Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:22 pm GMT

PDB ID	:	4BZJ
EMDB ID	:	EMD-2430
Title	:	The structure of the COPII coat assembled on membranes
Authors	:	Zanetti, G.; Prinz, S.; Daum, S.; Meister, A.; Schekman, R.; Bacia, K.; Briggs, J.A.G.
Deposited on	:	2013-07-26
Resolution	:	40.00 Å(reported)
Based on initial models	:	2PM6, 2PM9

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:

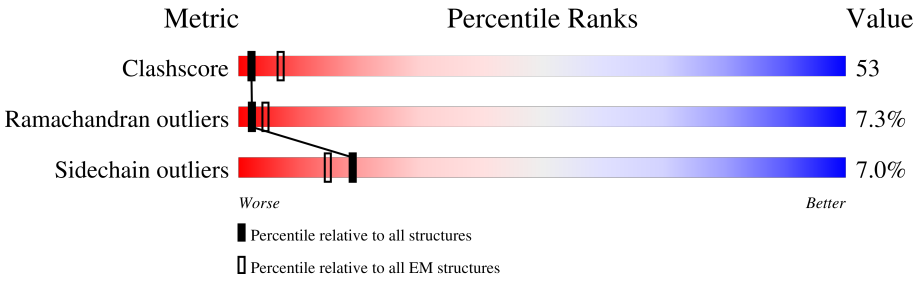
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 40.00 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	1273	7% 20% 29% 5% 46%
1	C	1273	5% 21% 27% 5% 46%
2	B	291	7% 43% 52%
3	F	291	8% 24% 61% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15423 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 Protein transport protein SEC31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	691	Total	C	N	O	S	0	0
			5410	3406	908	1084	12		
1	C	693	Total	C	N	O	S	0	0
			5427	3417	911	1087	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	SER	THR	conflict	UNP P38968
C	367	SER	THR	conflict	UNP P38968

- Molecule 2 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	279	Total	C	N	O	S	0	0
			2196	1403	375	415	3		

- Molecule 3 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	280	Total	C	N	O	S	0	0
			2205	1402	376	418	9		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	11	MET	LEU	conflict	UNP Q04491
F	17	MET	LEU	conflict	UNP Q04491
F	24	MET	LEU	conflict	UNP Q04491
F	80	MET	LEU	conflict	UNP Q04491
F	115	MET	LEU	conflict	UNP Q04491
F	222	MET	LEU	conflict	UNP Q04491

- Molecule 4 is water.

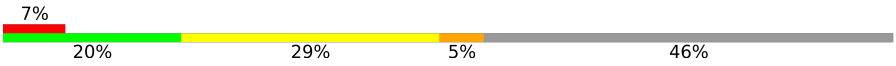
Mol	Chain	Residues	Atoms	AltConf
4	A	45	Total O 45 45	0
4	B	61	Total O 61 61	0
4	C	68	Total O 68 68	0
4	F	11	Total O 11 11	0

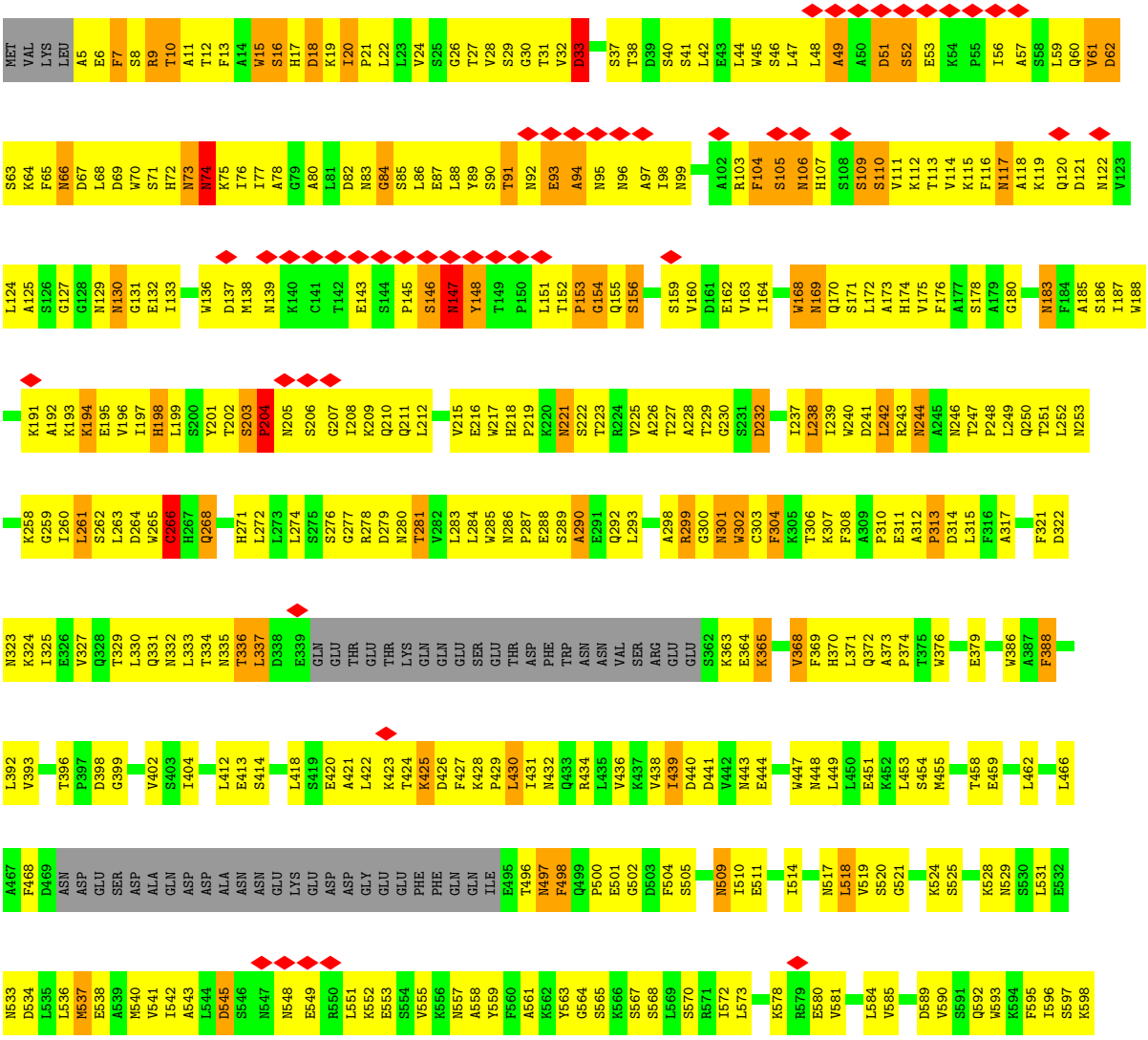
3 Residue-property plots (i)

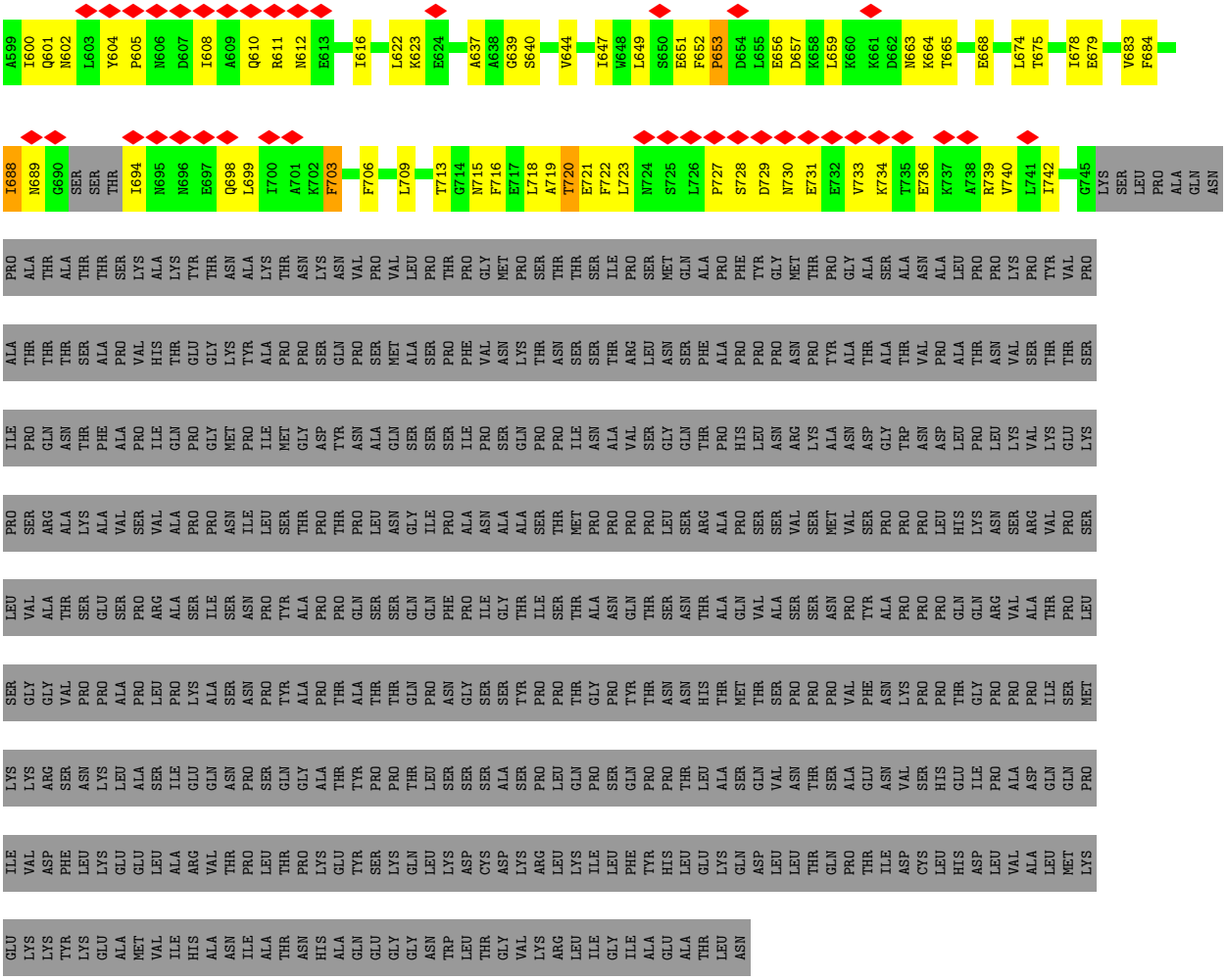
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Protein transport protein SEC31

Chain A:

