2:C:433:GLN:HB3	1.94	0.49
1:A:47:LYS:HB3	1:A:112:PHE:CE2	2.47	0.49
2:C:188:VAL:O	2:C:189:LYS:NZ	2.41	0.49
2:D:46:PHE:CE1	2:D:80:LYS:HB2	2.47	0.49
1:B:49:THR:HB	1:B:116:PHE:CB	2.42	0.49
2:D:247:ILE:HA	2:D:265:GLN:HB3	1.93	0.49
2:C:70:ILE:HD12	2:C:84:TYR:HD2	1.77	0.49
2:D:60:HIS:ND1	2:D:75:GLU:OE2	2.45	0.49
2:C:373:PHE:HA	2:C:377:ILE:HG22	1.94	0.49
2:C:48:ALA:HB1	2:C:71:TYR:HE1	1.78	0.49
2:D:90:LEU:HD11	2:D:107:LEU:HD11	1.94	0.49
2:D:430:PHE:HB3	2:D:433:GLN:HB3	1.94	0.49
1:A:176:TYR:O	1:A:178:ARG:HG2	2.13	0.49
1:B:47:LYS:HB3	1:B:112:PHE:CE2	2.48	0.49
2:D:48:ALA:HB1	2:D:71:TYR:HE1	1.78	0.49
2:D:325:PRO:HB3	2:D:341:ILE:HD12	1.95	0.49
2:D:523:PHE:HD2	2:D:528:GLN:HG3	1.78	0.49
1:A:158:HIS:HB3	1:A:197:ARG:NH1	2.28	0.48
2:C:46:PHE:CE1	2:C:80:LYS:HB2	2.47	0.48
2:C:379:ASN:ND2	2:C:382:ASN:OD1	2.41	0.48
2:D:373:PHE:HA	2:D:377:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:ILE:HD12	2:D:84:TYR:HD2	1.77	0.48
1:B:176:TYR:O	1:B:178:ARG:HG2	2.13	0.48
2:C:332:GLN:OE1	2:C:469:ARG:N	2.24	0.48
2:C:53:GLN:N	2:C:65:GLY:O	2.44	0.48
2:C:523:PHE:HD2	2:C:528:GLN:HG3	1.78	0.48
2:D:317:LEU:HD23	2:D:318:GLN:N	2.29	0.48
2:C:317:LEU:HD23	2:C:318:GLN:N	2.29	0.48
2:D:379:ASN:ND2	2:D:382:ASN:OD1	2.41	0.48
2:C:176:VAL:HA	2:C:217:ARG:NH1	2.29	0.48
2:C:325:PRO:HB3	2:C:341:ILE:HD12	1.95	0.48
2:D:176:VAL:HA	2:D:217:ARG:NH1	2.29	0.48
2:D:428:ASP:OD1	2:D:430:PHE:N	2.27	0.48
1:A:67:ALA:HB2	1:A:89:PHE:CD2	2.49	0.47
1:B:158:HIS:HB3	1:B:197:ARG:NH1	2.28	0.47
2:C:221:GLU:O	2:C:223:LYS:HE3	2.14	0.47
2:C:328:GLN:HA	2:C:331:ARG:HH22	1.79	0.47
2:C:359:ARG:HG2	2:C:435:SER:O	2.14	0.47
2:D:484:HIS:HB2	2:D:506:THR:HG22	1.96	0.47
2:C:90:LEU:HD11	2:C:107:LEU:HD11	1.94	0.47
2:D:221:GLU:O	2:D:223:LYS:HE3	2.14	0.47
2:D:359:ARG:HG2	2:D:435:SER:O	2.14	0.47
2:C:484:HIS:HB2	2:C:506:THR:HG22	1.96	0.47
2:D:329:LEU:HA	2:D:332:GLN:HB2	1.96	0.47
2:D:495:THR:HG22	2:D:496:LEU:HD23	1.97	0.47
1:A:152:TRP:CG	1:A:172:LEU:HD13	2.50	0.47
2:C:60:HIS:ND1	2:C:75:GLU:OE2	2.45	0.47
2:D:213:SER:OG	2:D:235:ILE:O	2.17	0.47
2:D:328:GLN:HA	2:D:331:ARG:HH22	1.79	0.47
2:D:267:GLU:HB3	2:D:273:THR:HG23	1.97	0.47
1:B:152:TRP:CG	1:B:172:LEU:HD13	2.50	0.47
2:D:53:GLN:N	2:D:65:GLY:O	2.44	0.47
2:C:329:LEU:HA	2:C:332:GLN:HB2	1.96	0.47
2:C:139:GLY:HA2	2:C:177:VAL:HG22	1.97	0.46
2:D:139:GLY:HA2	2:D:177:VAL:HG22	1.97	0.46
1:B:50:LEU:HD13	1:B:108:VAL:HG11	1.97	0.46
1:B:67:ALA:HB2	1:B:89:PHE:CD2	2.49	0.46
2:C:275:HIS:CE1	2:C:295:PRO:HB3	2.50	0.46
2:D:275:HIS:CE1	2:D:295:PRO:HB3	2.51	0.46
1:A:183:GLU:HG3	1:A:185:GLY:H	1.81	0.46
2:C:360:SER:OG	2:C:438:LEU:HA	2.16	0.46
1:B:83:THR:O	1:B:100:PRO:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:SER:OG	2:D:438:LEU:HA	2.16	0.46
1:A:73:ARG:HD3	1:A:98:TRP:CH2	2.51	0.46
1:A:83:THR:O	1:A:100:PRO:HA	2.15	0.46
1:B:73:ARG:HD3	1:B:98:TRP:CH2	2.51	0.46
1:B:183:GLU:HG3	1:B:185:GLY:H	1.81	0.46
2:C:426:ARG:HA	2:C:426:ARG:HD3	1.65	0.46
2:C:501:TYR:CG	2:C:512:LYS:HE3	2.51	0.46
1:B:99:PHE:HB3	1:B:101:PHE:CZ	2.51	0.46
1:B:152:TRP:CB	1:B:172:LEU:HD13	2.46	0.46
2:D:127:ASP:O	2:D:129:GLN:HG2	2.15	0.46
2:D:501:TYR:CG	2:D:512:LYS:HE3	2.51	0.46
1:A:156:ILE:HG13	2:D:373:PHE:HE1	1.81	0.46
2:C:127:ASP:O	2:C:129:GLN:HG2	2.15	0.46
2:C:495:THR:HG22	2:C:496:LEU:HD23	1.97	0.46
1:A:50:LEU:HD13	1:A:108:VAL:HG11	1.97	0.46
1:A:164:PRO:HG3	1:A:172:LEU:HD11	1.97	0.46
1:B:181:ARG:HG3	2:C:304:ARG:HG2	1.97	0.46
2:C:267:GLU:HB3	2:C:273:THR:HG23	1.97	0.46
2:D:448:GLY:N	2:D:498:GLN:OE1	2.49	0.46
