Full wwPDB EM Validation Report ⓘ

Aug 26, 2024 – 12:13 PM EDT

PDB ID	:	9C7V
EMDB ID	:	EMD-45295
Title	:	Structure of the human BOS:human EMC complex in GDN
Authors	:	Nguyen, V.N.; Tomaleri, G.P.; Voorhees, R.M.
Deposited on	:	2024-06-11
Resolution	:	6.60 Å(reported)
Based on initial models	:	9C7U, 8S9S

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:

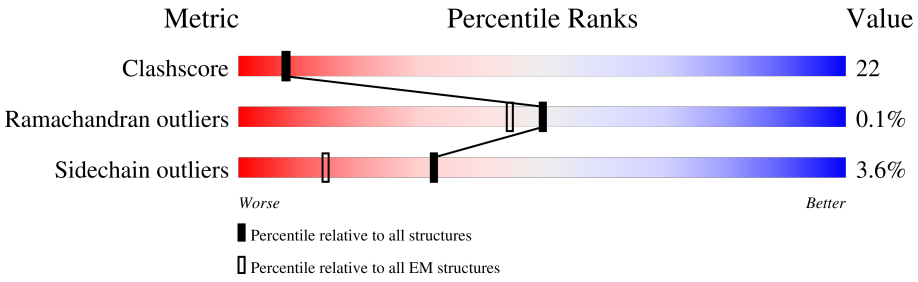
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	10	262	13% 30% 29% 41%
2	1	993	11% 51% 39% • 8%
3	2	297	8% 55% 38% • 5%
4	3	261	20% 46% 38% • 14%
5	4	183	55% 66% 12% • 21%
6	5	131	13% 40% 34% • 23%
7	6	110	5% 57% 33% 10%
8	7	242	20% 38% 19% 44%

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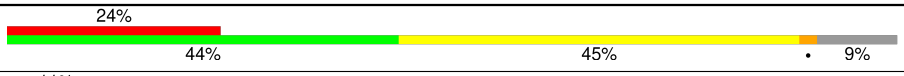
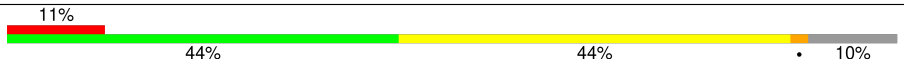
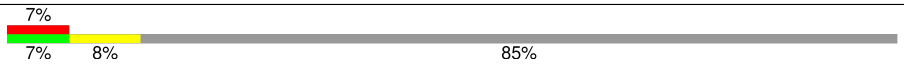
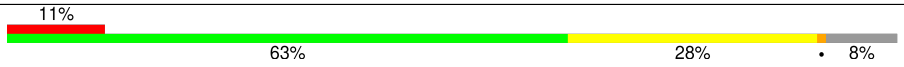
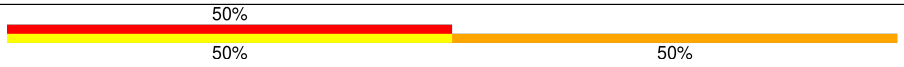
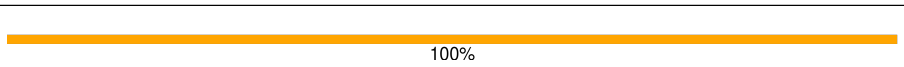
Mol	Chain	Length	Quality of chain
9	8	210	
10	A	563	
11	B	1267	
12	C	224	
13	D	2	
13	E	2	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 24532 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 ER membrane protein complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	10	154	1177	729	214	231	3	0	0

- Molecule 2 is a protein called ER membrane protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	916	7275	4668	1247	1336	24	0	0

- Molecule 3 is a protein called ER membrane protein complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	281	2306	1447	411	434	14	0	0

- Molecule 4 is a protein called ER membrane protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	225	1833	1194	298	332	9	0	0

- Molecule 5 is a protein called ER membrane protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	144	867	547	154	165	1	0	0

- Molecule 6 is a protein called Membrane magnesium transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	101	795	517	140	135	3	0	0

- Molecule 7 is a protein called ER membrane protein complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	99	Total	C	N	O	S	0	0
			774	521	126	125	2		

- Molecule 8 is a protein called ER membrane protein complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	136	Total	C	N	O	S	0	0
			1054	679	182	189	4		

- Molecule 9 is a protein called ER membrane protein complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	192	Total	C	N	O	S	0	0
			1533	968	266	287	12		

- Molecule 10 is a protein called Nicalin.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	505	Total	C	N	O	S	0	0
			3979	2521	703	738	17		

- Molecule 11 is a protein called BOS complex subunit NOMO2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	186	Total	C	N	O	S	0	0
			1482	942	251	286	3		

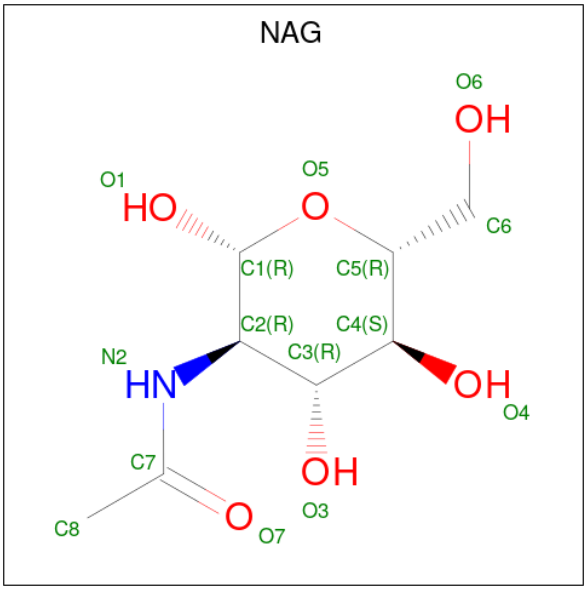
- Molecule 12 is a protein called Transmembrane protein 147.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	205	Total	C	N	O	S	0	0
			1373	885	234	247	7		

- Molecule 13 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
13	D	2	Total C N O 28 16 2 10	0	0
13	E	2	Total C N O 28 16 2 10	0	0

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



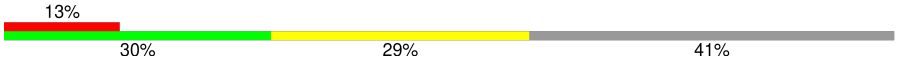
Mol	Chain	Residues	Atoms	AltConf
14	1	1	Total C N O 14 8 1 5	0
14	1	1	Total C N O 14 8 1 5	0

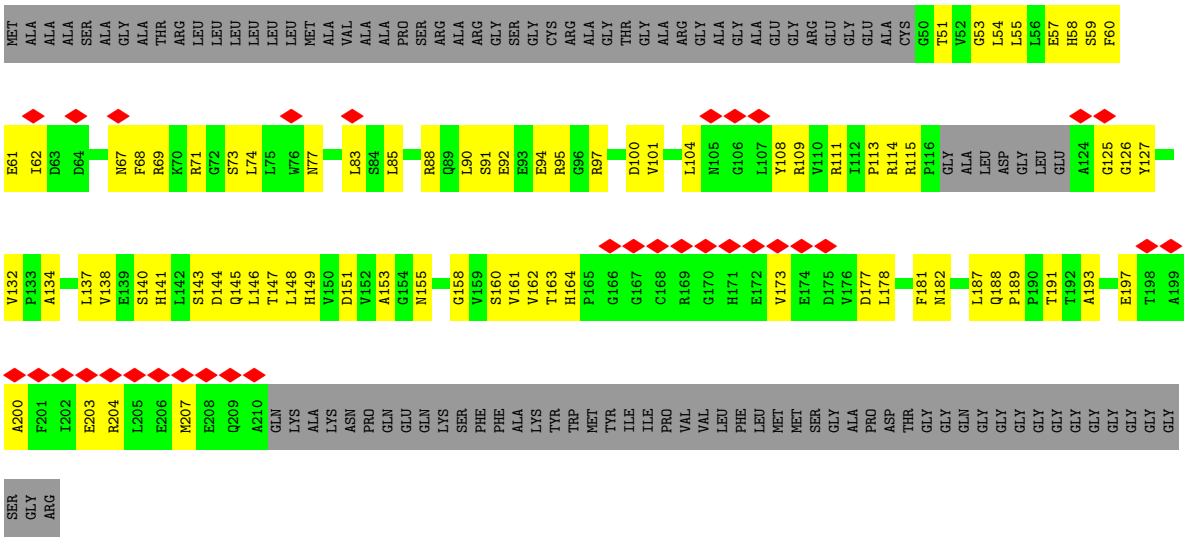
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ER membrane protein complex subunit 10

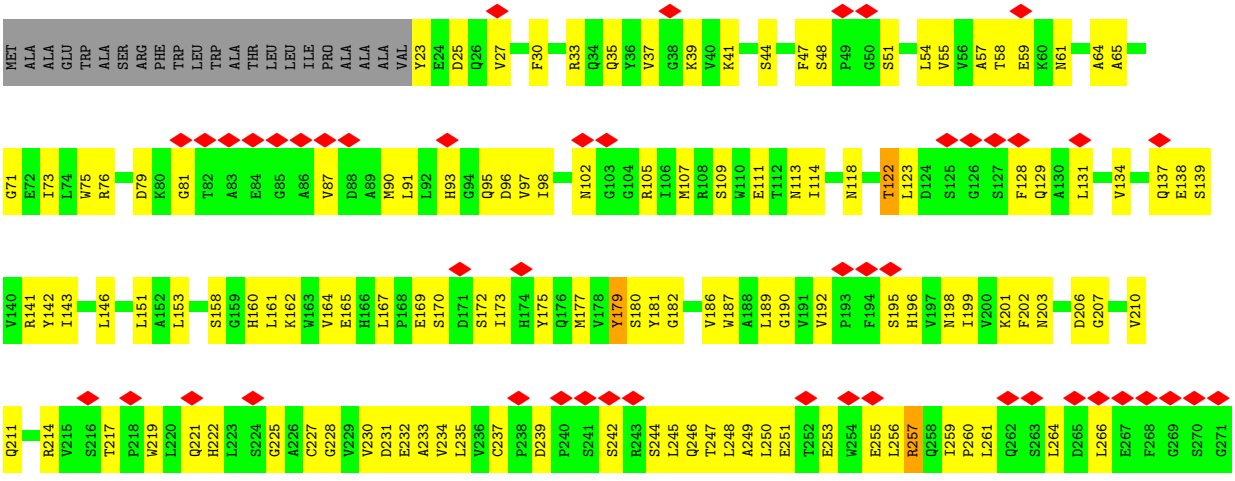
Chain 10:

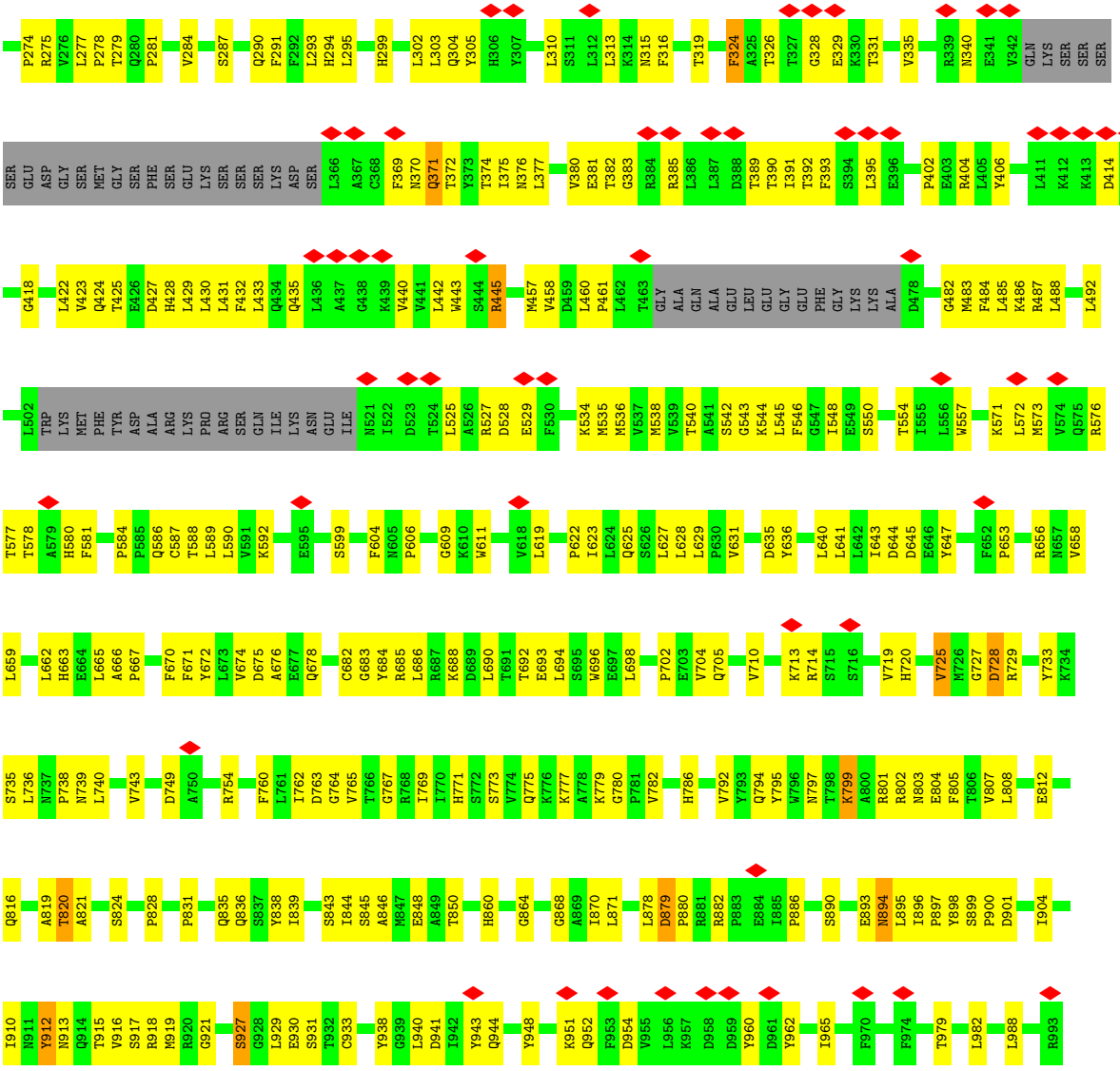




• Molecule 2: ER membrane protein complex subunit 1

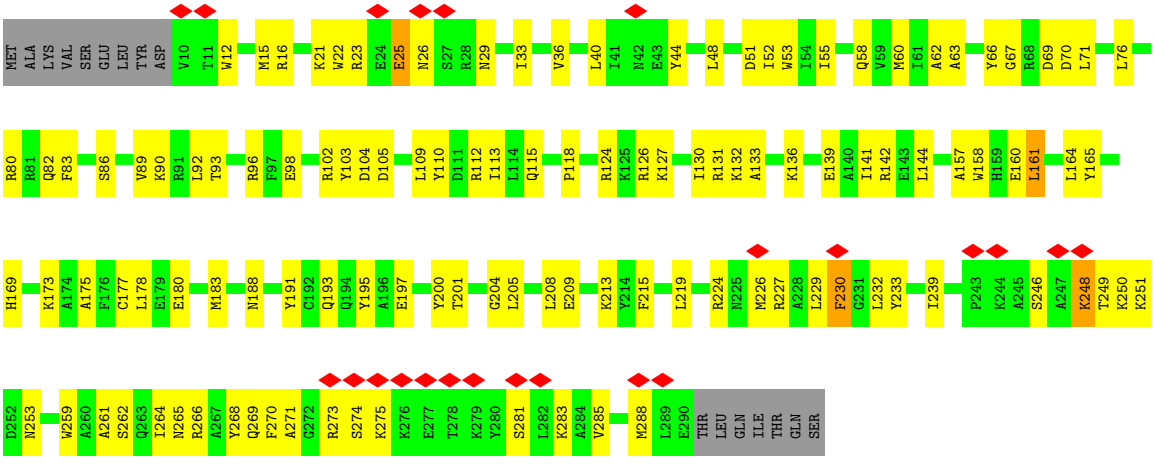
Chain 1:





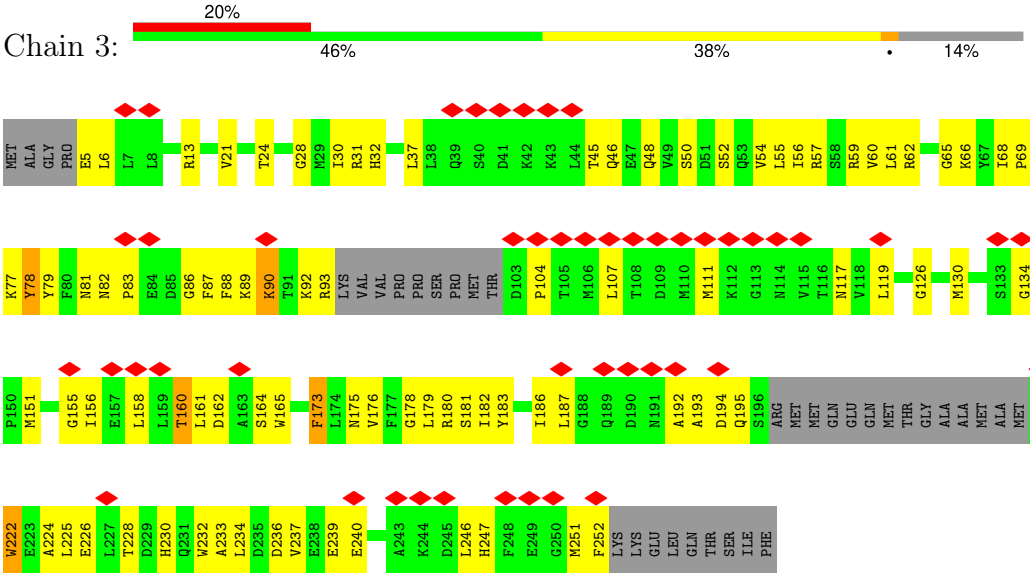
• Molecule 3: ER membrane protein complex subunit 2

Chain 2:



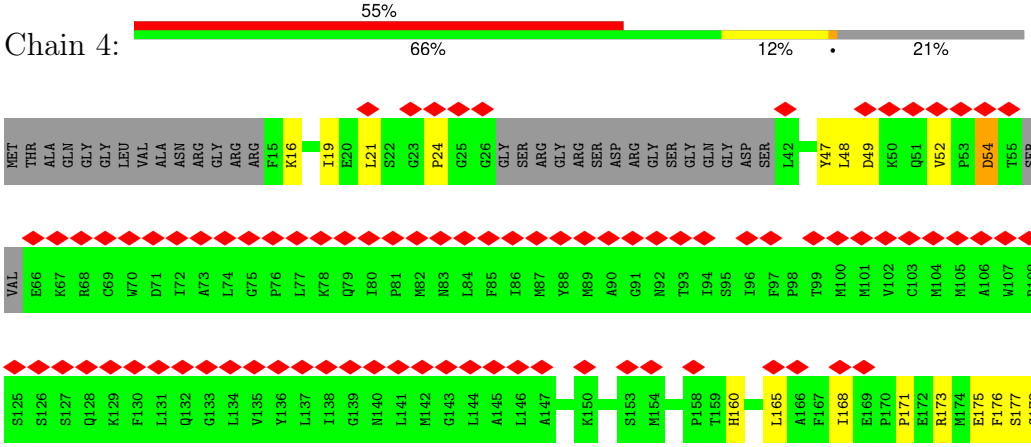
• Molecule 4: ER membrane protein complex subunit 3

Chain 3:



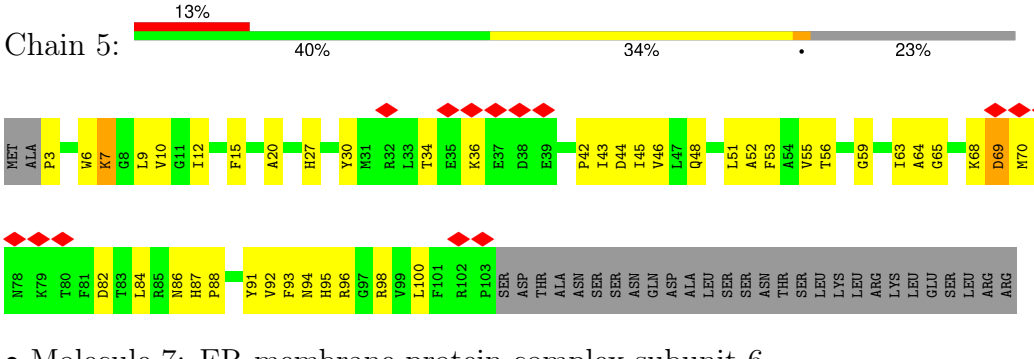
• Molecule 5: ER membrane protein complex subunit 4

Chain 4:



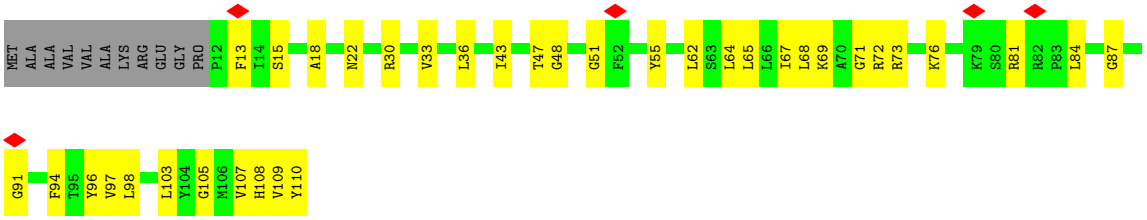
• Molecule 6: Membrane magnesium transporter 1

Chain 5:



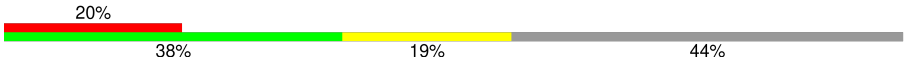
• Molecule 7: ER membrane protein complex subunit 6

