Full wwPDB EM Validation Report ⓘ

Mar 12, 2024 – 06:57 PM JST

PDB ID	:	8H3R
EMDB ID	:	EMD-34474
Title	:	Cryo-EM Structure of the KBTBD2-CRL3 N8 dimeric complex
Authors	:	Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on	:	2022-10-09
Resolution	:	6.36 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:

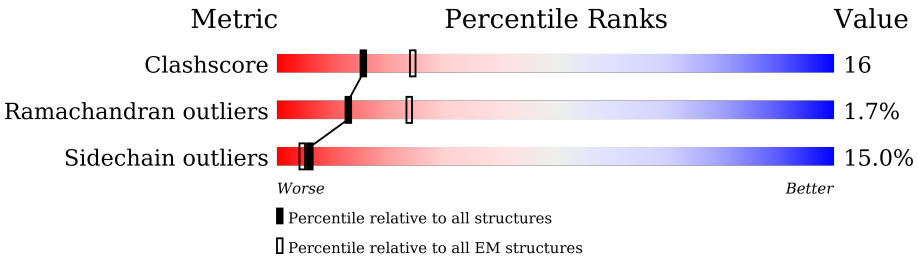
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 6.36 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	D	108	13% 29% 35% 15% • 18%
1	E	108	13% 34% 32% 13% • 18%
2	C	768	• 58% 31% 5% 6%
2	F	768	14% 57% 31% 5% • 6%
3	A	623	• 60% 28% • 10%
3	B	623	6% 61% 28% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22313 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 E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
1	D	89	Total	C	N	O	S	0	0
			737	466	135	127	9		

- Molecule 2 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	720	Total	C	N	O	S	0	0
			5866	3689	1037	1101	39		
2	F	720	Total	C	N	O	S	0	0
			5866	3689	1037	1101	39		

- Molecule 3 is a protein called Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	562	Total	C	N	O	S	0	0
			4544	2904	753	849	38		
3	B	564	Total	C	N	O	S	0	0
			4557	2911	758	850	38		

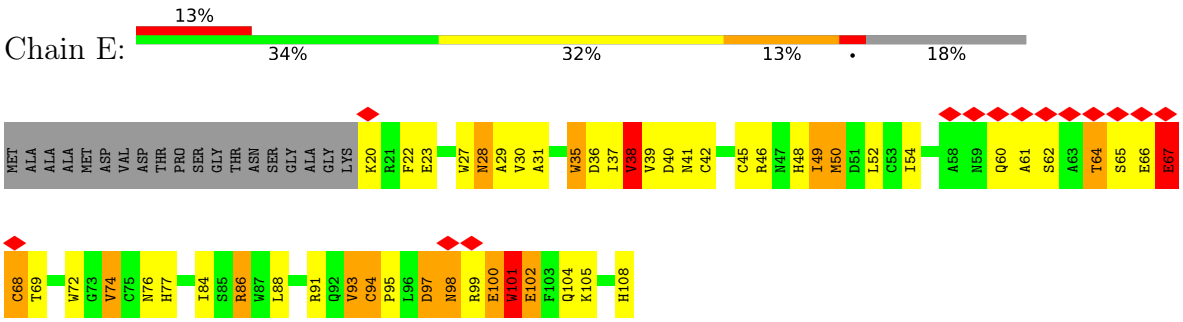
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	E	3	Total	Zn	0
			3	3	
4	D	3	Total	Zn	0
			3	3	

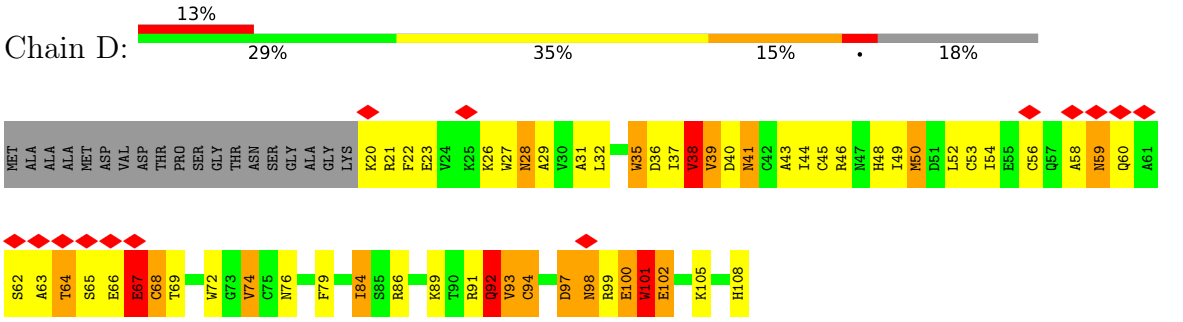
3 Residue-property plots (i)

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.

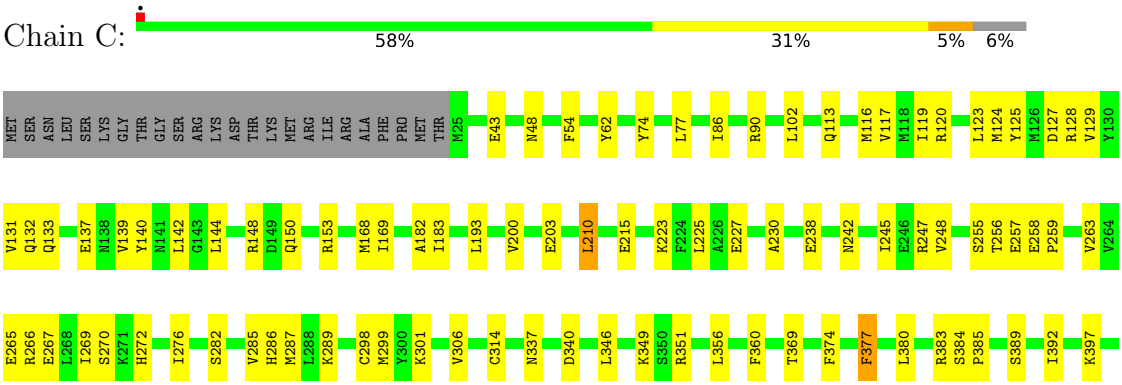
• Molecule 1: E3 ubiquitin-protein ligase RBX1

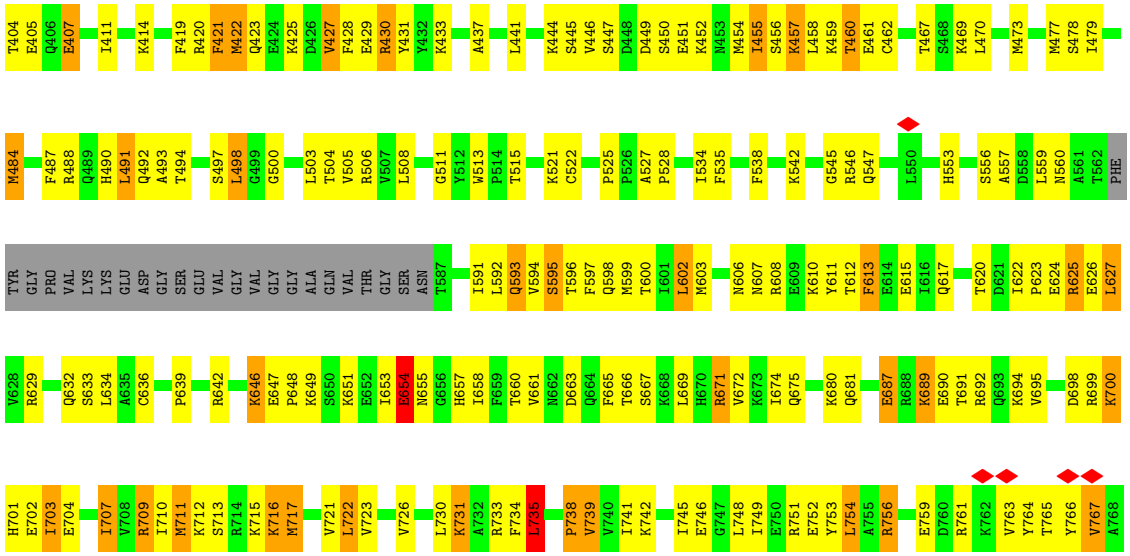


• Molecule 1: E3 ubiquitin-protein ligase RBX1



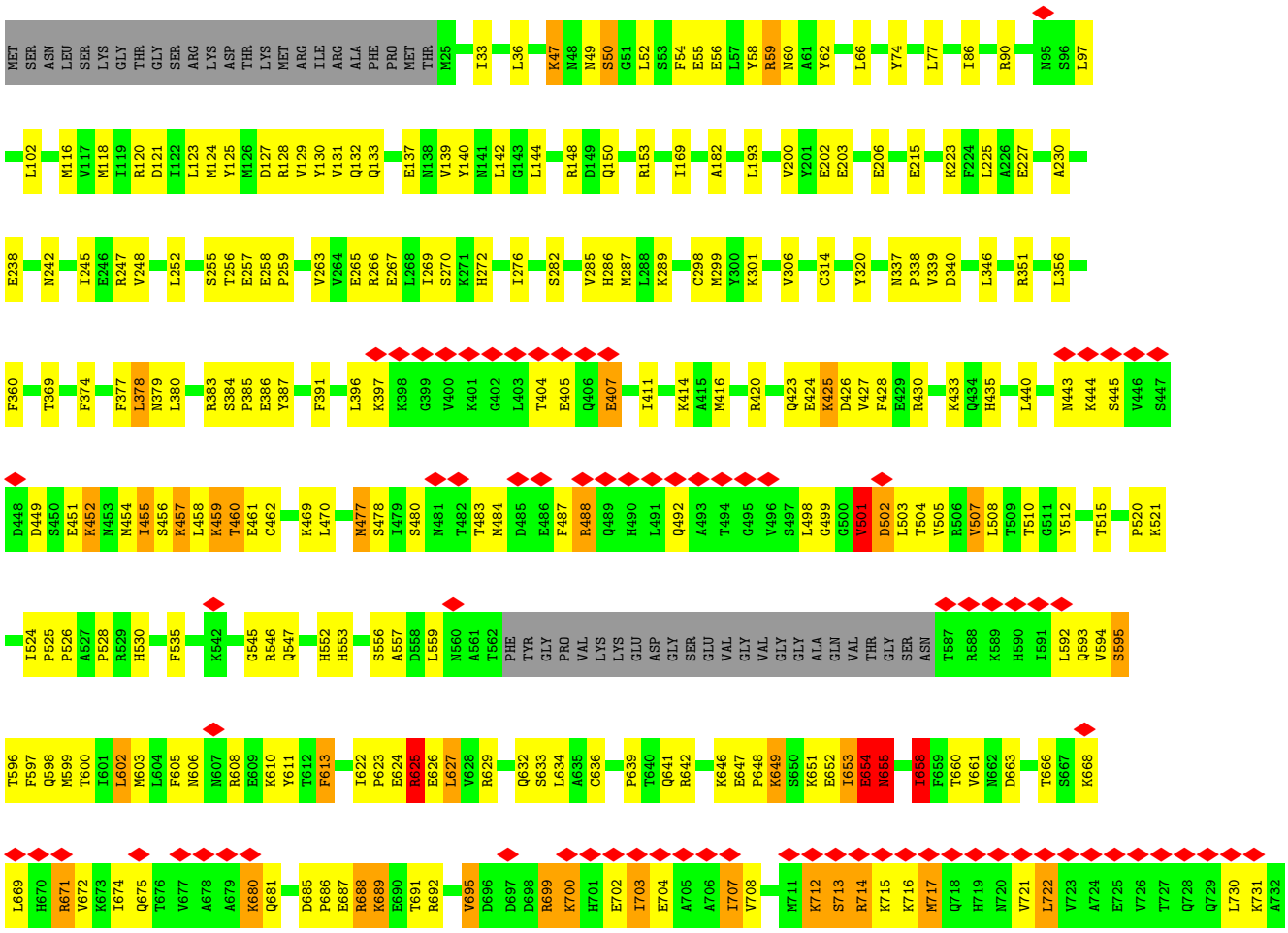
• Molecule 2: Cullin-3

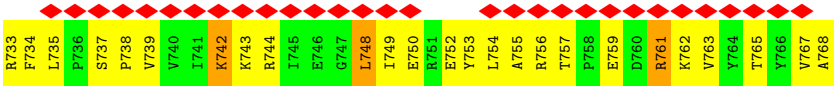




• Molecule 2: Cullin-3

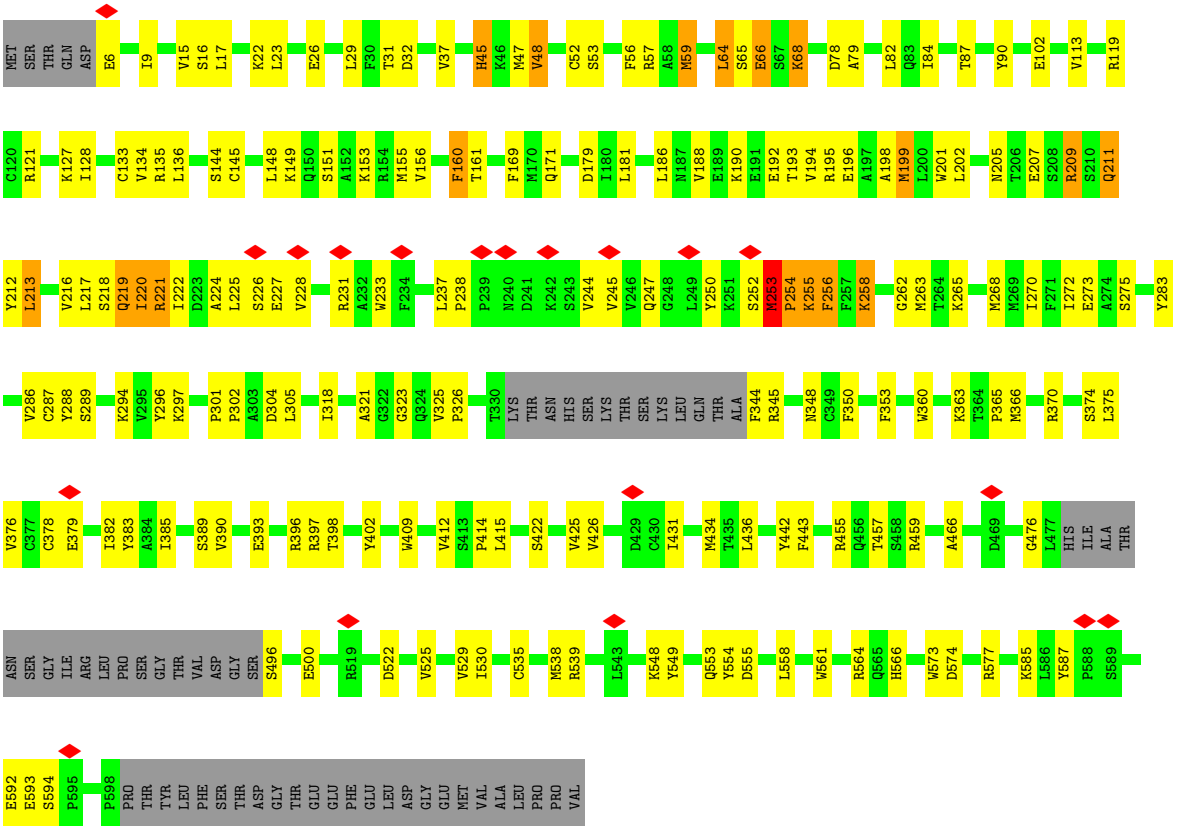
Chain F:





