Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 03:08 PM JST

PDB ID	:	7D44
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:

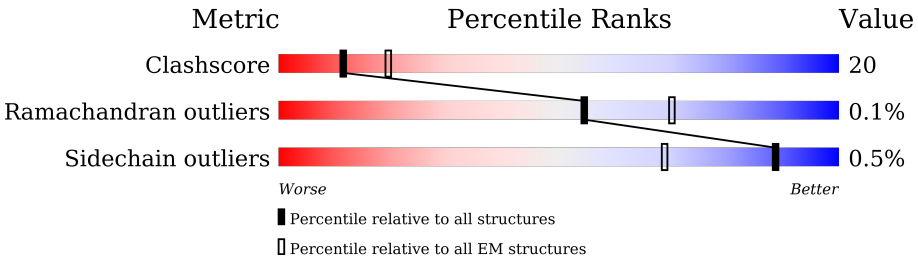
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	305	58% 38% ·
1	B	305	52% 42% · 5%
2	C	351	54% 36% 10%
2	D	351	56% 36% 8%
3	E	452	· 51% 25% 24%
3	F	452	· 45% 31% 24%
4	G	523	37% 31% 33%
4	H	523	41% 27% 33%

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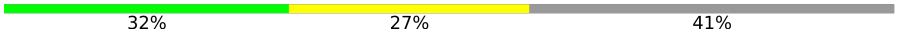
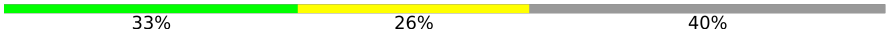
Mol	Chain	Length	Quality of chain
5	I	721	
5	J	721	
6	K	315	
6	L	315	

2 Entry composition (i)

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.

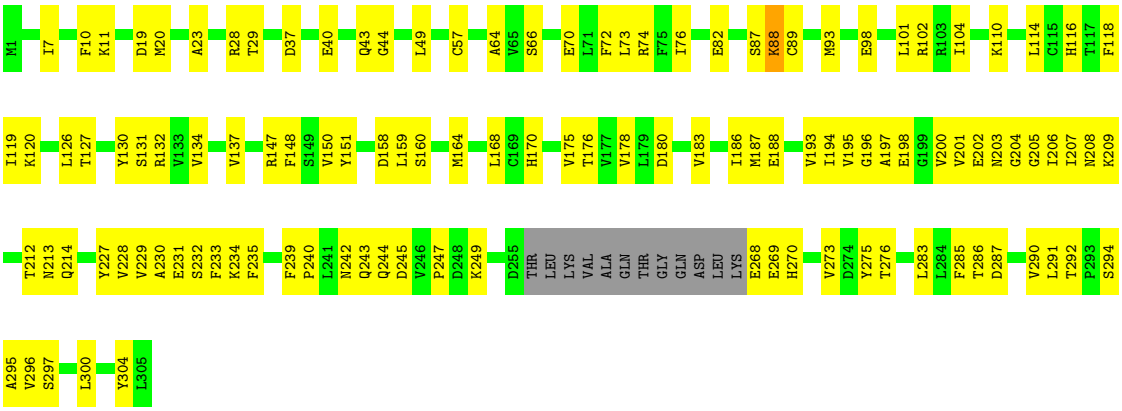
Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	176	Total	C	N	O	P	0	0
			889	529	179	180	1		
6	L	176	Total	C	N	O	P	0	0
			889	529	179	180	1		

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.

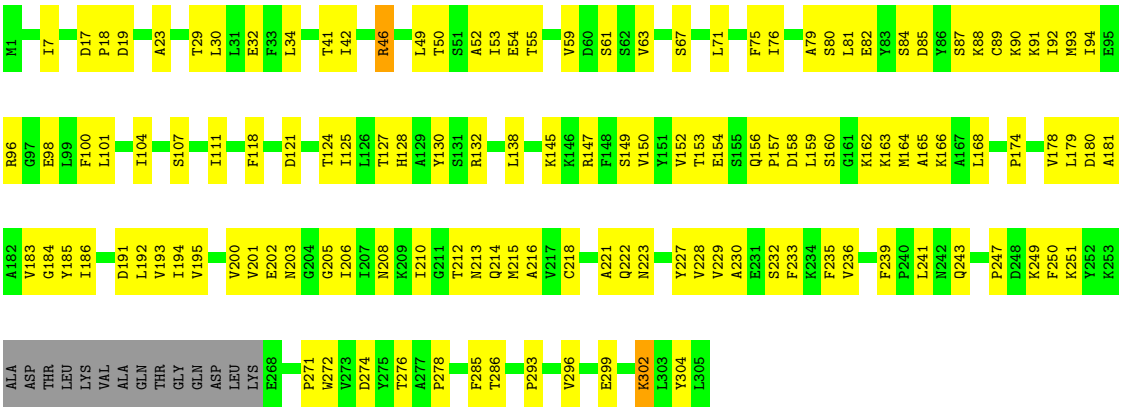
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A:



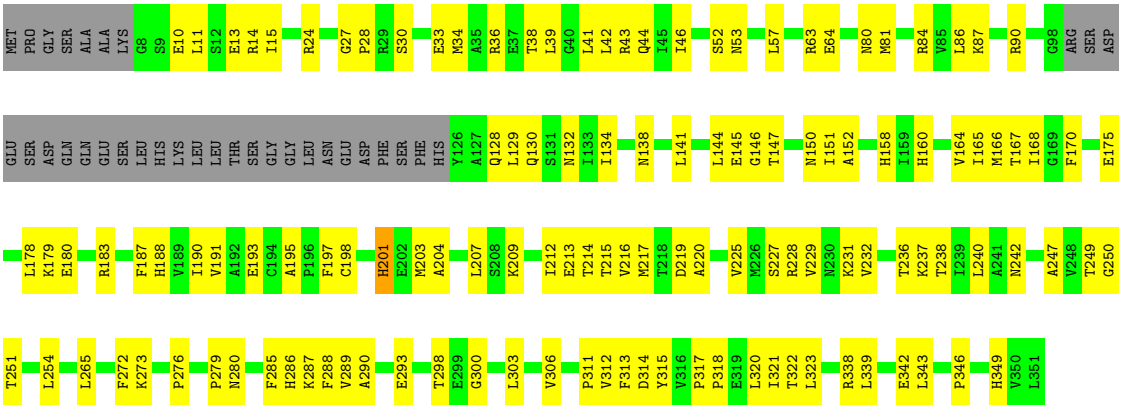
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain B:



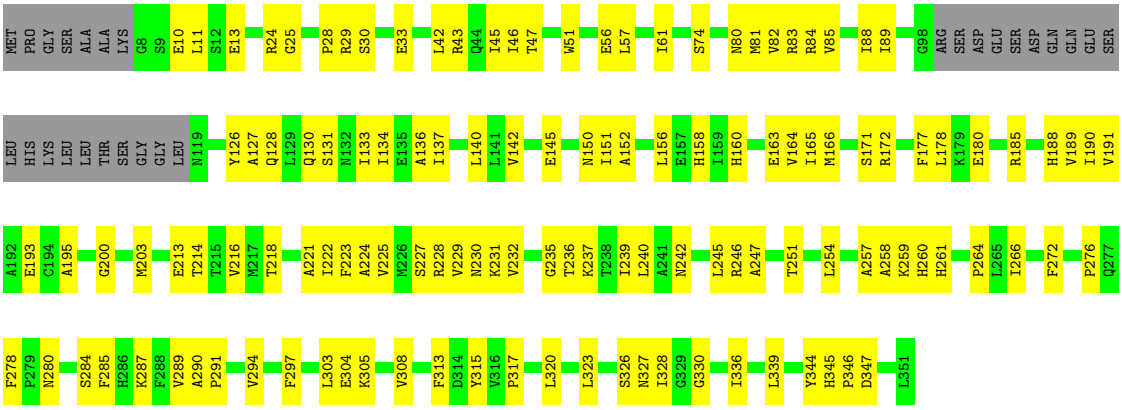
• Molecule 2: Translation initiation factor eIF-2B subunit beta