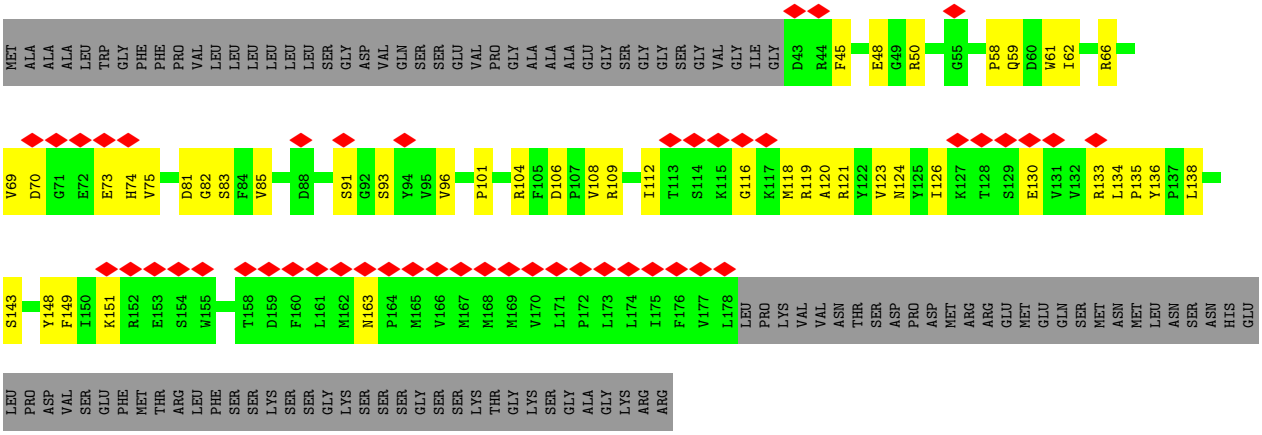
Chain 6:



• Molecule 8: ER membrane protein complex subunit 7

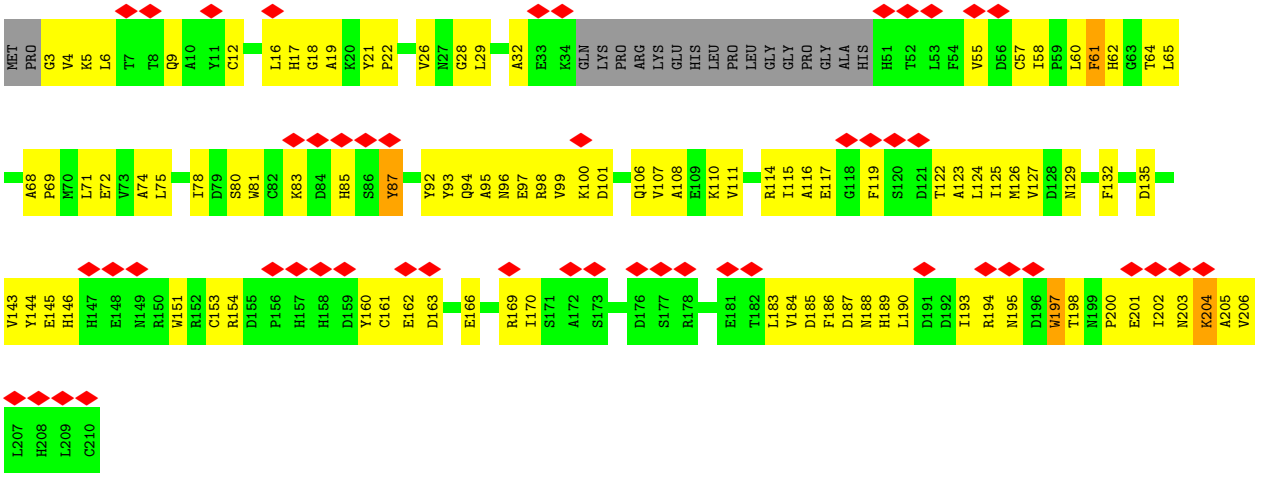
Chain 7:





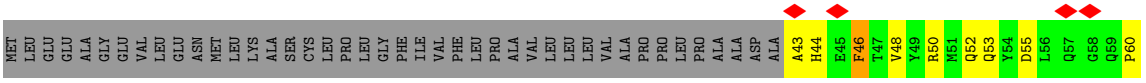
• Molecule 9: ER membrane protein complex subunit 8

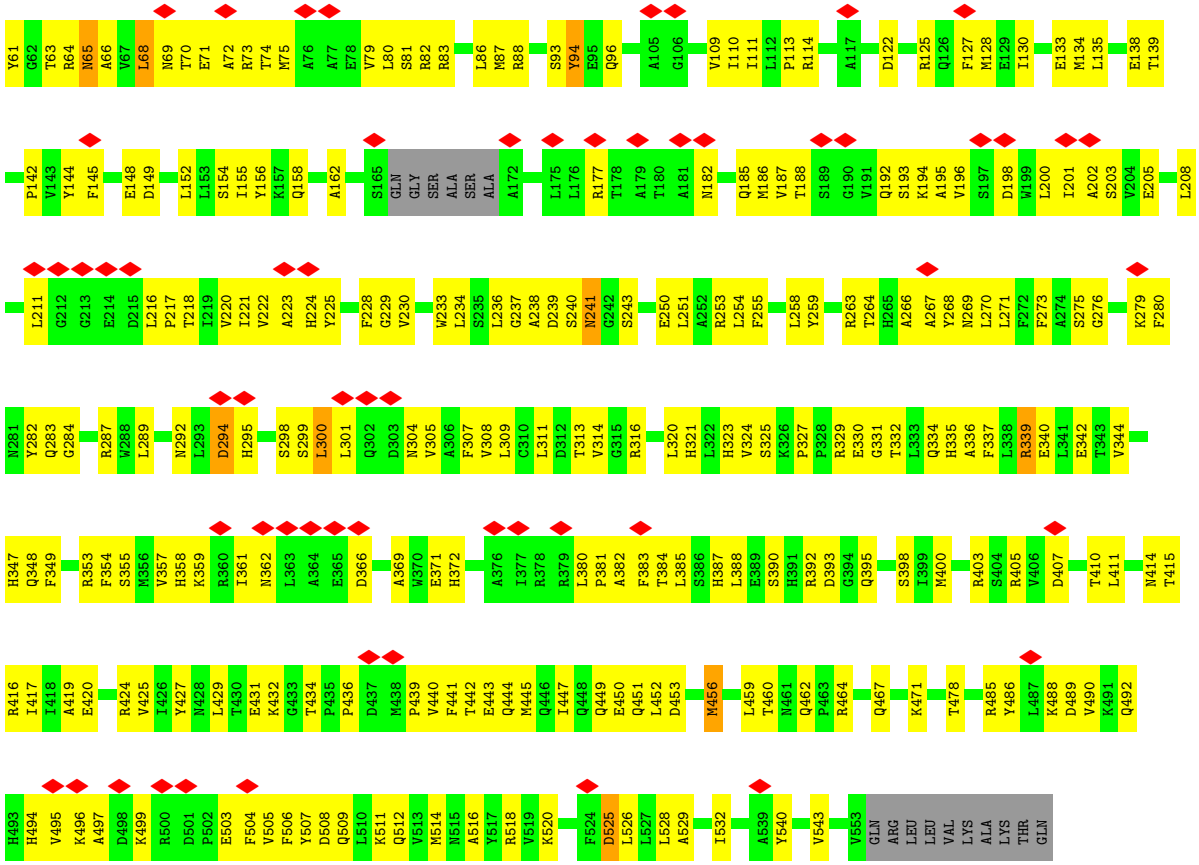
Chain 8:



• Molecule 10: Nicalin

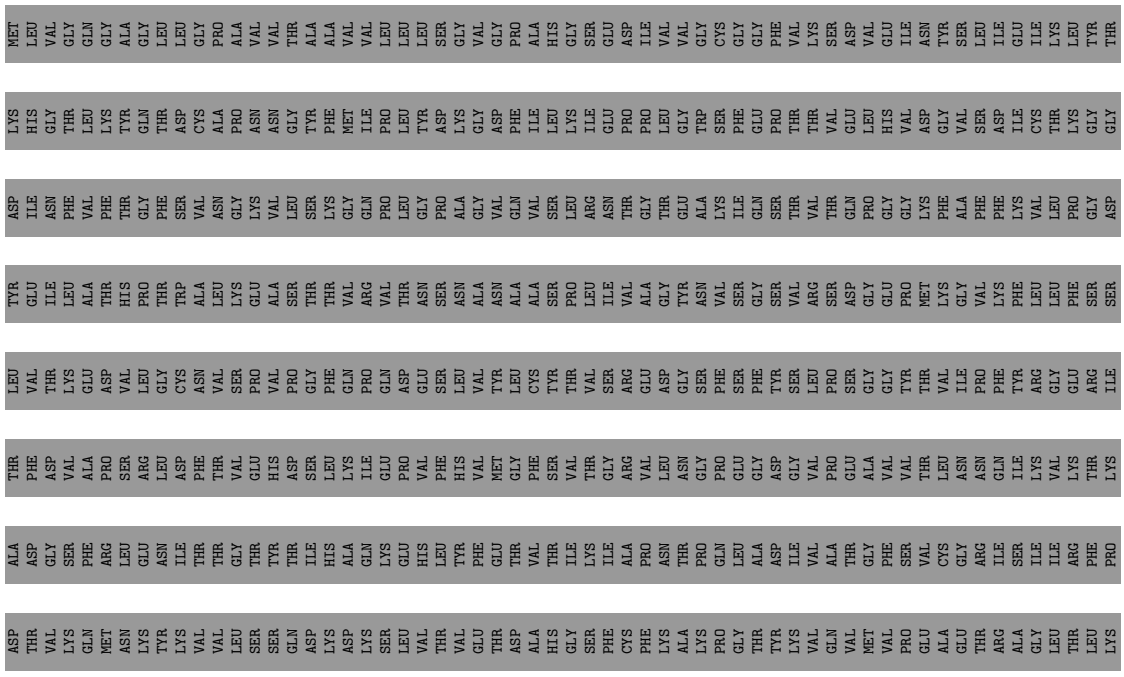
Chain A:

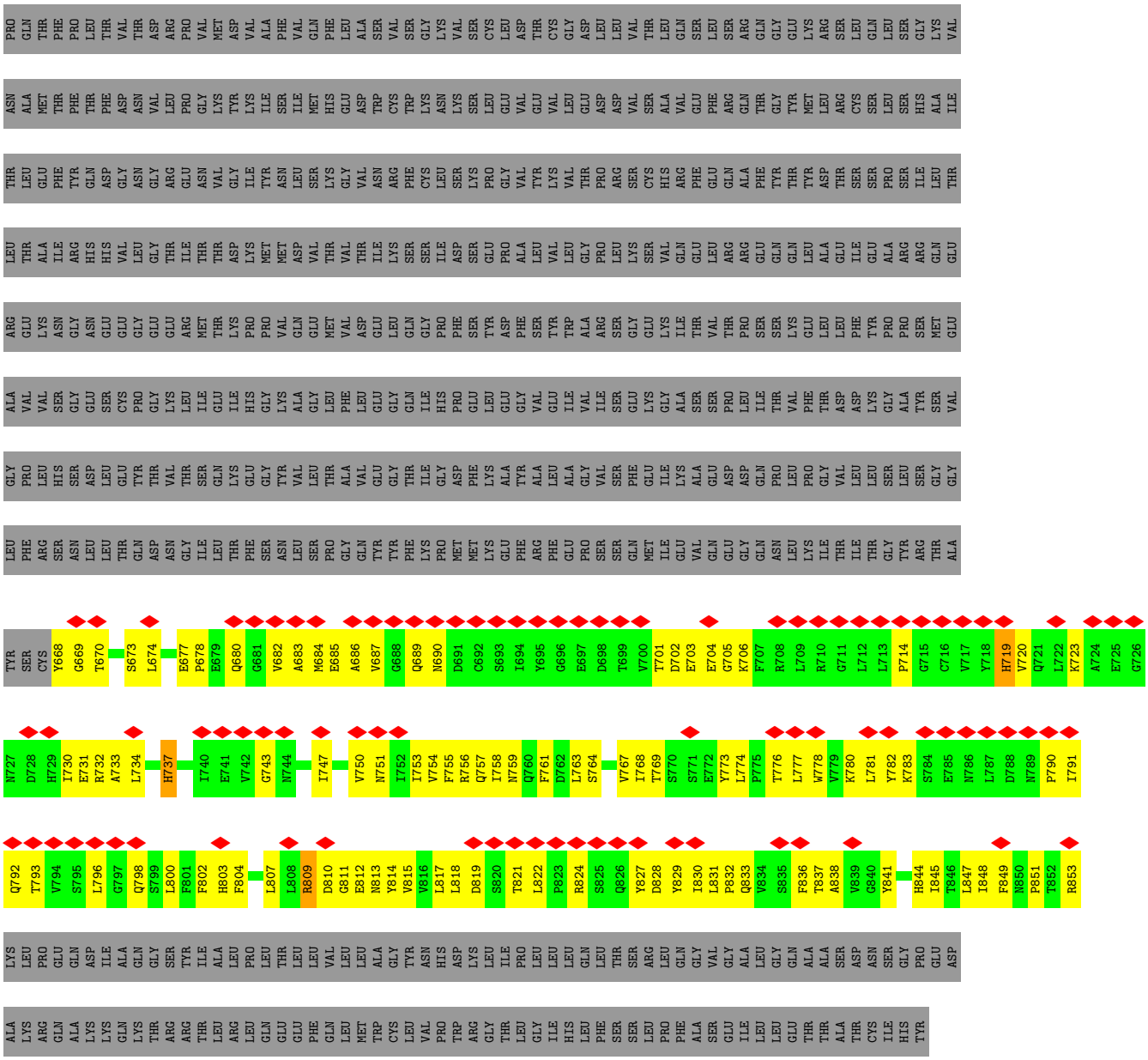




• Molecule 11: BOS complex subunit NOMO2

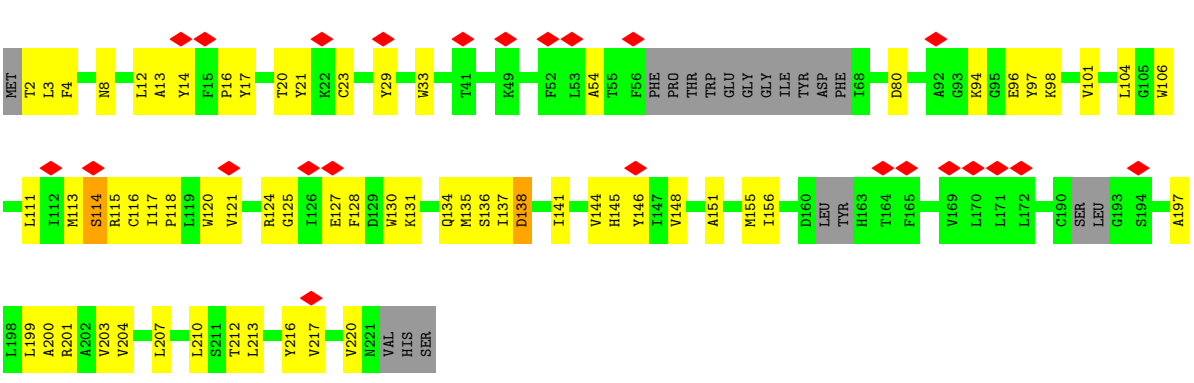
Chain B: 7% 7% 8% 85%





• Molecule 12: Transmembrane protein 147

Chain C:



• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45703	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.418	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0769	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

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	10	0.29	0/1197	0.60	0/1625
2	1	0.31	0/7439	0.56	1/10110 (0.0%)
3	2	0.28	0/2349	0.50	0/3158
4	3	0.30	0/1875	0.55	1/2537 (0.0%)
5	4	0.27	0/884	0.42	0/1219
6	5	0.34	0/816	0.56	0/1104
7	6	0.33	0/795	0.60	1/1077 (0.1%)
8	7	0.29	0/1084	0.58	0/1475
9	8	0.28	0/1572	0.52	0/2141
10	A	0.36	0/4059	0.63	1/5506 (0.0%)
11	B	0.31	0/1517	0.57	0/2067
12	C	0.31	0/1398	0.53	0/1915
All	All	0.31	0/24985	0.56	4/33934 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	728	ASP	CB-CG-OD1	5.64	123.37	118.30
4	3	83	PRO	CA-N-CD	-5.43	103.90	111.50
7	6	65	LEU	CA-CB-CG	-5.27	103.18	115.30
10	A	525	ASP	CB-CG-OD1	5.16	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10	1177	0	1146	65	0
2	1	7275	0	7334	319	0
3	2	2306	0	2241	109	0
4	3	1833	0	1842	94	0
5	4	867	0	623	31	0
6	5	795	0	793	39	0
7	6	774	0	803	34	0
8	7	1054	0	1014	27	0
9	8	1533	0	1470	91	0
10	A	3979	0	3935	229	0
11	B	1482	0	1433	87	0
12	C	1373	0	1162	55	0
13	D	28	0	25	3	0
13	E	28	0	25	3	0
14	1	28	0	26	3	0
All	All	24532	0	23872	1080	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 22.

