



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 07:41 AM UTC

PDB ID : 7MOA / pdb_00007moa
EMDB ID : EMD-23922
Title : Cryo-EM structure of the c-MET II/HGF I complex bound with HGF II in a rigid conformation
Authors : Uchikawa, E.; Chen, Z.M.; Xiao, G.Y.; Zhang, X.W.; Bai, X.C.
Deposited on : 2021-05-01
Resolution : 4.90 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:

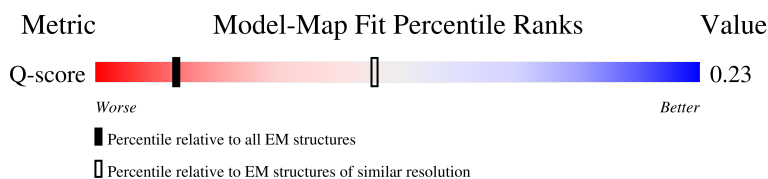
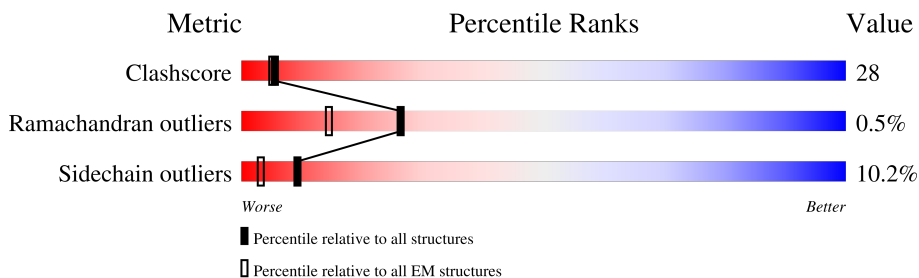
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.90 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.



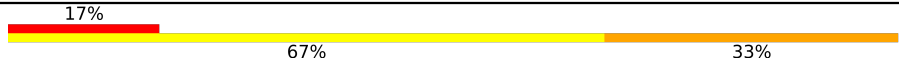
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1274 (4.40 - 5.40)

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 $\leq 5\%$. 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	728	<p>13% 20% 65%</p>
1	D	728	<p>11% 42% 42% 12%</p>
2	E	1390	<p>26% 22% 51%</p>
3	F	6	<p>33% 67% 33%</p>

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Mol	Chain	Length	Quality of chain
3	J	6	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '17%', a yellow segment in the middle labeled '67%', and an orange segment on the right labeled '33%'. The segments are stacked horizontally to total 100%.</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12511 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.

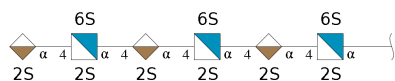
- Molecule 1 is a protein called Hepatocyte growth factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	254	Total	C	N	O	S	0	0
			2047	1283	370	373	21		
1	D	638	Total	C	N	O	S	0	0
			4946	3104	882	909	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	688	Total	C	N	O	S	0	0
			5324	3373	905	1006	40		

- Molecule 3 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	6	Total	C	N	O	S	0	0
			97	35	3	51	8		
3	J	6	Total	C	N	O	S	0	0
			97	35	3	51	8		

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

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

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

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose



SGN1
IDS2
SGN3
IDS4
SGN5
IDS6

- Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose



SGN1
IDS2
SGN3
IDS4
SGN5
IDS6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12513	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 ($e^-/\text{\AA}^2$)	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	0.041	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.52	0/2105	0.86	0/2840
1	D	0.59	0/5081	0.84	3/6901 (0.0%)
2	E	0.63	0/5444	0.84	1/7397 (0.0%)
All	All	0.60	0/12630	0.84	4/17138 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	88	PRO	N-CA-C	-5.83	101.94	111.21
1	D	352	ASN	N-CA-C	-5.33	106.61	113.01
1	D	368	THR	N-CA-C	-5.25	105.67	111.71
1	D	39	ILE	N-CA-C	-5.05	105.47	110.62

There are no chirality outliers.

There are no planarity outliers.

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	A	2047	0	1933	168	0
1	D	4946	0	4584	276	0
2	E	5324	0	5126	237	0
3	F	97	0	34	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	97	0	34	3	0
All	All	12511	0	11711	670	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 28.