Chain C:



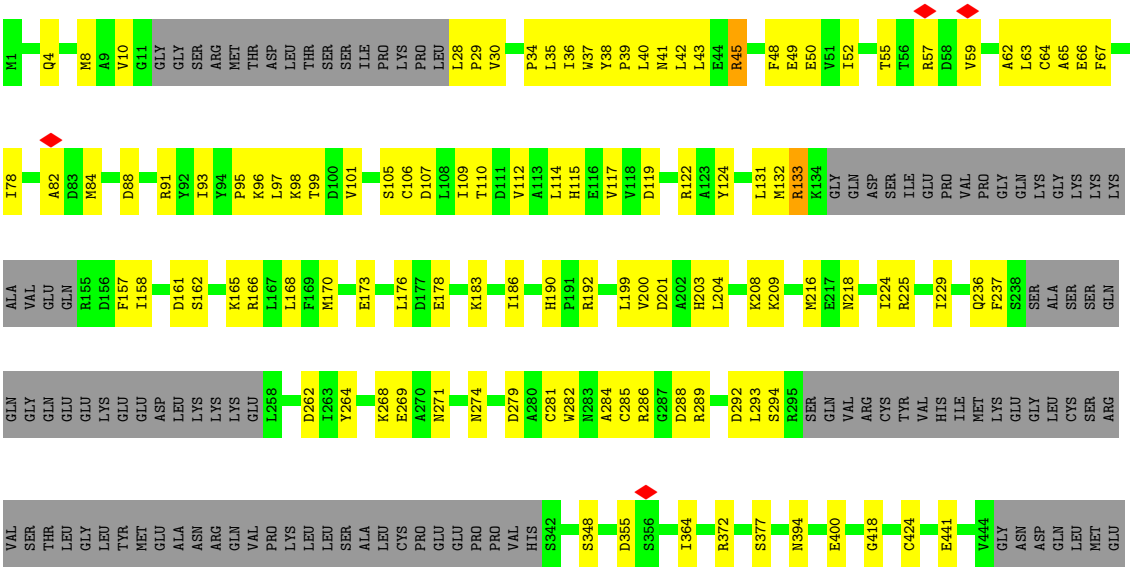
• Molecule 2: Translation initiation factor eIF-2B subunit beta

Chain D:



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

Chain E:



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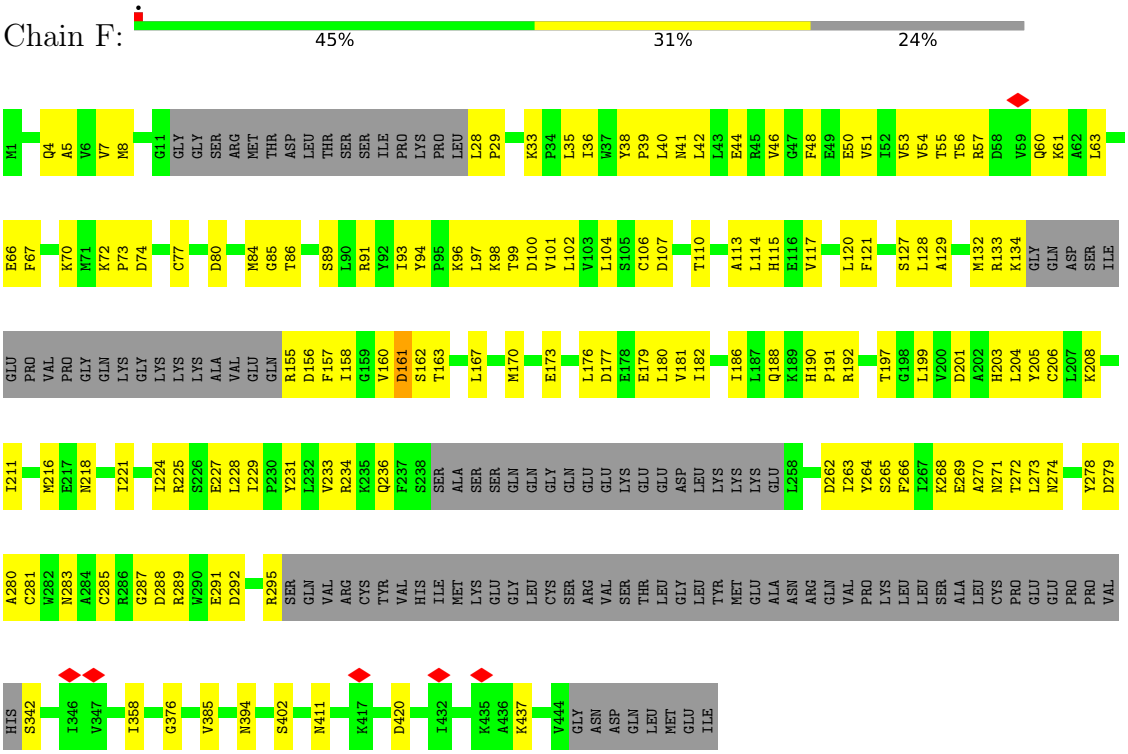
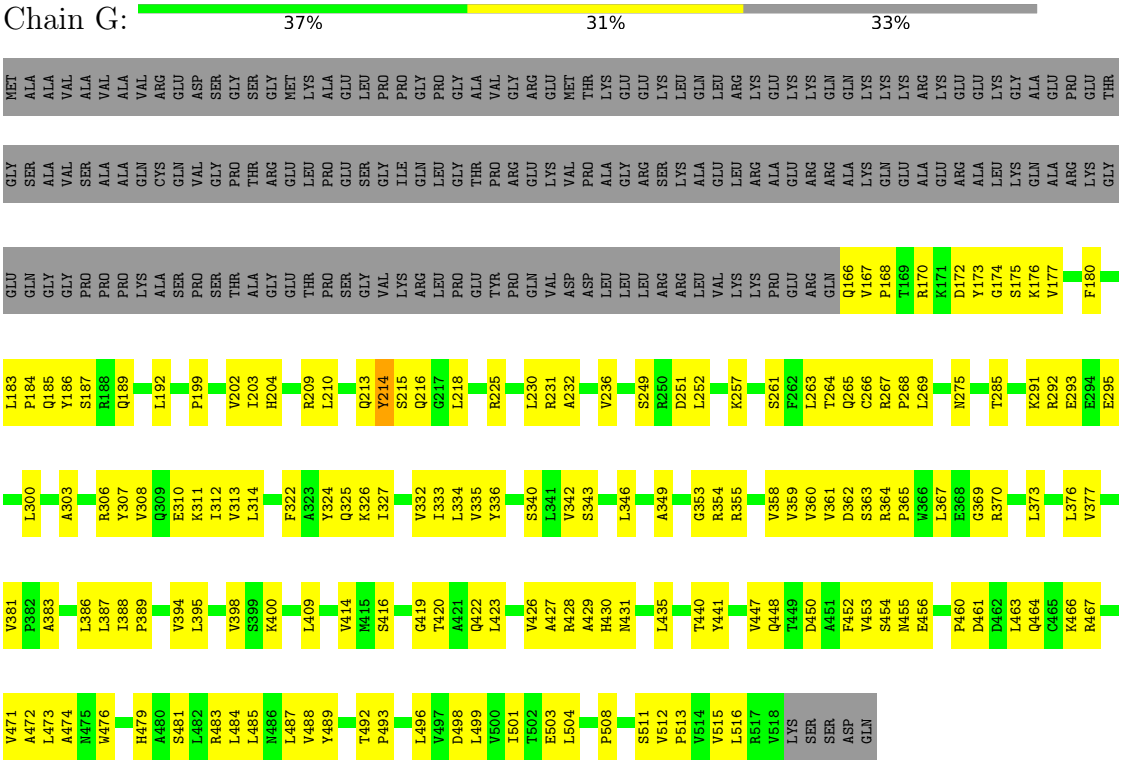
• Molecule 3: Translation initiation factor eIF-2B subunit gamma