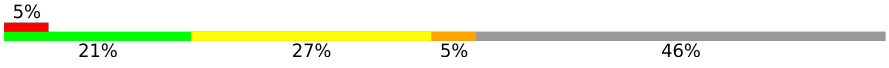


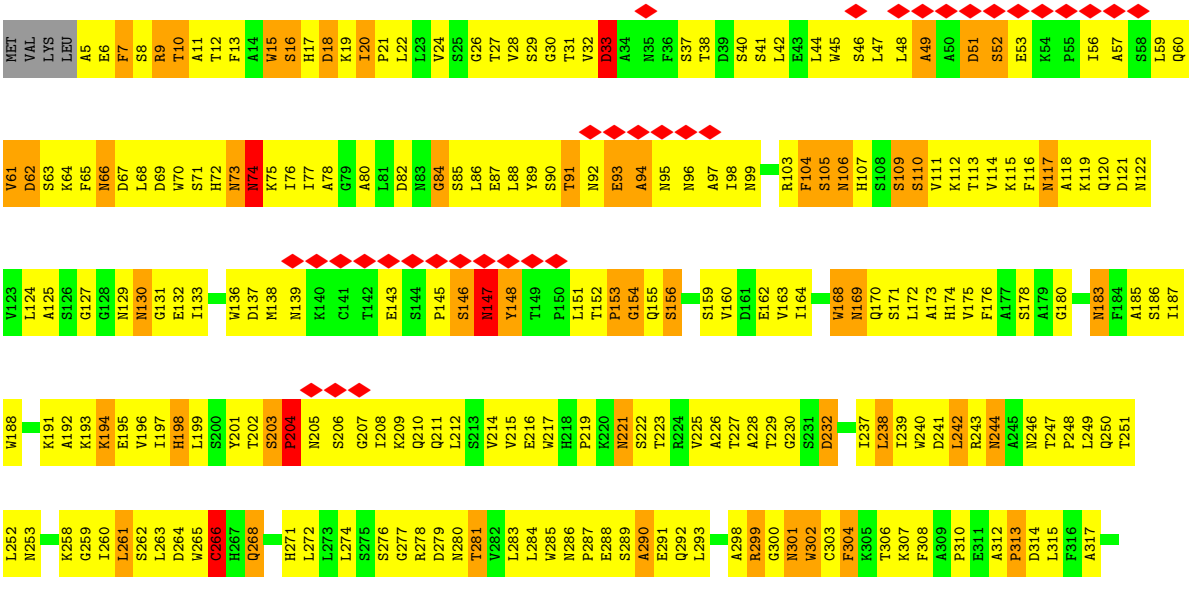


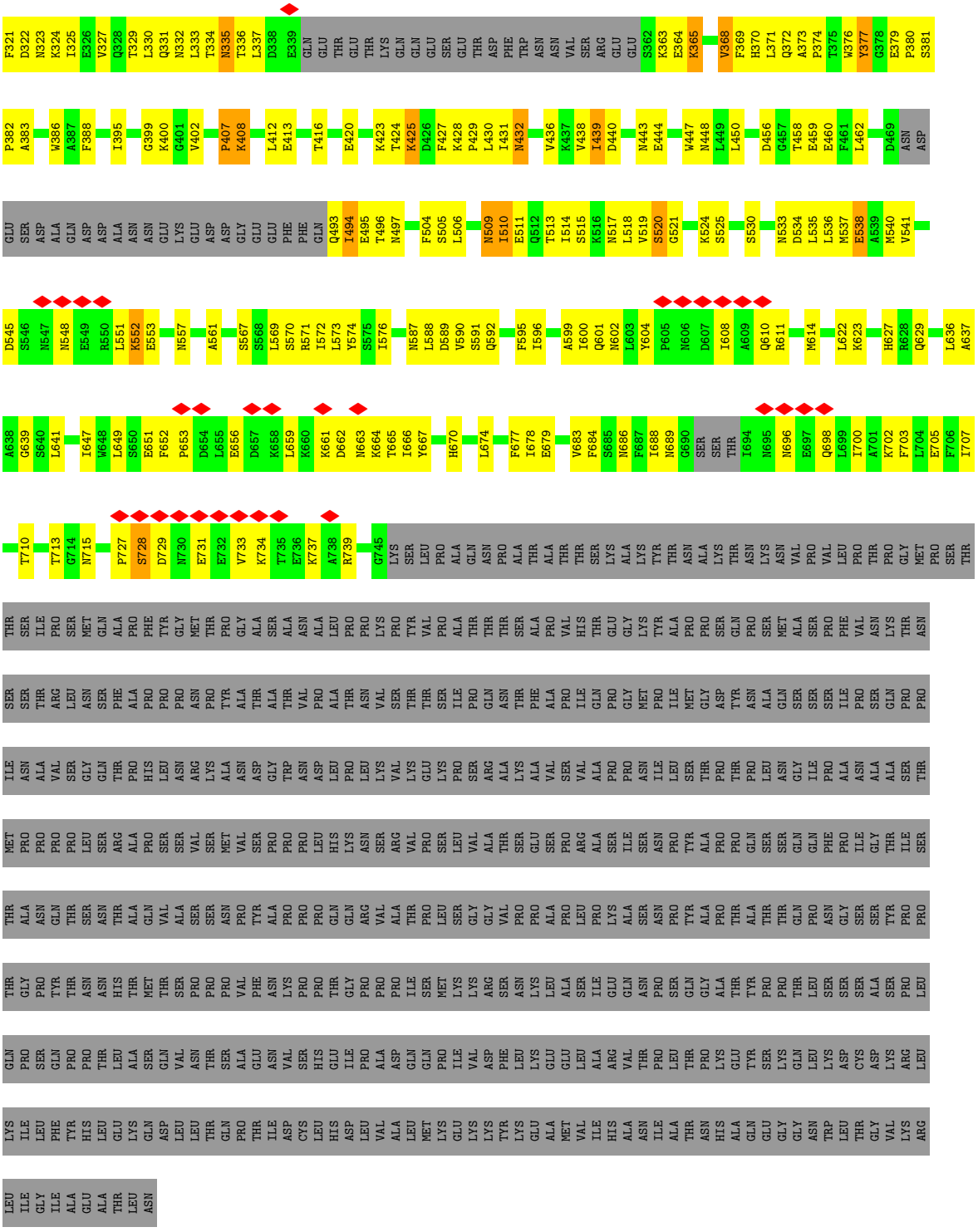


• Molecule 1: Protein transport protein SEC31

Chain C:

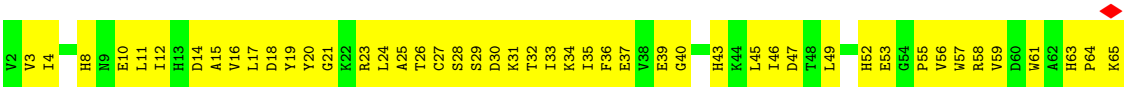


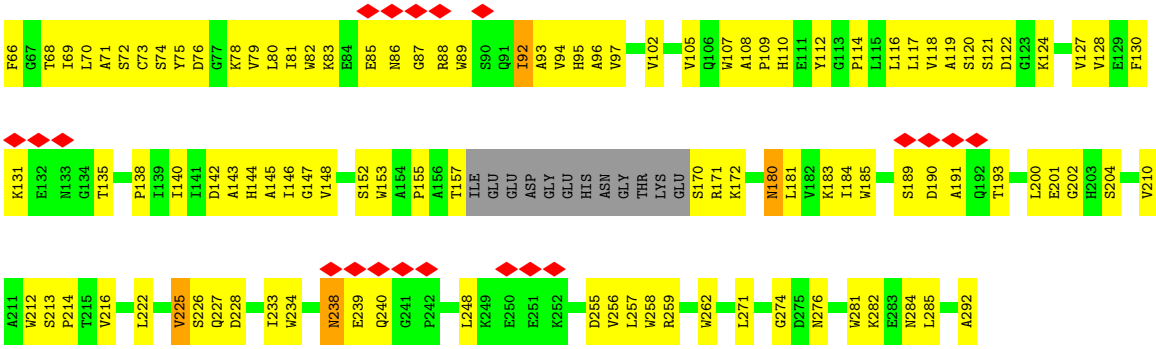




• Molecule 2: Protein transport protein SEC13

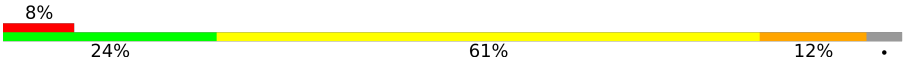
Chain B:

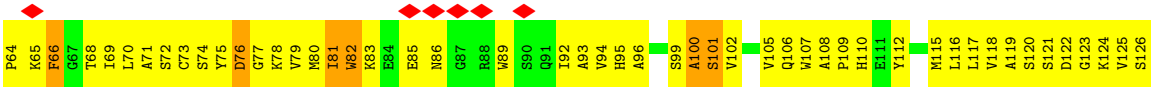


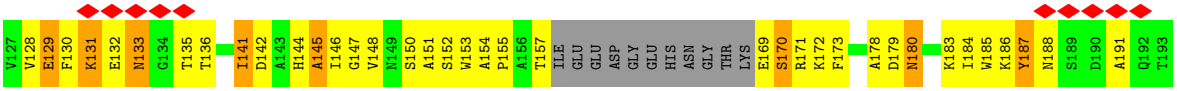


• Molecule 3: Protein transport protein SEC13

Chain F:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	182	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH TILTED IMAGE WITHIN TOMOGRAM	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	19500	Depositor
Image detector	GATAN MULTISCAN	Depositor
Maximum map value	6.137	Depositor
Minimum map value	-2.538	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	309.6, 309.6, 309.6	wwPDB
Map dimensions	72, 72, 72	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.3, 4.3, 4.3	Depositor

5 Model quality

5.1 Standard geometry

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	0.41	0/5516	0.70	2/7479 (0.0%)
1	C	0.44	0/5533	0.71	2/7502 (0.0%)
2	B	0.40	0/2256	0.68	0/3079
3	F	0.41	0/2265	0.67	0/3085
All	All	0.42	0/15570	0.69	4/21145 (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})
1	C	154	GLY	N-CA-C	5.10	125.85	113.10
1	A	156	SER	N-CA-C	5.10	124.76	111.00
1	A	154	GLY	N-CA-C	5.09	125.83	113.10
1	C	156	SER	N-CA-C	5.09	124.73	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5410	0	5272	605	0
1	C	5427	0	5289	609	0
2	B	2196	0	2138	189	0
3	F	2205	0	2131	304	0
4	A	45	0	0	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	61	0	0	26	0
4	C	68	0	0	25	0
4	F	11	0	0	4	0
All	All	15423	0	14830	1582	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 53.