1:A:170:LYS:HA	1:A:170:LYS:HD2	1.82	0.45
2:C:245:TYR:CD2	2:C:266:ARG:HB2	2.52	0.45
2:C:386:LEU:HD22	2:C:389:PHE:H	1.82	0.45
2:C:448:GLY:N	2:C:498:GLN:OE1	2.49	0.45
2:D:245:TYR:CD2	2:D:266:ARG:HB2	2.52	0.45
1:A:99:PHE:HB3	1:A:101:PHE:CZ	2.51	0.45
1:A:152:TRP:CB	1:A:172:LEU:HD13	2.46	0.45
1:A:198:TYR:CD2	2:D:305:LYS:HD2	2.52	0.45
2:D:267:GLU:N	2:D:273:THR:O	2.35	0.45
2:D:46:PHE:N	2:D:78:LEU:HD23	2.32	0.45
2:D:277:ARG:HD2	2:D:293:GLU:OE1	2.17	0.45
1:B:205:GLN:OE1	1:B:206:CYS:N	2.50	0.44
2:C:267:GLU:N	2:C:273:THR:O	2.35	0.44
2:C:277:ARG:HD2	2:C:293:GLU:OE1	2.17	0.44
2:D:386:LEU:HD22	2:D:389:PHE:H	1.81	0.44
2:C:88:PRO:HB3	2:C:114:ASP:HA	1.99	0.44
2:C:342:LEU:HD23	2:C:343:PHE:N	2.32	0.44
1:A:205:GLN:OE1	1:A:206:CYS:N	2.50	0.44
1:B:90:ASP:O	1:B:94:LYS:N	2.50	0.44
2:C:228:PHE:HD1	2:C:234:TYR:HD1	1.66	0.44
2:D:88:PRO:HB3	2:D:114:ASP:HA	1.99	0.44
2:D:219:LEU:HB2	2:D:226:PHE:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:342:LEU:HD23	2:D:343:PHE:N	2.32	0.44
1:A:90:ASP:O	1:A:94:LYS:N	2.50	0.44
1:B:164:PRO:HG3	1:B:172:LEU:HD11	1.97	0.44
1:B:170:LYS:HA	1:B:170:LYS:HD2	1.82	0.44
1:B:181:ARG:HA	1:B:181:ARG:HD3	1.76	0.44
2:D:228:PHE:HD1	2:D:234:TYR:HD1	1.66	0.44
1:A:83:THR:OG1	1:B:144:LYS:O	2.34	0.44
1:B:63:LYS:HA	1:B:95:GLN:HA	2.00	0.44
1:B:183:GLU:HB3	1:B:188:TRP:HE1	1.83	0.44
2:C:60:HIS:HA	2:C:75:GLU:CD	2.39	0.44
2:C:183:LYS:HA	2:C:183:LYS:HD3	1.77	0.43
2:D:267:GLU:HG3	2:D:275:HIS:ND1	2.33	0.43
2:C:441:SER:H	2:C:456:GLY:HA3	1.83	0.43
2:D:441:SER:H	2:D:456:GLY:HA3	1.83	0.43
2:C:46:PHE:N	2:C:78:LEU:HD23	2.32	0.43
2:D:55:VAL:HG23	2:D:505:ILE:HD11	1.99	0.43
2:C:546:VAL:O	2:C:556:TRP:NE1	2.51	0.43
2:D:379:ASN:OD1	2:D:382:ASN:N	2.51	0.43
2:D:70:ILE:O	2:D:83:GLU:HA	2.18	0.43
1:A:85:LYS:HG2	1:A:124:TYR:CD1	2.54	0.43
1:A:159:GLU:HG3	2:D:427:VAL:HG22	2.01	0.43
1:A:183:GLU:HB3	1:A:188:TRP:HE1	1.83	0.43
1:B:102:ASN:HB2	1:B:120:GLU:HG2	2.01	0.43
2:C:329:LEU:O	2:C:333:ILE:HG12	2.19	0.43
2:D:332:GLN:OE1	2:D:469:ARG:N	2.24	0.43
2:C:131:ILE:HG23	2:C:143:ARG:HB3	2.01	0.43
2:D:131:ILE:HG23	2:D:143:ARG:HB3	2.01	0.43
2:D:329:LEU:O	2:D:333:ILE:HG12	2.19	0.43
1:A:63:LYS:HA	1:A:95:GLN:HA	2.00	0.43
2:C:193:ILE:HG13	2:C:195:PHE:CZ	2.53	0.43
2:C:292:MET:HB2	2:C:374:PHE:CE2	2.54	0.43
2:D:193:ILE:HG13	2:D:195:PHE:CZ	2.53	0.43
2:D:277:ARG:HG2	2:D:295:PRO:HA	2.01	0.43
2:D:60:HIS:HA	2:D:75:GLU:OE1	2.19	0.43
1:A:183:GLU:HB2	2:D:304:ARG:HD3	2.00	0.43
2:C:55:VAL:HG23	2:C:505:ILE:HD11	1.99	0.43
2:C:328:GLN:HA	2:C:331:ARG:NH2	2.34	0.43
2:D:245:TYR:HA	2:D:266:ARG:HD2	2.01	0.43
2:D:461:ARG:HA	2:D:480:LEU:HA	2.01	0.43
2:C:267:GLU:HG3	2:C:275:HIS:ND1	2.33	0.42
2:C:386:LEU:HD21	2:C:388:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:461:ARG:HA	2:C:480:LEU:HA	2.01	0.42
2:C:476:HIS:HD2	2:C:477:VAL:HG23	1.84	0.42
1:A:170:LYS:HE2	1:A:178:ARG:HD2	2.01	0.42
2:C:219:LEU:HB2	2:C:226:PHE:HE2	1.83	0.42
1:B:170:LYS:HE2	1:B:178:ARG:HD2	2.01	0.42
2:C:70:ILE:O	2:C:83:GLU:HA	2.18	0.42
2:C:245:TYR:HA	2:C:266:ARG:HD2	2.01	0.42
2:D:60:HIS:HA	2:D:75:GLU:CD	2.39	0.42
2:D:85:LYS:HZ3	2:D:87:GLY:H	1.67	0.42
1:A:149:CYS:HB3	1:A:189:CYS:HB2	1.92	0.42
2:C:386:LEU:HD22	2:C:389:PHE:HB2	2.02	0.42
2:C:445:PHE:CZ	2:C:452:ILE:HB	2.54	0.42
2:D:90:LEU:HD13	2:D:112:TRP:CE2	2.54	0.42
2:D:445:PHE:CZ	2:D:452:ILE:HB	2.54	0.42
2:C:90:LEU:HD13	2:C:112:TRP:CE2	2.54	0.42
2:C:328:GLN:O	2:C:332:GLN:HG3	2.20	0.42
2:D:328:GLN:O	2:D:332:GLN:HG3	2.20	0.42
2:D:386:LEU:HD21	2:D:388:HIS:CE1	2.54	0.42
2:C:60:HIS:HA	2:C:75:GLU:OE1	2.19	0.42