All (670) 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:E:402:LEU:HB3	2:E:404:ARG:HG3	1.15	1.10
2:E:189:LYS:O	2:E:192:PHE:HB2	1.55	1.04
1:D:415:TRP:HB2	1:D:438:ASN:H	1.35	0.91
2:E:176:VAL:HA	2:E:217:ARG:HH21	1.35	0.91
2:E:402:LEU:HB3	2:E:404:ARG:CG	2.01	0.87
2:E:382:ASN:HD22	2:E:422:THR:HG21	1.40	0.86
2:E:65:GLY:HA3	2:E:117:ASN:HD22	1.42	0.85
1:D:657:ILE:HG12	1:D:708:ARG:HB2	1.57	0.84
1:A:66:THR:HG23	1:A:69:GLN:H	1.41	0.84
2:E:498:GLN:HE21	1:D:184:GLU:HB3	1.40	0.84
2:E:118:MET:HE1	2:E:179:ALA:HA	1.60	0.83
1:D:389:GLN:N	1:D:467:SER:HG	1.77	0.83
1:A:275:ASP:OD1	1:A:277:HIS:ND1	2.10	0.82
1:A:81:PRO:HG3	1:D:277:HIS:HB3	1.58	0.82
2:E:428:ASP:OD1	2:E:430:PHE:N	2.13	0.81
1:A:163:LEU:HD23	1:A:167:TYR:HE2	1.41	0.81
2:E:424:LEU:HD21	2:E:426:ARG:HH21	1.46	0.81
1:D:550:ILE:HD11	1:D:555:GLY:HA2	1.63	0.81
2:E:222:THR:OG1	2:E:224:ASP:OD1	1.98	0.81
1:A:243:HIS:NE2	1:A:245:PHE:O	2.14	0.80
1:D:552:ASP:OD1	1:D:556:ARG:NH2	2.15	0.80
2:E:247:ILE:HG22	2:E:265:GLN:HB3	1.63	0.80
2:E:62:ILE:HD13	2:E:503:LEU:HD21	1.64	0.80
1:D:653:ASN:OD1	1:D:654:GLU:N	2.16	0.78
2:E:666:TYR:HA	2:E:737:SER:HB3	1.64	0.78
2:E:498:GLN:NE2	1:D:184:GLU:CB	2.47	0.77
1:A:85:LYS:NZ	1:A:100:PRO:O	2.18	0.77
1:D:713:ALA:HA	1:D:716:ILE:HD12	1.67	0.77
1:A:64:VAL:HG11	1:A:69:GLN:HB3	1.68	0.76
1:D:73:ARG:HG2	3:J:3:SGN:H4	1.67	0.76
1:A:223:MET:HE1	1:A:260:CYS:HB2	1.68	0.76
1:D:126:ARG:O	1:D:127:ASN:OD1	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:640:GLU:O	1:D:644:GLN:NE2	2.18	0.75
1:D:177:CYS:HB3	1:D:189:CYS:HB3	1.66	0.75
1:D:76:ARG:HD2	3:J:4:IDS:H2	1.68	0.75
1:A:147:ILE:HG21	1:A:193:ASN:HB2	1.68	0.74
1:D:530:LEU:HD11	1:D:579:LEU:HD11	1.67	0.74
1:A:39:ILE:HA	1:A:42:PHE:HB2	1.70	0.74
2:E:547:ARG:NH1	2:E:548:SER:H	1.85	0.74
1:A:183:GLU:OE1	1:A:185:GLY:N	2.20	0.74
1:A:82:PHE:HZ	1:A:98:TRP:HB2	1.53	0.74
1:D:524:ILE:HG22	1:D:525:LYS:HD2	1.71	0.73
2:E:327:ALA:HB3	2:E:449:ASP:HB2	1.68	0.73
1:D:134:ARG:O	1:D:170:LYS:NZ	2.22	0.73
1:D:392:TYR:H	1:D:469:CYS:HB2	1.55	0.72
1:A:177:CYS:C	1:A:178:ARG:HD3	2.15	0.71
1:A:245:PHE:HA	1:A:250:TYR:HE2	1.54	0.71
1:D:602:TYR:HB2	1:D:714:LYS:HD3	1.72	0.71
2:E:358:ASP:HA	2:E:438:LEU:HB2	1.72	0.71
2:E:498:GLN:NE2	1:D:184:GLU:HB3	2.05	0.71
1:A:246:LEU:HG	1:A:249:ARG:HH11	1.56	0.71
1:A:96:CYS:SG	1:A:98:TRP:NE1	2.63	0.71
2:E:537:GLN:O	2:E:547:ARG:NH1	2.24	0.71
1:A:167:TYR:HB2	1:A:170:LYS:HG2	1.73	0.70
2:E:217:ARG:HD3	2:E:228:PHE:HE1	1.54	0.70
1:A:43:LYS:HB3	1:A:120:GLU:HB2	1.73	0.70
1:D:273:THR:HG22	1:D:275:ASP:H	1.57	0.70
1:D:310:GLY:HA2	1:D:313:TYR:HB3	1.74	0.69
2:E:379:ASN:HB2	2:E:380:LYS:HZ3	1.58	0.69
1:D:680:GLU:HA	1:D:685:ARG:HA	1.75	0.69
1:D:513:TYR:OH	1:D:514:ARG:NH2	2.25	0.69
1:A:88:VAL:HG23	1:A:99:PHE:CE2	2.28	0.69
1:A:227:GLU:HG3	1:A:284:ALA:HB2	1.75	0.69
2:E:91:GLU:O	2:E:110:GLY:N	2.26	0.69
1:D:507:TRP:CD1	1:D:597:ILE:HB	2.27	0.68
1:D:540:ASP:OD1	1:D:541:LEU:N	2.26	0.68
1:D:612:CYS:HB2	1:D:679:CYS:HA	1.76	0.68
1:A:234:ARG:NH2	1:A:236:ASP:OD2	2.27	0.68
2:E:343:PHE:HE2	2:E:444:THR:HG21	1.59	0.68
1:D:541:LEU:HD23	1:D:567:VAL:HG12	1.74	0.68
1:A:88:VAL:HG23	1:A:99:PHE:HE2	1.58	0.68
2:E:671:GLY:HA3	2:E:713:ALA:HA	1.75	0.68
1:D:214:CYS:HB3	1:D:348:ASP:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PHE:HD2	1:A:100:PRO:HB3	1.59	0.68
1:D:446:ASP:OD1	1:D:447:ALA:N	2.27	0.68
1:D:454:THR:OG1	1:D:459:ILE:O	2.11	0.68
2:E:60:HIS:HA	2:E:75:GLU:OE2	1.94	0.67
1:D:43:LYS:HG2	1:D:44:LYS:H	1.59	0.67
1:A:238:GLN:NE2	1:A:243:HIS:O	2.26	0.67
2:E:113:LYS:HG3	2:E:114:ASP:H	1.59	0.67
1:D:460:PRO:HB2	1:D:461:TRP:HD1	1.58	0.67
2:E:332:GLN:OE1	2:E:469:ARG:N	2.27	0.67
2:E:373:PHE:HA	2:E:377:ILE:HB	1.77	0.67
2:E:590:PHE:HB3	2:E:597:ASP:HB2	1.76	0.67
1:D:606:ILE:HD12	1:D:607:PRO:HD2	1.75	0.67
1:D:657:ILE:CG1	1:D:708:ARG:HB2	2.25	0.67
2:E:498:GLN:O	2:E:516:ASN:ND2	2.28	0.66
1:D:102:ASN:OD1	1:D:103:SER:N	2.28	0.66
2:E:27:LYS:H	2:E:27:LYS:HD2	1.60	0.66
2:E:498:GLN:NE2	1:D:184:GLU:HB2	2.11	0.66
2:E:213:SER:OG	2:E:235:ILE:O	2.13	0.66
1:D:561:CYS:HB3	1:D:593:PHE:CD2	2.31	0.66
2:E:46:PHE:HE2	2:E:80:LYS:HB3	1.60	0.66
1:D:90:ASP:OD1	1:D:115:GLU:HB2	1.96	0.65
1:D:524:ILE:HD12	1:D:599:LEU:HD21	1.79	0.65
2:E:211:LEU:O	2:E:212:HIS:ND1	2.29	0.65
1:D:279:ARG:HG3	1:D:280:TRP:HD1	1.60	0.65
1:A:144:LYS:HG2	1:A:202:ASP:HB3	1.77	0.65
1:D:540:ASP:OD1	1:D:542:LYS:N	2.27	0.64
1:A:223:MET:HE2	1:A:285:ILE:HD11	1.79	0.64
1:A:188:TRP:HA	1:A:200:VAL:HA	1.79	0.64
2:E:119:ALA:HB3	2:E:133:CYS:HB2	1.79	0.64
1:D:264:ASP:OD1	1:D:270:TRP:NE1	2.23	0.64
2:E:74:ASN:OD1	2:E:75:GLU:N	2.31	0.64
2:E:26:CYS:N	2:E:584:CYS:SG	2.70	0.64
2:E:498:GLN:HE22	1:D:184:GLU:HB2	1.63	0.64
1:A:90:ASP:HB3	1:A:93:ARG:HG2	1.79	0.64
1:D:496:VAL:O	1:D:666:SER:OG	2.13	0.63
1:D:152:TRP:N	1:D:174:GLU:O	2.28	0.63
1:D:606:ILE:HG12	1:D:636:ILE:HG13	1.80	0.63
1:D:318:ASN:HA	1:D:354:CYS:HB3	1.80	0.63
1:A:137:LYS:HD2	1:A:171:ASP:HB2	1.81	0.63
2:E:427:VAL:HG23	2:E:469:ARG:HH12	1.64	0.62
2:E:49:GLU:N	2:E:49:GLU:OE1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:261:PHE:HB2	2:E:279:ILE:HB	1.81	0.62
2:E:239:PRO:HA	2:E:242:ARG:NE	2.15	0.62
1:D:161:SER:C	1:D:163:LEU:H	2.06	0.62
2:E:46:PHE:CE2	2:E:80:LYS:HB3	2.35	0.62
1:A:150:GLN:NE2	1:A:154:SER:O	2.33	0.62
1:A:99:PHE:HB3	1:A:101:PHE:CE1	2.35	0.62
2:E:503:LEU:HB3	2:E:510:ILE:HD11	1.81	0.62
1:D:497:ASN:ND2	1:D:665:GLY:O	2.33	0.62
1:A:250:TYR:HB3	1:A:253:LYS:HD3	1.81	0.62
1:D:112:PHE:CZ	1:D:114:HIS:CE1	2.88	0.62
1:D:416:ASP:HA	1:D:419:MET:SD	2.40	0.61
2:E:126:TYR:OH	2:E:221:GLU:HG2	2.00	0.61
2:E:362:MET:HG2	2:E:430:PHE:CE2	2.35	0.61
1:A:87:PHE:HB2	1:A:98:TRP:HD1	1.65	0.61
1:A:85:LYS:HZ2	1:A:100:PRO:C	2.09	0.61
1:A:231:ILE:O	1:A:274:LEU:HD22	2.00	0.61
1:A:241:HIS:HB3	1:A:279:ARG:HH21	1.65	0.61
1:D:238:GLN:HB3	1:D:242:ARG:HG3	1.82	0.61
2:E:220:LYS:HE3	2:E:227:MET:SD	2.40	0.61
1:D:639:ASN:HB3	1:D:652:LEU:HD22	1.81	0.60
1:A:85:LYS:HB2	1:A:124:TYR:CE2	2.35	0.60
1:D:347:LYS:HB2	1:D:357:PRO:HB3	1.81	0.60
1:A:262:ASN:ND2	1:A:269:PRO:HA	2.16	0.60
2:E:149:ASN:OD1	2:E:150:HIS:N	2.34	0.60
1:A:188:TRP:HB3	1:A:200:VAL:HG22	1.82	0.60
1:A:219:TYR:CZ	1:A:221:GLY:HA3	2.37	0.60
1:D:87:PHE:CE2	1:D:89:PHE:HB2	2.36	0.60
1:A:73:ARG:NH2	3:F:3:SGN:O6S	2.35	0.60
1:A:102:ASN:OD1	1:A:104:MET:N	2.31	0.60
1:A:88:VAL:HG11	1:A:116:PHE:HB3	1.81	0.60
1:A:64:VAL:HG12	1:A:66:THR:H	1.65	0.60
1:A:150:GLN:NE2	1:A:156:ILE:O	2.35	0.60
1:D:538:SER:O	1:D:544:TYR:OH	2.10	0.60
1:A:220:ARG:HH21	1:A:261:ARG:HG3	1.67	0.60
1:D:43:LYS:HB2	1:D:122:LYS:HG2	1.84	0.60
1:A:35:ARG:HA	1:A:72:ASN:HD21	1.67	0.59
1:A:87:PHE:O	1:A:119:TYR:HB2	2.02	0.59
2:E:220:LYS:HG2	2:E:225:GLY:C	2.26	0.59
1:D:152:TRP:CH2	1:D:189:CYS:HA	2.37	0.59
1:A:108:VAL:C	1:A:109:LYS:HD3	2.28	0.59
1:A:163:LEU:HD12	1:A:163:LEU:H	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:TYR:HB3	1:A:261:ARG:NH1	2.16	0.59
2:E:196:PHE:CD1	2:E:216:VAL:HG22	2.37	0.59
1:D:508:MET:HA	1:D:508:MET:HE3	1.83	0.59
2:E:76:GLU:CD	2:E:76:GLU:H	2.10	0.59
2:E:80:LYS:O	2:E:80:LYS:HG3	2.02	0.59
1:D:85:LYS:NZ	1:D:100:PRO:O	2.36	0.59
1:D:103:SER:HA	1:D:108:VAL:HG21	1.84	0.59
1:A:164:PRO:HA	1:A:172:LEU:HD21	1.84	0.59
2:E:403:LEU:HD22	2:E:406:SER:HB2	1.85	0.59
1:A:207:SER:OG	1:A:208:GLU:OE2	2.16	0.59
2:E:238:LEU:HD12	2:E:240:GLU:H	1.68	0.59
2:E:196:PHE:HD1	2:E:216:VAL:HG22	1.68	0.59
1:D:579:LEU:HD12	1:D:580:VAL:H	1.68	0.59
2:E:623:LYS:HA	2:E:623:LYS:HE2	1.84	0.59
1:D:656:GLU:O	1:D:657:ILE:HD13	2.02	0.59
1:A:215:ASN:HD21	1:A:218:SER:H	1.51	0.58
2:E:341:ILE:HD13	2:E:366:PRO:HA	1.85	0.58
2:E:358:ASP:OD1	2:E:438:LEU:N	2.36	0.58
2:E:69:TYR:CD1	2:E:85:LYS:HG2	2.38	0.58
1:D:234:ARG:HG3	1:D:237:HIS:CE1	2.38	0.58
1:D:569:GLN:NE2	1:D:570:LEU:O	2.37	0.58
1:D:214:CYS:HB3	1:D:348:ASP:CB	2.34	0.58
1:D:217:GLU:HA	1:D:262:ASN:HB3	1.85	0.58
2:E:220:LYS:HG2	2:E:225:GLY:O	2.04	0.57
2:E:360:SER:OG	2:E:439:LEU:HG	2.05	0.57
1:D:452:CYS:SG	1:D:453:TYR:N	2.76	0.57
1:D:640:GLU:O	1:D:643:SER:OG	2.18	0.57
2:E:730:ASN:CG	2:E:731:ARG:H	2.12	0.57
1:D:554:HIS:HB2	1:D:556:ARG:HE	1.69	0.57
1:A:77:ASN:C	1:A:79:GLY:H	2.13	0.57
1:A:183:GLU:CD	1:A:185:GLY:H	2.11	0.57
1:D:85:LYS:HD2	1:D:101:PHE:HA	1.86	0.57
1:D:262:ASN:ND2	1:D:266:GLN:O	2.38	0.57
1:A:234:ARG:HE	1:A:237:HIS:CE1	2.23	0.56
2:E:113:LYS:HG3	2:E:114:ASP:N	2.19	0.56
1:D:191:THR:HG22	1:D:193:ASN:H	1.69	0.56
1:D:712:TYR:O	1:D:716:ILE:HG13	2.03	0.56
2:E:460:GLY:HA3	2:E:482:ASP:O	2.05	0.56
1:D:547:TRP:HD1	1:D:564:VAL:HA	1.69	0.56
1:A:125:ILE:HD12	1:A:125:ILE:H	1.70	0.56
1:D:228:SER:OG	1:D:281:GLU:OE1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:SER:OG	1:D:583:LYS:O	2.18	0.56
1:D:600:PRO:HG3	1:D:709:VAL:HG23	1.88	0.56
2:E:611:THR:OG1	2:E:625:THR:O	2.23	0.56
2:E:659:ILE:HD11	2:E:677:LEU:HD12	1.87	0.56
1:D:354:CYS:HB2	1:D:365:CYS:HB3	1.86	0.56
1:D:422:LEU:O	1:D:426:ILE:N	2.34	0.56
2:E:619:MET:SD	2:E:619:MET:N	2.78	0.56
1:D:556:ARG:NH2	1:D:626:ASP:O	2.38	0.56
1:D:717:HIS:O	1:D:720:ILE:HG22	2.05	0.56
2:E:69:TYR:CE1	2:E:85:LYS:HG2	2.41	0.56
2:E:190:ASP:HB3	1:D:534:GLN:HE22	1.71	0.56
1:D:88:VAL:HG22	1:D:118:LEU:HA	1.88	0.56
1:A:177:CYS:HB2	1:A:189:CYS:HB3	1.88	0.55
2:E:599:LYS:NZ	2:E:600:LYS:HE2	2.21	0.55
1:A:223:MET:SD	1:A:225:HIS:N	2.75	0.55
1:D:511:LEU:HD11	1:D:536:PHE:HE1	1.71	0.55
1:D:591:ASP:OD1	1:D:593:PHE:N	2.35	0.55
1:D:643:SER:OG	1:D:644:GLN:NE2	2.39	0.55
1:A:246:LEU:HB2	1:A:249:ARG:HD2	1.89	0.55
2:E:730:ASN:OD1	2:E:731:ARG:N	2.39	0.55
1:A:190:PHE:CD1	1:A:198:TYR:HB3	2.41	0.55
2:E:362:MET:HE2	2:E:429:LEU:HD12	1.88	0.55
1:A:89:PHE:CE1	1:A:96:CYS:HB3	2.42	0.55
1:A:259:TYR:HB3	1:A:261:ARG:HH12	1.71	0.55
2:E:101:CYS:HB2	2:E:104:LYS:HG3	1.88	0.55
2:E:123:ASP:OD2	2:E:129:GLN:NE2	2.39	0.55
1:D:89:PHE:CZ	1:D:94:LYS:HA	2.42	0.55
1:D:396:GLY:H	1:D:445:ASP:HA	1.71	0.55
2:E:63:PHE:HD1	2:E:72:VAL:HB	1.71	0.55
2:E:544:LYS:NZ	2:E:546:VAL:HG21	2.22	0.55