Chain F:



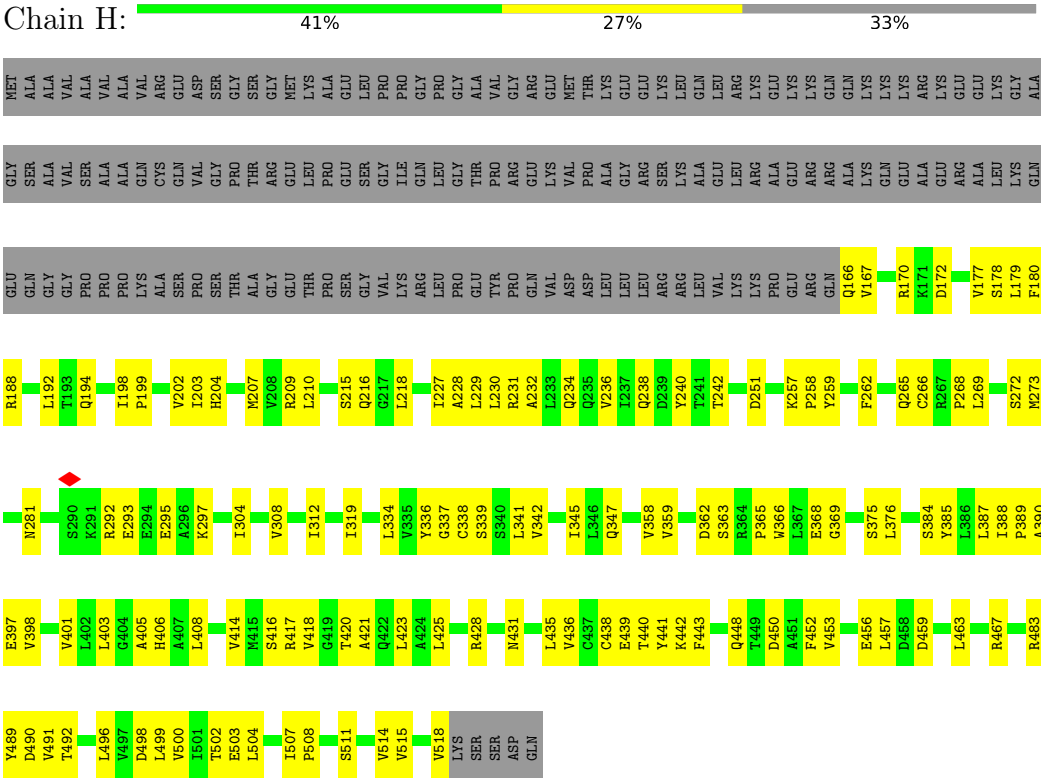
• Molecule 4: Translation initiation factor eIF-2B subunit delta

Chain G:



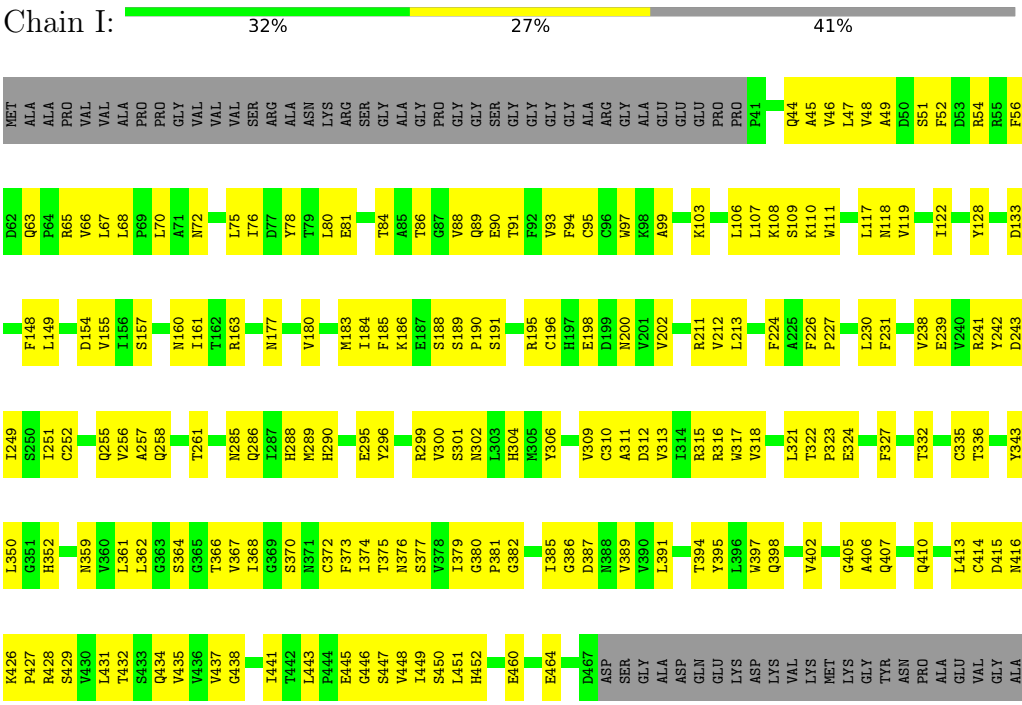
• Molecule 4: Translation initiation factor eIF-2B subunit delta

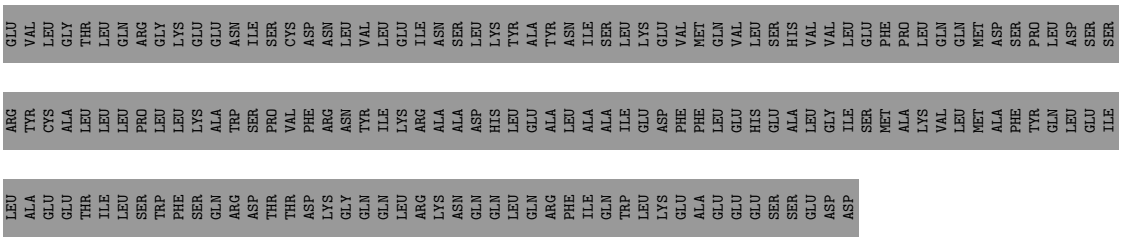
Chain H:



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

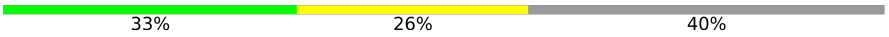
Chain I:

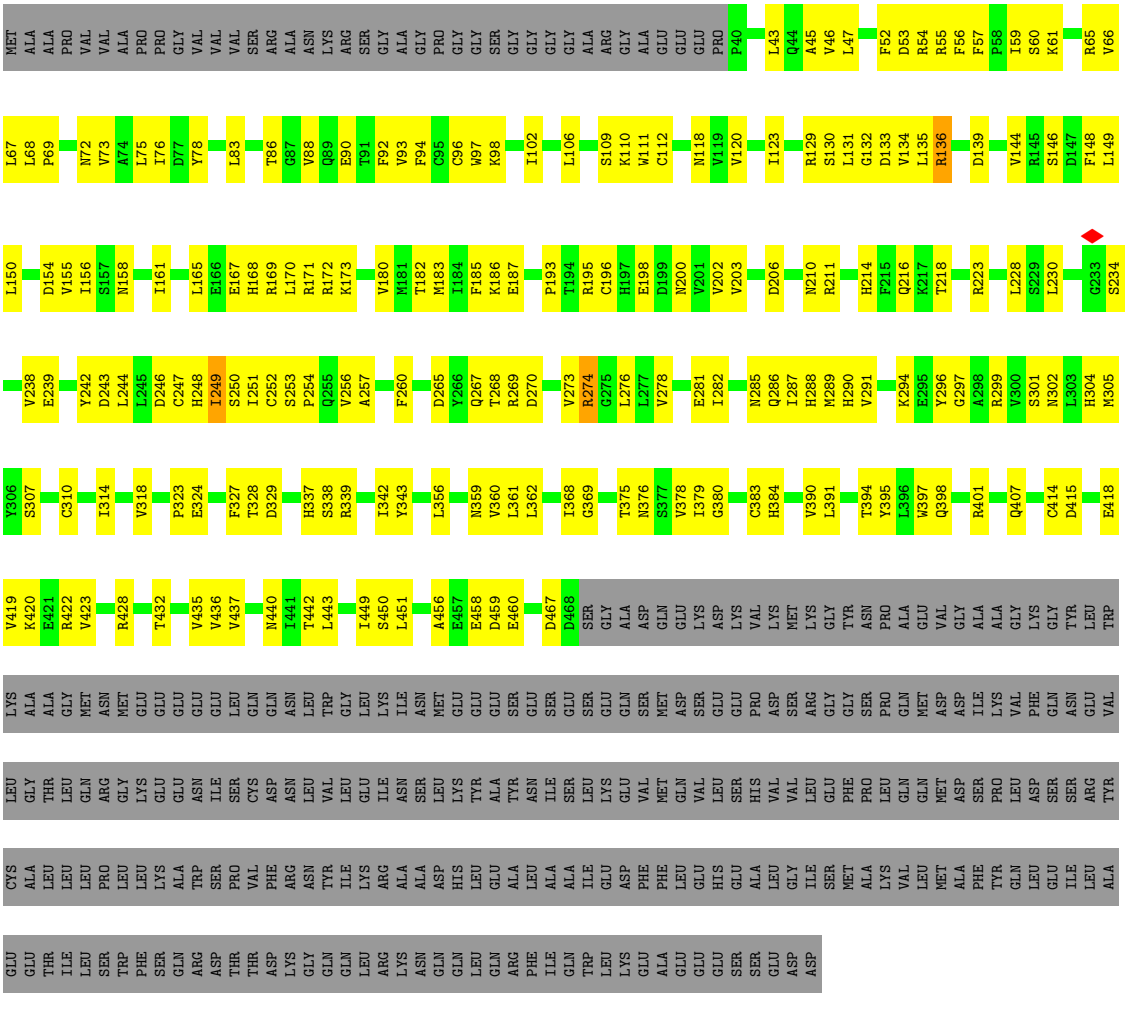




• Molecule 5: Translation initiation factor eIF-2B subunit epsilon

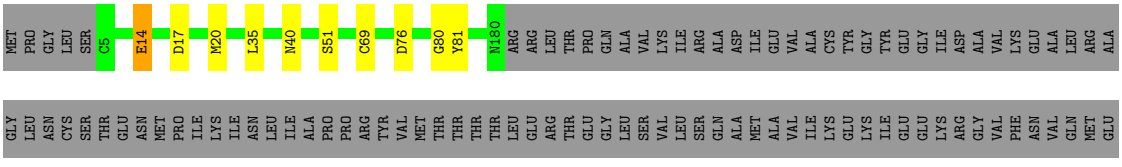
Chain J:



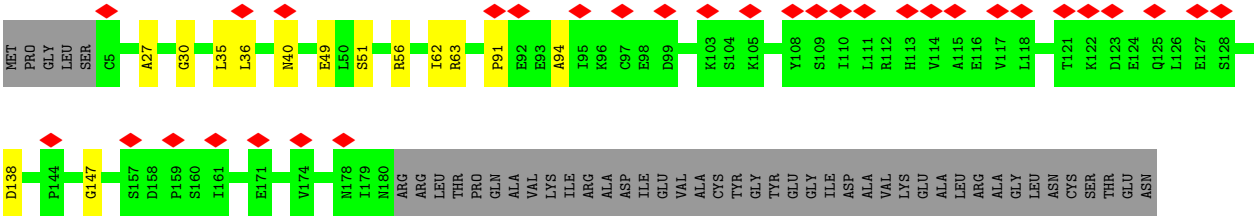


• Molecule 6: Eukaryotic translation initiation factor 2 subunit 1

Chain K:



• Molecule 6: Eukaryotic translation initiation factor 2 subunit 1



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	441.0, 441.0, 441.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.36	0/2296	0.51	0/3099
1	B	0.35	0/2281	0.50	0/3078
2	C	0.36	0/2522	0.51	0/3411
2	D	0.35	0/2587	0.52	0/3498
3	E	0.28	0/2464	0.48	0/3346
3	F	0.28	0/2463	0.50	0/3344
4	G	0.37	0/2802	0.52	0/3809
4	H	0.37	0/2802	0.51	0/3809
5	I	0.33	0/3427	0.50	0/4662
5	J	0.36	0/3443	0.52	0/4685
6	K	0.25	0/879	0.46	0/1224
6	L	0.24	0/879	0.43	0/1224
All	All	0.34	0/28845	0.51	0/39189

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.

There are no bond angle outliers.

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	103	0
2	C	2476	0	2493	108	0
2	D	2538	0	2538	101	0
3	E	2430	0	2197	91	0
3	F	2429	0	2196	105	0
4	G	2750	0	2811	133	0
4	H	2750	0	2811	125	0
5	I	3358	0	3325	151	0
5	J	3373	0	3336	151	0
6	K	889	0	401	5	0
6	L	889	0	401	11	0
All	All	28391	0	27162	1106	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 20.