2:D:176:VAL:HG21	2:D:226:PHE:HE1	1.84	0.42
2:D:292:MET:HB2	2:D:374:PHE:CE2	2.54	0.42
2:D:546:VAL:O	2:D:556:TRP:NE1	2.51	0.42
1:B:85:LYS:HG2	1:B:124:TYR:CD1	2.54	0.42
1:B:156:ILE:HG13	2:C:373:PHE:HE1	1.85	0.42
2:C:176:VAL:HG21	2:C:226:PHE:HE1	1.84	0.42
2:C:267:GLU:CA	2:C:275:HIS:HB2	2.47	0.42
2:C:368:LYS:HG3	2:C:369:TYR:HD1	1.85	0.42
2:D:443:SER:OG	2:D:454:ASN:ND2	2.53	0.42
2:D:470:SER:O	2:D:470:SER:OG	2.35	0.42
2:D:460:GLY:HA2	2:D:486:VAL:HG23	2.02	0.42
2:C:277:ARG:HG2	2:C:295:PRO:HA	2.01	0.42
2:D:368:LYS:HG3	2:D:369:TYR:HD1	1.85	0.42
2:D:476:HIS:HD2	2:D:477:VAL:HG23	1.84	0.42
2:D:386:LEU:HD22	2:D:389:PHE:HB2	2.02	0.42
2:D:553:SER:OG	2:D:555:THR:HG22	2.20	0.42
1:A:102:ASN:HB2	1:A:120:GLU:HG2	2.01	0.41
2:C:96:PHE:HB2	2:C:99:GLN:HE22	1.85	0.41
1:A:90:ASP:HA	1:A:115:GLU:O	2.20	0.41
1:A:178:ARG:O	1:A:187:PRO:HA	2.20	0.41
2:C:443:SER:OG	2:C:454:ASN:ND2	2.53	0.41
2:C:460:GLY:HA2	2:C:486:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:484:HIS:CG	2:D:507:GLY:HA3	2.56	0.41
2:C:315:ASN:OD1	2:C:316:ILE:HG12	2.20	0.41
2:C:553:SER:OG	2:C:555:THR:HG22	2.20	0.41
2:D:96:PHE:HB2	2:D:99:GLN:HE22	1.85	0.41
2:D:231:ASP:HA	2:D:234:TYR:CE1	2.56	0.41
2:D:328:GLN:HA	2:D:331:ARG:NH2	2.34	0.41
2:D:380:LYS:HD3	2:D:380:LYS:HA	1.74	0.41
1:B:129:ILE:HG23	1:B:203:ILE:HG21	2.03	0.41
2:C:265:GLN:NE2	2:C:277:ARG:HE	2.03	0.41
2:C:295:PRO:HB2	2:C:423:ALA:HB2	2.02	0.41
2:D:276:THR:OG1	2:D:315:ASN:O	2.28	0.41
2:D:329:LEU:HA	2:D:332:GLN:CG	2.51	0.41
2:D:548:SER:HB3	2:D:556:TRP:CE3	2.56	0.41
2:D:360:SER:OG	2:D:438:LEU:HD12	2.20	0.41
1:B:178:ARG:O	1:B:187:PRO:HA	2.20	0.41
2:D:118:MET:N	2:D:133:CYS:O	2.54	0.41
1:A:53:ILE:HD11	1:A:109:LYS:HB2	2.03	0.41
1:B:87:PHE:HA	1:B:97:LEU:O	2.21	0.41
1:B:90:ASP:HA	1:B:115:GLU:O	2.20	0.41
1:B:149:CYS:HB3	1:B:189:CYS:HB2	1.92	0.41
1:B:157:PRO:HB3	2:C:373:PHE:HZ	1.86	0.41
2:C:329:LEU:HA	2:C:332:GLN:CG	2.51	0.41
2:C:360:SER:OG	2:C:438:LEU:HD12	2.20	0.41
2:D:157:GLU:HG3	2:D:159:HIS:NE2	2.36	0.41
2:D:267:GLU:CB	2:D:273:THR:HG23	2.51	0.41
1:A:152:TRP:HH2	1:A:189:CYS:HA	1.85	0.41
2:D:426:ARG:HA	2:D:426:ARG:HD3	1.65	0.41
1:A:129:ILE:HG23	1:A:203:ILE:HG21	2.03	0.40
2:C:484:HIS:CG	2:C:507:GLY:HA3	2.56	0.40
2:D:315:ASN:OD1	2:D:316:ILE:HG12	2.20	0.40
2:C:118:MET:N	2:C:133:CYS:O	2.54	0.40
2:C:231:ASP:HA	2:C:234:TYR:CE1	2.56	0.40
1:A:144:LYS:O	1:B:83:THR:OG1	2.39	0.40
2:C:157:GLU:HG3	2:C:159:HIS:NE2	2.36	0.40
2:D:186:SER:HA	2:D:194:ASN:O	2.21	0.40
2:D:295:PRO:HB2	2:D:423:ALA:HB2	2.03	0.40
1:A:43:LYS:O	1:A:119:TYR:HA	2.21	0.40
2:C:34:GLU:C	2:C:524:GLN:HB2	2.41	0.40
2:C:186:SER:HA	2:C:194:ASN:O	2.21	0.40
2:C:267:GLU:CB	2:C:273:THR:HG23	2.51	0.40
2:C:548:SER:HB3	2:C:556:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:373:PHE:CD1	2:C:377:ILE:HG21	2.57	0.40
2:D:373:PHE:CD1	2:D:377:ILE:HG21	2.57	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	A	170/210 (81%)	159 (94%)	11 (6%)	0	100	100
1	B	170/210 (81%)	159 (94%)	11 (6%)	0	100	100
2	C	475/1390 (34%)	444 (94%)	31 (6%)	0	100	100
2	D	475/1390 (34%)	444 (94%)	31 (6%)	0	100	100
All	All	1290/3200 (40%)	1206 (94%)	84 (6%)	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	A	154/189 (82%)	154 (100%)	0	100	100
1	B	154/189 (82%)	154 (100%)	0	100	100
2	C	440/1246 (35%)	440 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	440/1246 (35%)	440 (100%)	0	100	100
All	All	1188/2870 (41%)	1188 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	45	ASN
2	C	117	ASN
2	D	45	ASN
2	D	117	ASN

