Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 05:24 PM EST

PDB ID	:	7MOA
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:

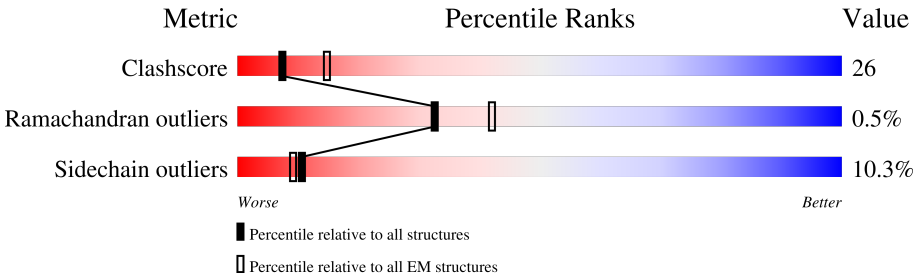
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 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)
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	728	14% 20% 65%
1	D	728	11% 43% 41% 12%
2	E	1390	27% 22% 51%
3	F	6	33% 67% 33%
3	J	6	17% 67% 33%

2 Entry composition

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.

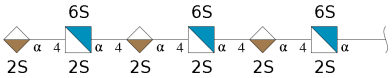
- Molecule 1 is a protein called Hepatocyte growth factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
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
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.



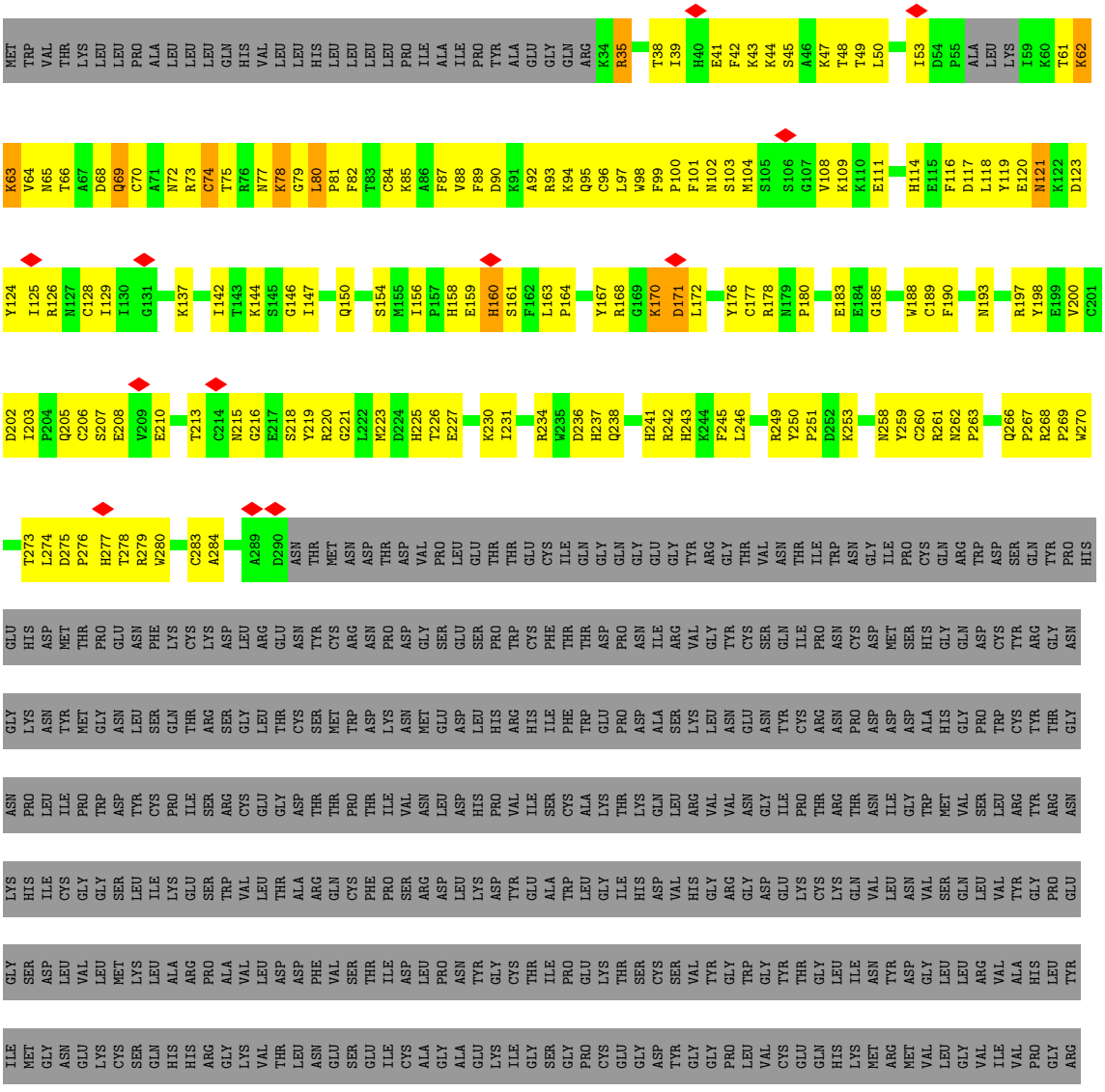
Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	6	Total	C	N	O	S	0	0
			97	35	3	51	8		
3	J	6	Total	C	N	O	S	0	0
			97	35	3	51	8		

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.