All (1582) 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)
1:C:739:ARG:HA	3:F:20:TYR:CE1	1.28	1.64
1:C:664:LYS:C	3:F:285:LEU:HD21	1.30	1.47
1:C:739:ARG:CA	3:F:20:TYR:HE1	1.28	1.45
1:A:314:ASP:OD2	1:A:376:TRP:CD2	1.64	1.44
1:A:314:ASP:OD2	1:A:376:TRP:CE2	1.76	1.38
1:C:665:THR:N	3:F:285:LEU:HD21	1.38	1.38
1:C:665:THR:HA	3:F:285:LEU:CD2	1.58	1.33
1:A:313:PRO:HG3	4:A:2118:HOH:O	1.14	1.30
1:C:313:PRO:HG3	4:C:1545:HOH:O	1.32	1.29
1:C:663:ASN:C	3:F:285:LEU:HD11	1.53	1.26
1:C:268:GLN:HB3	1:C:374:PRO:O	1.29	1.26
1:A:268:GLN:HB3	1:A:374:PRO:O	1.15	1.25
1:C:331:GLN:NE2	4:C:1544:HOH:O	1.74	1.21
1:A:268:GLN:HG3	4:A:2118:HOH:O	1.32	1.21
1:A:268:GLN:CB	1:A:374:PRO:O	1.87	1.21
1:C:314:ASP:OD2	1:C:376:TRP:CD2	1.95	1.20
1:C:665:THR:CA	3:F:285:LEU:CD2	2.19	1.20
1:C:663:ASN:C	3:F:285:LEU:CD1	2.13	1.16
1:C:314:ASP:OD1	4:C:1411:HOH:O	1.63	1.13
1:A:314:ASP:CG	1:A:376:TRP:CE2	2.22	1.13
1:C:664:LYS:N	3:F:285:LEU:HD11	1.65	1.12
1:C:314:ASP:OD2	1:C:376:TRP:CE2	2.01	1.11
1:C:665:THR:N	3:F:285:LEU:CD2	2.14	1.09
1:C:22:LEU:HD11	1:C:94:ALA:HB1	1.30	1.08
1:C:313:PRO:CG	4:C:1545:HOH:O	1.86	1.08
1:A:268:GLN:CG	4:A:2118:HOH:O	1.91	1.08
1:C:665:THR:CA	3:F:285:LEU:HD23	1.81	1.08
1:A:93:GLU:HB2	1:A:96:ASN:HD22	1.16	1.07
3:F:256:VAL:HG12	3:F:257:LEU:H	1.11	1.07
1:A:314:ASP:OD2	1:A:376:TRP:CE3	2.06	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:HB2	1:C:96:ASN:HD22	1.16	1.07
1:C:665:THR:HA	3:F:285:LEU:HD23	1.09	1.07
1:A:22:LEU:HD11	1:A:94:ALA:HB1	1.30	1.06
1:C:664:LYS:C	3:F:285:LEU:CD2	2.24	1.05
1:C:268:GLN:HA	1:C:373:ALA:HB1	1.34	1.05
1:C:665:THR:CA	3:F:285:LEU:HD21	1.83	1.05
1:C:408:LYS:HD3	1:C:408:LYS:H	1.22	1.05
1:C:268:GLN:NE2	4:C:1546:HOH:O	1.87	1.04
1:C:425:LYS:HE2	1:C:686:ASN:HD21	1.21	1.04
3:F:24:MET:HG2	3:F:25:ALA:H	1.18	1.03
1:A:268:GLN:HE21	1:A:313:PRO:HD3	1.19	1.03
3:F:46:ILE:HG22	3:F:47:ASP:H	1.20	1.02
1:C:268:GLN:HE21	1:C:313:PRO:HD3	1.19	1.02
1:C:739:ARG:CA	3:F:20:TYR:CE1	2.15	1.02
1:C:663:ASN:O	3:F:285:LEU:CD1	2.08	1.02
1:C:664:LYS:O	3:F:285:LEU:HD21	1.58	1.02
1:A:304:PHE:HD1	1:A:304:PHE:H	1.03	1.01
2:B:11:LEU:O	2:B:28:SER:HB2	1.61	1.01
1:C:688:ILE:HG13	1:C:689:ASN:H	1.20	1.01
2:B:128:VAL:HG22	2:B:138:PRO:HB3	1.43	1.00
1:C:154:GLY:O	1:C:155:GLN:HG2	1.61	1.00
1:A:431:ILE:HD11	1:A:683:VAL:HG11	1.42	0.99
1:C:623:LYS:HE3	1:C:647:ILE:HD12	1.44	0.99
3:F:69:ILE:HD11	3:F:83:LYS:HE2	1.43	0.99
1:A:154:GLY:O	1:A:155:GLN:HG2	1.61	0.99
3:F:80:MET:HG2	3:F:94:VAL:HG23	1.43	0.99
1:C:304:PHE:HD1	1:C:304:PHE:H	1.03	0.99
1:A:268:GLN:HA	1:A:373:ALA:HB1	1.45	0.98
3:F:69:ILE:HG12	3:F:83:LYS:HG2	1.45	0.97
1:C:377:TYR:CE2	3:F:75:TYR:HE1	1.80	0.97
1:C:268:GLN:CB	1:C:374:PRO:O	2.13	0.97
1:C:314:ASP:CG	4:C:1411:HOH:O	2.01	0.97
1:C:535:LEU:HB3	1:C:538:GLU:HG3	1.48	0.95
1:A:93:GLU:HB2	1:A:96:ASN:ND2	1.81	0.95
1:A:438:VAL:HG23	1:A:443:ASN:HD22	1.28	0.95
1:C:268:GLN:HA	1:C:373:ALA:CB	1.95	0.95
1:C:407:PRO:HD2	4:C:1614:HOH:O	1.67	0.94
1:A:299:ARG:HE	1:A:323:ASN:HB2	1.32	0.94
1:A:720:THR:HA	1:A:723:LEU:HD12	1.46	0.94
1:A:370:HIS:CE1	2:B:75:TYR:CE2	2.56	0.94
1:C:93:GLU:HB2	1:C:96:ASN:ND2	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:THR:HG23	1:A:28:VAL:HG12	1.50	0.93
1:C:16:SER:O	1:C:310:PRO:HG3	1.69	0.93
1:A:370:HIS:CE1	2:B:75:TYR:HE2	1.86	0.93
1:A:16:SER:O	1:A:310:PRO:HG3	1.69	0.93
1:A:72:HIS:CE1	1:A:118:ALA:HA	2.04	0.93
1:A:364:GLU:O	1:A:365:LYS:HB2	1.66	0.93
1:C:22:LEU:CD1	1:C:94:ALA:HB1	1.99	0.93
1:C:72:HIS:CE1	1:C:118:ALA:HA	2.04	0.92
1:A:268:GLN:HG3	4:A:2079:HOH:O	1.67	0.92
1:C:202:THR:C	1:C:204:PRO:HD2	1.90	0.92
1:C:10:THR:HG23	1:C:28:VAL:HG12	1.50	0.92
1:C:125:ALA:HB2	1:C:168:TRP:CH2	2.05	0.92
1:A:639:GLY:HA2	1:A:688:ILE:HD11	1.51	0.91
1:C:368:VAL:O	1:C:370:HIS:N	2.02	0.91
1:C:377:TYR:CE2	3:F:75:TYR:CE1	2.58	0.91
1:A:22:LEU:CD1	1:A:94:ALA:HB1	1.99	0.91
1:C:420:GLU:O	1:C:423:LYS:HG2	1.70	0.91
1:C:739:ARG:CB	3:F:20:TYR:HE1	1.83	0.91
1:A:368:VAL:O	1:A:370:HIS:N	2.02	0.91
3:F:233:ILE:H	3:F:233:ILE:HD12	1.33	0.91
1:A:125:ALA:HB2	1:A:168:TRP:CH2	2.05	0.91
1:A:202:THR:C	1:A:204:PRO:HD2	1.89	0.91
1:C:31:THR:HG22	1:C:32:VAL:H	1.33	0.91
1:C:664:LYS:CA	3:F:285:LEU:HD11	2.00	0.90
1:C:364:GLU:O	1:C:365:LYS:HB2	1.66	0.90
1:C:299:ARG:HE	1:C:323:ASN:HB2	1.33	0.90
1:C:244:ASN:HD21	1:C:246:ASN:ND2	1.70	0.90
1:A:314:ASP:N	1:A:376:TRP:HE1	1.69	0.90
1:A:31:THR:HG22	1:A:32:VAL:H	1.33	0.89
1:A:428:LYS:HB2	1:A:429:PRO:HD3	1.54	0.89
1:A:244:ASN:HD21	1:A:246:ASN:ND2	1.70	0.89
1:A:370:HIS:HE1	2:B:75:TYR:CE2	1.90	0.88
3:F:249:LYS:HE3	3:F:251:GLU:HB2	1.54	0.88
1:A:496:THR:HG23	1:C:557:ASN:HB3	1.54	0.88
1:A:202:THR:O	1:A:204:PRO:HD2	1.74	0.88
1:C:649:LEU:HD22	1:C:698:GLN:HG2	1.55	0.88
2:B:81:ILE:HB	4:B:1320:HOH:O	1.73	0.88
1:C:739:ARG:HA	3:F:20:TYR:CD1	2.08	0.87
1:A:268:GLN:HE21	1:A:313:PRO:CD	1.87	0.87
1:C:313:PRO:HG3	4:C:1480:HOH:O	1.73	0.87
2:B:81:ILE:HD13	2:B:93:ALA:HB3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:TYR:HB3	3:F:57:TRP:CH2	2.10	0.87
1:A:314:ASP:OD2	1:A:376:TRP:CZ2	2.28	0.86
1:A:592:GLN:HE21	1:C:506:LEU:HD12	1.40	0.86
1:C:268:GLN:HE21	1:C:313:PRO:CD	1.87	0.86
1:C:425:LYS:O	1:C:425:LYS:HD3	1.75	0.86
1:A:106:ASN:N	1:A:106:ASN:HD22	1.70	0.86
1:C:202:THR:O	1:C:204:PRO:HD2	1.74	0.86
1:A:75:LYS:NZ	1:A:94:ALA:H	1.74	0.86
1:C:106:ASN:N	1:C:106:ASN:HD22	1.70	0.86
4:A:2245:HOH:O	1:C:602:ASN:HB3	1.75	0.85
1:C:10:THR:CG2	1:C:28:VAL:HG12	2.06	0.85
1:C:663:ASN:O	3:F:285:LEU:HD11	1.69	0.85
1:C:377:TYR:HB3	3:F:57:TRP:CZ2	2.11	0.85
3:F:73:CYS:HB3	3:F:79:VAL:HG12	1.59	0.85
1:A:313:PRO:C	1:A:376:TRP:HE1	1.79	0.85
1:A:10:THR:CG2	1:A:28:VAL:HG12	2.06	0.85
1:C:314:ASP:OD2	1:C:376:TRP:CE3	2.30	0.85
1:C:663:ASN:O	3:F:285:LEU:HD12	1.74	0.84
3:F:180:ASN:HD22	3:F:180:ASN:N	1.72	0.84
2:B:257:LEU:HD13	2:B:271:LEU:HD21	1.59	0.84
1:C:75:LYS:NZ	1:C:94:ALA:H	1.74	0.84
1:A:412:LEU:HD21	1:A:713:THR:HG22	1.57	0.84
2:B:12:ILE:HA	2:B:28:SER:HB3	1.59	0.84
