



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:31 PM UTC

PDB ID : 7D44 / pdb_00007d44
EMDB ID : EMD-30569
Title : eIF2B-eIF2(aP), aP2 complex
Authors : Kashiwagi, K.; Ito, T.
Deposited on : 2020-09-22
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

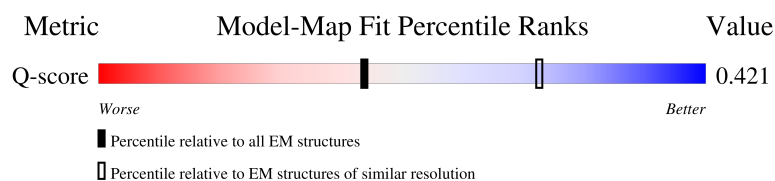
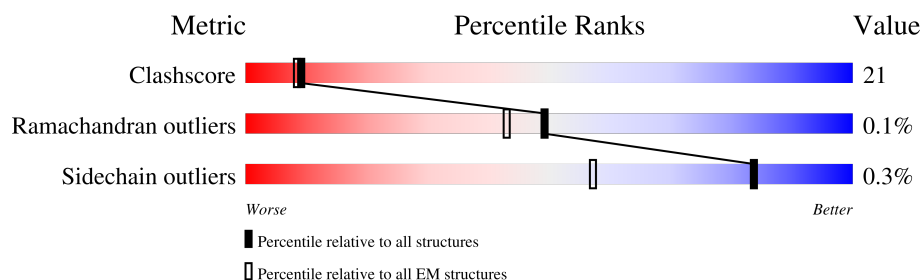
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



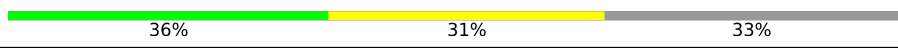
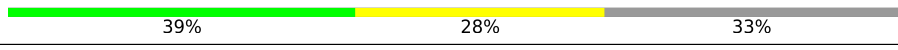
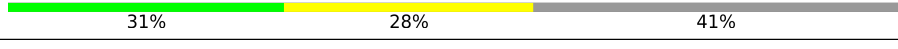
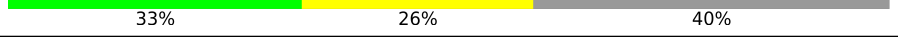
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	
1	B	305	
2	C	351	
2	D	351	

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Mol	Chain	Length	Quality of chain
3	E	452	
3	F	452	
4	G	523	
4	H	523	
5	I	721	
5	J	721	
6	K	315	
6	L	315	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28391 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	293	Total	C	N	O	S	0	0
			2262	1449	377	424	12		
1	B	291	Total	C	N	O	S	0	0
			2247	1442	373	420	12		

- Molecule 2 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	317	Total	C	N	O	S	0	0
			2476	1565	435	461	15		
2	D	324	Total	C	N	O	S	0	0
			2538	1605	445	473	15		

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	343	Total	C	N	O	S	0	0
			2430	1540	423	452	15		
3	F	343	Total	C	N	O	S	0	0
			2429	1540	423	451	15		

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	353	Total	C	N	O	S	0	0
			2750	1740	490	506	14		
4	H	353	Total	C	N	O	S	0	0
			2750	1740	490	506	14		

- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	427	Total	C	N	O	S	0	0
			3358	2115	591	637	15		
5	J	429	Total	C	N	O	S	0	0
			3373	2124	593	641	15		

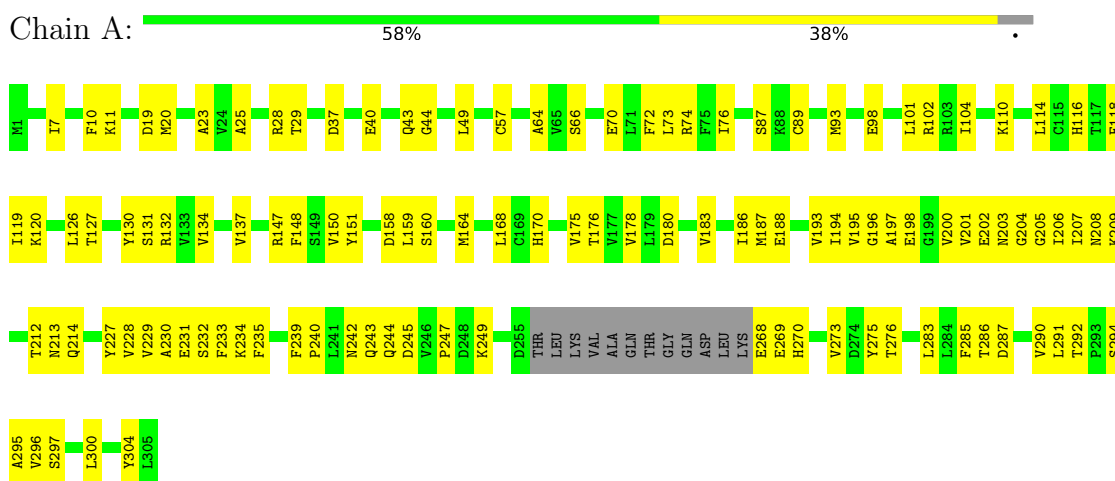
- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	176	Total	C	N	O	P	0	0
			889	529	179	180	1		
6	L	176	Total	C	N	O	P	0	0
			889	529	179	180	1		

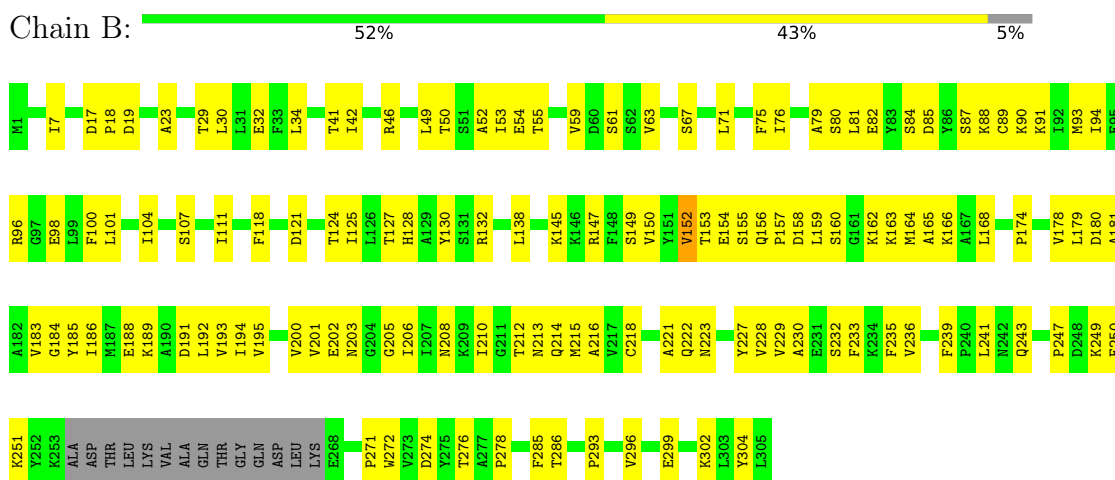
3 Residue-property plots

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: Translation initiation factor eIF-2B subunit alpha

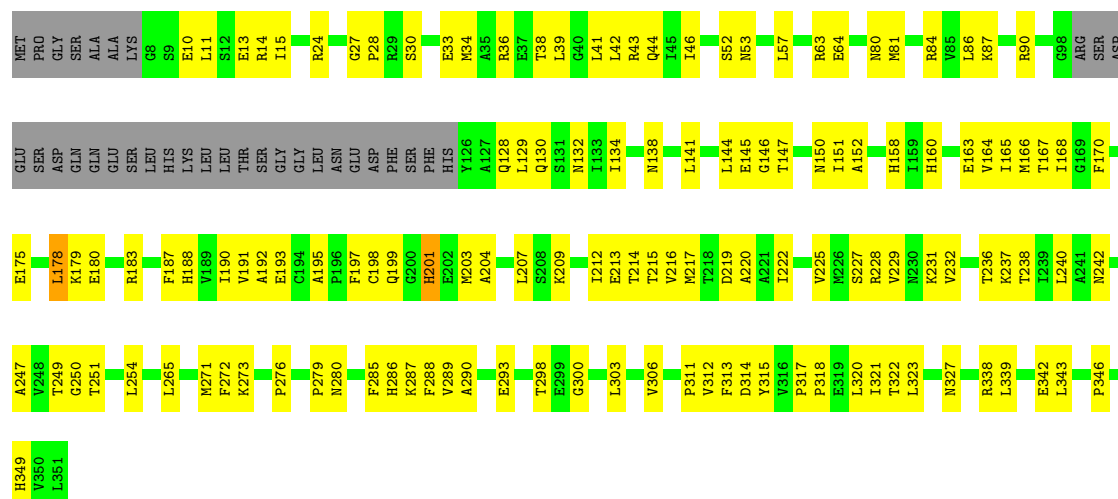


- Molecule 1: Translation initiation factor eIF-2B subunit alpha



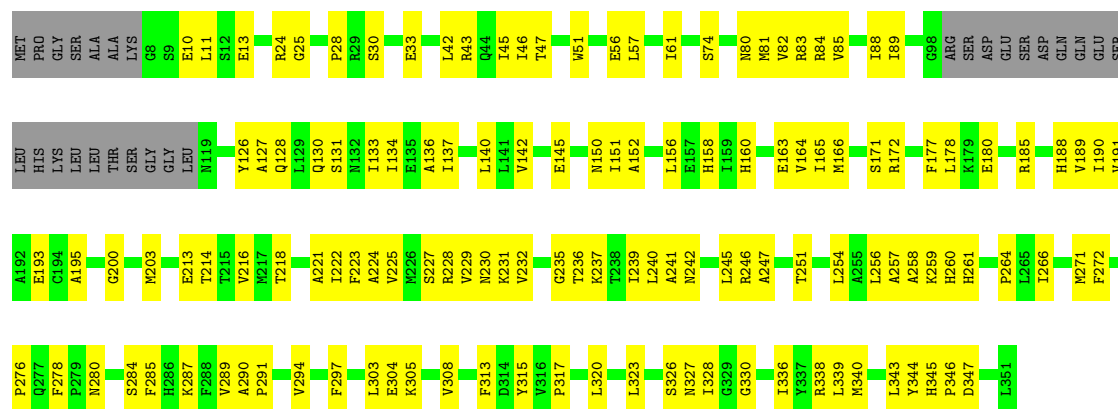
- Molecule 2: Translation initiation factor eIF-2B subunit beta





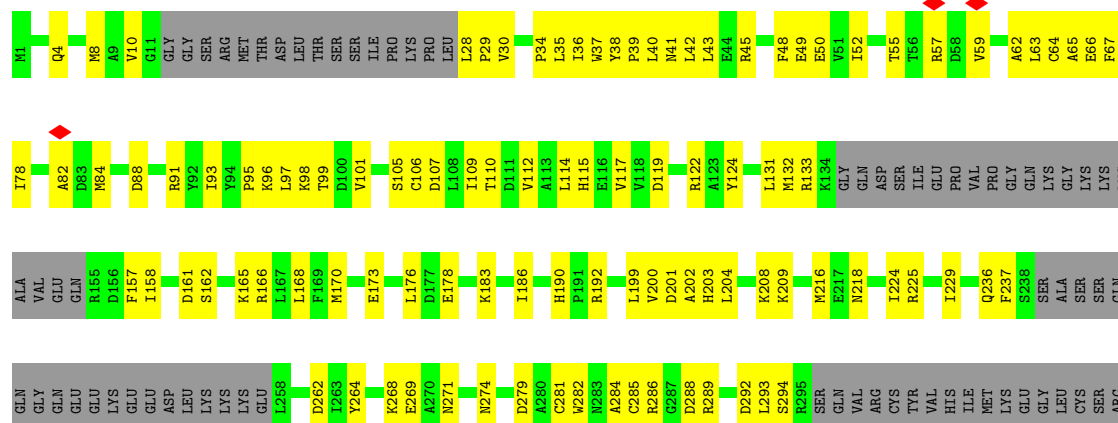
- Molecule 2: Translation initiation factor eIF-2B subunit beta

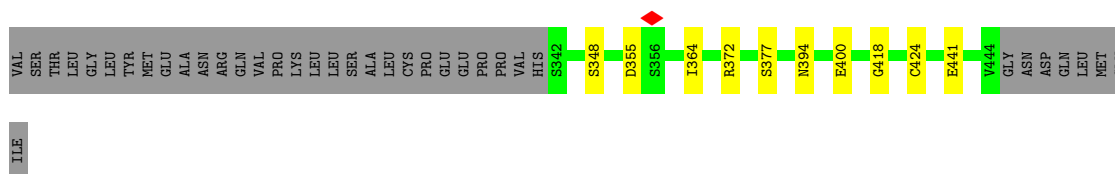
Chain D: 55% 38% 8%



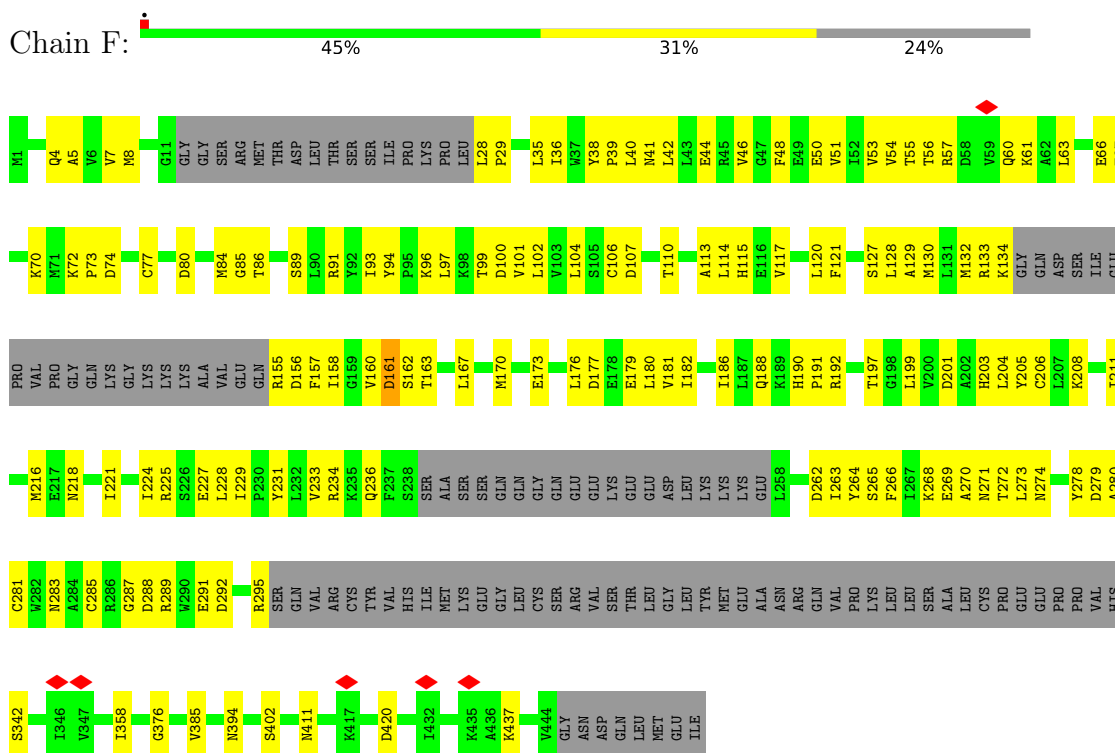
- Molecule 3: Translation initiation factor eIF-2B subunit gamma

Chain E: 51% 25% 24%

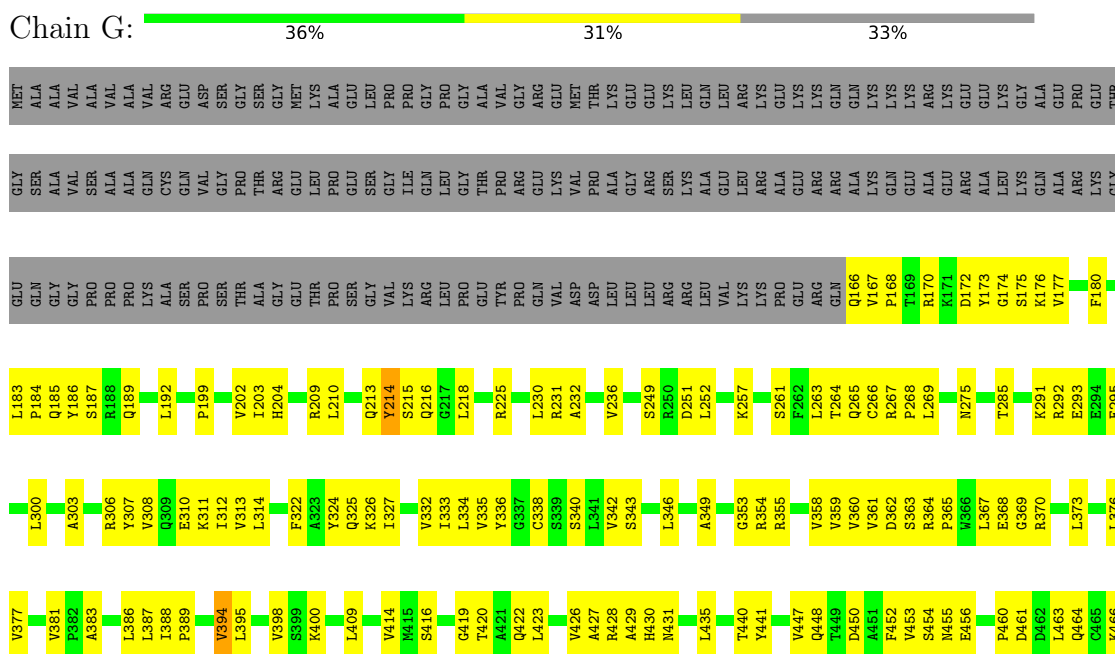


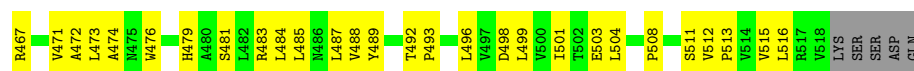


• Molecule 3: Translation initiation factor eIF-2B subunit gamma



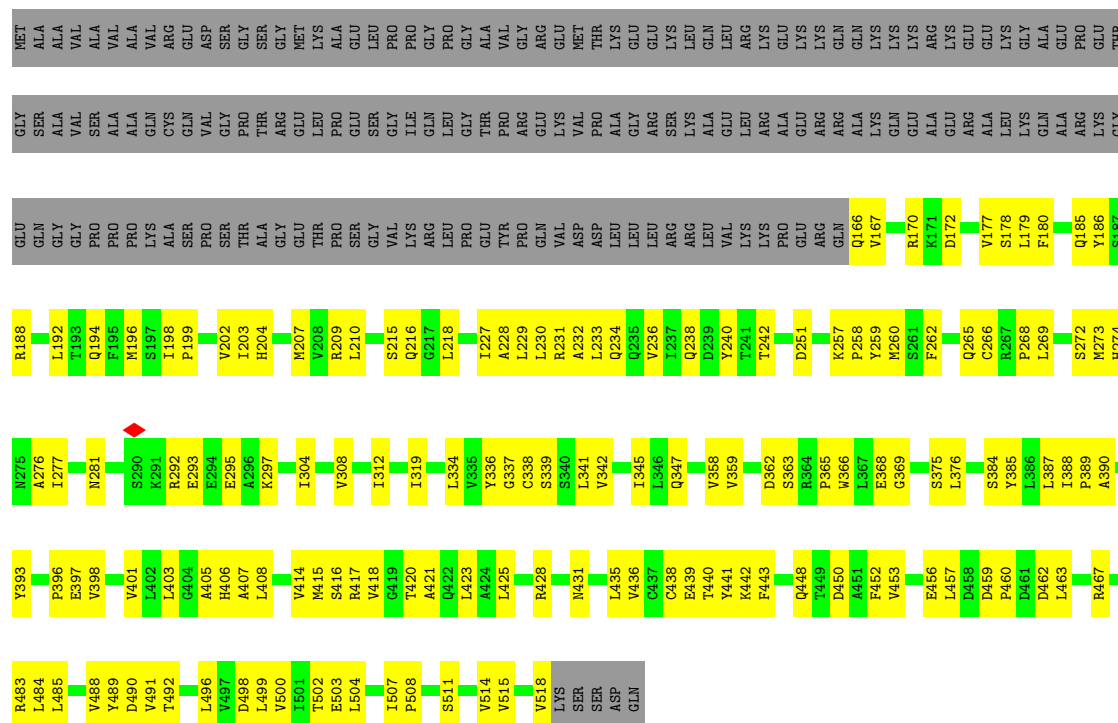
• Molecule 4: Translation initiation factor eIF-2B subunit delta