1:A:213:THR:O	1:A:216:GLY:N	2.39	0.55
1:D:396:GLY:N	1:D:445:ASP:OD1	2.40	0.54
2:E:526:CYS:HA	2:E:540:TRP:CE3	2.43	0.54
1:A:80:LEU:HD12	1:A:84:CYS:SG	2.48	0.54
1:A:215:ASN:OD1	1:A:218:SER:OG	2.24	0.54
1:D:708:ARG:HH21	1:D:711:TYR:HB2	1.72	0.54
1:D:305:CYS:SG	1:D:383:CYS:N	2.81	0.54
1:D:497:ASN:HD22	1:D:666:SER:HA	1.73	0.54
2:E:549:GLU:HB2	1:D:166:SER:HA	1.89	0.54
1:D:170:LYS:HD2	1:D:179:ASN:O	2.08	0.54
1:D:688:LEU:O	1:D:709:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:NH2	1:A:261:ARG:HG3	2.23	0.53
2:E:218:ARG:HG2	2:E:219:LEU:N	2.22	0.53
2:E:386:LEU:HB3	2:E:417:ARG:HB3	1.90	0.53
1:D:311:GLU:HA	1:D:356:ASN:HB3	1.90	0.53
2:E:35:MET:HA	2:E:524:GLN:OE1	2.08	0.53
1:D:539:ARG:HH11	1:D:539:ARG:HG2	1.72	0.53
1:A:63:LYS:HB3	1:A:95:GLN:HE22	1.74	0.53
2:E:181:GLY:N	2:E:200:THR:OG1	2.41	0.53
2:E:659:ILE:HD12	2:E:678:THR:O	2.08	0.53
1:D:47:LYS:HG2	1:D:114:HIS:HA	1.90	0.53
1:D:191:THR:H	1:D:198:TYR:HA	1.72	0.53
1:D:508:MET:HG3	1:D:629:LEU:HD11	1.90	0.53
1:D:512:ARG:HG3	1:D:512:ARG:HH11	1.74	0.53
1:D:612:CYS:CB	1:D:679:CYS:HA	2.38	0.53
1:A:72:ASN:ND2	3:F:4:IDS:O5	2.41	0.53
1:A:238:GLN:HG3	1:A:242:ARG:HG2	1.89	0.53
1:A:39:ILE:N	1:A:39:ILE:HD12	2.24	0.53
2:E:540:TRP:CD1	2:E:542:HIS:H	2.27	0.53
2:E:716:ILE:HG21	2:E:720:PHE:HZ	1.74	0.53
1:D:560:LYS:HD3	1:D:560:LYS:N	2.23	0.53
2:E:382:ASN:HD22	2:E:422:THR:CG2	2.18	0.53
2:E:726:ILE:C	2:E:728:LEU:H	2.15	0.53
2:E:409:CYS:SG	2:E:409:CYS:O	2.67	0.52
1:D:653:ASN:H	1:D:656:GLU:CD	2.18	0.52
1:A:246:LEU:O	1:A:249:ARG:HG2	2.08	0.52
1:D:508:MET:HG3	1:D:629:LEU:CD1	2.40	0.52
1:A:42:PHE:HD2	1:A:119:TYR:HB3	1.75	0.52
2:E:96:PHE:HB2	2:E:99:GLN:HG2	1.92	0.52
1:D:67:ALA:O	1:D:70:CYS:HB2	2.09	0.52
1:D:547:TRP:HA	1:D:563:GLN:O	2.10	0.52
2:E:546:VAL:HG12	2:E:547:ARG:O	2.10	0.52
1:D:141:SER:HB3	1:D:176:TYR:HA	1.90	0.52
1:D:564:VAL:C	1:D:565:LEU:HD12	2.34	0.52
2:E:77:ASP:HB2	2:E:79:GLN:HG2	1.92	0.52
2:E:635:ASN:OD1	2:E:635:ASN:O	2.28	0.52
1:D:279:ARG:HG3	1:D:280:TRP:CD1	2.43	0.52
1:D:626:ASP:OD1	1:D:626:ASP:N	2.40	0.52
1:A:93:ARG:HD2	1:A:95:GLN:HB3	1.92	0.51
1:A:159:GLU:OE2	2:E:333:ILE:HG22	2.10	0.51
2:E:339:ASP:OD2	2:E:368:LYS:HD3	2.10	0.51
2:E:396:HIS:HB3	2:E:400:ARG:HH21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:720:PHE:O	2:E:735:ILE:HA	2.11	0.51
1:D:579:LEU:HD12	1:D:580:VAL:N	2.25	0.51
2:E:261:PHE:O	2:E:262:LEU:HD23	2.10	0.51
2:E:566:TYR:N	2:E:584:CYS:O	2.42	0.51
1:D:510:SER:OG	1:D:547:TRP:HB2	2.11	0.51
2:E:253:PHE:CE1	2:E:260:TYR:HB2	2.46	0.51
1:D:442:ASN:HB2	1:D:451:TRP:CD1	2.45	0.51
1:D:714:LYS:HE3	1:D:714:LYS:HA	1.91	0.51
1:A:69:GLN:OE1	3:F:3:SGN:N2	2.44	0.51
2:E:225:GLY:O	2:E:226:PHE:HD1	1.93	0.51
1:D:422:LEU:HG	1:D:426:ILE:HB	1.93	0.51
1:D:568:SER:HB3	1:D:585:ALA:HA	1.93	0.51
1:D:76:ARG:NH1	3:J:4:IDS:H5	2.26	0.51
1:A:273:THR:OG1	1:A:278:THR:O	2.26	0.51
2:E:382:ASN:ND2	2:E:422:THR:HG21	2.18	0.51
1:A:176:TYR:HB2	1:A:178:ARG:HE	1.76	0.50
2:E:359:ARG:HG2	2:E:359:ARG:HH11	1.75	0.50
1:D:415:TRP:HB2	1:D:438:ASN:N	2.16	0.50
2:E:202:ASN:OD1	2:E:203:SER:N	2.44	0.50
2:E:445:PHE:CE1	2:E:452:ILE:HB	2.47	0.50
1:A:163:LEU:HD23	1:A:167:TYR:CE2	2.33	0.50
2:E:201:ILE:HB	2:E:206:PHE:HE1	1.75	0.50
2:E:217:ARG:HD3	2:E:228:PHE:CE1	2.42	0.50
1:D:312:GLY:O	1:D:314:ARG:NE	2.40	0.50
1:D:339:MET:HB2	1:D:366:PHE:HZ	1.74	0.50
1:A:126:ARG:HG2	1:A:128:CYS:HB2	1.94	0.50
2:E:117:ASN:HD21	2:E:120:LEU:HB2	1.76	0.50
2:E:296:LEU:HD22	2:E:365:PHE:CE2	2.46	0.50
1:A:35:ARG:HA	1:A:72:ASN:ND2	2.27	0.50
1:D:581:LEU:HD23	1:D:715:TRP:CH2	2.47	0.50
2:E:452:ILE:HD13	2:E:466:VAL:HA	1.94	0.50
1:A:142:ILE:HD11	1:A:146:GLY:C	2.37	0.50
2:E:30:LEU:HD23	2:E:584:CYS:HB3	1.94	0.50
2:E:88:PRO:O	2:E:112:TRP:HZ3	1.94	0.50
2:E:592:ARG:O	2:E:593:ASN:C	2.55	0.50
1:A:78:LYS:HE2	1:A:168:ARG:HD2	1.92	0.49
2:E:127:ASP:O	2:E:129:GLN:HG3	2.12	0.49
1:D:402:ASN:HA	1:D:439:TYR:CD2	2.47	0.49
1:D:552:ASP:HA	1:D:627:GLY:O	2.12	0.49
1:D:112:PHE:CZ	1:D:114:HIS:HE1	2.30	0.49
2:E:136:VAL:O	2:E:138:ARG:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:TRP:H	1:D:188:TRP:CD1	2.29	0.49
1:D:590:LEU:HD13	1:D:594:VAL:HG23	1.95	0.49
1:D:561:CYS:HB3	1:D:593:PHE:HD2	1.75	0.49
1:D:574:PRO:O	1:D:577:SER:OG	2.17	0.49
1:A:43:LYS:NZ	1:A:45:SER:HB3	2.27	0.49
2:E:422:THR:O	2:E:422:THR:OG1	2.28	0.49
1:D:157:PRO:HG2	1:D:158:HIS:CE1	2.48	0.49
1:D:717:HIS:O	1:D:721:LEU:HG	2.11	0.49
2:E:239:PRO:HA	2:E:242:ARG:CZ	2.41	0.49
1:A:69:GLN:HA	1:A:72:ASN:HB2	1.93	0.49
2:E:56:ILE:HG23	2:E:63:PHE:HD2	1.77	0.49
1:A:49:THR:HG23	1:A:111:GLU:OE1	2.13	0.49
2:E:174:ASP:O	2:E:176:VAL:HG23	2.12	0.49
1:D:127:ASN:HB2	1:D:140:VAL:HG23	1.95	0.49
1:A:93:ARG:HH21	1:A:96:CYS:HA	1.77	0.49
1:D:702:ARG:HG3	1:D:702:ARG:HH11	1.78	0.49
2:E:170:SER:HB2	2:E:171:GLN:NE2	2.27	0.48
2:E:218:ARG:CD	2:E:227:MET:HE2	2.43	0.48
2:E:335:ALA:HA	2:E:368:LYS:NZ	2.27	0.48
1:D:181:ARG:HB2	1:D:183:GLU:HG2	1.95	0.48
1:D:552:ASP:OD2	1:D:555:GLY:N	2.46	0.48
1:D:708:ARG:HE	1:D:711:TYR:HB2	1.77	0.48
2:E:659:ILE:HD11	2:E:677:LEU:HB3	1.95	0.48
1:A:88:VAL:HG22	1:A:118:LEU:HA	1.95	0.48
2:E:415:GLU:H	2:E:415:GLU:HG2	1.39	0.48
1:D:158:HIS:CD2	1:D:197:ARG:HG3	2.49	0.48
2:E:524:GLN:O	2:E:540:TRP:HH2	1.96	0.48
1:D:63:LYS:HG2	1:D:95:GLN:HG2	1.96	0.48
1:D:406:THR:C	1:D:465:PRO:HD3	2.39	0.48
1:A:109:LYS:HB2	1:A:111:GLU:OE2	2.14	0.48
2:E:224:ASP:OD1	2:E:224:ASP:N	2.45	0.48
2:E:28:GLU:CD	2:E:28:GLU:H	2.21	0.48
1:D:337:HIS:HB2	1:D:339:MET:HG3	1.95	0.48
1:D:406:THR:HG22	1:D:410:LEU:O	2.13	0.48
1:A:43:LYS:C	1:A:43:LYS:HD3	2.39	0.48
2:E:194:ASN:HA	2:E:217:ARG:O	2.13	0.48
2:E:219:LEU:HD11	2:E:223:LYS:HA	1.96	0.48
2:E:550:GLU:OE1	2:E:550:GLU:N	2.46	0.48
1:A:78:LYS:HE2	1:A:168:ARG:CD	2.44	0.47
1:A:39:ILE:C	1:A:41:GLU:N	2.70	0.47
2:E:384:ARG:NH1	2:E:387:GLN:OE1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:HIS:CD2	1:A:245:PHE:H	2.32	0.47
2:E:386:LEU:HD22	2:E:389:PHE:HB3	1.96	0.47
1:D:552:ASP:O	1:D:555:GLY:N	2.46	0.47
2:E:575:LEU:HD12	2:E:576:GLU:N	2.30	0.47
2:E:583:ILE:HB	2:E:622:LEU:HB2	1.96	0.47
2:E:697:CYS:HB3	2:E:712:PRO:HD3	1.96	0.47
2:E:726:ILE:C	2:E:728:LEU:N	2.73	0.47
1:D:149:CYS:HB3	1:D:189:CYS:HB2	1.64	0.47
1:D:190:PHE:HA	1:D:198:TYR:HA	1.96	0.47
1:D:126:ARG:O	1:D:127:ASN:CG	2.58	0.47
1:D:334:PRO:HG2	1:D:370:PRO:HA	1.97	0.47
1:A:38:THR:HG21	1:A:75:THR:OG1	2.14	0.47
1:A:88:VAL:HB	1:A:97:LEU:HD21	1.97	0.47
1:A:160:HIS:O	1:A:163:LEU:HD11	2.14	0.47
1:A:220:ARG:NH2	1:A:253:LYS:O	2.46	0.47
1:A:227:GLU:CD	1:A:268:ARG:HH21	2.21	0.47
1:A:263:PRO:HD2	1:A:270:TRP:NE1	2.29	0.47
2:E:544:LYS:HZ3	2:E:546:VAL:HG21	1.78	0.47
2:E:582:THR:O	2:E:583:ILE:HD13	2.14	0.47
1:D:60:LYS:HB2	1:D:60:LYS:HE2	1.43	0.47
1:D:351:GLU:HG2	1:D:352:ASN:H	1.80	0.47
1:D:600:PRO:HA	1:D:686:MET:HE1	1.96	0.47
1:A:137:LYS:HA	1:A:178:ARG:NH1	2.30	0.47
1:A:144:LYS:HG3	1:A:200:VAL:O	2.15	0.47
2:E:331:ARG:HB2	2:E:331:ARG:CZ	2.44	0.47
1:D:668:PRO:HG3	1:D:691:ILE:HG12	1.97	0.47
1:A:74:CYS:HA	1:A:80:LEU:HG	1.96	0.47
1:A:170:LYS:C	1:A:172:LEU:H	2.23	0.47
1:A:241:HIS:CB	1:A:279:ARG:HH21	2.27	0.46
1:A:245:PHE:O	1:A:246:LEU:HD23	2.15	0.46
2:E:137:ASN:O	2:E:140:THR:HG23	2.14	0.46
2:E:478:ASN:OD1	2:E:478:ASN:O	2.33	0.46
1:D:658:CYS:SG	1:D:703:PRO:HB2	2.55	0.46
2:E:540:TRP:HD1	2:E:542:HIS:H	1.62	0.46
2:E:617:SER:HB2	2:E:622:LEU:HD13	1.96	0.46
1:D:113:GLY:HA3	1:D:116:PHE:CD2	2.50	0.46
1:D:402:ASN:HA	1:D:439:TYR:CE2	2.51	0.46
2:E:130:LEU:HD12	2:E:130:LEU:HA	1.75	0.46
2:E:547:ARG:CZ	2:E:548:SER:H	2.29	0.46
1:A:160:HIS:HB2	1:A:197:ARG:NH2	2.31	0.46
2:E:46:PHE:HB3	2:E:510:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:266:ARG:H	2:E:266:ARG:HG3	1.55	0.46
2:E:692:ILE:HD13	2:E:722:VAL:HG22	1.97	0.46
1:A:44:LYS:HD2	1:A:44:LYS:HA	1.74	0.46
2:E:661:SER:O	2:E:677:LEU:HA	2.15	0.46
1:D:615:TYR:HB3	1:D:629:LEU:HD21	1.98	0.46
1:D:650:VAL:HG12	1:D:695:ARG:HD3	1.98	0.46
1:A:39:ILE:HD11	1:A:68:ASP:HA	1.98	0.46
1:A:238:GLN:HG3	1:A:238:GLN:O	2.15	0.46
1:D:524:ILE:C	1:D:525:LYS:HD2	2.40	0.46
2:E:718:THR:O	2:E:738:TYR:HB2	2.15	0.46
1:D:339:MET:HB2	1:D:366:PHE:CZ	2.50	0.46
2:E:580:ARG:C	2:E:623:LYS:HZ3	2.24	0.46
1:D:52:LYS:HG3	1:D:108:VAL:HG12	1.97	0.46
1:A:246:LEU:H	1:A:249:ARG:HD3	1.81	0.46
2:E:323:SER:OG	2:E:324:LYS:N	2.48	0.46
2:E:550:GLU:O	2:E:552:LEU:HD22	2.16	0.46
1:A:82:PHE:CD2	1:A:100:PRO:HB3	2.47	0.46
2:E:192:PHE:CZ	2:E:218:ARG:NH1	2.84	0.46
1:D:223:MET:HE3	1:D:223:MET:HB3	1.73	0.46
1:D:364:TRP:HB2	1:D:374:VAL:HG23	1.97	0.46
1:D:536:PHE:CE2	1:D:570:LEU:HD21	2.51	0.46
1:D:568:SER:OG	1:D:583:LYS:HG3	2.15	0.46
1:D:598:ASP:C	1:D:599:LEU:HD22	2.41	0.46
1:A:158:HIS:HD2	1:A:190:PHE:HB3	1.81	0.45
2:E:41:TYR:CD2	2:E:518:LEU:HD21	2.51	0.45
2:E:417:ARG:HA	2:E:417:ARG:HD3	1.57	0.45
1:D:62:LYS:HA	1:D:62:LYS:HD2	1.42	0.45
1:D:514:ARG:HB2	1:D:516:LYS:NZ	2.31	0.45
1:A:47:LYS:HA	1:A:114:HIS:HA	1.98	0.45
1:A:109:LYS:HD3	1:A:109:LYS:N	2.31	0.45
1:A:121:ASN:HB3	1:A:123:ASP:OD1	2.16	0.45
2:E:260:TYR:HA	2:E:279:ILE:O	2.17	0.45
2:E:463:MET:HA	2:E:477:VAL:O	2.16	0.45
1:D:598:ASP:OD1	1:D:686:MET:HB2	2.16	0.45
2:E:53:GLN:NE2	2:E:116:ILE:HB	2.31	0.45
1:D:66:THR:HG22	1:D:68:ASP:H	1.81	0.45
1:D:245:PHE:HA	1:D:250:TYR:CE2	2.51	0.45
1:A:190:PHE:CE1	1:A:198:TYR:HB3	2.50	0.45
1:A:273:THR:HG21	1:A:278:THR:HG23	1.98	0.45
2:E:53:GLN:HE21	2:E:116:ILE:HB	1.82	0.45
2:E:413:ARG:H	2:E:413:ARG:HG3	1.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:ILE:H	1:D:380:ILE:HG13	1.29	0.45
2:E:218:ARG:HD3	2:E:227:MET:HE2	1.97	0.45
2:E:580:ARG:HA	2:E:625:THR:HG22	1.98	0.45
2:E:597:ASP:C	2:E:599:LYS:H	2.24	0.45
1:D:249:ARG:HG3	1:D:250:TYR:CE1	2.51	0.45
1:A:260:CYS:O	1:A:261:ARG:NH2	2.49	0.45
2:E:279:ILE:CD1	2:E:293:GLU:HG2	2.47	0.45
1:D:155:MET:SD	1:D:161:SER:HB2	2.56	0.45
1:A:37:ASN:C	1:A:39:ILE:H	2.24	0.45
1:A:266:GLN:HB3	1:A:267:PRO:HD2	1.99	0.45
2:E:68:ASN:OD1	2:E:114:ASP:HB2	2.17	0.45