1:C:73:ASN:O	1:C:75:LYS:N	2.11	0.84
1:C:117:ASN:HD22	1:C:118:ALA:N	1.75	0.84
2:B:83:LYS:O	2:B:89:TRP:HA	1.76	0.84
1:C:314:ASP:CG	1:C:376:TRP:CE2	2.50	0.84
3:F:24:MET:CG	3:F:25:ALA:H	1.90	0.84
1:A:73:ASN:O	1:A:75:LYS:N	2.11	0.83
1:C:494:ILE:HG13	1:C:495:GLU:H	1.42	0.83
3:F:69:ILE:CD1	3:F:83:LYS:HE2	2.07	0.83
1:A:117:ASN:HD22	1:A:118:ALA:N	1.75	0.83
1:C:119:LYS:HB2	1:C:173:ALA:HB2	1.59	0.83
1:C:703:PHE:O	1:C:707:ILE:HG12	1.78	0.83
1:C:524:LYS:HG3	1:C:525:SER:H	1.43	0.83
3:F:79:VAL:HG23	3:F:95:HIS:HB3	1.60	0.83
1:A:119:LYS:HB2	1:A:173:ALA:HB2	1.59	0.82
1:C:74:ASN:HD22	1:C:74:ASN:N	1.77	0.82
1:C:75:LYS:HZ1	1:C:94:ALA:H	1.22	0.82
1:A:268:GLN:NE2	1:A:313:PRO:HD3	1.94	0.82
1:C:380:PRO:HG3	3:F:11:MET:CE	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ALA:HB1	4:F:1302:HOH:O	1.80	0.82
3:F:150:SER:OG	3:F:209:ASP:HA	1.79	0.82
3:F:46:ILE:HG22	3:F:47:ASP:N	1.95	0.82
1:A:336:THR:HB	2:B:96:ALA:O	1.80	0.82
1:C:268:GLN:NE2	1:C:313:PRO:HD3	1.94	0.82
1:C:30:GLY:HA3	1:C:321:PHE:HE2	1.44	0.81
1:C:665:THR:HG22	3:F:285:LEU:HA	1.61	0.81
1:A:314:ASP:CG	1:A:376:TRP:CD2	2.48	0.81
1:C:427:PHE:O	1:C:431:ILE:HG12	1.81	0.81
3:F:256:VAL:HG12	3:F:257:LEU:N	1.92	0.81
1:A:30:GLY:HA3	1:A:321:PHE:HE2	1.44	0.81
1:A:221:ASN:HD22	1:A:222:SER:N	1.79	0.81
1:A:370:HIS:CG	1:A:371:LEU:H	1.99	0.81
1:C:31:THR:HG22	1:C:32:VAL:N	1.95	0.81
1:A:74:ASN:N	1:A:74:ASN:HD22	1.77	0.80
1:A:314:ASP:N	1:A:376:TRP:NE1	2.29	0.80
1:A:31:THR:HG22	1:A:32:VAL:N	1.95	0.80
1:C:133:ILE:HD11	1:C:163:VAL:HG21	1.62	0.80
3:F:83:LYS:HG3	3:F:92:ILE:HD13	1.62	0.80
1:C:221:ASN:HD22	1:C:222:SER:N	1.78	0.80
1:C:74:ASN:HD22	1:C:74:ASN:H	1.30	0.80
1:C:314:ASP:H	1:C:376:TRP:HZ2	1.30	0.80
1:C:370:HIS:CG	1:C:371:LEU:H	1.99	0.80
1:A:133:ILE:HD11	1:A:163:VAL:HG21	1.62	0.80
1:A:505:SER:HB3	1:C:589:ASP:HB2	1.62	0.79
1:A:292:GLN:O	1:A:368:VAL:HG23	1.81	0.79
1:A:315:LEU:HD11	2:B:146:ILE:HD12	1.65	0.79
1:A:74:ASN:HD22	1:A:74:ASN:H	1.30	0.79
3:F:24:MET:HG2	3:F:25:ALA:N	1.96	0.79
1:A:518:LEU:HB3	1:C:576:ILE:HD13	1.63	0.79
1:C:300:GLY:O	1:C:301:ASN:HB2	1.81	0.79
1:C:439:ILE:HG21	1:C:659:LEU:HD21	1.63	0.79
1:A:80:ALA:HB1	1:A:111:VAL:HG12	1.65	0.79
1:A:300:GLY:O	1:A:301:ASN:HB2	1.81	0.79
1:C:292:GLN:O	1:C:368:VAL:HG23	1.82	0.79
1:A:19:LYS:O	1:A:21:PRO:HD3	1.82	0.79
1:A:250:GLN:NE2	1:A:251:THR:H	1.81	0.79
1:C:56:ILE:HD13	1:C:95:ASN:HA	1.65	0.79
1:A:420:GLU:HA	1:A:423:LYS:HE2	1.63	0.79
1:C:250:GLN:NE2	1:C:251:THR:H	1.81	0.79
1:A:56:ILE:HD13	1:A:95:ASN:HA	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLN:HG3	1:A:313:PRO:HG3	1.65	0.78
1:A:590:VAL:HG13	1:A:622:LEU:HD23	1.65	0.78
1:C:19:LYS:O	1:C:21:PRO:HD3	1.82	0.78
1:C:93:GLU:CB	1:C:96:ASN:HD22	1.97	0.78
1:C:652:PHE:HB3	1:C:653:PRO:HD3	1.64	0.78
1:C:513:THR:HB	4:C:1602:HOH:O	1.84	0.78
3:F:37:GLU:HG2	3:F:46:ILE:HD11	1.65	0.78
1:C:664:LYS:O	3:F:285:LEU:CD2	2.31	0.78
1:C:72:HIS:O	1:C:74:ASN:ND2	2.16	0.77
1:C:80:ALA:HB1	1:C:111:VAL:HG12	1.65	0.77
1:A:93:GLU:CB	1:A:96:ASN:HD22	1.97	0.77
1:A:72:HIS:O	1:A:74:ASN:ND2	2.16	0.77
1:C:739:ARG:HG3	3:F:20:TYR:CE1	2.20	0.77
1:A:304:PHE:CD1	1:A:304:PHE:N	2.52	0.77
3:F:71:ALA:HB2	3:F:81:ILE:HG22	1.67	0.77
1:C:196:VAL:HG23	1:C:197:ILE:HG13	1.66	0.77
1:C:268:GLN:HG3	1:C:313:PRO:HG3	1.65	0.76
1:A:75:LYS:HZ1	1:A:94:ALA:H	1.31	0.76
1:A:174:HIS:NE2	1:A:191:LYS:HB2	2.00	0.76
1:A:589:ASP:HB2	1:C:505:SER:HB3	1.67	0.76
1:C:80:ALA:HB2	1:C:114:VAL:HG23	1.67	0.76
1:A:80:ALA:HB2	1:A:114:VAL:HG23	1.67	0.76
1:C:174:HIS:NE2	1:C:191:LYS:HB2	1.99	0.76
1:A:372:GLN:O	1:A:372:GLN:HG3	1.86	0.76
1:C:372:GLN:O	1:C:372:GLN:HG3	1.86	0.76
1:A:196:VAL:HG23	1:A:197:ILE:HG13	1.66	0.76
1:C:151:LEU:HD12	1:C:152:THR:H	1.50	0.76
1:C:304:PHE:CD1	1:C:304:PHE:N	2.52	0.76
1:A:393:VAL:HG22	1:A:404:ILE:HG13	1.67	0.76
3:F:65:LYS:HD3	3:F:110:HIS:HB2	1.68	0.75
3:F:256:VAL:CG1	3:F:257:LEU:H	1.94	0.75
1:C:202:THR:C	1:C:204:PRO:CD	2.55	0.75
1:A:151:LEU:HD12	1:A:152:THR:H	1.51	0.75
1:C:524:LYS:HG3	1:C:525:SER:N	2.01	0.75
1:A:202:THR:C	1:A:204:PRO:CD	2.55	0.75
1:A:719:ALA:O	1:A:723:LEU:HG	1.87	0.75
2:B:10:GLU:HB2	4:B:1336:HOH:O	1.86	0.75
3:F:154:ALA:HB2	3:F:212:TRP:CZ3	2.21	0.75
1:A:652:PHE:HB3	1:A:653:PRO:HD3	1.69	0.74
1:C:428:LYS:HB2	1:C:429:PRO:HD3	1.69	0.74
3:F:33:ILE:HB	3:F:49:LEU:HD12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:GLN:HG3	1:C:595:PHE:HB3	1.69	0.74
1:C:688:ILE:HG13	1:C:689:ASN:N	1.98	0.74
1:C:133:ILE:CD1	1:C:163:VAL:HG21	2.17	0.74
1:A:723:LEU:HD11	1:A:740:VAL:HG21	1.69	0.74
1:C:739:ARG:CB	3:F:20:TYR:CE1	2.64	0.74
1:C:313:PRO:CD	4:C:1546:HOH:O	2.35	0.73
1:A:393:VAL:HG21	2:B:17:LEU:HG	1.69	0.73
3:F:83:LYS:HG3	3:F:92:ILE:HG21	1.68	0.73
3:F:282:LYS:HA	4:F:1298:HOH:O	1.87	0.73
1:C:548:ASN:O	1:C:552:LYS:HB2	1.89	0.73
3:F:117:LEU:HD23	3:F:151:ALA:O	1.86	0.73
2:B:117:LEU:HA	4:B:1340:HOH:O	1.86	0.73
1:A:31:THR:CG2	1:A:32:VAL:H	2.02	0.73
1:A:78:ALA:CB	1:A:114:VAL:HG11	2.19	0.73
1:A:10:THR:HG23	1:A:28:VAL:CG1	2.18	0.73
1:A:85:SER:HB2	1:A:104:PHE:O	1.88	0.73
1:C:377:TYR:CZ	3:F:75:TYR:HE1	2.06	0.73
1:A:276:SER:OG	1:A:303:CYS:HB2	1.88	0.73
1:C:31:THR:CG2	1:C:32:VAL:H	2.02	0.73
1:C:85:SER:HB2	1:C:104:PHE:O	1.88	0.73
1:A:578:LYS:O	1:A:580:GLU:HG3	1.88	0.73
1:C:408:LYS:HD3	1:C:408:LYS:N	1.97	0.73
1:A:133:ILE:CD1	1:A:163:VAL:HG21	2.17	0.72
1:C:10:THR:HG23	1:C:28:VAL:CG1	2.18	0.72
3:F:225:VAL:HG22	3:F:257:LEU:HD13	1.72	0.72
1:C:314:ASP:OD2	1:C:376:TRP:CZ2	2.42	0.72
1:C:93:GLU:CB	1:C:96:ASN:ND2	2.52	0.72
3:F:225:VAL:HG22	3:F:257:LEU:HB3	1.70	0.72
1:C:276:SER:OG	1:C:303:CYS:HB2	1.88	0.72
1:A:93:GLU:CB	1:A:96:ASN:ND2	2.52	0.72
1:A:73:ASN:C	1:A:75:LYS:H	1.92	0.71
1:A:171:SER:O	1:A:172:LEU:HD23	1.90	0.71
1:A:420:GLU:HG3	1:A:423:LYS:HE2	1.72	0.71
1:C:73:ASN:C	1:C:75:LYS:H	1.92	0.71
3:F:16:VAL:HG12	3:F:61:TRP:HD1	1.54	0.71
1:A:69:ASP:OD2	1:A:116:PHE:HB2	1.90	0.71
2:B:255:ASP:OD2	2:B:274:GLY:HA3	1.89	0.71
1:A:202:THR:OG1	1:A:209:LYS:HD3	1.90	0.71