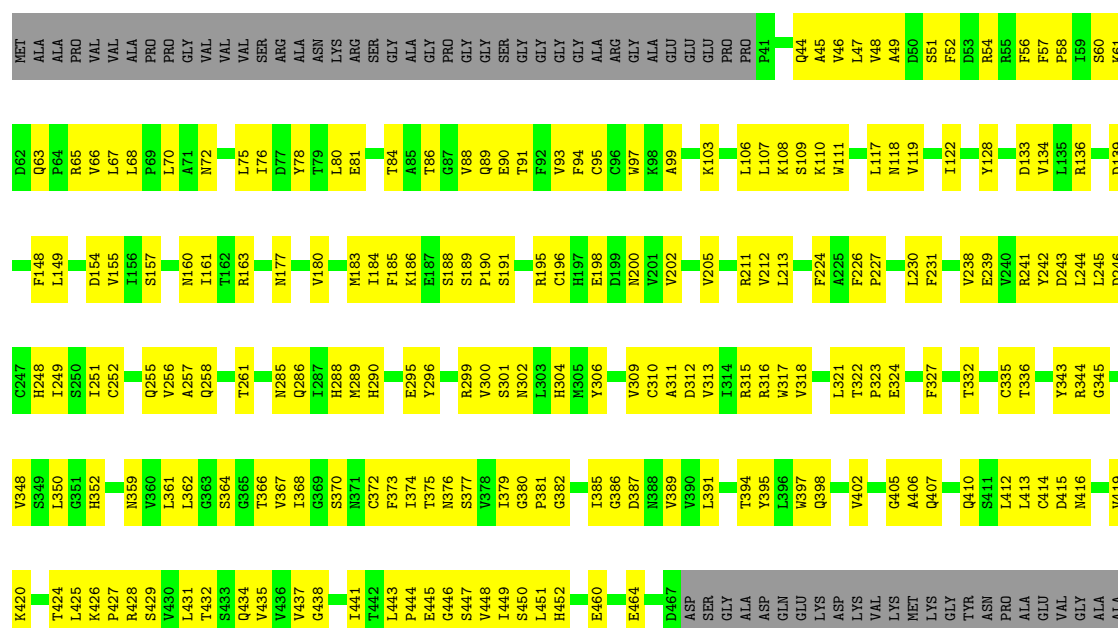
• Molecule 4: Translation initiation factor eIF-2B subunit delta

Chain H: 39% 28% 33%



• Molecule 5: Translation initiation factor eIF-2B subunit epsilon

Chain I: 31% 28% 41%



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

MET
GLU
PRO
LYS
LEU
VAL
SER
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ASP
THR
ASP
ASP
GLU
THR
THR
GLU
LEU
ALA
ARG
GLN
MET
GLU
GLY
ARG
ASN
ALA
ALA
THR

● Molecule 6: Eukaryotic translation initiation factor 2 subunit 1



MET
PRO
GLY
SER
G5
A27
G30
L35
L36
M40
E49
L50
S51
R56
I62
R63
P91
E92
E93
A94
I95
K96
C97
E98
D99
K103
S104
K105
Y108
S109
I110
L111
R112
H113
V114
A115
E116
V117
L118
T121
K122
D123
E124
Q125
L126
E127
S128

D138
P144
G147
S157
D158
P159
S160
I161
E171
V174
M178
I179
M190
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ASP
ALA
GLU
GLU
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GLU
ALA
LYS
ALA
GLU
ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.166	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	441.0, 441.0, 441.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.47, 1.47, 1.47	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/2296	0.54	0/3099
1	B	0.27	0/2281	0.50	0/3078
2	C	0.30	0/2522	0.54	2/3411 (0.1%)
2	D	0.32	0/2587	0.58	0/3498
3	E	0.22	0/2464	0.49	0/3346
3	F	0.23	0/2463	0.53	0/3344
4	G	0.30	0/2802	0.54	0/3809
4	H	0.30	0/2802	0.54	0/3809
5	I	0.26	0/3427	0.51	0/4662
5	J	0.29	0/3443	0.55	0/4685
6	K	0.23	0/879	0.68	5/1224 (0.4%)
6	L	0.17	0/879	0.43	0/1224
All	All	0.28	0/28845	0.53	7/39189 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	K	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	12	PHE	CA-C-N	8.94	131.02	119.84
6	K	12	PHE	C-N-CA	8.94	131.02	119.84
6	K	14	GLU	N-CA-C	5.79	116.72	108.74
6	K	14	GLU	CA-C-N	5.68	128.24	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	14	GLU	C-N-CA	5.68	128.24	120.35
2	C	178	LEU	CA-C-N	-5.36	111.23	121.94
2	C	178	LEU	C-N-CA	-5.36	111.23	121.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	K	14	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2262	0	2333	97	0
1	B	2247	0	2320	108	0
2	C	2476	0	2493	114	0
2	D	2538	0	2538	106	0
3	E	2430	0	2197	93	0
3	F	2429	0	2196	109	0
4	G	2750	0	2811	134	0
4	H	2750	0	2811	129	0
5	I	3358	0	3325	156	0
5	J	3373	0	3336	154	0
6	K	889	0	401	5	0
6	L	889	0	402	11	0
All	All	28391	0	27163	1140	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 21.