1:D:66:THR:HG22	1:D:69:GLN:H	1.81	0.45
1:D:512:ARG:HG2	1:D:515:ASN:HA	1.98	0.45
2:E:678:THR:OG1	2:E:705:SER:O	2.23	0.45
1:D:329:TRP:HZ2	1:D:355:ARG:H	1.65	0.45
1:D:499:ILE:O	1:D:631:VAL:HG12	2.17	0.45
1:D:523:LEU:HG	1:D:596:THR:HG22	1.98	0.45
1:D:529:VAL:HG21	1:D:582:MET:HE3	1.99	0.45
1:D:547:TRP:CD1	1:D:564:VAL:HA	2.51	0.45
1:A:93:ARG:NE	1:A:95:GLN:O	2.50	0.45
1:A:70:CYS:SG	1:A:89:PHE:HE1	2.40	0.44
1:A:90:ASP:OD2	1:A:92:ALA:HB3	2.17	0.44
2:E:67:THR:HG23	2:E:116:ILE:HG22	1.98	0.44
2:E:114:ASP:N	2:E:114:ASP:OD1	2.50	0.44
1:D:533:ARG:HH21	1:D:578:ASP:H	1.65	0.44
2:E:390:TYR:HD1	2:E:390:TYR:HA	1.62	0.44
1:D:652:LEU:HD12	1:D:652:LEU:H	1.82	0.44
2:E:515:LEU:C	2:E:517:GLY:H	2.26	0.44
1:D:456:ASN:OD1	1:D:458:LEU:N	2.50	0.44
1:D:513:TYR:O	1:D:516:LYS:NZ	2.50	0.44
1:D:543:ASP:OD1	1:D:543:ASP:N	2.37	0.44
2:E:463:MET:HE3	2:E:463:MET:HB2	1.87	0.44
2:E:533:PRO:HB2	2:E:535:PHE:CD1	2.53	0.44
1:D:87:PHE:CZ	1:D:89:PHE:HB2	2.52	0.44
1:D:232:CYS:O	1:D:258:ASN:HB3	2.17	0.44
1:D:309:GLN:O	1:D:356:ASN:ND2	2.49	0.44
1:D:313:TYR:OH	1:D:380:ILE:HD13	2.18	0.44
2:E:278:ILE:HB	2:E:296:LEU:HD12	1.98	0.44
1:D:84:CYS:SG	1:D:98:TRP:HB3	2.58	0.44
1:D:547:TRP:HE1	1:D:564:VAL:HG23	1.81	0.44
1:A:170:LYS:C	1:A:172:LEU:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:TRP:CE3	1:A:280:TRP:CE3	3.06	0.44
2:E:504:VAL:O	2:E:510:ILE:HD12	2.18	0.44
1:D:606:ILE:HG21	1:D:636:ILE:HG21	1.99	0.44
2:E:445:PHE:CZ	2:E:515:LEU:HB2	2.52	0.44
1:D:43:LYS:HG2	1:D:44:LYS:N	2.31	0.44
1:D:347:LYS:HD2	1:D:347:LYS:HA	1.48	0.44
1:D:403:LEU:HD23	1:D:405:GLN:H	1.82	0.44
1:D:598:ASP:OD1	1:D:686:MET:HE3	2.17	0.44
2:E:92:HIS:HE1	2:E:94:ASP:HB2	1.83	0.44
2:E:602:ARG:O	2:E:640:ILE:HD12	2.18	0.44
1:D:63:LYS:HA	1:D:94:LYS:O	2.17	0.44
1:D:497:ASN:HB2	1:D:666:SER:OG	2.17	0.44
1:D:542:LYS:O	1:D:542:LYS:HD3	2.18	0.44
1:D:640:GLU:C	1:D:644:GLN:HE21	2.20	0.44
1:A:44:LYS:NZ	1:A:117:ASP:HB3	2.33	0.44
1:A:63:LYS:CB	1:A:95:GLN:HE22	2.31	0.44
1:A:230:LYS:HE3	1:A:278:THR:HG21	2.00	0.44
1:A:234:ARG:HE	1:A:237:HIS:HE1	1.64	0.44
2:E:75:GLU:N	2:E:75:GLU:OE1	2.47	0.44
2:E:509:LYS:HD3	2:E:509:LYS:HA	1.89	0.44
1:A:64:VAL:HB	1:A:70:CYS:SG	2.58	0.43
1:D:438:ASN:O	1:D:439:TYR:CD1	2.71	0.43
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.88	0.43
1:A:102:ASN:CG	1:A:103:SER:N	2.76	0.43
1:D:530:LEU:HA	1:D:581:LEU:HD13	1.98	0.43
1:A:215:ASN:OD1	1:A:216:GLY:N	2.51	0.43
1:D:78:LYS:HB3	1:D:78:LYS:HE3	1.61	0.43
1:D:564:VAL:O	1:D:565:LEU:HD12	2.19	0.43
2:E:384:ARG:HH22	2:E:387:GLN:HG2	1.83	0.43
1:D:264:ASP:OD1	1:D:266:GLN:HG2	2.17	0.43
1:D:528:TRP:CH2	1:D:583:LYS:HB3	2.54	0.43
1:A:62:LYS:HB2	1:A:62:LYS:HE2	1.59	0.43
2:E:269:LEU:H	2:E:269:LEU:HG	1.35	0.43
1:D:407:ARG:N	1:D:463:TYR:O	2.49	0.43
1:D:708:ARG:NH2	1:D:711:TYR:HB2	2.34	0.43
1:A:160:HIS:HB2	1:A:197:ARG:HH22	1.82	0.43
1:A:223:MET:HE3	1:A:223:MET:HB3	1.88	0.43
2:E:48:ALA:HB3	2:E:52:ILE:HD11	2.00	0.43
2:E:76:GLU:CD	2:E:76:GLU:N	2.77	0.43
2:E:180:LEU:HB2	2:E:200:THR:OG1	2.18	0.43
2:E:200:THR:HG22	2:E:247:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:498:GLN:NE2	1:D:184:GLU:H	2.16	0.43
1:D:412:CYS:HB2	1:D:438:ASN:OD1	2.18	0.43
1:A:177:CYS:CB	1:A:189:CYS:HB3	2.47	0.43
1:A:215:ASN:ND2	1:A:218:SER:H	2.15	0.43
1:A:226:THR:HA	1:A:283:CYS:HA	2.01	0.43
1:A:251:PRO:O	1:A:253:LYS:HD2	2.18	0.43
1:A:262:ASN:HD21	1:A:268:ARG:C	2.27	0.43
2:E:539:GLY:H	2:E:556:TRP:HE1	1.67	0.43
1:A:48:THR:O	1:A:116:PHE:HB2	2.19	0.43
2:E:294:MET:HE1	2:E:373:PHE:HB3	2.00	0.43
2:E:540:TRP:CD1	2:E:542:HIS:N	2.87	0.43
1:D:248:GLU:O	1:D:251:PRO:HD3	2.19	0.43
1:D:679:CYS:N	1:D:686:MET:O	2.46	0.43
2:E:299:ILE:HG22	2:E:313:VAL:HB	2.00	0.43
2:E:343:PHE:CE2	2:E:444:THR:HG21	2.45	0.43
1:D:406:THR:OG1	1:D:407:ARG:N	2.52	0.43
1:A:137:LYS:HD2	1:A:171:ASP:CB	2.47	0.43
1:D:247:PRO:HB3	1:D:255:PHE:HB2	2.01	0.43
1:D:649:LYS:HD3	1:D:649:LYS:HA	1.90	0.43
2:E:36:ASN:OD1	2:E:36:ASN:N	2.52	0.42
2:E:229:LEU:HD23	2:E:229:LEU:HA	1.66	0.42
2:E:598:LEU:HD13	2:E:617:SER:O	2.19	0.42
2:E:599:LYS:HZ3	2:E:600:LYS:HG3	1.84	0.42
1:D:137:LYS:HB2	1:D:137:LYS:HE2	1.38	0.42
1:D:233:GLN:HE21	1:D:237:HIS:HB2	1.84	0.42
1:D:405:GLN:OE1	1:D:406:THR:N	2.52	0.42
1:D:436:ASN:OD1	1:D:439:TYR:HB2	2.19	0.42
1:A:220:ARG:HE	1:A:261:ARG:HD2	1.83	0.42
2:E:63:PHE:C	2:E:64:LEU:HD12	2.44	0.42
2:E:227:MET:HE3	2:E:229:LEU:HD21	2.00	0.42
2:E:537:GLN:O	2:E:547:ARG:HD2	2.19	0.42
1:D:329:TRP:HA	1:D:340:THR:HG22	2.01	0.42
1:D:612:CYS:HB2	1:D:678:VAL:O	2.20	0.42
1:D:651:THR:O	1:D:651:THR:OG1	2.32	0.42
2:E:46:PHE:CD1	2:E:46:PHE:C	2.97	0.42
1:D:451:TRP:HA	1:D:463:TYR:HA	2.01	0.42
1:D:528:TRP:CZ3	1:D:583:LYS:HB3	2.54	0.42
1:A:77:ASN:C	1:A:79:GLY:N	2.77	0.42
1:A:142:ILE:HD11	1:A:146:GLY:HA2	2.01	0.42
2:E:184:VAL:HG13	2:E:197:VAL:HG12	2.00	0.42
2:E:429:LEU:HA	2:E:429:LEU:HD23	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:505:ILE:HG13	2:E:510:ILE:HD13	2.00	0.42
1:D:73:ARG:HA	1:D:76:ARG:HE	1.84	0.42
1:D:125:ILE:H	1:D:125:ILE:HG13	1.67	0.42
1:D:151:PRO:HA	1:D:174:GLU:O	2.19	0.42
1:D:248:GLU:HG2	1:D:249:ARG:N	2.33	0.42
1:A:158:HIS:CE1	1:A:197:ARG:HA	2.53	0.42
2:E:238:LEU:HD12	2:E:241:PHE:H	1.84	0.42
1:D:569:GLN:CD	1:D:570:LEU:H	2.27	0.42
1:D:678:VAL:HA	1:D:687:VAL:HA	2.01	0.42
2:E:403:LEU:HD23	2:E:403:LEU:HA	1.75	0.42
2:E:462:PHE:HE2	2:E:513:ILE:HG21	1.84	0.42
1:D:713:ALA:HA	1:D:716:ILE:CD1	2.45	0.42
2:E:569:PHE:HA	2:E:570:PRO:HA	1.83	0.42
2:E:675:LEU:O	2:E:708:GLU:HA	2.20	0.42
1:D:66:THR:HB	1:D:69:GLN:HB3	2.02	0.42
2:E:119:ALA:HB3	2:E:133:CYS:CB	2.48	0.42
2:E:275:HIS:HA	2:E:315:ASN:O	2.20	0.42
2:E:714:GLN:HB2	2:E:738:TYR:CE2	2.55	0.42
1:D:524:ILE:HG22	1:D:525:LYS:CD	2.46	0.42
1:A:41:GLU:C	1:A:122:LYS:NZ	2.78	0.42
1:D:90:ASP:HB2	1:D:116:PHE:HD1	1.84	0.42
1:D:129:ILE:HA	1:D:129:ILE:HD13	1.66	0.42
1:A:144:LYS:NZ	1:A:200:VAL:O	2.44	0.41
1:A:219:TYR:C	1:A:220:ARG:HD2	2.45	0.41
2:E:549:GLU:CB	1:D:166:SER:HA	2.50	0.41
1:D:310:GLY:CA	1:D:313:TYR:HB3	2.48	0.41
1:A:84:CYS:HA	1:A:100:PRO:HA	2.03	0.41
1:A:102:ASN:OD1	1:A:103:SER:N	2.53	0.41
1:A:129:ILE:HD12	1:A:129:ILE:HA	1.80	0.41
1:A:170:LYS:HG3	1:A:180:PRO:HB3	2.02	0.41
2:E:206:PHE:CG	2:E:242:ARG:NH1	2.88	0.41
1:D:338:ASP:O	1:D:341:PRO:HD2	2.20	0.41
1:D:570:LEU:HD23	1:D:570:LEU:HA	1.69	0.41
1:A:39:ILE:HD12	1:A:39:ILE:H	1.85	0.41
1:A:41:GLU:C	1:A:122:LYS:HZ3	2.28	0.41
1:A:42:PHE:CD1	1:A:121:ASN:ND2	2.86	0.41
1:A:94:LYS:HD2	1:A:94:LYS:N	2.36	0.41
1:A:170:LYS:HD3	1:A:170:LYS:HA	1.28	0.41
2:E:39:MET:HG2	2:E:40:LYS:N	2.35	0.41
2:E:99:GLN:NE2	2:E:101:CYS:HB3	2.35	0.41
2:E:192:PHE:CE2	2:E:218:ARG:CZ	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:279:ILE:HD13	2:E:293:GLU:HG2	2.01	0.41
1:D:406:THR:HA	1:D:464:CYS:HA	2.02	0.41
1:D:512:ARG:NH2	1:D:547:TRP:CE3	2.87	0.41
2:E:61:HIS:NE2	2:E:151:THR:OG1	2.53	0.41
1:D:508:MET:HE1	1:D:676:PRO:CD	2.51	0.41
1:A:238:GLN:HG3	1:A:242:ARG:HA	2.02	0.41
2:E:618:THR:C	2:E:620:ASN:N	2.77	0.41
1:D:306:ILE:N	1:D:381:PRO:O	2.50	0.41
1:D:326:CYS:HB3	1:D:365:CYS:HB2	1.74	0.41
2:E:238:LEU:HD12	2:E:240:GLU:N	2.35	0.41
2:E:245:TYR:CE2	2:E:388:HIS:HB3	2.56	0.41
2:E:523:PHE:CD1	2:E:528:GLN:HB3	2.55	0.41
2:E:733:THR:OG1	2:E:734:SER:N	2.54	0.41
1:D:188:TRP:HE3	1:D:198:TYR:CD1	2.38	0.41
1:A:241:HIS:NE2	1:A:276:PRO:O	2.51	0.41
2:E:211:LEU:HD23	2:E:211:LEU:HA	1.74	0.41
2:E:671:GLY:HA3	2:E:713:ALA:CA	2.48	0.41
1:D:143:THR:HG21	1:D:191:THR:HG23	2.02	0.41
1:D:161:SER:C	1:D:163:LEU:N	2.73	0.41
1:D:442:ASN:HD22	1:D:450:PRO:HA	1.86	0.41
1:D:539:ARG:HG2	1:D:539:ARG:NH1	2.36	0.41
1:A:80:LEU:HD11	1:A:98:TRP:CE3	2.56	0.41
1:A:210:GLU:OE2	1:A:223:MET:N	2.54	0.41
2:E:329:LEU:O	2:E:333:ILE:HG12	2.20	0.41
1:D:217:GLU:CA	1:D:262:ASN:HB3	2.50	0.41
1:A:223:MET:SD	1:A:223:MET:C	3.04	0.41
1:D:143:THR:HB	1:D:199:GLU:HG2	2.02	0.41
1:D:233:GLN:OE1	1:D:240:PRO:HD2	2.21	0.41
1:D:686:MET:HB2	1:D:686:MET:HE3	1.84	0.41
1:D:688:LEU:C	1:D:709:VAL:HG22	2.46	0.41
1:A:178:ARG:HD3	1:A:178:ARG:N	2.36	0.41
2:E:452:ILE:HD13	2:E:452:ILE:HA	1.89	0.41
2:E:455:LEU:HD23	2:E:455:LEU:HA	1.68	0.41
1:D:252:ASP:C	1:D:253:LYS:HD3	2.46	0.41
1:D:522:SER:OG	1:D:676:PRO:HB3	2.21	0.41
1:D:656:GLU:H	1:D:656:GLU:HG2	1.73	0.41
1:D:720:ILE:HD12	1:D:720:ILE:HA	1.81	0.41
1:A:205:GLN:O	1:A:208:GLU:HG2	2.20	0.40
2:E:113:LYS:HE2	2:E:113:LYS:HB2	1.95	0.40
2:E:190:ASP:O	2:E:192:PHE:HD1	2.04	0.40
1:D:158:HIS:CE1	1:D:191:THR:O	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:HIS:NE2	1:D:197:ARG:HA	2.36	0.40
1:D:240:PRO:HG3	1:D:274:LEU:O	2.20	0.40
1:D:618:GLY:O	1:D:620:THR:HG23	2.21	0.40
2:E:285:ASN:OD1	2:E:286:SER:N	2.54	0.40
2:E:513:ILE:HD12	2:E:513:ILE:N	2.35	0.40
1:D:35:ARG:HB3	1:D:36:ARG:H	1.70	0.40
1:D:402:ASN:OD1	1:D:439:TYR:HE2	2.05	0.40
1:D:505:ILE:HG23	1:D:507:TRP:CE3	2.56	0.40
1:D:511:LEU:HD23	1:D:512:ARG:N	2.36	0.40
2:E:661:SER:O	2:E:677:LEU:HD13	2.21	0.40
1:D:44:LYS:HA	1:D:119:TYR:HA	2.03	0.40
1:A:215:ASN:HD21	1:A:218:SER:N	2.16	0.40
1:D:102:ASN:ND2	1:D:104:MET:HG2	2.36	0.40
1:D:112:PHE:CE2	1:D:114:HIS:HE1	2.39	0.40
1:D:634:LEU:HD12	1:D:635:TYR:H	1.87	0.40
2:E:275:HIS:NE2	2:E:295:PRO:HB3	2.36	0.40
2:E:461:ARG:NH2	2:E:478:ASN:O	2.54	0.40
2:E:730:ASN:CG	2:E:731:ARG:N	2.79	0.40
1:D:112:PHE:CE2	1:D:114:HIS:CE1	3.09	0.40
1:D:405:GLN:O	1:D:464:CYS:HB2	2.21	0.40
1:D:461:TRP:CZ2	1:D:718:LYS:HB2	2.57	0.40
1:D:606:ILE:HD12	1:D:607:PRO:CD	2.49	0.40
1:D:719:ILE:HD12	1:D:719:ILE:HA	1.88	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	250/728 (34%)	227 (91%)	23 (9%)	0	100 100
1	D	626/728 (86%)	569 (91%)	52 (8%)	5 (1%)	16 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	678/1390 (49%)	618 (91%)	58 (9%)	2 (0%)	36	71
All	All	1554/2846 (55%)	1414 (91%)	133 (9%)	7 (0%)	26	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	593	ASN
1	D	695	ARG
1	D	63	LYS
2	E	496	LEU
1	D	162	PHE
1	D	320	ILE
1	D	334	PRO