1:A:496:THR:O	1:A:497:ASN:HB2	1.89	0.71
1:C:78:ALA:CB	1:C:114:VAL:HG11	2.19	0.71
1:C:510:ILE:HD12	1:C:510:ILE:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:73:CYS:CB	3:F:79:VAL:HG12	2.20	0.71
3:F:196:LEU:HD11	3:F:198:SER:O	1.90	0.71
1:A:331:GLN:OE1	1:A:333:LEU:HD21	1.91	0.71
3:F:46:ILE:HD12	3:F:46:ILE:N	2.04	0.71
1:A:388:PHE:HB2	1:A:739:ARG:HH21	1.56	0.71
1:C:171:SER:O	1:C:172:LEU:HD23	1.90	0.71
1:C:202:THR:OG1	1:C:209:LYS:HD3	1.90	0.71
3:F:224:SER:HB2	3:F:234:TRP:HE1	1.53	0.70
1:A:665:THR:OG1	1:A:668:GLU:HG3	1.91	0.70
2:B:74:SER:HB3	2:B:76:ASP:OD1	1.91	0.70
3:F:154:ALA:HB2	3:F:212:TRP:CE3	2.26	0.70
1:A:431:ILE:HD13	1:A:447:TRP:HZ3	1.55	0.70
3:F:82:TRP:O	3:F:89:TRP:HZ3	1.74	0.70
1:C:331:GLN:OE1	1:C:333:LEU:HD21	1.91	0.70
1:A:164:ILE:HG12	1:A:180:GLY:HA2	1.74	0.70
1:A:94:ALA:O	1:A:95:ASN:HB2	1.92	0.70
1:A:518:LEU:HD13	1:C:576:ILE:HD12	1.73	0.70
1:C:212:LEU:HD13	1:C:227:THR:HG21	1.74	0.70
1:C:69:ASP:OD2	1:C:116:PHE:HB2	1.90	0.69
1:C:109:SER:O	1:C:110:SER:HB2	1.91	0.69
1:C:314:ASP:CB	4:C:1411:HOH:O	2.34	0.69
2:B:105:VAL:HG23	2:B:118:VAL:HG22	1.73	0.69
1:C:164:ILE:HG12	1:C:180:GLY:HA2	1.74	0.69
1:A:289:SER:OG	1:A:290:ALA:N	2.24	0.69
1:A:336:THR:CB	2:B:96:ALA:O	2.40	0.69
1:A:203:SER:O	1:A:205:ASN:N	2.26	0.69
1:A:595:PHE:CZ	1:C:515:SER:HB2	2.28	0.69
2:B:144:HIS:CE1	2:B:183:LYS:HD2	2.28	0.69
1:C:425:LYS:HE2	1:C:686:ASN:ND2	2.02	0.69
1:A:212:LEU:HD13	1:A:227:THR:HG21	1.74	0.69
1:A:314:ASP:CG	1:A:376:TRP:NE1	2.46	0.69
2:B:53:GLU:HG3	4:B:1337:HOH:O	1.93	0.69
1:C:203:SER:O	1:C:205:ASN:N	2.26	0.69
1:C:567:SER:HB3	1:C:570:SER:HB2	1.73	0.69
1:A:28:VAL:HG22	1:A:29:SER:H	1.58	0.69
1:A:428:LYS:NZ	1:A:455:MET:HG2	2.06	0.69
1:C:94:ALA:O	1:C:95:ASN:HB2	1.92	0.69
1:C:444:GLU:HG2	1:C:448:ASN:ND2	2.08	0.69
1:A:185:ALA:HB3	1:A:199:LEU:HB2	1.75	0.68
3:F:29:SER:C	3:F:31:LYS:H	1.95	0.68
1:C:19:LYS:HD2	3:F:206:TRP:HE1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:VAL:HG22	1:C:29:SER:H	1.58	0.68
3:F:233:ILE:HD12	3:F:233:ILE:N	2.05	0.68
1:C:185:ALA:HB3	1:C:199:LEU:HB2	1.75	0.68
3:F:16:VAL:HG12	3:F:61:TRP:CD1	2.29	0.68
1:C:314:ASP:HB3	4:C:1411:HOH:O	1.93	0.68
1:A:75:LYS:NZ	1:A:94:ALA:HB2	2.08	0.68
1:A:402:VAL:HG11	2:B:24:LEU:HD21	1.76	0.68
1:C:86:LEU:CD2	1:C:104:PHE:HB2	2.24	0.68
3:F:105:VAL:HG22	3:F:116:LEU:HD11	1.75	0.68
1:A:109:SER:O	1:A:110:SER:HB2	1.91	0.68
1:A:333:LEU:HD23	4:B:1298:HOH:O	1.59	0.68
1:C:75:LYS:NZ	1:C:94:ALA:HB2	2.08	0.68
1:A:736:GLU:O	1:A:740:VAL:HG23	1.93	0.68
1:C:289:SER:OG	1:C:290:ALA:N	2.24	0.68
3:F:227:GLN:HA	3:F:256:VAL:HG13	1.75	0.68
1:A:107:HIS:ND1	1:A:111:VAL:HG22	2.09	0.67
1:C:107:HIS:ND1	1:C:111:VAL:HG22	2.09	0.67
1:C:117:ASN:HD22	1:C:118:ALA:H	1.40	0.67
1:A:427:PHE:O	1:A:431:ILE:HG12	1.94	0.67
1:A:590:VAL:HG13	1:A:622:LEU:CD2	2.23	0.67
1:A:86:LEU:CD2	1:A:104:PHE:HB2	2.24	0.67
1:A:249:LEU:O	1:A:249:LEU:HD23	1.94	0.67
1:A:314:ASP:OD2	1:A:376:TRP:CZ3	2.46	0.67
1:A:528:LYS:HG3	1:C:493:GLN:HE22	1.58	0.67
1:A:557:ASN:HB3	1:C:496:THR:HG23	1.77	0.67
1:C:377:TYR:CB	3:F:57:TRP:CZ2	2.78	0.67
3:F:144:HIS:HB2	3:F:147:GLY:O	1.95	0.67
1:A:124:LEU:HG	1:A:125:ALA:N	2.10	0.67
1:A:314:ASP:H	1:A:376:TRP:HZ2	1.38	0.67
1:C:30:GLY:HA3	1:C:321:PHE:CE2	2.30	0.66
1:C:106:ASN:N	1:C:106:ASN:ND2	2.42	0.66
1:C:249:LEU:O	1:C:249:LEU:HD23	1.94	0.66
1:C:439:ILE:HG13	1:C:440:ASP:H	1.60	0.66
3:F:75:TYR:CD1	3:F:101:SER:HB2	2.31	0.66
1:A:117:ASN:HD22	1:A:118:ALA:H	1.39	0.66
2:B:24:LEU:HB3	2:B:36:PHE:HB2	1.76	0.66
3:F:153:TRP:O	3:F:212:TRP:HB3	1.95	0.66
3:F:200:LEU:HB3	3:F:234:TRP:CZ3	2.30	0.66
1:A:639:GLY:CA	1:A:688:ILE:HD11	2.25	0.66
1:C:535:LEU:HB3	1:C:538:GLU:CG	2.23	0.66
2:B:233:ILE:HD11	2:B:248:LEU:HD13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LYS:NZ	1:C:94:ALA:N	2.44	0.66
2:B:157:THR:OG1	2:B:170:SER:HB2	1.95	0.66
1:A:414:SER:OG	1:A:715:ASN:HB2	1.96	0.66
1:C:124:LEU:HG	1:C:125:ALA:N	2.10	0.66
1:A:304:PHE:HD1	1:A:304:PHE:N	1.87	0.66
1:A:536:LEU:O	1:A:540:MET:HG3	1.96	0.66
1:C:647:ILE:O	1:C:651:GLU:HG3	1.96	0.65
3:F:69:ILE:HD11	3:F:83:LYS:CE	2.25	0.65
3:F:225:VAL:CG2	3:F:257:LEU:HB3	2.26	0.65
1:C:250:GLN:HE21	1:C:251:THR:H	1.45	0.65
1:C:509:ASN:N	1:C:509:ASN:HD22	1.92	0.65
1:C:400:LYS:O	3:F:7:ALA:N	2.29	0.65
1:C:325:ILE:N	1:C:325:ILE:HD12	2.12	0.65
1:A:498:PHE:HB2	1:C:561:ALA:HA	1.77	0.65
2:B:102:VAL:CG2	4:B:1353:HOH:O	2.45	0.65
1:C:590:VAL:HG13	1:C:622:LEU:CD2	2.25	0.65
1:A:75:LYS:NZ	1:A:94:ALA:N	2.44	0.65
1:A:325:ILE:N	1:A:325:ILE:HD12	2.12	0.65
2:B:238:ASN:HD22	2:B:240:GLN:H	1.45	0.65
1:C:125:ALA:HB2	1:C:168:TRP:HH2	1.62	0.65
1:C:408:LYS:H	1:C:408:LYS:CD	2.05	0.65
1:A:557:ASN:HB3	1:C:496:THR:CG2	2.27	0.65
1:C:124:LEU:HG	1:C:125:ALA:H	1.62	0.65
3:F:2:VAL:HG13	3:F:41:GLU:HA	1.79	0.65
1:C:304:PHE:HD1	1:C:304:PHE:N	1.87	0.65
1:C:416:THR:HG22	1:C:420:GLU:OE2	1.96	0.65
3:F:207:VAL:HA	3:F:226:SER:HB2	1.78	0.65
1:A:96:ASN:HB2	4:A:1420:HOH:O	1.96	0.64
1:A:124:LEU:HG	1:A:125:ALA:H	1.62	0.64
1:A:20:ILE:O	1:A:20:ILE:HG13	1.97	0.64
1:A:337:LEU:HD21	2:B:97:VAL:CG1	2.26	0.64
1:A:427:PHE:CD2	1:A:683:VAL:HG22	2.31	0.64
1:A:438:VAL:HG23	1:A:443:ASN:ND2	2.07	0.64
1:A:592:GLN:HG3	1:A:595:PHE:HB3	1.80	0.64
2:B:40:GLY:N	4:B:1335:HOH:O	2.30	0.64
1:C:268:GLN:CA	1:C:373:ALA:HB1	2.21	0.64
3:F:52:HIS:N	4:F:1307:HOH:O	2.29	0.64
1:A:608:ILE:HB	1:A:611:ARG:HH12	1.62	0.64
1:C:20:ILE:O	1:C:20:ILE:HG13	1.97	0.64
1:C:96:ASN:HB2	4:C:2420:HOH:O	1.96	0.64
3:F:184:ILE:HD11	3:F:222:MET:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASN:HD22	1:A:221:ASN:C	2.01	0.64
1:A:519:VAL:HG13	1:C:599:ALA:HA	1.79	0.64
1:C:212:LEU:HD22	1:C:227:THR:CG2	2.28	0.64
1:A:78:ALA:HB3	1:A:114:VAL:HG11	1.80	0.64
1:A:212:LEU:HD22	1:A:227:THR:CG2	2.28	0.64
1:A:608:ILE:HD13	1:A:611:ARG:HH11	1.62	0.64
3:F:49:LEU:HD22	3:F:82:TRP:CD2	2.32	0.64
3:F:224:SER:CB	3:F:234:TRP:HE1	2.11	0.64
1:A:458:THR:HG23	1:A:459:GLU:N	2.14	0.64
1:A:727:PRO:C	1:A:729:ASP:H	2.01	0.64