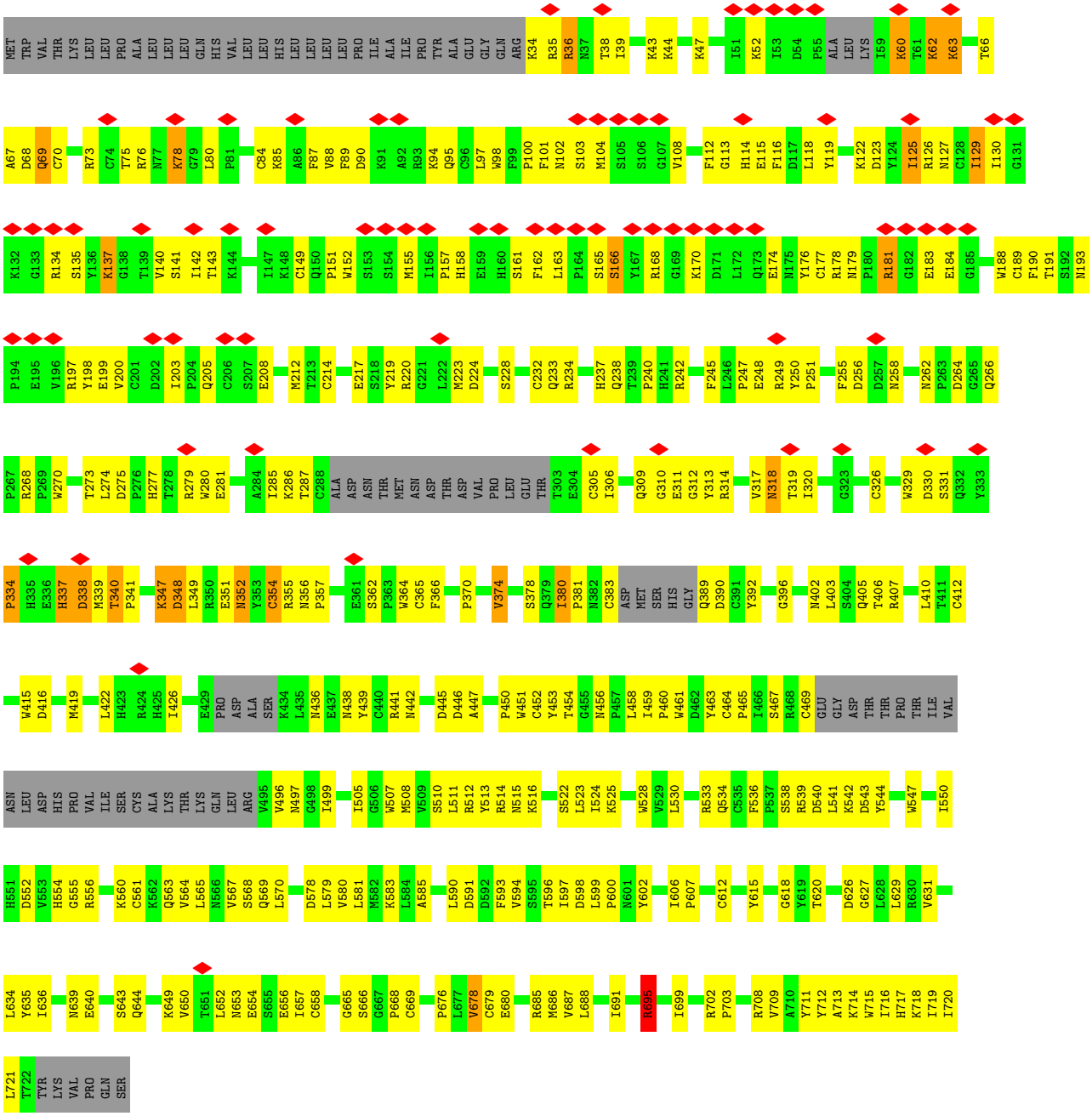
• Molecule 1: Hepatocyte growth factor

Chain A:



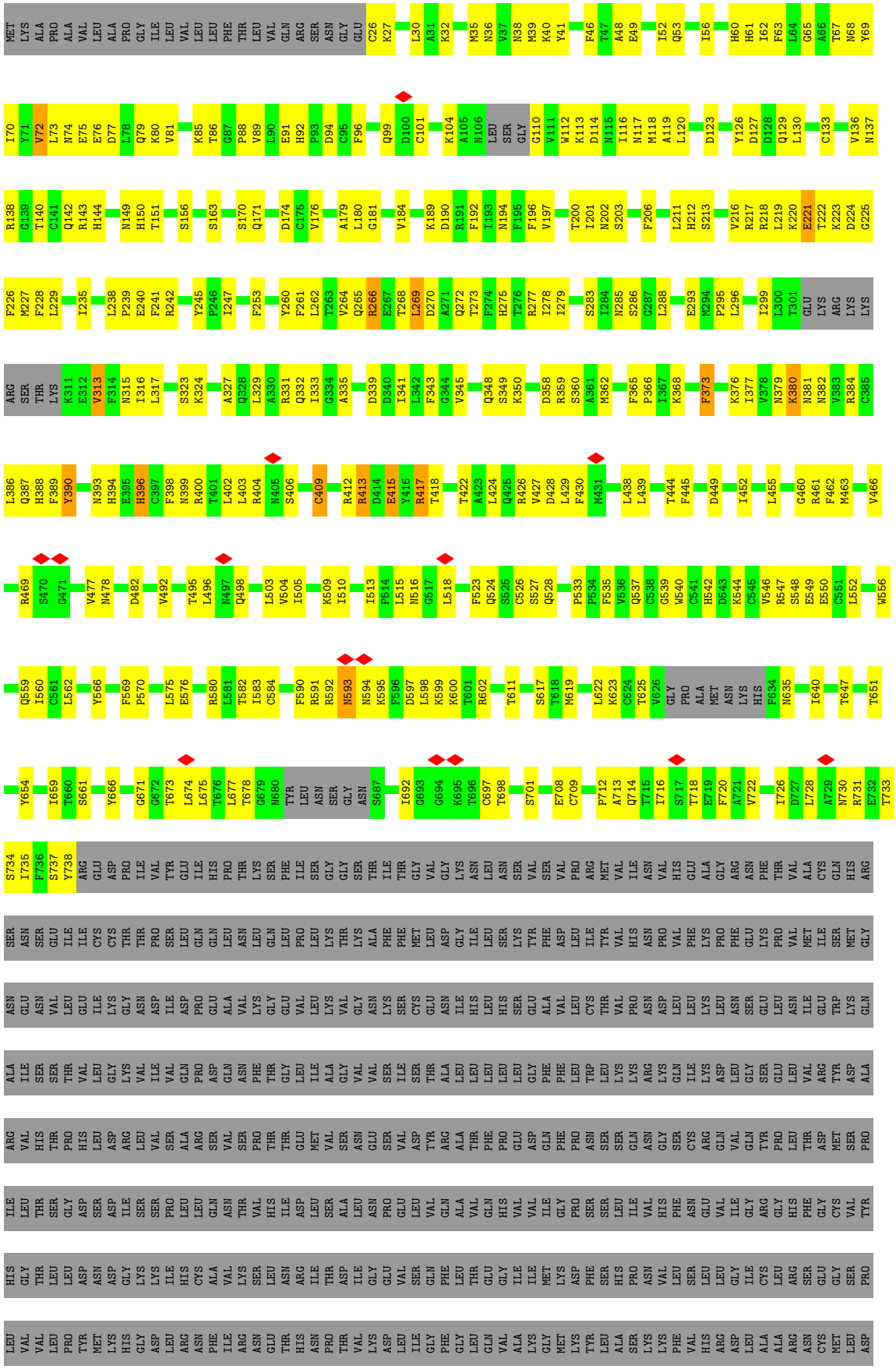
• Molecule 1: Hepatocyte growth factor

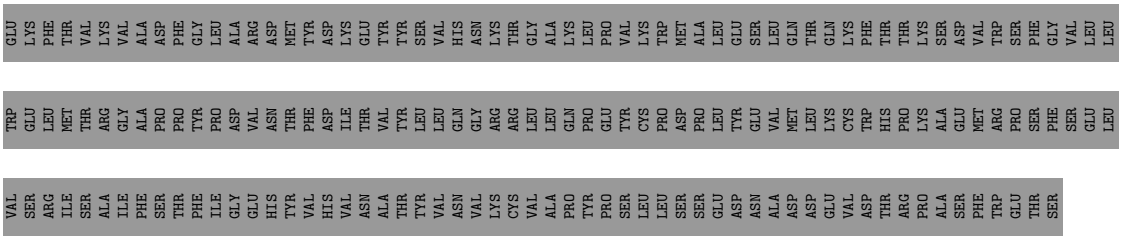
Chain D:



• Molecule 2: Hepatocyte growth factor receptor

Chain E:



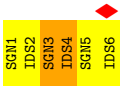


• Molecule 3: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain F:

• 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

Chain J:



4 Experimental information (i)

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 ($e^-/Å^2$)	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	0.041	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

5.1 Standard geometry

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	0.48	0/2105	0.68	0/2840
1	D	0.50	0/5081	0.62	2/6901 (0.0%)
2	E	0.53	0/5444	0.64	0/7397
All	All	0.51	0/12630	0.64	2/17138 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	441	ARG	C-N-CA	-5.66	107.56	121.70
1	D	390	ASP	CB-CG-OD2	5.18	122.97	118.30

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	2047	0	1933	155	0
1	D	4946	0	4584	265	0
2	E	5324	0	5126	224	0
3	F	97	0	34	3	0
3	J	97	0	34	3	0
All	All	12511	0	11711	633	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 26.