All (1080) 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)
8:7:134:LEU:HD12	8:7:135:PRO:HD2	1.46	0.93
10:A:205:GLU:O	10:A:490:VAL:HA	1.76	0.86
2:1:230:VAL:HG12	2:1:278:PRO:HB3	1.58	0.86
10:A:217:PRO:HA	10:A:304:ASN:HB3	1.58	0.85
10:A:403:ARG:NH2	10:A:453:ASP:OD1	2.08	0.85
10:A:65:ASN:OD1	10:A:192:GLN:NE2	2.10	0.84
5:4:19:ILE:HG22	9:8:114:ARG:HG3	1.58	0.82
10:A:307:PHE:HB3	10:A:334:GLN:HG2	1.62	0.81
12:C:94:LYS:HB3	12:C:97:TYR:HB2	1.62	0.81
10:A:429:LEU:HB3	10:A:434:THR:HG21	1.63	0.81
10:A:525:ASP:OD1	12:C:8:ASN:ND2	2.13	0.81
10:A:416:ARG:NH1	10:A:441:PHE:O	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:241:ASN:ND2	10:A:311:LEU:O	2.15	0.79
1:10:74:LEU:HB3	1:10:83:LEU:HD11	1.63	0.79
10:A:478:THR:OG1	11:B:800:LEU:N	2.14	0.79
10:A:114:ARG:NH2	10:A:149:ASP:OD1	2.16	0.79
10:A:65:ASN:HB3	10:A:142:PRO:HD3	1.65	0.78
10:A:442:THR:H	11:B:732:ARG:HH12	1.28	0.78
8:7:69:VAL:HB	8:7:74:HIS:HB2	1.62	0.78
2:1:281:PRO:HB3	2:1:326:THR:HG21	1.66	0.78
3:2:283:LYS:HD3	9:8:81:TRP:HA	1.67	0.77
2:1:432:PHE:O	2:1:442:LEU:N	2.14	0.77
4:3:149:LYS:NZ	4:3:161:LEU:O	2.17	0.76
6:5:64:ALA:HB3	7:6:69:LYS:HE2	1.67	0.76
4:3:89:LYS:O	4:3:92:LYS:NZ	2.17	0.76
10:A:424:ARG:NH1	10:A:434:THR:O	2.19	0.76
2:1:370:ASN:HB3	2:1:372:THR:HG23	1.67	0.76
2:1:161:LEU:HD21	2:1:164:VAL:HG23	1.69	0.75
10:A:263:ARG:NH2	11:B:677:GLU:OE1	2.18	0.75
11:B:782:TYR:HB2	11:B:815:VAL:HB	1.67	0.74
10:A:162:ALA:O	10:A:177:ARG:NH2	2.20	0.74
2:1:576:ARG:NE	2:1:584:PRO:O	2.20	0.74
10:A:344:VAL:HG13	10:A:348:GLN:HG3	1.70	0.74
4:3:87:PHE:O	4:3:89:LYS:NZ	2.20	0.73
12:C:2:THR:N	12:C:125:GLY:O	2.21	0.73
1:10:61:GLU:OE2	1:10:67:ASN:ND2	2.23	0.72
7:6:30:ARG:NH1	7:6:87:GLY:O	2.21	0.72
7:6:81:ARG:O	7:6:84:LEU:HB2	1.88	0.72
11:B:682:VAL:H	11:B:701:THR:HG22	1.52	0.72
10:A:149:ASP:HB2	10:A:152:LEU:HB2	1.70	0.72
11:B:776:THR:HB	11:B:821:THR:HG22	1.72	0.72
11:B:780:LYS:NZ	11:B:782:TYR:OH	2.20	0.72
2:1:427:ASP:OD2	2:1:544:LYS:NZ	2.20	0.72
10:A:258:LEU:O	10:A:264:THR:OG1	2.08	0.71
1:10:148:LEU:HD23	1:10:187:LEU:HD12	1.73	0.71
1:10:193:ALA:HB3	2:1:775:GLN:HG2	1.72	0.71
11:B:763:LEU:HD22	11:B:804:PHE:HD2	1.55	0.71
2:1:762:ILE:HG12	2:1:769:ILE:HG12	1.73	0.71
10:A:128:MET:SD	10:A:398:SER:OG	2.47	0.71
6:5:27:HIS:O	6:5:30:TYR:HB2	1.91	0.71
10:A:218:THR:HA	10:A:269:ASN:O	1.89	0.71
2:1:266:LEU:HD22	2:1:295:LEU:HD11	1.73	0.71
2:1:199:ILE:HG21	2:1:250:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:28:GLY:HA2	9:8:60:LEU:HG	1.73	0.70
2:1:98:ILE:HD13	2:1:143:ILE:HD11	1.73	0.70
9:8:57:CYS:SG	9:8:58:ILE:N	2.64	0.70
10:A:109:VAL:HA	10:A:144:TYR:O	1.92	0.70
2:1:667:PRO:O	2:1:685:ARG:NH2	2.25	0.70
10:A:236:LEU:O	10:A:464:ARG:NH1	2.24	0.70
3:2:270:PHE:HD2	3:2:273:ARG:HH21	1.38	0.69
3:2:26:ASN:O	6:5:86:ASN:ND2	2.25	0.69
2:1:234:VAL:HG13	2:1:249:ALA:HA	1.74	0.69
2:1:870:ILE:HB	2:1:910:ILE:HG12	1.72	0.69
10:A:46:PHE:HE1	10:A:514:MET:HB3	1.57	0.69
2:1:794:GLN:HE21	2:1:803:ASN:HB3	1.58	0.69
10:A:48:VAL:HB	10:A:144:TYR:HB3	1.75	0.69
2:1:248:LEU:HB2	2:1:256:LEU:HD23	1.75	0.69
2:1:625:GLN:NE2	5:4:181:LEU:O	2.24	0.69
10:A:203:SER:O	10:A:492:GLN:HA	1.93	0.69
2:1:487:ARG:NH2	6:5:44:ASP:OD1	2.23	0.69
1:10:55:LEU:HD21	1:10:57:GLU:HG3	1.73	0.68
3:2:205:LEU:HD11	3:2:239:ILE:HG23	1.76	0.68
10:A:224:HIS:ND1	10:A:371:GLU:OE1	2.22	0.68
1:10:90:LEU:O	1:10:95:ARG:NH2	2.27	0.68
4:3:75:THR:HB	5:4:48:LEU:HD21	1.76	0.68
2:1:845:SER:N	2:1:864:GLY:O	2.27	0.68
3:2:215:PHE:HB3	3:2:232:LEU:HB2	1.74	0.68
7:6:33:VAL:HG21	7:6:62:LEU:HD13	1.75	0.67
2:1:173:ILE:HD12	2:1:192:VAL:HG23	1.76	0.67
2:1:91:LEU:HG	2:1:98:ILE:HB	1.76	0.67
3:2:102:ARG:NH1	3:2:105:ASP:OD2	2.27	0.67
2:1:247:THR:HG21	2:1:305:TYR:CE2	2.30	0.67
5:4:173:ARG:HH11	5:4:176:PHE:HA	1.58	0.67
2:1:807:VAL:HG21	2:1:878:LEU:HB3	1.76	0.66
1:10:51:THR:HG22	1:10:77:ASN:HB2	1.77	0.66
3:2:285:VAL:HA	3:2:288:MET:HG2	1.77	0.66
3:2:273:ARG:HD2	3:2:274:SER:N	2.11	0.66
2:1:257:ARG:HH22	2:1:259:ILE:HB	1.60	0.66
2:1:316:PHE:HB3	2:1:319:THR:HG21	1.78	0.66
10:A:211:LEU:H	10:A:267:ALA:HA	1.60	0.66
4:3:180:ARG:NH1	4:3:181:SER:OG	2.28	0.66
10:A:200:LEU:HB2	10:A:471:LYS:HD2	1.78	0.65
2:1:765:VAL:HG22	5:4:177:SER:HB3	1.77	0.65
10:A:266:ALA:HB2	10:A:427:TYR:CZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:148:VAL:HG13	12:C:212:THR:HG21	1.78	0.65
10:A:218:THR:HG21	10:A:300:LEU:HB3	1.79	0.65
1:10:115:ARG:HH12	1:10:125:GLY:HA3	1.61	0.65
3:2:98:GLU:OE1	3:2:126:ARG:NH2	2.23	0.65
11:B:680:GLN:HG3	11:B:703:GLU:HG3	1.77	0.65
10:A:420:GLU:OE1	10:A:440:VAL:N	2.19	0.65
10:A:201:ILE:O	10:A:494:HIS:HA	1.97	0.65
2:1:203:ASN:HD21	2:1:206:ASP:HB3	1.62	0.64
2:1:836:GLN:NE2	2:1:880:PRO:O	2.31	0.64
10:A:114:ARG:NH2	10:A:148:GLU:O	2.31	0.64
12:C:127:GLU:OE1	12:C:127:GLU:N	2.25	0.64
2:1:674:VAL:HG21	2:1:710:VAL:HG11	1.79	0.64
4:3:180:ARG:HH22	7:6:91:GLY:HA2	1.61	0.64
2:1:663:HIS:CE1	2:1:688:LYS:HB3	2.33	0.64
10:A:50:ARG:NH1	10:A:53:GLN:OE1	2.29	0.64
10:A:416:ARG:HG2	10:A:447:ILE:HD13	1.79	0.64
2:1:247:THR:HG21	2:1:305:TYR:HE2	1.62	0.64
2:1:279:THR:HB	2:1:324:PHE:HD2	1.63	0.64
2:1:592:LYS:NZ	2:1:623:ILE:O	2.31	0.64
10:A:440:VAL:O	11:B:732:ARG:NH2	2.31	0.64
11:B:818:LEU:HB3	11:B:832:PRO:HD2	1.80	0.64
2:1:326:THR:HG22	2:1:328:GLY:H	1.61	0.64
9:8:17:HIS:ND1	9:8:93:TYR:OH	2.29	0.64
11:B:731:GLU:HB2	11:B:757:GLN:HA	1.80	0.64
11:B:769:THR:HB	11:B:849:PHE:HB3	1.80	0.64
1:10:187:LEU:HD23	1:10:189:PRO:HD3	1.80	0.63
10:A:46:PHE:CE1	10:A:514:MET:HB3	2.33	0.63
1:10:140:SER:OG	1:10:143:SER:OG	2.17	0.63
10:A:61:TYR:O	10:A:64:ARG:NH1	2.31	0.63
2:1:629:LEU:HB3	2:1:631:VAL:HG22	1.80	0.63
2:1:182:GLY:N	2:1:284:VAL:O	2.28	0.63
3:2:250:LYS:HA	3:2:253:ASN:HD21	1.63	0.63
2:1:777:LYS:HD3	2:1:799:LYS:HG3	1.81	0.63
10:A:222:VAL:HG12	10:A:273:PHE:HB3	1.81	0.62
11:B:730:ILE:HD11	11:B:754:VAL:HB	1.81	0.62
1:10:143:SER:OG	1:10:164:HIS:O	2.18	0.62
2:1:290:GLN:HE21	2:1:381:GLU:HA	1.64	0.62
9:8:125:ILE:HG22	9:8:143:VAL:HG22	1.81	0.62
12:C:3:LEU:HA	12:C:124:ARG:HA	1.81	0.62
2:1:105:ARG:NH2	2:1:122:THR:OG1	2.33	0.62
2:1:550:SER:O	2:1:944:GLN:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:266:ARG:NH2	4:3:246:LEU:O	2.28	0.62
10:A:339:ARG:NH2	10:A:342:GLU:OE1	2.33	0.62
2:1:33:ARG:HB2	2:1:943:TYR:HD2	1.62	0.62
2:1:765:VAL:HG21	5:4:175:GLU:HB3	1.81	0.62
4:3:140:VAL:N	4:3:164:SER:O	2.28	0.62
6:5:100:LEU:HB2	9:8:132:PHE:HD2	1.64	0.62
2:1:580:HIS:CE1	2:1:636:TYR:CD2	2.88	0.62
3:2:139:GLU:HB2	3:2:142:ARG:HH21	1.65	0.62
3:2:249:THR:O	3:2:253:ASN:ND2	2.32	0.62
6:5:59:GLY:O	6:5:63:ILE:HG12	2.00	0.62
11:B:813:ASN:OD1	11:B:837:THR:OG1	2.18	0.62
2:1:170:SER:HA	2:1:173:ILE:HG22	1.82	0.61
2:1:540:THR:HG22	2:1:542:SER:H	1.65	0.61
10:A:263:ARG:HD2	11:B:756:ARG:HD2	1.81	0.61
10:A:444:GLN:NE2	11:B:731:GLU:OE1	2.34	0.61
2:1:293:LEU:HD22	2:1:295:LEU:HD23	1.83	0.61
2:1:219:TRP:NE1	2:1:246:GLN:OE1	2.30	0.61
3:2:76:LEU:HD21	3:2:93:THR:HG22	1.81	0.61
4:3:93:ARG:NH2	4:3:213:ASP:OD1	2.33	0.61
8:7:104:ARG:NH1	8:7:143:SER:OG	2.34	0.61
10:A:307:PHE:HA	10:A:381:PRO:HB2	1.82	0.61
3:2:48:LEU:HD12	3:2:51:ASP:HB3	1.83	0.61
4:3:31:ARG:HH21	4:3:194:ASP:H	1.48	0.61
10:A:264:THR:O	10:A:427:TYR:OH	2.19	0.61
2:1:572:LEU:HD12	2:1:589:LEU:HB2	1.83	0.61
3:2:69:ASP:OD1	3:2:96:ARG:NH1	2.34	0.61
8:7:69:VAL:HG22	8:7:96:VAL:HG22	1.82	0.61
2:1:179:TYR:HB3	2:1:187:TRP:HB2	1.82	0.61
1:10:60:PHE:O	1:10:97:ARG:NH1	2.34	0.60
4:3:66:LYS:O	4:3:233:ALA:N	2.26	0.60
10:A:60:PRO:HG2	10:A:138:GLU:HG3	1.83	0.60
10:A:224:HIS:N	10:A:241:ASN:OD1	2.33	0.60
10:A:444:GLN:OE1	11:B:758:ILE:N	2.34	0.60
2:1:221:GLN:OE1	2:1:222:HIS:ND1	2.31	0.60
8:7:59:GLN:OE1	8:7:59:GLN:N	2.32	0.60
9:8:74:ALA:O	9:8:78:ILE:HG12	2.00	0.60
2:1:64:ALA:HB2	2:1:76:ARG:HG3	1.82	0.60
2:1:460:LEU:HB2	2:1:527:ARG:HA	1.83	0.60
2:1:217:THR:HG22	2:1:256:LEU:HD11	1.83	0.60
4:3:88:PHE:HB3	4:3:222:TRP:HD1	1.66	0.60
2:1:794:GLN:HB2	2:1:805:PHE:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:219:LEU:HD12	4:3:246:LEU:HD13	1.82	0.60
10:A:282:TYR:OH	10:A:369:ALA:O	2.14	0.60
10:A:431:GLU:O	10:A:431:GLU:HG2	2.00	0.60
2:1:683:GLY:HA3	2:1:696:TRP:NE1	2.16	0.60
2:1:739:ASN:OD1	2:1:824:SER:OG	2.18	0.60
2:1:169:GLU:OE2	2:1:172:SER:OG	2.19	0.60
2:1:313:LEU:HD12	2:1:383:GLY:H	1.66	0.60
2:1:901:ASP:HB2	8:7:126:ILE:HD11	1.83	0.60
2:1:290:GLN:OE1	2:1:290:GLN:N	2.33	0.60
3:2:62:ALA:O	3:2:66:TYR:N	2.31	0.60
2:1:868:GLY:HA3	2:1:915:THR:HB	1.84	0.60
9:8:110:LYS:HA	9:8:110:LYS:HE3	1.84	0.60
4:3:31:ARG:NH2	4:3:194:ASP:O	2.30	0.59
12:C:197:ALA:HB1	12:C:201:ARG:HH12	1.66	0.59
8:7:109:ARG:HB2	8:7:123:VAL:HG12	1.82	0.59
10:A:182:ASN:OD1	10:A:518:ARG:NE	2.35	0.59
1:10:182:ASN:OD1	13:D:1:NAG:N2	2.35	0.59
10:A:292:ASN:HB2	10:A:301:LEU:HD12	1.84	0.59
2:1:647:TYR:O	2:1:692:THR:OG1	2.16	0.59
10:A:485:ARG:HE	11:B:803:HIS:HB3	1.67	0.59
12:C:106:TRP:HB3	12:C:146:TYR:CE2	2.38	0.59
9:8:146:HIS:HB2	9:8:151:TRP:CE2	2.38	0.59
10:A:403:ARG:O	10:A:403:ARG:NH1	2.30	0.59
12:C:20:THR:HA	12:C:23:CYS:SG	2.43	0.59
2:1:275:ARG:HH21	2:1:277:LEU:HD11	1.68	0.59
11:B:815:VAL:HG13	11:B:833:GLN:HG3	1.84	0.59
8:7:101:PRO:O	8:7:148:TYR:OH	2.20	0.59
12:C:199:LEU:O	12:C:203:VAL:HG13	2.01	0.59
9:8:184:VAL:HG13	9:8:188:ASN:HB2	1.85	0.59
4:3:104:PRO:HG2	4:3:107:LEU:HB2	1.84	0.59
2:1:186:VAL:HB	2:1:202:PHE:HB2	1.85	0.58
10:A:314:VAL:O	10:A:414:ASN:ND2	2.32	0.58
1:10:68:PHE:HB2	1:10:111:ARG:HH21	1.67	0.58
11:B:763:LEU:HD22	11:B:804:PHE:CD2	2.38	0.58
13:E:1:NAG:H5	13:E:2:NAG:H83	1.84	0.58
2:1:290:GLN:NE2	2:1:381:GLU:HA	2.18	0.58
10:A:316:ARG:NE	10:A:405:ARG:O	2.34	0.58
1:10:58:HIS:ND1	1:10:71:ARG:HB2	2.19	0.58
2:1:105:ARG:NH1	2:1:123:LEU:O	2.35	0.58
3:2:90:LYS:HG2	3:2:112:ARG:HH12	1.69	0.58
2:1:528:ASP:OD1	2:1:529:GLU:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:237:GLY:O	10:A:464:ARG:NH1	2.31	0.58
1:10:164:HIS:HB3	13:D:1:NAG:H62	1.86	0.58
2:1:729:ARG:HG2	4:3:147:ARG:HH22	1.66	0.58
9:8:98:ARG:HB2	9:8:101:ASP:HB2	1.85	0.58
1:10:197:GLU:HB3	2:1:898:TYR:HE2	1.69	0.58
6:5:72:ALA:N	7:6:13:PHE:O	2.27	0.58
2:1:573:MET:HB2	2:1:588:THR:HG23	1.85	0.58
10:A:287:ARG:NH2	10:A:503:GLU:OE2	2.37	0.58
2:1:153:LEU:HB3	2:1:162:LYS:HB3	1.85	0.57
2:1:249:ALA:HB3	2:1:253:GLU:HB2	1.85	0.57
10:A:196:VAL:N	10:A:506:PHE:O	2.36	0.57
2:1:79:ASP:O	2:1:918:ARG:NH2	2.36	0.57
2:1:247:THR:HB	2:1:257:ARG:HG3	1.85	0.57
2:1:534:LYS:HE3	2:1:927:SER:HA	1.86	0.57
10:A:451:GLN:CD	11:B:844:HIS:HD1	2.07	0.57
2:1:685:ARG:HB2	2:1:693:GLU:HG2	1.86	0.57
2:1:896:ILE:H	2:1:896:ILE:HD12	1.69	0.57
4:3:31:ARG:NH1	4:3:117:ASN:O	2.37	0.57
1:10:149:HIS:HD2	1:10:188:GLN:HB3	1.68	0.57
8:7:91:SER:HA	8:7:112:ILE:HG13	1.86	0.57
10:A:372:HIS:ND1	10:A:384:THR:OG1	2.28	0.57
10:A:388:LEU:HD11	10:A:395:GLN:HB3	1.85	0.57
2:1:109:SER:O	2:1:118:ASN:N	2.34	0.57
2:1:179:TYR:HD1	2:1:180:SER:N	2.03	0.57
2:1:187:TRP:CH2	2:1:201:LYS:HD2	2.40	0.57
11:B:783:LYS:HE3	11:B:814:TYR:HE1	1.68	0.57
12:C:12:LEU:HD21	12:C:137:ILE:HD13	1.87	0.57
2:1:247:THR:O	2:1:257:ARG:N	2.30	0.57
2:1:457:MET:SD	2:1:536:MET:HG2	2.45	0.57
3:2:204:GLY:O	3:2:208:LEU:N	2.36	0.57
2:1:376:ASN:OD1	2:1:385:ARG:NH1	2.36	0.57
7:6:43:ILE:HD13	7:6:107:VAL:HG21	1.86	0.57
2:1:376:ASN:OD1	2:1:390:THR:OG1	2.16	0.57
9:8:170:ILE:HD11	9:8:206:VAL:HA	1.87	0.57
10:A:287:ARG:HG2	10:A:495:VAL:HB	1.86	0.57
2:1:819:ALA:H	14:1:1002:NAG:H83	1.70	0.56
9:8:143:VAL:HG23	9:8:160:TYR:CE2	2.39	0.56
1:10:197:GLU:HB3	2:1:898:TYR:CE2	2.40	0.56
3:2:226:MET:HA	3:2:229:LEU:HB2	1.86	0.56
10:A:416:ARG:CG	10:A:447:ILE:HD13	2.36	0.56
2:1:102:ASN:HB3	2:1:105:ARG:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:982:LEU:HB3	4:3:37:LEU:HD11	1.88	0.56
3:2:105:ASP:N	3:2:105:ASP:OD1	2.37	0.56
9:8:193:ILE:HD12	9:8:193:ILE:H	1.69	0.56
12:C:210:LEU:HA	12:C:213:LEU:HG	1.88	0.56
2:1:719:VAL:HG21	2:1:736:LEU:HD11	1.87	0.56
11:B:761:PHE:N	11:B:807:LEU:O	2.38	0.56
11:B:811:GLY:O	11:B:838:ALA:N	2.39	0.56
10:A:467:GLN:HG2	10:A:506:PHE:CG	2.41	0.56
11:B:687:VAL:O	11:B:689:GLN:NE2	2.39	0.56
2:1:233:ALA:O	2:1:250:LEU:HB3	2.05	0.56
1:10:143:SER:HA	1:10:182:ASN:HB3	1.88	0.56
6:5:52:ALA:O	6:5:56:THR:OG1	2.19	0.56
12:C:97:TYR:O	12:C:101:VAL:HG13	2.06	0.56
2:1:576:ARG:NH2	2:1:586:GLN:OE1	2.39	0.56
9:8:80:SER:HA	9:8:83:LYS:NZ	2.20	0.56
10:A:135:LEU:HG	10:A:230:VAL:HG23	1.87	0.56
3:2:246:SER:HB3	3:2:249:THR:HG23	1.88	0.56
10:A:339:ARG:HA	10:A:339:ARG:NE	2.20	0.56
9:8:16:LEU:HB3	9:8:183:LEU:HD22	1.87	0.55
10:A:202:ALA:HA	10:A:494:HIS:HD2	1.71	0.55
10:A:444:GLN:HG3	11:B:841:TYR:CZ	2.41	0.55
11:B:768:ILE:HB	11:B:848:ILE:HG12	1.87	0.55
10:A:202:ALA:HA	10:A:494:HIS:CD2	2.41	0.55
12:C:200:ALA:O	12:C:204:VAL:HG12	2.06	0.55
2:1:165:GLU:HG3	2:1:207:GLY:O	2.06	0.55
2:1:425:THR:OG1	2:1:427:ASP:OD1	2.22	0.55
2:1:71:GLY:HA3	2:1:443:TRP:CD2	2.42	0.55
2:1:850:THR:OG1	2:1:860:HIS:N	2.32	0.55
3:2:60:MET:HE1	3:2:76:LEU:HB2	1.89	0.55
3:2:76:LEU:HD11	3:2:93:THR:HG23	1.88	0.55
8:7:93:SER:OG	8:7:109:ARG:NH1	2.35	0.55
2:1:725:VAL:HG13	5:4:165:LEU:HD12	1.89	0.55
2:1:804:GLU:HG2	2:1:839:ILE:HD13	1.88	0.55
4:3:31:ARG:NH2	4:3:194:ASP:H	2.04	0.55
6:5:71:ASP:OD1	6:5:71:ASP:N	2.40	0.55
6:5:96:ARG:NH2	9:8:96:ASN:O	2.40	0.55
12:C:98:LYS:HA	12:C:101:VAL:HG22	1.89	0.55
2:1:666:ALA:O	2:1:686:LEU:HB3	2.07	0.55
1:10:145:GLN:OE1	1:10:164:HIS:NE2	2.39	0.55
1:10:162:VAL:HG21	2:1:828:PRO:HA	1.89	0.55
3:2:12:TRP:HB3	3:2:44:TYR:CG	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:94:TYR:HE2	10:A:133:GLU:HG2	1.72	0.55
2:1:733:TYR:O	2:1:812:GLU:N	2.30	0.54
2:1:604:PHE:HB3	2:1:611:TRP:CE3	2.42	0.54
10:A:220:VAL:HB	10:A:308:VAL:HG22	1.88	0.54
2:1:91:LEU:HD11	2:1:98:ILE:HD12	1.89	0.54
11:B:810:ASP:OD1	11:B:810:ASP:N	2.37	0.54
2:1:960:TYR:HB3	2:1:962:TYR:CE1	2.43	0.54
3:2:52:ILE:O	3:2:55:ILE:HB	2.08	0.54
10:A:79:VAL:HG12	10:A:81:SER:HB3	1.89	0.54
2:1:37:VAL:HB	2:1:58:THR:HG21	1.89	0.54
2:1:374:THR:HA	2:1:391:ILE:O	2.06	0.54
4:3:78:TYR:HD2	5:4:52:VAL:HG21	1.72	0.54
10:A:314:VAL:HA	10:A:387:HIS:H	1.72	0.54
11:B:730:ILE:HG13	11:B:755:PHE:O	2.08	0.54
2:1:720:HIS:ND1	4:3:160:THR:OG1	2.34	0.54
2:1:765:VAL:HG11	5:4:175:GLU:HG2	1.90	0.54
4:3:88:PHE:HB3	4:3:222:TRP:CD1	2.42	0.54
10:A:462:GLN:OE1	10:A:462:GLN:N	2.39	0.54
11:B:781:LEU:HD11	11:B:836:PHE:HZ	1.73	0.54
11:B:829:TYR:HB3	11:B:851:PRO:HB3	1.90	0.54
8:7:124:ASN:ND2	8:7:130:GLU:OE2	2.28	0.54
10:A:419:ALA:HB1	10:A:441:PHE:HE2	1.73	0.54
2:1:242:SER:OG	2:1:244:SER:OG	2.26	0.54
2:1:372:THR:HA	2:1:393:PHE:O	2.07	0.54
4:3:13:ARG:HH21	7:6:110:TYR:HB2	1.73	0.54
2:1:749:ASP:OD2	2:1:754:ARG:NE	2.40	0.53
4:3:56:ILE:HA	4:3:59:ARG:NH1	2.23	0.53
10:A:53:GLN:NE2	10:A:64:ARG:HA	2.23	0.53
10:A:52:GLN:NE2	10:A:229:GLY:O	2.41	0.53
10:A:520:LYS:HZ2	12:C:128:PHE:HE2	1.56	0.53
11:B:673:SER:N	11:B:677:GLU:O	2.38	0.53
11:B:767:VAL:HG21	11:B:796:LEU:HD11	1.90	0.53
2:1:402:PRO:HA	2:1:425:THR:HA	1.89	0.53
2:1:820:THR:HB	14:1:1002:NAG:O7	2.08	0.53
4:3:81:ASN:ND2	4:3:226:GLU:HG2	2.24	0.53
10:A:218:THR:HG22	10:A:269:ASN:HB2	1.90	0.53
2:1:488:LEU:O	2:1:492:LEU:HG	2.08	0.53
3:2:69:ASP:OD2	6:5:98:ARG:NH2	2.34	0.53
10:A:220:VAL:HG22	10:A:271:LEU:HB3	1.90	0.53
3:2:22:TRP:CE3	3:2:33:ILE:HG22	2.43	0.53
8:7:58:PRO:O	8:7:62:ILE:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:348:GLN:HG2	10:A:436:PRO:O	2.08	0.53
11:B:668:TYR:HD1	11:B:747:ILE:HG22	1.74	0.53
3:2:60:MET:SD	3:2:92:LEU:HD12	2.49	0.53
4:3:71:GLN:N	4:3:71:GLN:OE1	2.41	0.53
4:3:182:ILE:O	4:3:186:ILE:HG22	2.07	0.53
10:A:337:PHE:HD1	10:A:425:VAL:HG11	1.73	0.53
2:1:461:PRO:O	2:1:527:ARG:N	2.40	0.53
2:1:527:ARG:NH2	2:1:578:THR:OG1	2.42	0.53
2:1:819:ALA:O	5:4:171:PRO:HB3	2.09	0.53
2:1:27:VAL:HG13	2:1:912:TYR:CZ	2.43	0.53
2:1:371:GLN:HB3	2:1:395:LEU:HB2	1.91	0.53
2:1:573:MET:HB3	2:1:628:LEU:HD13	1.90	0.53
2:1:979:THR:HG21	4:3:30:ILE:HD13	1.90	0.53
3:2:270:PHE:HA	3:2:273:ARG:HG3	1.91	0.53
10:A:127:PHE:HD2	10:A:400:MET:HG2	1.74	0.53
1:10:146:LEU:HB3	1:10:161:VAL:HG22	1.90	0.53
1:10:158:GLY:HA3	2:1:698:LEU:HD22	1.90	0.53
6:5:42:PRO:HB2	6:5:45:ILE:HG23	1.91	0.53
10:A:313:THR:HG21	10:A:388:LEU:HD12	1.90	0.53
12:C:137:ILE:O	12:C:141:ILE:HG23	2.09	0.53
2:1:482:GLY:O	2:1:486:LYS:HG2	2.09	0.52
11:B:668:TYR:HA	11:B:706:LYS:NZ	2.24	0.52
9:8:163:ASP:HB3	9:8:166:GLU:HB3	1.92	0.52