1:A:241:ASP:C	1:A:243:ARG:H	2.02	0.63
1:C:193:LYS:O	1:C:194:LYS:HB3	1.99	0.63
1:A:250:GLN:HE21	1:A:251:THR:H	1.44	0.63
1:C:395:ILE:HD13	3:F:12:ILE:O	1.98	0.63
1:C:206:SER:O	1:C:208:ILE:HG13	1.98	0.63
1:A:280:ASN:C	1:A:298:ALA:HB3	2.19	0.63
1:A:592:GLN:HG3	1:A:592:GLN:O	1.99	0.63
2:B:18:ASP:HB2	4:B:1317:HOH:O	1.98	0.63
3:F:225:VAL:CG2	3:F:257:LEU:HD13	2.28	0.63
1:C:78:ALA:HB3	1:C:114:VAL:HG11	1.80	0.63
1:A:106:ASN:HD22	1:A:106:ASN:H	1.46	0.63
1:C:280:ASN:C	1:C:298:ALA:HB3	2.19	0.63
1:C:739:ARG:CG	3:F:20:TYR:CE1	2.82	0.63
1:A:206:SER:O	1:A:208:ILE:HG13	1.98	0.62
1:C:639:GLY:HA2	1:C:688:ILE:HD11	1.81	0.62
2:B:33:ILE:HD11	2:B:56:VAL:HG11	1.80	0.62
3:F:105:VAL:CG2	3:F:116:LEU:HD11	2.28	0.62
1:A:30:GLY:HA3	1:A:321:PHE:CE2	2.30	0.62
1:A:51:ASP:O	1:A:53:GLU:HG3	1.99	0.62
1:A:239:ILE:HB	1:A:250:GLN:HB3	1.81	0.62
1:C:192:ALA:O	1:C:194:LYS:HG2	2.00	0.62
3:F:249:LYS:CE	3:F:251:GLU:HB2	2.28	0.62
2:B:157:THR:HG22	2:B:157:THR:O	2.00	0.62
1:C:377:TYR:CB	3:F:57:TRP:CH2	2.82	0.62
1:C:239:ILE:HB	1:C:250:GLN:HB3	1.81	0.62
3:F:118:VAL:O	3:F:125:VAL:HG13	2.00	0.62
1:A:514:ILE:HA	1:A:517:ASN:HD22	1.65	0.62
2:B:23:ARG:NH1	2:B:68:THR:HG21	2.14	0.62
3:F:233:ILE:HD11	3:F:248:LEU:HD13	1.82	0.62
1:A:268:GLN:OE1	1:A:374:PRO:HD2	1.99	0.62
1:A:314:ASP:OD1	1:A:376:TRP:CD1	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:GLY:C	2:B:276:ASN:H	2.00	0.62
1:C:153:PRO:HB2	1:C:188:TRP:CZ3	2.35	0.62
1:A:192:ALA:O	1:A:194:LYS:HG2	2.00	0.61
1:A:392:LEU:HD13	4:A:2219:HOH:O	2.00	0.61
1:C:51:ASP:O	1:C:53:GLU:HG3	1.99	0.61
2:B:66:PHE:HE1	2:B:114:PRO:HD3	1.65	0.61
3:F:147:GLY:N	3:F:178:ALA:HB3	2.15	0.61
1:A:193:LYS:O	1:A:194:LYS:HB3	1.99	0.61
1:A:517:ASN:ND2	1:A:529:ASN:HD22	1.98	0.61
3:F:274:GLY:C	3:F:276:ASN:H	2.03	0.61
1:A:596:ILE:O	1:A:600:ILE:HG12	2.00	0.61
1:A:703:PHE:HA	4:A:2200:HOH:O	2.00	0.61
3:F:27:CYS:HB2	3:F:56:VAL:HG11	1.82	0.61
2:B:52:HIS:HA	4:B:1337:HOH:O	2.01	0.61
3:F:115:MET:HG2	3:F:129:GLU:HB2	1.82	0.61
1:A:370:HIS:HE1	2:B:75:TYR:CD2	2.18	0.61
1:C:314:ASP:N	1:C:376:TRP:CZ2	2.68	0.61
1:C:458:THR:HG23	1:C:459:GLU:H	1.65	0.61
1:C:519:VAL:C	1:C:521:GLY:H	2.02	0.61
1:A:241:ASP:OD1	1:A:243:ARG:HB2	2.00	0.61
2:B:155:PRO:HG3	2:B:214:PRO:HA	1.83	0.61
1:C:241:ASP:C	1:C:243:ARG:H	2.02	0.61
1:C:510:ILE:HA	4:C:1602:HOH:O	1.99	0.61
1:C:739:ARG:HG3	3:F:20:TYR:CD1	2.35	0.61
3:F:23:ARG:HA	3:F:36:PHE:O	2.01	0.61
1:C:106:ASN:HD22	1:C:106:ASN:H	1.45	0.61
1:C:313:PRO:HG2	1:C:376:TRP:CE2	2.36	0.61
1:C:641:LEU:HD13	1:C:688:ILE:HG21	1.82	0.61
3:F:172:LYS:HA	3:F:185:TRP:O	2.01	0.61
1:A:75:LYS:HZ1	1:A:94:ALA:HB2	1.66	0.61
1:A:559:TYR:CD2	1:C:541:VAL:HG21	2.35	0.61
2:B:30:ASP:OD1	2:B:32:THR:N	2.34	0.61
3:F:81:ILE:HD13	3:F:81:ILE:H	1.66	0.61
1:A:370:HIS:CG	1:A:371:LEU:N	2.68	0.61
2:B:102:VAL:HG23	4:B:1353:HOH:O	2.00	0.61
1:A:153:PRO:HB2	1:A:188:TRP:CZ3	2.35	0.60
1:A:396:THR:HG23	4:A:2251:HOH:O	2.01	0.60
1:A:675:THR:O	1:A:679:GLU:HG3	2.01	0.60
1:A:187:ILE:HG22	1:A:196:VAL:HG22	1.83	0.60
2:B:37:GLU:HG2	2:B:46:ILE:HG13	1.82	0.60
1:A:268:GLN:CA	1:A:373:ALA:HB1	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:ILE:HB	2:B:20:TYR:CD2	2.36	0.60
2:B:3:VAL:C	2:B:4:ILE:HD12	2.21	0.60
1:C:221:ASN:HD22	1:C:221:ASN:C	2.01	0.60
1:C:553:GLU:HG2	1:C:557:ASN:HD21	1.67	0.60
3:F:169:GLU:HG2	3:F:187:TYR:HD2	1.67	0.60
1:A:202:THR:O	1:A:202:THR:HG22	2.01	0.60
1:A:608:ILE:CD1	1:A:611:ARG:HH11	2.14	0.60
1:A:709:LEU:O	1:A:713:THR:HG23	2.02	0.60
1:A:537:MET:O	1:A:541:VAL:HG23	2.02	0.60
1:C:399:GLY:O	3:F:12:ILE:HG13	2.01	0.60
3:F:196:LEU:HD12	3:F:197:GLU:H	1.66	0.60
2:B:257:LEU:CD1	2:B:271:LEU:HD21	2.30	0.60
1:A:92:ASN:O	1:A:93:GLU:HB2	2.02	0.60
1:A:227:THR:HG22	1:A:227:THR:O	2.02	0.60
1:C:377:TYR:HB3	4:C:1513:HOH:O	2.02	0.60
1:C:604:TYR:CE1	1:C:610:GLN:HG2	2.36	0.60
1:C:667:TYR:CE2	3:F:266:GLY:HA2	2.37	0.60
2:B:12:ILE:HA	2:B:28:SER:CB	2.30	0.60
1:C:241:ASP:OD1	1:C:243:ARG:HB2	2.01	0.60
3:F:106:GLN:O	3:F:116:LEU:HD12	2.01	0.60
2:B:200:LEU:HB3	2:B:234:TRP:CZ3	2.36	0.60
1:C:75:LYS:HZ1	1:C:94:ALA:N	1.98	0.60
3:F:28:SER:OG	3:F:29:SER:N	2.35	0.60
2:B:4:ILE:HG13	2:B:43:HIS:ND1	2.16	0.60
1:C:202:THR:O	1:C:202:THR:HG22	2.01	0.60
3:F:14:ASP:OD2	3:F:59:VAL:HG22	2.01	0.60
1:A:272:LEU:HD22	1:A:284:LEU:HD11	1.83	0.59
1:C:71:SER:O	1:C:73:ASN:N	2.34	0.59
1:C:78:ALA:HB1	1:C:114:VAL:HG11	1.83	0.59
1:C:665:THR:HG22	3:F:285:LEU:CA	2.30	0.59
1:A:386:TRP:HA	4:A:2219:HOH:O	2.01	0.59
1:C:227:THR:HG22	1:C:227:THR:O	2.02	0.59
1:C:272:LEU:HD22	1:C:284:LEU:HD11	1.83	0.59
3:F:81:ILE:HD13	3:F:81:ILE:N	2.18	0.59
3:F:247:LEU:HD13	3:F:249:LYS:O	2.02	0.59
1:A:146:SER:O	1:A:147:ASN:HB2	2.02	0.59
1:C:129:ASN:HA	1:C:162:GLU:HB3	1.84	0.59
1:A:15:TRP:HB3	1:A:310:PRO:HD3	1.85	0.59
1:A:71:SER:O	1:A:73:ASN:N	2.34	0.59
1:C:187:ILE:HG22	1:C:196:VAL:HG22	1.83	0.59
1:C:330:LEU:O	1:C:371:LEU:HD21	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:O	1:A:371:LEU:HD21	2.02	0.59
1:A:388:PHE:CD1	1:A:739:ARG:CZ	2.86	0.59
2:B:225:VAL:HG13	2:B:257:LEU:HB2	1.84	0.59
1:C:386:TRP:CZ2	3:F:280:LEU:HD22	2.37	0.59
1:A:217:TRP:CD2	1:A:225:VAL:HG22	2.37	0.59
1:A:519:VAL:C	1:A:521:GLY:H	2.05	0.59
2:B:180:ASN:N	2:B:180:ASN:HD22	2.00	0.59
1:C:217:TRP:CD2	1:C:225:VAL:HG22	2.37	0.59
3:F:219:ARG:HG3	3:F:221:TYR:CE1	2.37	0.59
1:A:78:ALA:HB1	1:A:114:VAL:HG11	1.84	0.59
1:A:306:THR:HA	1:A:317:ALA:O	2.03	0.59
1:C:40:SER:OG	1:C:61:VAL:HG23	2.03	0.59
3:F:225:VAL:HG22	3:F:257:LEU:CD1	2.32	0.59
1:A:289:SER:O	1:A:290:ALA:HB2	2.03	0.59
1:A:584:LEU:HD12	1:A:584:LEU:N	2.18	0.59
1:C:727:PRO:C	1:C:729:ASP:H	2.06	0.59
3:F:249:LYS:HG2	3:F:251:GLU:OE1	2.03	0.59
1:C:15:TRP:HB3	1:C:310:PRO:HD3	1.85	0.59
1:C:244:ASN:ND2	1:C:246:ASN:ND2	2.47	0.59
3:F:4:ILE:N	3:F:4:ILE:HD12	2.18	0.59
1:A:88:LEU:HD13	1:A:138:MET:SD	2.43	0.59
1:C:84:GLY:HA3	1:C:110:SER:H	1.68	0.59
1:C:92:ASN:O	1:C:93:GLU:HB2	2.02	0.59
1:C:306:THR:HA	1:C:317:ALA:O	2.03	0.59