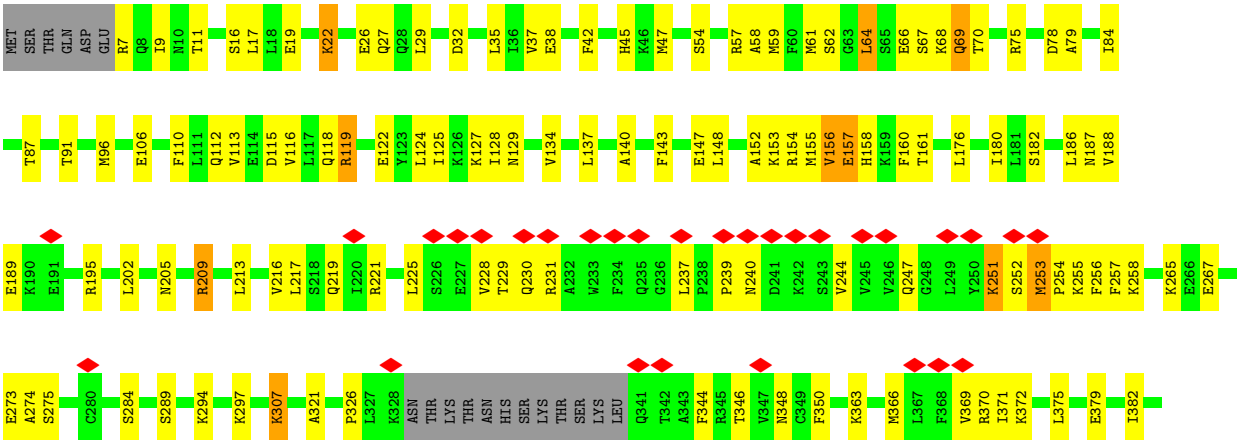
• Molecule 3: Kelch repeat and BTB domain-containing protein 2

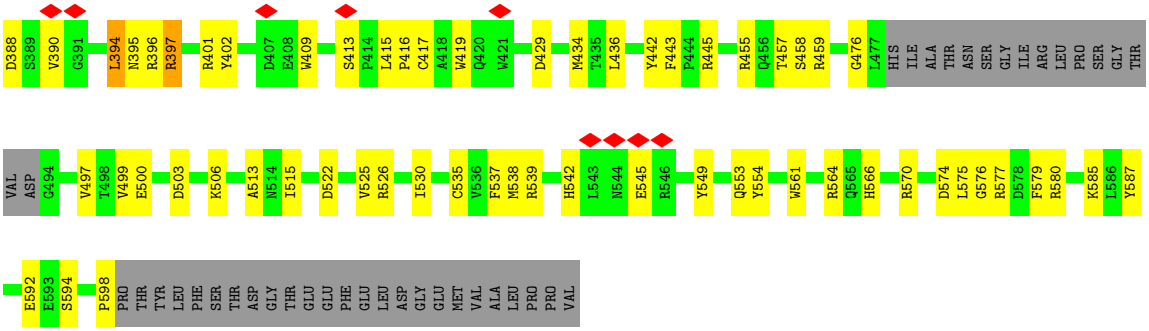
Chain A:



• Molecule 3: Kelch repeat and BTB domain-containing protein 2

Chain B:




D388 S389 V390 G391 L394 N395 R396 R397 R401 Y402 D407 E408 W409 S413 P414 L415 P416 C417 A418 W419 Q420 W421 D429 M434 T435 L436 Y442 F443 P444 R445 R455 Q456 T457 S458 R459 G476 L477 HIS ILE ALA THR ASN SER GLY ILE ARG LEU PRO SER GLY THR
VAL ASP G494 V497 T498 V499 E500 D503 K506 A513 N514 I515 D522 V525 R526 I530 C535 V536 F537 M538 R539 H542 L543 N544 E545 R546 Y549 Q553 Y554 W561 R564 Q565 H566 R570 D574 L575 G576 R577 D578 F579 R580 K585 L586 Y587
E592 E593 S594 P598 PRO THR TYR LEU PHE SER THR ASP GLY THR GLU GLU PHE GLU LEU ASP GLY GLU MET VAL ALA LEU PRO PRO VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	611847	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 ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.789	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	400.896, 400.896, 400.896	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.088, 2.088, 2.088	Depositor

5 Model quality

5.1 Standard geometry

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

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	D	0.51	0/759	0.58	0/1029
1	E	0.50	0/759	0.59	0/1029
2	C	0.42	0/5959	0.52	0/8006
2	F	0.44	0/5959	0.53	0/8006
3	A	0.40	0/4651	0.50	0/6308
3	B	0.35	0/4664	0.46	0/6324
All	All	0.42	0/22751	0.51	0/30702

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	737	0	686	56	0
1	E	737	0	686	54	0
2	C	5866	0	5904	181	0
2	F	5866	0	5904	203	0
3	A	4544	0	4453	148	0
3	B	4557	0	4473	167	0
4	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	3	0	0	0	0
All	All	22313	0	22106	729	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 16.