All (1140) 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)
6:L:35:LEU:O	6:L:40:ASN:HA	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:247:ALA:HB3	2:C:251:THR:HG21	1.52	0.91
1:B:205:GLY:HA3	1:B:276:THR:O	1.73	0.89
2:C:198:CYS:O	2:C:201:HIS:HB2	1.73	0.89
1:A:201:VAL:HG13	1:A:207:ILE:HD11	1.54	0.87
5:J:155:VAL:HG11	5:J:249:ILE:HD11	1.59	0.84
2:D:80:ASN:HA	2:D:83:ARG:HD2	1.60	0.82
1:A:203:ASN:ND2	1:A:275:TYR:OH	2.12	0.81
1:B:111:ILE:HD11	1:B:285:PHE:HB3	1.60	0.81
4:H:502:THR:HG23	4:H:504:LEU:H	1.45	0.81
3:F:288:ASP:O	3:F:292:ASP:N	2.11	0.80
2:D:304:GLU:HG3	2:D:305:LYS:HG3	1.62	0.80
1:A:203:ASN:HA	4:G:508:PRO:HG3	1.65	0.79
5:J:414:CYS:SG	5:J:415:ASP:N	2.56	0.78
3:E:133:ARG:HG2	3:E:269:GLU:HA	1.64	0.78
5:I:186:LYS:HE2	5:I:296:TYR:HA	1.65	0.78
4:G:275:ASN:ND2	4:G:441:TYR:O	2.17	0.78
5:I:413:LEU:HG	5:I:431:LEU:HD21	1.66	0.78
4:G:416:SER:HG	4:G:420:THR:HG1	1.28	0.77
5:J:172:ARG:NH2	5:J:252:CYS:O	2.17	0.77
5:J:65:ARG:HA	5:J:68:LEU:HG	1.67	0.77
1:B:81:LEU:HD21	1:B:93:MET:HE3	1.67	0.77
2:D:150:ASN:ND2	2:D:327:ASN:O	2.18	0.77
5:J:55:ARG:HH21	5:J:301:SER:HB2	1.51	0.76
5:J:111:TRP:HD1	5:J:118:ASN:HB3	1.49	0.76
2:D:130:GLN:HA	2:D:133:ILE:HD12	1.67	0.75
5:J:149:LEU:HD21	5:J:161:ILE:HD13	1.69	0.75
1:B:46:ARG:HH21	6:L:27:ALA:HB1	1.52	0.75
4:G:303:ALA:HA	4:G:306:ARG:HE	1.52	0.75
2:C:152:ALA:HB1	2:C:180:GLU:HG3	1.69	0.75
5:I:227:PRO:HG2	5:I:230:LEU:HB2	1.66	0.75
3:E:29:PRO:HA	3:E:35:LEU:HG	1.69	0.75
1:B:23:ALA:HB3	1:B:233:PHE:HE2	1.51	0.75
4:G:335:VAL:HG12	4:G:336:TYR:H	1.52	0.75
5:I:44:GLN:O	5:I:148:PHE:HA	1.86	0.75
4:H:362:ASP:OD1	4:H:363:SER:N	2.20	0.74
4:H:463:LEU:HD12	4:H:484:LEU:HD11	1.67	0.74
5:I:200:ASN:ND2	5:I:242:TYR:OH	2.20	0.74
1:A:126:LEU:HB3	1:A:193:VAL:HG22	1.69	0.74
2:C:288:PHE:HE1	2:C:311:PRO:HB3	1.53	0.74
5:J:356:LEU:HD22	5:J:360:VAL:HG21	1.69	0.74
4:G:170:ARG:NH1	4:G:187:SER:O	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4:GLN:HG3	3:F:97:LEU:HD11	1.68	0.73
5:J:59:ILE:HG12	5:J:432:THR:HG21	1.70	0.73
4:H:440:THR:HG21	4:H:504:LEU:HD23	1.69	0.73
5:J:43:LEU:HD22	5:J:88:VAL:HG22	1.71	0.72
5:J:83:LEU:HD22	5:J:88:VAL:HG21	1.72	0.72
4:G:267:ARG:HH11	4:G:268:PRO:HD2	1.52	0.72
5:I:372:CYS:SG	5:I:373:PHE:N	2.61	0.72
5:J:172:ARG:NH2	5:J:253:SER:HB2	2.04	0.72
4:G:168:PRO:HG2	4:G:192:LEU:HD23	1.71	0.72
4:H:240:TYR:O	4:H:297:LYS:NZ	2.21	0.72
1:B:87:SER:OG	1:B:91:LYS:NZ	2.23	0.72
1:A:196:GLY:O	1:A:208:ASN:ND2	2.23	0.72
1:B:30:LEU:HD11	1:B:53:ILE:HD11	1.71	0.72
5:I:63:GLN:HB2	5:I:67:LEU:HD23	1.71	0.71
4:H:403:LEU:HD21	4:H:423:LEU:HD23	1.72	0.71
5:J:53:ASP:O	5:J:55:ARG:NH1	2.24	0.70
2:C:165:ILE:HD12	2:C:231:LYS:HG2	1.73	0.70
2:D:166:MET:HE3	2:D:229:VAL:HG21	1.72	0.70
5:I:51:SER:HB2	5:I:65:ARG:HH22	1.57	0.70
4:H:448:GLN:HG3	4:H:453:VAL:HG22	1.74	0.70
3:F:57:ARG:NH2	3:F:80:ASP:OD2	2.24	0.69
2:C:237:LYS:HD3	2:C:313:PHE:HZ	1.57	0.69
5:I:441:ILE:HD13	5:I:464:GLU:HB2	1.74	0.69
3:F:158:ILE:HG22	3:F:170:MET:HB2	1.74	0.69
3:E:115:HIS:O	3:E:119:ASP:HB2	1.93	0.69
5:J:110:LYS:NZ	5:J:327:PHE:O	2.17	0.69
2:D:11:LEU:HD21	2:D:45:ILE:HG12	1.73	0.69
4:H:403:LEU:HD22	4:H:420:THR:HG23	1.73	0.69
4:H:421:ALA:HA	4:H:492:THR:HG22	1.75	0.69
4:G:455:ASN:ND2	4:G:489:TYR:O	2.26	0.69
1:B:147:ARG:HH22	5:I:350:LEU:HG	1.58	0.68
1:A:194:ILE:HD13	1:A:227:TYR:HB2	1.75	0.68
3:F:161:ASP:OD2	3:F:163:THR:OG1	2.09	0.68
3:F:236:GLN:HE21	3:F:262:ASP:HA	1.58	0.68
3:F:342:SER:N	3:F:358:ILE:O	2.26	0.68
4:G:231:ARG:HH12	4:G:308:VAL:HG11	1.58	0.68
5:J:273:VAL:HG13	5:J:287:ILE:HD12	1.75	0.68
5:I:56:PHE:O	5:I:60:SER:N	2.27	0.68
5:J:96:CYS:SG	5:J:129:ARG:NH1	2.67	0.68
2:D:164:VAL:HB	2:D:229:VAL:HA	1.75	0.68
4:G:177:VAL:HG21	4:G:485:LEU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:ALA:HB3	2:D:251:THR:HG21	1.75	0.68
3:F:231:TYR:HA	3:F:234:ARG:HH21	1.59	0.68
2:C:164:VAL:HG12	2:C:188:HIS:HB2	1.76	0.68
1:B:159:LEU:HD12	1:B:162:LYS:HE3	1.75	0.68
2:C:216:VAL:HB	4:G:484:LEU:HG	1.74	0.68
5:I:344:ARG:HG2	5:I:348:VAL:HG21	1.75	0.68
2:D:152:ALA:HB1	2:D:180:GLU:HG2	1.76	0.68
4:G:428:ARG:NH2	4:G:496:LEU:O	2.27	0.68
4:G:476:TRP:HE1	4:G:484:LEU:HB2	1.59	0.68
4:H:347:GLN:NE2	4:H:375:SER:O	2.27	0.68
1:B:205:GLY:CA	1:B:276:THR:O	2.43	0.67
5:I:133:ASP:OD1	5:I:136:ARG:NH2	2.27	0.67
5:I:47:LEU:HD22	5:I:93:VAL:HG12	1.75	0.67
3:F:86:THR:HG1	3:F:224:ILE:H	1.42	0.67
5:J:383:CYS:SG	5:J:384:HIS:N	2.66	0.67
3:E:132:MET:HA	3:E:201:ASP:HA	1.74	0.67
5:J:168:HIS:HD1	5:J:182:THR:HG1	1.42	0.67
1:A:291:LEU:HB3	1:A:295:ALA:HB3	1.76	0.67
2:C:146:GLY:O	2:C:150:ASN:ND2	2.27	0.67
5:J:106:LEU:HD21	5:J:120:VAL:HG21	1.76	0.67
1:A:23:ALA:HB2	1:A:64:ALA:HB1	1.78	0.66
2:C:250:GLY:N	2:C:314:ASP:OD2	2.26	0.66
3:E:115:HIS:CD2	4:H:194:GLN:HA	2.30	0.66
4:H:337:GLY:HA2	4:H:369:GLY:HA2	1.78	0.66
1:A:207:ILE:HG22	1:A:273:VAL:HG12	1.77	0.66
2:D:345:HIS:ND1	2:D:347:ASP:OD1	2.28	0.66
4:G:364:ARG:NH2	4:G:463:LEU:O	2.22	0.66
5:I:196:CYS:HB3	5:I:304:HIS:CE1	2.30	0.66
3:E:424:CYS:HA	3:E:441:GLU:HA	1.77	0.66
2:C:158:HIS:HE1	2:C:323:LEU:HD21	1.61	0.66
3:E:208:LYS:HG3	3:E:209:LYS:H	1.60	0.66
3:E:268:LYS:HD3	3:E:269:GLU:H	1.60	0.66
3:F:224:ILE:HA	3:F:228:LEU:HD13	1.76	0.65
3:F:376:GLY:HA3	3:F:394:ASN:HA	1.77	0.65
3:F:29:PRO:HA	3:F:35:LEU:H	1.61	0.65
5:J:205:VAL:HG11	5:J:289:MET:HE3	1.78	0.65
2:C:288:PHE:CE1	2:C:311:PRO:HB3	2.32	0.65
1:A:70:GLU:OE2	1:A:74:ARG:NE	2.29	0.65
5:I:241:ARG:HD3	5:I:244:LEU:HD21	1.79	0.65
5:I:155:VAL:HG11	5:I:249:ILE:HD11	1.79	0.65
3:E:91:ARG:HG3	3:E:216:MET:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:170:ARG:H	4:H:265:GLN:HE21	1.44	0.64
5:J:195:ARG:NH1	5:J:243:ASP:O	2.30	0.64
1:B:223:ASN:ND2	4:G:429:ALA:O	2.30	0.64
2:C:170:PHE:CD1	2:C:203:MET:HB2	2.32	0.64
3:E:186:ILE:HD11	3:E:237:PHE:CD1	2.32	0.64
1:B:214:GLN:HG3	1:B:215:MET:H	1.62	0.64
4:H:405:ALA:HB3	4:H:438:CYS:HB2	1.80	0.64
1:A:208:ASN:OD1	1:A:209:LYS:N	2.31	0.64
2:C:134:ILE:O	2:C:138:ASN:ND2	2.31	0.64
5:I:70:LEU:HD12	5:I:75:LEU:HD21	1.80	0.64
2:D:46:ILE:HD12	2:D:57:LEU:HD21	1.80	0.63
5:J:139:ASP:HB2	5:J:257:ALA:HB1	1.80	0.63
5:I:44:GLN:HA	5:I:90:GLU:HB2	1.81	0.63
3:F:127:SER:N	3:F:262:ASP:O	2.31	0.63
4:H:397:GLU:OE2	5:J:339:ARG:NH1	2.32	0.63
5:I:211:ARG:HD2	5:I:286:GLN:HG3	1.80	0.63
1:B:121:ASP:OD1	1:B:147:ARG:N	2.31	0.63
2:D:284:SER:HB3	5:J:337:HIS:HB3	1.79	0.63
4:G:362:ASP:OD1	4:G:363:SER:N	2.30	0.63
3:E:91:ARG:NH2	3:E:218:ASN:O	2.31	0.63
4:H:504:LEU:HD11	6:L:56:ARG:HA	1.81	0.62
5:I:139:ASP:HB2	5:I:257:ALA:HB1	1.81	0.62
4:G:291:LYS:HB3	4:G:295:GLU:HB2	1.81	0.62
5:J:110:LYS:HD3	5:J:328:THR:HA	1.79	0.62
2:C:11:LEU:HA	2:C:44:GLN:HE21	1.64	0.62
2:D:241:ALA:HA	2:D:340:MET:HE3	1.82	0.62
3:E:64:CYS:SG	3:E:65:ALA:N	2.73	0.62
4:G:416:SER:O	4:G:489:TYR:HA	1.99	0.62
5:I:435:VAL:HG21	5:I:450:SER:HA	1.81	0.62
3:F:39:PRO:HG2	3:F:106:CYS:HA	1.82	0.62
5:I:255:GLN:HA	5:I:258:GLN:HB3	1.81	0.62
2:D:195:ALA:HB3	4:H:389:PRO:HG2	1.82	0.62
4:G:214:TYR:OH	4:G:225:ARG:O	2.17	0.62
5:J:195:ARG:NH1	5:J:244:LEU:O	2.33	0.62
1:B:202:GLU:HB2	1:B:239:PHE:HD1	1.65	0.62
1:A:214:GLN:NE2	1:B:181:ALA:O	2.33	0.62
5:I:359:ASN:HB2	5:I:376:ASN:HA	1.79	0.62
5:J:130:SER:OG	5:J:267:GLN:OE1	2.11	0.62
4:G:202:VAL:HG13	4:G:203:ILE:HG12	1.81	0.62
2:C:80:ASN:ND2	2:C:272:PHE:O	2.24	0.61
4:G:333:ILE:HG22	4:G:334:LEU:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HD21	1:B:49:LEU:HD21	1.81	0.61
5:J:168:HIS:ND1	5:J:182:THR:OG1	2.34	0.61
1:A:20:MET:HE3	1:A:25:ALA:HB2	1.83	0.61
1:B:293:PRO:O	1:B:296:VAL:HG12	2.01	0.61
5:I:70:LEU:HD21	5:I:310:CYS:HA	1.82	0.61
2:C:225:VAL:HA	4:G:452:PHE:HZ	1.66	0.61
3:F:72:LYS:HD2	3:F:73:PRO:HD2	1.81	0.61
5:I:61:LYS:HD2	5:I:452:HIS:CE1	2.35	0.61
1:B:67:SER:OG	1:B:235:PHE:O	2.18	0.61
3:E:157:PHE:O	3:E:170:MET:HA	2.00	0.61
6:K:76:ASP:O	6:K:80:GLY:N	2.32	0.61
4:H:490:ASP:OD2	4:H:491:VAL:N	2.30	0.61
1:B:222:GLN:HB3	4:G:431:ASN:ND2	2.16	0.60
3:E:178:GLU:HA	5:J:228:LEU:HD23	1.83	0.60
4:G:362:ASP:OD2	4:G:369:GLY:N	2.34	0.60
5:I:451:LEU:HA	5:I:460:GLU:HB2	1.83	0.60
2:D:85:VAL:HG13	2:D:137:ILE:HD11	1.83	0.60
5:J:368:ILE:HG22	5:J:369:GLY:H	1.65	0.60
1:A:57:CYS:HG	1:A:66:SER:HG	1.48	0.60
5:I:286:GLN:OE1	5:I:286:GLN:N	2.30	0.60
3:F:233:VAL:HG22	3:F:263:ILE:HG21	1.84	0.60
2:C:46:ILE:HG13	2:C:57:LEU:HD11	1.82	0.60
5:J:435:VAL:HG22	5:J:460:GLU:HB3	1.84	0.60
3:F:157:PHE:HB2	3:F:197:THR:HG22	1.82	0.60
3:F:179:GLU:HA	5:I:226:PHE:O	2.02	0.60
3:E:114:LEU:HD13	3:E:204:LEU:HD11	1.83	0.60
4:G:214:TYR:HD2	4:G:263:LEU:HD11	1.67	0.60
4:H:358:VAL:HG11	4:H:376:LEU:HD13	1.84	0.60
4:H:365:PRO:HD2	4:H:366:TRP:HD1	1.66	0.60
6:L:138:ASP:HA	6:L:147:GLY:HA3	1.83	0.60
1:A:19:ASP:OD1	1:A:20:MET:N	2.35	0.60
2:C:217:MET:HB3	4:G:485:LEU:HD21	1.84	0.60
3:E:57:ARG:HB2	3:E:82:ALA:HA	1.83	0.60
4:H:435:LEU:HG	4:H:499:LEU:HB2	1.84	0.60
4:H:227:ILE:HD11	4:H:312:ILE:HD11	1.83	0.59
5:I:84:THR:OG1	5:I:111:TRP:NE1	2.32	0.59
5:I:374:ILE:HD13	5:I:391:LEU:HB2	1.83	0.59
3:F:224:ILE:HG12	3:F:228:LEU:HD22	1.83	0.59
4:H:347:GLN:NE2	4:H:375:SER:OG	2.28	0.59
4:H:362:ASP:OD2	4:H:368:GLU:N	2.36	0.59
1:A:89:CYS:O	1:A:93:MET:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:237:LYS:HD3	2:C:313:PHE:CZ	2.36	0.59
5:I:316:ARG:NH2	5:I:324:GLU:OE2	2.26	0.59
1:B:213:ASN:O	1:B:216:ALA:HB3	2.03	0.59
5:J:132:GLY:C	5:J:136:ARG:HE	2.10	0.59
2:D:164:VAL:HA	2:D:188:HIS:HB2	1.83	0.59
5:J:47:LEU:HD23	5:J:93:VAL:HG22	1.85	0.59
4:G:336:TYR:HE1	4:G:388:ILE:HD12	1.67	0.59
5:I:359:ASN:ND2	5:I:376:ASN:OD1	2.36	0.59
5:J:248:HIS:C	5:J:250:SER:H	2.10	0.59
3:E:110:THR:HA	3:E:271:ASN:HB2	1.84	0.59
5:I:54:ARG:HH21	5:I:97:TRP:HD1	1.49	0.59
5:I:414:CYS:HB3	5:I:432:THR:HA	1.84	0.59
2:D:189:VAL:HG13	2:D:214:THR:HA	1.83	0.59
3:F:157:PHE:CE2	3:F:180:LEU:HD11	2.38	0.59
5:I:160:ASN:O	5:I:163:ARG:NH2	2.35	0.59
5:J:307:SER:HA	5:J:395:TYR:HE2	1.66	0.59
1:A:37:ASP:OD1	1:A:37:ASP:N	2.34	0.58
5:J:214:HIS:NE2	5:J:216:GLN:OE1	2.33	0.58
3:E:110:THR:HG23	3:E:271:ASN:HB2	1.85	0.58
3:E:377:SER:H	3:E:394:ASN:HA	1.68	0.58
5:J:61:LYS:O	5:J:98:LYS:NZ	2.33	0.58
3:F:91:ARG:HG3	3:F:216:MET:HG2	1.86	0.58
3:F:120:LEU:HD21	3:F:266:PHE:HB2	1.85	0.58
1:B:208:ASN:ND2	1:B:212:THR:OG1	2.37	0.58
2:C:192:ALA:HB2	2:C:217:MET:HE3	1.83	0.58
2:C:225:VAL:HA	4:G:452:PHE:CZ	2.38	0.58
5:I:381:PRO:HG2	5:I:398:GLN:HG2	1.84	0.58
2:D:223:PHE:HD2	4:H:421:ALA:HB1	1.68	0.58
3:F:91:ARG:NH2	3:F:218:ASN:O	2.30	0.58
5:J:67:LEU:HD23	5:J:102:ILE:HG12	1.85	0.58
1:A:287:ASP:OD1	1:A:287:ASP:N	2.32	0.58
5:J:302:ASN:OD1	5:J:305:MET:N	2.34	0.58
5:J:165:LEU:HD21	5:J:169:ARG:HH22	1.68	0.58
3:F:157:PHE:HE2	3:F:180:LEU:HD11	1.68	0.58
4:G:349:ALA:O	4:G:354:ARG:HB3	2.04	0.58
5:I:84:THR:HA	5:I:118:ASN:HD22	1.69	0.58
2:C:158:HIS:CE1	2:C:323:LEU:HD21	2.39	0.57
2:C:180:GLU:HG2	2:C:183:ARG:HH12	1.69	0.57
4:G:322:PHE:O	4:G:325:GLN:NE2	2.36	0.57
5:J:130:SER:N	5:J:133:ASP:OD2	2.37	0.57
1:B:80:SER:OG	6:L:49:GLU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:279:PRO:HB3	2:C:315:TYR:CE2	2.39	0.57
2:D:43:ARG:HB2	2:D:137:ILE:HG21	1.86	0.57
2:D:51:TRP:CE2	2:D:57:LEU:HD22	2.39	0.57
4:H:341:LEU:O	4:H:345:ILE:HG12	2.04	0.57
2:C:207:LEU:HB3	2:C:212:ILE:HG21	1.87	0.57
1:A:98:GLU:HB3	1:A:102:ARG:HH12	1.68	0.57
4:G:334:LEU:HB2	4:G:398:VAL:HG11	1.86	0.57
4:H:207:MET:HG3	4:H:259:TYR:CG	2.40	0.57
4:H:215:SER:OG	4:H:216:GLN:OE1	2.17	0.57
1:B:118:PHE:O	2:C:280:ASN:ND2	2.36	0.57
3:F:93:ILE:HD11	3:F:96:LYS:HD3	1.87	0.57
4:H:334:LEU:HD12	4:H:398:VAL:HG21	1.87	0.57
2:D:227:SER:OG	2:D:228:ARG:NH1	2.38	0.57
2:D:271:MET:HE3	2:D:343:LEU:HD11	1.87	0.57
3:E:84:MET:HG2	3:E:88:ASP:HB3	1.86	0.57
5:I:364:SER:O	5:I:382:GLY:N	2.38	0.57
5:I:420:LYS:HD2	5:I:438:GLY:HA2	1.86	0.57
5:I:426:LYS:HG2	5:I:427:PRO:HD2	1.86	0.57
1:A:43:GLN:HG2	1:A:44:GLY:H	1.70	0.57
1:B:203:ASN:HA	4:H:508:PRO:HG3	1.86	0.57
5:J:171:ARG:HD3	5:J:288:HIS:CD2	2.39	0.57
3:E:186:ILE:O	3:E:190:HIS:N	2.34	0.57
4:G:340:SER:O	4:G:343:SER:OG	2.21	0.57
5:I:149:LEU:HD23	5:I:251:ILE:HG23	1.86	0.57
2:C:306:VAL:HG11	4:G:373:LEU:HD21	1.87	0.56
2:C:338:ARG:HH11	4:H:518:VAL:HG21	1.70	0.56
3:E:132:MET:HE3	3:E:201:ASP:HB3	1.86	0.56
4:H:408:LEU:HD22	4:H:414:VAL:HG22	1.86	0.56
5:J:94:PHE:HE1	5:J:123:ILE:HD12	1.69	0.56
1:A:49:LEU:HB3	1:A:73:LEU:HD21	1.86	0.56
3:E:285:CYS:O	3:E:288:ASP:HB3	2.04	0.56
4:G:440:THR:OG1	4:G:503:GLU:OE1	2.21	0.56
1:B:81:LEU:O	1:B:88:LYS:NZ	2.39	0.56
5:I:239:GLU:OE2	5:I:241:ARG:NH2	2.37	0.56
5:J:72:ASN:HD21	5:J:380:GLY:HA2	1.69	0.56
1:B:163:LYS:HA	1:B:166:LYS:HE2	1.88	0.56
3:F:41:ASN:HA	3:F:44:GLU:HG2	1.87	0.56
3:F:133:ARG:HE	3:F:269:GLU:C	2.14	0.56
5:J:307:SER:HA	5:J:395:TYR:CE2	2.41	0.56
1:B:213:ASN:HA	1:B:276:THR:HG22	1.87	0.56