All (1106) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:168:HIS:HD1	5:J:182:THR:HG1	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
4:H:240:TYR:O	4:H:297:LYS:NZ	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:34:LEU:HD21	1:B:49:LEU:HD21	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:E:55:THR:OG1	3:E:78:ILE:O	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
1:B:92:ILE:HG23	1:B:93:MET:HE2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:J:248:HIS:C	5:J:250:SER:H	2.10	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
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
5:J:132:GLY:C	5:J:136:ARG:HE	2.10	0.54
4:H:272:SER:HG	4:H:441:TYR:HE2	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:A:158:ASP:OD1	1:A:209:LYS:NZ	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:236:THR:OG1	2:C:238:THR:O	2.27	0.51
3:F:33:LYS:H	3:F:38:TYR:HH	1.57	0.51
3:F:133:ARG:HE	3:F:269:GLU:C	2.14	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:82:GLU:OE2	1:A:88:LYS:NZ	2.36	0.50
3:F:94:TYR:CG	3:F:216:MET:HG3	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:27:GLY:HA2	2:C:28:PRO:C	2.32	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:C:227:SER:C	2:C:228:ARG:HD2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:84:THR:HG1	5:I:111:TRP:HE1	1.57	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
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:C:219:ASP:OD1	2:C:219:ASP:N	2.47	0.47
2:D:51:TRP:CE3	2:D:57:LEU:HB2	2.48	0.47
3:F:8:MET:HE2	3:F:86:THR:HA	1.97	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
5:J:265:ASP:OD1	5:J:265:ASP:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:J:286:GLN:H	5:J:286:GLN:CD	2.18	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
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
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
2:D:166:MET:CE	2:D:229:VAL:HG21	2.46	0.46
4:G:435:LEU:HD23	4:G:501:ILE:HD11	1.97	0.46
1:A:197:ALA:HA	1:A:208:ASN:HD22	1.80	0.46
1:B:80:SER:HG	6:L:49:GLU:H	1.61	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:231:GLU:CD	1:A:231:GLU:H	2.17	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:D:61:ILE:HD13	2:D:61:ILE:HA	1.82	0.45
3:E:95:PRO:O	3:E:98:LYS:NZ	2.36	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
4:H:511:SER:O	4:H:511:SER:OG	2.30	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:229:LEU:HD22	4:H:273:MET:HE3	1.98	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
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
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
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
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
1:A:43:GLN:H	1:A:43:GLN:CD	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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
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: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
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
4:G:367:LEU:HD23	4:G:370:ARG:CZ	2.48	0.43
5:I:231:PHE:CD1	5:I:238:VAL:HG11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:SER:HG	5:J:112:CYS:H	1.66	0.43
5:J:200:ASN:HB2	5:J:218:THR:CG2	2.48	0.43
6:L:62:ILE:O	6:L:63:ARG:HB2	2.18	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
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
4:G:362:ASP:CG	4:G:369:GLY:H	2.21	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:HG13	5:J:282:ILE:O	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
2:C:249:THR:HA	2:C:314:ASP:CG	2.39	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:N	3:E:107:ASP:OD1	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: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)
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
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
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: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
2:C:166:MET:HE3	2:C:254:LEU:HD11	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:456:GLU:C	4:H:457:LEU:HD12	2.40	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:166:MET:HE2	2:C:229:VAL:HG21	2.00	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: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
4:H:272:SER:OG	4:H:441:TYR:HE2	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:472:ALA:C	4:G:473:LEU:HD12	2.40	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
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:A:208:ASN:CG	1:A:209:LYS:H	2.23	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
5:I:108:LYS:HE2	5:I:108:LYS:HB2	1.93	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:57:PHE:HE1	5:J:61:LYS:HD3	1.86	0.41
5:J:168:HIS:ND1	5:J:182:THR:OG1	2.34	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:E:133:ARG:C	3:E:199:LEU:HD13	2.42	0.41
3:F:60:GLN:C	3:F:61:LYS:HD3	2.41	0.41
3:F:102:LEU:HD13	3:F:206:CYS:HB2	2.03	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
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
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:B:156:GLN:N	1:B:157:PRO:HD2	2.36	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:388:ILE:C	4:H:390:ALA:H	2.25	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
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
5:J:248:HIS:C	5:J:250:SER:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/305 (95%)	254 (88%)	35 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	41 75
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%)	47 79
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%)	54 84

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	248/260 (95%)	247 (100%)	1 (0%)	91 94
1	B	247/260 (95%)	245 (99%)	2 (1%)	81 89
2	C	269/298 (90%)	268 (100%)	1 (0%)	91 94
2	D	276/298 (93%)	275 (100%)	1 (0%)	91 94
3	E	214/398 (54%)	212 (99%)	2 (1%)	78 88
3	F	214/398 (54%)	212 (99%)	2 (1%)	78 88
4	G	309/444 (70%)	308 (100%)	1 (0%)	92 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	378 (99%)	5 (1%)	69 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%)	2841 (100%)	15 (0%)	89 93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	B	46	ARG
1	B	302	LYS
2	C	201	HIS
2	D	29	ARG
3	E	45	ARG
3	E	133	ARG
3	F	98	LYS
3	F	161	ASP
4	G	214	TYR
5	J	54	ARG
5	J	136	ARG
5	J	223	ARG
5	J	274	ARG
5	J	428	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	B	13	GLN
1	B	156	GLN
1	B	208	ASN
1	B	213	ASN
1	B	223	ASN
2	C	49	HIS
2	C	132	ASN
2	C	138	ASN
2	C	154	GLN

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Mol	Chain	Res	Type
2	C	158	HIS
2	C	160	HIS
2	C	252	HIS
2	C	261	HIS
2	C	331	ASN
2	D	97	HIS
2	D	119	ASN
2	D	158	HIS
2	D	199	GLN
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	283	ASN
4	G	166	GLN
4	G	189	GLN
4	G	213	GLN
4	G	216	GLN
4	G	254	ASN
4	G	265	GLN
4	G	281	ASN
4	G	325	GLN
4	G	406	HIS
4	G	430	HIS
4	G	455	ASN
4	G	479	HIS
4	H	194	GLN
4	H	234	GLN
4	H	265	GLN
4	H	274	HIS
4	H	281	ASN
4	H	347	GLN
4	H	430	HIS
5	I	197	HIS
5	I	200	ASN
5	I	214	HIS
5	I	248	HIS
5	I	255	GLN
5	I	304	HIS

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Mol	Chain	Res	Type
5	I	388	ASN
5	J	44	GLN
5	J	72	ASN
5	J	279	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	1.55	1 (12%)	8,12,14	1.53	2 (25%)
6	SEP	L	51	6	8,9,10	1.54	1 (12%)	8,12,14	1.66	2 (25%)

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	-	2/5/8/10	-
6	SEP	L	51	6	-	4/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	51	SEP	P-O1P	3.39	1.61	1.50
6	L	51	SEP	P-O1P	3.35	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	51	SEP	P-OG-CB	-3.39	108.96	118.30
6	K	51	SEP	P-OG-CB	-3.07	109.83	118.30
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

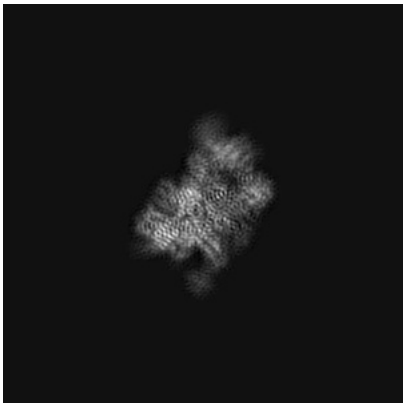
6 Map visualisation

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

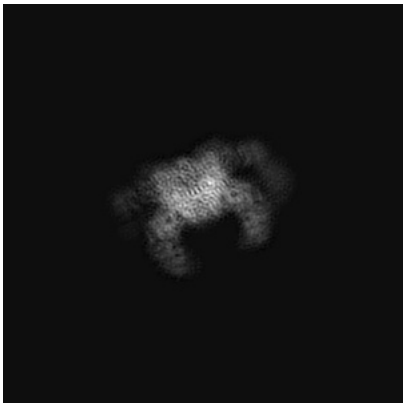
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