2:1:684:TYR:CE1	2:1:694:LEU:HD12	2.44	0.52
3:2:175:ALA:HB1	3:2:195:TYR:HE1	1.74	0.52
3:2:205:LEU:HA	3:2:208:LEU:HB2	1.92	0.52
3:2:246:SER:N	3:2:249:THR:OG1	2.42	0.52
4:3:141:PRO:O	7:6:48:GLY:N	2.41	0.52
3:2:15:MET:HB3	3:2:36:VAL:HG13	1.90	0.52
4:3:139:LYS:HB2	4:3:165:TRP:CZ3	2.44	0.52
6:5:88:PRO:HA	6:5:91:TYR:CE1	2.44	0.52
1:10:138:VAL:HG22	1:10:173:VAL:HG11	1.90	0.52
2:1:623:ILE:HA	2:1:644:ASP:HA	1.91	0.52
4:3:140:VAL:O	4:3:164:SER:HB2	2.10	0.52
4:3:232:TRP:CE2	4:3:234:LEU:HB2	2.45	0.52
8:7:66:ARG:HH11	8:7:75:VAL:HG21	1.75	0.52
9:8:29:LEU:HD11	9:8:75:LEU:HD23	1.91	0.52
1:10:62:ILE:HG23	1:10:104:LEU:HD12	1.92	0.52
12:C:151:ALA:O	12:C:155:MET:HG2	2.10	0.52
2:1:61:ASN:HB3	2:1:79:ASP:HB3	1.91	0.52
2:1:622:PRO:O	2:1:645:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:136:TYR:O	8:7:138:LEU:N	2.42	0.52
10:A:411:LEU:HG	10:A:452:LEU:HD13	1.92	0.52
1:10:149:HIS:HE1	1:10:160:SER:HB3	1.75	0.52
3:2:23:ARG:HB2	3:2:58:GLN:NE2	2.25	0.52
3:2:90:LYS:HG3	3:2:109:LEU:HD11	1.90	0.52
9:8:116:ALA:HA	9:8:122:THR:HB	1.92	0.52
10:A:69:ASN:HB2	10:A:187:VAL:HG23	1.92	0.52
10:A:440:VAL:HG22	11:B:734:LEU:HD11	1.92	0.52
1:10:193:ALA:HB2	2:1:773:SER:OG	2.09	0.52
2:1:702:PRO:HA	2:1:705:GLN:O	2.10	0.52
2:1:739:ASN:O	2:1:764:GLY:N	2.41	0.52
3:2:144:LEU:HD23	3:2:161:LEU:HB2	1.91	0.52
6:5:53:PHE:HE1	7:6:36:LEU:HB3	1.74	0.52
10:A:154:SER:O	10:A:158:GLN:HG3	2.09	0.52
10:A:228:PHE:CD1	10:A:279:LYS:HB2	2.45	0.52
10:A:331:GLY:H	10:A:335:HIS:CD2	2.27	0.52
2:1:663:HIS:HE1	2:1:688:LYS:HB3	1.75	0.51
3:2:266:ARG:O	3:2:270:PHE:HD1	1.92	0.51
4:3:54:VAL:HG11	4:3:87:PHE:HZ	1.75	0.51
10:A:70:THR:O	10:A:185:GLN:HG3	2.10	0.51
10:A:55:ASP:OD1	10:A:64:ARG:NH2	2.42	0.51
2:1:838:TYR:OH	2:1:879:ASP:O	2.28	0.51
3:2:261:ALA:O	3:2:265:ASN:ND2	2.44	0.51
10:A:208:LEU:HB2	10:A:270:LEU:HB2	1.91	0.51
2:1:201:LYS:O	2:1:210:VAL:N	2.43	0.51
4:3:252:PHE:HA	9:8:194:ARG:NE	2.24	0.51
6:5:82:ASP:OD1	9:8:62:HIS:NE2	2.44	0.51
10:A:255:PHE:HA	10:A:258:LEU:HB2	1.93	0.51
10:A:347:HIS:HB2	10:A:436:PRO:HB2	1.91	0.51
10:A:529:ALA:O	10:A:532:ILE:HG12	2.10	0.51
2:1:81:GLY:HA2	2:1:918:ARG:HH21	1.76	0.51
2:1:423:VAL:HG13	2:1:431:LEU:HB2	1.93	0.51
2:1:571:LYS:HB3	2:1:590:LEU:HB3	1.91	0.51
2:1:713:LYS:HB3	2:1:786:HIS:CD2	2.45	0.51
3:2:246:SER:O	3:2:250:LYS:N	2.38	0.51
4:3:21:VAL:HA	4:3:175:ASN:ND2	2.26	0.51
4:3:81:ASN:HA	4:3:89:LYS:HZ1	1.76	0.51
10:A:308:VAL:H	10:A:382:ALA:HA	1.74	0.51
10:A:429:LEU:HA	10:A:432:LYS:HB2	1.91	0.51
2:1:370:ASN:O	2:1:372:THR:N	2.42	0.51
3:2:239:ILE:HG22	3:2:253:ASN:ND2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:45:THR:HG22	4:3:46:GLN:H	1.76	0.51
9:8:85:HIS:HB3	9:8:87:TYR:CE2	2.45	0.51
1:10:140:SER:O	1:10:143:SER:OG	2.24	0.51
4:3:21:VAL:HA	4:3:175:ASN:HD21	1.75	0.51
10:A:69:ASN:OD1	10:A:185:GLN:NE2	2.42	0.51
10:A:308:VAL:N	10:A:381:PRO:O	2.43	0.51
10:A:336:ALA:O	10:A:340:GLU:HG2	2.11	0.51
11:B:782:TYR:CE1	11:B:790:PRO:HB3	2.45	0.51
2:1:234:VAL:HG11	2:1:305:TYR:CZ	2.46	0.51
2:1:313:LEU:HD12	2:1:383:GLY:N	2.25	0.51
9:8:17:HIS:CE1	9:8:26:VAL:HB	2.46	0.51
3:2:63:ALA:O	3:2:67:GLY:N	2.44	0.51
4:3:158:LEU:HD12	4:3:161:LEU:HD22	1.92	0.51
9:8:124:LEU:HD21	9:8:126:MET:HG3	1.91	0.51
9:8:189:HIS:NE2	9:8:193:ILE:HG23	2.25	0.51
11:B:774:LEU:HD13	11:B:800:LEU:HD23	1.93	0.50
2:1:675:ASP:OD2	2:1:678:GLN:NE2	2.28	0.50
4:3:78:TYR:CE2	5:4:52:VAL:HG11	2.45	0.50
8:7:119:ARG:HD2	8:7:133:ARG:HD2	1.93	0.50
10:A:63:THR:HA	10:A:139:THR:O	2.11	0.50
10:A:68:LEU:HD11	10:A:514:MET:SD	2.52	0.50
10:A:325:SER:HA	10:A:359:LYS:O	2.11	0.50
11:B:683:ALA:HB3	11:B:723:LYS:HB2	1.93	0.50
2:1:192:VAL:HG12	2:1:195:SER:HB3	1.92	0.50
4:3:89:LYS:HZ1	4:3:222:TRP:HE1	1.59	0.50
9:8:99:VAL:HA	9:8:129:ASN:OD1	2.11	0.50
10:A:308:VAL:HB	10:A:382:ALA:HB2	1.94	0.50
12:C:124:ARG:O	12:C:124:ARG:HG2	2.11	0.50
2:1:146:LEU:HB2	2:1:151:LEU:HD12	1.93	0.50
2:1:540:THR:O	2:1:543:GLY:N	2.44	0.50
11:B:822:LEU:HD11	11:B:827:TYR:HD2	1.76	0.50
2:1:111:GLU:HG2	2:1:114:ILE:HG12	1.92	0.50
3:2:112:ARG:O	3:2:115:GLN:HG2	2.11	0.50
3:2:230:PHE:HA	3:2:233:TYR:HB3	1.94	0.50
11:B:773:TYR:O	11:B:777:LEU:HD13	2.10	0.50
2:1:169:GLU:OE2	2:1:173:ILE:HB	2.11	0.50
2:1:175:TYR:HA	2:1:190:GLY:HA2	1.91	0.50
2:1:222:HIS:HD2	2:1:225:GLY:H	1.58	0.50
4:3:89:LYS:CE	4:3:222:TRP:HE1	2.24	0.50
9:8:26:VAL:HG22	9:8:95:ALA:HB3	1.94	0.50
2:1:573:MET:SD	2:1:640:LEU:HD13	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:28:GLY:HA3	4:3:183:TYR:CZ	2.46	0.50
10:A:50:ARG:HG2	10:A:63:THR:HG21	1.93	0.50
2:1:635:ASP:OD1	2:1:635:ASP:N	2.45	0.50
10:A:233:TRP:NE1	10:A:511:LYS:HB2	2.27	0.50
2:1:199:ILE:HG21	2:1:250:LEU:CD1	2.41	0.50
2:1:458:VAL:HB	2:1:535:MET:HG2	1.94	0.50
2:1:577:THR:OG1	2:1:578:THR:N	2.45	0.50
1:10:132:VAL:HG21	1:10:163:THR:HG23	1.94	0.49
2:1:219:TRP:HH2	2:1:237:CYS:HB3	1.76	0.49
10:A:221:ILE:HG12	10:A:309:LEU:HB3	1.93	0.49
12:C:94:LYS:HZ2	12:C:96:GLU:H	1.60	0.49
2:1:629:LEU:HD13	2:1:641:LEU:HD13	1.94	0.49
10:A:239:ASP:O	10:A:313:THR:HA	2.11	0.49
1:10:57:GLU:OE1	1:10:111:ARG:NE	2.45	0.49
2:1:404:ARG:NH2	2:1:406:TYR:OH	2.46	0.49
2:1:672:TYR:HA	2:1:682:CYS:O	2.12	0.49
5:4:16:LYS:O	9:8:114:ARG:NH2	2.45	0.49
12:C:29:TYR:HE2	12:C:97:TYR:HB3	1.77	0.49
2:1:335:VAL:O	2:1:375:ILE:HA	2.11	0.49
2:1:763:ASP:OD2	2:1:824:SER:HB3	2.11	0.49
2:1:912:TYR:HD1	2:1:913:ASN:H	1.60	0.49
10:A:529:ALA:HB2	12:C:8:ASN:HD21	1.77	0.49
10:A:111:ILE:HD13	10:A:152:LEU:HG	1.95	0.49
2:1:295:LEU:HD12	2:1:299:HIS:CD2	2.48	0.49
3:2:262:SER:HA	3:2:265:ASN:HD22	1.78	0.49
11:B:818:LEU:O	11:B:831:LEU:HB2	2.12	0.49
1:10:88:ARG:NH2	1:10:94:GLU:OE2	2.46	0.49
3:2:132:LYS:O	9:8:98:ARG:NH1	2.45	0.49
4:3:79:TYR:O	4:3:87:PHE:HB3	2.12	0.49
2:1:249:ALA:O	2:1:253:GLU:N	2.42	0.49
10:A:424:ARG:HG3	10:A:429:LEU:HB2	1.95	0.49
2:1:663:HIS:ND1	2:1:688:LYS:O	2.46	0.49
5:4:52:VAL:HB	5:4:54:ASP:OD1	2.13	0.49
7:6:67:ILE:O	7:6:71:GLY:N	2.36	0.49
7:6:105:GLY:HA2	7:6:109:VAL:CG2	2.42	0.49
2:1:670:PHE:CE2	2:1:685:ARG:HG2	2.48	0.49
4:3:46:GLN:O	4:3:50:SER:OG	2.20	0.49
11:B:669:GLY:HA3	11:B:750:VAL:O	2.12	0.49
1:10:140:SER:OG	1:10:140:SER:O	2.31	0.48
2:1:713:LYS:HD2	2:1:738:PRO:HA	1.93	0.48
3:2:224:ARG:NH2	4:3:251:MET:HA	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:69:PRO:HB2	4:3:71:GLN:OE1	2.13	0.48
10:A:82:ARG:O	10:A:82:ARG:HG2	2.12	0.48
10:A:88:ARG:HD3	10:A:156:TYR:CE2	2.48	0.48
10:A:320:LEU:HB3	10:A:354:PHE:HD1	1.78	0.48
10:A:327:PRO:HD3	10:A:358:HIS:NE2	2.28	0.48
11:B:783:LYS:HG2	11:B:814:TYR:CE1	2.48	0.48
11:B:812:GLU:HB3	11:B:814:TYR:CZ	2.48	0.48
2:1:592:LYS:HD3	5:4:183:LEU:HB3	1.95	0.48
8:7:70:ASP:O	8:7:73:GLU:HB2	2.14	0.48
10:A:415:THR:HG22	10:A:447:ILE:HG12	1.95	0.48
1:10:151:ASP:OD1	1:10:153:ALA:N	2.46	0.48
2:1:261:LEU:HB3	2:1:266:LEU:HB2	1.94	0.48
2:1:890:SER:O	2:1:894:ASN:N	2.46	0.48
4:3:134:GLY:HA2	4:3:155:GLY:O	2.13	0.48
10:A:313:THR:O	10:A:387:HIS:ND1	2.37	0.48
11:B:720:VAL:O	11:B:737:HIS:HA	2.13	0.48
11:B:774:LEU:HD11	11:B:796:LEU:HB3	1.94	0.48
1:10:143:SER:HB2	1:10:182:ASN:HD22	1.77	0.48
2:1:257:ARG:HH12	2:1:259:ILE:HG22	1.78	0.48
2:1:931:SER:O	2:1:948:TYR:HA	2.13	0.48
3:2:29:ASN:OD1	3:2:29:ASN:N	2.46	0.48
3:2:248:LYS:HG3	3:2:249:THR:N	2.29	0.48
4:3:72:SER:O	4:3:76:ARG:HG2	2.13	0.48
9:8:92:TYR:OH	9:8:94:GLN:NE2	2.46	0.48
10:A:53:GLN:HG3	10:A:63:THR:O	2.14	0.48
2:1:35:GLN:O	2:1:445:ARG:NH2	2.46	0.48
2:1:158:SER:OG	2:1:160:HIS:ND1	2.44	0.48
9:8:135:ASP:OD1	9:8:135:ASP:N	2.35	0.48
10:A:195:ALA:HA	10:A:507:TYR:CD1	2.49	0.48
10:A:228:PHE:HD1	10:A:279:LYS:HB2	1.79	0.48
2:1:41:LYS:HD3	2:1:59:GLU:HG2	1.95	0.48
2:1:55:VAL:HG11	2:1:97:VAL:HG21	1.95	0.48
4:3:65:GLY:HA2	4:3:68:ILE:HD13	1.95	0.48
10:A:135:LEU:HD21	10:A:230:VAL:HA	1.95	0.48
2:1:882:ARG:HH11	2:1:896:ILE:HB	1.78	0.48
3:2:205:LEU:O	3:2:209:GLU:HG2	2.13	0.48
6:5:3:PRO:HD2	6:5:6:TRP:HE1	1.79	0.48
6:5:68:LYS:HB3	7:6:18:ALA:HB1	1.94	0.48
2:1:303:LEU:HD13	2:1:310:LEU:HD12	1.95	0.48
2:1:659:LEU:O	2:1:663:HIS:HB3	2.14	0.48
2:1:820:THR:H	14:1:1002:NAG:H81	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:24:THR:HG22	4:3:179:LEU:HD12	1.96	0.48
4:3:45:THR:H	4:3:48:GLN:NE2	2.11	0.48
8:7:48:GLU:HG2	8:7:85:VAL:HG22	1.96	0.48
3:2:248:LYS:HE3	3:2:249:THR:HG22	1.96	0.48
4:3:126:GLY:O	4:3:130:MET:HG2	2.14	0.48
6:5:9:LEU:O	6:5:12:ILE:HG12	2.13	0.48
9:8:146:HIS:HB2	9:8:151:TRP:CZ2	2.48	0.48
4:3:180:ARG:HD3	4:3:195:GLN:HE22	1.79	0.48
10:A:55:ASP:HB2	10:A:505:VAL:HG23	1.96	0.48
11:B:767:VAL:HG12	11:B:769:THR:HG22	1.96	0.48
3:2:12:TRP:O	3:2:16:ARG:HB2	2.14	0.47
5:4:24:PRO:HD3	9:8:106:GLN:HE22	1.78	0.47
10:A:55:ASP:O	10:A:504:PHE:HA	2.14	0.47
1:10:108:TYR:HB2	1:10:134:ALA:HB2	1.94	0.47
1:10:149:HIS:CE1	1:10:160:SER:HB3	2.49	0.47
2:1:96:ASP:OD1	2:1:96:ASP:N	2.46	0.47
2:1:247:THR:HB	2:1:257:ARG:HH11	1.79	0.47
2:1:792:VAL:HG22	2:1:807:VAL:HG22	1.96	0.47
9:8:98:ARG:O	9:8:129:ASN:ND2	2.48	0.47
10:A:332:THR:HG23	10:A:334:GLN:H	1.80	0.47
10:A:349:PHE:CD2	10:A:417:ILE:HG12	2.49	0.47
12:C:118:PRO:HA	12:C:121:VAL:HG12	1.96	0.47
2:1:418:GLY:HA2	2:1:435:GLN:OE1	2.15	0.47
2:1:422:LEU:HD11	2:1:430:LEU:HD22	1.96	0.47
9:8:145:GLU:HB3	9:8:154:ARG:NH1	2.29	0.47
9:8:201:GLU:HB3	9:8:204:LYS:HZ1	1.79	0.47
10:A:324:VAL:HG23	10:A:358:HIS:HA	1.97	0.47
13:E:1:NAG:O3	13:E:2:NAG:O5	2.31	0.47
2:1:177:MET:HG3	2:1:189:LEU:HB2	1.96	0.47
2:1:808:LEU:HG	2:1:835:GLN:HG2	1.95	0.47
3:2:21:LYS:O	3:2:25:GLU:HG3	2.14	0.47
3:2:60:MET:CE	3:2:76:LEU:HB2	2.45	0.47
10:A:87:MET:O	10:A:110:ILE:HA	2.13	0.47
2:1:698:LEU:HD11	2:1:767:GLY:O	2.14	0.47
2:1:728:ASP:OD1	2:1:728:ASP:O	2.33	0.47
2:1:782:VAL:HA	2:1:794:GLN:O	2.14	0.47
3:2:193:GLN:O	3:2:197:GLU:HG3	2.15	0.47
3:2:288:MET:SD	3:2:288:MET:N	2.87	0.47
1:10:137:LEU:HA	1:10:163:THR:HG21	1.96	0.47
1:10:203:GLU:O	1:10:207:MET:HG3	2.15	0.47
2:1:44:SER:OG	2:1:55:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:88:PRO:HA	6:5:91:TYR:CD1	2.49	0.47
6:5:96:ARG:NH1	9:8:21:TYR:O	2.47	0.47
9:8:94:GLN:NE2	9:8:108:ALA:HB2	2.30	0.47
11:B:782:TYR:CD2	11:B:817:LEU:HB2	2.48	0.47
11:B:832:PRO:HB2	11:B:847:LEU:HD22	1.95	0.47
13:E:1:NAG:H3	13:E:2:NAG:H2	1.95	0.47
2:1:246:GLN:HG2	2:1:256:LEU:HD22	1.97	0.47
2:1:381:GLU:OE2	2:1:382:THR:OG1	2.28	0.47
3:2:90:LYS:HB3	3:2:113:ILE:HD11	1.97	0.47
3:2:248:LYS:HA	3:2:251:LYS:HE3	1.97	0.47
6:5:94:ASN:O	9:8:99:VAL:N	2.48	0.47
8:7:58:PRO:HA	8:7:61:TRP:NE1	2.28	0.47
9:8:60:LEU:HD22	9:8:74:ALA:HB1	1.97	0.47
10:A:43:ALA:HA	10:A:516:ALA:O	2.14	0.47
10:A:449:GLN:O	10:A:449:GLN:NE2	2.48	0.47
11:B:783:LYS:HG3	11:B:791:ILE:HG21	1.97	0.47
1:10:147:THR:OG1	1:10:160:SER:OG	2.19	0.47
3:2:90:LYS:HE2	3:2:112:ARG:HH22	1.79	0.47
10:A:113:PRO:HA	10:A:148:GLU:HG3	1.97	0.47
10:A:407:ASP:HB3	10:A:410:THR:HG23	1.96	0.47
11:B:802:PHE:HZ	11:B:845:ILE:HB	1.79	0.47
11:B:817:LEU:HA	11:B:832:PRO:O	2.15	0.47
2:1:340:ASN:N	2:1:340:ASN:OD1	2.47	0.47
11:B:689:GLN:HE22	11:B:719:HIS:HB2	1.80	0.47
4:3:77:LYS:NZ	4:3:225:LEU:O	2.30	0.47
4:3:81:ASN:HB2	4:3:222:TRP:CE2	2.50	0.47
10:A:73:ARG:HG3	10:A:83:ARG:HD2	1.96	0.47
10:A:218:THR:O	10:A:218:THR:OG1	2.32	0.47
10:A:254:LEU:HA	10:A:254:LEU:HD23	1.60	0.47
10:A:321:HIS:CE1	10:A:355:SER:HB2	2.50	0.47
10:A:324:VAL:HG12	10:A:383:PHE:HB3	1.97	0.47
10:A:456:MET:HA	10:A:459:LEU:HD12	1.96	0.47
11:B:836:PHE:O	11:B:837:THR:C	2.54	0.47
12:C:12:LEU:HB3	12:C:136:SER:OG	2.15	0.47
2:1:627:LEU:HD23	5:4:176:PHE:HE1	1.80	0.46
12:C:113:MET:HG3	12:C:114:SER:H	1.79	0.46
12:C:141:ILE:O	12:C:144:VAL:HG12	2.15	0.46
9:8:80:SER:HA	9:8:83:LYS:HZ3	1.77	0.46
10:A:64:ARG:HD2	10:A:138:GLU:HG2	1.97	0.46
10:A:130:ILE:HG12	10:A:134:MET:HE2	1.95	0.46
10:A:276:GLY:O	10:A:284:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:339:ARG:HA	10:A:339:ARG:HE	1.80	0.46
10:A:509:GLN:OE1	10:A:512:GLN:NE2	2.43	0.46
11:B:763:LEU:HB3	11:B:804:PHE:HB2	1.97	0.46
2:1:484:PHE:CZ	12:C:54:ALA:HB1	2.50	0.46
2:1:733:TYR:CD2	2:1:816:GLN:HB3	2.51	0.46
6:5:51:LEU:O	6:5:55:VAL:HG12	2.15	0.46
9:8:106:GLN:O	9:8:110:LYS:HG2	2.15	0.46
9:8:201:GLU:HA	9:8:204:LYS:HD3	1.96	0.46
10:A:127:PHE:CD2	10:A:400:MET:HG2	2.50	0.46
2:1:743:VAL:HG13	2:1:760:PHE:HB2	1.97	0.46
3:2:110:TYR:HA	3:2:113:ILE:HD12	1.96	0.46
4:3:82:ASN:H	4:3:89:LYS:HZ3	1.63	0.46
4:3:236:ASP:OD1	4:3:239:GLU:HB2	2.16	0.46
6:5:20:ALA:HB2	6:5:48:GLN:OE1	2.16	0.46
10:A:528:LEU:O	10:A:532:ILE:HG23	2.16	0.46
3:2:131:ARG:NH1	3:2:139:GLU:OE2	2.33	0.46
3:2:141:ILE:HD11	3:2:164:LEU:HB3	1.97	0.46
3:2:178:LEU:HD23	3:2:178:LEU:HA	1.74	0.46
4:3:73:PHE:CD2	4:3:230:HIS:HB2	2.51	0.46
7:6:64:LEU:O	7:6:68:LEU:N	2.45	0.46
4:3:156:ILE:HG22	4:3:158:LEU:H	1.81	0.46
5:4:109:PRO:O	5:4:111:GLN:N	2.45	0.46
10:A:127:PHE:HA	10:A:130:ILE:HG22	1.97	0.46
10:A:194:LYS:N	10:A:508:ASP:OD1	2.30	0.46
10:A:280:PHE:O	10:A:283:GLN:HG2	2.15	0.46
2:1:39:LYS:HD2	2:1:428:HIS:CD2	2.50	0.46
9:8:29:LEU:HD12	9:8:78:ILE:HG13	1.98	0.46
10:A:203:SER:HB3	10:A:273:PHE:CZ	2.51	0.46
2:1:138:GLU:HA	2:1:284:VAL:HG21	1.98	0.46
6:5:96:ARG:HH11	9:8:22:PRO:HA	1.80	0.46
12:C:131:LYS:O	12:C:135:MET:HG3	2.16	0.46
2:1:590:LEU:HD21	2:1:623:ILE:HD11	1.98	0.46
2:1:710:VAL:HG21	5:4:181:LEU:HG	1.98	0.46
2:1:779:LYS:HG2	2:1:780:GLY:N	2.31	0.46
3:2:40:LEU:HA	3:2:44:TYR:HD2	1.80	0.46
4:3:93:ARG:NH2	4:3:213:ASP:HA	2.31	0.46
7:6:73:ARG:HH12	7:6:76:LYS:HD3	1.80	0.46
7:6:105:GLY:HA2	7:6:109:VAL:HG23	1.98	0.46
1:10:104:LEU:HD23	1:10:104:LEU:HA	1.80	0.46
3:2:200:TYR:HD2	9:8:69:PRO:HD3	1.81	0.46
11:B:714:PRO:HB3	11:B:743:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:160:GLU:OE1	6:5:87:HIS:ND1	2.48	0.45
4:3:5:GLU:HB3	4:3:6:LEU:H	1.64	0.45
4:3:89:LYS:NZ	4:3:222:TRP:HE1	2.13	0.45
8:7:106:ASP:OD1	8:7:106:ASP:N	2.46	0.45
9:8:93:TYR:HA	9:8:125:ILE:HG13	1.99	0.45
10:A:471:LYS:HE3	10:A:471:LYS:HB2	1.85	0.45
1:10:62:ILE:HD12	1:10:62:ILE:H	1.82	0.45
1:10:73:SER:O	1:10:85:LEU:HA	2.16	0.45
2:1:129:GLN:HB2	2:1:146:LEU:HD23	1.97	0.45
2:1:871:LEU:HD11	2:1:904:ILE:HA	1.98	0.45
2:1:917:SER:O	2:1:940:LEU:HB2	2.17	0.45
3:2:82:GLN:O	3:2:82:GLN:NE2	2.50	0.45
4:3:62:ARG:HH22	4:3:221:GLU:CD	2.20	0.45
1:10:91:SER:O	1:10:95:ARG:HB2	2.17	0.45
2:1:671:PHE:O	2:1:683:GLY:HA2	2.16	0.45
2:1:846:ALA:O	2:1:864:GLY:N	2.49	0.45
3:2:259:TRP:HH2	4:3:246:LEU:HD21	1.81	0.45
4:3:13:ARG:HB2	7:6:110:TYR:CE2	2.52	0.45
1:10:95:ARG:HD3	1:10:178:LEU:HB2	1.99	0.45
2:1:73:ILE:HG21	2:1:76:ARG:HB2	1.99	0.45
2:1:587:CYS:SG	2:1:606:PRO:HB3	2.56	0.45
9:8:115:ILE:HG23	9:8:122:THR:HG21	1.98	0.45
10:A:443:GLU:C	10:A:445:MET:H	2.19	0.45
12:C:213:LEU:O	12:C:217:VAL:HG12	2.16	0.45
2:1:107:MET:HE3	2:1:123:LEU:HD11	1.99	0.45
10:A:72:ALA:HB2	10:A:186:MET:HG3	1.99	0.45
10:A:449:GLN:HE21	10:A:453:ASP:HB2	1.82	0.45
11:B:763:LEU:HD23	11:B:764:SER:N	2.32	0.45
12:C:197:ALA:O	12:C:201:ARG:HG3	2.16	0.45
2:1:674:VAL:O	5:4:181:LEU:HD23	2.15	0.45
3:2:104:ASP:OD1	3:2:104:ASP:N	2.49	0.45
4:3:24:THR:O	4:3:183:TYR:OH	2.35	0.45
4:3:55:LEU:HD13	4:3:59:ARG:HH22	1.81	0.45
7:6:107:VAL:HG12	7:6:108:HIS:CD2	2.52	0.45
9:8:12:CYS:O	9:8:16:LEU:HD23	2.17	0.45
9:8:32:ALA:HA	9:8:55:VAL:HG12	1.99	0.45
2:1:370:ASN:C	2:1:372:THR:H	2.20	0.45
2:1:389:THR:HA	2:1:435:GLN:HE21	1.81	0.45
2:1:483:MET:HA	2:1:486:LYS:HE3	1.99	0.45
10:A:152:LEU:HD12	10:A:152:LEU:HA	1.62	0.45
10:A:320:LEU:O	10:A:354:PHE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:824:ARG:O	11:B:853:ARG:NH2	2.50	0.45
2:1:377:LEU:HB2	2:1:389:THR:OG1	2.17	0.45
2:1:576:ARG:HD3	2:1:635:ASP:O	2.17	0.45
4:3:71:GLN:O	4:3:74:LEU:HD12	2.17	0.45
4:3:173:PHE:O	4:3:176:VAL:HG12	2.17	0.45
10:A:217:PRO:CA	10:A:304:ASN:HB3	2.39	0.45
12:C:80:ASP:HA	12:C:106:TRP:CH2	2.52	0.45
12:C:197:ALA:HB1	12:C:201:ARG:NH1	2.30	0.45
1:10:51:THR:HA	1:10:77:ASN:HA	1.98	0.45
1:10:58:HIS:CE1	1:10:71:ARG:HB2	2.52	0.45
2:1:460:LEU:HD22	2:1:525:LEU:HG	1.98	0.45
10:A:152:LEU:HA	10:A:155:ILE:HG22	1.99	0.45
10:A:200:LEU:HB3	10:A:494:HIS:HB3	1.98	0.45
10:A:329:ARG:O	10:A:332:THR:HG22	2.16	0.45
11:B:815:VAL:HG12	11:B:817:LEU:H	1.82	0.45
1:10:143:SER:CB	1:10:182:ASN:HD22	2.30	0.45
1:10:144:ASP:HA	1:10:163:THR:HA	1.98	0.45
2:1:203:ASN:ND2	2:1:206:ASP:HB3	2.28	0.45
2:1:231:ASP:O	2:1:287:SER:OG	2.25	0.45
3:2:110:TYR:CE2	3:2:126:ARG:HB3	2.52	0.45
4:3:162:ASP:HB3	4:3:165:TRP:CD1	2.52	0.45