2:C:188:HIS:HA	2:C:213:GLU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:293:GLU:HG3	4:G:467:ARG:NH1	2.21	0.56
5:I:311:ALA:O	5:I:315:ARG:NH1	2.38	0.56
5:J:459:ASP:HB3	5:J:467:ASP:HB3	1.87	0.56
4:H:366:TRP:CD1	4:H:366:TRP:H	2.24	0.56
5:J:72:ASN:ND2	5:J:380:GLY:HA2	2.21	0.56
2:C:84:ARG:HH22	2:C:272:PHE:HA	1.71	0.56
4:H:414:VAL:HG21	4:H:436:VAL:HG21	1.88	0.56
3:E:97:LEU:HD12	3:E:101:VAL:HG12	1.87	0.56
4:G:335:VAL:HG13	4:G:342:VAL:HG11	1.86	0.56
4:H:177:VAL:HG21	4:H:485:LEU:HD13	1.87	0.56
5:J:391:LEU:HD23	5:J:394:THR:HG21	1.88	0.56
2:D:158:HIS:HE1	2:D:323:LEU:HD21	1.71	0.56
5:J:43:LEU:HD21	5:J:149:LEU:HD13	1.87	0.56
5:J:111:TRP:CD1	5:J:118:ASN:HB3	2.36	0.56
5:J:132:GLY:O	5:J:136:ARG:NE	2.26	0.56
3:F:72:LYS:HG3	3:F:74:ASP:H	1.71	0.55
3:E:4:GLN:HE22	3:E:98:LYS:H	1.54	0.55
4:G:170:ARG:NH2	4:G:266:CYS:O	2.39	0.55
1:A:64:ALA:HB2	1:A:234:LYS:HE2	1.88	0.55
1:B:202:GLU:HB2	1:B:239:PHE:CD1	2.42	0.55
2:C:87:LYS:NZ	2:C:342:GLU:O	2.39	0.55
2:C:265:LEU:N	2:C:322:THR:OG1	2.39	0.55
3:E:95:PRO:O	3:E:98:LYS:NZ	2.36	0.55
3:F:167:LEU:HB3	3:F:265:SER:OG	2.05	0.55
2:C:15:ILE:HD13	2:C:41:LEU:HD21	1.88	0.55
3:F:40:LEU:HD22	3:F:70:LYS:HD3	1.88	0.55
5:I:183:MET:N	5:I:288:HIS:O	2.27	0.55
5:I:312:ASP:O	5:I:317:TRP:HB2	2.06	0.55
5:J:310:CYS:SG	5:J:378:VAL:HG21	2.47	0.55
1:A:195:VAL:O	1:A:228:VAL:HA	2.06	0.55
2:C:178:LEU:HD22	2:C:187:PHE:CZ	2.42	0.55
2:C:346:PRO:HA	2:C:349:HIS:NE2	2.21	0.55
2:D:51:TRP:CG	2:D:57:LEU:HD13	2.42	0.55
4:G:324:TYR:CE1	4:G:354:ARG:HD2	2.42	0.55
1:B:200:VAL:HG13	1:B:206:ILE:HG22	1.88	0.55
4:G:322:PHE:HA	4:G:325:GLN:HE22	1.71	0.55
5:I:426:LYS:HB3	5:I:445:GLU:HA	1.87	0.55
2:C:167:THR:OG1	2:C:168:ILE:N	2.40	0.55
2:C:193:GLU:OE1	2:C:201:HIS:NE2	2.40	0.55
2:D:131:SER:HA	2:D:134:ILE:HG22	1.89	0.55
3:E:29:PRO:HB2	3:E:34:PRO:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:187:SER:OG	4:G:189:GLN:NE2	2.40	0.55
5:I:332:THR:O	5:I:364:SER:OG	2.23	0.55
5:J:449:ILE:HG12	5:J:458:GLU:HB2	1.87	0.55
3:F:167:LEU:HD21	3:F:263:ILE:HG12	1.89	0.55
4:H:240:TYR:OH	4:H:251:ASP:OD2	2.25	0.55
1:A:134:VAL:HA	1:A:137:VAL:HG12	1.88	0.54
2:D:42:LEU:HD11	2:D:82:VAL:HG22	1.89	0.54
5:J:375:THR:HG22	5:J:376:ASN:HD22	1.72	0.54
1:A:231:GLU:HG3	1:A:233:PHE:CE2	2.42	0.54
1:A:296:VAL:O	1:A:300:LEU:HB2	2.08	0.54
2:C:27:GLY:HA2	2:C:28:PRO:C	2.32	0.54
3:E:225:ARG:HA	3:E:229:ILE:HD12	1.88	0.54
3:F:4:GLN:HB2	3:F:101:VAL:HA	1.89	0.54
4:G:174:GLY:HA3	4:G:476:TRP:HZ3	1.73	0.54
5:I:443:LEU:HD23	5:I:447:SER:HB3	1.88	0.54
1:A:70:GLU:O	1:A:74:ARG:HG2	2.08	0.54
1:A:202:GLU:O	1:A:297:SER:OG	2.15	0.54
3:F:48:PHE:H	4:G:199:PRO:CG	2.21	0.54
2:D:165:ILE:HG21	2:D:178:LEU:HD11	1.90	0.54
3:E:117:VAL:HG21	3:E:131:LEU:HD12	1.88	0.54
3:F:86:THR:OG1	3:F:224:ILE:N	2.32	0.54
1:B:19:ASP:HA	1:B:132:ARG:HG3	1.90	0.54
3:E:40:LEU:HA	3:E:43:LEU:HD23	1.89	0.54
3:F:176:LEU:HD21	3:F:181:VAL:HG23	1.90	0.54
1:B:150:VAL:HG11	1:B:168:LEU:HD21	1.89	0.54
3:F:110:THR:HG23	3:F:271:ASN:HB2	1.89	0.54
5:I:386:GLY:N	5:I:402:VAL:O	2.41	0.54
5:J:133:ASP:OD1	5:J:136:ARG:NH2	2.41	0.54
1:A:131:SER:O	1:A:134:VAL:HG12	2.08	0.54
2:C:11:LEU:HA	2:C:44:GLN:NE2	2.23	0.54
2:C:129:LEU:HA	2:C:132:ASN:ND2	2.23	0.53
3:E:279:ASP:O	3:E:282:TRP:HB3	2.09	0.53
3:F:160:VAL:HA	3:F:167:LEU:HA	1.89	0.53
2:D:266:ILE:HD12	2:D:323:LEU:HD23	1.90	0.53
4:G:333:ILE:HG22	4:G:334:LEU:N	2.23	0.53
4:G:512:VAL:N	4:G:513:PRO:HD2	2.23	0.53
4:H:416:SER:OG	4:H:417:ARG:N	2.41	0.53
5:I:323:PRO:HD2	5:I:343:TYR:HE2	1.73	0.53
2:D:239:ILE:HG22	2:D:240:LEU:H	1.73	0.53
3:E:37:TRP:HE3	3:E:38:TYR:HD1	1.55	0.53
3:E:282:TRP:O	3:E:286:ARG:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:133:ARG:HE	3:F:270:ALA:N	2.06	0.53
3:F:133:ARG:HH21	3:F:272:THR:HG23	1.72	0.53
5:I:295:GLU:OE1	5:I:295:GLU:N	2.39	0.53
1:A:205:GLY:HA3	1:A:276:THR:O	2.09	0.53
1:B:188:GLU:OE2	1:B:189:LYS:NZ	2.29	0.53
4:G:426:VAL:HG12	4:G:430:HIS:HD2	1.73	0.53
4:H:238:GLN:HA	4:H:297:LYS:HD3	1.90	0.53
5:I:377:SER:HB2	5:I:394:THR:HG23	1.89	0.53
5:I:416:ASN:HB3	5:I:434:GLN:HG3	1.90	0.53
5:J:342:ILE:HG22	5:J:360:VAL:HG22	1.90	0.53
2:D:304:GLU:OE2	2:D:305:LYS:NZ	2.36	0.53
4:G:365:PRO:O	4:G:367:LEU:N	2.41	0.53
4:H:319:ILE:HG22	4:H:345:ILE:HD11	1.89	0.53
5:I:86:THR:OG1	5:I:161:ILE:HG12	2.09	0.53
3:E:124:TYR:OH	3:E:165:LYS:NZ	2.38	0.53
3:F:132:MET:HG2	3:F:201:ASP:HA	1.90	0.53
5:I:410:GLN:HB3	5:I:427:PRO:HA	1.90	0.53
5:I:205:VAL:HG21	5:I:289:MET:HE3	1.89	0.53
2:C:130:GLN:O	2:C:134:ILE:HG12	2.08	0.53
4:G:249:SER:OG	4:G:285:THR:HA	2.09	0.53
5:J:247:CYS:HB3	5:J:249:ILE:HG12	1.91	0.53
2:D:156:LEU:O	2:D:185:ARG:NH2	2.41	0.53
4:H:503:GLU:OE1	4:H:503:GLU:N	2.36	0.53
1:B:214:GLN:HG3	1:B:215:MET:N	2.24	0.53
2:C:28:PRO:HB3	2:C:33:GLU:HG2	1.91	0.53
2:C:166:MET:O	2:C:232:VAL:HA	2.09	0.53
2:C:317:PRO:HG2	2:C:320:LEU:HG	1.91	0.53
2:D:223:PHE:CD2	4:H:421:ALA:HB1	2.44	0.52
3:E:162:SER:HB2	3:E:192:ARG:HB2	1.90	0.52
4:G:261:SER:O	4:G:265:GLN:HG2	2.09	0.52
4:H:210:LEU:HD11	4:H:228:ALA:HB1	1.89	0.52
5:I:48:VAL:HG12	5:I:134:VAL:HG11	1.90	0.52
5:I:54:ARG:HH21	5:I:97:TRP:CD1	2.26	0.52
5:I:212:VAL:HG23	5:I:289:MET:HB2	1.91	0.52
5:J:146:SER:HA	5:J:254:PRO:HD3	1.89	0.52
5:J:268:THR:HG22	5:J:270:ASP:H	1.74	0.52
5:J:401:ARG:HB3	5:J:418:GLU:HG2	1.91	0.52
2:C:227:SER:C	2:C:228:ARG:HD2	2.34	0.52
3:F:8:MET:HE2	3:F:86:THR:HA	1.91	0.52
4:G:336:TYR:CE1	4:G:419:GLY:HA3	2.44	0.52
6:K:20:MET:HA	6:K:69:CYS:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:PRO:HB3	2:D:308:VAL:HB	1.92	0.52
5:I:435:VAL:HG22	5:I:460:GLU:HG3	1.91	0.52
2:D:80:ASN:OD1	2:D:81:MET:N	2.42	0.52
2:D:88:ILE:HD12	2:D:136:ALA:HB1	1.89	0.52
3:F:280:ALA:HA	3:F:283:ASN:HD21	1.74	0.52
3:F:420:ASP:O	3:F:437:LYS:N	2.41	0.52
5:I:189:SER:O	5:I:191:SER:N	2.43	0.52
1:A:10:PHE:HD1	1:A:29:THR:HG21	1.74	0.52
3:E:4:GLN:HE21	3:E:99:THR:HG22	1.75	0.52
3:E:289:ARG:HD3	3:E:372:ARG:HA	1.92	0.52
3:E:50:GLU:OE2	3:E:52:ILE:N	2.42	0.52
3:E:173:GLU:N	3:E:173:GLU:OE1	2.42	0.52
5:I:70:LEU:HD11	5:I:309:VAL:HG13	1.92	0.52
1:B:130:TYR:HA	1:B:164:MET:HB2	1.90	0.52
2:D:164:VAL:HG12	2:D:229:VAL:HG13	1.92	0.52
4:G:261:SER:O	4:G:264:THR:OG1	2.24	0.52
4:G:463:LEU:HD12	4:G:484:LEU:HD23	1.92	0.52
5:I:89:GLN:O	5:I:119:VAL:HG22	2.10	0.52
5:I:202:VAL:HG21	5:I:224:PHE:CE1	2.45	0.52
5:J:144:VAL:HG11	5:J:148:PHE:CD1	2.45	0.52
3:F:5:ALA:HB2	3:F:48:PHE:CD1	2.45	0.52
5:J:323:PRO:HG2	5:J:343:TYR:HE2	1.74	0.52
2:D:228:ARG:HD3	4:H:452:PHE:CE2	2.45	0.52
3:E:183:LYS:HD3	3:E:237:PHE:HE2	1.75	0.52
4:G:376:LEU:HD22	4:G:381:VAL:HG11	1.91	0.52
5:I:128:TYR:HB2	5:I:133:ASP:OD2	2.10	0.52
1:B:158:ASP:N	1:B:158:ASP:OD1	2.42	0.51
2:C:204:ALA:HA	2:C:214:THR:HG21	1.91	0.51
3:E:50:GLU:OE2	3:E:52:ILE:HG13	2.10	0.51
3:F:162:SER:OG	3:F:192:ARG:O	2.20	0.51
5:I:368:ILE:HD13	5:I:385:ILE:HG13	1.92	0.51
1:A:231:GLU:CD	1:A:231:GLU:H	2.17	0.51
2:C:236:THR:OG1	2:C:238:THR:O	2.27	0.51
4:H:336:TYR:HE1	4:H:388:ILE:HD12	1.75	0.51
1:A:203:ASN:HB3	1:A:239:PHE:CZ	2.46	0.51
1:B:71:LEU:HB2	1:B:304:TYR:HE1	1.76	0.51
5:I:188:SER:OG	5:I:189:SER:N	2.43	0.51
5:J:286:GLN:H	5:J:286:GLN:CD	2.18	0.51
1:B:125:ILE:HG21	1:B:138:LEU:HD11	1.92	0.51
3:E:133:ARG:N	3:E:200:VAL:O	2.43	0.51
4:H:312:ILE:HG22	4:H:441:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:TYR:O	2:D:128:GLN:N	2.44	0.51
3:E:40:LEU:O	3:E:43:LEU:HB2	2.10	0.51
3:F:36:ILE:HG23	3:F:106:CYS:SG	2.50	0.51
5:I:394:THR:OG1	5:I:395:TYR:N	2.43	0.51
2:C:228:ARG:HH12	2:D:160:HIS:CE1	2.29	0.51
5:I:117:LEU:HD23	5:I:117:LEU:H	1.76	0.51
1:A:283:LEU:HD11	2:D:242:ASN:HD21	1.74	0.51
3:F:107:ASP:O	3:F:273:LEU:HB2	2.10	0.51
4:G:307:TYR:CE1	4:G:311:LYS:HG3	2.46	0.51
5:I:78:TYR:HD1	5:I:321:LEU:HD23	1.76	0.51
5:I:375:THR:HG22	5:I:376:ASN:HD22	1.75	0.51
2:C:228:ARG:HH12	2:D:160:HIS:HE1	1.57	0.51
2:D:84:ARG:CZ	2:D:140:LEU:HD11	2.41	0.51
3:F:291:GLU:HA	3:F:295:ARG:NH2	2.26	0.51
4:H:438:CYS:SG	4:H:442:LYS:HB2	2.50	0.51
1:A:206:ILE:HD11	1:A:212:THR:HG21	1.93	0.51
1:B:23:ALA:HB3	1:B:233:PHE:CE2	2.41	0.51
1:B:203:ASN:HB3	1:B:239:PHE:CZ	2.46	0.51
3:E:41:ASN:O	3:E:45:ARG:N	2.44	0.51
4:G:251:ASP:OD1	4:G:252:LEU:N	2.43	0.51
5:J:167:GLU:OE1	5:J:290:HIS:NE2	2.42	0.51
5:J:185:PHE:HB2	5:J:291:VAL:HG22	1.92	0.51
6:K:14:GLU:O	6:K:17:ASP:CB	2.59	0.51
1:A:131:SER:O	1:A:134:VAL:N	2.44	0.51
4:G:174:GLY:HA3	4:G:476:TRP:CZ3	2.46	0.51
5:J:158:ASN:ND2	5:J:318:VAL:O	2.44	0.51
3:E:91:ARG:HG3	3:E:216:MET:HA	1.93	0.50
3:F:203:HIS:HA	3:F:205:TYR:CZ	2.45	0.50
3:F:221:ILE:HG23	3:F:227:GLU:HB2	1.93	0.50
5:I:425:LEU:HB3	5:I:429:SER:OG	2.11	0.50
5:J:61:LYS:HA	5:J:97:TRP:HH2	1.75	0.50
2:C:10:GLU:O	2:C:13:GLU:HG3	2.11	0.50
3:E:55:THR:OG1	3:E:78:ILE:O	2.22	0.50
2:C:63:ARG:NE	2:C:64:GLU:OE2	2.40	0.50
2:C:220:ALA:HB2	4:G:388:ILE:HG21	1.94	0.50
4:H:456:GLU:HB2	4:H:488:VAL:HG22	1.94	0.50
1:A:19:ASP:HB2	1:A:132:ARG:CZ	2.41	0.50
3:F:155:ARG:HA	3:F:173:GLU:OE1	2.12	0.50
5:J:73:VAL:HB	5:J:78:TYR:HE1	1.76	0.50
3:F:42:LEU:O	3:F:46:VAL:HG12	2.11	0.50
3:F:121:PHE:HB2	3:F:129:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:257:LYS:NZ	4:H:281:ASN:HD21	2.09	0.50
5:I:88:VAL:O	5:I:118:ASN:ND2	2.45	0.50
1:B:104:ILE:HD12	1:B:233:PHE:CD1	2.46	0.50
2:C:188:HIS:HB3	2:C:213:GLU:OE1	2.12	0.50
2:C:286:HIS:ND1	2:C:313:PHE:O	2.39	0.50
3:F:94:TYR:CG	3:F:216:MET:HG3	2.46	0.50
3:F:130:MET:HE2	3:F:132:MET:HE3	1.93	0.50
3:F:285:CYS:SG	3:F:289:ARG:NE	2.82	0.50
5:I:95:CYS:HB2	5:I:99:ALA:HB1	1.93	0.50
1:A:213:ASN:ND2	1:B:184:GLY:O	2.45	0.50
2:D:225:VAL:HA	4:H:452:PHE:HZ	1.76	0.50
3:F:56:THR:H	3:F:67:PHE:HE2	1.60	0.50
4:G:416:SER:OG	4:G:420:THR:OG1	2.05	0.50
1:A:43:GLN:NE2	6:K:81:TYR:O	2.36	0.50
1:A:229:VAL:HA	1:A:285:PHE:HB2	1.92	0.50
3:E:28:LEU:O	3:E:30:VAL:N	2.45	0.50
4:G:511:SER:O	4:G:511:SER:OG	2.30	0.50
1:A:74:ARG:NH2	1:A:304:TYR:O	2.45	0.49
1:A:292:THR:O	1:A:294:SER:N	2.45	0.49
4:H:166:GLN:HE21	4:H:258:PRO:HB3	1.75	0.49
4:H:388:ILE:HG22	4:H:389:PRO:HD3	1.93	0.49
5:I:52:PHE:HD1	5:I:54:ARG:HH12	1.58	0.49
1:A:197:ALA:HB3	1:A:230:ALA:HB2	1.94	0.49
1:B:128:HIS:HB2	1:B:215:MET:HE1	1.95	0.49
4:H:204:HIS:CD2	4:H:236:VAL:HG22	2.47	0.49
5:I:89:GLN:HA	5:I:118:ASN:HA	1.93	0.49
1:B:29:THR:O	1:B:32:GLU:HG3	2.13	0.49
3:E:10:VAL:HG22	3:E:106:CYS:SG	2.51	0.49
3:F:55:THR:CG2	3:F:77:CYS:HB2	2.42	0.49
3:F:394:ASN:O	3:F:411:ASN:HA	2.12	0.49
4:G:176:LYS:HD3	4:G:180:PHE:O	2.12	0.49
4:H:269:LEU:HB3	4:H:273:MET:HB2	1.95	0.49
1:B:210:ILE:HD13	1:B:271:PRO:HG2	1.93	0.49
2:D:74:SER:HA	2:D:246:ARG:HH22	1.77	0.49
2:D:225:VAL:HA	4:H:452:PHE:CZ	2.48	0.49
3:F:203:HIS:O	3:F:203:HIS:ND1	2.44	0.49
4:G:409:LEU:HD13	4:G:448:GLN:HB3	1.94	0.49
5:J:170:LEU:HA	5:J:173:LYS:HG2	1.94	0.49
1:B:124:THR:OG1	1:B:191:ASP:N	2.35	0.49
2:C:300:GLY:HA2	5:I:189:SER:HB2	1.94	0.49
1:A:147:ARG:NH1	1:A:148:PHE:O	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LEU:HD22	1:B:89:CYS:SG	2.53	0.49
2:C:195:ALA:HB1	4:G:387:LEU:HD13	1.94	0.49
3:F:117:VAL:O	3:F:120:LEU:HG	2.12	0.49
5:J:269:ARG:O	5:J:273:VAL:HG23	2.12	0.49
1:A:235:PHE:HZ	1:A:286:THR:HG21	1.78	0.49
4:H:204:HIS:CG	4:H:236:VAL:HG22	2.47	0.49
5:I:352:HIS:H	5:I:370:SER:HA	1.77	0.49
5:I:426:LYS:HD3	5:I:445:GLU:N	2.28	0.49
5:J:248:HIS:CD2	5:J:299:ARG:HD2	2.48	0.49
1:A:159:LEU:HD12	1:A:159:LEU:H	1.78	0.49
1:B:90:LYS:O	1:B:94:ILE:HG12	2.12	0.49
2:C:191:VAL:HG11	2:C:204:ALA:HB2	1.94	0.49
2:D:42:LEU:O	2:D:46:ILE:HG12	2.12	0.49
3:F:191:PRO:HB2	5:I:243:ASP:HB3	1.95	0.49
3:F:201:ASP:OD1	3:F:225:ARG:NH2	2.32	0.49
5:J:281:GLU:HG2	5:J:282:ILE:N	2.27	0.49
1:A:57:CYS:SG	1:A:66:SER:OG	2.60	0.49
2:D:289:VAL:HG22	2:D:290:ALA:H	1.77	0.49
3:F:99:THR:OG1	3:F:100:ASP:N	2.43	0.49
4:H:204:HIS:N	4:H:259:TYR:OH	2.46	0.49
2:C:175:GLU:O	2:C:179:LYS:HG2	2.13	0.49
4:H:196:MET:HE3	4:H:203:ILE:HG13	1.94	0.49
5:I:49:ALA:HB3	5:I:95:CYS:HA	1.95	0.49
5:I:361:LEU:HD23	5:I:362:LEU:N	2.28	0.49
1:B:183:VAL:HG11	1:B:215:MET:HB2	1.95	0.48
3:F:85:GLY:O	3:F:89:SER:N	2.35	0.48
3:F:113:ALA:HB1	3:F:115:HIS:CE1	2.47	0.48
4:H:269:LEU:HB2	4:H:274:HIS:CE1	2.48	0.48
1:A:43:GLN:H	1:A:43:GLN:CD	2.17	0.48
1:A:151:TYR:CD1	1:A:176:THR:HB	2.48	0.48
1:B:201:VAL:HG22	1:B:205:GLY:O	2.13	0.48
3:F:28:LEU:HD23	3:F:35:LEU:HB3	1.95	0.48
4:H:362:ASP:OD2	4:H:369:GLY:N	2.26	0.48
5:J:390:VAL:HB	5:J:407:GLN:HG3	1.94	0.48
1:A:232:SER:HB2	1:A:287:ASP:OD1	2.13	0.48
1:A:242:ASN:HD21	1:A:244:GLN:HB2	1.78	0.48
2:C:24:ARG:NH2	5:I:81:GLU:OE2	2.44	0.48
4:G:471:VAL:HG23	4:G:474:ALA:HB2	1.95	0.48
5:J:109:SER:HB2	5:J:111:TRP:HE3	1.77	0.48
1:A:206:ILE:HG21	1:A:228:VAL:HG11	1.96	0.48
5:J:56:PHE:O	5:J:60:SER:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:203:VAL:HG11	5:J:244:LEU:HD12	1.95	0.48
4:G:175:SER:HB3	4:G:483:ARG:HG2	1.95	0.48