All (729) 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:C:594:VAL:CG1	2:C:598:GLN:HB2	1.68	1.23
3:B:110:PHE:CD1	2:F:62:TYR:CD1	2.27	1.22
3:B:110:PHE:HD1	2:F:62:TYR:CD1	1.55	1.22
2:F:594:VAL:CG1	2:F:598:GLN:HB2	1.68	1.21
3:A:160:PHE:CE1	3:A:169:PHE:CE2	2.30	1.19
3:B:366:MET:CE	3:B:370:ARG:HE	1.56	1.19
2:F:594:VAL:HA	2:F:598:GLN:OE1	1.47	1.13
2:C:594:VAL:HA	2:C:598:GLN:OE1	1.47	1.13
3:B:366:MET:HE3	3:B:370:ARG:NE	1.62	1.12
2:F:594:VAL:HG12	2:F:598:GLN:CB	1.80	1.12
2:C:594:VAL:HG12	2:C:598:GLN:CB	1.80	1.09
3:B:110:PHE:HD1	2:F:62:TYR:CE1	1.72	1.07
3:B:189:GLU:HB3	3:B:265:LYS:HE3	1.33	1.06
2:F:263:VAL:HG22	2:F:267:GLU:OE2	1.58	1.02
2:F:594:VAL:CG2	2:F:599:MET:HG2	1.88	1.02
2:C:594:VAL:CG2	2:C:599:MET:HG2	1.88	1.02
3:A:233:TRP:CH2	3:A:245:VAL:HA	1.95	1.01
3:B:366:MET:HE3	3:B:370:ARG:HE	0.88	1.01
3:B:156:VAL:HG13	3:B:160:PHE:CE1	1.97	0.99
3:B:156:VAL:HG13	3:B:160:PHE:CD1	1.97	0.99
3:A:379:GLU:O	3:A:379:GLU:HG3	1.63	0.98
3:A:233:TRP:HH2	3:A:245:VAL:CA	1.76	0.98
3:A:233:TRP:HH2	3:A:245:VAL:HA	1.26	0.98
3:B:110:PHE:CD1	2:F:62:TYR:CE1	2.51	0.97
3:A:190:LYS:HB2	3:A:192:GLU:OE2	1.65	0.97
3:A:160:PHE:CE1	3:A:169:PHE:CZ	2.53	0.97
3:B:110:PHE:CD1	2:F:62:TYR:CG	2.52	0.96
2:C:248:VAL:HG22	2:C:256:THR:HG23	1.47	0.96
3:A:233:TRP:CH2	3:A:245:VAL:HG22	2.02	0.95
2:C:263:VAL:HG22	2:C:267:GLU:OE2	1.66	0.94
1:E:104:GLN:NE2	2:C:511:GLY:CA	2.31	0.94
3:B:110:PHE:HD1	2:F:62:TYR:CG	1.87	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:415:LEU:HD22	3:B:417:CYS:O	1.67	0.93
2:F:559:LEU:HD22	2:F:602:LEU:HD23	1.51	0.92
1:E:72:TRP:HB2	1:E:105:LYS:HB3	1.52	0.91
2:C:634:LEU:HD23	2:C:674:ILE:HG21	1.52	0.91
2:C:559:LEU:HD22	2:C:602:LEU:HD23	1.51	0.90
3:A:151:SER:O	3:A:155:MET:HG2	1.71	0.90
1:E:104:GLN:HE22	2:C:511:GLY:HA3	1.36	0.90
3:B:394:LEU:HD12	3:B:395:ASN:N	1.87	0.90
3:B:415:LEU:CD2	3:B:417:CYS:H	1.84	0.90
2:F:33:ILE:HG23	2:F:60:ASN:HB3	1.54	0.89
2:F:127:ASP:O	2:F:131:VAL:HG22	1.72	0.89
1:E:104:GLN:NE2	2:C:511:GLY:HA3	1.88	0.89
2:F:553:HIS:CE1	2:F:623:PRO:HG3	2.06	0.89
2:F:594:VAL:HG23	2:F:599:MET:HG2	1.54	0.89
2:F:634:LEU:HD23	2:F:674:ILE:HG21	1.52	0.89
1:D:72:TRP:HB2	1:D:105:LYS:HB3	1.52	0.89
1:D:22:PHE:HD2	2:F:606:ASN:HD21	1.19	0.88
2:C:553:HIS:CE1	2:C:623:PRO:HG3	2.06	0.88
2:C:594:VAL:HG23	2:C:599:MET:HG2	1.54	0.87
3:A:233:TRP:NE1	3:A:237:LEU:HB3	1.89	0.87
3:B:379:GLU:HG3	3:B:379:GLU:O	1.74	0.86
2:C:505:VAL:HG11	2:C:535:PHE:CE2	2.10	0.85
3:A:160:PHE:CE1	3:A:169:PHE:CD2	2.63	0.85
2:C:553:HIS:HE1	2:C:623:PRO:HG3	1.41	0.85
3:A:161:THR:HB	3:A:188:VAL:HG13	1.59	0.85
1:E:30:VAL:HG22	2:C:506:ARG:HB2	1.59	0.84
3:B:189:GLU:HB3	3:B:265:LYS:CE	2.07	0.84
2:F:594:VAL:HG21	2:F:599:MET:HG2	1.58	0.84
2:C:594:VAL:HG21	2:C:599:MET:HG2	1.58	0.83
2:F:553:HIS:HE1	2:F:623:PRO:HG3	1.41	0.83
2:C:248:VAL:HG22	2:C:256:THR:CG2	2.08	0.83
2:C:594:VAL:CA	2:C:598:GLN:OE1	2.26	0.83
3:A:160:PHE:CZ	3:A:169:PHE:CZ	2.65	0.83
2:C:490:HIS:HB2	2:C:538:PHE:CE1	2.13	0.82
3:B:110:PHE:HA	2:F:62:TYR:CE1	2.15	0.82
2:F:594:VAL:CA	2:F:598:GLN:OE1	2.26	0.82
2:C:346:LEU:HD11	2:C:414:LYS:HB3	1.62	0.81
2:F:559:LEU:CD2	2:F:602:LEU:HD23	2.10	0.81
3:B:122:GLU:O	3:B:125:ILE:HG22	1.79	0.81
2:C:127:ASP:O	2:C:131:VAL:HG22	1.79	0.81
2:C:559:LEU:CD2	2:C:602:LEU:HD23	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:346:LEU:HD11	2:F:414:LYS:HB3	1.63	0.80
1:D:36:ASP:HA	1:D:72:TRP:HH2	1.44	0.80
2:C:700:LYS:HA	2:C:703:ILE:HG13	1.63	0.80
1:E:36:ASP:HA	1:E:72:TRP:HH2	1.47	0.80
2:F:700:LYS:HA	2:F:703:ILE:HG13	1.64	0.80
2:F:594:VAL:HG12	2:F:598:GLN:HB2	0.84	0.79
3:B:189:GLU:CB	3:B:265:LYS:HE3	2.11	0.79
3:B:110:PHE:CB	2:F:62:TYR:CE1	2.66	0.79
3:B:156:VAL:O	3:B:157:GLU:C	2.21	0.79
3:A:160:PHE:HE1	3:A:169:PHE:CE2	1.95	0.79
3:B:112:GLN:HG3	2:F:125:TYR:HD1	1.48	0.78
3:A:390:VAL:HG12	3:A:393:GLU:HG3	1.66	0.78
1:E:104:GLN:NE2	2:C:511:GLY:HA2	1.96	0.78
3:A:262:GLY:O	3:A:265:LYS:HG2	1.82	0.78
1:D:22:PHE:HD2	2:F:606:ASN:ND2	1.80	0.78
2:F:263:VAL:CG2	2:F:267:GLU:OE2	2.32	0.78
3:B:110:PHE:HB2	2:F:62:TYR:CE1	2.19	0.77
3:B:394:LEU:HD12	3:B:395:ASN:H	1.46	0.76
3:A:160:PHE:HE1	3:A:169:PHE:CD2	2.02	0.76
3:B:161:THR:HB	3:B:188:VAL:HG13	1.67	0.76
2:C:490:HIS:HB3	2:C:542:LYS:HZ2	1.50	0.75
2:C:594:VAL:HG12	2:C:598:GLN:HB2	0.84	0.75
3:B:415:LEU:HD23	3:B:416:PRO:N	2.02	0.74
3:B:134:VAL:HB	3:B:160:PHE:CZ	2.22	0.74
2:F:120:ARG:HG3	2:F:140:TYR:HB2	1.68	0.74
2:F:633:SER:O	2:F:674:ILE:CG2	2.36	0.74
2:C:120:ARG:HG3	2:C:140:TYR:HB2	1.68	0.73
2:C:124:MET:HA	2:C:127:ASP:HB2	1.70	0.73
2:C:633:SER:O	2:C:674:ILE:CG2	2.36	0.73
2:F:124:MET:HA	2:F:127:ASP:HB2	1.70	0.73
1:E:36:ASP:HA	1:E:72:TRP:CH2	2.25	0.72
2:F:622:ILE:HG12	2:F:627:LEU:HD13	1.73	0.71
2:C:245:ILE:HA	2:C:248:VAL:HG12	1.72	0.71
2:C:556:SER:HA	2:C:595:SER:HA	1.73	0.71
2:C:622:ILE:HG12	2:C:627:LEU:HD13	1.73	0.70
3:A:233:TRP:CH2	3:A:245:VAL:CG2	2.74	0.70
2:F:556:SER:HA	2:F:595:SER:HA	1.73	0.70
3:A:233:TRP:CD1	3:A:237:LEU:HB3	2.26	0.70
2:F:248:VAL:HG22	2:F:256:THR:HG23	1.72	0.70
3:B:143:PHE:HE1	2:F:66:LEU:CD1	2.05	0.69
3:B:366:MET:CE	3:B:370:ARG:NE	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:110:PHE:CE1	2:F:62:TYR:CG	2.81	0.69
2:C:123:LEU:HB3	2:C:139:VAL:HG11	1.75	0.69
3:B:110:PHE:HA	2:F:62:TYR:HE1	1.55	0.68
3:B:189:GLU:HB2	3:B:265:LYS:HZ1	1.58	0.68
3:A:53:SER:HA	3:A:113:VAL:HG22	1.74	0.68
2:F:123:LEU:HB3	2:F:139:VAL:HG11	1.75	0.68
2:C:210:LEU:CD1	2:C:263:VAL:HG11	2.23	0.68
2:C:437:ALA:HA	2:C:513:TRP:HZ3	1.58	0.68
3:B:110:PHE:CA	2:F:62:TYR:CE1	2.76	0.68
1:E:35:TRP:HE1	1:E:37:ILE:HA	1.58	0.68
3:B:161:THR:HG21	3:B:186:LEU:HB2	1.75	0.68
1:D:36:ASP:HA	1:D:72:TRP:CH2	2.28	0.68
3:B:110:PHE:HD1	2:F:62:TYR:CZ	2.12	0.67
1:E:62:SER:HB2	1:E:64:THR:HG22	1.77	0.67
2:C:437:ALA:HA	2:C:513:TRP:CZ3	2.30	0.67
2:F:338:PRO:HB3	2:F:387:TYR:CG	2.30	0.66
1:D:62:SER:HB2	1:D:64:THR:HG22	1.77	0.66
2:C:522:CYS:SG	2:C:620:THR:HG22	2.35	0.66
2:C:90:ARG:NH2	2:C:150:GLN:OE1	2.29	0.66
3:B:187:ASN:ND2	3:B:587:TYR:OH	2.28	0.66
3:B:66:GLU:HA	3:B:69:GLN:HB2	1.78	0.66
3:B:110:PHE:CA	2:F:62:TYR:HE1	2.09	0.66
2:F:90:ARG:NH2	2:F:150:GLN:OE1	2.29	0.66
3:B:379:GLU:O	3:B:379:GLU:CG	2.43	0.65
1:E:72:TRP:HB2	1:E:105:LYS:CB	2.25	0.65
3:B:64:LEU:HD23	2:F:54:PHE:HD1	1.60	0.65
3:B:58:ALA:HB1	2:F:121:ASP:HB3	1.79	0.65
3:B:225:LEU:O	3:B:230:GLN:NE2	2.30	0.65
2:F:557:ALA:HB2	2:F:599:MET:SD	2.36	0.65
3:A:47:MET:HB2	3:B:45:HIS:HD2	1.61	0.65
2:C:557:ALA:HB2	2:C:599:MET:SD	2.36	0.65
1:D:72:TRP:HB2	1:D:105:LYS:CB	2.25	0.65
3:B:539:ARG:HH22	3:B:577:ARG:HD3	1.62	0.65
1:D:66:GLU:C	1:D:68:CYS:H	2.00	0.65
2:C:525:PRO:HB3	2:C:603:MET:HG3	1.79	0.65
3:A:207:GLU:HG3	3:A:238:PRO:HG3	1.79	0.65
3:A:436:LEU:O	3:A:455:ARG:NH2	2.30	0.64
2:F:396:LEU:HB2	2:F:454:MET:HE3	1.79	0.64
3:A:378:CYS:HB2	3:A:426:VAL:HG21	1.77	0.64
2:F:248:VAL:HG22	2:F:256:THR:CG2	2.28	0.64
3:B:415:LEU:HD22	3:B:417:CYS:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:GLU:C	1:E:68:CYS:H	2.00	0.64
2:C:491:LEU:C	2:C:493:ALA:H	2.02	0.64
3:B:436:LEU:O	3:B:455:ARG:NH2	2.31	0.64
3:A:202:LEU:HD13	3:A:213:LEU:HD12	1.79	0.63
1:E:28:ASN:HA	2:C:504:THR:O	1.97	0.63
3:A:47:MET:HB2	3:B:45:HIS:CD2	2.33	0.63
3:A:233:TRP:CH2	3:A:245:VAL:CA	2.64	0.63
3:A:273:GLU:HA	3:A:283:TYR:HB3	1.82	0.62
3:B:553:GLN:HB2	3:B:564:ARG:HB2	1.81	0.62
1:E:67:GLU:O	1:E:69:THR:N	2.33	0.62
3:B:189:GLU:CB	3:B:265:LYS:CE	2.74	0.62
1:E:39:VAL:HG11	1:E:108:HIS:HE1	1.65	0.62
3:B:415:LEU:HD23	3:B:417:CYS:H	1.63	0.62
2:F:215:GLU:HA	2:F:215:GLU:OE2	1.98	0.62
2:F:632:GLN:HB2	2:F:636:CYS:HB3	1.82	0.62
1:D:67:GLU:O	1:D:69:THR:N	2.33	0.62
2:C:210:LEU:HD12	2:C:263:VAL:HG11	1.81	0.61
1:D:32:LEU:HD23	2:F:510:THR:HA	1.81	0.61
1:D:45:CYS:HB2	1:D:54:ILE:HG12	1.81	0.61
2:F:338:PRO:HB3	2:F:387:TYR:CD1	2.35	0.61
1:D:35:TRP:HA	2:F:546:ARG:HB3	1.82	0.61
3:A:231:ARG:H	3:A:231:ARG:HD2	1.66	0.61
2:F:487:PHE:CD1	2:F:535:PHE:HD2	2.18	0.61
2:F:520:PRO:HG2	2:F:552:HIS:H	1.66	0.61
3:A:289:SER:HG	3:A:294:LYS:H	1.46	0.60
3:B:217:LEU:HD13	3:B:225:LEU:HD11	1.82	0.60
3:A:56:PHE:HA	3:A:59:MET:HB3	1.81	0.60
3:A:127:LYS:HG3	3:A:127:LYS:O	2.02	0.60
3:B:153:LYS:HE2	3:B:180:ILE:HA	1.82	0.60
2:C:632:GLN:HB2	2:C:636:CYS:HB3	1.82	0.60
3:B:397:ARG:HG2	3:B:415:LEU:HB3	1.84	0.60
2:C:337:ASN:ND2	2:C:340:ASP:OD1	2.35	0.60
2:F:699:ARG:HD3	2:F:700:LYS:CD	2.32	0.60
2:F:245:ILE:HA	2:F:248:VAL:HG12	1.84	0.59
2:F:337:ASN:ND2	2:F:340:ASP:OD1	2.35	0.59
2:F:712:LYS:HB3	2:F:768:ALA:HA	1.83	0.59
2:F:282:SER:HA	2:F:286:HIS:HB3	1.85	0.59
2:C:43:GLU:OE2	2:C:48:ASN:ND2	2.32	0.59
2:C:525:PRO:HB2	2:C:528:PRO:HD2	1.85	0.59
2:F:356:LEU:HD12	2:F:360:PHE:HB2	1.84	0.59
2:F:557:ALA:CB	2:F:599:MET:SD	2.91	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:356:LEU:HD12	2:C:360:PHE:HB2	1.84	0.59
1:E:35:TRP:HA	2:C:546:ARG:HB3	1.83	0.59
3:A:196:GLU:HA	3:A:199:MET:HB2	1.85	0.59
2:F:102:LEU:HD21	2:F:182:ALA:HB1	1.83	0.59
2:F:594:VAL:HG23	2:F:599:MET:CG	2.30	0.59
3:B:112:GLN:CG	2:F:125:TYR:HD1	2.15	0.58
3:B:140:ALA:HB2	3:B:148:LEU:HD23	1.85	0.58
2:C:490:HIS:O	2:C:493:ALA:HB3	2.03	0.58
3:B:143:PHE:HE1	2:F:66:LEU:HD11	1.68	0.58
2:C:557:ALA:CB	2:C:599:MET:SD	2.91	0.58
3:A:535:CYS:SG	3:A:564:ARG:NH1	2.76	0.58
1:E:41:ASN:HA	1:E:48:HIS:HA	1.86	0.58
2:F:452:LYS:HA	2:F:455:ILE:HG23	1.85	0.58
2:C:594:VAL:HG23	2:C:599:MET:CG	2.29	0.58
3:A:153:LYS:HE3	3:A:179:ASP:OD1	2.02	0.58
3:A:186:LEU:HD13	3:A:194:VAL:HG11	1.85	0.58
3:B:228:VAL:HG12	3:B:229:THR:N	2.18	0.58
1:E:35:TRP:HB3	1:E:76:ASN:HD21	1.69	0.57
3:A:379:GLU:O	3:A:379:GLU:CG	2.40	0.57
3:A:382:ILE:HB	3:A:402:TYR:HB3	1.85	0.57
3:B:110:PHE:CD1	2:F:62:TYR:CD2	2.92	0.57
3:B:110:PHE:HD1	2:F:62:TYR:CD2	2.22	0.57
3:A:459:ARG:HB3	3:A:476:GLY:HA3	1.86	0.57
3:B:195:ARG:HD3	3:B:229:THR:HG21	1.86	0.57
2:C:282:SER:HA	2:C:286:HIS:HB3	1.85	0.57
3:A:233:TRP:CZ3	3:A:245:VAL:HA	2.38	0.57
2:F:289:LYS:O	2:F:351:ARG:NH2	2.38	0.57
2:C:289:LYS:O	2:C:351:ARG:NH2	2.38	0.57
3:A:127:LYS:O	3:A:127:LYS:CG	2.51	0.57
3:B:35:LEU:HB2	3:B:42:PHE:HB2	1.87	0.57
3:B:152:ALA:O	3:B:156:VAL:N	2.30	0.57
2:C:612:THR:H	2:C:615:GLU:HB2	1.70	0.57
3:B:350:PHE:HD1	3:B:363:LYS:HB2	1.69	0.57
2:C:648:PRO:HG2	2:C:657:HIS:HA	1.87	0.56
2:F:129:VAL:O	2:F:133:GLN:NE2	2.34	0.56
2:C:238:GLU:O	2:C:242:ASN:ND2	2.32	0.56
3:A:202:LEU:HD22	3:A:213:LEU:HB2	1.86	0.56
3:A:476:GLY:O	3:A:496:SER:N	2.38	0.56
2:C:102:LEU:HD11	2:C:182:ALA:HB1	1.85	0.56
2:C:557:ALA:HB3	2:C:594:VAL:HG23	1.88	0.56
3:A:160:PHE:HE1	3:A:169:PHE:CZ	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:415:LEU:HD22	3:B:417:CYS:N	2.21	0.56
1:D:27:TRP:CZ2	1:D:29:ALA:HB2	2.40	0.56
2:C:245:ILE:HA	2:C:248:VAL:CG1	2.35	0.56
2:C:594:VAL:CG1	2:C:598:GLN:CB	2.61	0.56
2:C:144:LEU:HD12	2:C:193:LEU:HA	1.88	0.56
2:F:385:PRO:HB3	2:F:428:PHE:HB2	1.88	0.56
2:C:248:VAL:CG2	2:C:256:THR:HG23	2.28	0.56
2:C:594:VAL:CG2	2:C:599:MET:CG	2.76	0.56
3:A:398:THR:HG22	3:A:414:PRO:HB3	1.88	0.56
3:B:297:LYS:HZ1	3:B:594:SER:HA	1.71	0.56
3:A:525:VAL:HA	3:A:538:MET:HG2	1.88	0.55
1:D:35:TRP:HE1	1:D:37:ILE:HA	1.71	0.55
3:A:233:TRP:HH2	3:A:245:VAL:N	2.04	0.55
3:B:19:GLU:HA	3:B:22:LYS:HE3	1.88	0.55
1:D:22:PHE:HB2	2:F:606:ASN:ND2	2.22	0.55
2:F:416:MET:HG2	2:F:457:LYS:HE3	1.87	0.55
2:F:557:ALA:HB3	2:F:594:VAL:HG23	1.88	0.55
1:E:31:ALA:N	2:C:506:ARG:O	2.33	0.55
1:D:22:PHE:HB2	2:F:606:ASN:HD21	1.72	0.55
3:A:305:LEU:HD21	3:A:323:GLY:HA3	1.88	0.55
1:E:27:TRP:CZ2	1:E:29:ALA:HB2	2.40	0.55
3:B:415:LEU:CD2	3:B:417:CYS:O	2.50	0.55
2:F:699:ARG:HD3	2:F:700:LYS:HD3	1.89	0.55
3:B:153:LYS:O	3:B:157:GLU:N	2.39	0.55
2:F:102:LEU:CD2	2:F:182:ALA:HB1	2.37	0.55
2:F:680:LYS:NZ	2:F:680:LYS:H	2.04	0.55
1:D:35:TRP:HB3	1:D:76:ASN:HD21	1.71	0.55
2:C:129:VAL:O	2:C:133:GLN:NE2	2.34	0.55
2:F:144:LEU:HD12	2:F:193:LEU:HA	1.88	0.55
2:C:385:PRO:HB3	2:C:428:PHE:HB2	1.89	0.54
2:C:594:VAL:HG11	2:C:602:LEU:HD22	1.89	0.54
3:B:134:VAL:HB	3:B:160:PHE:CE1	2.41	0.54
3:B:415:LEU:HD23	3:B:416:PRO:CD	2.37	0.54
2:C:314:CYS:HB3	2:C:369:THR:HG21	1.89	0.54
3:B:137:LEU:HB2	3:B:156:VAL:HG21	1.89	0.54
2:F:594:VAL:HG11	2:F:602:LEU:HD22	1.89	0.54
1:D:26:LYS:HG2	2:F:502:ASP:HB2	1.90	0.54
3:A:160:PHE:HE1	3:A:169:PHE:CG	2.25	0.54
3:B:275:SER:OG	3:B:574:ASP:O	2.25	0.54
2:F:680:LYS:H	2:F:680:LYS:HZ2	1.56	0.54
3:B:267:GLU:HG2	3:B:530:ILE:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:348:ASN:ND2	3:B:366:MET:O	2.40	0.54
1:E:104:GLN:HE22	2:C:511:GLY:CA	2.02	0.54
3:A:286:VAL:HG11	3:A:573:TRP:HH2	1.71	0.54
2:F:314:CYS:HB3	2:F:369:THR:HG21	1.89	0.54
2:C:633:SER:O	2:C:674:ILE:HG21	2.08	0.54
3:B:37:VAL:HG12	3:B:38:GLU:HG2	1.88	0.54
1:D:37:ILE:O	1:D:38:VAL:C	2.46	0.53
3:B:570:ARG:HA	3:B:598:PRO:HB3	1.90	0.53
2:F:594:VAL:CG2	2:F:599:MET:CG	2.76	0.53
1:D:62:SER:HB2	1:D:64:THR:CG2	2.38	0.53
3:A:198:ALA:O	3:A:202:LEU:HG	2.09	0.53
2:C:116:MET:HA	2:C:119:ILE:HB	1.90	0.53
2:C:505:VAL:HG11	2:C:535:PHE:CD2	2.43	0.53
3:B:110:PHE:CD1	2:F:62:TYR:CZ	2.92	0.53
3:B:530:ILE:HG23	3:B:564:ARG:HH12	1.73	0.53
1:E:49:ILE:HG22	1:E:50:MET:HG3	1.91	0.53
2:C:427:VAL:HA	2:C:430:ARG:HB3	1.90	0.53
2:F:238:GLU:O	2:F:242:ASN:ND2	2.32	0.53
2:C:169:ILE:HD11	2:C:247:ARG:HD3	1.91	0.53
2:C:487:PHE:CD1	2:C:535:PHE:HD2	2.27	0.53
2:F:404:THR:OG1	2:F:407:GLU:OE2	2.20	0.53
1:D:66:GLU:C	1:D:68:CYS:N	2.62	0.53
3:A:555:ASP:HB3	3:A:558:LEU:HB2	1.90	0.53
3:B:156:VAL:HG12	3:B:157:GLU:N	2.24	0.53
3:A:365:PRO:O	3:A:409:TRP:NE1	2.41	0.53
3:B:110:PHE:HA	2:F:62:TYR:CD1	2.43	0.53
1:E:66:GLU:C	1:E:68:CYS:N	2.62	0.53
3:A:233:TRP:HE1	3:A:237:LEU:HB3	1.68	0.53
3:A:397:ARG:HG3	3:A:415:LEU:O	2.09	0.52
3:B:455:ARG:NH1	3:B:500:GLU:OE2	2.42	0.52
2:F:700:LYS:HE2	2:F:703:ILE:HD11	1.90	0.52
2:C:491:LEU:HD12	2:C:534:ILE:HG21	1.92	0.52
2:C:700:LYS:O	2:C:704:GLU:HG2	2.09	0.52
1:E:37:ILE:O	1:E:38:VAL:C	2.47	0.52
1:E:62:SER:HB2	1:E:64:THR:CG2	2.38	0.52
3:A:263:MET:SD	3:A:263:MET:N	2.83	0.52
3:A:297:LYS:NZ	3:A:593:GLU:O	2.42	0.52
3:B:526:ARG:HB2	3:B:537:PHE:HB3	1.90	0.52
2:C:102:LEU:CD1	2:C:182:ALA:HB1	2.40	0.52
2:C:437:ALA:O	2:C:441:LEU:HB2	2.10	0.52
3:B:202:LEU:HD13	3:B:213:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:TRP:CD1	1:D:76:ASN:ND2	2.78	0.52
3:A:348:ASN:ND2	3:A:366:MET:O	2.42	0.52
3:B:366:MET:HG3	3:B:409:TRP:CZ2	2.44	0.52
2:F:169:ILE:HD11	2:F:247:ARG:HD3	1.91	0.52
1:E:30:VAL:HG21	2:C:441:LEU:HD22	1.91	0.52
2:F:374:PHE:O	2:F:378:LEU:HB2	2.10	0.52
3:A:321:ALA:HB3	3:A:375:LEU:HD11	1.92	0.51
1:D:49:ILE:HG22	1:D:50:MET:HG3	1.92	0.51
2:C:441:LEU:HD21	2:C:508:LEU:HD11	1.91	0.51
3:A:301:PRO:HG3	3:A:360:TRP:CE2	2.45	0.51
3:B:127:LYS:O	3:B:129:ASN:ND2	2.43	0.51
2:F:633:SER:O	2:F:674:ILE:HG21	2.08	0.51
2:F:499:GLY:HA3	2:F:530:HIS:HB2	1.92	0.51
3:B:366:MET:HE3	3:B:370:ARG:CZ	2.36	0.51
2:C:647:GLU:HB2	2:C:648:PRO:HD3	1.93	0.51
3:A:370:ARG:HG2	3:A:389:SER:HA	1.90	0.51
3:A:553:GLN:HB2	3:A:564:ARG:HB2	1.91	0.51
2:F:605:PHE:HE2	2:F:611:TYR:HB2	1.76	0.51
1:D:53:CYS:H	1:D:56:CYS:HB2	1.76	0.51
2:C:419:PHE:HA	2:C:422:MET:HG3	1.93	0.51
2:C:258:GLU:HB2	2:C:259:PRO:HD3	1.93	0.51
3:A:522:ASP:OD1	3:A:522:ASP:N	2.43	0.51
2:C:490:HIS:HB3	2:C:542:LYS:NZ	2.23	0.50
3:A:275:SER:OG	3:A:573:TRP:NE1	2.44	0.50
3:A:548:LYS:NZ	3:A:549:TYR:O	2.42	0.50
2:C:508:LEU:HD13	2:C:513:TRP:CE2	2.46	0.50
2:C:717:MET:HG3	2:C:764:TYR:HE2	1.76	0.50
3:B:189:GLU:CB	3:B:265:LYS:NZ	2.75	0.50
3:B:189:GLU:HB2	3:B:265:LYS:NZ	2.26	0.50
2:F:58:TYR:C	2:F:60:ASN:N	2.64	0.50
2:F:298:CYS:HA	2:F:301:LYS:HG2	1.93	0.50
2:C:553:HIS:HE1	2:C:623:PRO:CG	2.20	0.50
3:B:228:VAL:HG12	3:B:229:THR:H	1.77	0.50
1:E:22:PHE:HB3	2:C:559:LEU:HD11	1.94	0.50
1:D:22:PHE:HB2	2:F:606:ASN:OD1	2.12	0.50
3:B:110:PHE:CG	2:F:62:TYR:CE1	2.97	0.50
1:E:27:TRP:O	2:C:504:THR:OG1	2.30	0.50
1:D:20:LYS:HE3	1:D:23:GLU:HG2	1.93	0.50
3:A:181:LEU:HD22	3:A:219:GLN:HB3	1.94	0.50
2:F:58:TYR:C	2:F:60:ASN:H	2.15	0.50
2:F:258:GLU:HB2	2:F:259:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:685:ASP:HA	2:F:688:ARG:HE	1.75	0.50
1:D:35:TRP:CB	1:D:76:ASN:HD21	2.25	0.50
2:C:447:SER:HB2	2:C:450:SER:HB3	1.93	0.50
2:F:634:LEU:HD23	2:F:674:ILE:CG2	2.35	0.50
3:B:118:GLN:OE1	3:B:119:ARG:NH1	2.45	0.49
1:E:20:LYS:HE3	1:E:23:GLU:HG2	1.93	0.49