6:5:65:GLY:O	7:6:69:LYS:NZ	2.42	0.45
10:A:238:ALA:O	10:A:243:SER:HB3	2.17	0.45
11:B:774:LEU:HD22	11:B:800:LEU:HG	1.99	0.45
3:2:133:ALA:HB2	6:5:92:VAL:HG23	1.99	0.44
6:5:69:ASP:HB2	6:5:71:ASP:OD1	2.17	0.44
7:6:64:LEU:O	7:6:67:ILE:HB	2.17	0.44
2:1:139:SER:OG	2:1:141:ARG:NH1	2.50	0.44
2:1:299:HIS:CE1	2:1:315:ASN:HD21	2.35	0.44
2:1:331:THR:HB	2:1:380:VAL:HB	1.99	0.44
2:1:771:HIS:NE2	2:1:773:SER:HB2	2.33	0.44
3:2:60:MET:O	3:2:63:ALA:HB3	2.17	0.44
8:7:50:ARG:HA	8:7:83:SER:HA	1.98	0.44
9:8:28:GLY:HA3	9:8:93:TYR:CE2	2.52	0.44
9:8:143:VAL:HG12	9:8:154:ARG:NH1	2.32	0.44
10:A:208:LEU:HD23	10:A:488:LYS:HZ2	1.82	0.44
11:B:678:PRO:HB3	11:B:704:GLU:O	2.18	0.44
11:B:678:PRO:HB2	11:B:703:GLU:O	2.16	0.44
11:B:824:ARG:NE	11:B:828:ASP:HA	2.32	0.44
2:1:48:SER:O	2:1:51:SER:OG	2.30	0.44
2:1:65:ALA:HB2	2:1:75:TRP:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:109:SER:OG	2:1:118:ASN:HB2	2.17	0.44
2:1:219:TRP:CH2	2:1:237:CYS:HB3	2.52	0.44
2:1:538:MET:SD	2:1:548:ILE:HD12	2.56	0.44
10:A:321:HIS:ND1	10:A:355:SER:O	2.40	0.44
1:10:91:SER:OG	1:10:92:GLU:N	2.51	0.44
2:1:802:ARG:HD2	2:1:839:ILE:HD12	1.98	0.44
3:2:250:LYS:HA	3:2:253:ASN:ND2	2.32	0.44
4:3:89:LYS:HE3	4:3:222:TRP:HE1	1.83	0.44
4:3:224:ALA:O	4:3:228:THR:HG23	2.17	0.44
8:7:136:TYR:O	8:7:138:LEU:HD12	2.18	0.44
9:8:5:LYS:HD3	9:8:6:LEU:N	2.32	0.44
1:10:191:THR:O	2:1:773:SER:HA	2.18	0.44
2:1:245:LEU:HB3	2:1:259:ILE:HG23	2.00	0.44
2:1:274:PRO:HA	2:1:294:HIS:O	2.18	0.44
2:1:302:LEU:HD23	2:1:302:LEU:HA	1.83	0.44
2:1:666:ALA:HA	2:1:686:LEU:HD23	1.99	0.44
2:1:893:GLU:HG3	2:1:895:LEU:HG	2.00	0.44
5:4:21:LEU:HD11	9:8:107:VAL:HG13	1.99	0.44
5:4:165:LEU:HD23	5:4:168:ILE:HD12	1.99	0.44
7:6:72:ARG:O	7:6:73:ARG:HG2	2.18	0.44
1:10:138:VAL:HG23	1:10:178:LEU:HD21	2.00	0.44
2:1:128:PHE:CE1	2:1:131:LEU:HB2	2.52	0.44
2:1:432:PHE:HB3	2:1:442:LEU:HB3	2.00	0.44
2:1:740:LEU:HD12	2:1:740:LEU:HA	1.73	0.44
3:2:118:PRO:HB2	4:3:46:GLN:OE1	2.17	0.44
3:2:144:LEU:HD11	3:2:157:ALA:HB1	1.99	0.44
6:5:93:PHE:HA	6:5:95:HIS:CE1	2.52	0.44
7:6:103:LEU:O	7:6:107:VAL:HB	2.18	0.44
9:8:68:ALA:N	9:8:69:PRO:HD2	2.33	0.44
9:8:94:GLN:O	9:8:126:MET:HA	2.18	0.44
10:A:289:LEU:HD12	10:A:301:LEU:HD13	2.00	0.44
10:A:390:SER:HB2	10:A:392:ARG:NH1	2.32	0.44
12:C:3:LEU:CA	12:C:124:ARG:HA	2.47	0.44
12:C:113:MET:O	12:C:115:ARG:N	2.51	0.44
3:2:90:LYS:CG	3:2:112:ARG:HH12	2.29	0.44
5:4:19:ILE:HD11	9:8:71:LEU:HB3	1.99	0.44
10:A:110:ILE:HD12	10:A:145:PHE:CE2	2.53	0.44
10:A:321:HIS:HB2	10:A:388:LEU:O	2.17	0.44
10:A:330:GLU:HG2	10:A:335:HIS:CE1	2.53	0.44
11:B:670:THR:HA	11:B:705:GLY:O	2.18	0.44
12:C:94:LYS:C	12:C:98:LYS:HE3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:389:THR:HA	2:1:435:GLN:NE2	2.33	0.44
2:1:714:ARG:NH2	2:1:848:GLU:OE2	2.51	0.44
2:1:819:ALA:O	2:1:821:ALA:N	2.51	0.44
6:5:68:LYS:HE3	7:6:18:ALA:HA	2.00	0.44
10:A:60:PRO:HB2	10:A:64:ARG:HD2	1.99	0.44
10:A:305:VAL:HG11	10:A:380:LEU:HG	2.00	0.44
2:1:180:SER:OG	2:1:186:VAL:HA	2.17	0.44
2:1:879:ASP:O	2:1:882:ARG:HG3	2.18	0.44
3:2:33:ILE:HD11	3:2:62:ALA:HB2	1.99	0.44
3:2:271:ALA:O	3:2:275:LYS:HG2	2.18	0.44
9:8:96:ASN:OD1	9:8:97:GLU:N	2.48	0.44
10:A:201:ILE:HB	10:A:495:VAL:HG13	1.99	0.44
10:A:269:ASN:HB3	10:A:300:LEU:HD22	2.00	0.44
11:B:830:ILE:HD13	11:B:830:ILE:HA	1.82	0.44
12:C:13:ALA:HB1	12:C:111:LEU:HD11	1.99	0.44
1:10:67:ASN:OD1	1:10:69:ARG:NH1	2.50	0.43
2:1:167:LEU:HD22	2:1:175:TYR:CZ	2.52	0.43
2:1:329:GLU:N	2:1:329:GLU:OE1	2.51	0.43
2:1:571:LYS:O	2:1:590:LEU:N	2.41	0.43
3:2:12:TRP:HB3	3:2:44:TYR:CD1	2.52	0.43
9:8:123:ALA:HB1	9:8:144:TYR:O	2.18	0.43
10:A:298:SER:O	10:A:299:SER:HB3	2.17	0.43
11:B:731:GLU:HB2	11:B:757:GLN:CA	2.48	0.43
1:10:113:PRO:HA	1:10:127:TYR:CD1	2.53	0.43
2:1:653:PRO:HG2	2:1:658:VAL:HG21	2.00	0.43
2:1:797:ASN:HD22	2:1:804:GLU:CD	2.21	0.43
2:1:916:VAL:HG13	2:1:941:ASP:HB2	2.00	0.43
3:2:133:ALA:O	9:8:98:ARG:NH2	2.50	0.43
4:3:92:LYS:HB2	4:3:215:ASN:OD1	2.18	0.43
9:8:19:ALA:O	9:8:22:PRO:HD3	2.18	0.43
10:A:193:SER:HB2	10:A:507:TYR:HB3	2.00	0.43
10:A:208:LEU:HD23	10:A:488:LYS:NZ	2.33	0.43
10:A:216:LEU:HD13	10:A:216:LEU:HA	1.67	0.43
10:A:309:LEU:HD21	10:A:385:LEU:HD12	2.00	0.43
12:C:13:ALA:O	12:C:16:PRO:HD2	2.18	0.43
2:1:921:GLY:HA3	2:1:938:TYR:CZ	2.53	0.43
3:2:180:GLU:O	3:2:183:MET:HB2	2.17	0.43
11:B:817:LEU:HD23	11:B:832:PRO:O	2.17	0.43
2:1:23:TYR:CB	8:7:149:PHE:HA	2.48	0.43
8:7:108:VAL:HG13	8:7:121:ARG:O	2.19	0.43
9:8:161:CYS:SG	9:8:162:GLU:N	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:72:ALA:HB2	10:A:186:MET:CG	2.47	0.43
10:A:393:ASP:OD2	10:A:395:GLN:HB2	2.18	0.43
12:C:17:TYR:HE2	12:C:111:LEU:HB2	1.82	0.43
2:1:143:ILE:O	2:1:153:LEU:HD13	2.18	0.43
2:1:219:TRP:CZ2	2:1:239:ASP:HB2	2.53	0.43
2:1:424:GLN:HA	2:1:429:LEU:O	2.19	0.43
2:1:627:LEU:HD22	2:1:671:PHE:HE1	1.83	0.43
2:1:843:SER:OG	2:1:844:ILE:N	2.50	0.43
2:1:882:ARG:NH2	2:1:899:SER:H	2.16	0.43
3:2:201:THR:HG23	9:8:68:ALA:HB2	2.01	0.43
7:6:72:ARG:HE	12:C:33:TRP:CB	2.32	0.43
10:A:440:VAL:HG13	11:B:755:PHE:HZ	1.83	0.43
10:A:529:ALA:HB2	12:C:8:ASN:ND2	2.33	0.43
6:5:96:ARG:HB3	9:8:129:ASN:HB2	1.99	0.43
10:A:110:ILE:HD12	10:A:145:PHE:CZ	2.54	0.43
10:A:253:ARG:HB2	10:A:486:TYR:CE2	2.53	0.43
2:1:198:ASN:HB2	2:1:214:ARG:HG2	2.00	0.43
2:1:485:LEU:O	2:1:488:LEU:HG	2.19	0.43
2:1:760:PHE:HA	2:1:771:HIS:O	2.19	0.43
3:2:227:ARG:HA	3:2:230:PHE:CZ	2.53	0.43
6:5:68:LYS:O	7:6:22:ASN:ND2	2.44	0.43
7:6:55:TYR:HB2	7:6:96:TYR:CE2	2.53	0.43
9:8:198:THR:OG1	9:8:200:PRO:HD3	2.18	0.43
10:A:250:GLU:CD	10:A:253:ARG:HE	2.22	0.43
1:10:59:SER:HB3	1:10:68:PHE:HA	1.99	0.43
2:1:929:LEU:HG	2:1:954:ASP:OD2	2.18	0.43
3:2:15:MET:HB2	3:2:40:LEU:HD21	2.00	0.43
3:2:52:ILE:HA	3:2:55:ILE:HD12	2.01	0.43
3:2:70:ASP:OD1	3:2:71:LEU:N	2.52	0.43
3:2:136:LYS:HD2	3:2:139:GLU:OE1	2.19	0.43
3:2:213:LYS:HD2	4:3:232:TRP:CH2	2.53	0.43
4:3:57:ARG:HA	4:3:60:VAL:HG12	2.00	0.43
4:3:141:PRO:O	7:6:47:THR:HG23	2.19	0.43
9:8:60:LEU:HD12	9:8:60:LEU:O	2.19	0.43
1:10:200:ALA:O	1:10:204:ARG:HB2	2.19	0.43
2:1:940:LEU:HD23	2:1:940:LEU:HA	1.81	0.43
3:2:268:TYR:HB3	3:2:281:SER:HB3	2.01	0.43
10:A:216:LEU:HD12	10:A:267:ALA:O	2.19	0.43
10:A:543:VAL:HG11	12:C:23:CYS:HB2	1.99	0.43
11:B:685:GLU:OE1	11:B:723:LYS:HG2	2.18	0.43
11:B:686:ALA:HA	11:B:719:HIS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:702:ASP:OD1	11:B:706:LYS:N	2.47	0.43
2:1:656:ARG:NH2	11:B:798:GLN:OE1	2.52	0.43
2:1:965:ILE:HD13	2:1:965:ILE:HA	1.90	0.43
3:2:173:LYS:HG2	5:4:47:TYR:CE2	2.54	0.43
4:3:86:GLY:O	4:3:90:LYS:HG2	2.19	0.43
4:3:119:LEU:HD12	4:3:119:LEU:HA	1.90	0.43
6:5:74:SER:OG	6:5:75:GLU:N	2.52	0.43
11:B:780:LYS:HE2	11:B:793:THR:HG23	2.01	0.43
1:10:200:ALA:O	1:10:203:GLU:HG3	2.19	0.42
2:1:57:ALA:HB1	2:1:87:VAL:HG21	2.01	0.42
3:2:188:ASN:HB3	3:2:191:TYR:CD2	2.54	0.42
9:8:204:LYS:HG2	9:8:205:ALA:N	2.33	0.42
10:A:122:ASP:N	10:A:122:ASP:OD1	2.52	0.42
10:A:440:VAL:HG22	11:B:734:LEU:CD1	2.49	0.42
11:B:783:LYS:HE2	11:B:783:LYS:HB3	1.80	0.42
2:1:231:ASP:OD1	2:1:232:GLU:N	2.52	0.42
3:2:23:ARG:HB2	3:2:58:GLN:HE22	1.83	0.42
3:2:110:TYR:CZ	3:2:126:ARG:HB3	2.53	0.42
12:C:138:ASP:O	12:C:141:ILE:HG12	2.18	0.42
2:1:47:PHE:HB3	2:1:51:SER:OG	2.19	0.42
2:1:179:TYR:HD1	2:1:180:SER:H	1.67	0.42
2:1:483:MET:H	2:1:483:MET:HG2	1.62	0.42
2:1:674:VAL:HB	5:4:181:LEU:HA	2.00	0.42
10:A:74:THR:OG1	10:A:75:MET:N	2.51	0.42
12:C:200:ALA:O	12:C:203:VAL:HG22	2.19	0.42
1:10:141:HIS:HA	1:10:177:ASP:OD2	2.20	0.42
1:10:153:ALA:HB2	2:1:704:VAL:HG21	2.01	0.42
2:1:545:LEU:HB3	2:1:557:TRP:CH2	2.54	0.42
2:1:662:LEU:HD11	2:1:690:LEU:HD11	2.02	0.42
2:1:683:GLY:HA3	2:1:696:TRP:CE2	2.54	0.42
5:4:19:ILE:HG12	9:8:72:GLU:HG2	2.01	0.42
8:7:151:LYS:HE2	8:7:151:LYS:HB2	1.76	0.42
10:A:61:TYR:H	10:A:64:ARG:NH1	2.18	0.42
11:B:733:ALA:HA	11:B:754:VAL:HA	2.01	0.42
2:1:95:GLN:HG2	2:1:113:ASN:ND2	2.34	0.42
2:1:230:VAL:HG11	2:1:291:PHE:CG	2.55	0.42
2:1:392:THR:O	2:1:440:VAL:HG21	2.19	0.42
2:1:676:ALA:HB2	5:4:181:LEU:HD21	2.02	0.42
3:2:283:LYS:HE3	3:2:283:LYS:HB2	1.84	0.42
6:5:7:LYS:O	6:5:10:VAL:HG12	2.19	0.42
9:8:21:TYR:HE2	9:8:185:ASP:OD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:100:LYS:HD3	9:8:100:LYS:HA	1.73	0.42
10:A:250:GLU:HG2	10:A:447:ILE:HG23	2.01	0.42
10:A:450:GLU:H	10:A:450:GLU:HG3	1.72	0.42
2:1:232:GLU:HG3	2:1:251:GLU:HG3	2.01	0.42
2:1:264:LEU:HD23	2:1:264:LEU:HA	1.85	0.42
3:2:270:PHE:HD2	3:2:273:ARG:NH2	2.13	0.42
4:3:52:SER:O	4:3:55:LEU:HG	2.20	0.42
10:A:194:LYS:HB2	10:A:194:LYS:HE2	1.74	0.42
12:C:216:TYR:O	12:C:220:VAL:HG13	2.20	0.42
2:1:433:LEU:HA	2:1:440:VAL:O	2.20	0.42
2:1:544:LYS:HE2	2:1:546:PHE:CZ	2.55	0.42
2:1:735:SER:HB2	2:1:831:PRO:HB3	2.02	0.42
3:2:165:TYR:CZ	3:2:173:LYS:HD3	2.55	0.42
2:1:302:LEU:HG	2:1:316:PHE:HE1	1.84	0.42
2:1:931:SER:OG	2:1:952:GLN:HA	2.20	0.42
5:4:54:ASP:OD1	5:4:54:ASP:N	2.52	0.42
6:5:96:ARG:HG2	9:8:22:PRO:O	2.20	0.42
10:A:66:ALA:HB3	10:A:192:GLN:HA	2.01	0.42
12:C:94:LYS:O	12:C:98:LYS:HE3	2.20	0.42
12:C:156:ILE:HD13	12:C:156:ILE:HA	1.89	0.42
1:10:53:GLY:HA2	1:10:74:LEU:O	2.19	0.42
1:10:97:ARG:O	1:10:101:VAL:HG23	2.20	0.42
2:1:141:ARG:HD3	2:1:142:TYR:CZ	2.55	0.42
2:1:713:LYS:HB3	2:1:713:LYS:HE2	1.77	0.42
2:1:795:TYR:CZ	2:1:804:GLU:HB2	2.55	0.42
3:2:164:LEU:HD23	3:2:164:LEU:HA	1.84	0.42
3:2:224:ARG:HE	3:2:224:ARG:HB3	1.75	0.42
9:8:108:ALA:HB1	9:8:124:LEU:HD11	2.02	0.42
11:B:747:ILE:HD12	11:B:747:ILE:HA	1.87	0.42
12:C:120:TRP:CE3	12:C:120:TRP:HA	2.55	0.42
1:10:71:ARG:NH1	1:10:108:TYR:OH	2.52	0.42
2:1:228:GLY:O	2:1:235:LEU:HD12	2.20	0.42
2:1:672:TYR:O	5:4:180:GLY:N	2.50	0.42
2:1:727:GLY:C	2:1:729:ARG:H	2.23	0.42
4:3:237:VAL:O	4:3:240:GLU:HG2	2.19	0.42
6:5:70:MET:O	7:6:15:SER:N	2.47	0.42
8:7:45:PHE:CE2	8:7:116:GLY:HA2	2.55	0.42
10:A:80:LEU:HD12	10:A:80:LEU:HA	1.88	0.42
12:C:12:LEU:HD22	12:C:136:SER:OG	2.19	0.42
2:1:134:VAL:HG12	2:1:180:SER:OG	2.20	0.41
7:6:94:PHE:O	7:6:97:VAL:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:10:59:SER:OG	1:10:109:ARG:HB2	2.20	0.41
2:1:217:THR:O	2:1:217:THR:OG1	2.35	0.41
3:2:229:LEU:HD22	3:2:264:ILE:HG13	2.02	0.41
4:3:32:HIS:HD2	4:3:192:ALA:H	1.69	0.41
4:3:78:TYR:O	4:3:82:ASN:HB3	2.21	0.41
4:3:178:GLY:HA3	7:6:98:LEU:HD22	2.02	0.41
9:8:166:GLU:HA	9:8:169:ARG:HG2	2.02	0.41
10:A:182:ASN:OD1	10:A:520:LYS:NZ	2.45	0.41
11:B:824:ARG:HD2	11:B:824:ARG:HA	1.86	0.41
2:1:73:ILE:CG2	2:1:76:ARG:HB2	2.50	0.41
2:1:196:HIS:CD2	2:1:214:ARG:HD2	2.55	0.41
2:1:627:LEU:HD11	5:4:178:GLY:C	2.40	0.41
2:1:930:GLU:HB2	4:3:6:LEU:HD11	2.02	0.41
3:2:165:TYR:O	3:2:169:HIS:N	2.53	0.41
7:6:55:TYR:HB2	7:6:96:TYR:CZ	2.55	0.41
10:A:55:ASP:HB2	10:A:505:VAL:CG2	2.49	0.41
10:A:74:THR:HA	10:A:86:LEU:H	1.85	0.41
10:A:234:LEU:HD23	10:A:234:LEU:HA	1.82	0.41
10:A:251:LEU:HD22	10:A:255:PHE:HE2	1.85	0.41
10:A:420:GLU:OE2	10:A:439:PRO:HB3	2.20	0.41
10:A:526:LEU:HD12	12:C:4:PHE:CE1	2.55	0.41
11:B:674:LEU:HD12	11:B:674:LEU:HA	1.85	0.41
11:B:831:LEU:H	11:B:831:LEU:HD23	1.84	0.41
12:C:111:LEU:HD23	12:C:116:CYS:HB2	2.02	0.41
2:1:143:ILE:O	2:1:153:LEU:HA	2.21	0.41
2:1:727:GLY:C	2:1:729:ARG:N	2.73	0.41
3:2:83:PHE:HB3	3:2:86:SER:OG	2.20	0.41
4:3:59:ARG:NH1	4:3:59:ARG:HB3	2.35	0.41
10:A:485:ARG:HD3	10:A:485:ARG:HA	1.92	0.41
2:1:181:TYR:HB2	2:1:284:VAL:O	2.20	0.41
2:1:729:ARG:HD3	5:4:160:HIS:CE1	2.56	0.41
3:2:127:LYS:O	3:2:131:ARG:HG2	2.20	0.41
8:7:81:ASP:OD1	8:7:82:GLY:N	2.53	0.41
9:8:169:ARG:HG3	9:8:170:ILE:N	2.35	0.41
10:A:75:MET:CE	10:A:96:GLN:HB3	2.50	0.41
10:A:220:VAL:HG13	10:A:271:LEU:O	2.21	0.41
11:B:781:LEU:HD23	11:B:792:GLN:NE2	2.35	0.41
2:1:625:GLN:H	2:1:643:ILE:HG23	1.86	0.41
3:2:103:TYR:CD1	3:2:130:ILE:HG23	2.55	0.41
4:3:68:ILE:O	4:3:230:HIS:HE1	2.03	0.41
4:3:77:LYS:HG2	4:3:225:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:145:GLU:HB3	9:8:154:ARG:CZ	2.50	0.41
9:8:202:ILE:HG13	9:8:203:ASN:N	2.34	0.41
10:A:93:SER:HB2	10:A:96:GLN:HG2	2.02	0.41
10:A:403:ARG:HB2	10:A:460:THR:HG21	2.02	0.41
11:B:734:LEU:HB3	11:B:753:ILE:HG13	2.02	0.41
12:C:14:TYR:O	12:C:17:TYR:HB2	2.20	0.41
1:10:114:ARG:CZ	1:10:126:GLY:HA3	2.50	0.41
8:7:120:ALA:HB3	8:7:134:LEU:O	2.21	0.41
9:8:58:ILE:HD11	9:8:197:TRP:O	2.21	0.41
12:C:207:LEU:O	12:C:210:LEU:HG	2.20	0.41
13:D:1:NAG:H61	13:D:2:NAG:C7	2.50	0.41
2:1:54:LEU:O	2:1:65:ALA:HA	2.21	0.41
2:1:557:TRP:CE3	2:1:609:GLY:HA3	2.55	0.41
2:1:839:ILE:N	2:1:900:PRO:O	2.36	0.41
2:1:886:PRO:HG3	2:1:897:PRO:HB3	2.02	0.41
9:8:4:VAL:HB	9:8:143:VAL:HG11	2.03	0.41
10:A:65:ASN:HB3	10:A:142:PRO:CD	2.45	0.41
10:A:325:SER:HB2	10:A:361:ILE:HG12	2.02	0.41
11:B:814:TYR:HB2	11:B:836:PHE:CE1	2.56	0.41
2:1:253:GLU:HG2	2:1:255:GLU:O	2.21	0.41
2:1:627:LEU:HD22	2:1:671:PHE:CE1	2.56	0.41
2:1:870:ILE:O	2:1:910:ILE:HG23	2.21	0.41
3:2:21:LYS:HE3	3:2:21:LYS:HB3	1.83	0.41
6:5:96:ARG:HD2	9:8:18:GLY:O	2.21	0.41
7:6:36:LEU:HD12	7:6:36:LEU:HA	1.85	0.41
7:6:105:GLY:O	7:6:109:VAL:HB	2.21	0.41
9:8:3:GLY:N	9:8:154:ARG:HE	2.18	0.41
9:8:64:THR:O	9:8:65:LEU:HD23	2.21	0.41
9:8:111:VAL:O	9:8:115:ILE:HG22	2.20	0.41
9:8:186:PHE:O	9:8:190:LEU:HG	2.19	0.41
10:A:48:VAL:CG2	10:A:514:MET:HB2	2.51	0.41
10:A:69:ASN:CB	10:A:187:VAL:HG23	2.50	0.41
10:A:71:GLU:HA	10:A:185:GLN:HA	2.03	0.41
10:A:225:TYR:O	10:A:464:ARG:NE	2.40	0.41
10:A:292:ASN:CB	10:A:301:LEU:HD12	2.50	0.41
10:A:321:HIS:HE1	10:A:355:SER:HB2	1.85	0.41
10:A:323:HIS:HA	10:A:357:VAL:O	2.21	0.41
11:B:759:ASN:O	11:B:809:ARG:HG2	2.21	0.41
12:C:117:ILE:O	12:C:121:VAL:HG12	2.21	0.41
12:C:130:TRP:O	12:C:134:GLN:HG3	2.21	0.41
1:10:54:LEU:HB2	1:10:74:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:4:VAL:HG21	9:8:123:ALA:HB3	2.03	0.41
10:A:224:HIS:HA	10:A:275:SER:O	2.21	0.41
3:2:183:MET:SD	4:3:61:LEU:HD13	2.61	0.40
4:3:158:LEU:HD23	4:3:158:LEU:HA	1.86	0.40
7:6:51:GLY:O	7:6:96:TYR:OH	2.24	0.40
9:8:124:LEU:H	9:8:151:TRP:HZ3	1.68	0.40
10:A:63:THR:HA	10:A:139:THR:OG1	2.21	0.40
10:A:68:LEU:H	10:A:188:THR:HG22	1.86	0.40
10:A:223:ALA:HB1	10:A:241:ASN:HD21	1.85	0.40
10:A:366:ASP:OD1	10:A:366:ASP:N	2.54	0.40
12:C:146:TYR:HD1	12:C:146:TYR:HA	1.67	0.40
2:1:279:THR:HB	2:1:324:PHE:CD2	2.50	0.40
2:1:685:ARG:HB2	2:1:693:GLU:CG	2.51	0.40
2:1:836:GLN:HG2	2:1:838:TYR:CE1	2.56	0.40
2:1:988:LEU:HD21	3:2:53:TRP:CZ3	2.56	0.40
3:2:80:ARG:HG2	3:2:89:VAL:HG11	2.03	0.40
4:3:32:HIS:ND1	4:3:187:LEU:HD21	2.36	0.40
10:A:65:ASN:CB	10:A:142:PRO:HD3	2.44	0.40
10:A:217:PRO:HB2	10:A:268:TYR:CE1	2.56	0.40
10:A:337:PHE:HB2	10:A:425:VAL:HG21	2.03	0.40
2:1:244:SER:HA	2:1:260:PRO:HA	2.03	0.40
2:1:548:ILE:HA	2:1:554:THR:O	2.21	0.40
2:1:882:ARG:O	2:1:898:TYR:HB2	2.21	0.40
4:3:62:ARG:HG3	4:3:228:THR:HG21	2.03	0.40
10:A:255:PHE:O	10:A:259:TYR:N	2.50	0.40
10:A:294:ASP:OD1	10:A:295:HIS:N	2.55	0.40
10:A:509:GLN:HB3	10:A:512:GLN:NE2	2.37	0.40
11:B:768:ILE:HD12	11:B:848:ILE:HG12	2.04	0.40
2:1:425:THR:HG21	2:1:429:LEU:HD23	2.02	0.40
5:4:47:TYR:CD1	5:4:48:LEU:N	2.89	0.40
6:5:43:ILE:HA	6:5:46:VAL:HG22	2.04	0.40
9:8:61:PHE:HZ	9:8:74:ALA:HB2	1.86	0.40
9:8:95:ALA:HB2	9:8:127:VAL:HB	2.04	0.40
9:8:114:ARG:O	9:8:117:GLU:HB2	2.22	0.40
9:8:144:TYR:HA	9:8:153:CYS:HA	2.03	0.40
10:A:122:ASP:HA	10:A:125:ARG:NH1	2.36	0.40
2:1:259:ILE:HG21	2:1:310:LEU:HD22	2.03	0.40
2:1:572:LEU:HD11	2:1:604:PHE:HZ	1.86	0.40
2:1:599:SER:O	2:1:619:LEU:HB2	2.22	0.40
3:2:124:ARG:O	3:2:127:LYS:HG2	2.22	0.40
4:3:32:HIS:HB2	4:3:193:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:34:THR:HG22	6:5:36:LYS:HB3	2.02	0.40
10:A:497:ALA:C	10:A:499:LYS:H	2.25	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	10	150/262 (57%)	145 (97%)	5 (3%)	0	100	100
2	1	908/993 (91%)	844 (93%)	61 (7%)	3 (0%)	37	73
3	2	279/297 (94%)	273 (98%)	6 (2%)	0	100	100
4	3	219/261 (84%)	207 (94%)	12 (6%)	0	100	100
5	4	138/183 (75%)	127 (92%)	11 (8%)	0	100	100
6	5	99/131 (76%)	94 (95%)	5 (5%)	0	100	100
7	6	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
8	7	134/242 (55%)	123 (92%)	11 (8%)	0	100	100
9	8	188/210 (90%)	179 (95%)	9 (5%)	0	100	100
10	A	501/563 (89%)	450 (90%)	51 (10%)	0	100	100
11	B	184/1267 (14%)	167 (91%)	17 (9%)	0	100	100
12	C	197/224 (88%)	186 (94%)	10 (5%)	1 (0%)	25	64
All	All	3094/4743 (65%)	2891 (93%)	199 (6%)	4 (0%)	50	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	820	THR
2	1	369	PHE