5:J:135:LEU:HD23	5:J:260:PHE:CD2	2.49	0.48
5:J:276:LEU:HD11	5:J:285:ASN:HB2	1.94	0.48
1:B:61:SER:OG	1:B:249:LYS:O	2.20	0.48
1:B:118:PHE:CD2	2:C:280:ASN:HB3	2.49	0.48
1:B:156:GLN:HB2	1:B:180:ASP:OD2	2.14	0.48
1:B:229:VAL:HG12	1:B:285:PHE:HB2	1.95	0.48
4:H:198:ILE:HB	4:H:199:PRO:HD3	1.95	0.48
5:J:47:LEU:HD21	5:J:76:ILE:HD11	1.95	0.48
5:J:185:PHE:CD1	5:J:246:ASP:HA	2.49	0.48
6:L:36:LEU:HA	6:L:40:ASN:H	1.79	0.48
1:B:41:THR:OG1	1:B:42:ILE:N	2.47	0.48
1:B:94:ILE:O	1:B:98:GLU:HG2	2.12	0.48
2:C:271:MET:HE2	2:C:327:ASN:HD21	1.79	0.48
5:J:286:GLN:HG2	5:J:288:HIS:HE1	1.79	0.48
2:D:171:SER:OG	2:D:235:GLY:HA3	2.14	0.48
2:D:336:ILE:O	2:D:339:LEU:N	2.47	0.48
5:I:72:ASN:ND2	5:I:381:PRO:HD3	2.29	0.48
5:J:52:PHE:HD1	5:J:129:ARG:NH2	2.11	0.48
1:B:230:ALA:O	1:B:286:THR:HG22	2.13	0.48
3:E:38:TYR:HB2	3:E:39:PRO:HD3	1.95	0.48
4:G:334:LEU:HD22	4:G:423:LEU:HD21	1.94	0.48
4:G:362:ASP:CG	4:G:369:GLY:H	2.21	0.48
4:H:406:HIS:HB2	4:H:416:SER:HA	1.95	0.48
5:J:419:VAL:HG12	5:J:423:VAL:HG11	1.96	0.48
1:B:241:LEU:HD21	4:H:499:LEU:HD21	1.96	0.48
2:D:28:PRO:HG2	2:D:33:GLU:HG2	1.96	0.48
3:E:166:ARG:HE	3:E:236:GLN:NE2	2.12	0.48
5:J:361:LEU:HD23	5:J:362:LEU:N	2.29	0.48
1:B:218:CYS:O	1:B:221:ALA:HB3	2.14	0.47
2:C:236:THR:OG1	2:C:237:LYS:N	2.47	0.47
2:C:236:THR:HG23	2:C:273:LYS:HD3	1.95	0.47
2:D:24:ARG:HG3	2:D:25:GLY:H	1.79	0.47
3:E:183:LYS:HE2	3:E:183:LYS:HB3	1.67	0.47
1:A:227:TYR:CE1	1:A:283:LEU:HB2	2.49	0.47
3:F:291:GLU:OE1	3:F:295:ARG:NH2	2.42	0.47
5:I:368:ILE:HA	5:I:385:ILE:HB	1.96	0.47
4:G:185:GLN:NE2	4:G:460:PRO:HG3	2.29	0.47
4:G:324:TYR:HE1	4:G:354:ARG:HD2	1.79	0.47
4:H:207:MET:HG3	4:H:259:TYR:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:HG2	1:A:87:SER:HA	1.96	0.47
3:E:281:CYS:O	3:E:284:ALA:HB3	2.14	0.47
4:G:335:VAL:HG12	4:G:336:TYR:N	2.25	0.47
4:G:386:LEU:HD12	4:G:386:LEU:O	2.15	0.47
4:H:186:TYR:HE2	4:H:268:PRO:HG3	1.78	0.47
5:J:131:LEU:HD11	5:J:150:LEU:HD21	1.95	0.47
5:J:360:VAL:HG23	5:J:360:VAL:O	2.15	0.47
2:C:249:THR:HA	2:C:314:ASP:CG	2.39	0.47
3:E:122:ARG:HG2	4:H:209:ARG:NH2	2.30	0.47
4:H:514:VAL:HG23	4:H:515:VAL:HG23	1.97	0.47
5:I:248:HIS:CE1	5:I:299:ARG:HH21	2.33	0.47
5:J:52:PHE:HD1	5:J:129:ARG:HH21	1.62	0.47
1:A:23:ALA:HB3	1:A:233:PHE:CE1	2.50	0.47
1:B:152:VAL:HG11	1:B:165:ALA:HB2	1.96	0.47
1:B:156:GLN:NE2	1:B:156:GLN:O	2.48	0.47
2:D:51:TRP:CE3	2:D:57:LEU:HB2	2.48	0.47
5:J:185:PHE:HD1	5:J:246:ASP:HA	1.80	0.47
1:A:104:ILE:HD12	1:A:233:PHE:HD2	1.80	0.47
2:D:236:THR:OG1	2:D:245:LEU:HD13	2.15	0.47
4:G:326:LYS:O	4:G:400:LYS:HE3	2.15	0.47
4:G:346:LEU:HD13	4:G:358:VAL:HG21	1.97	0.47
5:I:68:LEU:HD22	5:I:397:TRP:HH2	1.80	0.47
5:I:88:VAL:HB	5:I:118:ASN:HD21	1.80	0.47
2:C:52:SER:OG	2:C:53:ASN:N	2.47	0.47
2:D:24:ARG:HG3	2:D:25:GLY:N	2.30	0.47
2:D:158:HIS:CE1	2:D:323:LEU:HD21	2.50	0.47
3:F:104:LEU:HG	3:F:204:LEU:HD12	1.97	0.47
3:F:190:HIS:O	3:F:192:ARG:N	2.48	0.47
4:G:386:LEU:HD11	4:G:394:VAL:HG21	1.97	0.47
4:H:456:GLU:C	4:H:457:LEU:HD12	2.40	0.47
5:I:58:PRO:HG3	5:I:450:SER:OG	2.15	0.47
5:I:133:ASP:N	5:I:136:ARG:HH21	2.13	0.47
2:C:287:LYS:O	2:C:312:VAL:HG22	2.14	0.47
4:H:405:ALA:HB2	4:H:436:VAL:HB	1.97	0.47
1:A:178:VAL:HG11	1:A:186:ILE:HD12	1.97	0.46
1:A:206:ILE:HD12	1:A:208:ASN:HB2	1.96	0.46
2:C:128:GLN:OE1	2:C:128:GLN:N	2.48	0.46
2:D:223:PHE:CD1	4:H:425:LEU:HD22	2.50	0.46
2:D:230:ASN:O	2:D:264:PRO:HD2	2.15	0.46
2:D:276:PRO:HD3	2:D:344:TYR:CE2	2.50	0.46
4:G:264:THR:HG22	4:G:269:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:80:LEU:HD11	5:I:106:LEU:HD11	1.96	0.46
5:I:213:LEU:HB3	5:I:230:LEU:HD21	1.97	0.46
5:J:248:HIS:O	5:J:250:SER:N	2.48	0.46
5:J:302:ASN:HD21	5:J:304:HIS:HB3	1.81	0.46
3:F:38:TYR:HB2	3:F:39:PRO:HD3	1.97	0.46
4:H:170:ARG:NH2	4:H:266:CYS:O	2.37	0.46
4:H:233:LEU:HD21	4:H:260:MET:HE1	1.97	0.46
1:B:52:ALA:HA	1:B:55:THR:HG22	1.97	0.46
2:D:188:HIS:HA	2:D:213:GLU:OE1	2.16	0.46
5:I:180:VAL:HG23	5:I:285:ASN:HB3	1.96	0.46
1:A:243:GLN:HB3	1:B:185:TYR:CD1	2.51	0.46
2:D:191:VAL:HG13	2:D:216:VAL:HA	1.97	0.46
5:I:66:VAL:HA	5:I:154:ASP:OD2	2.16	0.46
5:J:94:PHE:CE1	5:J:123:ILE:HD12	2.48	0.46
5:J:339:ARG:O	5:J:342:ILE:HG12	2.16	0.46
1:A:243:GLN:HB3	1:B:185:TYR:CE1	2.51	0.46
2:C:43:ARG:HA	2:C:46:ILE:HG22	1.97	0.46
2:C:303:LEU:HD22	5:I:317:TRP:HZ2	1.80	0.46
4:G:435:LEU:HD23	4:G:501:ILE:HD11	1.97	0.46
4:G:472:ALA:C	4:G:473:LEU:HD12	2.40	0.46
1:A:197:ALA:HA	1:A:208:ASN:HD22	1.80	0.46
3:F:55:THR:HG23	3:F:77:CYS:HB2	1.98	0.46
4:H:230:LEU:HD21	4:H:276:ALA:HB1	1.98	0.46
5:J:397:TRP:HB2	5:J:414:CYS:HA	1.97	0.46
1:A:208:ASN:CG	1:A:209:LYS:H	2.23	0.46
2:C:86:LEU:O	2:C:90:ARG:HG3	2.16	0.46
2:C:190:ILE:HG12	2:C:215:THR:OG1	2.15	0.46
2:C:197:PHE:HE2	2:C:312:VAL:HG11	1.80	0.46
2:C:265:LEU:HD22	2:C:321:ILE:HD13	1.97	0.46
3:E:105:SER:HB2	3:E:203:HIS:HB3	1.97	0.46
3:E:131:LEU:HD23	3:E:132:MET:N	2.30	0.46
5:J:379:ILE:HG22	5:J:380:GLY:H	1.80	0.46
2:C:170:PHE:HD1	2:C:203:MET:HB2	1.79	0.46
3:E:292:ASP:OD1	3:E:293:LEU:N	2.48	0.46
3:F:134:LYS:HB2	3:F:269:GLU:HG3	1.97	0.46
3:F:182:ILE:HG23	3:F:186:ILE:HD11	1.97	0.46
4:G:327:ILE:O	4:G:354:ARG:HD3	2.16	0.46
5:I:195:ARG:NH2	5:I:200:ASN:OD1	2.49	0.46
5:J:380:GLY:HA3	5:J:398:GLN:HA	1.97	0.46
3:E:224:ILE:HG23	3:E:225:ARG:H	1.80	0.46
4:G:185:GLN:HE21	4:G:460:PRO:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:292:ARG:HG2	4:G:293:GLU:H	1.80	0.46
4:H:251:ASP:N	4:H:251:ASP:OD1	2.49	0.46
4:H:438:CYS:SG	4:H:439:GLU:N	2.89	0.46
5:J:183:MET:HA	5:J:250:SER:HA	1.98	0.46
2:C:298:THR:O	5:I:189:SER:OG	2.34	0.46
3:F:278:TYR:HB3	3:F:281:CYS:HB3	1.97	0.46
1:A:207:ILE:HG22	1:A:273:VAL:CG1	2.45	0.45
3:E:8:MET:O	3:E:106:CYS:HA	2.16	0.45
3:F:63:LEU:HA	3:F:66:GLU:OE1	2.15	0.45
3:F:72:LYS:HE3	3:F:74:ASP:HB3	1.98	0.45
5:I:316:ARG:NH1	5:I:343:TYR:OH	2.48	0.45
5:J:45:ALA:HB3	5:J:88:VAL:HG11	1.97	0.45
1:A:72:PHE:CZ	1:A:76:ILE:HD11	2.51	0.45
1:A:240:PRO:HG2	1:A:275:TYR:CD2	2.51	0.45
1:B:132:ARG:HA	1:B:132:ARG:HD3	1.73	0.45
3:F:60:GLN:C	3:F:61:LYS:HD3	2.41	0.45
4:G:225:ARG:NH2	4:G:489:TYR:OH	2.44	0.45
5:I:300:VAL:HG23	5:I:306:TYR:HB2	1.97	0.45
3:E:132:MET:HB3	3:E:199:LEU:HD12	1.99	0.45
3:E:133:ARG:C	3:E:199:LEU:HD13	2.42	0.45
4:H:202:VAL:HG13	4:H:203:ILE:HG12	1.99	0.45
4:H:393:TYR:O	4:H:396:PRO:HD2	2.16	0.45
4:H:431:ASN:ND2	4:H:431:ASN:O	2.50	0.45
2:D:30:SER:HB3	2:D:172:ARG:NH1	2.32	0.45
2:D:232:VAL:HG21	2:D:258:ALA:HB1	1.98	0.45
2:D:345:HIS:CG	2:D:346:PRO:HD2	2.51	0.45
3:F:288:ASP:HA	3:F:291:GLU:HB2	1.98	0.45
4:G:395:LEU:HD13	4:G:427:ALA:HA	1.98	0.45
4:H:439:GLU:HG2	4:H:442:LYS:HD2	1.98	0.45
4:H:498:ASP:O	4:H:499:LEU:HD22	2.17	0.45
5:I:185:PHE:CE1	5:I:246:ASP:HA	2.52	0.45
5:I:336:THR:O	5:I:336:THR:OG1	2.31	0.45
1:B:104:ILE:HD12	1:B:233:PHE:HD1	1.80	0.45
1:B:145:LYS:HE3	1:B:145:LYS:HB2	1.78	0.45
2:C:339:LEU:HD23	2:C:339:LEU:HA	1.73	0.45
2:D:216:VAL:HB	4:H:484:LEU:CD1	2.47	0.45
3:F:50:GLU:OE2	3:F:51:VAL:N	2.42	0.45
3:F:177:ASP:OD1	3:F:177:ASP:N	2.49	0.45
4:G:180:PHE:CE2	4:G:487:LEU:HD11	2.52	0.45
4:G:387:LEU:HB3	4:G:389:PRO:HD2	1.98	0.45
1:A:200:VAL:HG12	1:A:296:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLU:HA	1:B:302:LYS:HG3	1.97	0.45
2:C:39:LEU:HD12	2:C:39:LEU:HA	1.85	0.45
2:C:180:GLU:HG2	2:C:183:ARG:NH1	2.31	0.45
3:E:209:LYS:HB2	3:E:209:LYS:HE2	1.78	0.45
3:F:279:ASP:OD1	3:F:280:ALA:N	2.48	0.45
4:G:414:VAL:HB	4:G:492:THR:CG2	2.46	0.45
4:H:359:VAL:HG12	4:H:384:SER:OG	2.17	0.45
4:H:366:TRP:CE3	4:H:368:GLU:HG2	2.51	0.45
5:I:444:PRO:O	5:I:447:SER:OG	2.28	0.45
2:D:165:ILE:O	2:D:190:ILE:N	2.45	0.45
1:A:130:TYR:HD1	1:A:164:MET:HB2	1.81	0.45
1:A:180:ASP:OD1	1:A:180:ASP:N	2.48	0.45
2:C:39:LEU:HD23	2:C:141:LEU:HB2	1.99	0.45
2:C:219:ASP:OD1	2:C:219:ASP:N	2.47	0.45
2:D:61:ILE:HD13	2:D:61:ILE:HA	1.82	0.45
3:F:107:ASP:HB3	3:F:274:ASN:O	2.16	0.45
3:F:229:ILE:O	3:F:233:VAL:HG23	2.17	0.45
4:G:422:GLN:O	4:G:426:VAL:HG23	2.17	0.45
4:G:476:TRP:NE1	4:G:484:LEU:HD13	2.32	0.45
4:H:231:ARG:HA	4:H:231:ARG:HD3	1.70	0.45
4:H:366:TRP:CZ3	4:H:368:GLU:HG2	2.52	0.45
5:I:431:LEU:O	5:I:432:THR:OG1	2.34	0.45
5:J:165:LEU:HG	5:J:169:ARG:HH12	1.81	0.45
5:J:248:HIS:C	5:J:250:SER:N	2.74	0.45
5:J:186:LYS:HD2	5:J:187:GLU:O	2.17	0.45
1:A:183:VAL:O	1:A:187:MET:HB2	2.17	0.45
4:G:388:ILE:N	4:G:389:PRO:HD2	2.31	0.45
4:H:308:VAL:O	4:H:312:ILE:HG12	2.17	0.45
4:H:388:ILE:C	4:H:390:ALA:H	2.25	0.45
4:H:456:GLU:HB2	4:H:488:VAL:CG2	2.46	0.45
5:I:136:ARG:HG2	5:I:261:THR:HG23	1.98	0.45
2:D:74:SER:HB2	2:D:287:LYS:HD3	1.98	0.44
3:E:262:ASP:HB3	3:E:264:TYR:CE1	2.52	0.44
3:F:57:ARG:HD3	3:F:84:MET:HB2	1.99	0.44
4:G:485:LEU:HD23	4:G:485:LEU:H	1.82	0.44
5:I:177:ASN:HB3	5:I:255:GLN:HE22	1.82	0.44
5:J:144:VAL:HG11	5:J:148:PHE:HD1	1.82	0.44
1:A:158:ASP:O	1:A:160:SER:N	2.48	0.44
2:C:287:LYS:HE2	2:C:312:VAL:HG21	2.00	0.44
4:G:381:VAL:O	4:G:383:ALA:N	2.51	0.44
4:H:188:ARG:NH1	4:H:459:ASP:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:269:LEU:HD12	4:H:274:HIS:CE1	2.52	0.44
5:J:75:LEU:HD23	5:J:156:ILE:HD11	1.97	0.44
5:J:244:LEU:HD11	5:J:289:MET:HE2	2.00	0.44
2:C:228:ARG:HH22	2:D:160:HIS:CE1	2.35	0.44
2:D:304:GLU:HB3	5:J:193:PRO:HG2	1.98	0.44
3:F:60:GLN:NE2	3:F:63:LEU:HG	2.31	0.44
3:F:130:MET:HE1	3:F:229:ILE:HG21	1.98	0.44
5:I:103:LYS:O	5:I:106:LEU:N	2.50	0.44
1:B:149:SER:HA	1:B:174:PRO:HG2	1.99	0.44
2:C:175:GLU:HB2	2:C:179:LYS:NZ	2.33	0.44
2:D:259:LYS:HD3	2:D:320:LEU:HD22	1.99	0.44
2:D:330:GLY:HA3	4:G:447:VAL:HG11	1.99	0.44
5:J:55:ARG:H	5:J:65:ARG:NH1	2.15	0.44
6:L:91:PRO:HA	6:L:94:ALA:HB3	1.99	0.44
2:D:142:VAL:O	2:D:145:GLU:HG3	2.17	0.44
5:J:450:SER:OG	5:J:456:ALA:HB2	2.17	0.44
1:A:180:ASP:O	1:A:183:VAL:HG23	2.18	0.44
1:B:18:PRO:HB2	1:B:130:TYR:OH	2.17	0.44
1:B:158:ASP:O	1:B:160:SER:N	2.50	0.44
1:B:205:GLY:H	1:B:278:PRO:HB3	1.83	0.44
3:E:4:GLN:NE2	3:E:99:THR:H	2.16	0.44
3:F:7:VAL:HG13	3:F:54:VAL:HG12	1.99	0.44
4:H:172:ASP:OD1	4:H:185:GLN:HB3	2.17	0.44
4:H:334:LEU:HB3	4:H:401:VAL:HG22	2.00	0.44
1:A:118:PHE:HZ	2:D:278:PHE:HB3	1.83	0.44
2:D:89:ILE:HD13	2:D:133:ILE:HG12	1.99	0.44
2:D:166:MET:SD	2:D:222:ILE:HD12	2.58	0.44
2:D:224:ALA:HB2	4:H:490:ASP:OD1	2.18	0.44
3:E:42:LEU:HA	3:E:45:ARG:HB2	2.00	0.44
3:E:202:ALA:C	3:E:204:LEU:H	2.26	0.44
4:H:500:VAL:HB	4:H:507:ILE:HG13	2.00	0.44
5:I:184:ILE:HA	5:I:290:HIS:O	2.18	0.44
5:I:196:CYS:SG	5:I:198:GLU:HG2	2.57	0.44
5:J:90:GLU:HB3	5:J:92:PHE:CE1	2.52	0.44
5:J:265:ASP:OD1	5:J:265:ASP:N	2.48	0.44
1:A:198:GLU:HA	1:A:234:LYS:HD3	1.99	0.44
1:A:231:GLU:OE1	1:A:231:GLU:N	2.50	0.44
3:E:132:MET:SD	3:E:158:ILE:HD13	2.58	0.44
4:G:170:ARG:NH1	4:G:186:TYR:HB3	2.33	0.44
4:G:493:PRO:HD2	4:G:496:LEU:HD12	2.00	0.44
5:I:45:ALA:O	5:I:91:THR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:61:LYS:HA	5:J:61:LYS:HD2	1.75	0.44
5:J:180:VAL:HG13	5:J:256:VAL:HG22	1.99	0.44
1:B:50:THR:O	1:B:54:GLU:HG2	2.17	0.44
2:C:28:PRO:HG2	2:C:34:MET:HG2	1.98	0.44
2:C:209:LYS:NZ	4:G:479:HIS:HE1	2.16	0.44
2:C:271:MET:HE2	2:C:271:MET:HB3	1.77	0.44
2:D:43:ARG:O	2:D:47:THR:HG22	2.18	0.44
3:E:294:SER:O	3:E:294:SER:OG	2.36	0.44
3:F:94:TYR:CE2	3:F:216:MET:HE2	2.52	0.44
4:H:428:ARG:HH22	4:H:498:ASP:HB2	1.83	0.44
5:J:218:THR:O	5:J:218:THR:OG1	2.32	0.44
1:A:268:GLU:N	1:A:269:GLU:OE1	2.51	0.43
1:B:84:SER:OG	1:B:85:ASP:N	2.51	0.43
2:C:80:ASN:OD1	2:C:81:MET:N	2.51	0.43
2:C:166:MET:HE3	2:C:254:LEU:HD11	1.99	0.43
2:C:249:THR:N	2:C:312:VAL:O	2.50	0.43
3:E:97:LEU:O	3:E:209:LYS:NZ	2.51	0.43
4:G:450:ASP:OD2	4:G:453:VAL:HG13	2.17	0.43
5:I:54:ARG:HB3	5:I:57:PHE:CE2	2.53	0.43
5:I:180:VAL:HG12	5:I:256:VAL:HG22	2.00	0.43
5:I:379:ILE:HG22	5:I:380:GLY:H	1.83	0.43
5:J:270:ASP:C	5:J:274:ARG:HH21	2.25	0.43
1:A:7:ILE:O	1:A:11:LYS:HG2	2.19	0.43
1:A:150:VAL:HG11	1:A:168:LEU:HD21	1.99	0.43
1:A:245:ASP:OD1	4:G:326:LYS:NZ	2.45	0.43
3:E:36:ILE:O	3:E:39:PRO:HD2	2.18	0.43
4:G:183:LEU:HD21	4:G:454:SER:HA	2.00	0.43
4:G:440:THR:HG23	4:G:516:LEU:HD22	1.99	0.43
4:H:180:PHE:HZ	4:H:452:PHE:CD1	2.36	0.43
4:H:488:VAL:HG23	4:H:489:TYR:CD2	2.53	0.43
5:J:329:ASP:OD1	5:J:329:ASP:N	2.49	0.43
1:B:80:SER:HG	6:L:49:GLU:H	1.63	0.43
1:B:195:VAL:HG23	1:B:228:VAL:HG12	2.01	0.43
3:E:59:VAL:HG23	3:E:63:LEU:HD21	2.00	0.43
4:G:456:GLU:HB2	4:G:488:VAL:HG21	2.00	0.43
4:H:277:ILE:HD13	4:H:277:ILE:HA	1.82	0.43
5:I:72:ASN:CG	5:I:381:PRO:HD3	2.44	0.43
1:A:116:HIS:HA	1:A:119:ILE:HD12	2.00	0.43
1:A:150:VAL:O	1:A:175:VAL:HA	2.18	0.43
2:D:80:ASN:OD1	2:D:80:ASN:C	2.61	0.43
4:G:367:LEU:HD23	4:G:370:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:231:PHE:CD1	5:I:238:VAL:HG11	2.53	0.43
5:I:370:SER:OG	5:I:387:ASP:OD1	2.29	0.43
5:J:46:VAL:HG13	5:J:150:LEU:HA	2.01	0.43
5:J:200:ASN:HB2	5:J:218:THR:CG2	2.48	0.43
2:C:286:HIS:HA	2:C:313:PHE:HB2	2.00	0.43