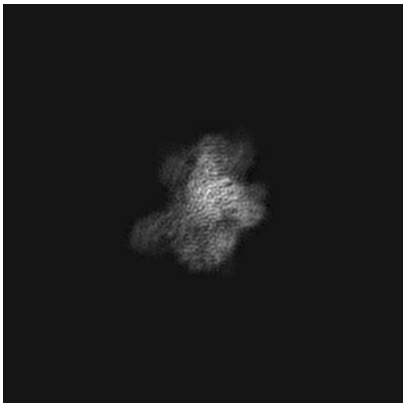
6.1.1 Primary map



X



Y

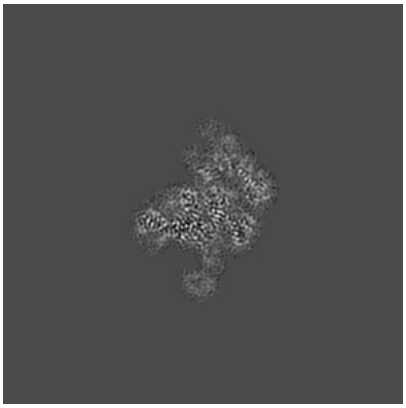


Z

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

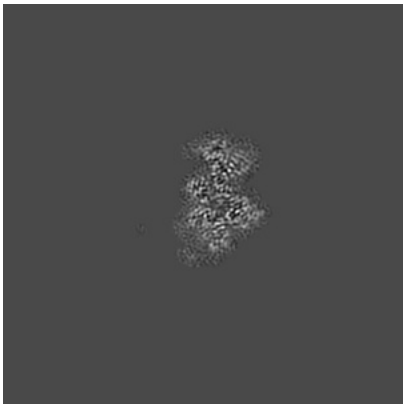
6.2 Central slices

6.2.1 Primary map



X Index: 150

Y Index: 150

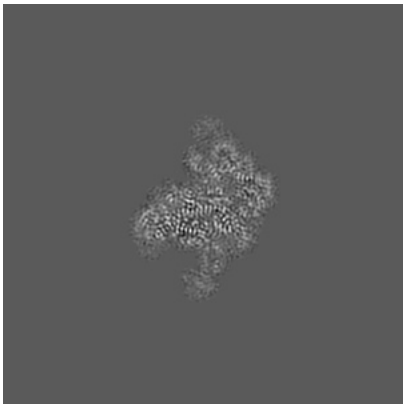


Z Index: 150

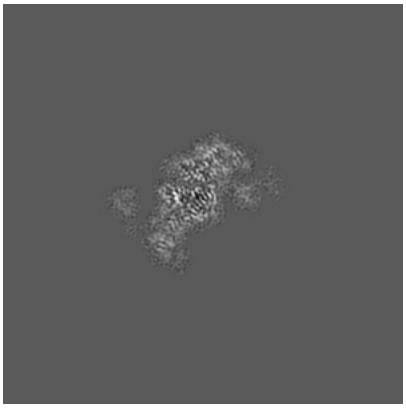
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

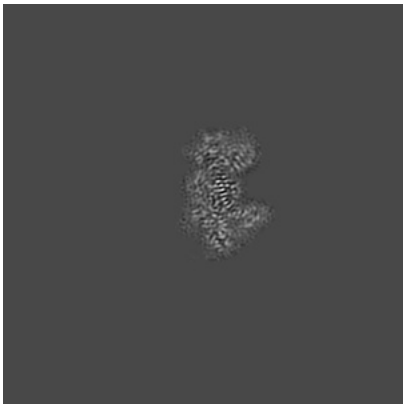
6.3.1 Primary map



X Index: 154



Y Index: 140



Z Index: 157

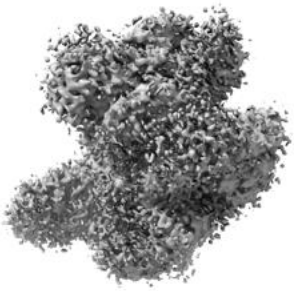
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

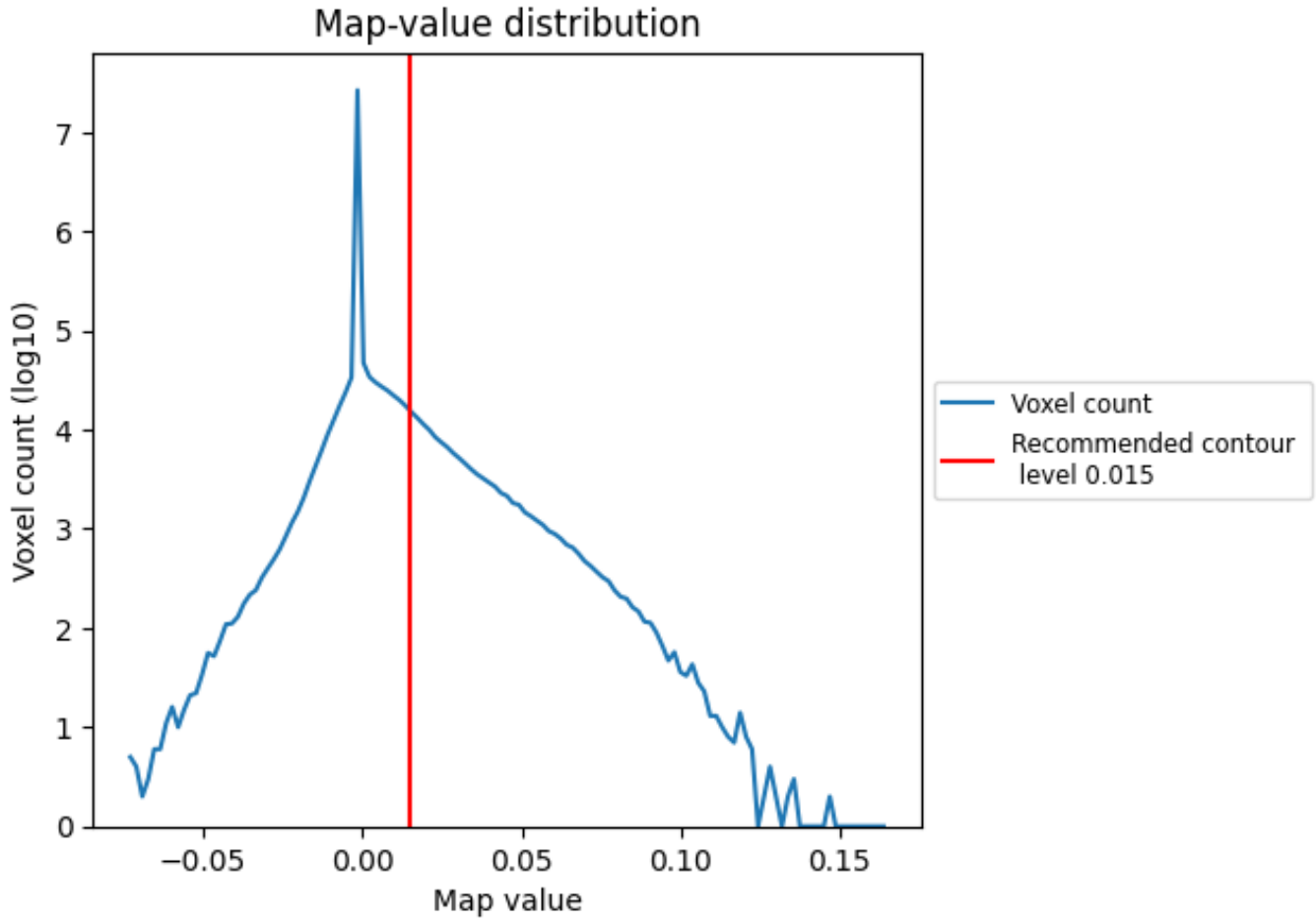
6.5 Mask visualisation (i)