All (633) 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	0.84
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:D:126:ARG:O	1:D:127:ASN:OD1	2.04	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:600:PRO:HA	1:D:686:MET:HE1	1.71	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:177:CYS:C	1:A:178:ARG:HD3	2.15	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:80:LYS:O	2:E:80:LYS:HG3	2.02	0.59
1:D:152:TRP:CH2	1:D:189:CYS:HA	2.37	0.59
1:A:163:LEU:HD12	1:A:163:LEU:H	1.65	0.59
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:161:SER:C	1:D:163:LEU:H	2.06	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
1:D:554:HIS:HB2	1:D:556:ARG:HE	1.69	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:85:LYS:HZ2	1:A:100:PRO:C	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:220:LYS:HG2	2:E:225:GLY:C	2.26	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
1:A:89:PHE:CE1	1:A:96:CYS:HB3	2.42	0.55
1:A:108:VAL:C	1:A:109:LYS:HD3	2.28	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
2:E:76:GLU:CD	2:E:76:GLU:H	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:409:CYS:SG	2:E:409:CYS:O	2.67	0.52
2:E:730:ASN:CG	2:E:731:ARG:H	2.12	0.52
1:A:77:ASN:C	1:A:79:GLY:H	2.13	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
1:A:183:GLU:CD	1:A:185:GLY:H	2.11	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:D:590:LEU:HD13	1:D:594:VAL:HG23	1.95	0.49
2:E:224:ASP:OD1	2:E:224:ASP:N	2.45	0.49
1:D:561:CYS:HB3	1:D:593:PHE:HD2	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:170:SER:HB2	2:E:171:GLN:NE2	2.27	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:A:109:LYS:HB2	1:A:111:GLU:OE2	2.14	0.48
2:E:726:ILE:C	2:E:728:LEU:H	2.15	0.48
1:D:564:VAL:C	1:D:565:LEU:HD12	2.34	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
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
2:E:384:ARG:NH1	2:E:387:GLN:OE1	2.41	0.47
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
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: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:263:PRO:HD2	1:A:270:TRP:NE1	2.29	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: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
1:D:653:ASN:H	1:D:656:GLU:CD	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:323:SER:OG	2:E:324:LYS:N	2.48	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
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
2:E:163:SER:OG	2:E:174:ASP:OD2	2.30	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:380:ILE:H	1:D:380:ILE:HG13	1.29	0.45
2:E:580:ARG:HA	2:E:625:THR:HG22	1.98	0.45
1:D:249:ARG:HG3	1:D:250:TYR:CE1	2.51	0.45
1:A:142:ILE:HD11	1:A:146:GLY:C	2.37	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
2:E:592:ARG:O	2:E:593:ASN:C	2.55	0.45
1:D:155:MET:SD	1:D:161:SER:HB2	2.56	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
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: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
1:D:456:ASN:OD1	1:D:458:LEU:N	2.50	0.44
1:D:543:ASP:OD1	1:D:543:ASP:N	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:514:ARG:HB2	1:D:516:LYS:HZ2	1.83	0.44
2:E:278:ILE:HB	2:E:296:LEU:HD12	1.98	0.44
2:E:379:ASN:HB2	2:E:380:LYS:HZ1	1.82	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: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
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: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: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:406:THR:C	1:D:465:PRO:HD3	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:HIS:HB2	1:A:197:ARG:HH22	1.82	0.43
2:E:48:ALA:HB3	2:E:52:ILE:HD11	2.00	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
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:43:LYS:C	1:A:43:LYS:HD3	2.39	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
2:E:539:GLY:H	2:E:556:TRP:HE1	1.67	0.43
1:A:39:ILE:C	1:A:41:GLU:N	2.70	0.43
1:A:48:THR:O	1:A:116:PHE:HB2	2.19	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
2:E:599:LYS:HZ3	2:E:600:LYS:HG3	1.84	0.43
1:D:406:THR:OG1	1:D:407:ARG:N	2.52	0.43
1:D:513:TYR:O	1:D:516:LYS:NZ	2.50	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
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:726:ILE:C	2:E:728:LEU:N	2.73	0.42
1:D:126:ARG:O	1:D:127:ASN:CG	2.58	0.42
1:A:170:LYS:C	1:A:172:LEU:H	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HD11	1:A:146:GLY:HA2	2.01	0.42
1:A:227:GLU:CD	1:A:268:ARG:HH21	2.21	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
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: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:379:ASN:HB2	2:E:380:LYS:NZ	2.34	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: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:D:524:ILE:C	1:D:525:LYS:HD2	2.40	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:PHE:CE2	2:E:218:ARG:CZ	3.03	0.41
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:A:238:GLN:HG3	1:A:242:ARG:HA	2.02	0.41
2:E:181:GLY:N	2:E:200:THR:HG1	2.17	0.41
2:E:580:ARG:C	2:E:623:LYS:HZ3	2.24	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:D:598:ASP:C	1:D:599:LEU:HD22	2.41	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: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:85:LYS:HZ2	1:D:101:PHE:HA	1.85	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
1:D:158:HIS:NE2	1:D:197:ARG:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:597:ASP:C	2:E:599:LYS:H	2.24	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
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%)	19	60
2	E	678/1390 (49%)	618 (91%)	58 (9%)	2 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1554/2846 (55%)	1414 (91%)	133 (9%)	7 (0%)	32 68

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%)	12 37
1	D	525/646 (81%)	467 (89%)	58 (11%)	6 25
2	E	598/1246 (48%)	535 (90%)	63 (10%)	7 26
All	All	1347/2538 (53%)	1208 (90%)	139 (10%)	11 27

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	53	ILE
1	A	61	THR
1	A	62	LYS
1	A	63	LYS
1	A	65	ASN
1	A	69	GLN
1	A	74	CYS
1	A	78	LYS

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Mol	Chain	Res	Type
1	A	80	LEU
1	A	121	ASN
1	A	160	HIS
1	A	161	SER
1	A	170	LYS
1	A	171	ASP
1	A	203	ILE
1	A	206	CYS
1	A	258	ASN
2	E	32	LYS
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	144	HIS
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	277	ARG
2	E	283	SER
2	E	288	LEU
2	E	313	VAL
2	E	316	ILE
2	E	317	LEU
2	E	345	VAL
2	E	348	GLN
2	E	349	SER
2	E	350	LYS
2	E	373	PHE
2	E	376	LYS
2	E	380	LYS

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Mol	Chain	Res	Type
2	E	381	ASN
2	E	390	TYR
2	E	393	ASN
2	E	394	HIS
2	E	396	HIS
2	E	398	PHE
2	E	399	ASN
2	E	409	CYS
2	E	412	ARG
2	E	413	ARG
2	E	415	GLU
2	E	417	ARG
2	E	418	THR
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	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	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	60	LYS
1	D	62	LYS
1	D	69	GLN
1	D	75	THR
1	D	78	LYS
1	D	80	LEU
1	D	97	LEU
1	D	123	ASP