2:D:254:LEU:HD12	2:D:254:LEU:O	2.19	0.43
3:E:348:SER:HA	3:E:364:ILE:O	2.18	0.43
3:F:48:PHE:H	4:G:199:PRO:HG3	1.82	0.43
4:G:166:GLN:OE1	4:G:166:GLN:N	2.51	0.43
4:G:360:VAL:HG12	4:G:361:VAL:O	2.19	0.43
4:H:273:MET:HE2	4:H:273:MET:HB3	1.85	0.43
4:H:460:PRO:C	4:H:462:ASP:H	2.25	0.43
5:J:238:VAL:HG22	5:J:239:GLU:N	2.34	0.43
1:B:125:ILE:HG13	1:B:138:LEU:HD21	2.01	0.43
3:E:49:GLU:HG2	3:E:50:GLU:H	1.83	0.43
3:F:385:VAL:HA	3:F:402:SER:N	2.34	0.43
6:K:35:LEU:O	6:K:40:ASN:HA	2.18	0.43
1:B:75:PHE:CE2	1:B:100:PHE:HB2	2.54	0.43
1:B:111:ILE:HD12	1:B:111:ILE:HA	1.76	0.43
4:H:167:VAL:HG21	4:H:262:PHE:HD1	1.84	0.43
4:H:192:LEU:HD12	4:H:192:LEU:H	1.83	0.43
4:H:339:SER:O	4:H:342:VAL:HG22	2.19	0.43
5:I:324:GLU:HA	5:I:335:CYS:HB2	2.00	0.43
5:J:196:CYS:O	5:J:198:GLU:N	2.52	0.43
5:J:282:ILE:O	5:J:282:ILE:HG13	2.17	0.43
1:A:292:THR:O	1:A:295:ALA:N	2.47	0.43
2:C:36:ARG:NE	2:C:145:GLU:OE2	2.52	0.43
2:C:215:THR:HA	4:G:483:ARG:O	2.19	0.43
3:E:93:ILE:O	3:E:96:LYS:HG2	2.18	0.43
3:E:161:ASP:OD1	3:E:168:LEU:HD11	2.19	0.43
4:H:216:GLN:O	4:H:218:LEU:HD12	2.19	0.43
5:J:289:MET:SD	5:J:291:VAL:HG23	2.59	0.43
5:J:338:SER:HB2	5:J:342:ILE:HG13	1.99	0.43
1:A:205:GLY:CA	1:A:276:THR:O	2.67	0.43
1:B:17:ASP:HB3	1:B:19:ASP:OD1	2.18	0.43
2:D:303:LEU:HD23	2:D:303:LEU:HA	1.83	0.43
3:E:107:ASP:OD1	3:E:107:ASP:N	2.52	0.43
5:J:202:VAL:HG22	5:J:242:TYR:HD1	1.83	0.43
1:B:127:THR:OG1	1:B:128:HIS:N	2.52	0.43
2:C:217:MET:HE1	2:C:222:ILE:HA	2.01	0.43
2:D:294:VAL:HG13	4:H:387:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:407:ALA:HB3	4:H:415:MET:HE2	2.01	0.43
5:I:65:ARG:NH1	5:I:299:ARG:HE	2.16	0.43
1:B:160:SER:O	1:B:163:LYS:HB3	2.19	0.42
2:C:84:ARG:NH2	2:C:272:PHE:HA	2.32	0.42
2:C:163:GLU:CD	2:C:165:ILE:HD11	2.43	0.42
4:G:204:HIS:CD2	4:G:236:VAL:HG23	2.54	0.42
4:G:373:LEU:O	4:G:377:VAL:HG22	2.19	0.42
4:G:515:VAL:HG12	4:G:516:LEU:HD23	2.01	0.42
5:I:109:SER:OG	5:I:110:LYS:N	2.52	0.42
5:J:211:ARG:HA	5:J:288:HIS:HA	2.01	0.42
6:L:62:ILE:O	6:L:63:ARG:HB2	2.18	0.42
2:D:294:VAL:HG12	4:H:385:TYR:CE2	2.54	0.42
3:E:281:CYS:O	3:E:285:CYS:N	2.32	0.42
3:F:173:GLU:OE1	3:F:173:GLU:N	2.50	0.42
4:G:230:LEU:HD23	4:G:230:LEU:HA	1.78	0.42
5:I:51:SER:HB2	5:I:65:ARG:NH2	2.30	0.42
5:I:405:GLY:O	5:I:407:GLN:NE2	2.52	0.42
5:J:418:GLU:O	5:J:436:VAL:HA	2.18	0.42
1:A:28:ARG:HH12	1:A:101:LEU:HD21	1.82	0.42
2:D:200:GLY:O	2:D:203:MET:HB3	2.19	0.42
3:E:110:THR:HB	3:E:112:VAL:HG13	2.00	0.42
3:E:186:ILE:HD13	3:E:186:ILE:HA	1.86	0.42
3:F:208:LYS:O	3:F:211:ILE:HG22	2.20	0.42
4:H:272:SER:OG	4:H:441:TYR:HE2	2.02	0.42
4:H:443:PHE:CG	4:H:443:PHE:O	2.72	0.42
5:I:93:VAL:HG23	5:I:122:ILE:HA	2.00	0.42
5:I:446:GLY:O	5:I:448:VAL:N	2.49	0.42
5:J:251:ILE:HG22	5:J:252:CYS:H	1.84	0.42
5:J:422:ARG:HB2	5:J:440:ASN:H	1.84	0.42
2:C:38:THR:O	2:C:42:LEU:HD23	2.19	0.42
4:G:461:ASP:O	4:G:464:GLN:NE2	2.52	0.42
4:G:481:SER:O	4:G:481:SER:OG	2.22	0.42
4:H:334:LEU:HA	4:H:359:VAL:HG23	2.00	0.42
4:H:496:LEU:HD12	4:H:496:LEU:H	1.84	0.42
5:I:66:VAL:HG11	5:I:76:ILE:HD13	2.01	0.42
5:I:389:VAL:HG12	5:I:406:ALA:N	2.35	0.42
5:I:447:SER:O	5:I:449:ILE:HG23	2.19	0.42
5:J:86:THR:OG1	5:J:88:VAL:HG23	2.19	0.42
1:A:120:LYS:HE2	2:D:280:ASN:HB3	2.00	0.42
4:G:210:LEU:HD22	4:G:232:ALA:HB3	2.01	0.42
1:B:247:PRO:HD2	1:B:250:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:ILE:HG22	2:D:177:PHE:HD2	1.84	0.42
3:F:132:MET:SD	3:F:158:ILE:HD13	2.60	0.42
4:G:209:ARG:HG2	4:G:213:GLN:HE21	1.85	0.42
5:I:318:VAL:HG23	5:I:321:LEU:O	2.19	0.42
5:J:75:LEU:HD22	5:J:154:ASP:HB2	2.01	0.42
5:J:131:LEU:HA	5:J:134:VAL:HB	2.01	0.42
5:J:230:LEU:O	5:J:234:SER:N	2.52	0.42
1:B:7:ILE:HG23	1:B:59:VAL:HG21	2.01	0.42
1:B:178:VAL:HG11	1:B:186:ILE:HD13	2.02	0.42
3:F:128:LEU:O	3:F:263:ILE:HG13	2.19	0.42
4:G:498:ASP:O	4:G:499:LEU:HG	2.20	0.42
4:H:210:LEU:HD22	4:H:232:ALA:HB3	2.01	0.42
5:I:76:ILE:O	5:I:80:LEU:HG	2.20	0.42
6:L:27:ALA:HB3	6:L:30:GLY:O	2.20	0.42
1:A:203:ASN:OD1	1:A:204:GLY:N	2.52	0.42
2:C:188:HIS:HD2	2:C:213:GLU:HG3	1.85	0.42
2:D:284:SER:O	2:D:284:SER:OG	2.31	0.42
3:E:400:GLU:O	3:E:418:GLY:N	2.46	0.42
3:F:268:LYS:HE3	3:F:270:ALA:HB2	2.01	0.42
4:G:336:TYR:CZ	4:G:419:GLY:HA3	2.55	0.42
5:I:157:SER:HA	5:I:296:TYR:O	2.20	0.42
5:I:313:VAL:HG23	5:I:318:VAL:CG2	2.50	0.42
5:I:424:THR:C	5:I:425:LEU:HD12	2.45	0.42
5:J:66:VAL:HG12	5:J:76:ILE:HB	2.02	0.42
5:J:314:ILE:HG21	5:J:359:ASN:O	2.20	0.42
1:A:283:LEU:HD22	1:A:290:VAL:HG12	2.00	0.42
2:D:228:ARG:NH2	4:H:450:ASP:OD2	2.53	0.42
3:E:43:LEU:HD12	3:E:48:PHE:CD1	2.55	0.42
3:E:62:ALA:HB3	3:E:66:GLU:HG2	2.02	0.42
3:E:109:ILE:HG22	3:E:274:ASN:HD21	1.85	0.42
4:G:440:THR:HG21	4:G:504:LEU:HD11	2.02	0.42
4:G:476:TRP:HE1	4:G:484:LEU:HD13	1.85	0.42
5:I:345:GLY:O	5:I:348:VAL:HG23	2.19	0.42
5:J:436:VAL:HG12	5:J:437:VAL:N	2.35	0.42
1:B:79:ALA:HB2	1:B:96:ARG:HH21	1.85	0.42
1:B:183:VAL:HG12	1:B:183:VAL:O	2.20	0.42
1:B:194:ILE:HD13	1:B:227:TYR:HB2	2.01	0.42
1:B:203:ASN:HB3	1:B:239:PHE:CE1	2.55	0.42
2:D:10:GLU:O	2:D:13:GLU:HG3	2.20	0.42
2:D:317:PRO:HD2	2:D:320:LEU:HD12	2.02	0.42
2:D:336:ILE:C	2:D:338:ARG:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:109:ILE:HG22	3:E:274:ASN:ND2	2.34	0.42
3:F:134:LYS:HG3	3:F:199:LEU:HD13	2.01	0.42
4:G:332:VAL:CG2	4:G:398:VAL:HA	2.50	0.42
4:H:292:ARG:HB3	4:H:295:GLU:HG2	2.02	0.42
5:I:300:VAL:HG13	5:I:300:VAL:O	2.20	0.42
5:I:304:HIS:HB2	5:I:428:ARG:HH12	1.85	0.42
5:J:247:CYS:SG	5:J:297:GLY:HA3	2.60	0.42
1:B:82:GLU:O	1:B:88:LYS:NZ	2.47	0.41
1:B:274:ASP:N	1:B:274:ASP:OD1	2.53	0.41
2:D:51:TRP:HA	2:D:56:GLU:OE2	2.20	0.41
2:D:163:GLU:HA	2:D:230:ASN:OD1	2.19	0.41
3:F:188:GLN:OE1	5:I:190:PRO:HB2	2.19	0.41
5:J:420:LYS:HB2	5:J:437:VAL:O	2.19	0.41
1:A:247:PRO:HB2	1:A:249:LYS:HG2	2.02	0.41
2:C:87:LYS:NZ	2:C:343:LEU:O	2.39	0.41
2:D:228:ARG:HG2	4:H:179:LEU:HD21	2.01	0.41
3:E:355:ASP:O	3:E:372:ARG:N	2.34	0.41
4:G:310:GLU:HA	4:G:314:LEU:HD12	2.01	0.41
1:B:76:ILE:HG12	1:B:93:MET:SD	2.60	0.41
2:D:285:PHE:CE2	2:D:315:TYR:HB2	2.55	0.41
2:D:326:SER:OG	2:D:328:ILE:HG12	2.20	0.41
3:E:161:ASP:OD2	3:E:162:SER:N	2.52	0.41
4:G:257:LYS:HA	4:G:257:LYS:HD3	1.74	0.41
4:G:359:VAL:HG23	4:G:359:VAL:O	2.20	0.41
4:H:242:THR:N	4:H:293:GLU:OE2	2.53	0.41
4:H:397:GLU:OE2	5:J:339:ARG:HD2	2.20	0.41
1:B:46:ARG:NH2	6:L:27:ALA:HB1	2.28	0.41
1:B:98:GLU:O	1:B:101:LEU:HG	2.20	0.41
3:F:156:ASP:OD1	3:F:201:ASP:HB3	2.20	0.41
3:F:288:ASP:C	3:F:291:GLU:H	2.29	0.41
4:G:177:VAL:CG2	4:G:485:LEU:HB3	2.47	0.41
4:H:230:LEU:HD13	4:H:304:ILE:HG23	2.02	0.41
1:B:111:ILE:HD13	1:B:286:THR:C	2.45	0.41
1:B:193:VAL:HG12	1:B:195:VAL:HG13	2.02	0.41
2:C:180:GLU:HA	2:C:183:ARG:NH1	2.35	0.41
2:D:257:ALA:O	2:D:260:HIS:N	2.53	0.41
3:E:52:ILE:HD11	3:E:96:LYS:HE2	2.02	0.41
4:G:167:VAL:HG23	4:G:167:VAL:O	2.20	0.41
4:G:184:PRO:HB2	4:G:186:TYR:HE2	1.84	0.41
4:G:338:CYS:H	4:G:368:GLU:CD	2.28	0.41
5:I:108:LYS:HE2	5:I:108:LYS:HB2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:321:LEU:HG	5:I:327:PHE:CE2	2.55	0.41
5:I:419:VAL:HG22	5:I:437:VAL:HG12	2.02	0.41
5:J:131:LEU:HD21	5:J:150:LEU:HD11	2.02	0.41
5:J:390:VAL:C	5:J:391:LEU:HD12	2.45	0.41
1:A:127:THR:HA	1:A:194:ILE:O	2.20	0.41
1:A:188:GLU:OE1	1:B:243:GLN:HG2	2.20	0.41
1:B:128:HIS:ND1	1:B:153:THR:OG1	2.53	0.41
2:C:28:PRO:HB2	2:C:34:MET:HG2	2.02	0.41
2:C:289:VAL:HG22	2:C:290:ALA:H	1.86	0.41
2:D:237:LYS:HG2	2:D:313:PHE:CZ	2.56	0.41
4:G:353:GLY:HA2	4:G:355:ARG:NH2	2.35	0.41
5:I:91:THR:HG23	5:I:118:ASN:OD1	2.20	0.41
5:I:211:ARG:HA	5:I:288:HIS:HA	2.01	0.41
5:J:129:ARG:NE	5:J:129:ARG:O	2.53	0.41
5:J:135:LEU:HD12	5:J:135:LEU:HA	1.83	0.41
5:J:248:HIS:CE1	5:J:269:ARG:HH11	2.38	0.41
2:C:14:ARG:HD2	2:C:44:GLN:OE1	2.21	0.41
2:D:227:SER:HB3	2:D:261:HIS:CE1	2.56	0.41
3:F:114:LEU:HA	3:F:117:VAL:HG23	2.03	0.41
5:I:415:ASP:OD1	5:I:416:ASN:N	2.53	0.41
1:B:154:GLU:HG2	1:B:180:ASP:H	1.86	0.41
2:C:30:SER:O	2:C:33:GLU:N	2.52	0.41
2:C:242:ASN:O	2:C:318:PRO:HB3	2.20	0.41
2:C:276:PRO:HB2	2:C:349:HIS:CG	2.55	0.41
3:E:35:LEU:O	3:E:39:PRO:HD3	2.20	0.41
3:E:63:LEU:HA	3:E:67:PHE:HD2	1.85	0.41
3:F:287:GLY:O	3:F:291:GLU:HG2	2.19	0.41
4:G:312:ILE:HG13	4:G:313:VAL:N	2.36	0.41
4:G:466:LYS:HD2	4:G:466:LYS:HA	1.90	0.41
4:H:366:TRP:CH2	4:H:417:ARG:HD2	2.56	0.41
5:I:245:LEU:HD12	5:I:246:ASP:H	1.86	0.41
5:J:132:GLY:HA2	5:J:260:PHE:CD1	2.56	0.41
5:J:442:THR:O	5:J:443:LEU:HD12	2.21	0.41
1:A:43:GLN:HG2	1:A:44:GLY:N	2.34	0.41
1:A:170:HIS:ND1	1:A:170:HIS:O	2.54	0.41
1:A:270:HIS:HB3	1:B:179:LEU:HG	2.03	0.41
1:B:63:VAL:HG13	1:B:236:VAL:HG11	2.02	0.41
1:B:125:ILE:HD13	1:B:192:LEU:HD21	2.02	0.41
2:C:144:LEU:O	2:C:147:THR:HG22	2.20	0.41
2:C:166:MET:HE2	2:C:229:VAL:HG21	2.02	0.41
2:C:197:PHE:C	2:C:199:GLN:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:ILE:HA	2:D:231:LYS:O	2.20	0.41
3:E:176:LEU:HD23	3:E:176:LEU:HA	1.91	0.41
3:F:192:ARG:HG2	5:I:241:ARG:HG3	2.03	0.41
3:F:224:ILE:HG23	3:F:228:LEU:HD22	2.03	0.41
4:G:172:ASP:OD2	4:G:173:TYR:N	2.47	0.41
5:I:107:LEU:HD23	5:I:107:LEU:HA	1.75	0.41
5:J:57:PHE:HE1	5:J:61:LYS:HD3	1.86	0.41
5:J:337:HIS:CD2	5:J:338:SER:H	2.39	0.41
1:A:104:ILE:HD12	1:A:233:PHE:CD2	2.56	0.41
2:D:80:ASN:ND2	2:D:272:PHE:O	2.25	0.41
3:F:102:LEU:HD13	3:F:206:CYS:HB2	2.03	0.41
3:F:161:ASP:CG	3:F:163:THR:H	2.29	0.41
4:G:215:SER:OG	4:G:216:GLN:N	2.54	0.41
4:H:403:LEU:HB2	4:H:436:VAL:HG12	2.03	0.41
5:I:90:GLU:HA	5:I:119:VAL:HG22	2.02	0.41
5:I:213:LEU:HD12	5:I:238:VAL:HG23	2.03	0.41
5:J:274:ARG:O	5:J:278:VAL:HG13	2.21	0.41
5:J:324:GLU:OE2	5:J:337:HIS:HB2	2.21	0.41
1:B:107:SER:OG	1:B:232:SER:HB3	2.20	0.40
2:C:240:LEU:HD11	2:C:285:PHE:CZ	2.56	0.40
2:D:166:MET:CE	2:D:229:VAL:HG21	2.46	0.40
3:F:53:VAL:O	3:F:77:CYS:HA	2.21	0.40
4:H:210:LEU:HD21	4:H:229:LEU:HA	2.02	0.40
4:H:234:GLN:HE21	4:H:304:ILE:CG2	2.34	0.40
4:H:511:SER:O	4:H:511:SER:OG	2.30	0.40
5:I:46:VAL:HG23	5:I:94:PHE:CE2	2.56	0.40
5:I:48:VAL:O	5:I:48:VAL:HG23	2.21	0.40
5:I:149:LEU:HD11	5:I:161:ILE:HD13	2.03	0.40
1:A:110:LYS:HG3	1:A:114:LEU:HD23	2.03	0.40
1:B:130:TYR:OH	1:B:132:ARG:NH1	2.53	0.40
1:B:251:LYS:O	1:B:272:TRP:HB2	2.21	0.40
2:C:151:ILE:HD13	2:C:151:ILE:HA	1.91	0.40
2:D:221:ALA:HB2	4:H:418:VAL:HB	2.03	0.40
2:D:297:PHE:HE2	5:J:296:TYR:HE1	1.70	0.40
3:E:262:ASP:HB3	3:E:264:TYR:HE1	1.87	0.40
3:F:53:VAL:HB	3:F:77:CYS:HB3	2.02	0.40
4:G:170:ARG:CZ	4:G:186:TYR:HB3	2.51	0.40
4:G:216:GLN:HB2	4:G:218:LEU:CD1	2.51	0.40
4:H:365:PRO:HD2	4:H:366:TRP:CD1	2.52	0.40
1:A:243:GLN:HB2	1:B:188:GLU:CD	2.46	0.40
1:B:156:GLN:N	1:B:157:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:GLU:OE1	2:D:218:THR:HA	2.22	0.40
3:E:42:LEU:HD22	3:E:112:VAL:HG23	2.03	0.40
4:G:300:LEU:HD23	4:G:300:LEU:HA	1.94	0.40
4:H:467:ARG:HH22	5:J:294:LYS:HE2	1.87	0.40
5:I:252:CYS:SG	5:I:256:VAL:HG11	2.62	0.40
5:I:301:SER:OG	5:I:302:ASN:ND2	2.55	0.40
5:I:321:LEU:O	5:I:322:THR:OG1	2.35	0.40
5:J:451:LEU:HA	5:J:460:GLU:OE1	2.22	0.40
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.94	0.40
1:A:283:LEU:HD21	2:D:242:ASN:OD1	2.21	0.40
2:C:134:ILE:HG22	2:C:138:ASN:HD21	1.85	0.40
2:C:160:HIS:HE1	4:H:179:LEU:HD11	1.87	0.40
2:D:216:VAL:HB	4:H:484:LEU:HD13	2.02	0.40
3:E:4:GLN:OE1	3:E:97:LEU:HA	2.20	0.40
3:F:120:LEU:HD13	3:F:264:TYR:HB3	2.02	0.40
4:G:455:ASN:ND2	4:G:489:TYR:HB2	2.36	0.40
4:H:178:SER:H	4:H:483:ARG:HH11	1.70	0.40
4:H:338:CYS:N	4:H:368:GLU:OE1	2.32	0.40
5:I:412:LEU:C	5:I:413:LEU:HD12	2.47	0.40
5:J:53:ASP:O	5:J:55:ARG:HD3	2.21	0.40
5:J:69:PRO:HG2	5:J:397:TRP:CG	2.57	0.40
5:J:180:VAL:HG21	5:J:285:ASN:HB3	2.04	0.40
5:J:206:ASP:O	5:J:210:ASN:N	2.52	0.40
5:J:368:ILE:HG22	5:J:369:GLY:N	2.35	0.40
1:B:104:ILE:HG23	1:B:233:PHE:CE1	2.56	0.40
1:B:155:SER:C	1:B:157:PRO:HD2	2.46	0.40
3:E:4:GLN:OE1	3:E:97:LEU:HD13	2.22	0.40
4:G:180:PHE:CZ	4:G:452:PHE:HD2	2.40	0.40
4:G:363:SER:O	4:G:367:LEU:HD12	2.20	0.40
5:I:183:MET:O	5:I:290:HIS:N	2.55	0.40
5:I:245:LEU:HD12	5:I:246:ASP:N	2.37	0.40
5:I:366:THR:OG1	5:I:367:VAL:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	289/305 (95%)	254 (88%)	35 (12%)	0	100	100
1	B	287/305 (94%)	259 (90%)	28 (10%)	0	100	100
2	C	313/351 (89%)	271 (87%)	42 (13%)	0	100	100
2	D	320/351 (91%)	271 (85%)	48 (15%)	1 (0%)	36	70
3	E	333/452 (74%)	260 (78%)	73 (22%)	0	100	100
3	F	333/452 (74%)	262 (79%)	71 (21%)	0	100	100
4	G	351/523 (67%)	299 (85%)	52 (15%)	0	100	100
4	H	351/523 (67%)	305 (87%)	46 (13%)	0	100	100
5	I	425/721 (59%)	345 (81%)	80 (19%)	0	100	100
5	J	427/721 (59%)	344 (81%)	82 (19%)	1 (0%)	43	75
6	K	173/315 (55%)	144 (83%)	29 (17%)	0	100	100
6	L	173/315 (55%)	143 (83%)	30 (17%)	0	100	100
All	All	3775/5334 (71%)	3157 (84%)	616 (16%)	2 (0%)	49	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	127	ALA
5	J	249	ILE