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

7 Map analysis

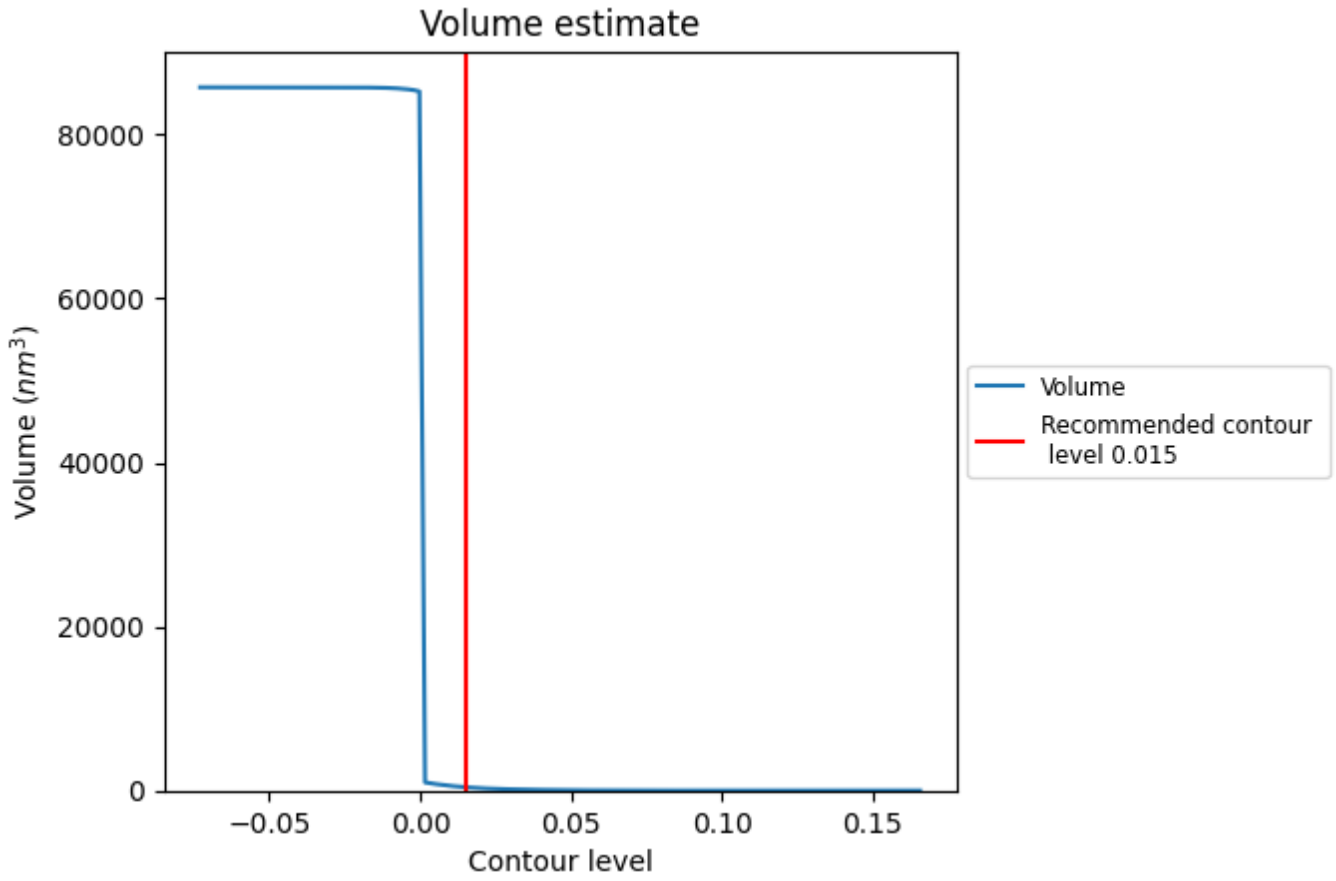
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

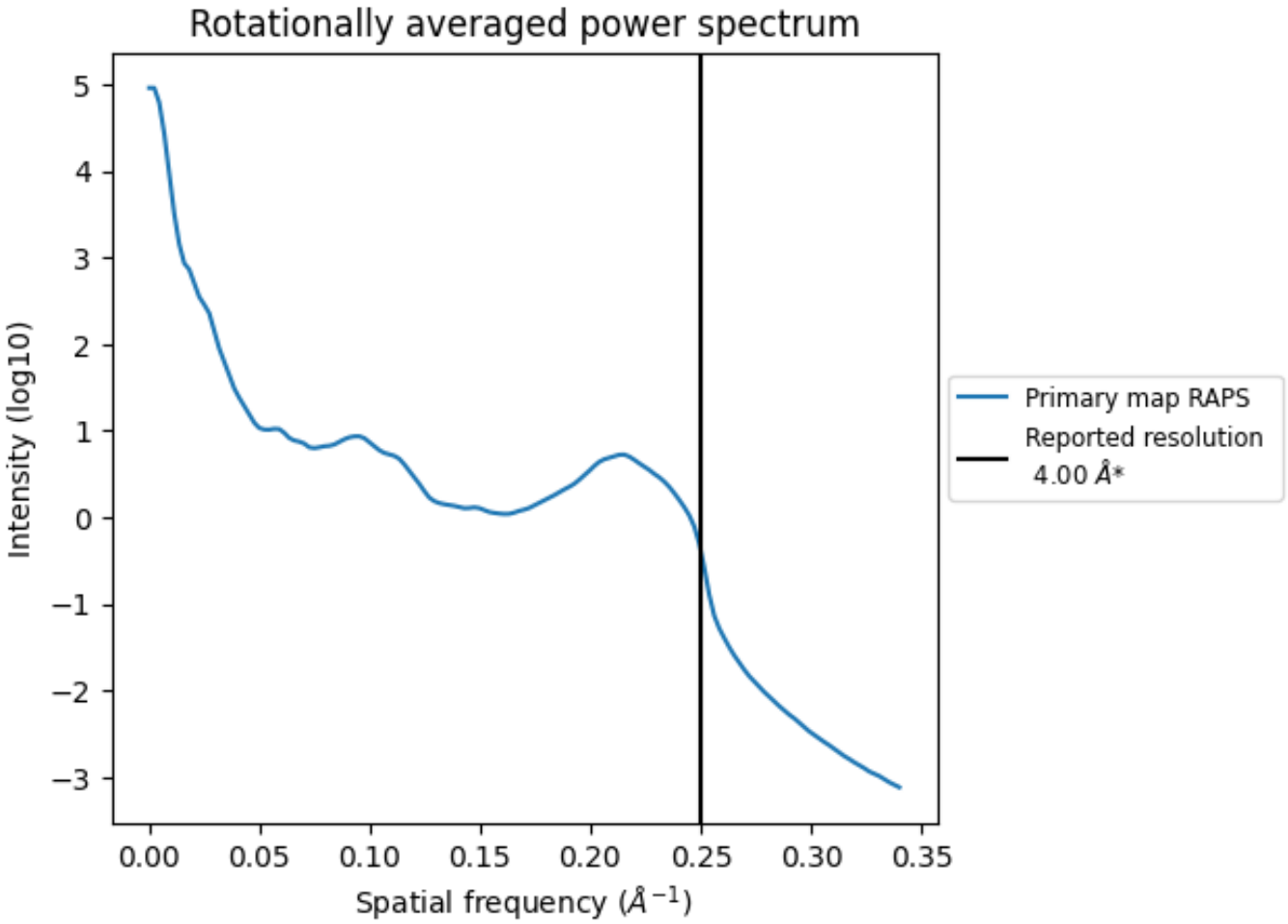
7.2 Volume estimate



The volume at the recommended contour level is 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}

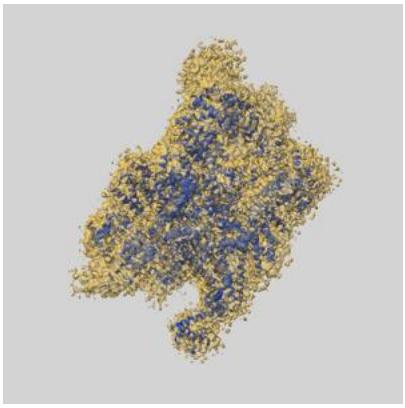
8 Fourier-Shell correlation

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

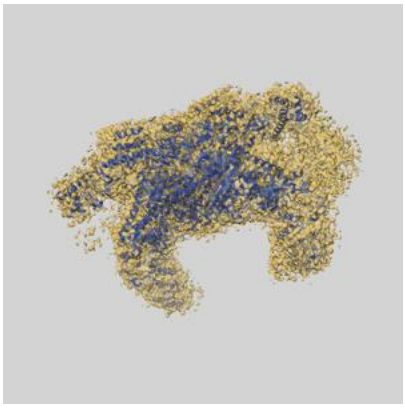
9 Map-model fit

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.