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	224/646 (35%)	206 (92%)	18 (8%)	11	31
1	D	525/646 (81%)	466 (89%)	59 (11%)	6	20
2	E	598/1246 (48%)	537 (90%)	61 (10%)	7	23
All	All	1347/2538 (53%)	1209 (90%)	138 (10%)	9	23

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	52	LYS
1	A	53	ILE
1	A	61	THR
1	A	62	LYS
1	A	63	LYS
1	A	65	ASN
1	A	69	GLN

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Mol	Chain	Res	Type
1	A	74	CYS
1	A	78	LYS
1	A	80	LEU
1	A	121	ASN
1	A	160	HIS
1	A	161	SER
1	A	170	LYS
1	A	203	ILE
1	A	206	CYS
1	A	258	ASN
2	E	38	ASN
2	E	70	ILE
2	E	72	VAL
2	E	73	LEU
2	E	81	VAL
2	E	86	THR
2	E	89	VAL
2	E	142	GLN
2	E	143	ARG
2	E	156	SER
2	E	221	GLU
2	E	264	VAL
2	E	266	ARG
2	E	268	THR
2	E	269	LEU
2	E	270	ASP
2	E	272	GLN
2	E	273	THR
2	E	283	SER
2	E	288	LEU
2	E	313	VAL
2	E	316	ILE
2	E	345	VAL
2	E	348	GLN
2	E	349	SER
2	E	350	LYS
2	E	376	LYS
2	E	378	VAL
2	E	380	LYS
2	E	381	ASN
2	E	390	TYR
2	E	393	ASN

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Mol	Chain	Res	Type
2	E	395	GLU
2	E	396	HIS
2	E	398	PHE
2	E	399	ASN
2	E	412	ARG
2	E	413	ARG
2	E	415	GLU
2	E	417	ARG
2	E	418	THR
2	E	491	ILE
2	E	492	VAL
2	E	495	THR
2	E	527	SER
2	E	559	GLN
2	E	560	ILE
2	E	562	LEU
2	E	565	ILE
2	E	591	ARG
2	E	594	ASN
2	E	595	LYS
2	E	647	THR
2	E	651	THR
2	E	654	TYR
2	E	673	THR
2	E	674	LEU
2	E	690	ILE
2	E	698	THR
2	E	701	SER
2	E	709	CYS
1	D	34	LYS
1	D	36	ARG
1	D	38	THR
1	D	39	ILE
1	D	59	ILE
1	D	60	LYS
1	D	62	LYS
1	D	63	LYS
1	D	69	GLN
1	D	75	THR
1	D	78	LYS
1	D	80	LEU
1	D	97	LEU

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Mol	Chain	Res	Type
1	D	123	ASP
1	D	125	ILE
1	D	126	ARG
1	D	129	ILE
1	D	130	ILE
1	D	135	SER
1	D	137	LYS
1	D	142	ILE
1	D	165	SER
1	D	166	SER
1	D	168	ARG
1	D	178	ARG
1	D	200	VAL
1	D	203	ILE
1	D	205	GLN
1	D	208	GLU
1	D	212	MET
1	D	219	TYR
1	D	220	ARG
1	D	223	MET
1	D	224	ASP
1	D	256	ASP
1	D	285	ILE
1	D	286	LYS
1	D	287	THR
1	D	317	VAL
1	D	318	ASN
1	D	319	THR
1	D	330	ASP
1	D	331	SER
1	D	337	HIS
1	D	338	ASP
1	D	340	THR
1	D	347	LYS
1	D	348	ASP
1	D	349	LEU
1	D	352	ASN
1	D	354	CYS
1	D	362	SER
1	D	374	VAL
1	D	378	SER
1	D	380	ILE

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Mol	Chain	Res	Type
1	D	669	CYS
1	D	678	VAL
1	D	695	ARG
1	D	699	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	158	HIS
1	A	160	HIS
2	E	142	GLN
2	E	289	HIS
2	E	318	GLN
2	E	379	ASN
2	E	381	ASN
2	E	382	ASN
2	E	393	ASN
2	E	498	GLN
2	E	607	ASN
2	E	635	ASN
1	D	114	HIS
1	D	158	HIS
1	D	233	GLN
1	D	258	ASN
1	D	497	ASN
1	D	504	ASN
1	D	644	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](#)

12 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SGN	F	1	3	15,18,20	0.93	0	20,26,31	1.30	2 (10%)
3	IDS	F	2	3	16,16,17	1.20	1 (6%)	16,24,26	0.89	1 (6%)
3	SGN	F	3	3	19,19,20	3.35	3 (15%)	23,29,31	1.63	2 (8%)
3	IDS	F	4	3	16,16,17	0.96	0	16,24,26	0.93	1 (6%)
3	SGN	F	5	3	13,13,20	3.98	2 (15%)	12,19,31	1.64	1 (8%)
3	IDS	F	6	3	15,15,17	1.19	1 (6%)	14,22,26	1.48	2 (14%)
3	SGN	J	1	3	15,18,20	0.95	0	20,26,31	1.46	3 (15%)
3	IDS	J	2	3	16,16,17	0.99	0	16,24,26	1.24	2 (12%)
3	SGN	J	3	3	19,19,20	3.38	2 (10%)	23,29,31	1.82	5 (21%)
3	IDS	J	4	3	16,16,17	1.16	1 (6%)	16,24,26	0.91	0
3	SGN	J	5	3	13,13,20	3.97	2 (15%)	12,19,31	1.63	2 (16%)
3	IDS	J	6	3	15,15,17	1.18	1 (6%)	14,22,26	1.40	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SGN	F	1	3	-	5/8/27/31	0/1/1/1
3	IDS	F	2	3	-	3/9/26/29	0/1/1/1
3	SGN	F	3	3	-	6/11/28/31	0/1/1/1
3	IDS	F	4	3	-	3/9/26/29	0/1/1/1
3	SGN	F	5	3	-	3/5/19/31	1/1/1/1
3	IDS	F	6	3	-	4/9/22/29	1/1/1/1
3	SGN	J	1	3	-	6/8/27/31	0/1/1/1
3	IDS	J	2	3	-	1/9/26/29	0/1/1/1
3	SGN	J	3	3	-	2/11/28/31	0/1/1/1
3	IDS	J	4	3	-	0/9/26/29	0/1/1/1
3	SGN	J	5	3	-	2/5/19/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IDS	J	6	3	-	1/9/22/29	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	5	SGN	O1S-S1	10.04	1.53	1.42
3	J	3	SGN	O1S-S1	9.96	1.53	1.42
3	J	5	SGN	O2S-S1	9.95	1.53	1.42
3	F	3	SGN	O1S-S1	9.90	1.53	1.42
3	F	5	SGN	O1S-S1	9.90	1.53	1.42
3	F	5	SGN	O2S-S1	9.89	1.53	1.42
3	F	3	SGN	O2S-S1	9.83	1.53	1.42
3	J	3	SGN	O2S-S1	9.80	1.53	1.42
3	F	2	IDS	O2-C2	-2.84	1.43	1.47
3	J	6	IDS	O2-C2	-2.60	1.43	1.47
3	F	6	IDS	O2-C2	-2.58	1.43	1.47
3	J	4	IDS	O2-C2	-2.45	1.43	1.47
3	F	3	SGN	S1-N2	2.34	1.62	1.59