3:B:459:ARG:HB3	3:B:476:GLY:HA3	1.93	0.49
3:B:274:ALA:N	3:B:284:SER:O	2.46	0.49
3:B:522:ASP:OD1	3:B:522:ASP:N	2.45	0.49
3:A:431:ILE:HB	3:A:442:TYR:HB3	1.95	0.49
2:C:298:CYS:HA	2:C:301:LYS:HG2	1.93	0.49
3:A:45:HIS:HB2	3:B:47:MET:SD	2.52	0.49
3:A:160:PHE:HE1	3:A:169:PHE:CE1	2.31	0.49
3:A:161:THR:HB	3:A:188:VAL:CG1	2.37	0.49
3:B:458:SER:O	3:B:459:ARG:NH1	2.42	0.49
1:E:45:CYS:HB2	1:E:54:ILE:HG12	1.93	0.49
2:F:547:GLN:N	2:F:547:GLN:OE1	2.46	0.49
2:C:547:GLN:N	2:C:547:GLN:OE1	2.46	0.49
3:A:209:ARG:HB3	3:A:212:TYR:HB2	1.95	0.49
2:F:717:MET:HA	2:F:722:LEU:HD23	1.94	0.49
3:A:455:ARG:NH1	3:A:500:GLU:OE2	2.46	0.49
3:B:273:GLU:OE2	3:B:307:LYS:N	2.45	0.49
3:B:297:LYS:HZ2	3:B:592:GLU:HG2	1.78	0.49
2:F:128:ARG:O	2:F:132:GLN:HB2	2.13	0.49
2:C:255:SER:O	2:C:257:GLU:N	2.45	0.49
1:D:22:PHE:HB3	2:F:559:LEU:HD11	1.94	0.49
2:C:491:LEU:C	2:C:493:ALA:N	2.65	0.49
3:B:78:ASP:OD1	3:B:79:ALA:N	2.46	0.49
2:C:245:ILE:CA	2:C:248:VAL:HG12	2.41	0.48
2:C:593:GLN:HB2	2:C:671:ARG:HH12	1.77	0.48
3:A:47:MET:HB3	3:B:47:MET:SD	2.52	0.48
3:B:415:LEU:HD23	3:B:415:LEU:C	2.32	0.48
3:B:513:ALA:HB3	3:B:561:TRP:HZ3	1.78	0.48
2:C:457:LYS:HD2	2:C:457:LYS:HA	1.50	0.48
2:C:671:ARG:HD2	2:C:671:ARG:HA	1.59	0.48
3:A:318:ILE:HB	3:A:353:PHE:HB3	1.95	0.48
3:B:413:SER:HB3	3:B:442:TYR:HE2	1.78	0.48
2:F:596:THR:HA	2:F:599:MET:HE2	1.95	0.48
1:D:39:VAL:HA	1:D:49:ILE:HG13	1.96	0.48
3:B:297:LYS:HB3	3:B:594:SER:HB2	1.94	0.48
3:B:455:ARG:NH1	3:B:457:THR:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:703:ILE:O	2:F:707:ILE:HG22	2.12	0.48
1:D:29:ALA:O	2:F:505:VAL:HA	2.14	0.48
1:D:39:VAL:HG12	1:D:108:HIS:HE1	1.78	0.48
3:A:374:SER:OG	3:A:385:ILE:O	2.28	0.48
3:A:425:VAL:HB	3:A:466:ALA:HB2	1.96	0.48
3:B:154:ARG:O	3:B:155:MET:C	2.52	0.48
3:B:321:ALA:HB3	3:B:375:LEU:HD11	1.95	0.48
2:F:559:LEU:O	2:F:592:LEU:N	2.39	0.48
2:F:699:ARG:HD3	2:F:700:LYS:CE	2.43	0.48
2:F:708:VAL:HG11	2:F:748:LEU:HD22	1.94	0.48
1:E:35:TRP:CB	1:E:76:ASN:HD21	2.25	0.48
2:C:634:LEU:HD23	2:C:674:ILE:CG2	2.35	0.48
3:A:304:ASP:OD1	3:A:304:ASP:N	2.47	0.48
3:A:434:MET:HE2	3:A:455:ARG:HG3	1.96	0.48
3:A:455:ARG:NH1	3:A:457:THR:O	2.47	0.48
3:B:112:GLN:CG	2:F:125:TYR:CD1	2.97	0.48
2:F:440:LEU:HD13	2:F:477:MET:HG3	1.94	0.48
1:E:35:TRP:NE1	1:E:37:ILE:HA	2.27	0.48
2:F:77:LEU:HD22	2:F:123:LEU:HD22	1.95	0.48
2:C:596:THR:HA	2:C:599:MET:HE2	1.94	0.48
2:F:255:SER:O	2:F:257:GLU:N	2.46	0.48
2:F:285:VAL:HG23	2:F:320:TYR:CD1	2.49	0.48
1:E:94:CYS:HB2	1:E:101:TRP:HB2	1.96	0.47
2:C:77:LEU:HD22	2:C:123:LEU:HD22	1.95	0.47
3:A:305:LEU:HB2	3:A:325:VAL:HB	1.96	0.47
2:F:62:TYR:HD1	2:F:125:TYR:HH	1.62	0.47
3:B:155:MET:O	3:B:156:VAL:O	2.32	0.47
3:B:265:LYS:CG	3:B:265:LYS:O	2.61	0.47
2:F:594:VAL:CG1	2:F:598:GLN:CB	2.61	0.47
1:E:35:TRP:HB3	1:E:76:ASN:ND2	2.29	0.47
3:B:128:ILE:HG13	3:B:155:MET:HG2	1.94	0.47
3:B:346:THR:HG22	3:B:369:VAL:HB	1.95	0.47
1:E:27:TRP:CE2	1:E:29:ALA:HB2	2.49	0.47
2:C:349:LYS:HE3	2:C:421:PHE:HZ	1.79	0.47
1:D:27:TRP:CE2	1:D:29:ALA:HB2	2.49	0.47
2:C:128:ARG:O	2:C:132:GLN:HB2	2.13	0.47
3:A:171:GLN:OE1	3:A:171:GLN:HA	2.14	0.47
3:A:228:VAL:HG22	3:A:231:ARG:HB2	1.96	0.47
2:F:248:VAL:HG23	2:F:252:LEU:HD12	1.96	0.47
2:F:680:LYS:HZ3	2:F:680:LYS:C	2.17	0.47
1:D:41:ASN:HA	1:D:48:HIS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:394:LEU:CD1	3:B:395:ASN:N	2.70	0.47
1:D:22:PHE:CD2	2:F:606:ASN:ND2	2.60	0.47
3:A:134:VAL:HG21	3:A:169:PHE:HA	1.96	0.47
3:A:160:PHE:CZ	3:A:169:PHE:CE2	2.93	0.47
2:F:259:PRO:O	2:F:263:VAL:HG12	2.15	0.47
2:F:386:GLU:OE1	2:F:386:GLU:N	2.44	0.47
3:A:302:PRO:HG2	3:A:305:LEU:HB3	1.97	0.47
3:B:382:ILE:HB	3:B:402:TYR:HB3	1.96	0.47
2:F:647:GLU:HB2	2:F:648:PRO:HD3	1.96	0.47
1:D:43:ALA:HB3	1:D:79:PHE:HE1	1.78	0.47
3:B:415:LEU:HD23	3:B:416:PRO:HD2	1.96	0.47
3:A:265:LYS:HD3	3:A:587:TYR:OH	2.15	0.47
3:B:228:VAL:CG1	3:B:229:THR:H	2.28	0.47
2:F:501:VAL:HB	2:F:502:ASP:H	1.58	0.47
1:E:49:ILE:HD13	1:E:49:ILE:HA	1.67	0.46
3:B:395:ASN:O	3:B:395:ASN:ND2	2.48	0.46
1:E:39:VAL:CG1	1:E:108:HIS:HE1	2.28	0.46
3:B:247:GLN:O	3:B:251:LYS:HB2	2.15	0.46
1:D:94:CYS:HB2	1:D:101:TRP:HB2	1.96	0.46
3:A:66:GLU:H	3:A:66:GLU:HG3	1.43	0.46
3:A:350:PHE:HD1	3:A:363:LYS:HB2	1.80	0.46
2:F:245:ILE:O	2:F:248:VAL:HG12	2.15	0.46
2:F:525:PRO:HB2	2:F:528:PRO:HD2	1.96	0.46
2:C:210:LEU:HD13	2:C:210:LEU:HA	1.76	0.46
2:C:613:PHE:HB2	2:C:657:HIS:CE1	2.51	0.46
3:A:275:SER:OG	3:A:574:ASP:O	2.26	0.46
3:A:529:VAL:O	3:A:530:ILE:HG13	2.14	0.46
3:B:124:LEU:HB3	3:B:148:LEU:HD11	1.98	0.46
2:F:435:HIS:CE1	2:F:681:GLN:HG3	2.50	0.46
2:F:457:LYS:HD2	2:F:457:LYS:HA	1.68	0.46
2:F:742:LYS:HA	2:F:742:LYS:HD3	1.68	0.46
3:A:353:PHE:HB2	3:A:360:TRP:CH2	2.51	0.46
3:B:542:HIS:HB2	3:B:545:GLU:HB2	1.96	0.46
2:C:215:GLU:OE1	2:C:215:GLU:N	2.49	0.46
3:B:371:ILE:HB	3:B:388:ASP:HB2	1.98	0.46
1:E:35:TRP:HB2	2:C:546:ARG:NE	2.31	0.46
1:E:35:TRP:CD1	1:E:76:ASN:ND2	2.84	0.46
1:D:35:TRP:HB3	1:D:76:ASN:ND2	2.30	0.46
3:A:48:VAL:HG21	3:A:90:TYR:CZ	2.51	0.46
2:F:148:ARG:HH11	2:F:200:VAL:HG21	1.80	0.46
2:F:722:LEU:HD13	2:F:722:LEU:HA	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:553:HIS:CE1	2:C:623:PRO:CG	2.92	0.46
3:A:160:PHE:CE1	3:A:169:PHE:CE1	3.02	0.46
3:B:64:LEU:HD23	2:F:54:PHE:CD1	2.47	0.46
3:B:112:GLN:HG3	2:F:125:TYR:CD1	2.40	0.46
2:F:553:HIS:HE1	2:F:623:PRO:CG	2.20	0.46
2:C:646:LYS:HB3	2:C:646:LYS:HE3	1.57	0.45
2:C:716:LYS:H	2:C:716:LYS:HG3	1.63	0.45
3:A:301:PRO:HB2	3:A:302:PRO:HD3	1.98	0.45
3:B:106:GLU:HG2	3:B:143:PHE:HE2	1.81	0.45
3:B:202:LEU:HD11	3:B:216:VAL:HG11	1.98	0.45
2:C:148:ARG:HH11	2:C:200:VAL:HG21	1.80	0.45
2:C:559:LEU:O	2:C:592:LEU:N	2.39	0.45
3:B:84:ILE:HA	3:B:87:THR:HG22	1.98	0.45
2:F:595:SER:C	2:F:597:PHE:N	2.67	0.45
1:D:35:TRP:HB2	2:F:546:ARG:NE	2.31	0.45
3:B:265:LYS:HG3	3:B:585:LYS:HD3	1.98	0.45
2:C:595:SER:C	2:C:597:PHE:N	2.67	0.45
3:B:275:SER:N	3:B:575:LEU:O	2.49	0.45
3:B:115:ASP:OD1	3:B:116:VAL:N	2.48	0.45
2:C:223:LYS:HE3	2:C:227:GLU:HG3	1.99	0.45
3:A:156:VAL:O	3:A:160:PHE:HB3	2.17	0.45
3:B:75:ARG:HB3	2:F:59:ARG:HD3	1.98	0.45
2:C:735:LEU:HD22	2:C:735:LEU:HA	1.77	0.45
3:A:84:ILE:HA	3:A:87:THR:HG22	1.99	0.45
3:A:231:ARG:HD2	3:A:231:ARG:N	2.32	0.45
3:A:265:LYS:HE2	3:A:265:LYS:HA	1.98	0.45
3:B:228:VAL:CG1	3:B:229:THR:N	2.79	0.45
2:C:54:PHE:HB3	3:A:66:GLU:HG2	1.99	0.45
3:A:128:ILE:HG12	3:A:136:LEU:HD21	1.99	0.45
3:A:268:MET:HB3	3:A:287:CYS:SG	2.56	0.45
3:B:221:ARG:NE	3:B:258:LYS:O	2.50	0.45
3:A:326:PRO:HA	3:A:344:PHE:HA	1.97	0.45
2:F:423:GLN:HG2	2:F:424:GLU:H	1.82	0.45
2:C:153:ARG:HH21	2:C:200:VAL:HG13	1.82	0.44
2:C:441:LEU:HA	2:C:506:ARG:NH1	2.32	0.44
2:C:687:GLU:O	2:C:690:GLU:HG3	2.18	0.44
3:A:422:SER:OG	3:A:434:MET:O	2.24	0.44
2:C:700:LYS:N	2:C:700:LYS:HD2	2.32	0.44
3:B:110:PHE:HB2	2:F:62:TYR:CZ	2.52	0.44
2:C:62:TYR:HD1	2:C:125:TYR:HH	1.61	0.44
2:C:723:VAL:HA	2:C:726:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:78:ASP:OD1	3:A:79:ALA:N	2.51	0.44
3:A:265:LYS:CD	3:A:587:TYR:CZ	3.00	0.44
2:F:425:LYS:HE3	2:F:425:LYS:HB2	1.47	0.44
1:D:31:ALA:O	2:F:507:VAL:HA	2.17	0.44
2:C:129:VAL:HG23	3:A:144:SER:HB2	2.00	0.44
3:A:265:LYS:HD2	3:A:587:TYR:CZ	2.53	0.44
3:B:434:MET:HE2	3:B:455:ARG:HG3	1.99	0.44
2:F:86:ILE:HG23	2:F:90:ARG:HD2	2.00	0.44
3:A:287:CYS:SG	3:A:288:TYR:N	2.90	0.44
3:B:372:LYS:NZ	3:B:580:ARG:HE	2.16	0.44
2:F:265:GLU:HB3	2:F:306:VAL:HG22	2.00	0.44
2:F:596:THR:HA	2:F:599:MET:CE	2.48	0.44
2:C:113:GLN:O	2:C:117:VAL:HG23	2.18	0.44
3:A:160:PHE:CD1	3:A:169:PHE:CD2	3.06	0.44
3:B:29:LEU:HD12	3:B:29:LEU:HA	1.82	0.44
3:B:128:ILE:CG1	3:B:155:MET:HG2	2.48	0.44
2:F:613:PHE:HB3	2:F:655:ASN:HD22	1.81	0.44
1:E:35:TRP:CA	2:C:546:ARG:HB3	2.47	0.44
2:C:86:ILE:HG23	2:C:90:ARG:HD2	1.99	0.44
2:C:527:ALA:HB3	2:C:528:PRO:HD3	2.00	0.44
3:A:121:ARG:HD3	3:A:145:CYS:SG	2.58	0.44
3:A:566:HIS:O	3:A:566:HIS:ND1	2.50	0.44
2:F:595:SER:O	2:F:596:THR:C	2.56	0.44
3:A:325:VAL:O	3:A:345:ARG:N	2.50	0.44
3:B:87:THR:O	3:B:91:THR:HG22	2.18	0.44
2:F:689:LYS:HD2	2:F:689:LYS:HA	1.60	0.44
1:D:21:ARG:HG3	2:F:606:ASN:ND2	2.32	0.44
2:C:265:GLU:HB3	2:C:306:VAL:HG22	2.00	0.44
2:C:404:THR:OG1	2:C:407:GLU:OE2	2.20	0.44
2:C:451:GLU:O	2:C:455:ILE:HG23	2.17	0.44
3:A:37:VAL:HG21	3:A:82:LEU:HD23	1.99	0.44
3:A:258:LYS:HE2	3:A:258:LYS:HB2	1.44	0.44
3:B:110:PHE:HD1	2:F:62:TYR:CE2	2.35	0.44
2:F:47:LYS:HD2	2:F:47:LYS:HA	1.41	0.44
2:F:488:ARG:HD2	2:F:488:ARG:HA	1.47	0.43
2:F:655:ASN:HD22	2:F:655:ASN:HA	1.51	0.43
1:D:92:GLN:HE21	1:D:92:GLN:HB2	1.59	0.43
2:C:596:THR:HA	2:C:599:MET:CE	2.48	0.43
2:C:691:THR:O	2:C:695:VAL:HG23	2.19	0.43
3:A:128:ILE:HG23	3:A:136:LEU:HD21	1.99	0.43
3:B:499:VAL:HG21	3:B:561:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:225:LEU:HB3	2:C:272:HIS:CE1	2.54	0.43
2:C:230:ALA:HB2	2:C:276:ILE:HG13	1.99	0.43
2:C:505:VAL:CG1	2:C:535:PHE:CE2	2.94	0.43
2:F:230:ALA:HB2	2:F:276:ILE:HG13	1.99	0.43
2:C:689:LYS:HA	2:C:689:LYS:HD2	1.49	0.43
2:C:722:LEU:HD13	2:C:722:LEU:HA	1.73	0.43
3:B:182:SER:HB3	3:B:219:GLN:HB3	2.01	0.43
3:B:239:PRO:O	3:B:240:ASN:OD1	2.35	0.43
1:D:21:ARG:HG3	2:F:606:ASN:HD22	1.84	0.43
3:A:68:LYS:HB3	3:A:68:LYS:HE3	1.82	0.43
3:B:415:LEU:CD2	3:B:417:CYS:N	2.64	0.43
3:B:503:ASP:HB3	3:B:506:LYS:HB2	2.00	0.43
2:F:647:GLU:HB2	2:F:658:ILE:HG13	1.99	0.43
2:F:248:VAL:O	2:F:256:THR:HG21	2.18	0.43
2:F:658:ILE:H	2:F:658:ILE:HG12	1.43	0.43
2:F:744:ARG:HA	2:F:744:ARG:HD2	1.69	0.43
1:E:39:VAL:HG11	1:E:108:HIS:CE1	2.49	0.43
3:A:160:PHE:HE1	3:A:169:PHE:CD1	2.37	0.43
3:A:221:ARG:HB2	3:A:255:LYS:HG3	2.00	0.43
3:A:265:LYS:HE2	3:A:585:LYS:HB3	1.99	0.43
3:A:286:VAL:HA	3:A:297:LYS:HA	2.01	0.43
3:A:539:ARG:HH22	3:A:577:ARG:HD3	1.83	0.43
2:F:605:PHE:CE2	2:F:611:TYR:HB2	2.54	0.43
2:C:374:PHE:HA	2:C:377:PHE:CD2	2.53	0.43
3:A:133:CYS:SG	3:A:134:VAL:N	2.92	0.43
3:B:535:CYS:SG	3:B:564:ARG:NH1	2.86	0.43
2:F:223:LYS:HE3	2:F:227:GLU:HG3	1.99	0.43
1:E:93:VAL:HG12	1:E:100:GLU:HA	2.01	0.43
2:C:248:VAL:O	2:C:256:THR:HG21	2.18	0.43
2:C:269:ILE:HB	2:C:306:VAL:HG21	2.01	0.43
3:A:48:VAL:HG13	3:B:47:MET:HE1	2.01	0.43
3:A:193:THR:HG23	3:A:194:VAL:N	2.34	0.43
2:F:74:TYR:OH	2:F:137:GLU:OE2	2.37	0.43
2:F:225:LEU:HB3	2:F:272:HIS:CE1	2.54	0.43
1:D:58:ALA:O	1:D:59:ASN:C	2.56	0.43
3:A:297:LYS:HZ2	3:A:594:SER:HA	1.84	0.43
3:B:554:TYR:HA	3:B:561:TRP:HA	2.01	0.43
2:F:36:LEU:HD11	2:F:60:ASN:HD22	1.84	0.43
2:F:153:ARG:HH21	2:F:200:VAL:HG13	1.83	0.43
1:E:35:TRP:CE3	2:C:545:GLY:HA3	2.54	0.42
2:C:703:ILE:O	2:C:707:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:730:LEU:O	2:C:734:PHE:HB2	2.19	0.42
3:A:376:VAL:N	3:A:383:TYR:O	2.45	0.42
2:C:490:HIS:HB2	2:C:538:PHE:CD1	2.53	0.42
3:B:137:LEU:HG	3:B:176:LEU:HD21	1.99	0.42
3:B:525:VAL:HA	3:B:538:MET:HG2	2.00	0.42
2:C:74:TYR:OH	2:C:137:GLU:OE2	2.37	0.42
2:C:285:VAL:CG2	2:C:286:HIS:N	2.83	0.42
2:C:498:LEU:C	2:C:500:GLY:H	2.23	0.42
1:E:22:PHE:HB2	2:C:606:ASN:HD21	1.84	0.42
1:D:35:TRP:CE3	2:F:545:GLY:HA3	2.54	0.42
2:C:102:LEU:HD12	2:C:102:LEU:C	2.40	0.42
2:C:595:SER:O	2:C:596:THR:C	2.56	0.42
3:B:143:PHE:HE1	2:F:66:LEU:HD13	1.84	0.42
2:F:202:GLU:HA	2:F:206:GLU:HB2	2.00	0.42
2:F:717:MET:HG3	2:F:722:LEU:H	1.84	0.42
2:C:487:PHE:O	2:C:488:ARG:C	2.58	0.42
2:C:654:GLU:HB2	2:C:655:ASN:H	1.60	0.42
3:B:497:VAL:HB	3:B:515:ILE:H	1.84	0.42
2:F:118:MET:H	2:F:118:MET:HG3	1.71	0.42
2:F:649:LYS:HB3	2:F:649:LYS:HE3	1.37	0.42
1:E:37:ILE:HG12	1:E:77:HIS:HA	2.02	0.42
2:F:715:LYS:HB3	2:F:715:LYS:HE2	1.89	0.42
1:D:84:ILE:HD13	1:D:84:ILE:O	2.20	0.42
1:D:93:VAL:HG12	1:D:100:GLU:HA	2.01	0.42
2:C:484:MET:HB2	2:C:505:VAL:O	2.19	0.42
2:C:613:PHE:O	2:C:617:GLN:HG2	2.20	0.42
2:F:713:SER:HB3	2:F:714:ARG:H	1.66	0.42
1:E:86:ARG:HE	1:E:86:ARG:HB3	1.61	0.42
3:A:402:TYR:HB2	3:A:409:TRP:CZ3	2.54	0.42
3:B:539:ARG:HH21	3:B:579:PHE:HE1	1.66	0.42
3:B:566:HIS:O	3:B:566:HIS:ND1	2.53	0.42
2:F:269:ILE:HB	2:F:306:VAL:HG21	2.01	0.42
2:C:54:PHE:HD1	3:A:64:LEU:HD23	1.85	0.42
2:C:287:MET:HE1	2:C:299:MET:SD	2.60	0.42
3:A:457:THR:HG22	3:A:459:ARG:HG2	2.02	0.42
2:F:700:LYS:N	2:F:700:LYS:HD2	2.34	0.42
1:D:32:LEU:CD2	2:F:510:THR:HA	2.48	0.41
2:C:479:ILE:HD13	2:C:479:ILE:HA	1.90	0.41
2:C:500:GLY:HA2	2:C:503:LEU:HD23	2.01	0.41
3:B:237:LEU:HD11	3:B:244:VAL:HB	2.02	0.41
2:F:339:VAL:HG23	2:F:391:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ASN:HA	1:E:48:HIS:CA	2.49	0.41
1:D:22:PHE:HB2	2:F:606:ASN:CG	2.41	0.41
2:C:266:ARG:O	2:C:270:SER:HB2	2.21	0.41
2:C:592:LEU:HD23	2:C:672:VAL:HG13	2.03	0.41
3:A:287:CYS:N	3:A:296:TYR:O	2.41	0.41
3:A:426:VAL:O	3:A:426:VAL:CG1	2.68	0.41
3:A:554:TYR:HB2	3:A:561:TRP:CD1	2.55	0.41
2:F:287:MET:HE1	2:F:299:MET:SD	2.60	0.41
2:F:592:LEU:HD23	2:F:672:VAL:HG13	2.03	0.41
1:D:35:TRP:CA	2:F:546:ARG:HB3	2.47	0.41
2:C:210:LEU:HD11	2:C:263:VAL:HG11	1.99	0.41
2:C:710:ILE:HG22	2:C:711:MET:HE3	2.02	0.41
2:C:731:LYS:HA	2:C:731:LYS:HD3	1.73	0.41
3:A:253:MET:H	3:A:254:PRO:HD2	1.84	0.41
3:B:205:ASN:HB2	3:B:209:ARG:HG2	2.01	0.41
2:C:285:VAL:HG23	2:C:286:HIS:N	2.35	0.41
3:A:212:TYR:O	3:A:216:VAL:HG23	2.20	0.41
3:A:390:VAL:CG1	3:A:393:GLU:HG3	2.43	0.41
2:F:129:VAL:CG2	2:F:130:TYR:N	2.84	0.41
1:E:97:ASP:N	1:E:97:ASP:OD1	2.54	0.41
3:B:415:LEU:CD2	3:B:415:LEU:C	2.89	0.41
2:F:426:ASP:HB2	2:F:695:VAL:HG11	2.02	0.41
2:F:654:GLU:H	2:F:654:GLU:HG3	1.38	0.41
3:B:326:PRO:HA	3:B:344:PHE:HA	2.01	0.41
2:F:761:ARG:H	2:F:761:ARG:HG2	1.53	0.41
2:C:74:TYR:CZ	2:C:142:LEU:HD22	2.56	0.41
3:A:382:ILE:O	3:A:402:TYR:N	2.44	0.41
3:A:397:ARG:HB2	3:A:415:LEU:CB	2.51	0.41
3:B:228:VAL:O	3:B:229:THR:OG1	2.23	0.41
3:B:539:ARG:NH2	3:B:576:GLY:O	2.54	0.41
2:F:266:ARG:O	2:F:270:SER:HB2	2.21	0.41
2:F:668:LYS:HA	2:F:668:LYS:HD3	1.89	0.41
1:E:35:TRP:HA	2:C:545:GLY:O	2.21	0.41
3:A:211:GLN:H	3:A:211:GLN:HG3	1.38	0.41
3:A:539:ARG:HD3	3:A:549:TYR:CZ	2.55	0.41
3:B:415:LEU:HD11	3:B:419:TRP:CE3	2.55	0.41
2:F:624:GLU:HB3	2:F:625:ARG:H	1.76	0.41
2:F:671:ARG:HA	2:F:671:ARG:HD2	1.55	0.41
1:E:64:THR:O	1:E:65:SER:C	2.58	0.41
1:E:94:CYS:HA	1:E:95:PRO:HD3	1.87	0.41
1:D:28:ASN:ND2	2:F:556:SER:OG	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:CYS:HA	1:D:60:GLN:OE1	2.21	0.41
1:D:60:GLN:HE21	1:D:63:ALA:CA	2.34	0.41
1:D:64:THR:O	1:D:65:SER:C	2.58	0.41
1:D:89:LYS:NZ	2:F:752:GLU:HB2	2.35	0.41
1:D:97:ASP:N	1:D:97:ASP:OD1	2.54	0.41
2:C:498:LEU:HD22	2:C:498:LEU:HA	1.86	0.41
2:C:624:GLU:O	2:C:627:LEU:N	2.38	0.41
2:C:709:ARG:HE	2:C:709:ARG:HB2	1.35	0.41
2:C:754:LEU:HD11	2:C:756:ARG:HE	1.86	0.41
3:A:220:ILE:HD13	3:A:220:ILE:HA	1.66	0.41
3:A:297:LYS:HZ3	3:A:592:GLU:HG2	1.86	0.41
3:B:539:ARG:HD3	3:B:549:TYR:CZ	2.56	0.41
1:E:28:ASN:ND2	2:C:556:SER:OG	2.54	0.41
3:B:289:SER:HG	3:B:294:LYS:H	1.60	0.41
3:B:429:ASP:O	3:B:445:ARG:NH2	2.43	0.41
2:F:526:PRO:HD2	2:F:603:MET:HG3	2.01	0.41
2:F:595:SER:N	2:F:598:GLN:OE1	2.53	0.41
2:F:749:ILE:HA	2:F:755:ALA:HA	2.03	0.41
1:D:74:VAL:HB	1:D:102:GLU:HG3	2.03	0.40
2:C:168:MET:SD	2:C:183:ILE:HD11	2.62	0.40
3:A:195:ARG:HB2	3:A:224:ALA:HB1	2.03	0.40
3:B:156:VAL:O	3:B:158:HIS:N	2.54	0.40
1:E:61:ALA:O	1:E:62:SER:C	2.60	0.40
2:C:560:ASN:HA	2:C:591:ILE:HG13	2.03	0.40
3:A:148:LEU:O	3:A:149:LYS:C	2.60	0.40
3:B:113:VAL:HB	3:B:116:VAL:HG12	2.04	0.40
2:F:762:LYS:HD3	2:F:762:LYS:HA	1.62	0.40
2:C:54:PHE:CD1	3:A:64:LEU:HD23	2.56	0.40
2:C:389:SER:O	2:C:392:ILE:HG22	2.21	0.40
2:C:738:PRO:HB2	2:C:739:VAL:H	1.55	0.40
3:A:244:VAL:O	3:A:247:GLN:HG3	2.21	0.40
2:F:74:TYR:CZ	2:F:142:LEU:HD22	2.56	0.40
2:F:129:VAL:HG23	2:F:130:TYR:N	2.36	0.40
2:F:653:ILE:H	2:F:653:ILE:HG12	1.81	0.40
1:E:74:VAL:HB	1:E:102:GLU:HG3	2.03	0.40
2:C:392:ILE:HD11	2:C:454:MET:HE1	2.03	0.40
2:C:595:SER:N	2:C:598:GLN:OE1	2.53	0.40
3:A:102:GLU:HG3	3:A:135:ARG:HH12	1.85	0.40
3:A:194:VAL:HG23	3:A:220:ILE:HD11	2.04	0.40
3:A:265:LYS:HD3	3:A:587:TYR:CZ	2.57	0.40
3:B:64:LEU:HD12	3:B:64:LEU:HA	1.97	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	D	87/108 (81%)	60 (69%)	19 (22%)	8 (9%)	1 10
1	E	87/108 (81%)	63 (72%)	17 (20%)	7 (8%)	1 12
2	C	716/768 (93%)	628 (88%)	78 (11%)	10 (1%)	11 46
2	F	716/768 (93%)	624 (87%)	79 (11%)	13 (2%)	8 40
3	A	556/623 (89%)	502 (90%)	50 (9%)	4 (1%)	22 63
3	B	558/623 (90%)	508 (91%)	45 (8%)	5 (1%)	17 56
All	All	2720/2998 (91%)	2385 (88%)	288 (11%)	47 (2%)	13 42