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.

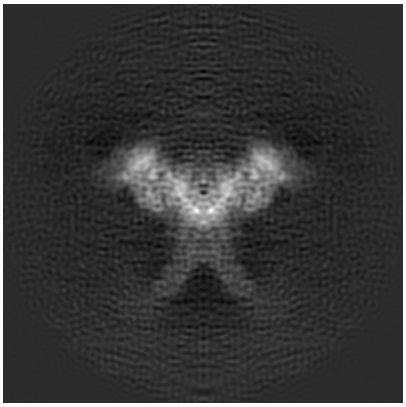
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23923. These allow visual inspection of the internal detail of the map and identification of artifacts.

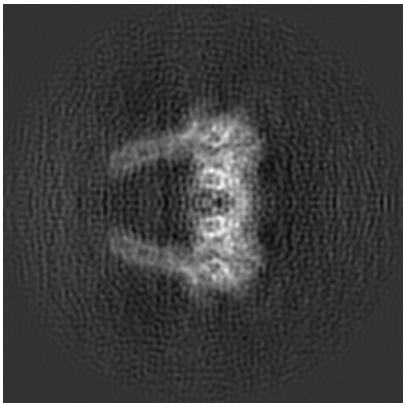
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

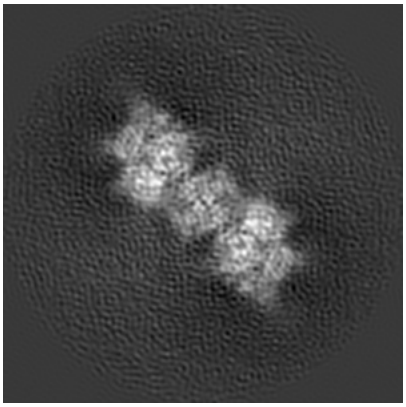
6.1.1 Primary map



X



Y

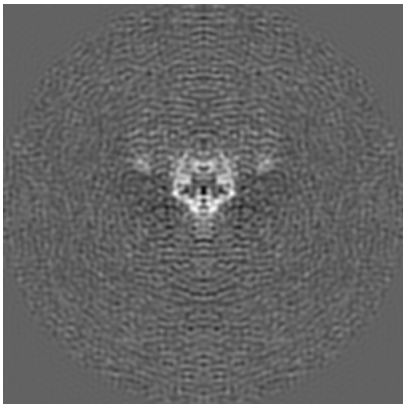


Z

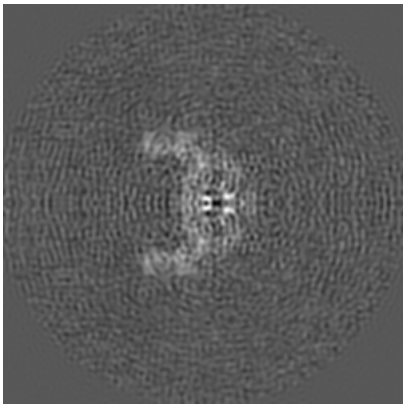
The images above show the map projected in three orthogonal directions.