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	SGN	O1S-S1-O2S	-5.08	109.07	120.36
3	J	5	SGN	O1S-S1-O2S	-4.92	109.41	120.36
3	F	5	SGN	O1S-S1-O2S	-4.84	109.59	120.36
3	J	3	SGN	O1S-S1-O2S	-4.82	109.64	120.36
3	J	3	SGN	C1-O5-C5	-4.01	106.81	112.19
3	F	3	SGN	C4-C3-C2	-4.00	105.15	111.02
3	J	2	IDS	O2-C2-C3	3.59	111.96	106.95
3	J	1	SGN	C4-C3-C2	-3.55	105.81	111.02
3	F	6	IDS	C1-O5-C5	-3.51	108.11	113.81
3	F	1	SGN	C2-N2-S1	-3.43	108.11	116.99
3	J	3	SGN	O5-C1-C2	-3.27	106.23	111.29
3	J	6	IDS	C1-O5-C5	-3.25	108.54	113.81
3	J	3	SGN	C3-C4-C5	3.21	116.06	110.23
3	F	1	SGN	C4-C3-C2	-2.96	106.68	111.02
3	J	6	IDS	O6A-C6-C5	-2.71	117.00	122.85
3	J	1	SGN	C2-N2-S1	-2.70	110.02	116.99
3	F	6	IDS	O6A-C6-C5	-2.69	117.04	122.85
3	J	1	SGN	C3-C4-C5	-2.61	105.51	110.23
3	J	3	SGN	C4-C3-C2	2.38	114.50	111.02
3	F	2	IDS	O2-C2-C3	2.26	110.11	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	IDS	O3S-S-O2	2.16	111.33	106.37
3	F	4	IDS	O2-C2-C3	2.08	109.86	106.95
3	J	5	SGN	C5-O5-C1	-2.08	108.06	111.42

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	IDS	C2-O2-S-O2S
3	F	2	IDS	C2-O2-S-O3S
3	F	3	SGN	O5-C5-C6-O6
3	F	3	SGN	C2-N2-S1-O2S
3	F	4	IDS	C1-C2-O2-S
3	F	5	SGN	C2-N2-S1-O2S
3	F	5	SGN	C2-N2-S1-O3S
3	F	6	IDS	C2-O2-S-O1S
3	F	6	IDS	C2-O2-S-O2S
3	F	6	IDS	C2-O2-S-O3S
3	J	1	SGN	C1-C2-N2-S1
3	J	1	SGN	C6-O6-S2-O6S
3	J	2	IDS	C3-C2-O2-S
3	J	3	SGN	C4-C5-C6-O6
3	J	5	SGN	C2-N2-S1-O3S
3	F	3	SGN	C6-O6-S2-O4S
3	F	2	IDS	C2-O2-S-O1S
3	J	1	SGN	C5-C6-O6-S2
3	F	1	SGN	C6-O6-S2-O5S
3	J	1	SGN	C6-O6-S2-O4S
3	J	1	SGN	C6-O6-S2-O5S
3	F	1	SGN	C6-O6-S2-O4S
3	F	3	SGN	C6-O6-S2-O5S
3	F	1	SGN	O5-C5-C6-O6
3	F	5	SGN	C2-N2-S1-O1S
3	J	1	SGN	O5-C5-C6-O6
3	J	3	SGN	O5-C5-C6-O6
3	F	3	SGN	C4-C5-C6-O6
3	F	4	IDS	C2-O2-S-O3S
3	J	6	IDS	O5-C5-C6-O6A
3	F	1	SGN	C6-O6-S2-O6S
3	F	3	SGN	C6-O6-S2-O6S
3	F	4	IDS	C3-C2-O2-S
3	J	5	SGN	C2-N2-S1-O2S

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Mol	Chain	Res	Type	Atoms
3	F	1	SGN	C5-C6-O6-S2
3	F	6	IDS	O5-C5-C6-O6A

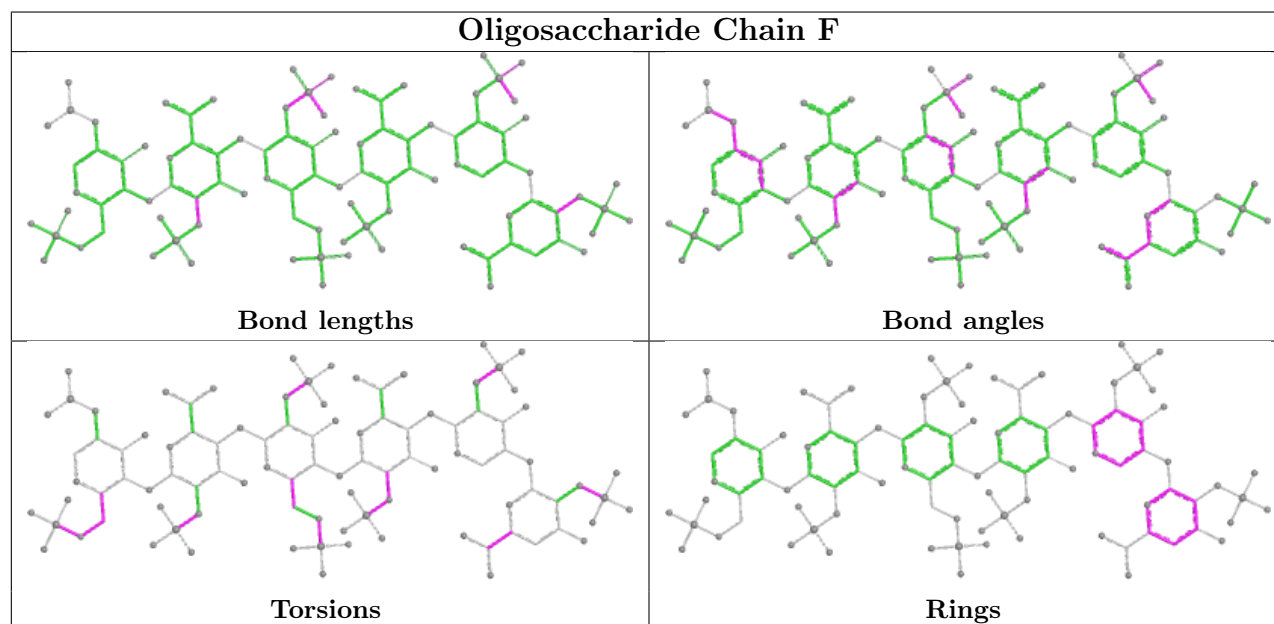
All (2) ring outliers are listed below:

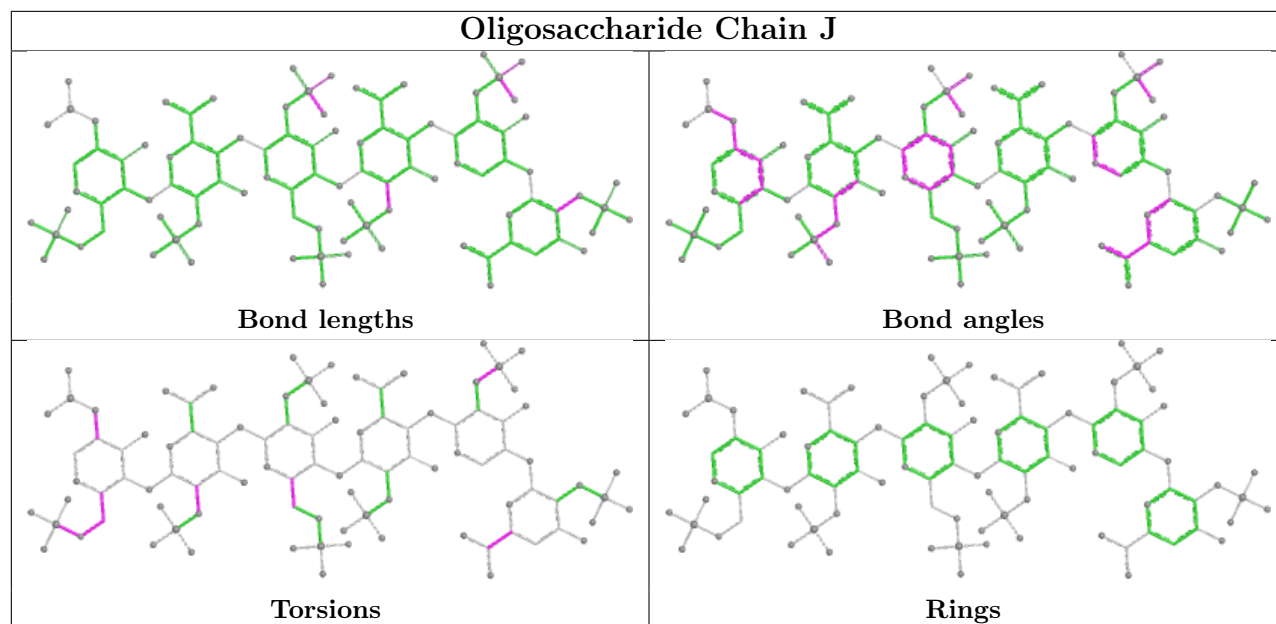
Mol	Chain	Res	Type	Atoms
3	F	6	IDS	C1-C2-C3-C4-C5-O5
3	F	5	SGN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	SGN	2	0
3	F	4	IDS	1	0
3	J	4	IDS	2	0
3	J	3	SGN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





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.

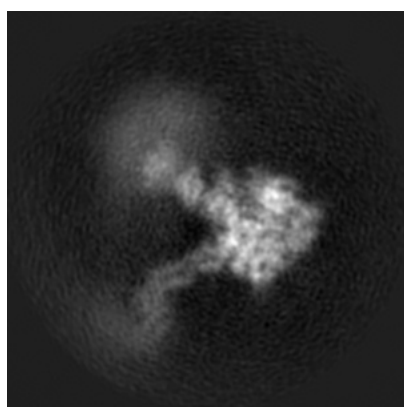
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23922. These allow visual inspection of the internal detail of the map and identification of artifacts.

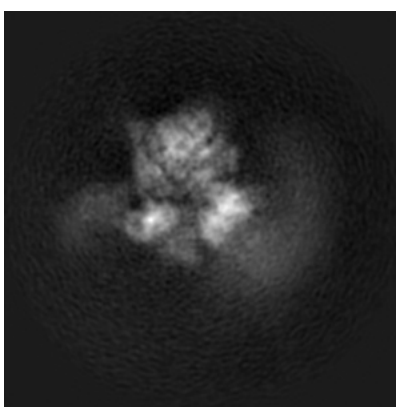
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

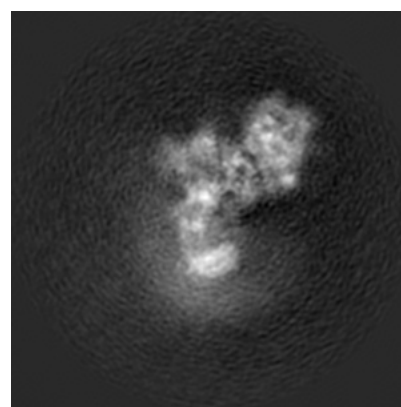
6.1.1 Primary map



X



Y

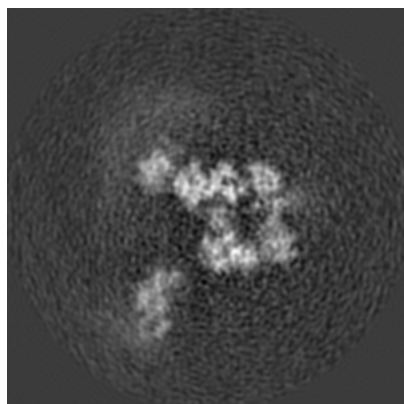


Z

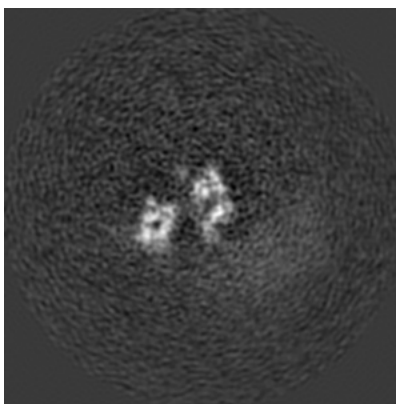
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