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	38	VAL
1	E	68	CYS
1	D	38	VAL
1	D	68	CYS
1	D	92	GLN
3	B	156	VAL
3	B	157	GLU
2	F	639	PRO
2	F	735	LEU
2	F	738	PRO
1	E	94	CYS
1	D	94	CYS
2	C	639	PRO
2	C	738	PRO
3	A	254	PRO
3	B	254	PRO
2	F	459	LYS

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Mol	Chain	Res	Type
2	F	501	VAL
2	C	460	THR
2	C	492	GLN
2	C	625	ARG
2	C	654	GLU
3	A	252	SER
3	A	253	MET
3	A	256	PHE
2	F	460	THR
2	F	625	ARG
1	E	67	GLU
1	E	97	ASP
1	E	98	ASN
1	D	67	GLU
1	D	97	ASP
1	D	98	ASN
3	B	62	SER
3	B	253	MET
2	F	50	SER
1	E	101	TRP
1	D	101	TRP
2	C	715	LYS
2	C	749	ILE
2	C	767	VAL
2	F	449	ASP
2	F	654	GLU
2	F	655	ASN
2	F	658	ILE
2	C	735	LEU
2	F	686	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	D	78/90 (87%)	54 (69%)	24 (31%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	78/90 (87%)	55 (70%)	23 (30%)	0 2
2	C	652/693 (94%)	536 (82%)	116 (18%)	2 10
2	F	652/693 (94%)	527 (81%)	125 (19%)	1 8
3	A	506/560 (90%)	459 (91%)	47 (9%)	9 28
3	B	507/560 (90%)	471 (93%)	36 (7%)	14 39
All	All	2473/2686 (92%)	2102 (85%)	371 (15%)	6 15