3:F:80:MET:CG	3:F:94:VAL:HG23	2.27	0.59
2:B:19:TYR:CD2	2:B:64:PRO:HG2	2.38	0.58
1:C:112:LYS:HG3	1:C:164:ILE:HG22	1.85	0.58
1:C:268:GLN:HG3	1:C:313:PRO:CG	2.33	0.58
1:C:509:ASN:N	1:C:509:ASN:ND2	2.51	0.58
1:A:40:SER:OG	1:A:61:VAL:HG23	2.02	0.58
1:A:228:ALA:HB1	1:A:260:ILE:HG21	1.85	0.58
1:A:370:HIS:CE1	2:B:75:TYR:CD2	2.90	0.58
2:B:120:SER:HB3	2:B:122:ASP:OD1	2.03	0.58
1:C:175:VAL:HG12	1:C:176:PHE:N	2.18	0.58
1:C:592:GLN:HG3	1:C:595:PHE:CB	2.33	0.58
1:C:665:THR:CG2	3:F:285:LEU:HD23	2.33	0.58
1:A:84:GLY:HA3	1:A:110:SER:H	1.68	0.58
1:A:458:THR:HG23	1:A:459:GLU:H	1.66	0.58
1:A:509:ASN:N	1:A:509:ASN:HD22	2.01	0.58
1:A:518:LEU:HB3	1:C:576:ILE:CD1	2.31	0.58
1:A:112:LYS:HG3	1:A:164:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ASN:N	1:C:74:ASN:ND2	2.50	0.58
1:C:438:VAL:HG23	1:C:443:ASN:HD22	1.68	0.58
1:C:670:HIS:HE1	1:C:705:GLU:OE1	1.86	0.58
3:F:187:TYR:CG	3:F:188:ASN:N	2.71	0.58
2:B:68:THR:C	2:B:69:ILE:HD12	2.23	0.58
2:B:83:LYS:HB2	2:B:92:ILE:HD13	1.85	0.58
2:B:216:VAL:HG12	2:B:216:VAL:O	2.03	0.58
1:C:661:LYS:C	1:C:663:ASN:H	2.06	0.58
1:C:280:ASN:HB3	1:C:300:GLY:C	2.24	0.58
3:F:147:GLY:H	3:F:178:ALA:HB3	1.66	0.58
1:A:280:ASN:HB3	1:A:300:GLY:C	2.24	0.58
1:A:314:ASP:OD2	1:A:376:TRP:CH2	2.55	0.58
1:A:496:THR:O	1:A:497:ASN:CB	2.51	0.58
1:C:88:LEU:HD13	1:C:138:MET:SD	2.43	0.58
1:C:146:SER:O	1:C:147:ASN:HB2	2.02	0.58
1:C:289:SER:O	1:C:290:ALA:HB2	2.03	0.58
3:F:29:SER:O	3:F:31:LYS:N	2.37	0.58
3:F:37:GLU:HB2	3:F:44:LYS:HB3	1.85	0.58
1:A:175:VAL:HG12	1:A:176:PHE:N	2.18	0.58
1:A:228:ALA:HB2	1:A:263:LEU:HD11	1.85	0.58
1:A:314:ASP:N	1:A:376:TRP:CE2	2.72	0.58
1:A:612:ASN:O	1:A:616:ILE:HG12	2.03	0.58
1:A:129:ASN:HA	1:A:162:GLU:HB3	1.84	0.58
1:A:306:THR:O	1:A:307:LYS:HD3	2.04	0.58
1:A:329:THR:HB	1:A:331:GLN:O	2.04	0.58
1:A:511:GLU:HG3	4:A:2107:HOH:O	2.03	0.58
1:C:147:ASN:O	1:C:148:TYR:C	2.42	0.58
1:C:228:ALA:HB2	1:C:263:LEU:HD11	1.85	0.58
1:A:365:LYS:HD2	1:A:365:LYS:O	2.04	0.58
1:C:21:PRO:HB2	1:C:47:LEU:HD11	1.86	0.58
1:C:306:THR:O	1:C:307:LYS:HD3	2.04	0.58
1:A:283:LEU:HD22	1:A:292:GLN:HE21	1.69	0.57
3:F:25:ALA:HB1	3:F:70:LEU:HD21	1.86	0.57
3:F:130:PHE:HA	3:F:136:THR:HG22	1.86	0.57
1:C:11:ALA:HB1	1:C:26:GLY:O	2.04	0.57
1:C:380:PRO:HG3	3:F:11:MET:SD	2.43	0.57
1:A:674:LEU:O	1:A:678:ILE:HG12	2.03	0.57
1:A:11:ALA:HB1	1:A:26:GLY:O	2.04	0.57
1:A:315:LEU:HD11	2:B:146:ILE:CD1	2.33	0.57
1:A:731:GLU:O	1:A:734:LYS:HB3	2.04	0.57
2:B:4:ILE:HG13	2:B:43:HIS:CG	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ALA:HB1	1:C:260:ILE:HG21	1.85	0.57
1:C:370:HIS:CG	1:C:371:LEU:N	2.68	0.57
1:C:656:GLU:OE2	1:C:670:HIS:HA	2.04	0.57
1:A:147:ASN:O	1:A:148:TYR:C	2.42	0.57
1:A:221:ASN:ND2	1:A:223:THR:H	2.03	0.57
1:A:423:LYS:HG3	1:A:424:THR:HG23	1.86	0.57
1:A:647:ILE:O	1:A:651:GLU:HG3	2.04	0.57
1:A:730:ASN:O	1:A:733:VAL:HB	2.03	0.57
2:B:29:SER:HA	2:B:55:PRO:HB3	1.84	0.57
1:C:221:ASN:ND2	1:C:223:THR:H	2.02	0.57
1:C:329:THR:HB	1:C:331:GLN:O	2.04	0.57
1:C:386:TRP:HZ2	3:F:280:LEU:HD22	1.68	0.57
1:A:72:HIS:ND1	1:A:118:ALA:HA	2.19	0.57
1:A:468:PHE:CE1	1:A:598:LYS:HE3	2.40	0.57
2:B:108:ALA:HB1	2:B:109:PRO:CD	2.34	0.57
1:C:75:LYS:HZ1	1:C:94:ALA:HB2	1.69	0.57
3:F:180:ASN:N	3:F:180:ASN:ND2	2.46	0.57
1:A:71:SER:HA	1:A:116:PHE:CG	2.40	0.57
1:C:62:ASP:CG	1:C:103:ARG:HH12	2.08	0.57
1:A:155:GLN:CB	1:A:195:GLU:HB3	2.35	0.57
1:A:262:SER:HB2	1:A:304:PHE:O	2.05	0.57
1:A:268:GLN:HB2	1:A:374:PRO:O	1.98	0.57
1:C:44:LEU:HD23	1:C:56:ILE:HB	1.87	0.57
1:C:241:ASP:O	1:C:243:ARG:N	2.38	0.57
1:C:155:GLN:CB	1:C:195:GLU:HB3	2.35	0.56
3:F:239:GLU:N	4:F:1304:HOH:O	2.38	0.56
1:A:62:ASP:CG	1:A:103:ARG:HH12	2.08	0.56
1:A:106:ASN:N	1:A:106:ASN:ND2	2.42	0.56
1:A:268:GLN:HG3	1:A:313:PRO:CG	2.34	0.56
1:A:292:GLN:O	1:A:368:VAL:CG2	2.53	0.56
1:C:71:SER:HA	1:C:116:PHE:CG	2.40	0.56
1:C:72:HIS:ND1	1:C:118:ALA:HA	2.19	0.56
1:C:145:PRO:O	1:C:147:ASN:N	2.39	0.56
1:C:283:LEU:HD22	1:C:292:GLN:HE21	1.69	0.56
3:F:10:GLU:HG3	3:F:30:ASP:HB3	1.87	0.56
1:A:241:ASP:O	1:A:243:ARG:N	2.38	0.56
1:A:431:ILE:HD13	1:A:447:TRP:CZ3	2.40	0.56
1:A:496:THR:HG23	1:C:557:ASN:CB	2.32	0.56
2:B:222:LEU:HB2	2:B:234:TRP:HB2	1.85	0.56
4:C:1535:HOH:O	3:F:282:LYS:NZ	2.38	0.56
3:F:29:SER:C	3:F:31:LYS:N	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:79:VAL:CG2	3:F:95:HIS:HB3	2.35	0.56
3:F:196:LEU:HG	3:F:197:GLU:N	2.21	0.56
1:C:365:LYS:HD2	1:C:365:LYS:O	2.04	0.56
1:C:494:ILE:HG13	1:C:495:GLU:N	2.18	0.56
1:A:21:PRO:HB2	1:A:47:LEU:HD11	1.86	0.56
1:A:113:THR:HG22	1:A:114:VAL:N	2.20	0.56
2:B:4:ILE:HD12	2:B:4:ILE:N	2.20	0.56
2:B:56:VAL:HA	2:B:74:SER:HB2	1.87	0.56
1:C:113:THR:HG22	1:C:114:VAL:N	2.20	0.56
1:C:430:LEU:HD11	1:C:679:GLU:HG2	1.86	0.56
2:B:24:LEU:HG	2:B:25:ALA:N	2.20	0.56
2:B:180:ASN:N	2:B:180:ASN:ND2	2.53	0.56
3:F:4:ILE:HG22	3:F:4:ILE:O	2.04	0.56
1:A:74:ASN:O	1:A:76:ILE:HG12	2.06	0.56
1:A:244:ASN:ND2	1:A:246:ASN:ND2	2.47	0.56
1:C:280:ASN:HB3	1:C:300:GLY:O	2.06	0.56
1:C:87:GLU:HG2	1:C:89:TYR:CE1	2.41	0.56
3:F:184:ILE:HG12	3:F:198:SER:HB2	1.88	0.56
3:F:257:LEU:HD23	3:F:273:GLY:HA2	1.87	0.56
1:A:74:ASN:H	1:A:74:ASN:ND2	2.02	0.56
1:A:120:GLN:HG3	1:A:122:ASN:OD1	2.06	0.56
1:A:153:PRO:HB2	1:A:188:TRP:CE3	2.41	0.56
1:A:438:VAL:HG22	1:A:439:ILE:N	2.20	0.56
1:A:584:LEU:HD12	1:A:584:LEU:H	1.71	0.56
1:C:120:GLN:HG3	1:C:122:ASN:OD1	2.06	0.56
1:C:260:ILE:CG2	1:C:261:LEU:N	2.69	0.56
1:A:42:LEU:HD21	1:A:89:TYR:CD2	2.41	0.56
1:A:280:ASN:HB3	1:A:300:GLY:O	2.06	0.56
1:A:365:LYS:NZ	1:A:371:LEU:HD22	2.21	0.56
2:B:66:PHE:CE1	2:B:114:PRO:HD3	2.41	0.56
2:B:189:SER:C	2:B:191:ALA:H	2.09	0.56
1:C:17:HIS:HB2	1:C:73:ASN:HB2	1.87	0.56
1:C:178:SER:HB2	1:C:186:SER:HB2	1.88	0.56
1:C:268:GLN:HG3	4:C:1545:HOH:O	2.06	0.56
1:C:444:GLU:HG2	1:C:448:ASN:HD21	1.71	0.56
1:A:74:ASN:N	1:A:74:ASN:ND2	2.50	0.55
1:A:80:ALA:CB	1:A:111:VAL:HG12	2.37	0.55
1:C:153:PRO:HB2	1:C:188:TRP:CE3	2.41	0.55
1:C:203:SER:N	1:C:204:PRO:CD	2.69	0.55
1:C:262:SER:HB2	1:C:304:PHE:O	2.05	0.55