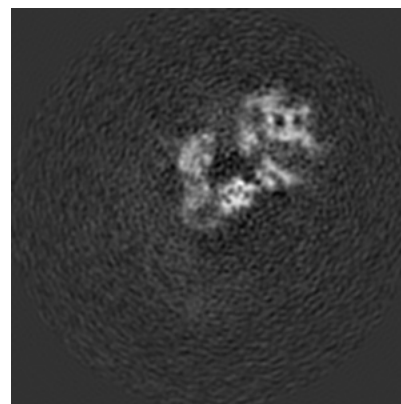
6.2.1 Primary map



X Index: 135



Y Index: 135

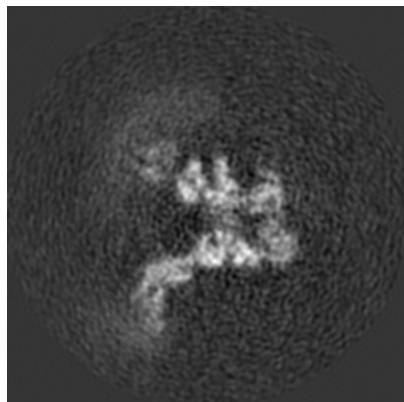


Z Index: 135

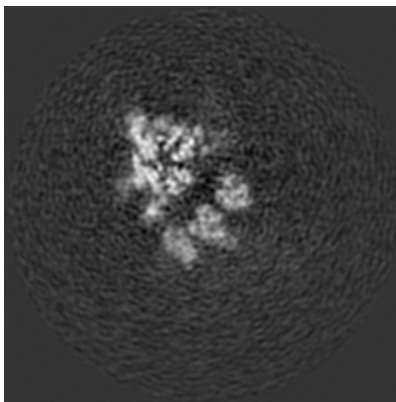
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

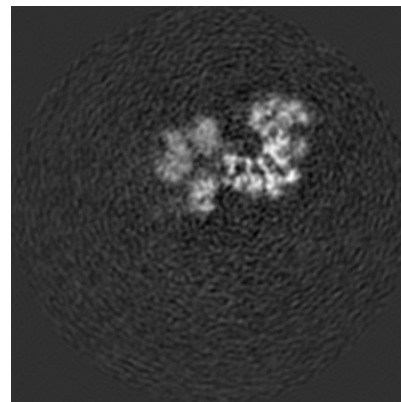
6.3.1 Primary map



X Index: 129



Y Index: 167

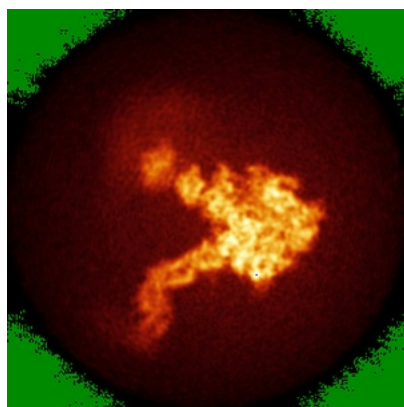


Z Index: 113

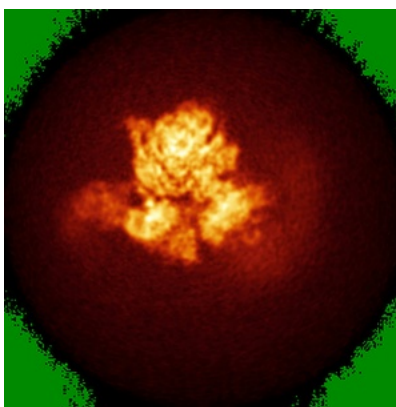
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

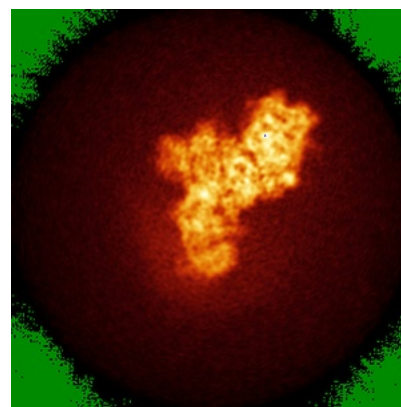
6.4.1 Primary map



X



Y

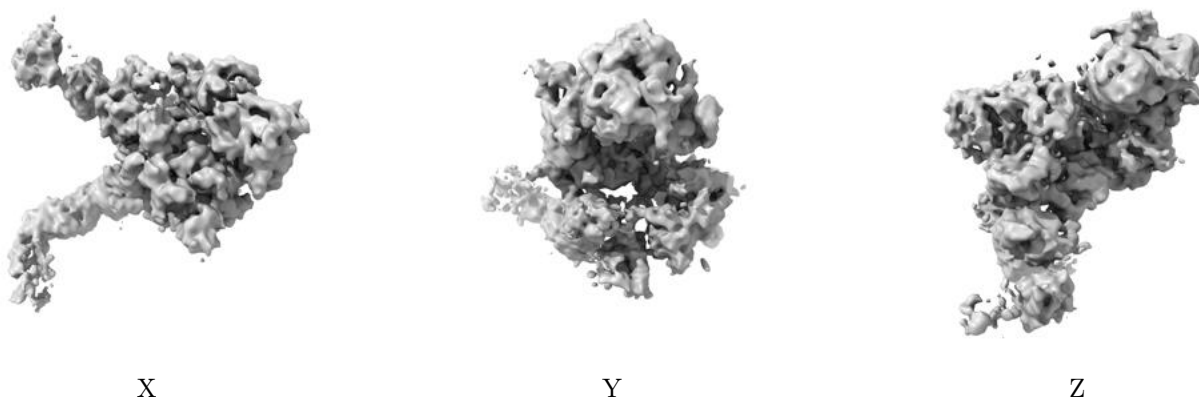


Z

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 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

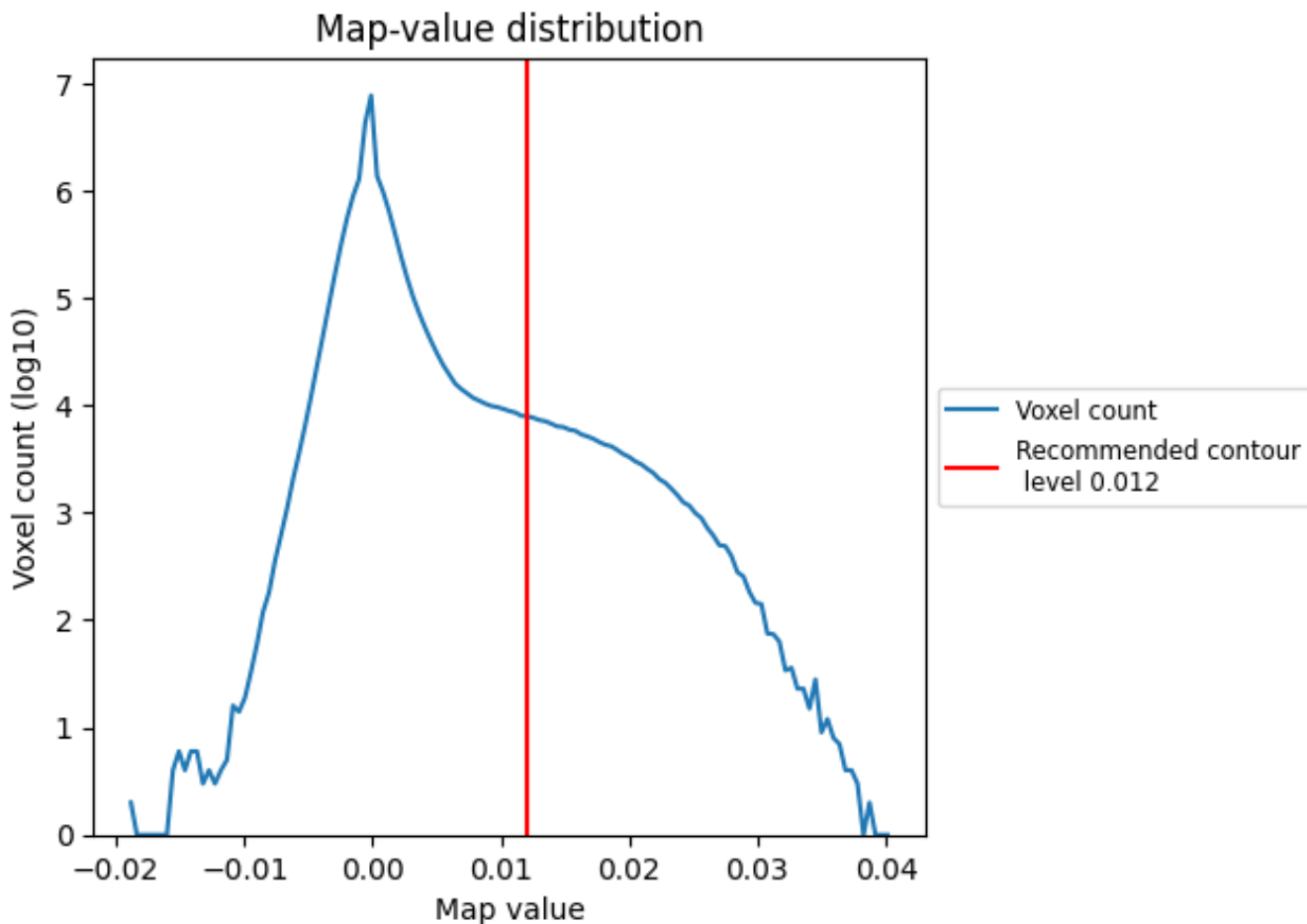
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

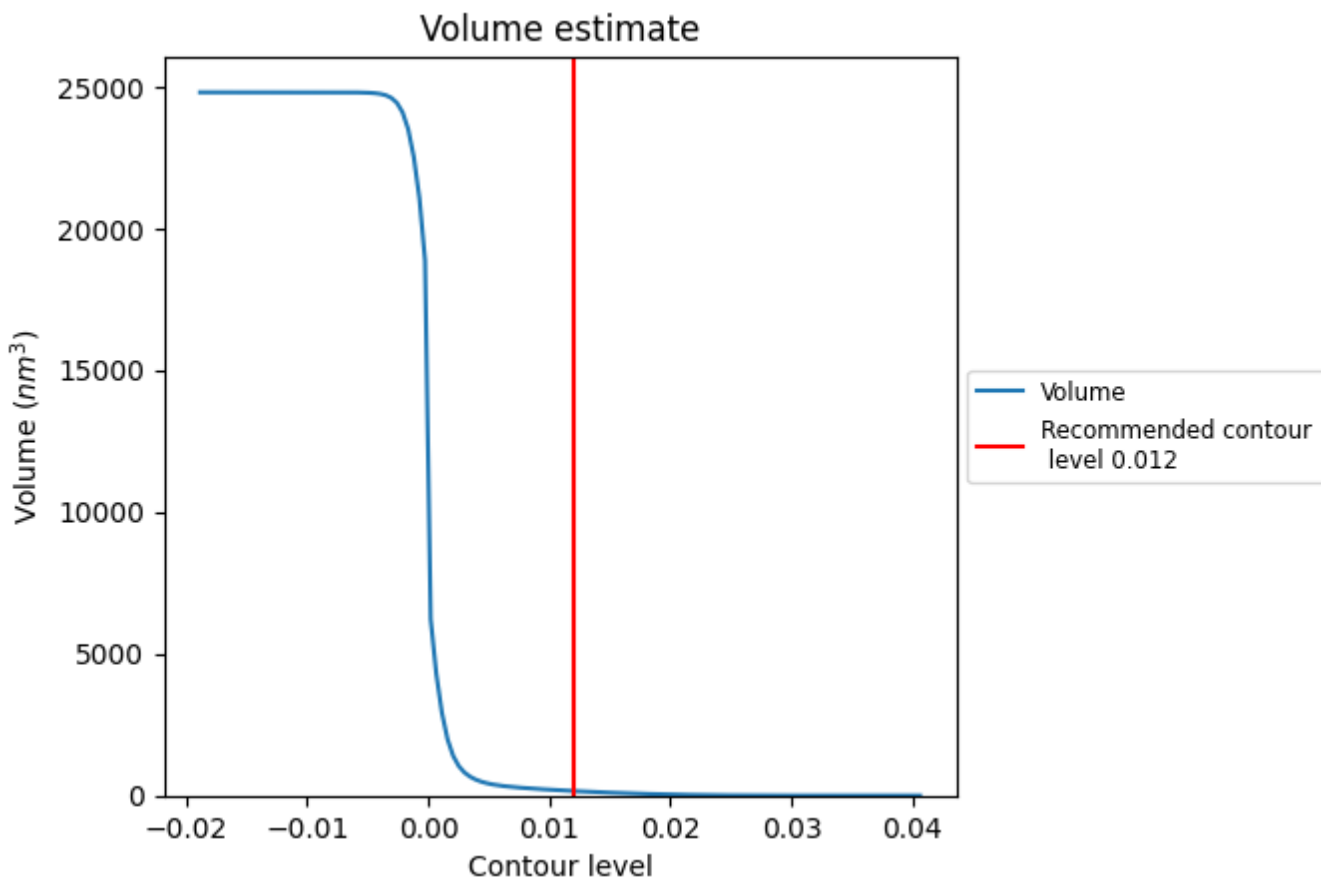
This section contains the results of statistical analysis of the map.