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	28	ASN
1	E	35	TRP
1	E	38	VAL
1	E	40	ASP
1	E	42	CYS
1	E	46	ARG
1	E	49	ILE
1	E	50	MET
1	E	52	LEU
1	E	60	GLN
1	E	64	THR
1	E	67	GLU
1	E	74	VAL
1	E	84	ILE
1	E	86	ARG
1	E	88	LEU
1	E	91	ARG
1	E	93	VAL
1	E	98	ASN
1	E	99	ARG
1	E	100	GLU
1	E	101	TRP
1	E	102	GLU
1	D	28	ASN
1	D	35	TRP
1	D	38	VAL
1	D	39	VAL
1	D	40	ASP
1	D	41	ASN
1	D	44	ILE

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Mol	Chain	Res	Type
1	D	46	ARG
1	D	50	MET
1	D	52	LEU
1	D	59	ASN
1	D	64	THR
1	D	67	GLU
1	D	74	VAL
1	D	84	ILE
1	D	86	ARG
1	D	91	ARG
1	D	92	GLN
1	D	93	VAL
1	D	98	ASN
1	D	99	ARG
1	D	100	GLU
1	D	101	TRP
1	D	102	GLU
2	C	203	GLU
2	C	210	LEU
2	C	377	PHE
2	C	380	LEU
2	C	383	ARG
2	C	384	SER
2	C	397	LYS
2	C	405	GLU
2	C	407	GLU
2	C	411	ILE
2	C	420	ARG
2	C	421	PHE
2	C	422	MET
2	C	423	GLN
2	C	425	LYS
2	C	427	VAL
2	C	429	GLU
2	C	430	ARG
2	C	431	TYR
2	C	433	LYS
2	C	444	LYS
2	C	445	SER
2	C	446	VAL
2	C	449	ASP
2	C	452	LYS

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Mol	Chain	Res	Type
2	C	455	ILE
2	C	456	SER
2	C	457	LYS
2	C	458	LEU
2	C	459	LYS
2	C	460	THR
2	C	461	GLU
2	C	462	CYS
2	C	467	THR
2	C	469	LYS
2	C	470	LEU
2	C	473	MET
2	C	477	MET
2	C	478	SER
2	C	484	MET
2	C	491	LEU
2	C	494	THR
2	C	497	SER
2	C	498	LEU
2	C	515	THR
2	C	521	LYS
2	C	593	GLN
2	C	595	SER
2	C	600	THR
2	C	602	LEU
2	C	607	ASN
2	C	608	ARG
2	C	610	LYS
2	C	611	TYR
2	C	613	PHE
2	C	625	ARG
2	C	626	GLU
2	C	627	LEU
2	C	629	ARG
2	C	642	ARG
2	C	646	LYS
2	C	649	LYS
2	C	651	LYS
2	C	653	ILE
2	C	654	GLU
2	C	658	ILE
2	C	660	THR

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Mol	Chain	Res	Type
2	C	661	VAL
2	C	663	ASP
2	C	665	PHE
2	C	666	THR
2	C	667	SER
2	C	669	LEU
2	C	671	ARG
2	C	675	GLN
2	C	680	LYS
2	C	681	GLN
2	C	687	GLU
2	C	689	LYS
2	C	692	ARG
2	C	694	LYS
2	C	698	ASP
2	C	699	ARG
2	C	700	LYS
2	C	701	HIS
2	C	702	GLU
2	C	703	ILE
2	C	707	ILE
2	C	709	ARG
2	C	711	MET
2	C	712	LYS
2	C	713	SER
2	C	716	LYS
2	C	717	MET
2	C	721	VAL
2	C	722	LEU
2	C	731	LYS
2	C	733	ARG
2	C	735	LEU
2	C	739	VAL
2	C	741	ILE
2	C	742	LYS
2	C	745	ILE
2	C	746	GLU
2	C	748	LEU
2	C	751	ARG
2	C	752	GLU
2	C	753	TYR
2	C	754	LEU

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Mol	Chain	Res	Type
2	C	756	ARG
2	C	759	GLU
2	C	761	ARG
2	C	763	VAL
2	C	765	THR
2	C	766	TYR
2	C	767	VAL
3	A	6	GLU
3	A	9	ILE
3	A	15	VAL
3	A	16	SER
3	A	17	LEU
3	A	22	LYS
3	A	23	LEU
3	A	26	GLU
3	A	29	LEU
3	A	31	THR
3	A	32	ASP
3	A	45	HIS
3	A	48	VAL
3	A	52	CYS
3	A	57	ARG
3	A	59	MET
3	A	64	LEU
3	A	65	SER
3	A	66	GLU
3	A	68	LYS
3	A	119	ARG
3	A	160	PHE
3	A	199	MET
3	A	201	TRP
3	A	205	ASN
3	A	209	ARG
3	A	211	GLN
3	A	213	LEU
3	A	217	LEU
3	A	218	SER
3	A	219	GLN
3	A	220	ILE
3	A	221	ARG
3	A	222	ILE
3	A	225	LEU

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Mol	Chain	Res	Type
3	A	226	SER
3	A	227	GLU
3	A	250	TYR
3	A	253	MET
3	A	255	LYS
3	A	256	PHE
3	A	258	LYS
3	A	270	ILE
3	A	272	ILE
3	A	396	ARG
3	A	412	VAL
3	A	443	PHE
3	B	7	ARG
3	B	9	ILE
3	B	11	THR
3	B	16	SER
3	B	17	LEU
3	B	22	LYS
3	B	26	GLU
3	B	27	GLN
3	B	32	ASP
3	B	54	SER
3	B	57	ARG
3	B	59	MET
3	B	61	MET
3	B	64	LEU
3	B	67	SER
3	B	68	LYS
3	B	69	GLN
3	B	70	THR
3	B	96	MET
3	B	119	ARG
3	B	147	GLU
3	B	209	ARG
3	B	231	ARG
3	B	251	LYS
3	B	252	SER
3	B	253	MET
3	B	255	LYS
3	B	256	PHE
3	B	257	PHE
3	B	307	LYS

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Mol	Chain	Res	Type
3	B	390	VAL
3	B	394	LEU
3	B	396	ARG
3	B	397	ARG
3	B	401	ARG
3	B	443	PHE
2	F	47	LYS
2	F	49	ASN
2	F	50	SER
2	F	52	LEU
2	F	55	GLU
2	F	56	GLU
2	F	59	ARG
2	F	97	LEU
2	F	116	MET
2	F	203	GLU
2	F	377	PHE
2	F	378	LEU
2	F	379	ASN
2	F	380	LEU
2	F	383	ARG
2	F	384	SER
2	F	397	LYS
2	F	405	GLU
2	F	407	GLU
2	F	411	ILE
2	F	420	ARG
2	F	425	LYS
2	F	427	VAL
2	F	430	ARG
2	F	433	LYS
2	F	443	ASN
2	F	444	LYS
2	F	445	SER
2	F	451	GLU
2	F	452	LYS
2	F	455	ILE
2	F	456	SER
2	F	457	LYS
2	F	458	LEU
2	F	459	LYS
2	F	460	THR

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Mol	Chain	Res	Type
2	F	461	GLU
2	F	462	CYS
2	F	469	LYS
2	F	470	LEU
2	F	477	MET
2	F	478	SER
2	F	480	SER
2	F	483	THR
2	F	484	MET
2	F	488	ARG
2	F	492	GLN
2	F	498	LEU
2	F	501	VAL
2	F	502	ASP
2	F	503	LEU
2	F	504	THR
2	F	507	VAL
2	F	508	LEU
2	F	512	TYR
2	F	515	THR
2	F	521	LYS
2	F	524	ILE
2	F	593	GLN
2	F	595	SER
2	F	600	THR
2	F	602	LEU
2	F	608	ARG
2	F	610	LYS
2	F	613	PHE
2	F	625	ARG
2	F	626	GLU
2	F	627	LEU
2	F	629	ARG
2	F	641	GLN
2	F	642	ARG
2	F	646	LYS
2	F	649	LYS
2	F	651	LYS
2	F	652	GLU
2	F	653	ILE
2	F	654	GLU
2	F	655	ASN

Continued on next page...

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Mol	Chain	Res	Type
2	F	658	ILE
2	F	660	THR
2	F	661	VAL
2	F	663	ASP
2	F	666	THR
2	F	669	LEU
2	F	671	ARG
2	F	675	GLN
2	F	680	LYS
2	F	687	GLU
2	F	688	ARG
2	F	689	LYS
2	F	691	THR
2	F	692	ARG
2	F	695	VAL
2	F	699	ARG
2	F	700	LYS
2	F	702	GLU
2	F	703	ILE
2	F	704	GLU
2	F	707	ILE
2	F	712	LYS
2	F	713	SER
2	F	714	ARG
2	F	716	LYS
2	F	717	MET
2	F	721	VAL
2	F	722	LEU
2	F	730	LEU
2	F	731	LYS
2	F	733	ARG
2	F	734	PHE
2	F	737	SER
2	F	739	VAL
2	F	742	LYS
2	F	743	LYS
2	F	748	LEU
2	F	750	GLU
2	F	753	TYR
2	F	754	LEU
2	F	756	ARG
2	F	757	THR

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Mol	Chain	Res	Type
2	F	759	GLU
2	F	761	ARG
2	F	763	VAL
2	F	765	THR
2	F	767	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	28	ASN
1	E	41	ASN
1	E	76	ASN
1	E	92	GLN
1	E	98	ASN
1	E	104	GLN
1	E	108	HIS
1	D	28	ASN
1	D	60	GLN
1	D	76	ASN
1	D	92	GLN
1	D	98	ASN
1	D	108	HIS
2	C	163	GLN
2	C	443	ASN
2	C	481	ASN
2	C	553	HIS
2	C	606	ASN
2	C	618	GLN
2	C	655	ASN
2	C	681	GLN
3	A	69	GLN
3	A	71	HIS
3	A	166	GLN
3	A	356	GLN
3	A	357	GLN
3	B	129	ASN
3	B	150	GLN
3	B	166	GLN
3	B	187	ASN
3	B	219	GLN
3	B	230	GLN
3	B	235	GLN

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Mol	Chain	Res	Type
2	F	49	ASN
2	F	60	ASN
2	F	163	GLN
2	F	381	ASN
2	F	481	ASN
2	F	553	HIS
2	F	618	GLN
2	F	641	GLN
2	F	655	ASN
2	F	664	GLN
2	F	718	GLN
2	F	729	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

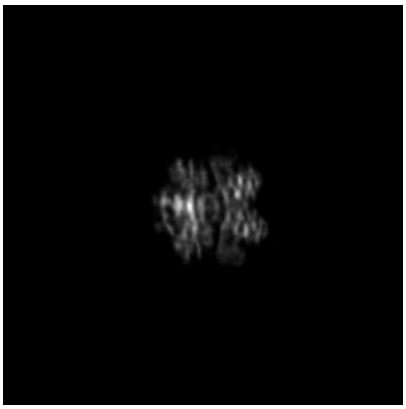
This section contains visualisations of the EMDB entry EMD-34474. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

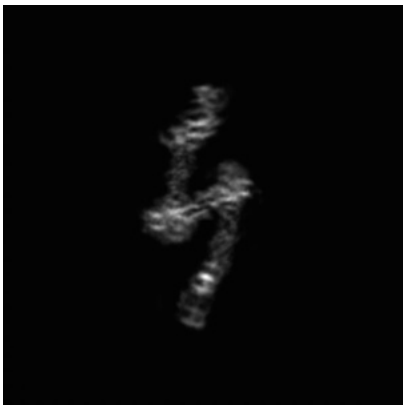
6.1 Orthogonal projections

6.1.1 Primary map

X

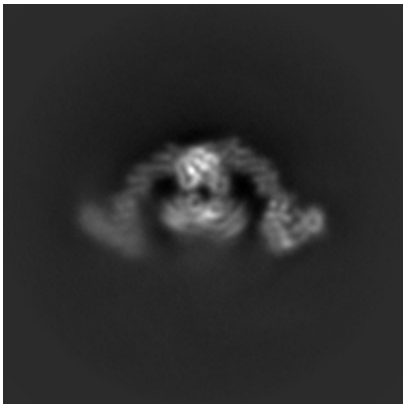


Y

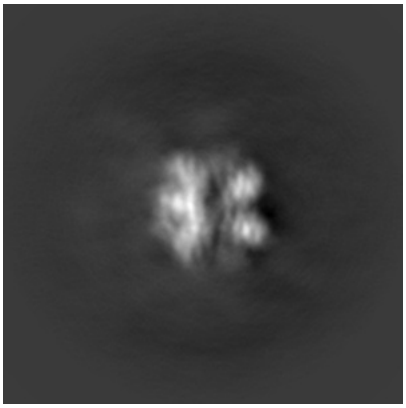


Z

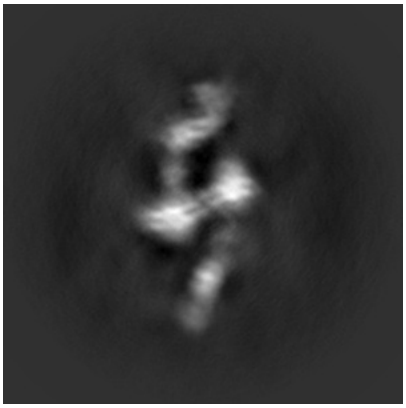
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

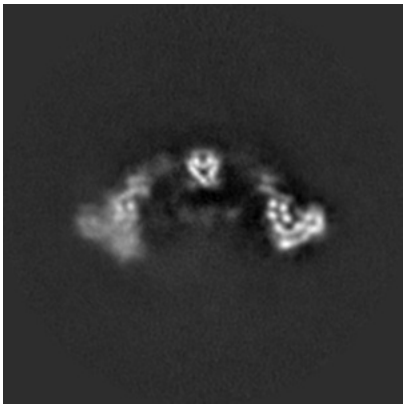
6.2.1 Primary map

X Index: 96

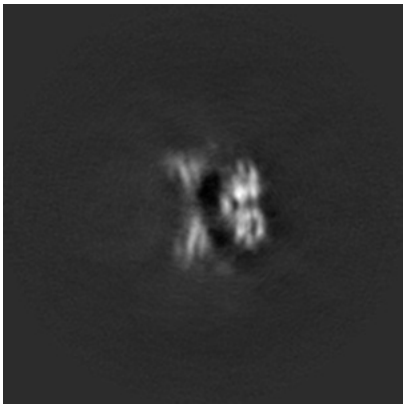
Y Index: 96

Z Index: 96

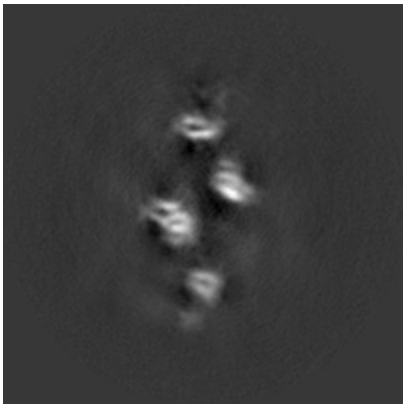
6.2.2 Raw map



X Index: 96



Y Index: 96



Z Index: 96

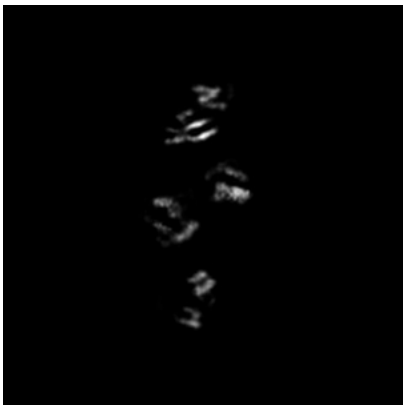
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