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Mol	Chain	Res	Type
2	1	371	GLN
12	C	114	SER

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	10	129/194 (66%)	126 (98%)	3 (2%)	45	64
2	1	809/872 (93%)	783 (97%)	26 (3%)	34	53
3	2	236/255 (92%)	229 (97%)	7 (3%)	36	55
4	3	204/235 (87%)	194 (95%)	10 (5%)	21	42
5	4	46/149 (31%)	44 (96%)	2 (4%)	25	46
6	5	82/112 (73%)	76 (93%)	6 (7%)	11	31
7	6	78/85 (92%)	78 (100%)	0	100	100
8	7	110/207 (53%)	108 (98%)	2 (2%)	54	71
9	8	168/182 (92%)	160 (95%)	8 (5%)	21	43
10	A	421/475 (89%)	404 (96%)	17 (4%)	27	47
11	B	167/1097 (15%)	159 (95%)	8 (5%)	21	43
12	C	100/186 (54%)	96 (96%)	4 (4%)	27	47
All	All	2550/4049 (63%)	2457 (96%)	93 (4%)	32	50

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	10	100	ASP
1	10	155	ASN
1	10	181	PHE
2	1	25	ASP
2	1	30	PHE
2	1	90	MET
2	1	93	HIS
2	1	122	THR

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Mol	Chain	Res	Type
2	1	137	GLN
2	1	179	TYR
2	1	211	GLN
2	1	227	CYS
2	1	257	ARG
2	1	304	GLN
2	1	324	PHE
2	1	414	ASP
2	1	445	ARG
2	1	581	PHE
2	1	665	LEU
2	1	725	VAL
2	1	799	LYS
2	1	801	ARG
2	1	879	ASP
2	1	894	ASN
2	1	912	TYR
2	1	919	MET
2	1	927	SER
2	1	933	CYS
2	1	951	LYS
3	2	25	GLU
3	2	158	TRP
3	2	161	LEU
3	2	177	CYS
3	2	230	PHE
3	2	248	LYS
3	2	269	GLN
4	3	74	LEU
4	3	78	TYR
4	3	90	LYS
4	3	111	MET
4	3	151	MET
4	3	160	THR
4	3	173	PHE
4	3	216	LYS
4	3	222	TRP
4	3	247	HIS
5	4	49	ASP
5	4	54	ASP
6	5	7	LYS
6	5	15	PHE

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Mol	Chain	Res	Type
6	5	69	ASP
6	5	75	GLU
6	5	76	LEU
6	5	84	LEU
8	7	118	MET
8	7	163	ASN
9	8	9	GLN
9	8	61	PHE
9	8	87	TYR
9	8	119	PHE
9	8	187	ASP
9	8	195	ASN
9	8	197	TRP
9	8	204	LYS
10	A	44	HIS
10	A	46	PHE
10	A	65	ASN
10	A	68	LEU
10	A	94	TYR
10	A	198	ASP
10	A	240	SER
10	A	241	ASN
10	A	294	ASP
10	A	300	LEU
10	A	339	ARG
10	A	353	ARG
10	A	362	ASN
10	A	456	MET
10	A	489	ASP
10	A	496	LYS
10	A	540	TYR
11	B	684	MET
11	B	690	ASN
11	B	719	HIS
11	B	737	HIS
11	B	751	ASN
11	B	778	TRP
11	B	809	ARG
11	B	819	ASP
12	C	21	TYR
12	C	104	LEU
12	C	138	ASP

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Mol	Chain	Res	Type
12	C	145	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	10	149	HIS
2	1	198	ASN
2	1	299	HIS
2	1	315	ASN
2	1	739	ASN
2	1	786	HIS
2	1	794	GLN
2	1	860	HIS
3	2	253	ASN
4	3	175	ASN
10	A	192	GLN
10	A	335	HIS
11	B	689	GLN
12	C	8	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	D	1	13,1	14,14,15	0.70	0	17,19,21	1.20	2 (11%)
13	NAG	D	2	13	14,14,15	0.73	0	17,19,21	0.85	0
13	NAG	E	1	13,2	14,14,15	0.80	0	17,19,21	0.83	1 (5%)
13	NAG	E	2	13	14,14,15	0.95	1 (7%)	17,19,21	0.86	0

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
13	NAG	D	1	13,1	-	1/6/23/26	0/1/1/1
13	NAG	D	2	13	-	2/6/23/26	0/1/1/1
13	NAG	E	1	13,2	-	0/6/23/26	0/1/1/1
13	NAG	E	2	13	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	2	NAG	C1-C2	2.88	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	D	1	NAG	C2-N2-C7	3.25	127.25	122.90
13	E	1	NAG	C1-O5-C5	2.51	115.55	112.19
13	D	1	NAG	C1-O5-C5	2.31	115.28	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	2	NAG	C8-C7-N2-C2
13	D	2	NAG	O7-C7-N2-C2
13	E	2	NAG	C8-C7-N2-C2
13	E	2	NAG	O7-C7-N2-C2
13	E	2	NAG	O5-C5-C6-O6
13	D	1	NAG	C3-C2-N2-C7

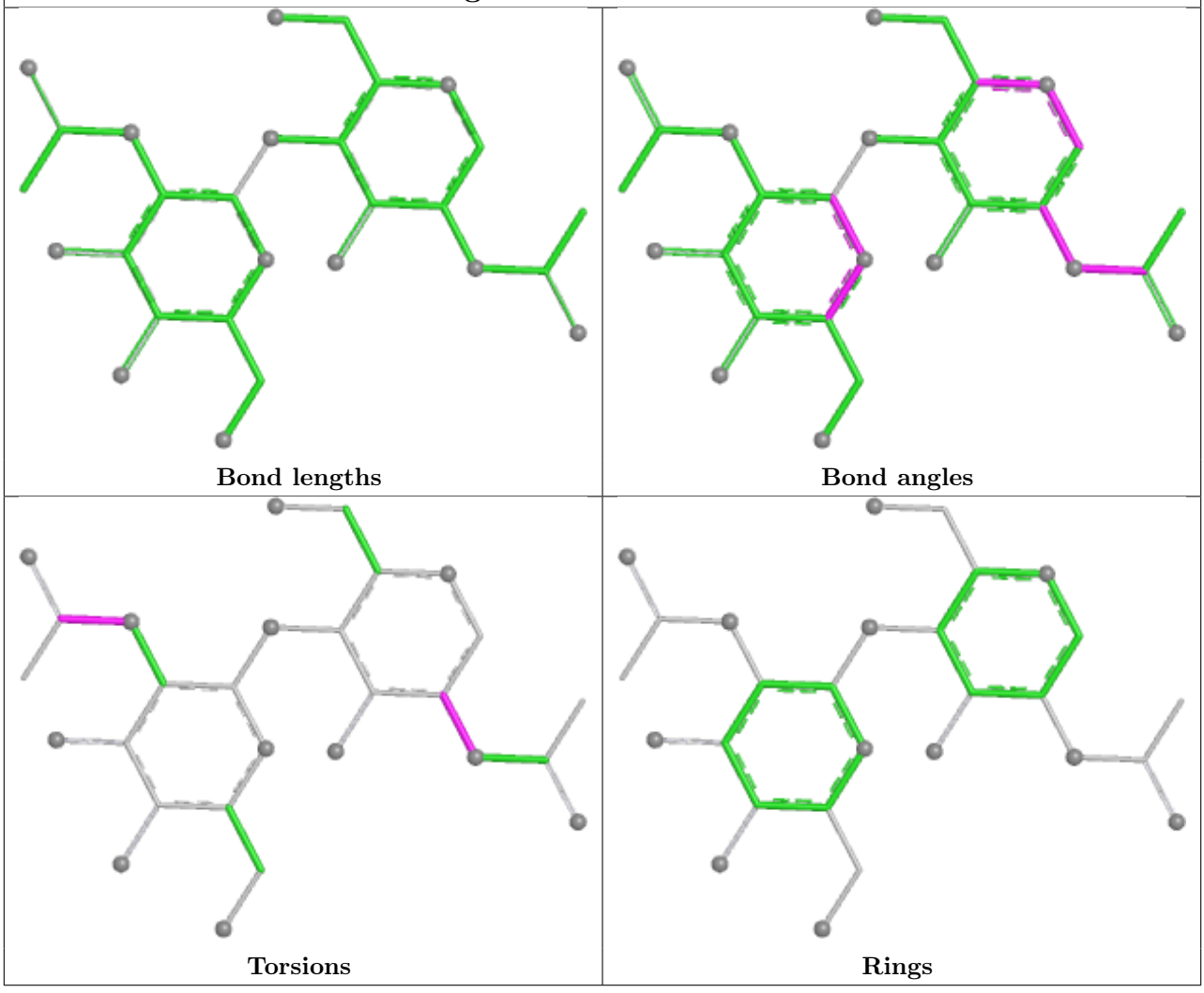
There are no ring outliers.