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.

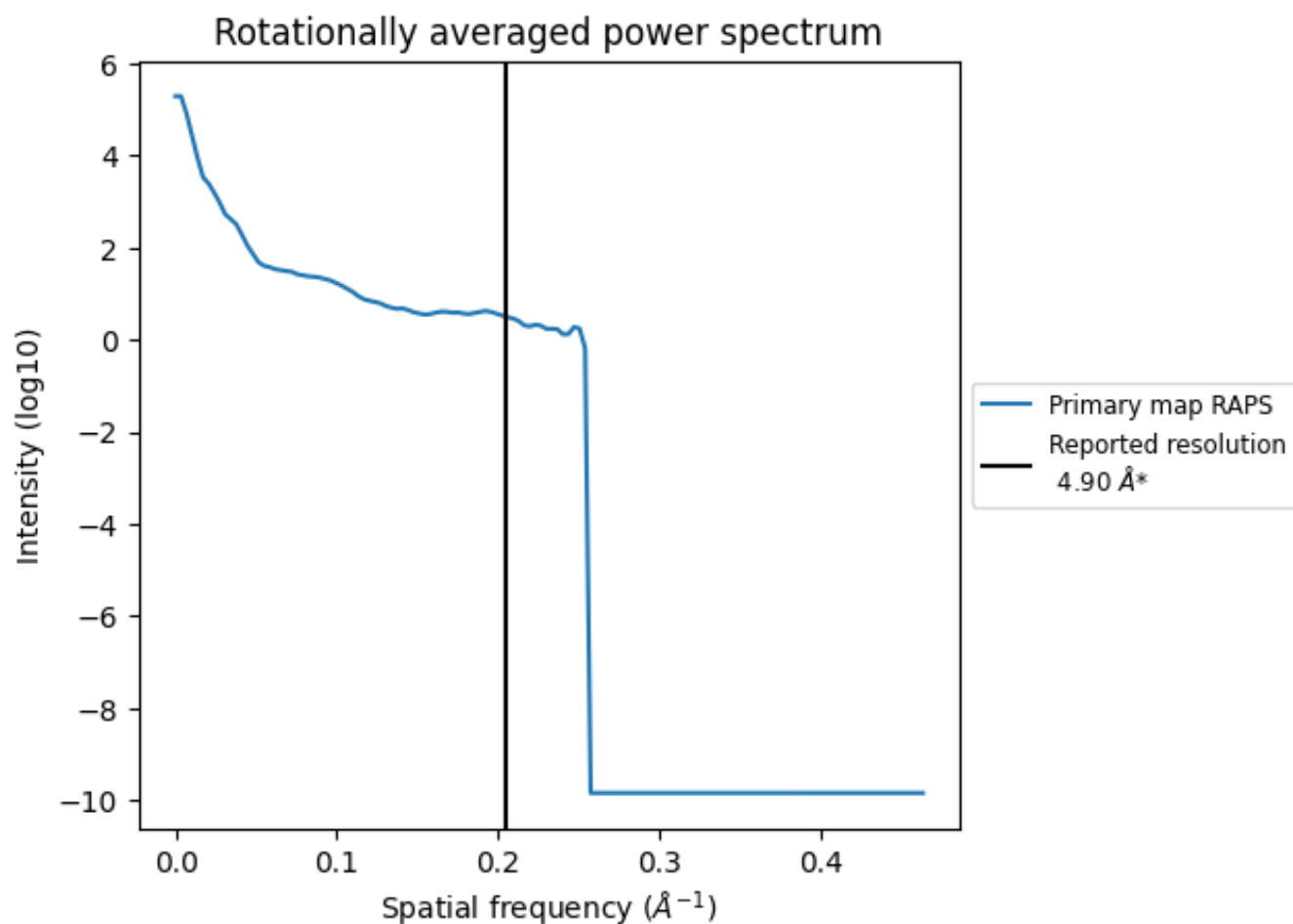
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 161 nm³; 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 [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

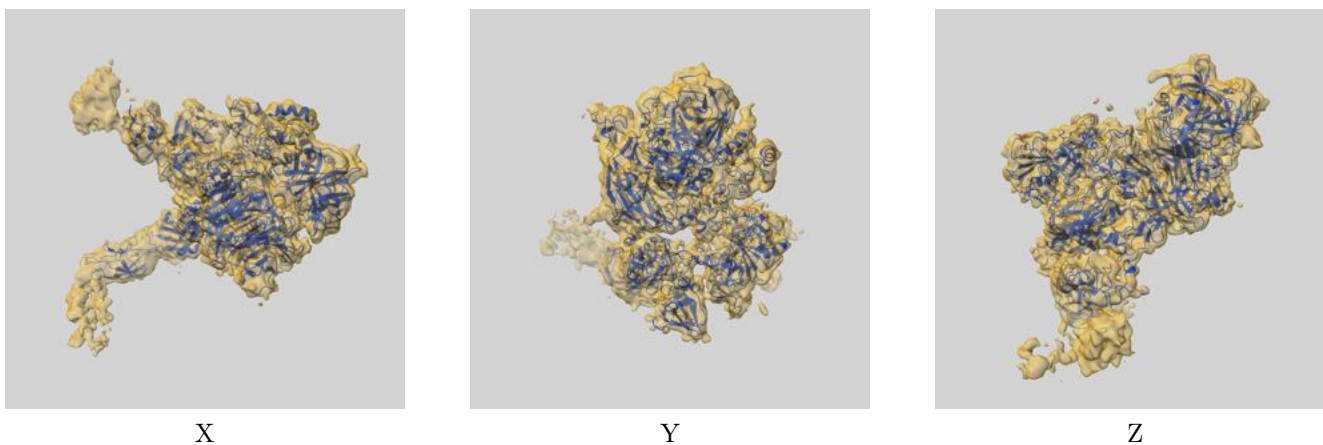
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

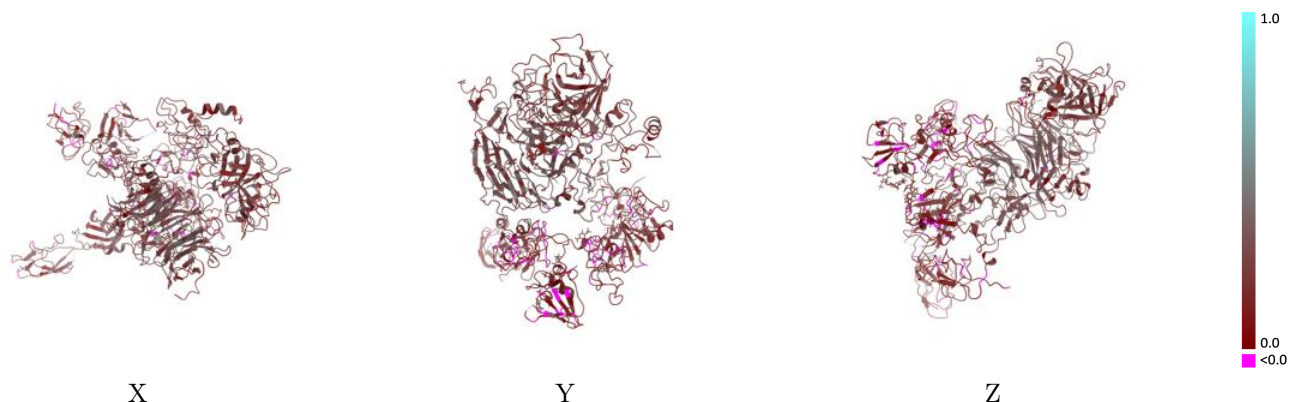
This section contains information regarding the fit between EMDB map EMD-23922 and PDB model 7MOA. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



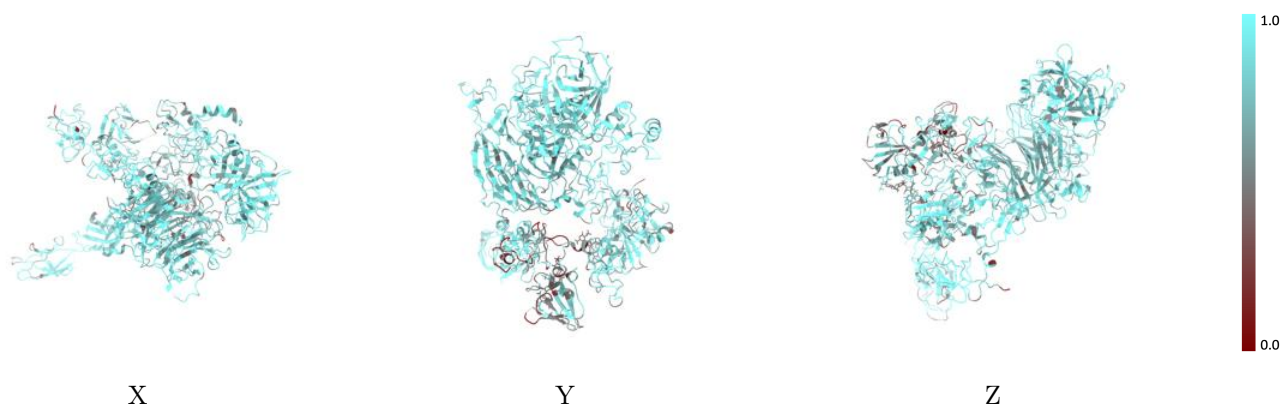
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



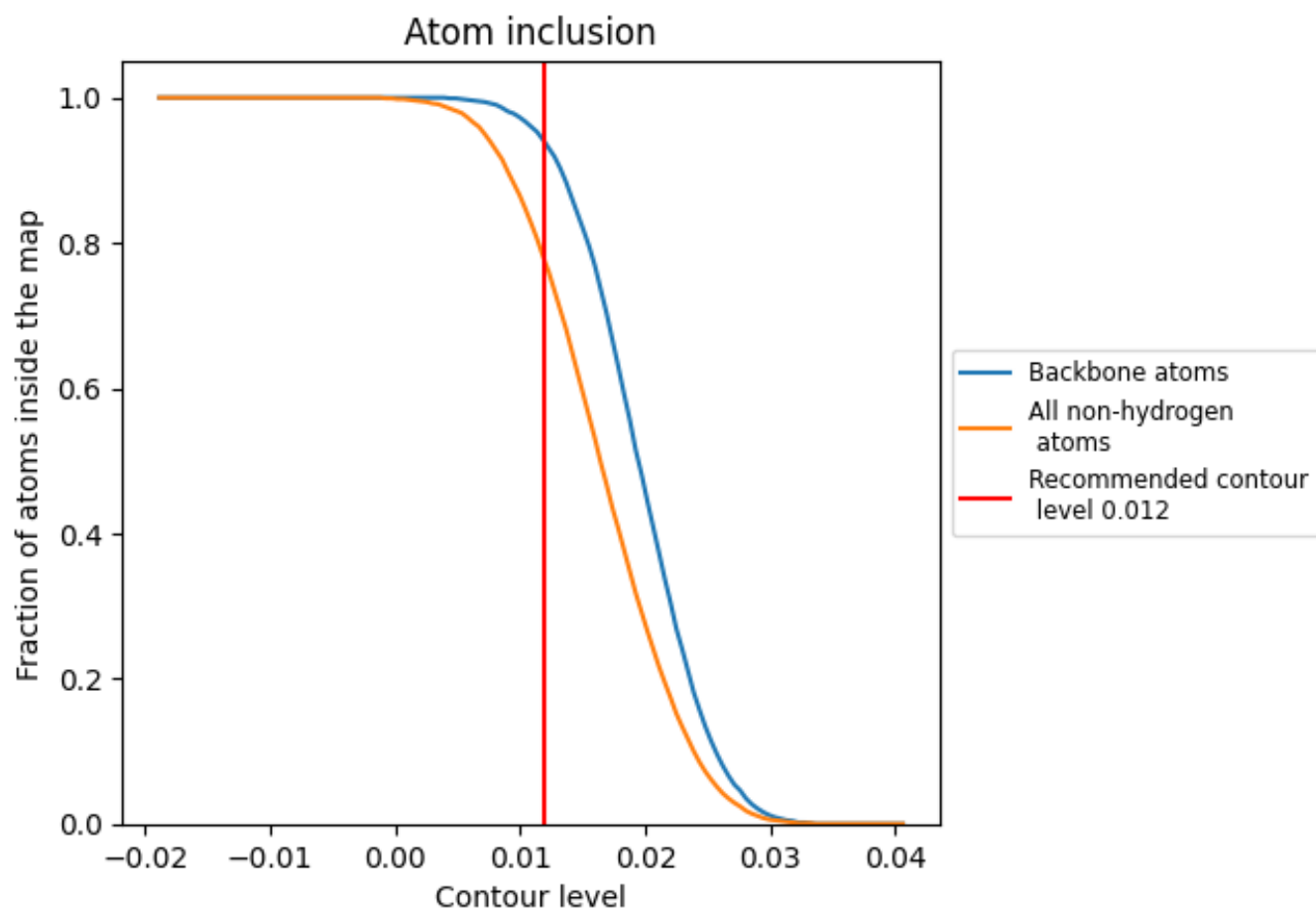
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.012).













9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 77% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.2300
A	 0.8140	 0.2030
D	 0.7160	 0.2020
E	 0.8170	 0.2670
F	 0.6800	 0.1190
J	 0.5570	 0.2360