6.2 Central slices

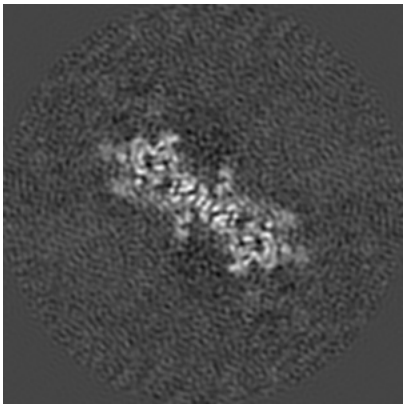
6.2.1 Primary map



X Index: 135



Y Index: 135

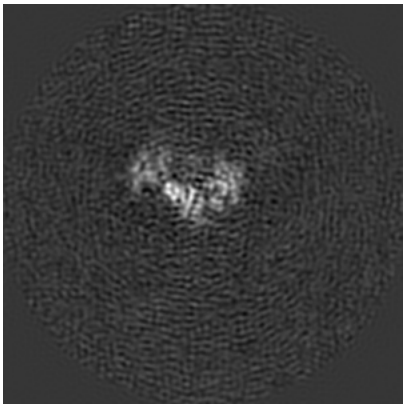


Z Index: 135

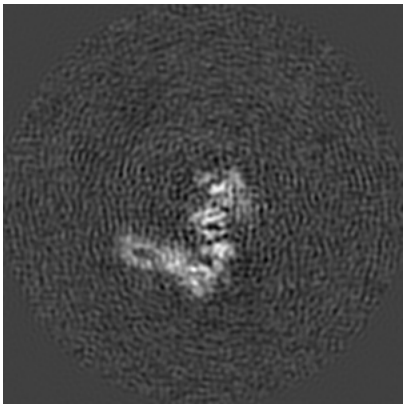
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

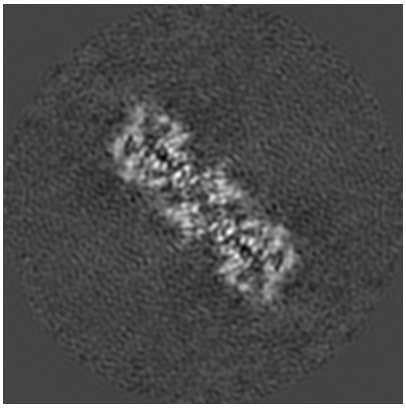
6.3.1 Primary map



X Index: 146



Y Index: 149



Z Index: 148

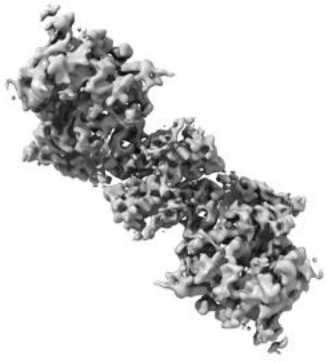
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

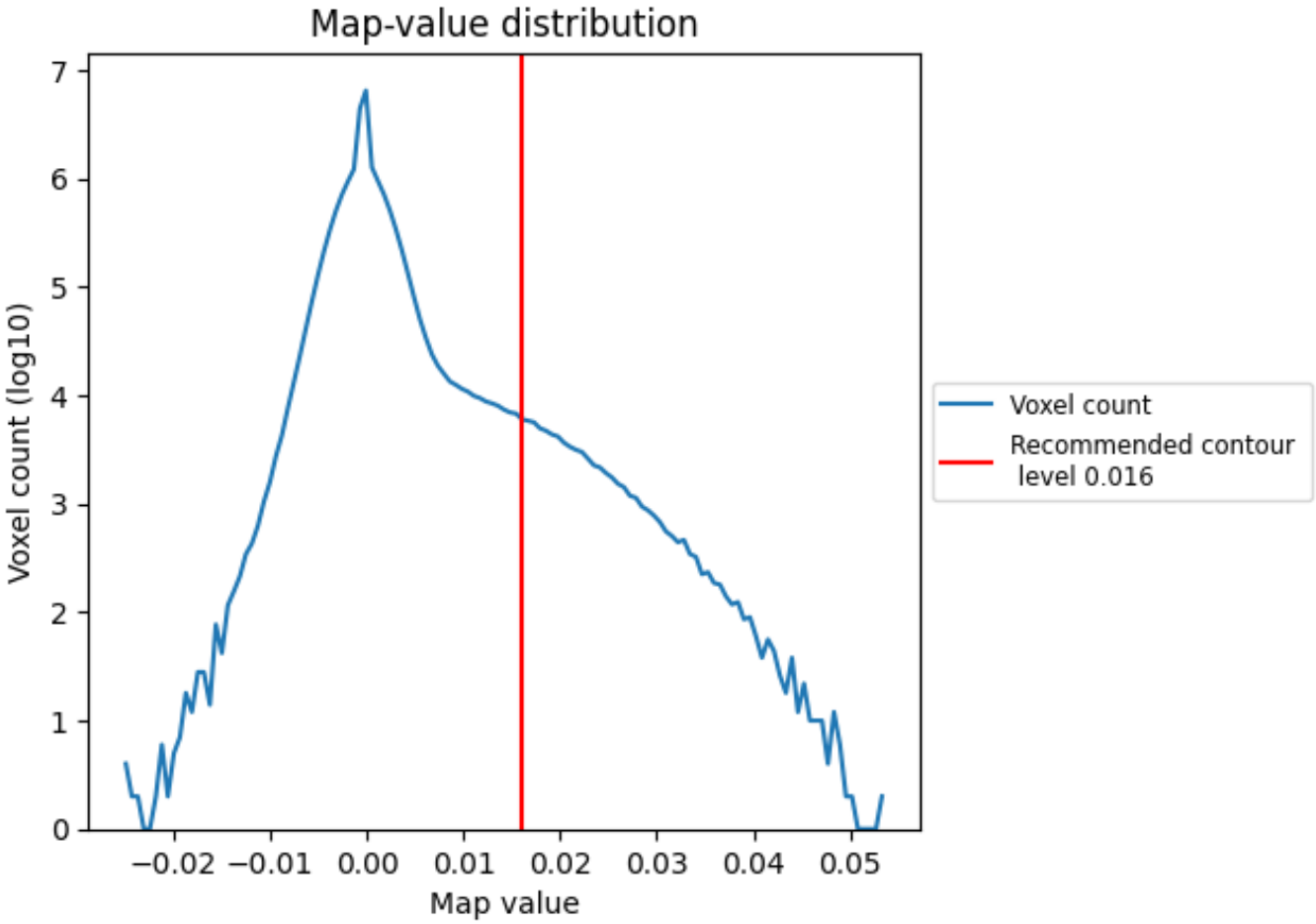
6.5 Mask visualisation (i)