4 monomers are involved in 6 short contacts:

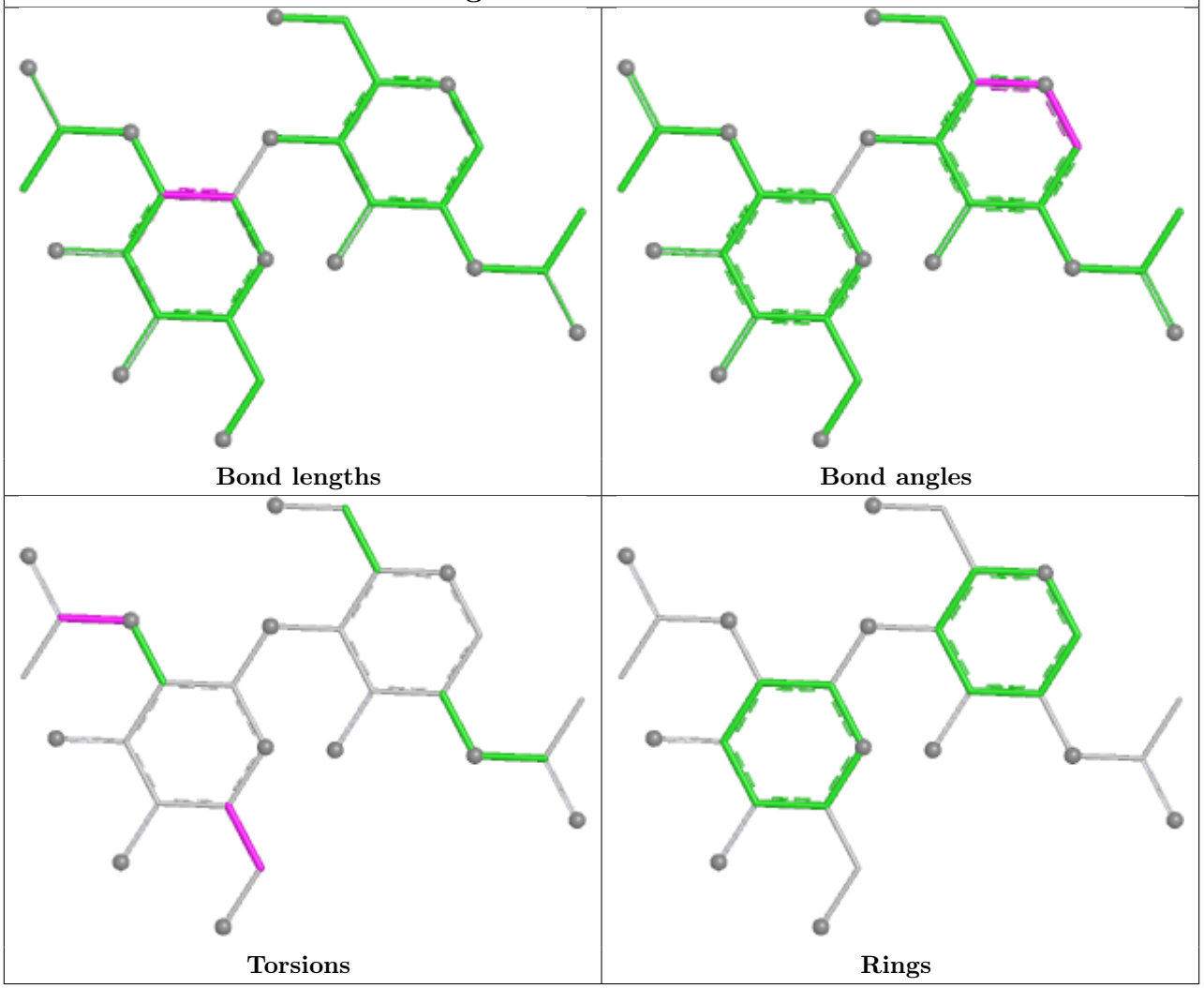
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	1	NAG	3	0
13	D	2	NAG	1	0
13	E	1	NAG	3	0
13	E	2	NAG	3	0

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

Oligosaccharide Chain D



Oligosaccharide Chain E



5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
14	NAG	1	1001	2	14,14,15	0.55	0	17,19,21	1.33	2 (11%)
14	NAG	1	1002	2	14,14,15	0.62	0	17,19,21	0.78	1 (5%)

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
14	NAG	1	1001	2	-	1/6/23/26	0/1/1/1
14	NAG	1	1002	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1	1001	NAG	C2-N2-C7	4.27	128.63	122.90
14	1	1001	NAG	C1-C2-N2	2.10	113.74	110.43
14	1	1002	NAG	C2-N2-C7	2.02	125.60	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	1	1001	NAG	C3-C2-N2-C7
14	1	1002	NAG	C3-C2-N2-C7
14	1	1002	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	1002	NAG	3	0

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.

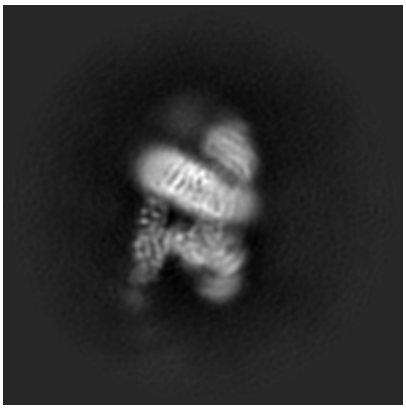
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45295. These allow visual inspection of the internal detail of the map and identification of artifacts.

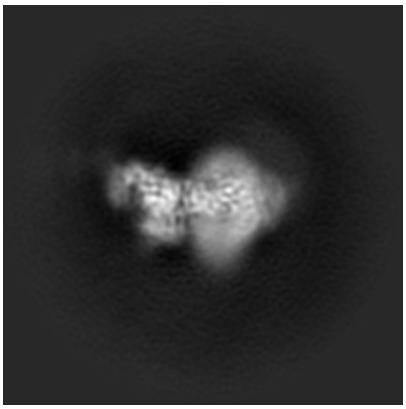
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

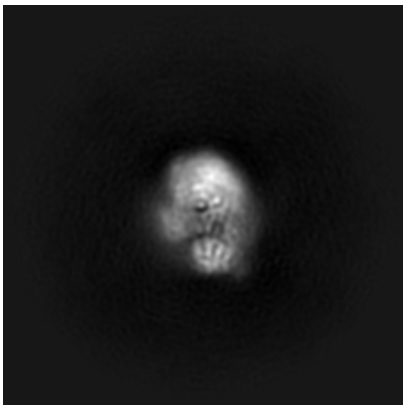
6.1.1 Primary map



X

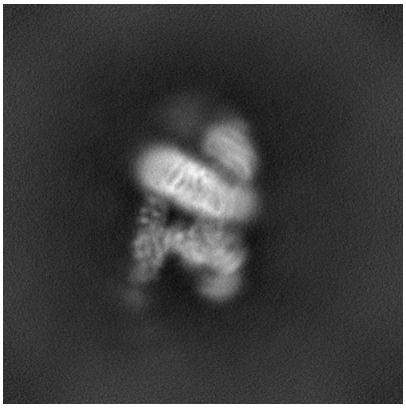


Y

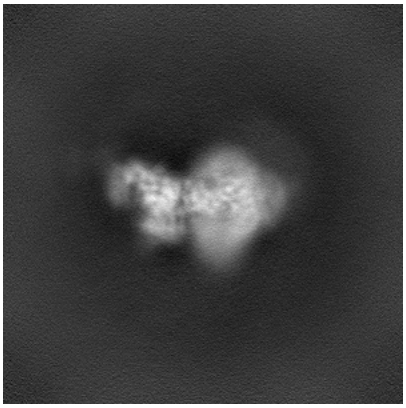


Z

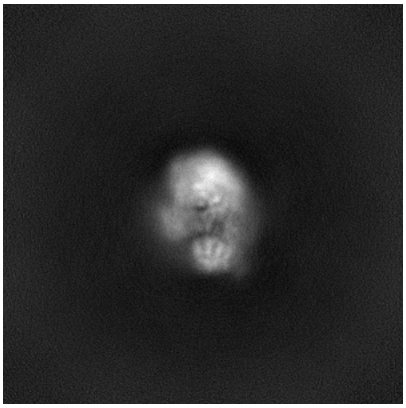
6.1.2 Raw map



X



Y

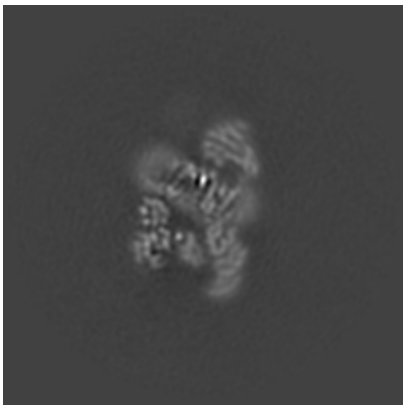


Z

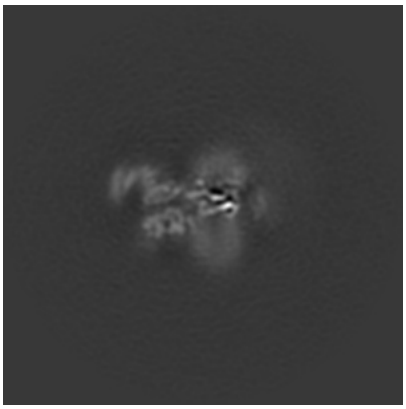
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

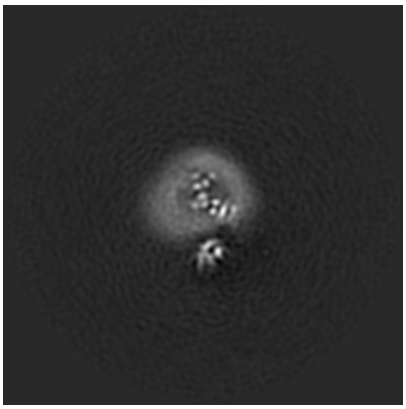
6.2.1 Primary map



X Index: 256

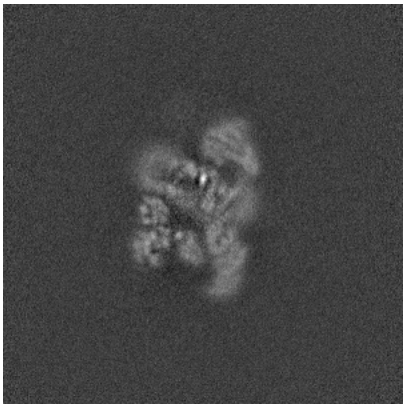


Y Index: 256

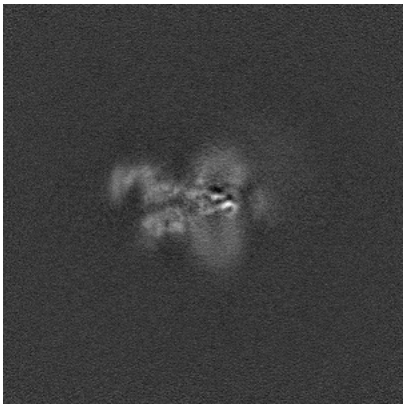


Z Index: 256

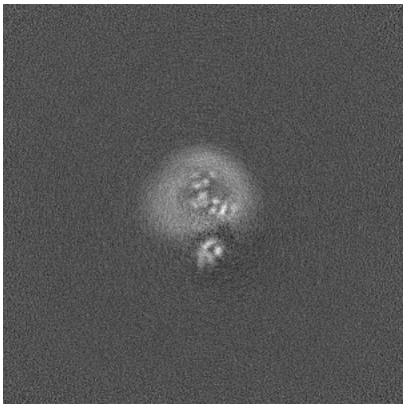
6.2.2 Raw map



X Index: 256



Y Index: 256

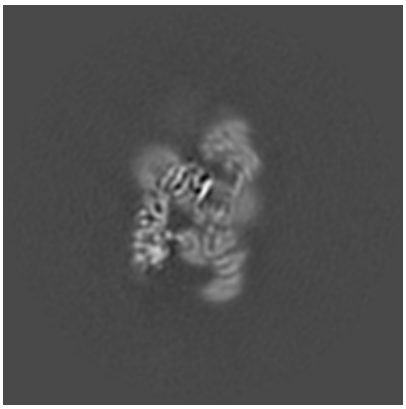


Z Index: 256

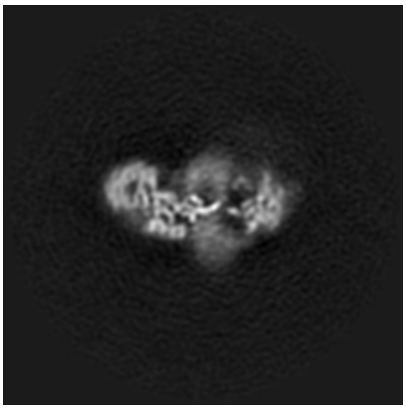
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

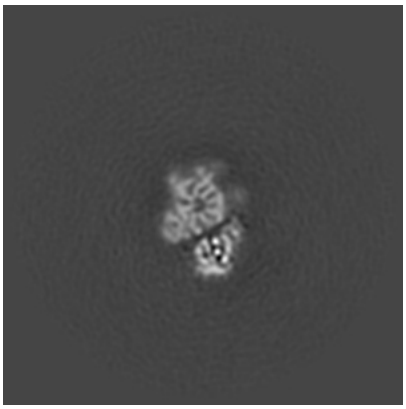
6.3.1 Primary map



X Index: 264

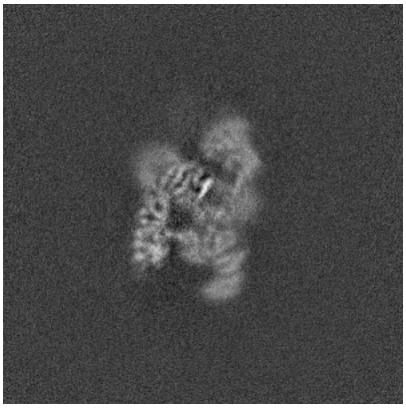


Y Index: 278

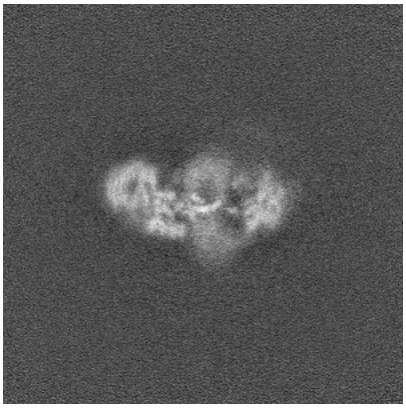


Z Index: 205

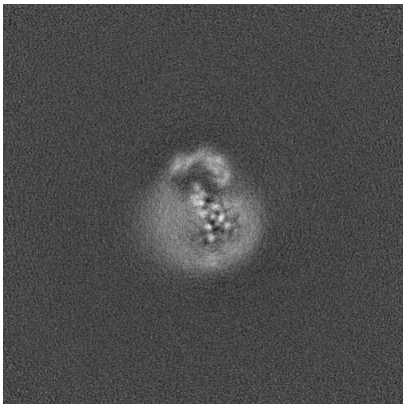
6.3.2 Raw map



X Index: 264



Y Index: 279



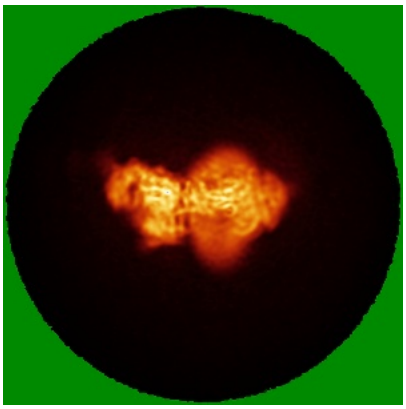
Z Index: 295

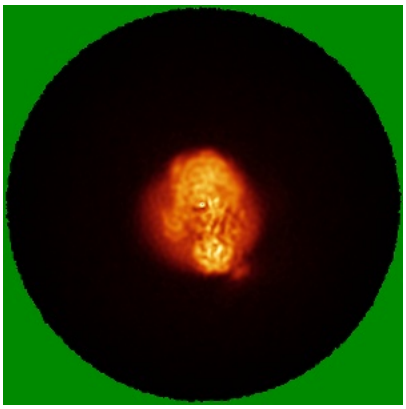
The images above show the largest variance slices of the map in three orthogonal directions.

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

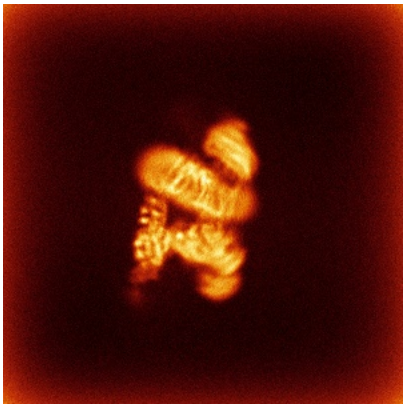
6.4.1 Primary map

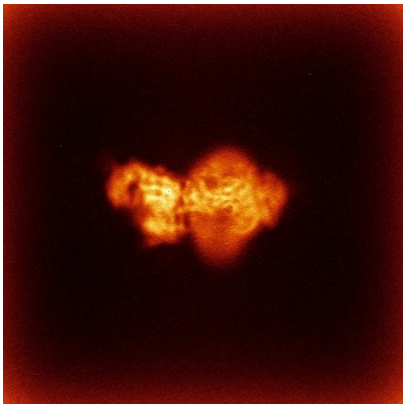

X

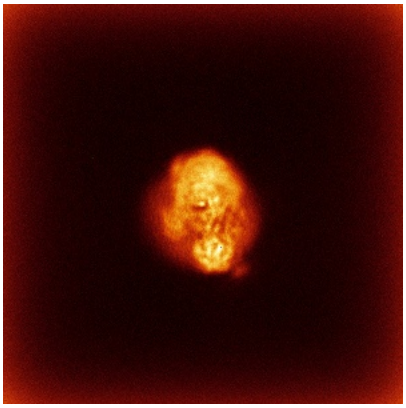

Y


Z

6.4.2 Raw map


X

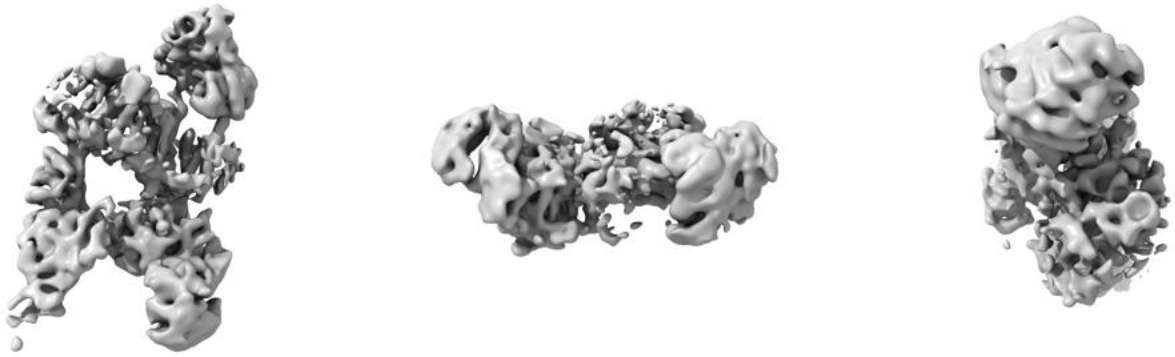

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0769. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