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Mol	Chain	Res	Type
1	D	125	ILE
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	181	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	268	ARG
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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	HIS
2	E	498	GLN
2	E	635	ASN
1	D	114	HIS
1	D	158	HIS
1	D	233	GLN
1	D	497	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	0.94	0	19,26,31	1.30	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	IDS	F	2	3	16,16,17	1.19	1 (6%)	17,24,26	0.82	1 (5%)
3	SGN	F	3	3	18,19,20	3.41	3 (16%)	22,29,31	1.59	3 (13%)
3	IDS	F	4	3	16,16,17	0.97	0	17,24,26	1.84	2 (11%)
3	SGN	F	5	3	12,13,20	4.10	2 (16%)	12,19,31	1.59	2 (16%)
3	IDS	F	6	3	15,15,17	1.18	1 (6%)	15,22,26	1.44	2 (13%)
3	SGN	J	1	3	15,18,20	0.97	0	19,26,31	1.48	3 (15%)
3	IDS	J	2	3	16,16,17	0.99	0	17,24,26	2.14	2 (11%)
3	SGN	J	3	3	18,19,20	3.44	2 (11%)	22,29,31	1.80	5 (22%)
3	IDS	J	4	3	16,16,17	1.16	1 (6%)	17,24,26	0.97	1 (5%)
3	SGN	J	5	3	12,13,20	4.09	2 (16%)	12,19,31	1.56	2 (16%)
3	IDS	J	6	3	15,15,17	1.18	1 (6%)	15,22,26	1.38	2 (13%)

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	-	4/7/27/31	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	-	4/7/27/31	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
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	9.99	1.53	1.42
3	J	3	SGN	O1S-S1	9.91	1.53	1.42
3	J	5	SGN	O2S-S1	9.90	1.53	1.42
3	F	3	SGN	O1S-S1	9.85	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	SGN	O1S-S1	9.85	1.53	1.42
3	F	5	SGN	O2S-S1	9.84	1.53	1.42
3	F	3	SGN	O2S-S1	9.78	1.53	1.42
3	J	3	SGN	O2S-S1	9.75	1.53	1.42
3	F	2	IDS	O2-C2	-2.75	1.43	1.47
3	J	6	IDS	O2-C2	-2.51	1.43	1.47
3	F	6	IDS	O2-C2	-2.50	1.43	1.47
3	J	4	IDS	O2-C2	-2.38	1.43	1.47
3	F	3	SGN	S1-N2	2.11	1.62	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	2	IDS	C2-O2-S	7.50	127.70	117.91
3	F	4	IDS	C2-O2-S	6.70	126.65	117.91
3	F	3	SGN	O1S-S1-O2S	-4.69	109.07	120.16
3	J	5	SGN	O1S-S1-O2S	-4.55	109.41	120.16
3	F	5	SGN	O1S-S1-O2S	-4.47	109.59	120.16
3	J	3	SGN	O1S-S1-O2S	-4.45	109.64	120.16
3	F	3	SGN	C4-C3-C2	-4.00	105.15	111.02
3	J	3	SGN	C1-O5-C5	-3.97	106.81	112.19
3	F	6	IDS	C1-O5-C5	-3.80	108.11	113.92
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	J	6	IDS	C1-O5-C5	-3.52	108.54	113.92
3	F	1	SGN	C2-N2-S1	-3.46	108.11	117.07
3	J	3	SGN	C3-C4-C5	3.26	116.06	110.24
3	J	3	SGN	O5-C1-C2	-3.21	106.23	111.29
3	F	1	SGN	C4-C3-C2	-2.96	106.68	111.02
3	J	1	SGN	C2-N2-S1	-2.73	110.02	117.07
3	J	1	SGN	C3-C4-C5	-2.65	105.51	110.24
3	J	3	SGN	C4-C3-C2	2.38	114.50	111.02
3	J	6	IDS	O6A-C6-C5	-2.36	117.00	122.57
3	F	6	IDS	O6A-C6-C5	-2.34	117.04	122.57
3	F	2	IDS	O2-C2-C3	2.26	110.11	106.95
3	J	5	SGN	C5-O5-C1	-2.25	108.06	111.52
3	J	4	IDS	C2-O2-S	2.12	120.68	117.91
3	F	4	IDS	O2-C2-C3	2.08	109.86	106.95
3	F	5	SGN	C5-O5-C1	-2.06	108.36	111.52
3	F	3	SGN	C3-C4-C5	-2.04	106.61	110.24

There are no chirality outliers.

All (33) torsion outliers are listed below:

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

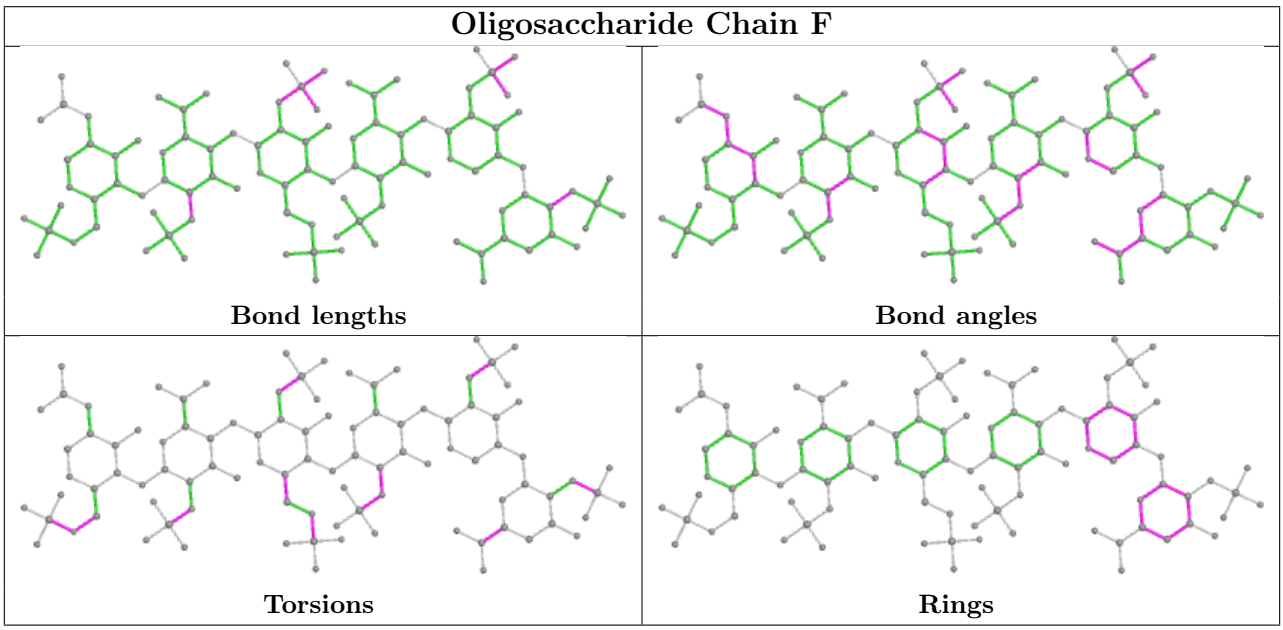
All (2) ring outliers are listed below:

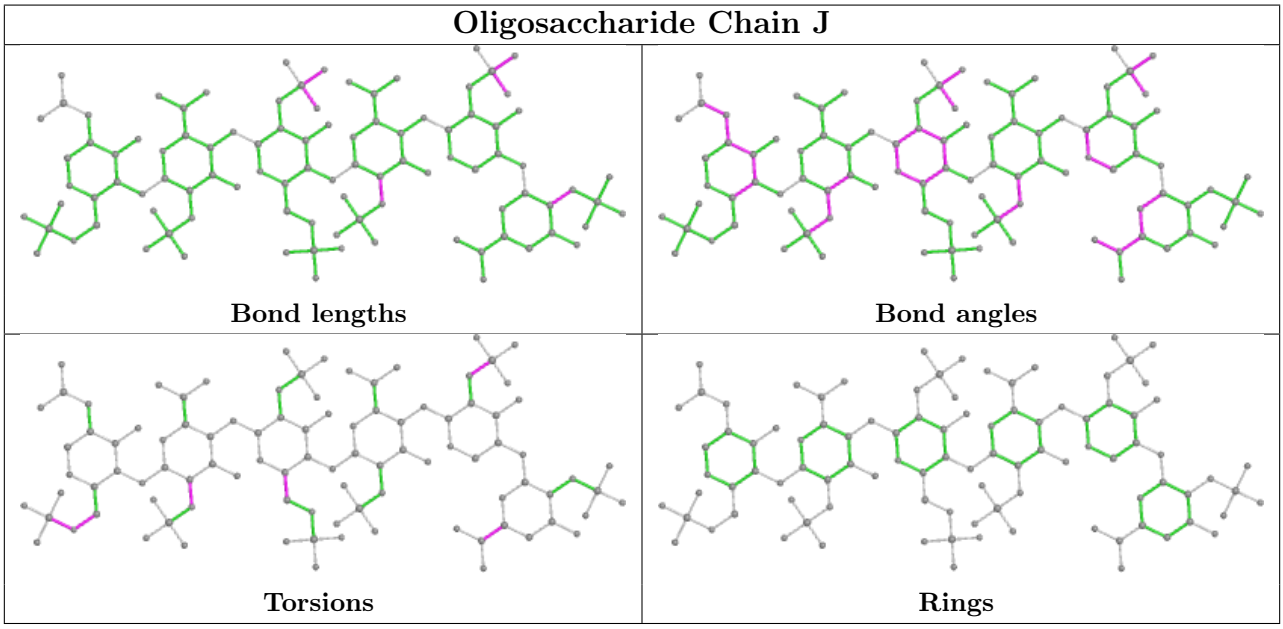
Mol	Chain	Res	Type	Atoms
3	F	6	IDS	C1-C2-C3-C4-C5-O5
3	F	5	SGN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 6 short contacts:

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

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





5.6 Ligand geometry

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.

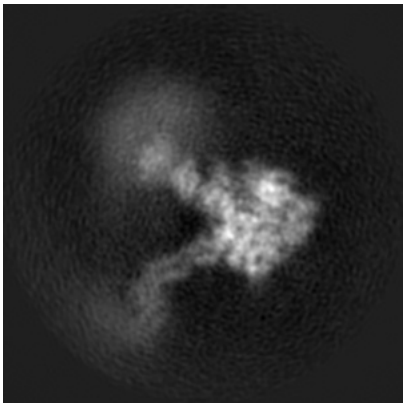
6 Map visualisation

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

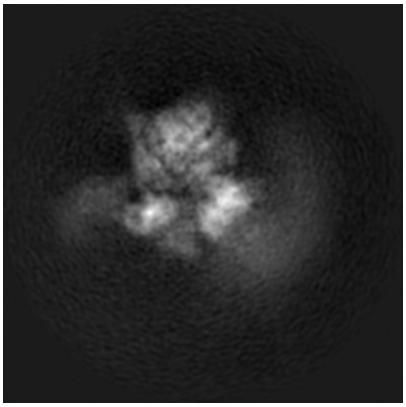
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

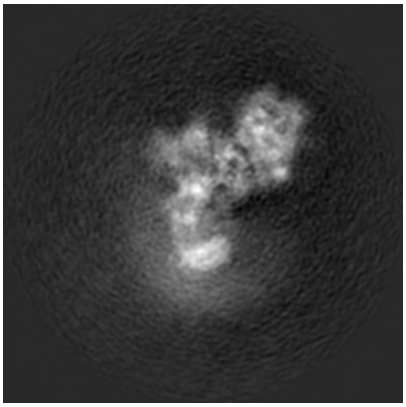
6.1.1 Primary map



X



Y

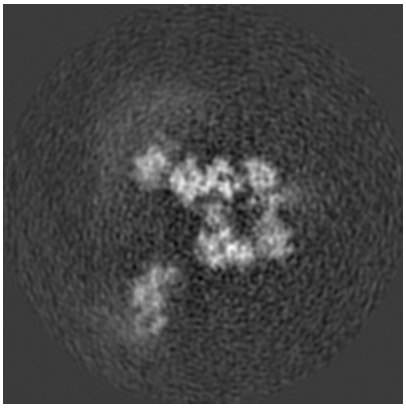


Z

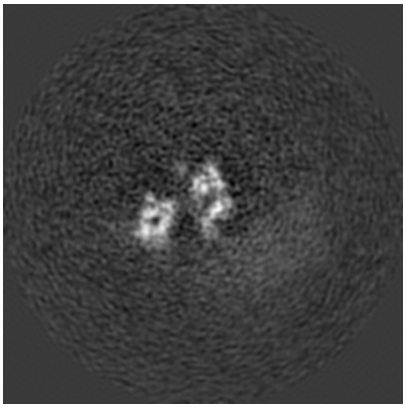
The images above show the map projected in three orthogonal directions.

6.2 Central slices

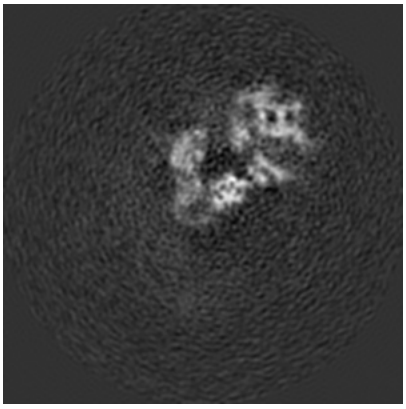
6.2.1 Primary map



X Index: 135



Y Index: 135

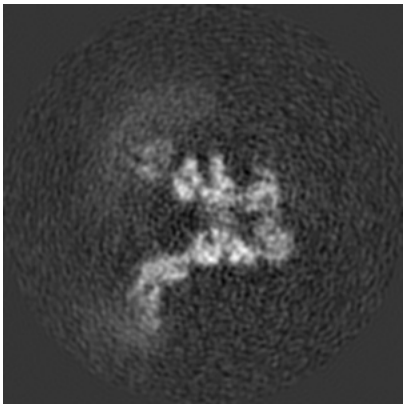


Z Index: 135

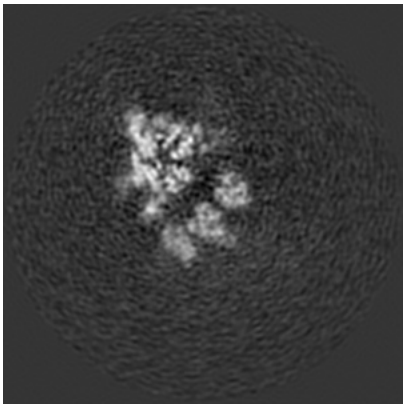
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