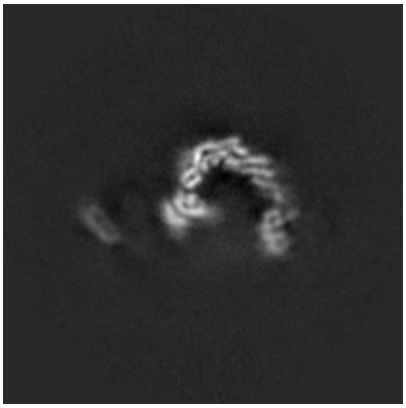
X Index: 96

Y Index: 90

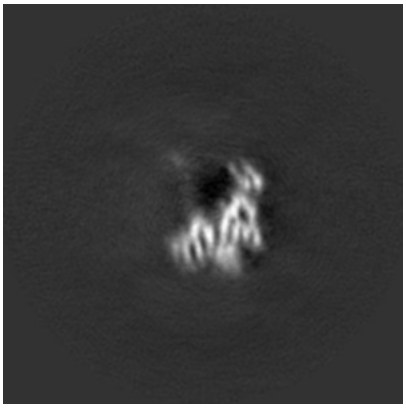


Z Index: 90

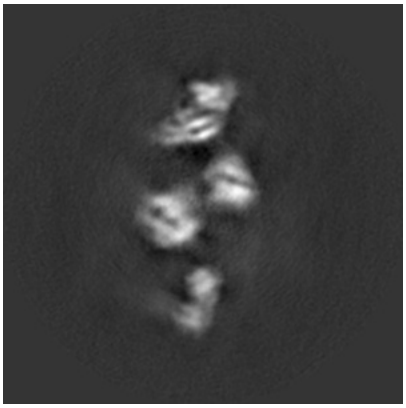
6.3.2 Raw map



X Index: 84



Y Index: 91

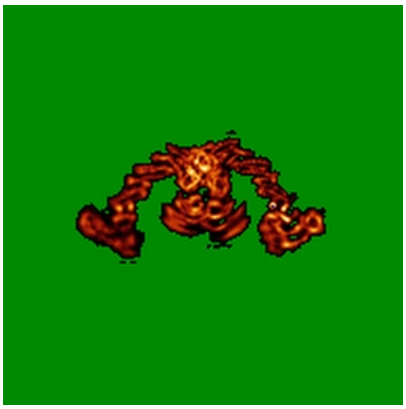


Z Index: 90

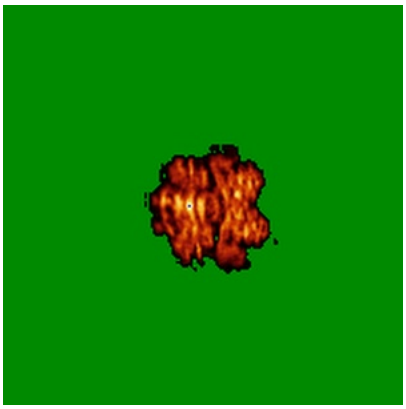
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



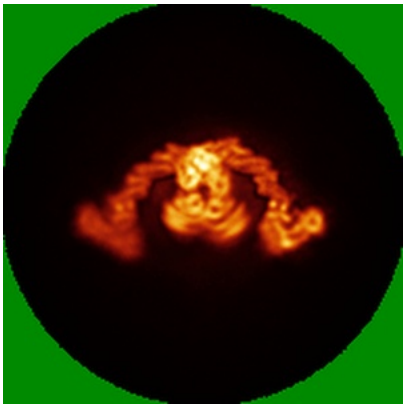
X



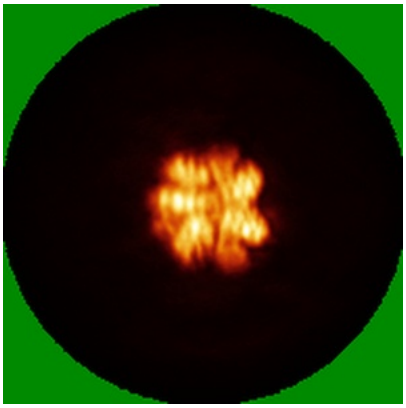
Y

Z

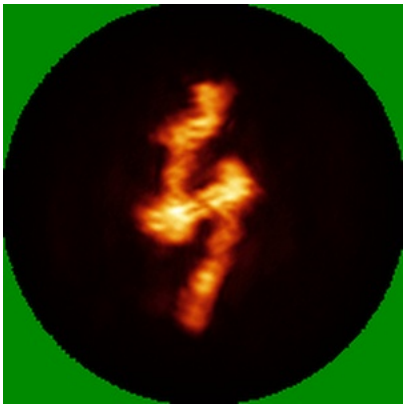
6.4.2 Raw map



X



Y

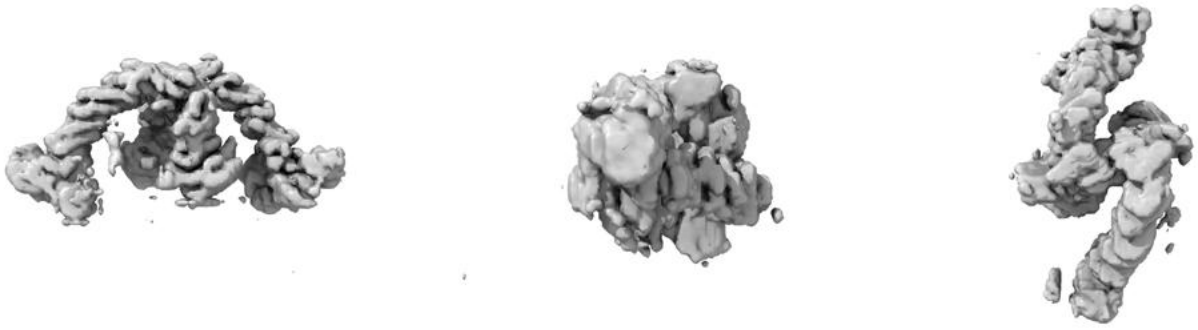


Z

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)

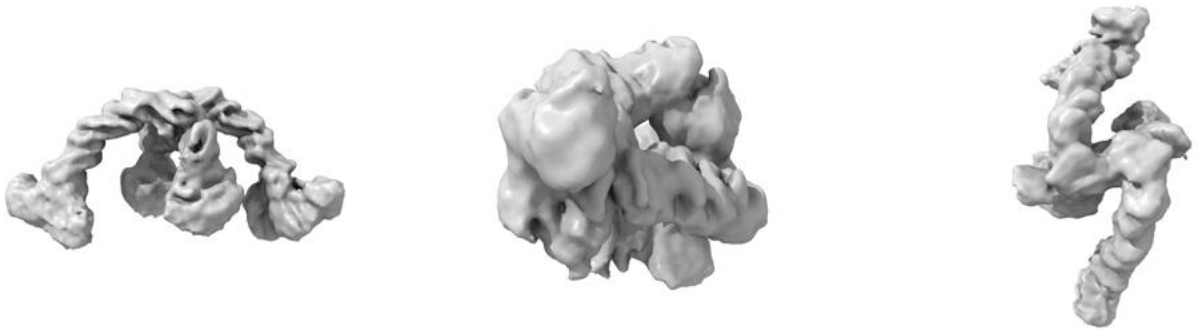
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

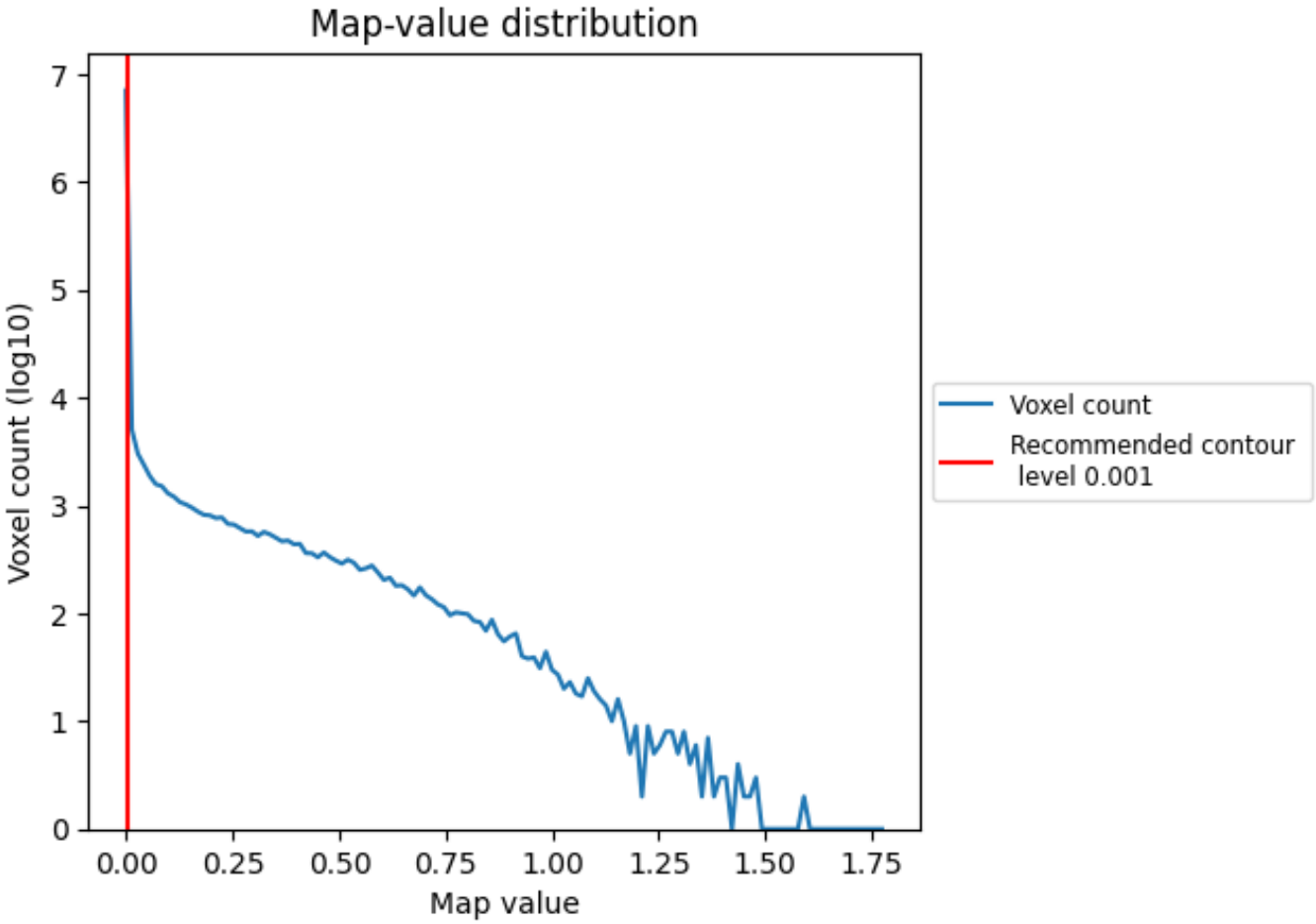
6.6 Mask visualisation (i)

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

7 Map analysis

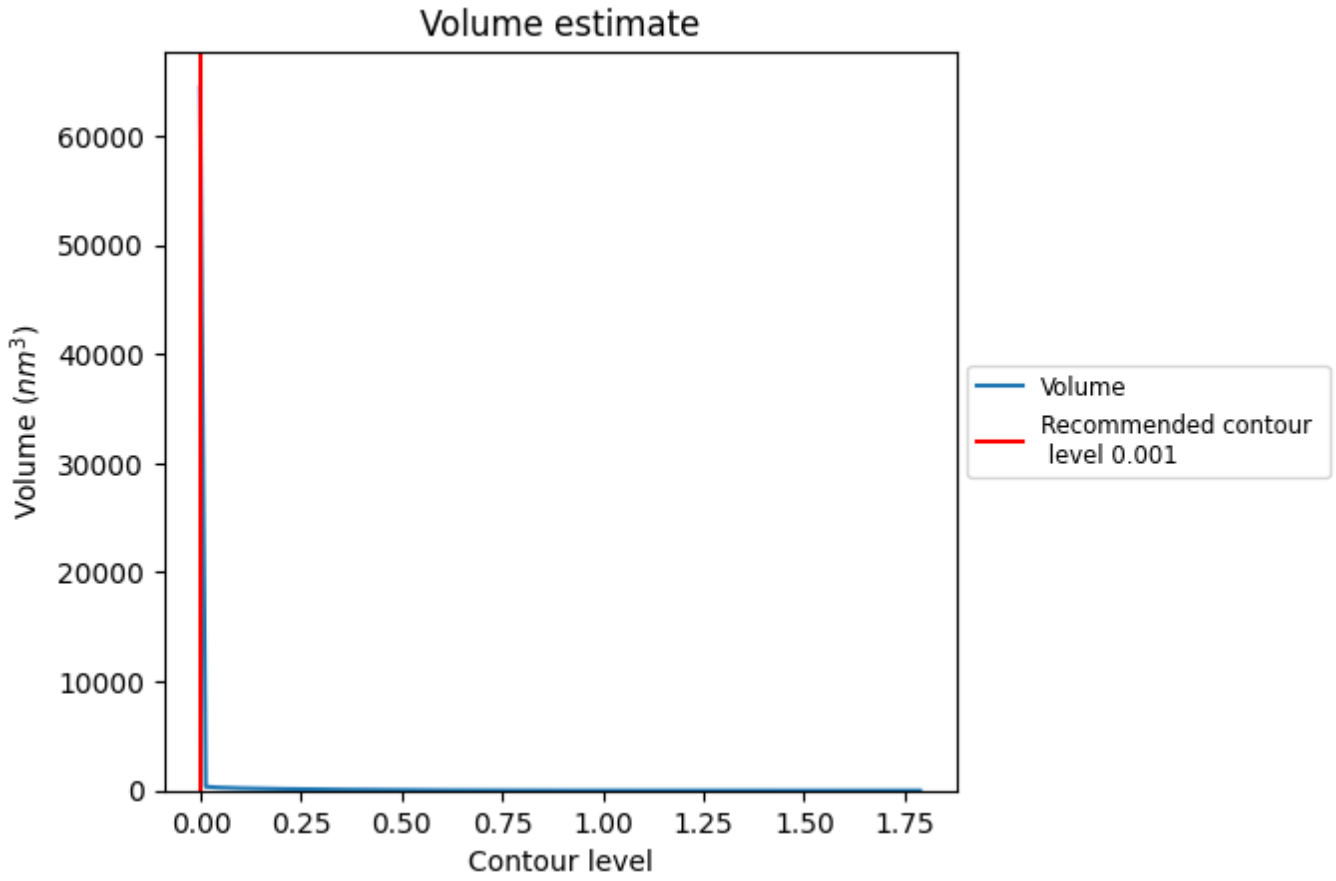
This section contains the results of statistical analysis of the map.

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.