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

7 Map analysis

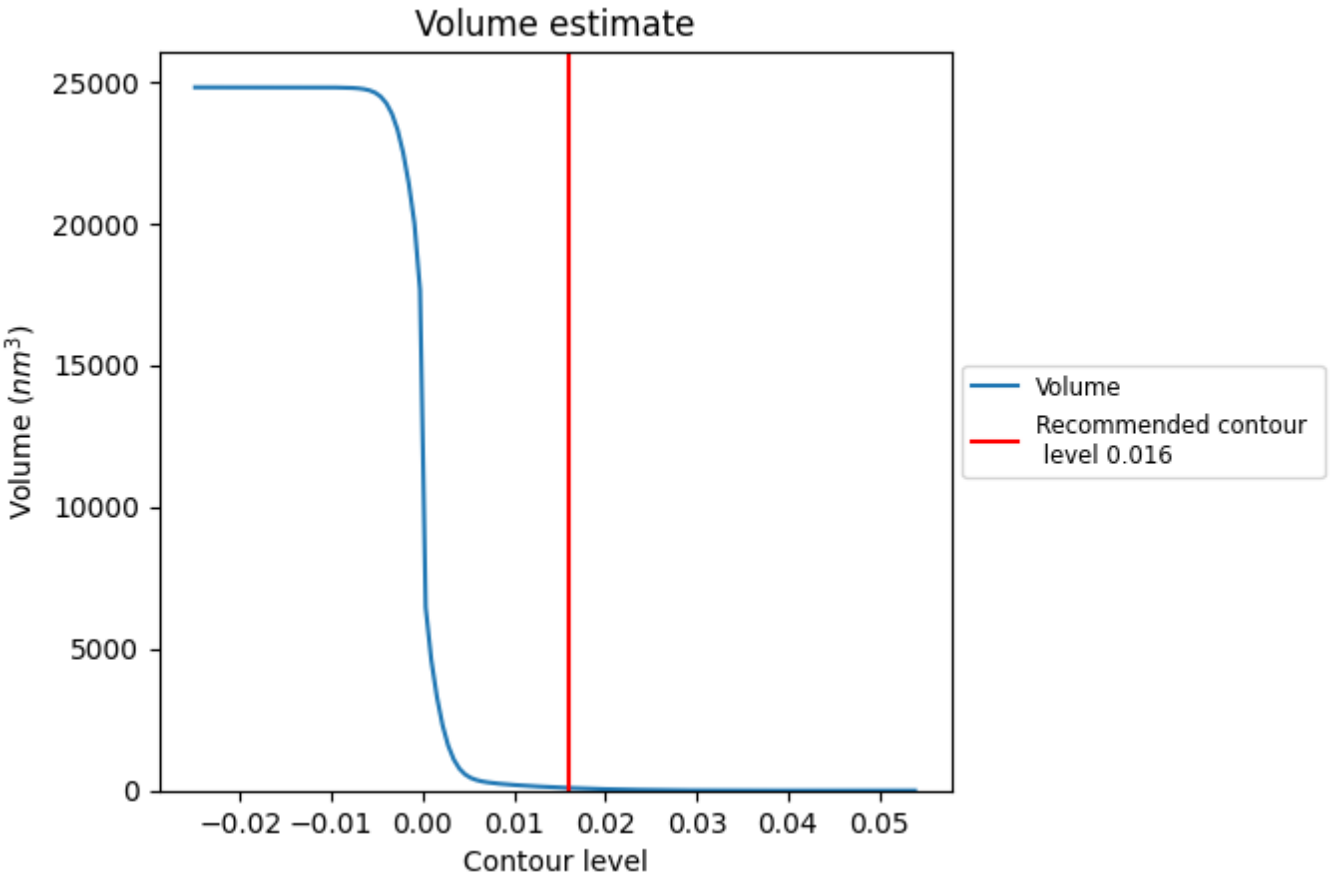
This section contains the results of statistical analysis of the map.

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.