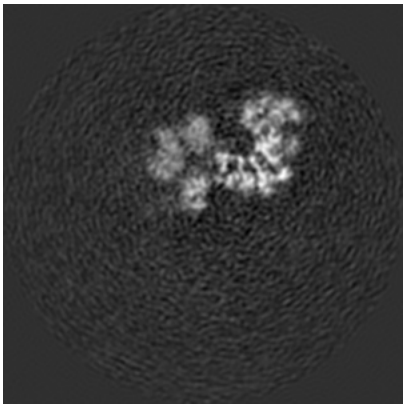
6.3.1 Primary map



X Index: 129



Y Index: 167

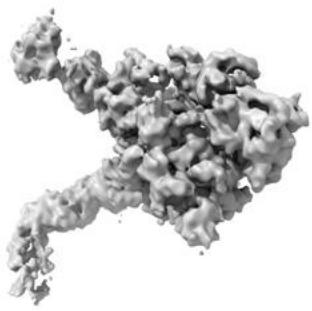


Z Index: 113

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

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

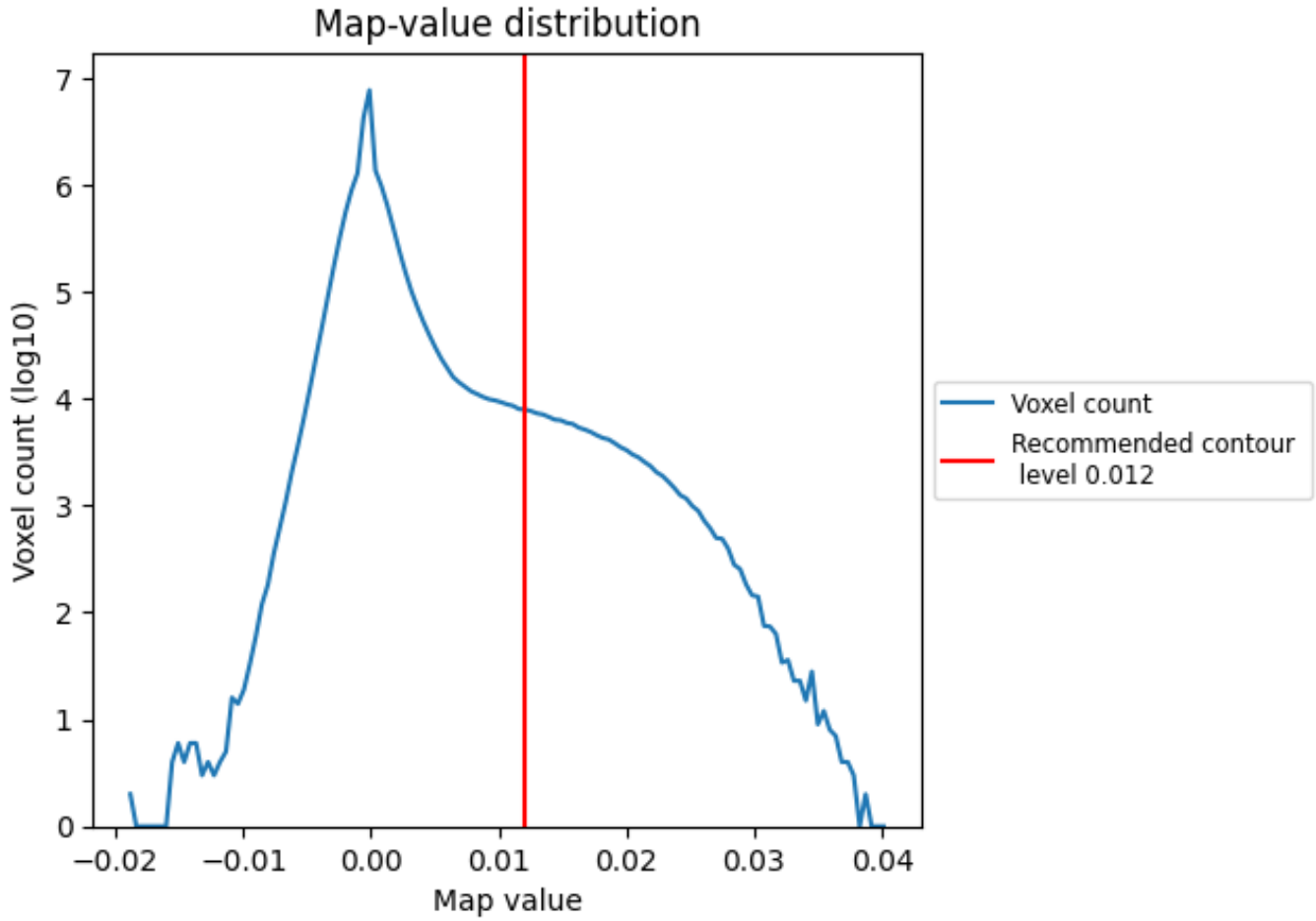
6.5 Mask visualisation (i)

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

7 Map analysis

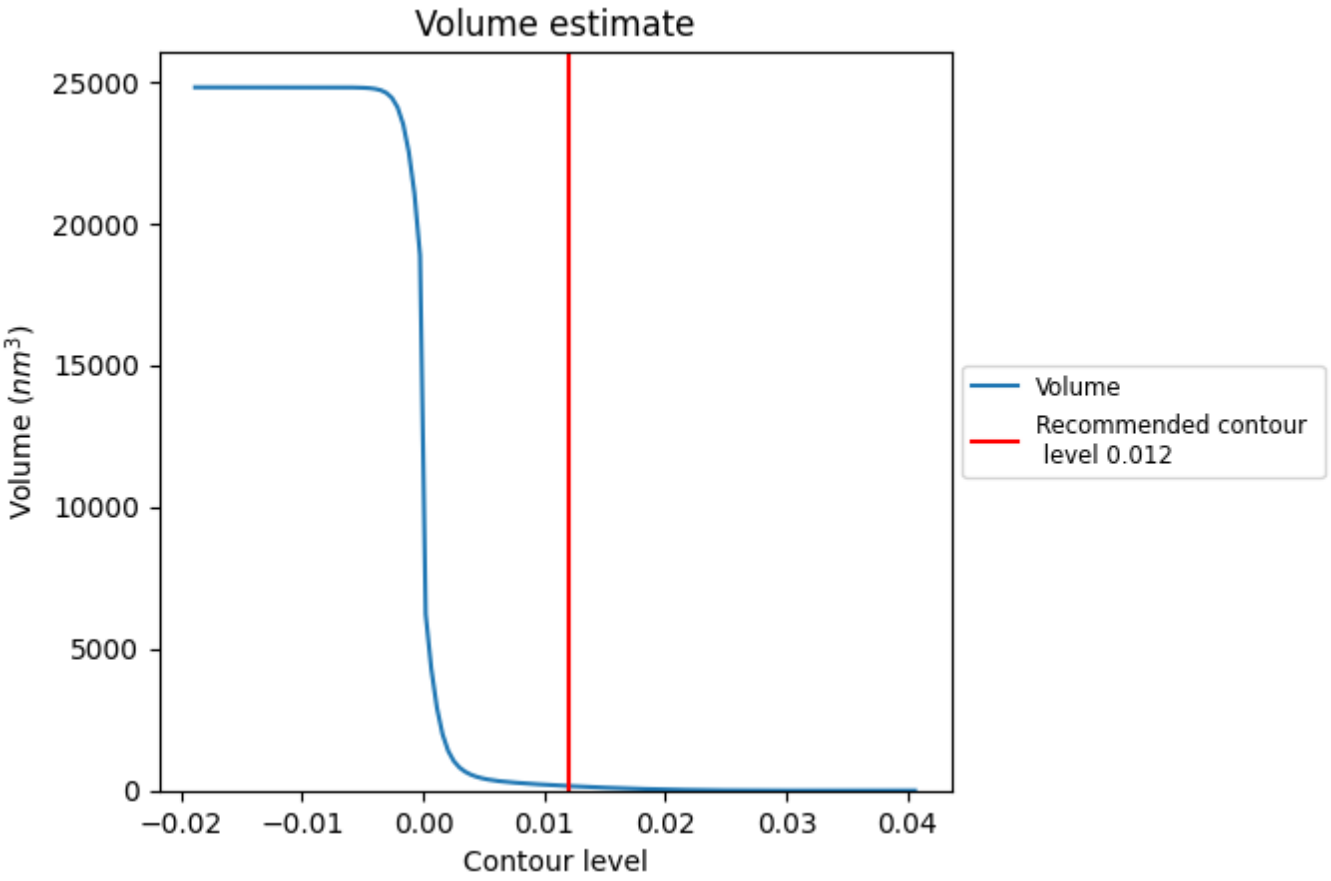
This section contains the results of statistical analysis of the map.