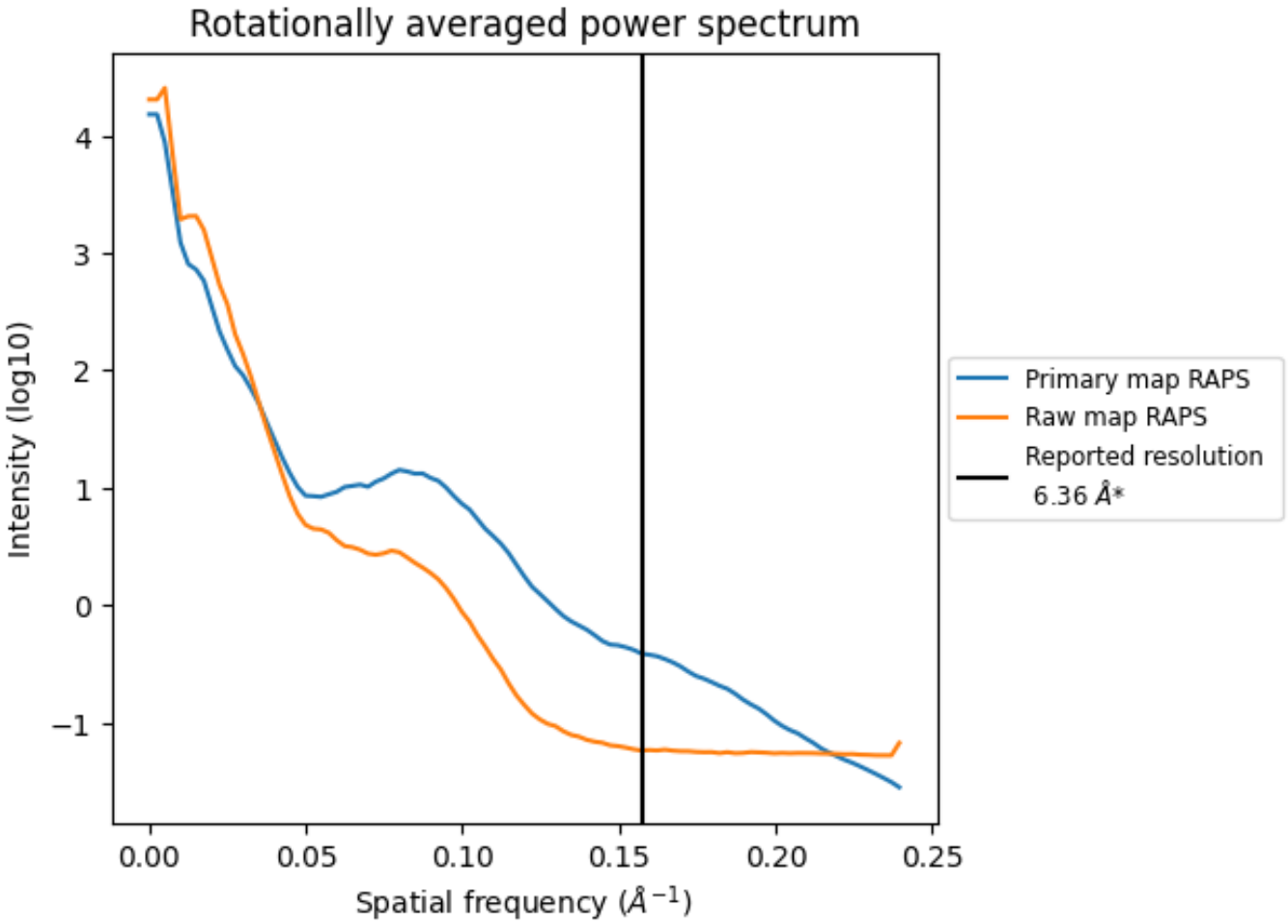
7.2 Volume estimate



The volume at the recommended contour level is 52999 nm^3; this corresponds to an approximate mass of 47875 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)

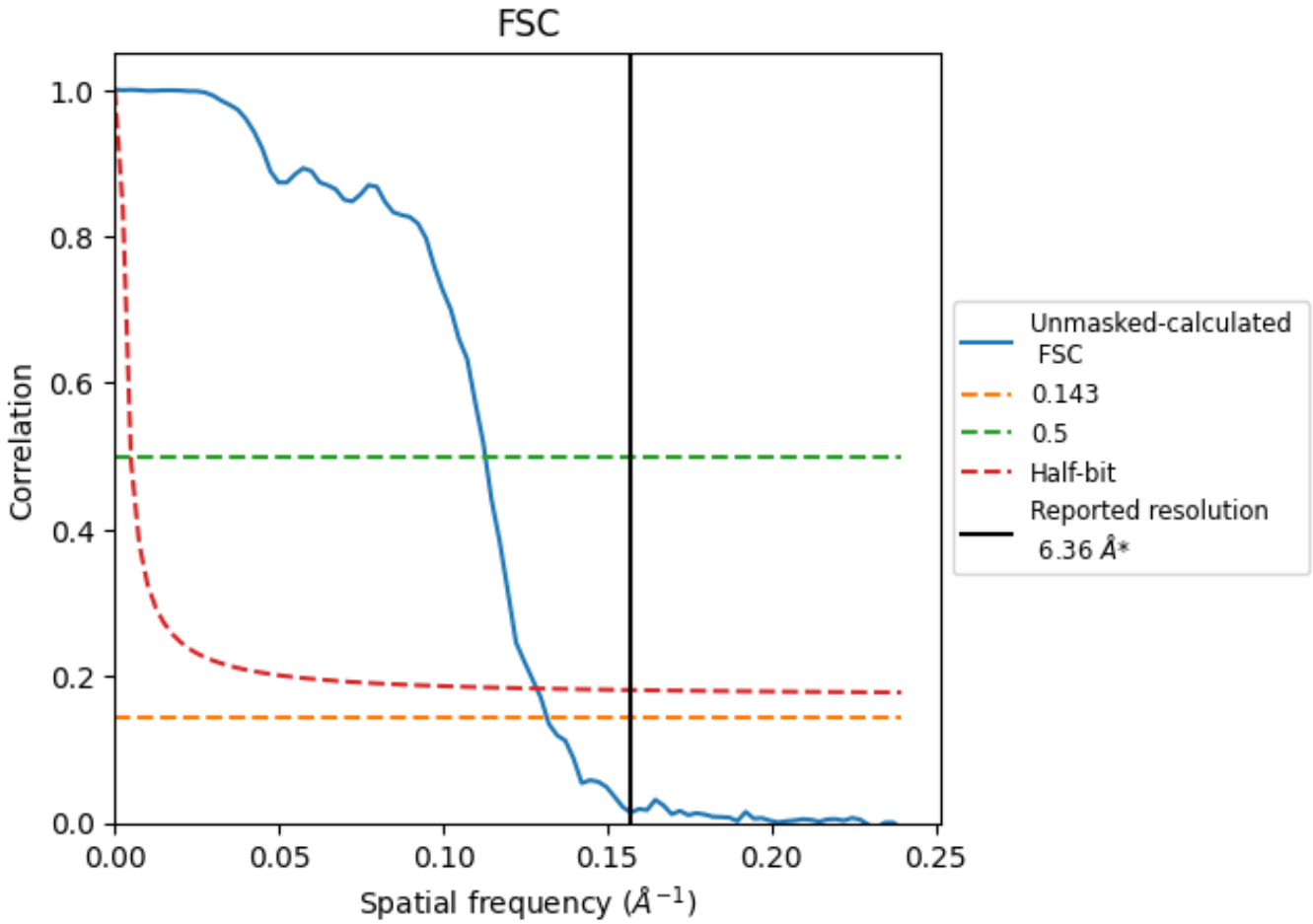


*Reported resolution corresponds to spatial frequency of 0.157 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.157 Å^{-1}

8.2 Resolution estimates (i)

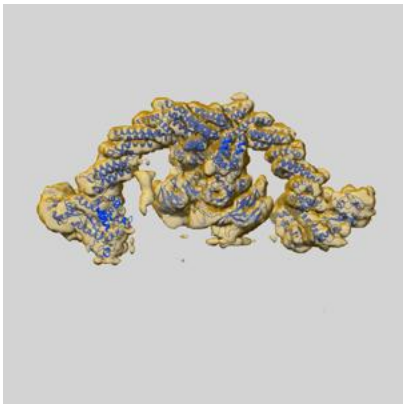
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.36	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.60	8.86	7.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.60 differs from the reported value 6.36 by more than 10 %

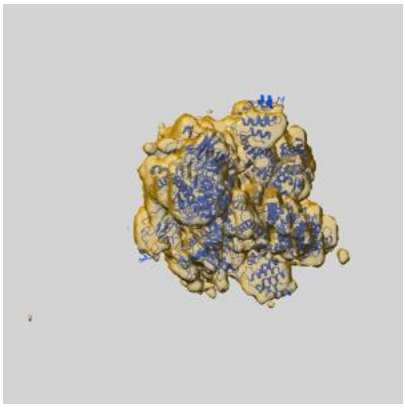
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34474 and PDB model 8H3R. Per-residue inclusion information can be found in section 3 on page 4.

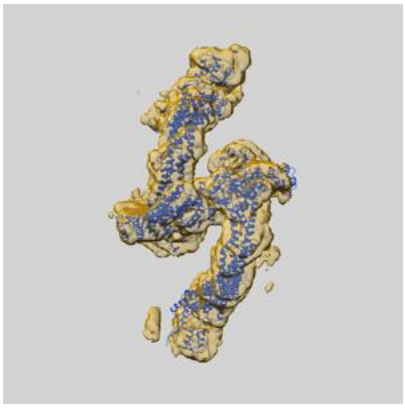
9.1 Map-model overlay



X



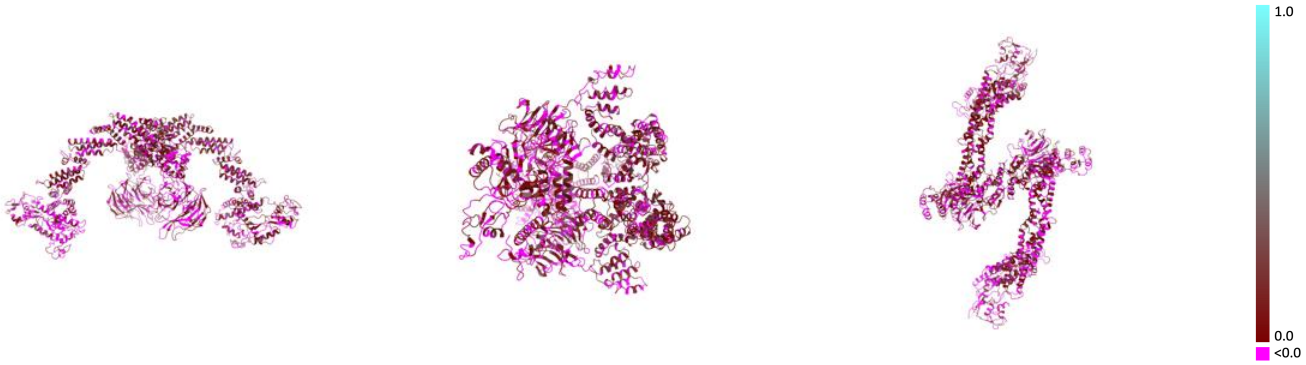
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.001 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.

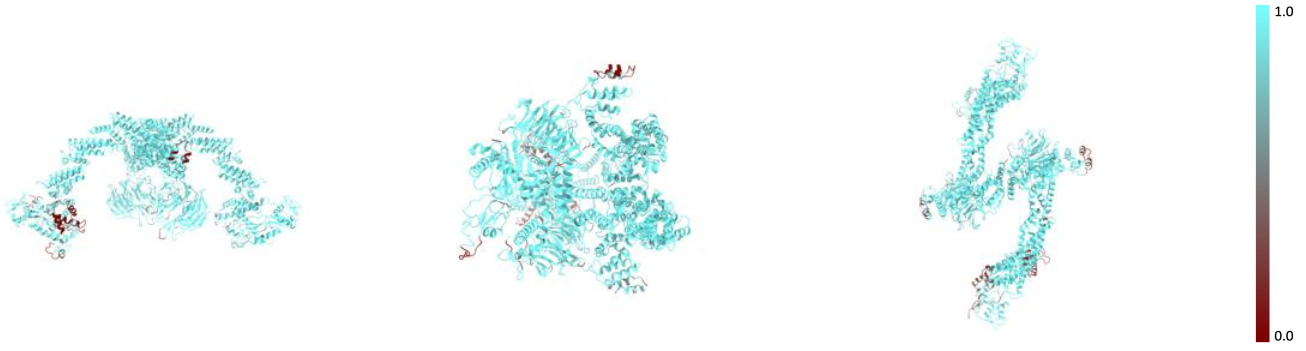
9.2 Q-score mapped to coordinate model (i)



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.

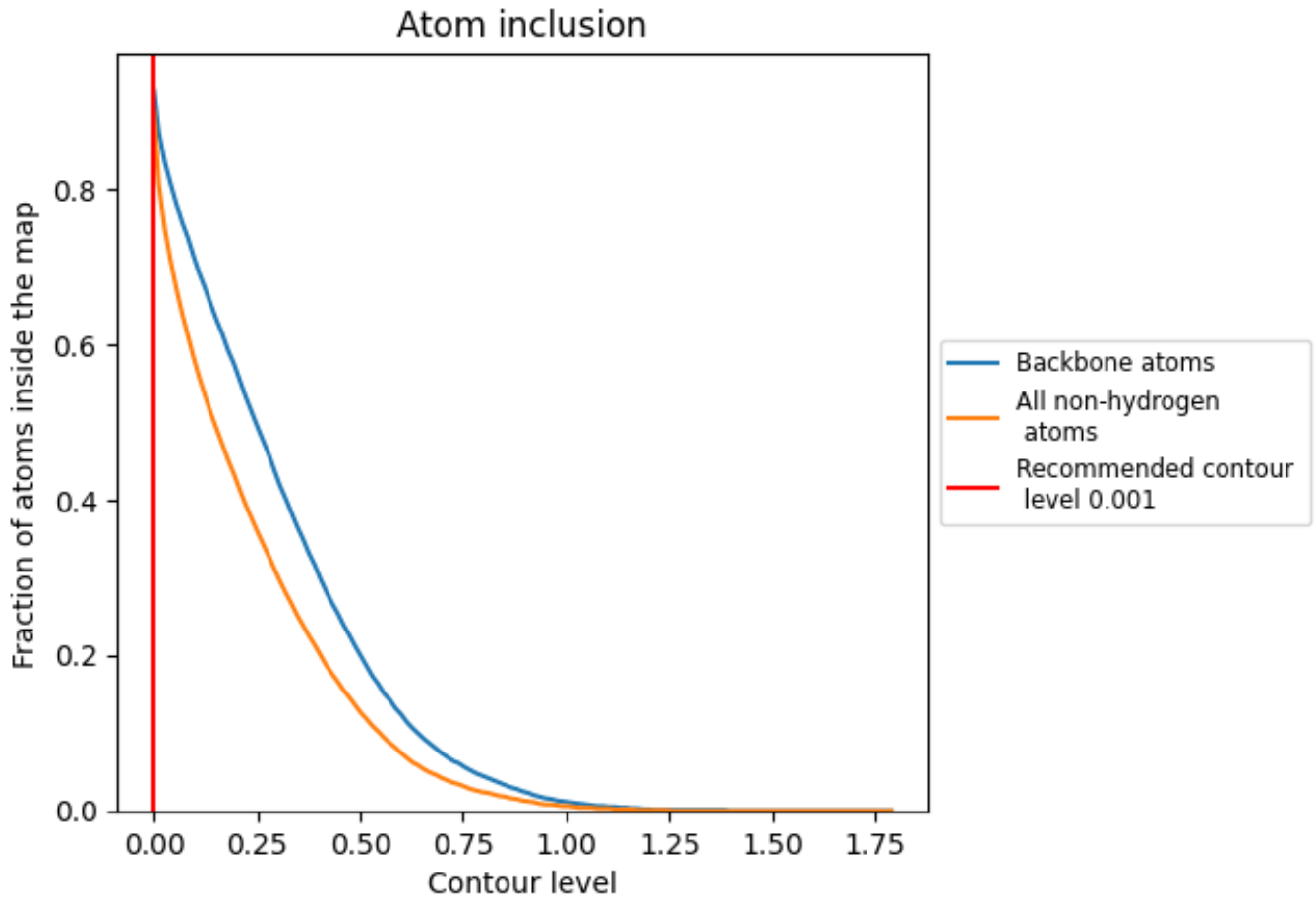
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.001).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8990	0.0400
A	0.9350	0.0480
B	0.8970	0.0330
C	0.9580	0.0680
D	0.8230	-0.0240
E	0.8510	-0.0180
F	0.8290	0.0260