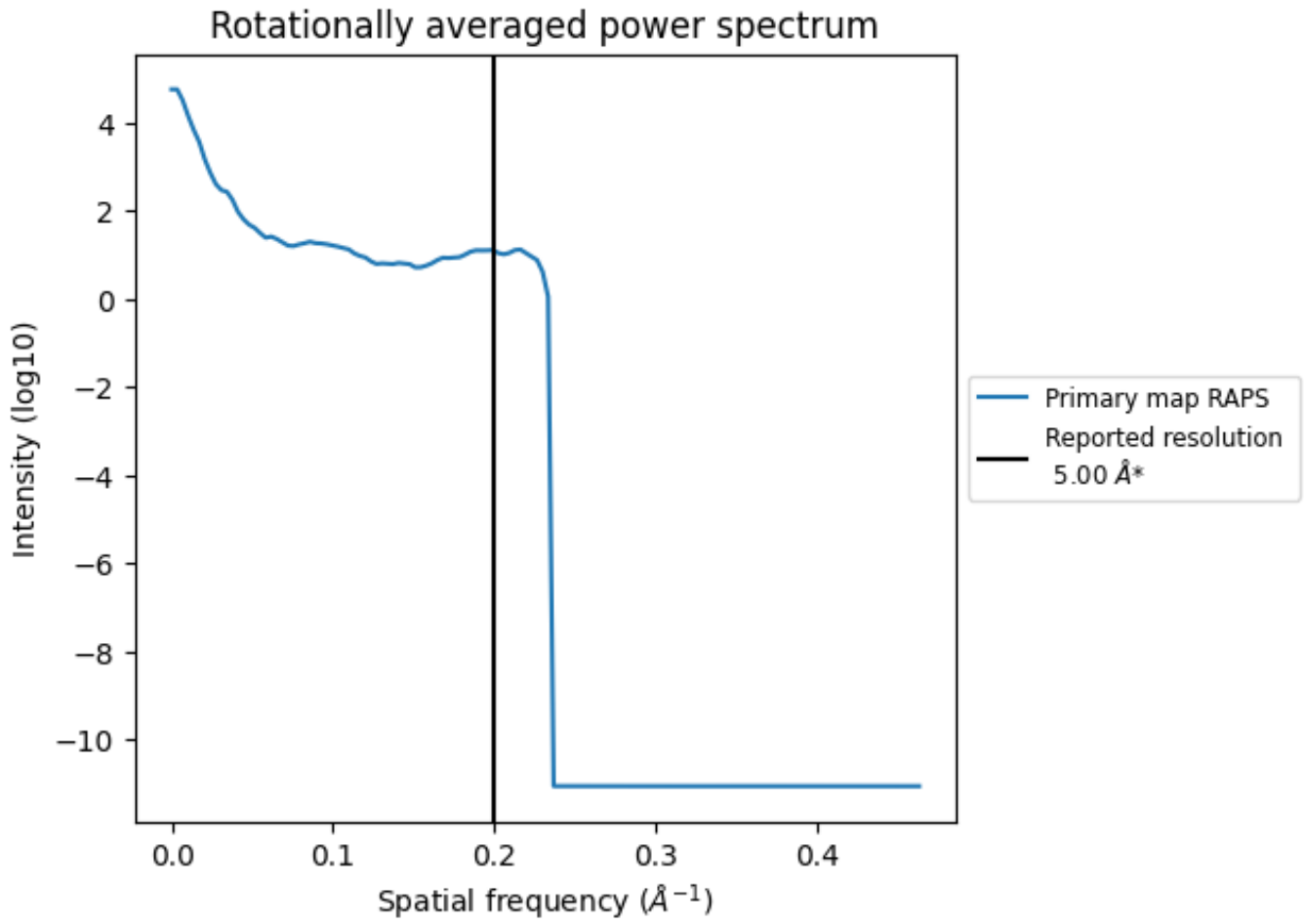
7.2 Volume estimate



The volume at the recommended contour level is 92 nm^3; this corresponds to an approximate mass of 83 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 0.200 Å^{-1}

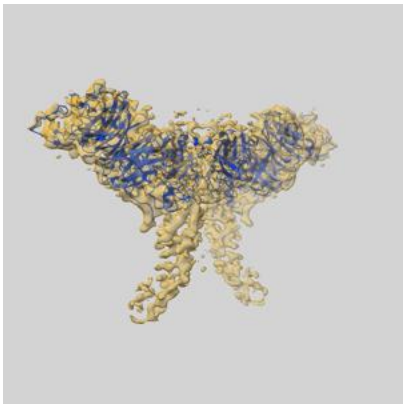
8 Fourier-Shell correlation (i)

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

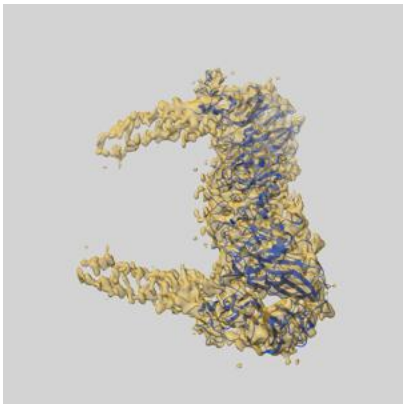
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23923 and PDB model 7MOB. Per-residue inclusion information can be found in section 3 on page 4.

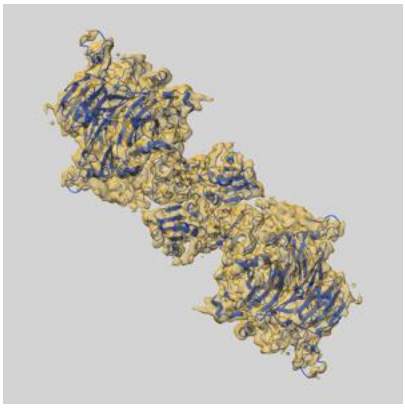
9.1 Map-model overlay



X



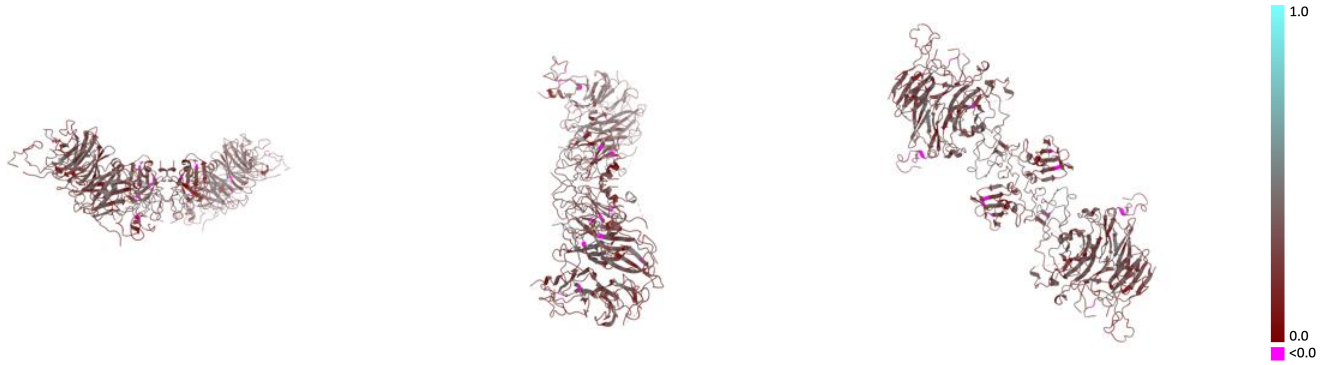
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