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.

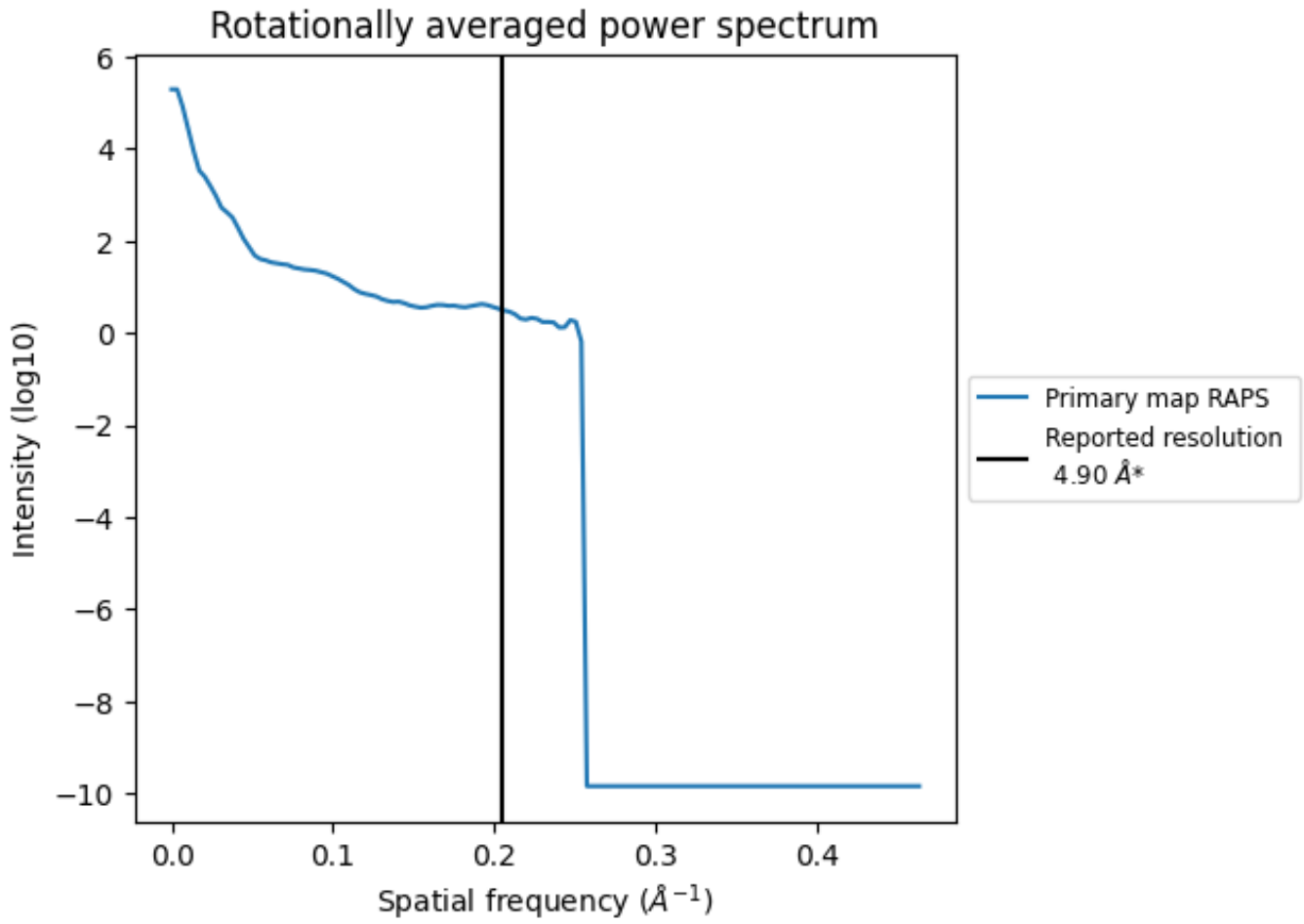
7.2 Volume estimate



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

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.204 Å^{-1}

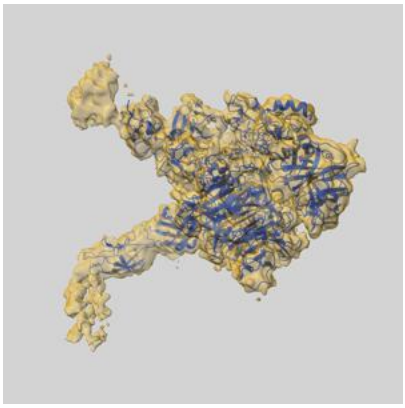
8 Fourier-Shell correlation (i)

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

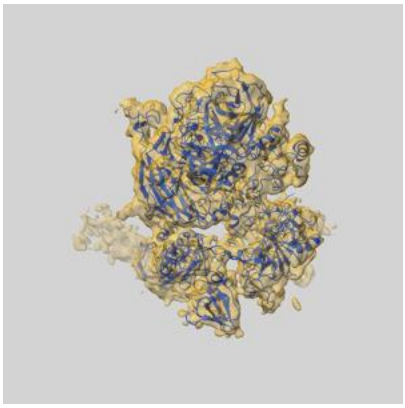
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23922 and PDB model 7MOA. Per-residue inclusion information can be found in section 3 on page 4.