5.3.2 Protein sidechains ⓘ

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	248/260 (95%)	248 (100%)	0	100	100
1	B	247/260 (95%)	246 (100%)	1 (0%)	84	84
2	C	269/298 (90%)	268 (100%)	1 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	276/298 (93%)	275 (100%)	1 (0%)	84	84
3	E	214/398 (54%)	214 (100%)	0	100	100
3	F	214/398 (54%)	213 (100%)	1 (0%)	81	82
4	G	309/444 (70%)	307 (99%)	2 (1%)	78	81
4	H	309/444 (70%)	309 (100%)	0	100	100
5	I	381/626 (61%)	381 (100%)	0	100	100
5	J	383/626 (61%)	381 (100%)	2 (0%)	81	82
6	K	3/279 (1%)	3 (100%)	0	100	100
6	L	3/279 (1%)	3 (100%)	0	100	100
All	All	2856/4610 (62%)	2848 (100%)	8 (0%)	84	85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	152	VAL
2	C	201	HIS
2	D	256	LEU
3	F	161	ASP
4	G	214	TYR
4	G	394	VAL
5	J	133	ASP
5	J	400	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	B	13	GLN
1	B	156	GLN
1	B	208	ASN
1	B	223	ASN
2	C	49	HIS
2	C	132	ASN
2	C	138	ASN
2	C	154	GLN
2	C	158	HIS
2	C	160	HIS
2	C	252	HIS

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Mol	Chain	Res	Type
2	D	97	HIS
2	D	119	ASN
2	D	158	HIS
3	E	4	GLN
3	E	115	HIS
3	E	196	HIS
3	E	274	ASN
3	F	60	GLN
3	F	115	HIS
3	F	236	GLN
3	F	271	ASN
3	F	283	ASN
4	G	166	GLN
4	G	185	GLN
4	G	189	GLN
4	G	213	GLN
4	G	254	ASN
4	G	265	GLN
4	G	274	HIS
4	G	281	ASN
4	G	325	GLN
4	G	347	GLN
4	G	406	HIS
4	G	430	HIS
4	G	478	ASN
4	G	479	HIS
4	H	194	GLN
4	H	265	GLN
4	H	274	HIS
4	H	275	ASN
4	H	281	ASN
4	H	347	GLN
4	H	430	HIS
4	H	478	ASN
5	I	118	ASN
5	I	197	HIS
5	I	200	ASN
5	I	214	HIS
5	I	232	GLN
5	I	248	HIS
5	I	255	GLN
5	I	304	HIS

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Mol	Chain	Res	Type
5	I	371	ASN
5	I	388	ASN
5	I	410	GLN
5	I	416	ASN
5	J	44	GLN
5	J	72	ASN
5	J	158	ASN
5	J	279	ASN
5	J	359	ASN
5	J	376	ASN
5	J	416	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
6	SEP	K	51	6	8,9,10	1.61	1 (12%)	7,12,14	1.18	1 (14%)
6	SEP	L	51	6	8,9,10	1.60	1 (12%)	7,12,14	1.25	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SEP	K	51	6	-	2/6/8/10	-
6	SEP	L	51	6	-	4/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	51	SEP	P-O1P	3.54	1.61	1.50
6	L	51	SEP	P-O1P	3.50	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	51	SEP	OG-CB-CA	2.64	110.72	108.14
6	K	51	SEP	OG-CB-CA	2.47	110.55	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	51	SEP	N-CA-CB-OG
6	L	51	SEP	N-CA-CB-OG
6	L	51	SEP	CB-OG-P-O1P
6	L	51	SEP	CB-OG-P-O2P
6	L	51	SEP	CB-OG-P-O3P
6	K	51	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

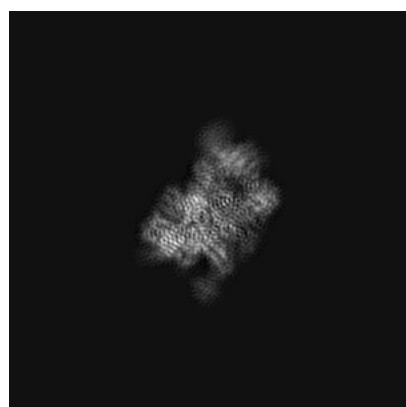
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30569. These allow visual inspection of the internal detail of the map and identification of artifacts.

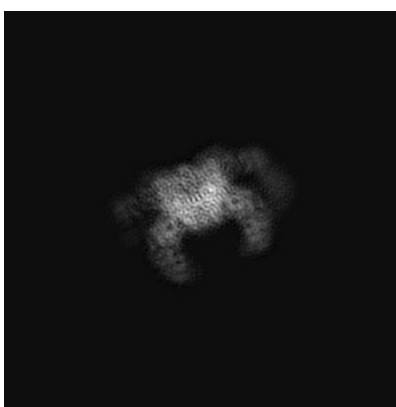
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

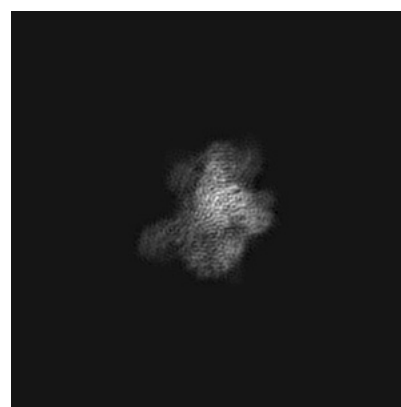
6.1.1 Primary map



X



Y

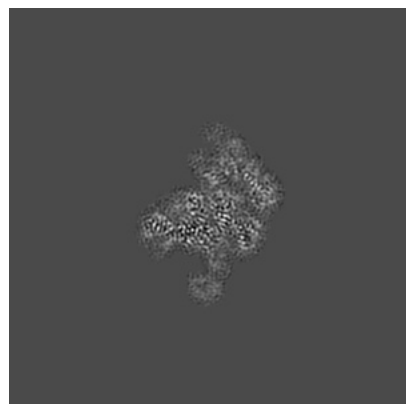


Z

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

6.2 Central slices [i](#)

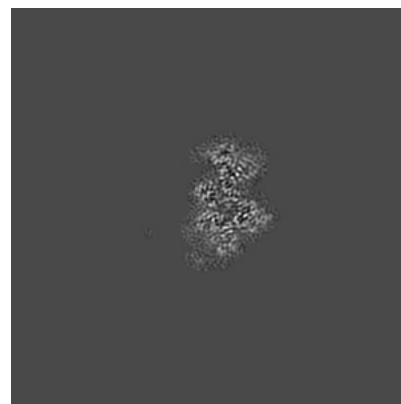
6.2.1 Primary map



X Index: 150



Y Index: 150

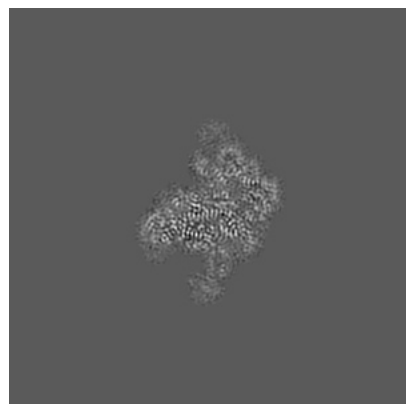


Z Index: 150

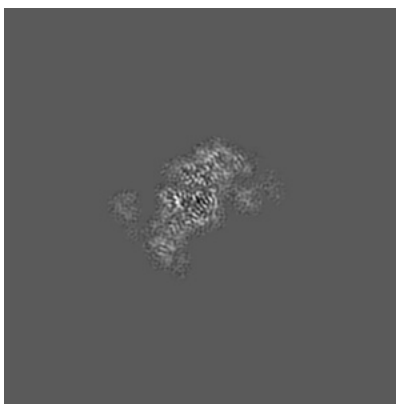
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

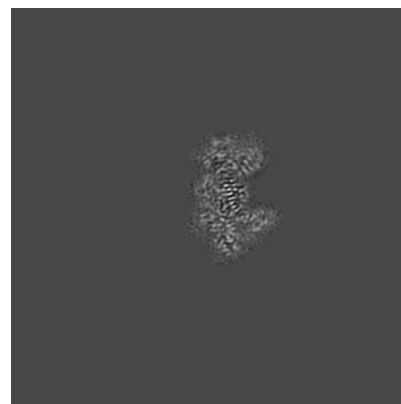
6.3.1 Primary map



X Index: 154



Y Index: 140

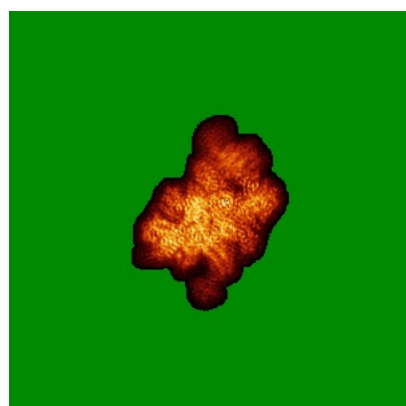


Z Index: 157

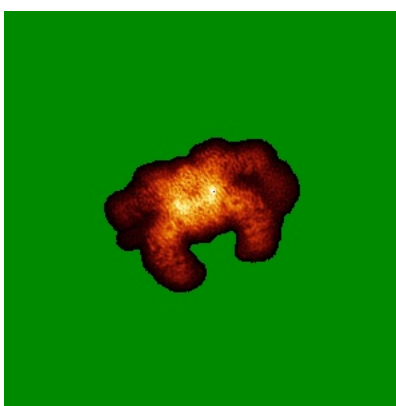
The images above show the largest variance slices of the map in three orthogonal directions.