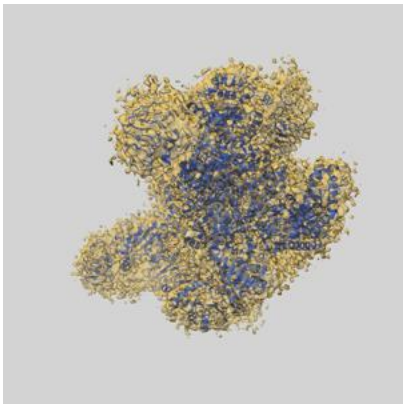
9.1 Map-model overlay



X



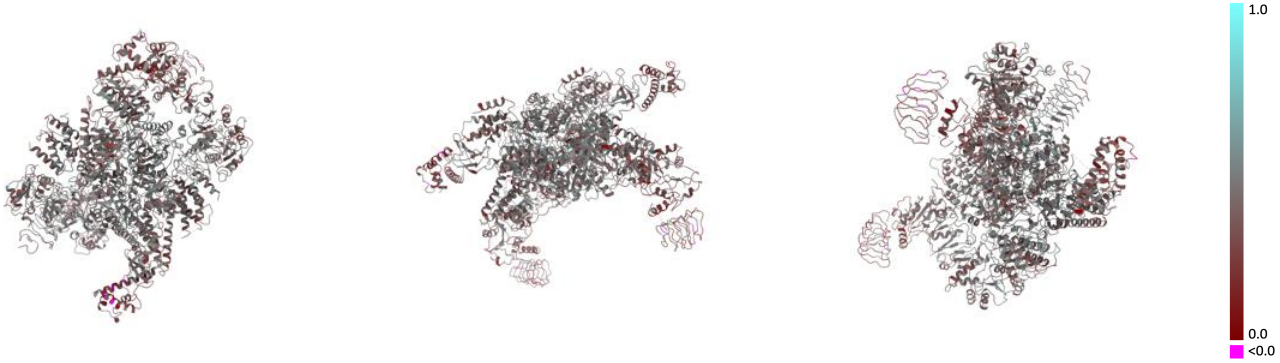
Y



Z

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.

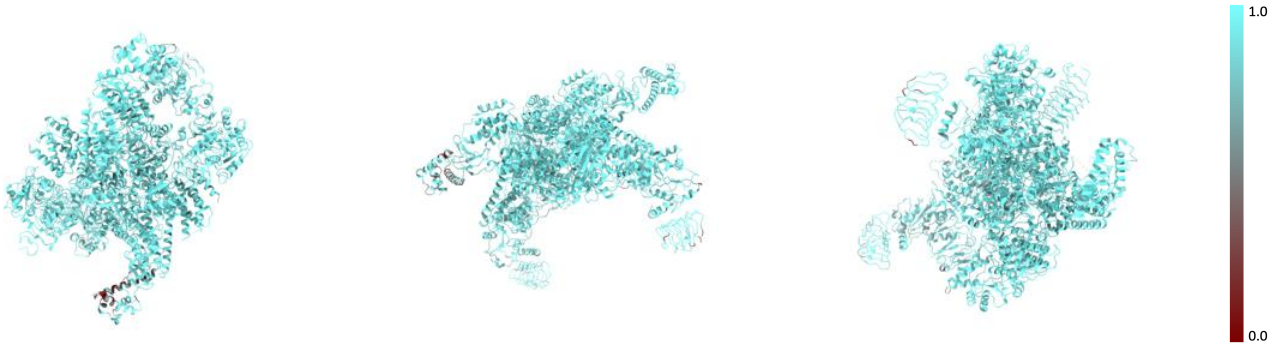
9.2 Q-score mapped to coordinate model (i)



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.

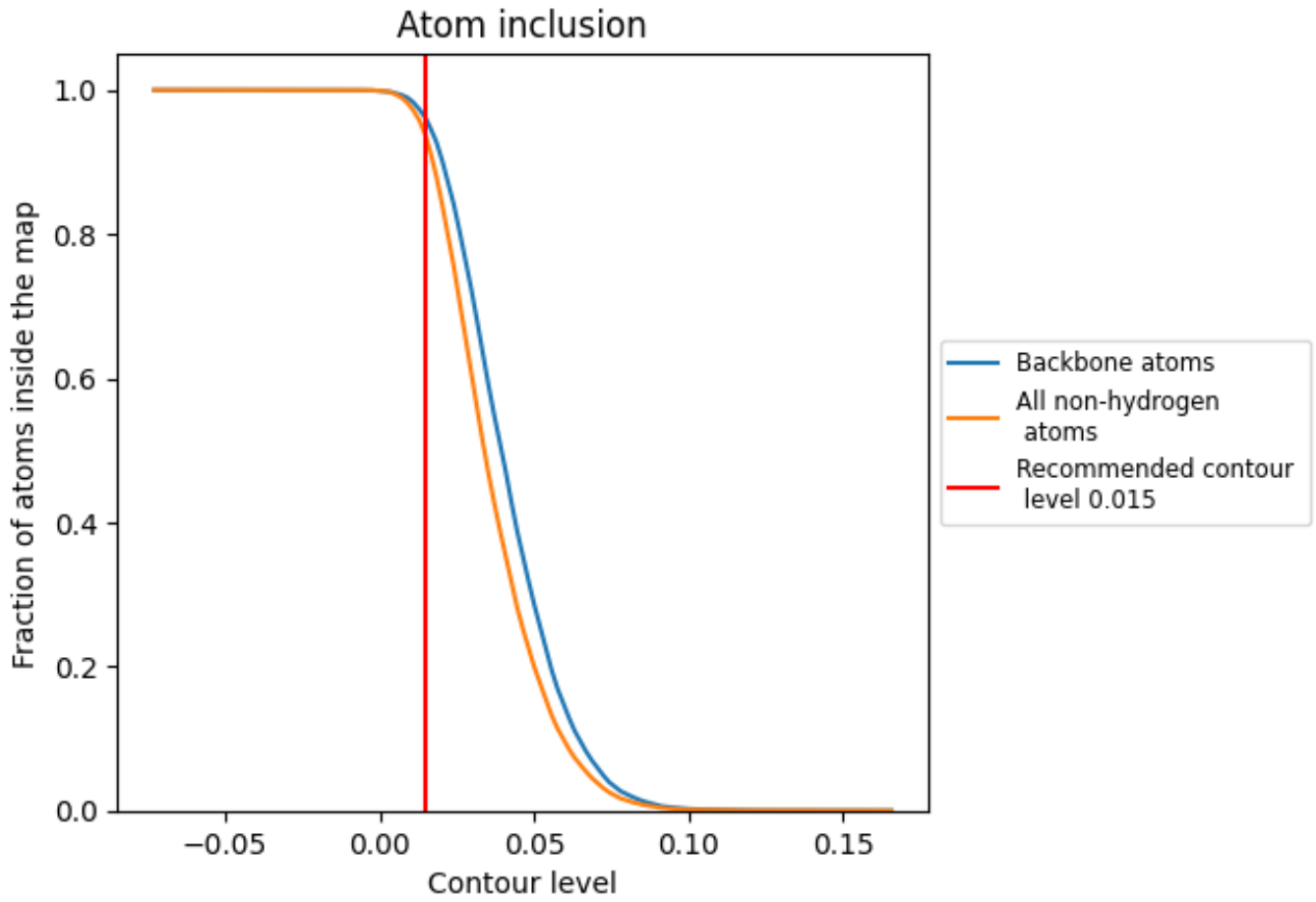
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



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	0.9358	0.4210
A	0.9583	0.4330
B	0.9463	0.4380
C	0.9457	0.4460
D	0.9571	0.4470
E	0.8904	0.3600
F	0.9163	0.3530
G	0.9494	0.4450
H	0.9341	0.4420
I	0.9502	0.4290
J	0.9543	0.4400
K	0.9526	0.3840
L	0.7655	0.3590