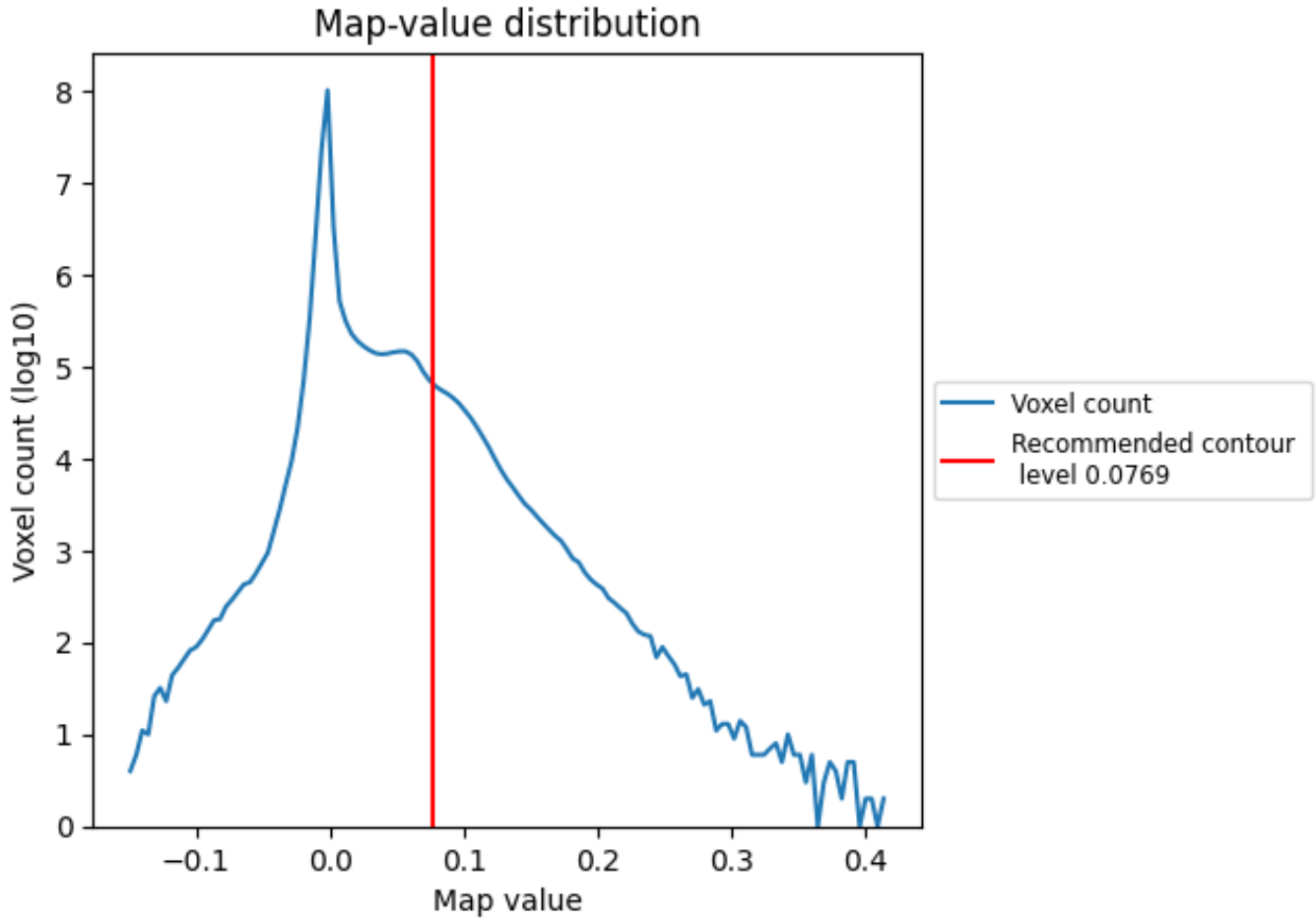
6.6 Mask visualisation (i)

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

7 Map analysis

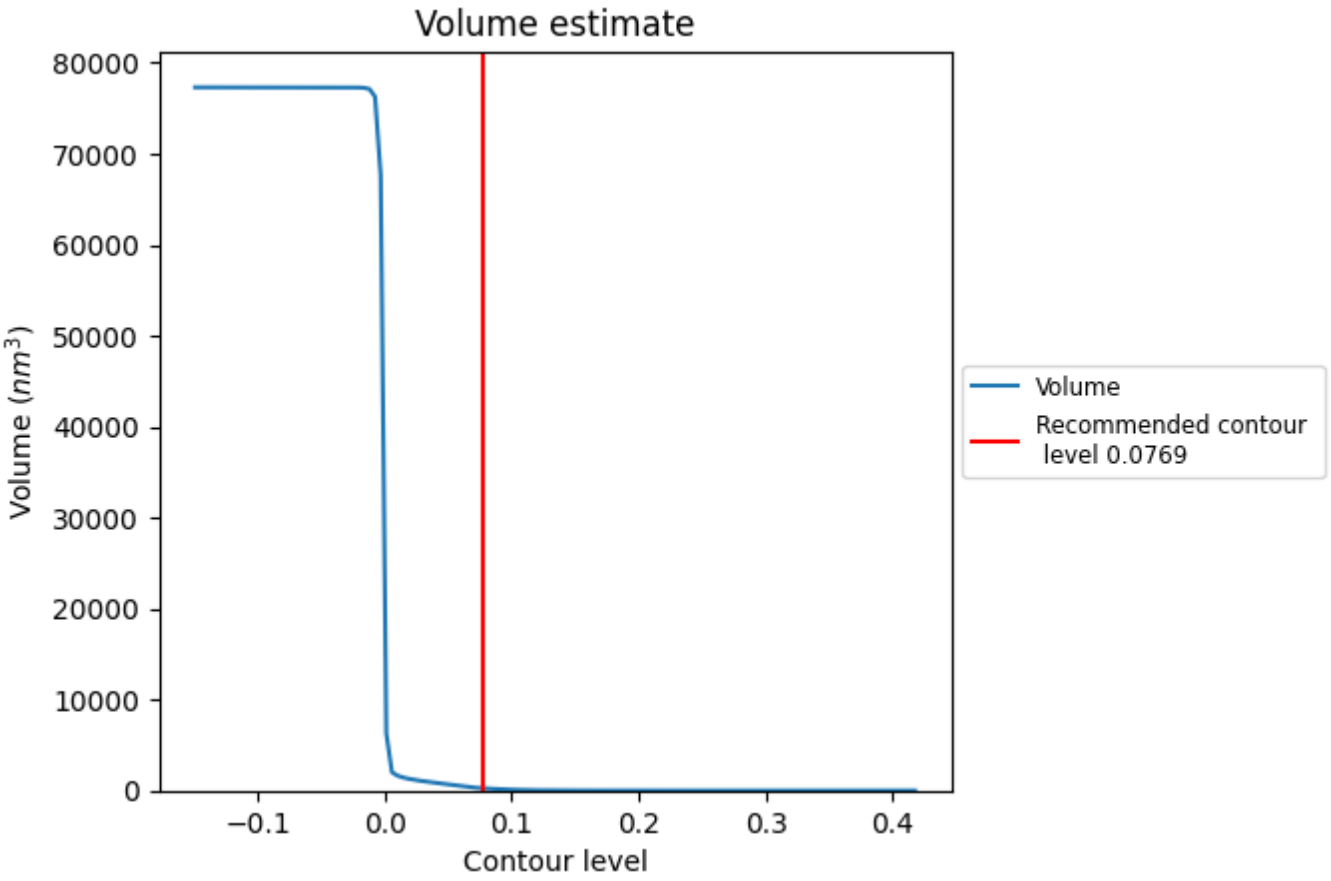
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

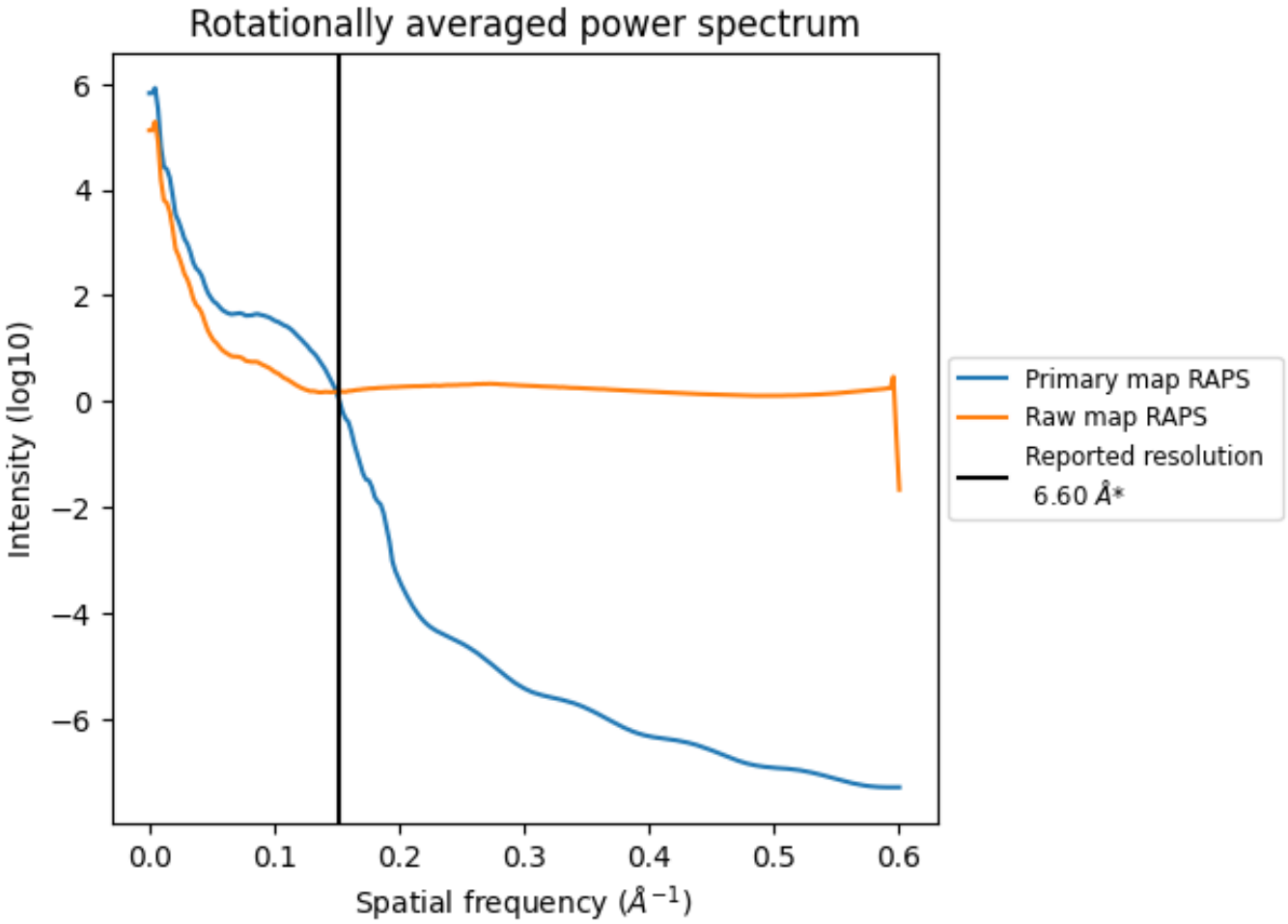
7.2 Volume estimate



The volume at the recommended contour level is 255 nm^3; this corresponds to an approximate mass of 231 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)

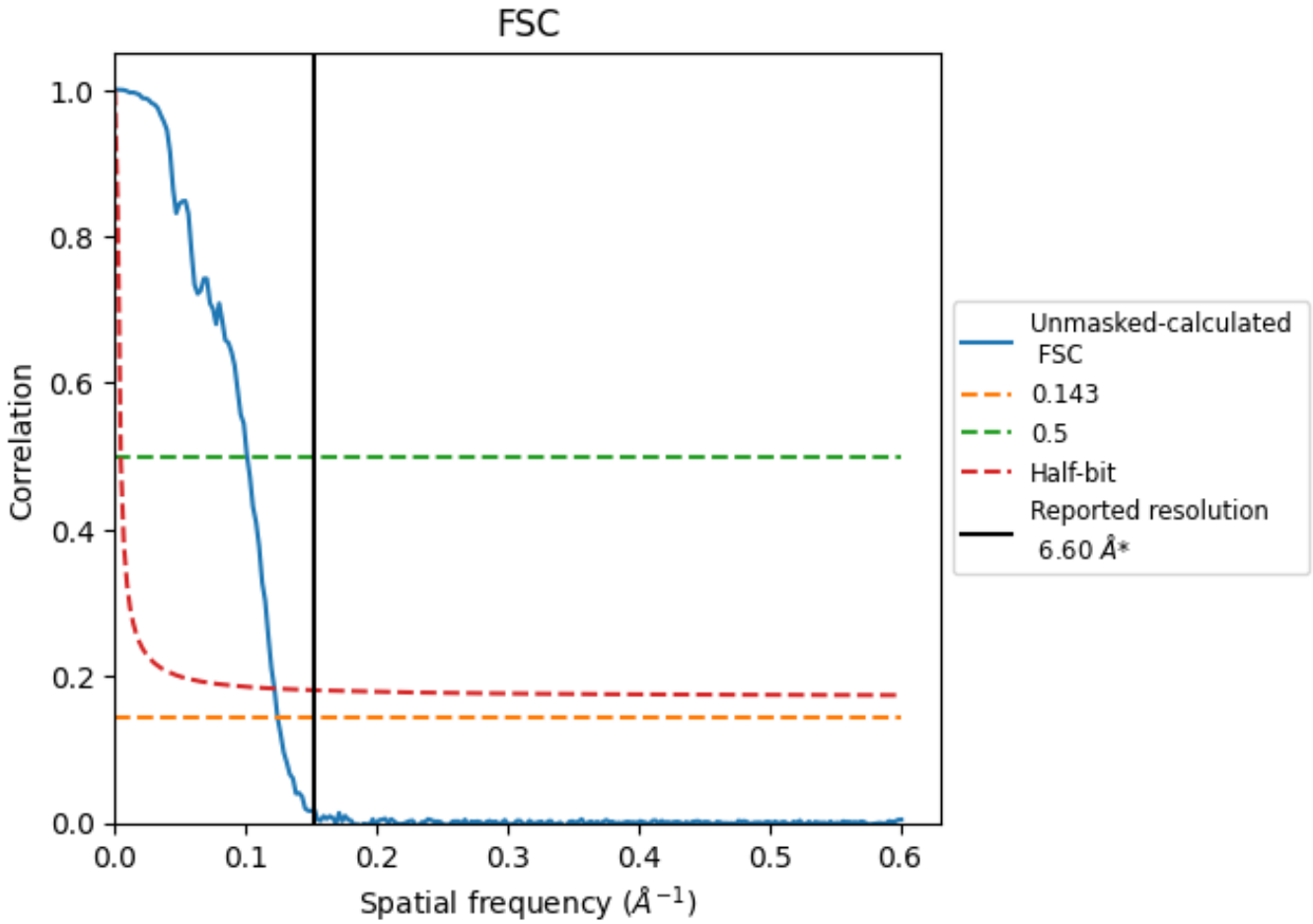


*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8.2 Resolution estimates (i)

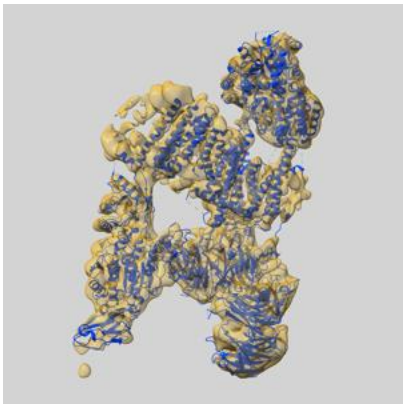
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.03	9.89	8.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.03 differs from the reported value 6.6 by more than 10 %

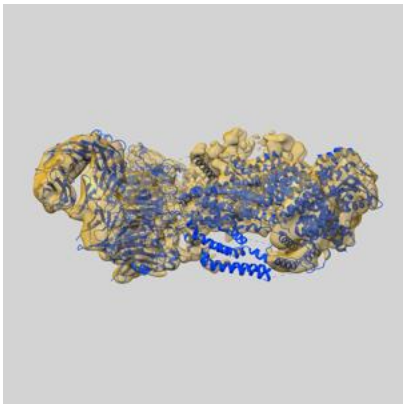
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45295 and PDB model 9C7V. Per-residue inclusion information can be found in section 3 on page 7.

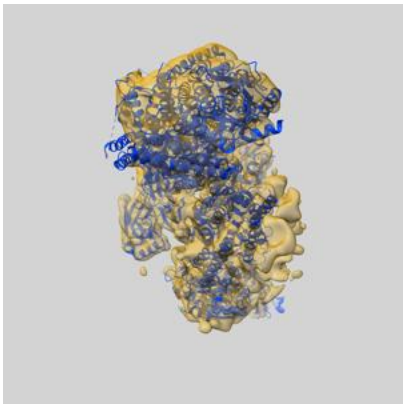
9.1 Map-model overlay



X



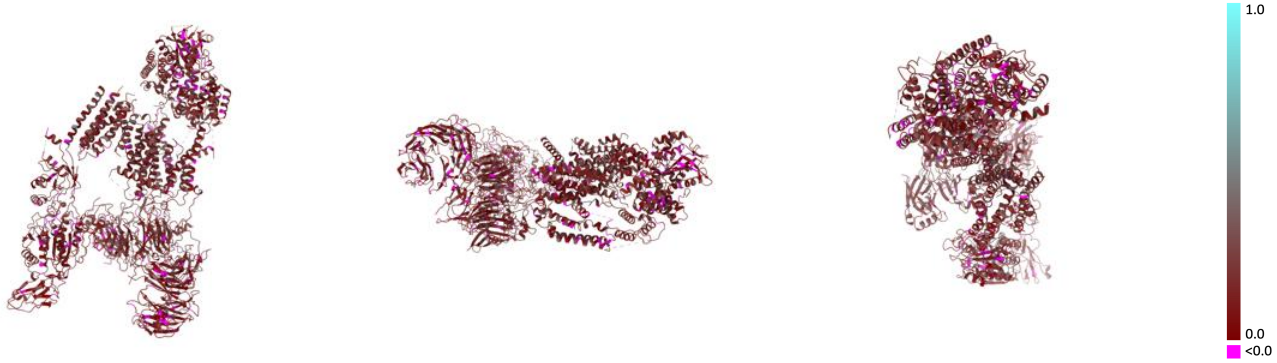
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0769 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.

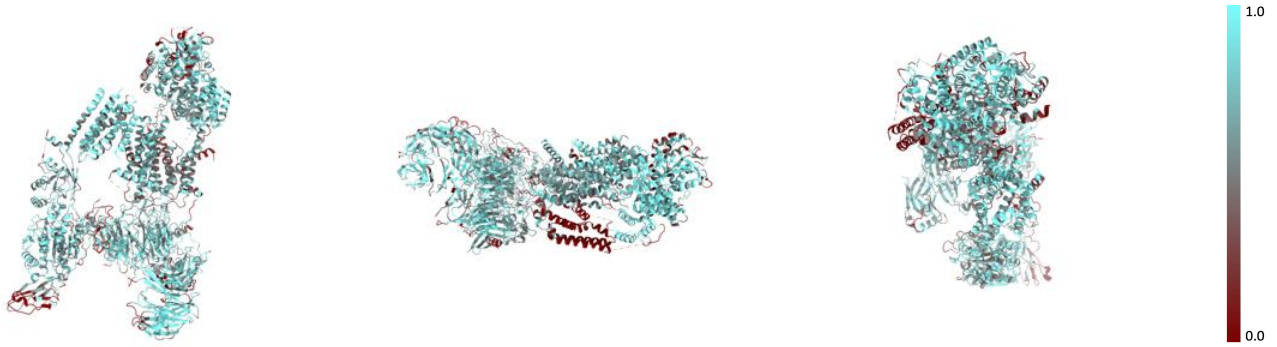
9.2 Q-score mapped to coordinate model (i)



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.

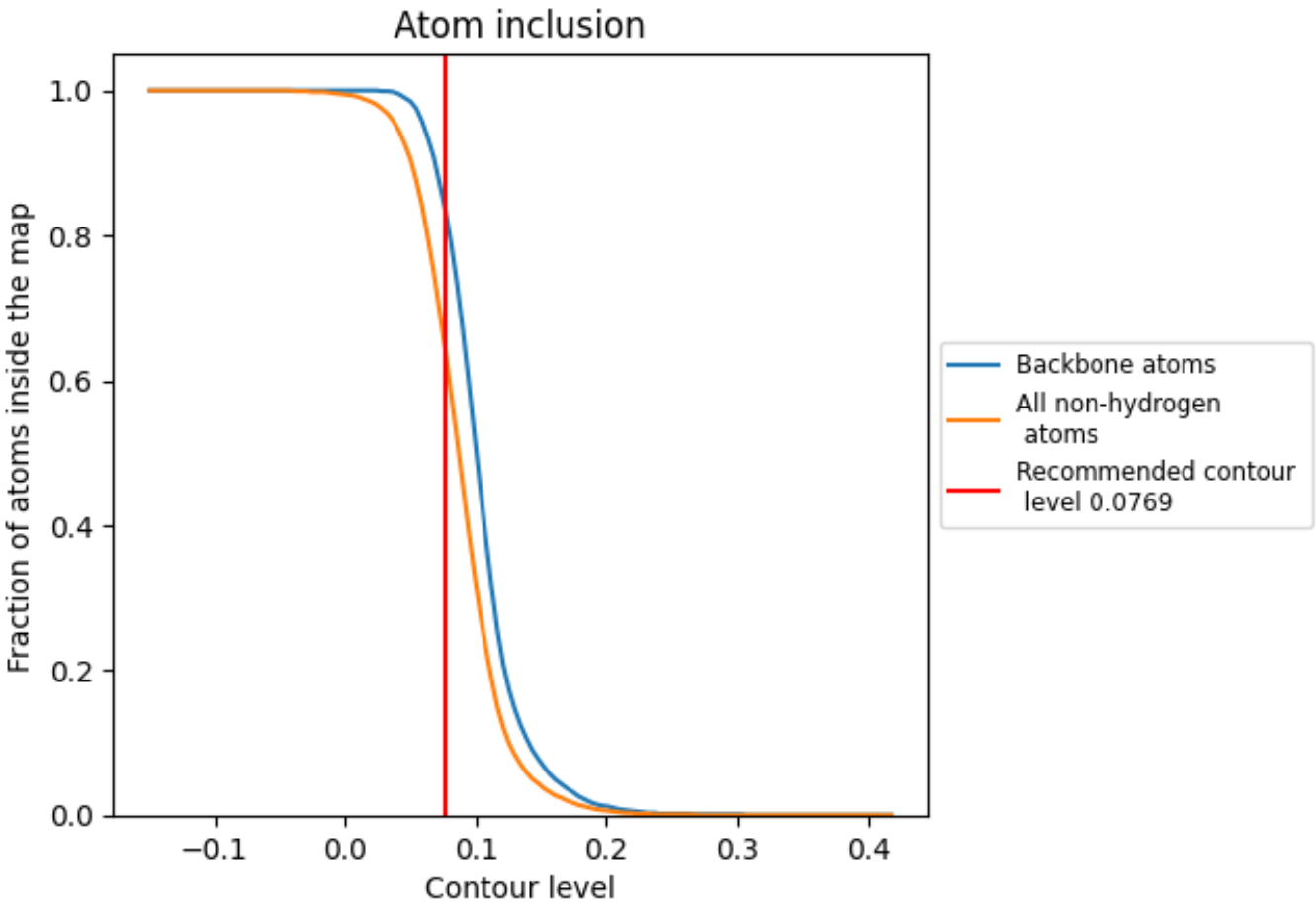
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0769).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 64% 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 (0.0769) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6400	0.1660
1	0.6950	0.1630
10	0.6360	0.1800
2	0.7370	0.1670
3	0.5940	0.1690
4	0.3180	0.1760
5	0.6520	0.1830
6	0.6440	0.1700
7	0.5420	0.1660
8	0.6310	0.1450
A	0.6770	0.1590
B	0.3850	0.1500
C	0.7050	0.1980
D	0.5000	0.2730
E	0.5360	0.2360