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

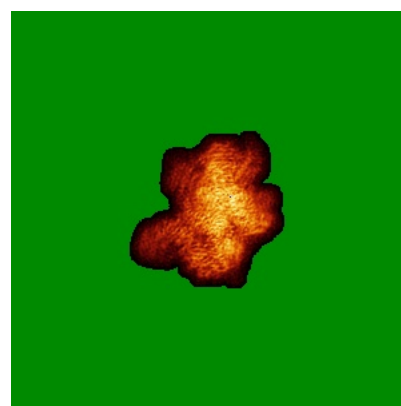
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

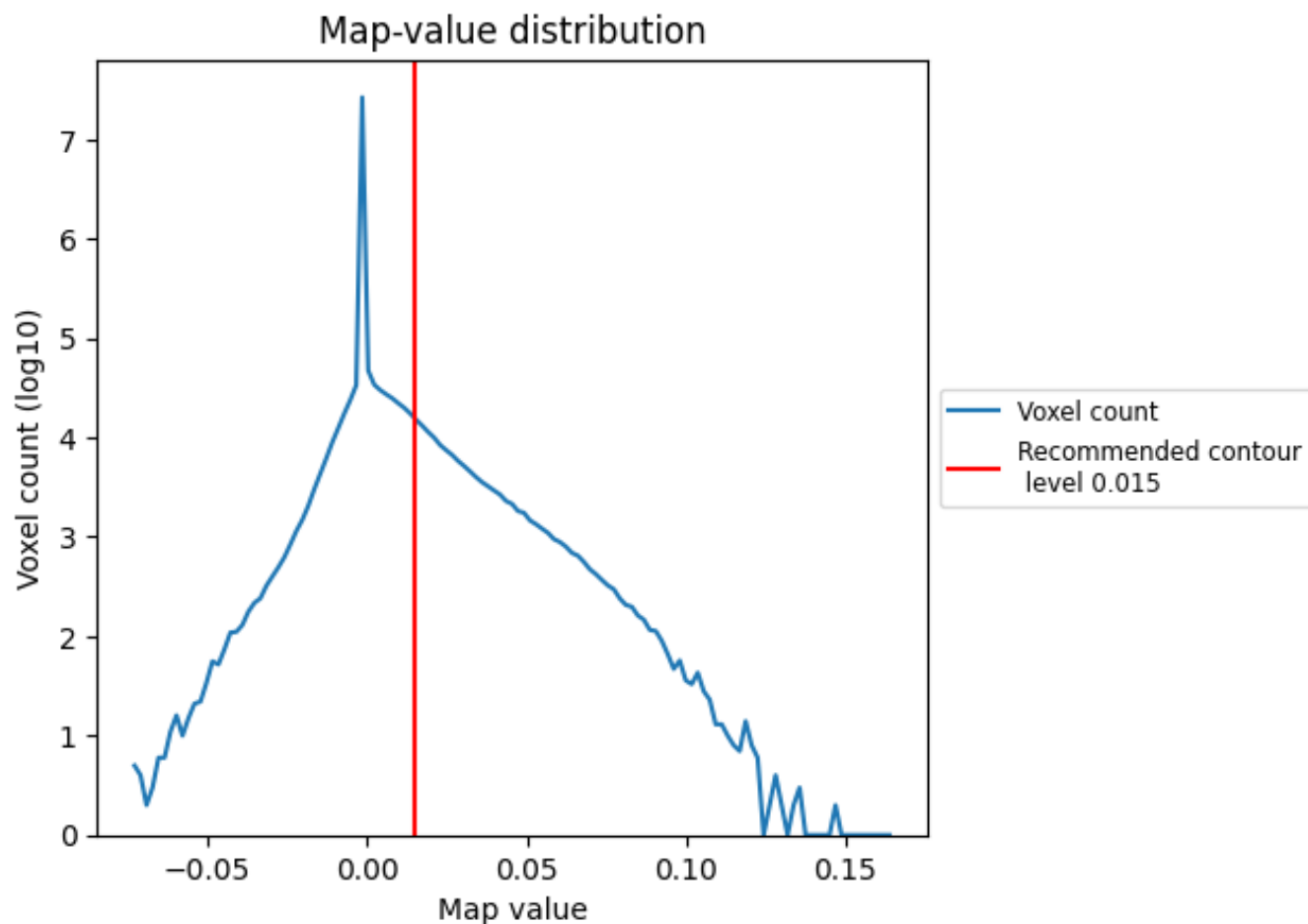
6.6 Mask visualisation

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

7 Map analysis [i](#)

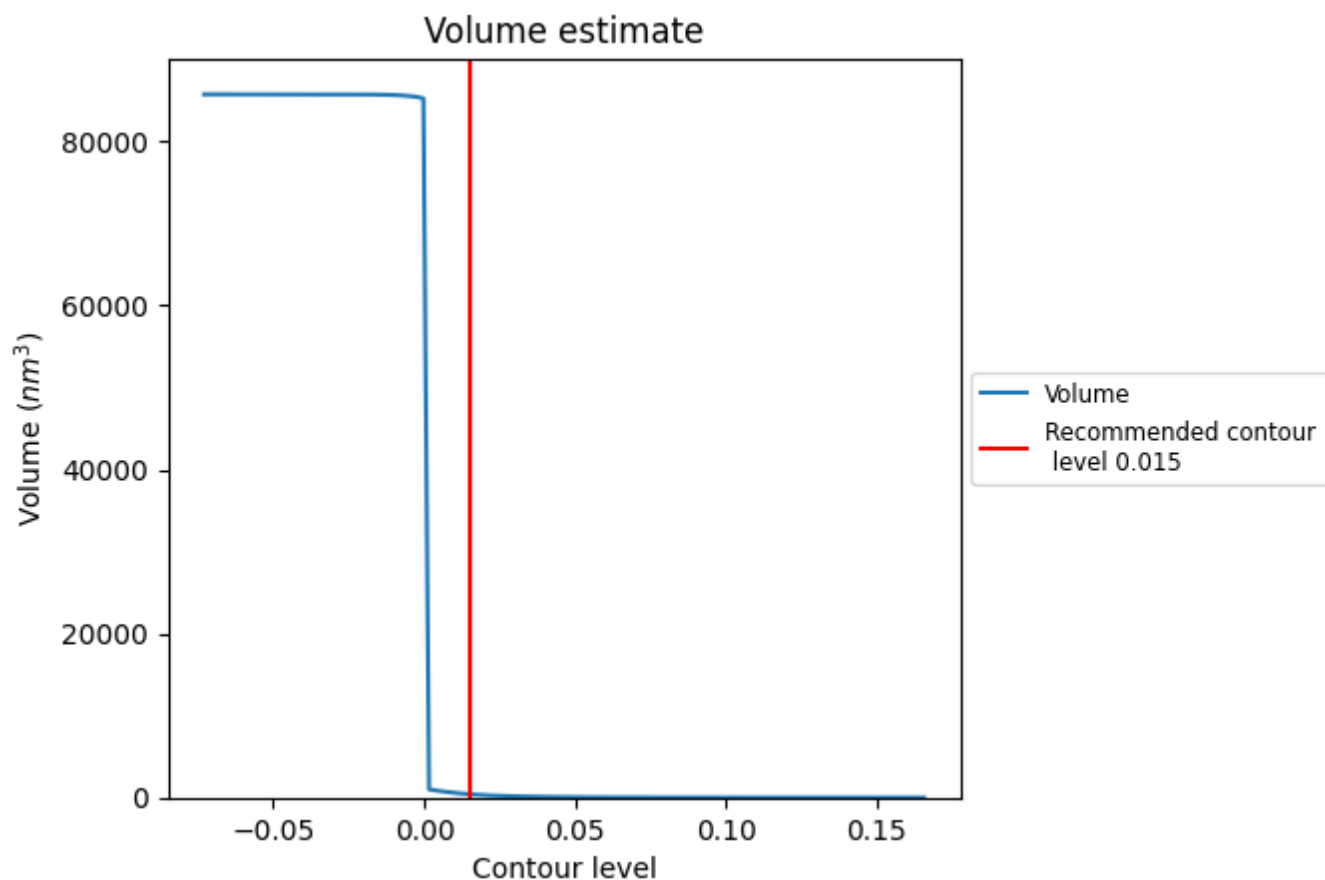
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

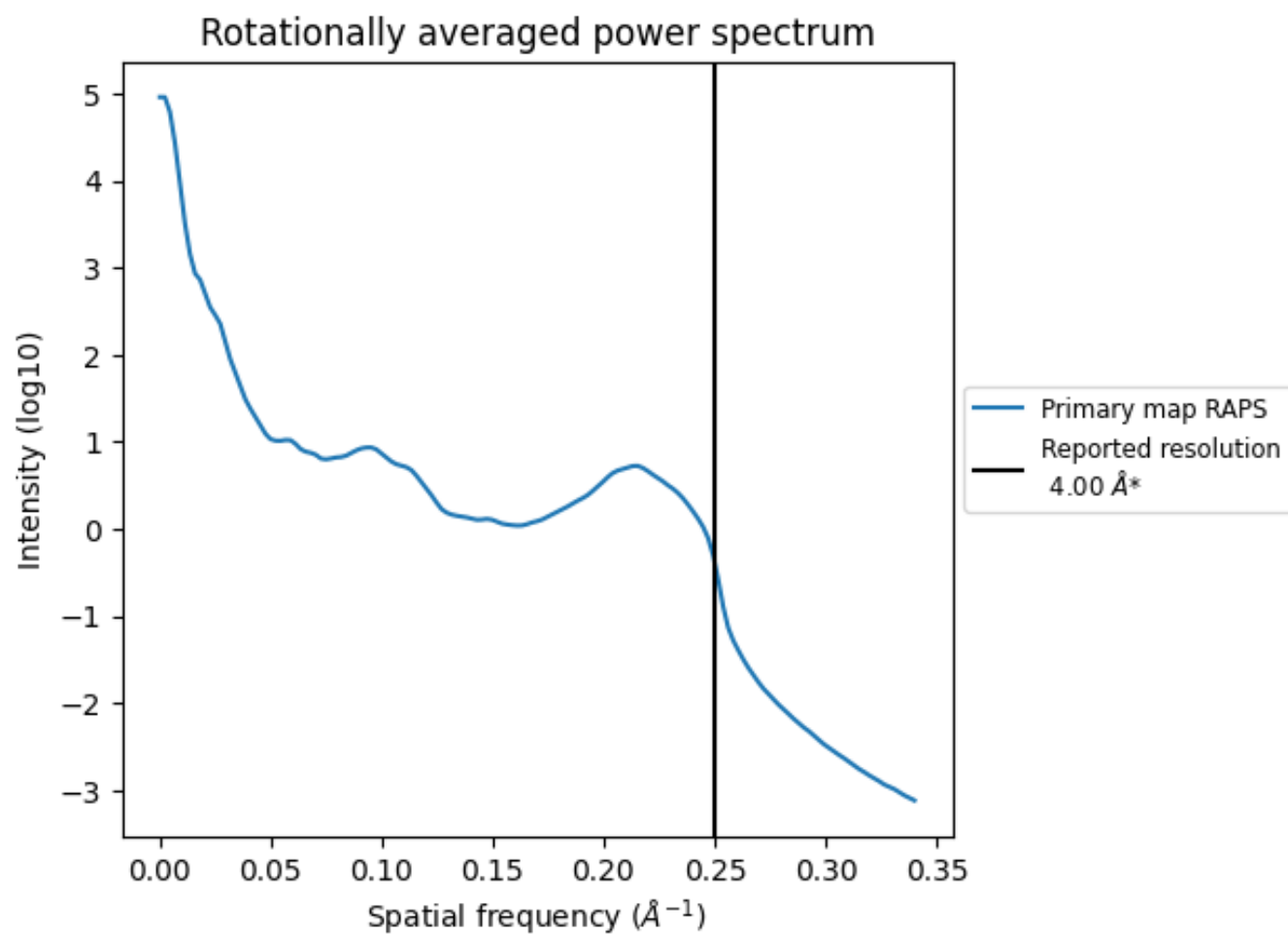
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 410 nm^3 ; this corresponds to an approximate mass of 370 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 0.250 Å⁻¹

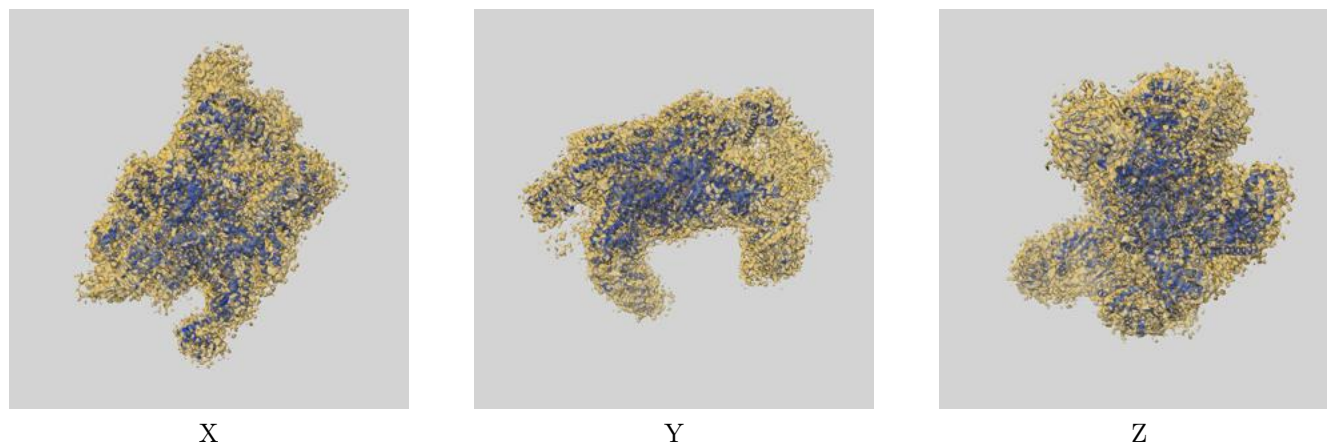
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

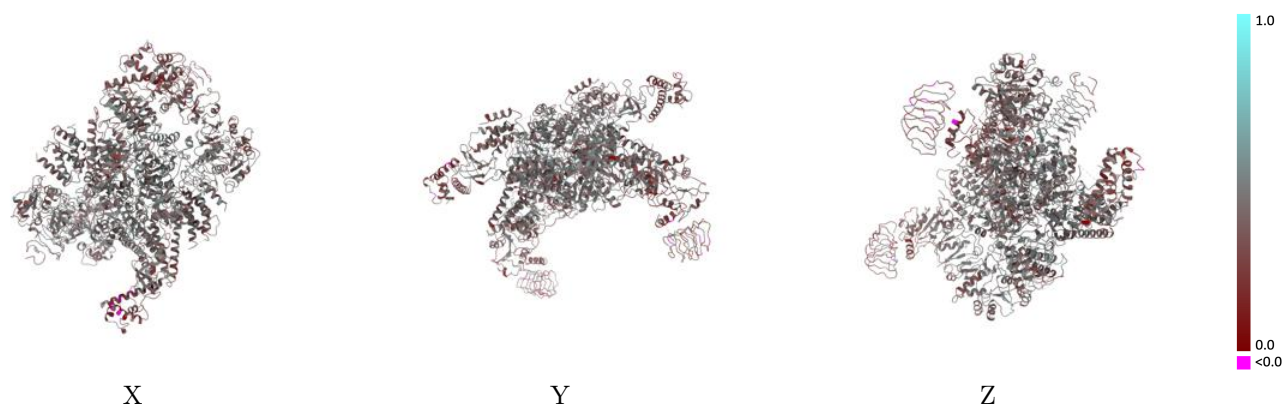
This section contains information regarding the fit between EMDB map EMD-30569 and PDB model 7D44. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



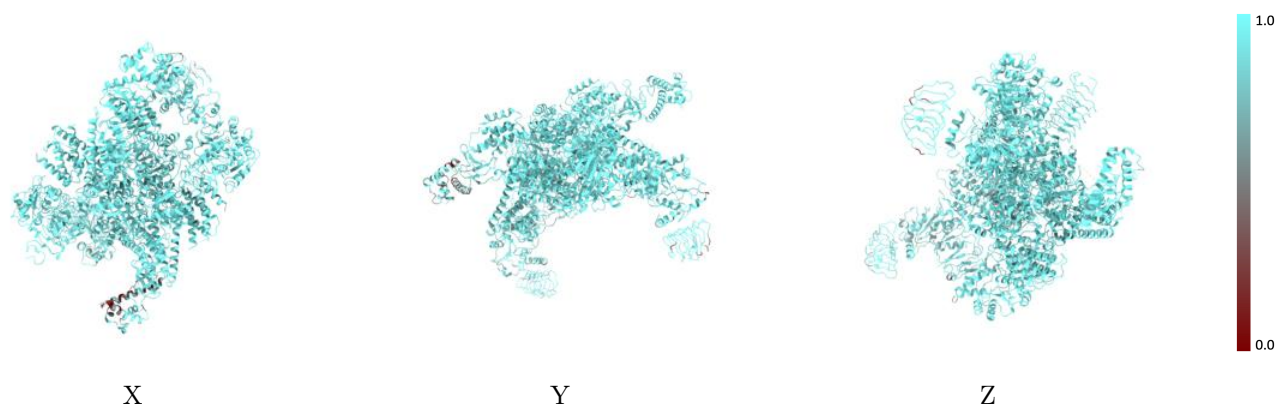
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



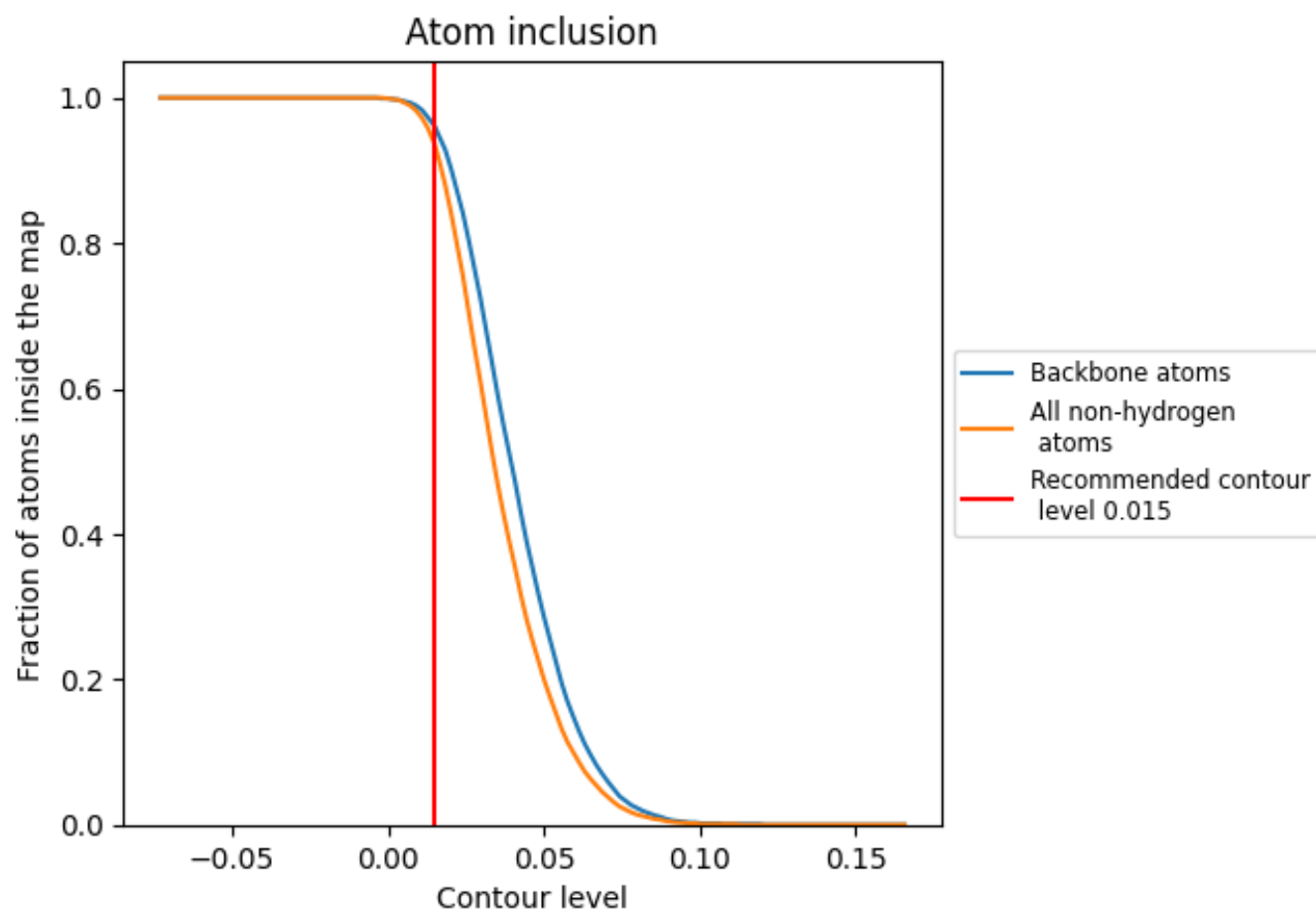
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9360	0.4210
A	0.9580	0.4330
B	0.9460	0.4380
C	0.9460	0.4460
D	0.9570	0.4470
E	0.8900	0.3600
F	0.9160	0.3530
G	0.9490	0.4450
H	0.9340	0.4420
I	0.9500	0.4290
J	0.9540	0.4400
K	0.9530	0.3840
L	0.7650	0.3590

1.0

0.0

<0.0