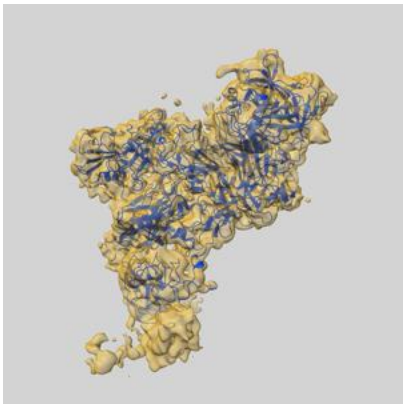
9.1 Map-model overlay



X



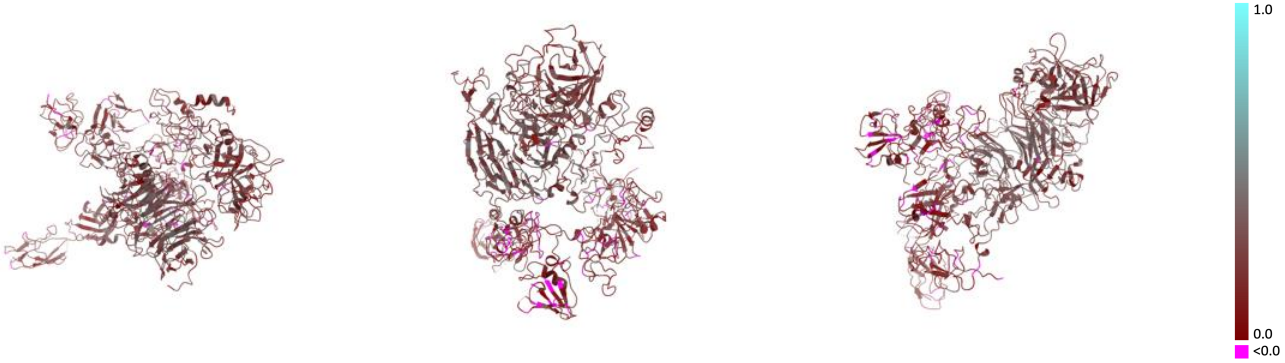
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

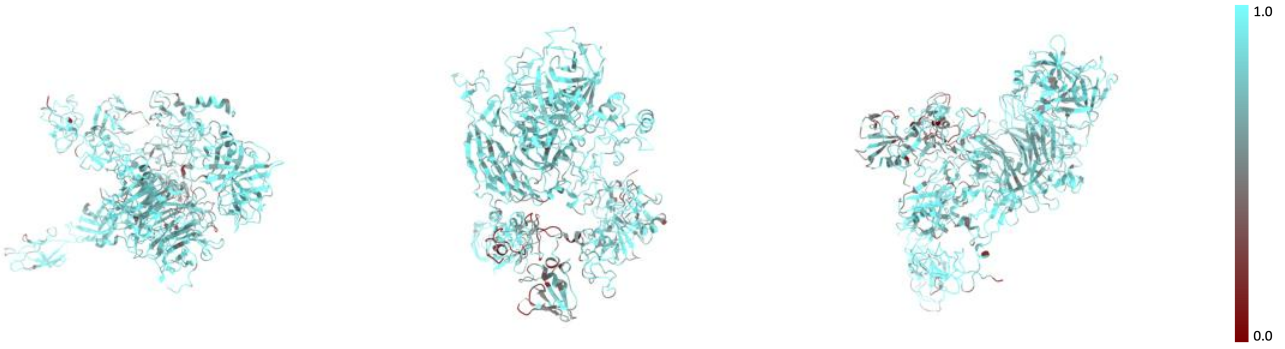
9.2 Q-score mapped to coordinate model (i)



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.

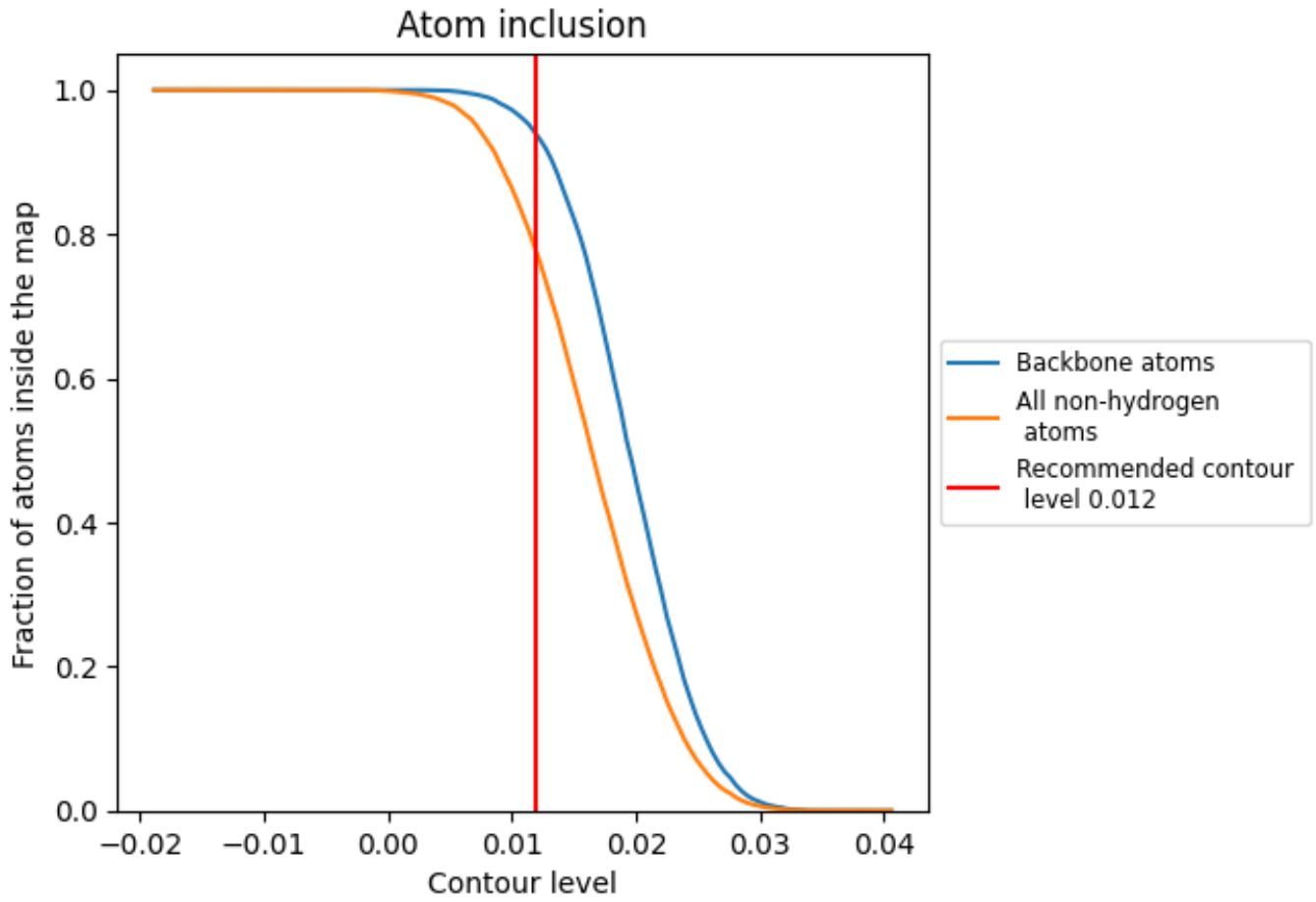
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.012).

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	0.7735	0.2300
A	0.8141	0.2030
D	0.7160	0.2020
E	0.8166	0.2670
F	0.6804	0.1190
J	0.5567	0.2360