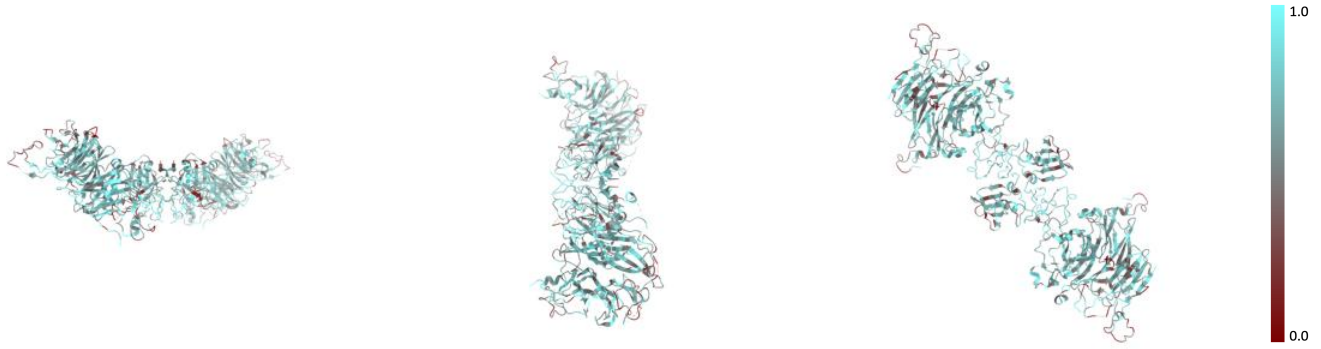
9.2 Q-score mapped to coordinate model (i)



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.

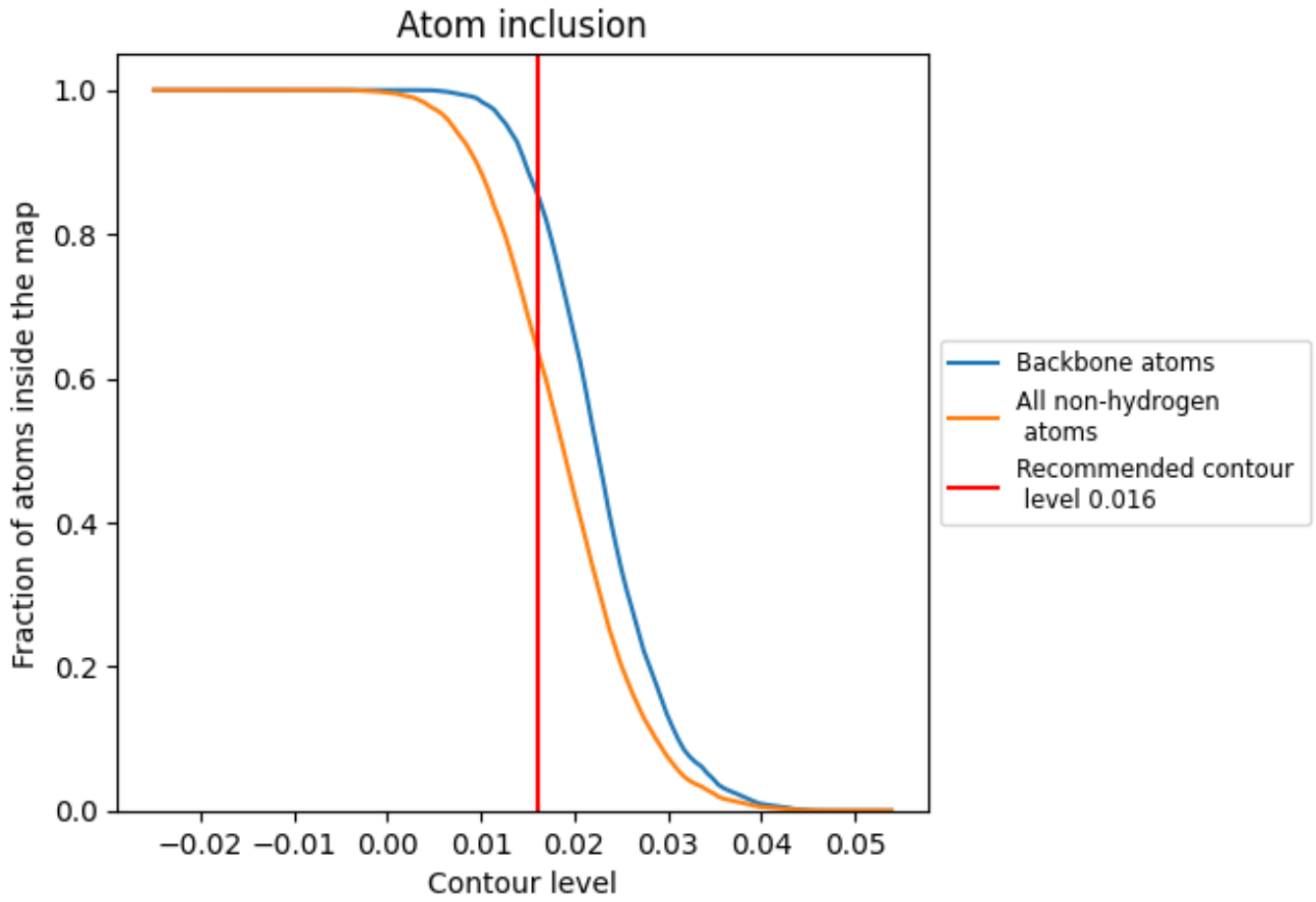
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6411	0.2960
A	0.6657	0.3040
B	0.6694	0.3030
C	0.6321	0.2920
D	0.6313	0.2930