2:B:8:HIS:ND1	2:B:30:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LEU:HD21	1:C:89:TYR:CD2	2.41	0.55
1:C:292:GLN:O	1:C:368:VAL:CG2	2.53	0.55
1:C:365:LYS:NZ	1:C:371:LEU:HD22	2.21	0.55
1:A:162:GLU:O	1:A:164:ILE:HG23	2.06	0.55
1:A:616:ILE:HD11	1:A:640:SER:HB2	1.88	0.55
1:A:17:HIS:HB2	1:A:73:ASN:HB2	1.87	0.55
1:A:730:ASN:HB3	1:A:733:VAL:CG2	2.36	0.55
1:C:313:PRO:HD2	4:C:1546:HOH:O	2.00	0.55
1:C:462:LEU:HD22	1:C:637:ALA:HB2	1.87	0.55
1:A:12:THR:HG23	1:A:12:THR:O	2.06	0.55
1:A:44:LEU:HD23	1:A:56:ILE:HB	1.87	0.55
1:A:106:ASN:H	1:A:106:ASN:ND2	2.05	0.55
1:A:420:GLU:HG3	1:A:423:LYS:CE	2.37	0.55
1:C:535:LEU:HD22	1:C:538:GLU:HG3	1.88	0.55
3:F:71:ALA:CB	3:F:81:ILE:HG22	2.37	0.55
1:A:87:GLU:HG2	1:A:89:TYR:CE1	2.41	0.55
1:A:260:ILE:CG2	1:A:261:LEU:N	2.69	0.55
1:C:431:ILE:HD11	1:C:683:VAL:HG11	1.88	0.55
1:C:667:TYR:CD2	3:F:266:GLY:HA2	2.41	0.55
3:F:155:PRO:HG2	3:F:214:PRO:HA	1.88	0.55
1:A:199:LEU:HD13	1:A:240:TRP:CG	2.42	0.55
1:A:517:ASN:HD21	1:A:529:ASN:ND2	2.04	0.55
2:B:69:ILE:HD12	2:B:69:ILE:N	2.22	0.55
1:A:38:THR:O	1:A:64:LYS:HE2	2.07	0.55
1:A:312:ALA:CB	1:A:315:LEU:HD12	2.36	0.55
1:A:623:LYS:HE3	1:A:647:ILE:HD12	1.89	0.55
3:F:2:VAL:HG12	3:F:2:VAL:O	2.07	0.55
3:F:74:SER:HB3	3:F:76:ASP:OD1	2.06	0.55
3:F:81:ILE:HG12	3:F:92:ILE:HG13	1.88	0.55
3:F:150:SER:HB2	3:F:210:VAL:HG22	1.88	0.55
1:A:105:SER:C	1:A:107:HIS:H	2.09	0.55
1:A:145:PRO:O	1:A:147:ASN:N	2.38	0.55
1:A:247:THR:CG2	1:A:248:PRO:HD2	2.37	0.55
1:C:105:SER:C	1:C:107:HIS:H	2.09	0.55
3:F:145:ALA:HB3	3:F:179:ASP:HB3	1.89	0.55
1:A:41:SER:O	1:A:42:LEU:HB3	2.07	0.55
1:A:80:ALA:HB2	1:A:114:VAL:CG2	2.36	0.55
1:A:203:SER:N	1:A:204:PRO:CD	2.69	0.55
1:A:418:LEU:HD23	1:A:718:LEU:HD21	1.89	0.55
1:A:129:ASN:ND2	1:A:162:GLU:OE1	2.38	0.54
1:A:418:LEU:HG	1:A:718:LEU:HD11	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ARG:HG3	1:A:447:TRP:CZ2	2.41	0.54
1:C:519:VAL:HG23	1:C:520:SER:N	2.21	0.54
1:C:733:VAL:O	1:C:737:LYS:HG3	2.07	0.54
3:F:260:ALA:HA	3:F:271:LEU:HD12	1.89	0.54
1:C:12:THR:HG23	1:C:12:THR:O	2.06	0.54
1:C:162:GLU:O	1:C:164:ILE:HG23	2.06	0.54
1:C:199:LEU:HD13	1:C:240:TRP:CG	2.42	0.54
1:C:312:ALA:CB	1:C:315:LEU:HD12	2.36	0.54
1:A:46:SER:HB2	1:A:56:ILE:HD11	1.90	0.54
2:B:73:CYS:HB2	2:B:102:VAL:CG1	2.37	0.54
1:C:38:THR:O	1:C:64:LYS:HE2	2.07	0.54
1:C:59:LEU:HD22	1:C:98:ILE:HG12	1.90	0.54
1:C:247:THR:CG2	1:C:248:PRO:HD2	2.37	0.54
1:A:66:ASN:N	1:A:80:ALA:O	2.39	0.54
1:A:337:LEU:CD2	2:B:97:VAL:HG12	2.36	0.54
1:A:510:ILE:HB	4:A:2107:HOH:O	2.06	0.54
1:C:26:GLY:HA2	1:C:42:LEU:HA	1.89	0.54
1:C:244:ASN:HD21	1:C:246:ASN:HD22	1.49	0.54
3:F:183:LYS:HB2	3:F:185:TRP:HE1	1.72	0.54
1:C:104:PHE:N	1:C:104:PHE:CD1	2.75	0.54
1:C:590:VAL:HG13	1:C:622:LEU:HD23	1.90	0.54
1:C:696:ASN:O	1:C:700:ILE:HG13	2.08	0.54
3:F:92:ILE:HG13	3:F:93:ALA:H	1.72	0.54
3:F:208:ARG:H	3:F:226:SER:HA	1.72	0.54
1:A:178:SER:HB2	1:A:186:SER:HB2	1.88	0.54
1:A:244:ASN:HD21	1:A:246:ASN:HD22	1.49	0.54
2:B:45:LEU:O	2:B:46:ILE:HD13	2.08	0.54
1:C:74:ASN:O	1:C:76:ILE:HG12	2.06	0.54
1:C:129:ASN:ND2	1:C:162:GLU:OE1	2.38	0.54
3:F:184:ILE:CG1	3:F:198:SER:HB2	2.38	0.54
1:C:41:SER:O	1:C:42:LEU:HB3	2.07	0.54
1:C:402:VAL:HG11	3:F:24:MET:SD	2.47	0.54
1:A:26:GLY:HA2	1:A:42:LEU:HA	1.89	0.54
1:A:73:ASN:C	1:A:75:LYS:N	2.59	0.54
1:C:66:ASN:N	1:C:80:ALA:O	2.39	0.54
1:C:80:ALA:HB2	1:C:114:VAL:CG2	2.36	0.54
3:F:225:VAL:HG22	3:F:257:LEU:CB	2.37	0.54
3:F:283:GLU:HA	3:F:288:LYS:O	2.07	0.54
1:C:73:ASN:C	1:C:75:LYS:N	2.58	0.54
3:F:39:GLU:O	3:F:41:GLU:N	2.33	0.54
1:A:314:ASP:CG	1:A:376:TRP:CD1	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:LEU:HD23	2:B:94:VAL:HG23	1.90	0.54
1:C:510:ILE:HG21	1:C:533:ASN:ND2	2.23	0.54
3:F:25:ALA:HA	3:F:34:LYS:O	2.08	0.54
1:A:48:LEU:O	1:A:49:ALA:O	2.25	0.53
1:A:509:ASN:N	1:A:509:ASN:ND2	2.54	0.53
2:B:80:LEU:CD2	2:B:94:VAL:HG23	2.38	0.53
1:A:154:GLY:O	1:A:155:GLN:CG	2.48	0.53
2:B:25:ALA:HB2	2:B:61:TRP:CZ2	2.44	0.53
1:C:48:LEU:O	1:C:49:ALA:O	2.25	0.53
1:C:74:ASN:H	1:C:74:ASN:ND2	2.02	0.53
3:F:155:PRO:CG	3:F:214:PRO:HA	2.37	0.53
3:F:229:ARG:HG2	3:F:256:VAL:HA	1.90	0.53
3:F:236:GLN:HG2	3:F:237:ASP:N	2.22	0.53
1:A:528:LYS:HG3	1:C:493:GLN:NE2	2.22	0.53
1:A:551:LEU:C	1:A:553:GLU:H	2.11	0.53
1:C:259:GLY:HA3	1:C:278:ARG:HH11	1.74	0.53
1:C:46:SER:HB2	1:C:56:ILE:HD11	1.90	0.53
1:C:707:ILE:O	1:C:710:THR:HB	2.09	0.53
3:F:17:MET:C	3:F:61:TRP:CD1	2.81	0.53
1:A:59:LEU:HD22	1:A:98:ILE:HG12	1.90	0.53
1:A:110:SER:OG	1:A:129:ASN:ND2	2.41	0.53
1:A:125:ALA:HB2	1:A:168:TRP:HH2	1.62	0.53
1:A:175:VAL:HG13	1:A:188:TRP:O	2.08	0.53
1:A:439:ILE:HG21	1:A:659:LEU:HD21	1.90	0.53
2:B:39:GLU:HB2	4:B:1335:HOH:O	2.08	0.53
1:C:423:LYS:CG	1:C:424:THR:N	2.71	0.53
1:A:285:TRP:CZ3	1:A:292:GLN:HG3	2.44	0.53
1:C:604:TYR:CZ	1:C:610:GLN:HG2	2.43	0.53
3:F:215:THR:HG23	3:F:215:THR:O	2.08	0.53
1:A:13:PHE:HA	1:A:24:VAL:O	2.09	0.53
2:B:33:ILE:CD1	2:B:56:VAL:HG11	2.39	0.53
2:B:49:LEU:HB3	2:B:82:TRP:CZ3	2.44	0.53
1:C:665:THR:HG22	3:F:285:LEU:HD23	1.91	0.53
3:F:46:ILE:CG2	3:F:47:ASP:H	1.99	0.53
1:C:80:ALA:CB	1:C:111:VAL:HG12	2.37	0.53
1:C:386:TRP:NE1	3:F:270:ALA:HB2	2.24	0.53
1:A:57:ALA:O	1:A:98:ILE:HG22	2.09	0.53
1:A:337:LEU:HD11	2:B:97:VAL:HB	1.91	0.53
1:A:723:LEU:HA	4:A:2255:HOH:O	2.08	0.53
1:C:13:PHE:HA	1:C:24:VAL:O	2.09	0.53
1:C:535:LEU:CB	1:C:538:GLU:HG3	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:SER:OG	1:C:129:ASN:ND2	2.42	0.53
1:C:199:LEU:HD13	1:C:240:TRP:CD2	2.44	0.53
1:C:313:PRO:C	1:C:376:TRP:HE1	2.12	0.53
1:C:408:LYS:HE2	3:F:292:ALA:O	2.09	0.53
3:F:119:ALA:HB2	3:F:151:ALA:HB2	1.91	0.53
1:A:104:PHE:CD1	1:A:104:PHE:N	2.75	0.52
1:A:451:GLU:O	1:A:454:SER:HB3	2.09	0.52
1:A:7:PHE:O	1:A:324:LYS:HD3	2.09	0.52
1:A:129:ASN:C	1:A:131:GLY:H	2.11	0.52
1:A:199:LEU:HD13	1:A:240:TRP:CD2	2.44	0.52
1:C:286:ASN:HB2	1:C:293:LEU:HD11	1.92	0.52
3:F:108:ALA:HB2	3:F:153:TRP:CZ2	2.44	0.52
3:F:184:ILE:HD11	3:F:222:MET:HE3	1.89	0.52
1:A:90:SER:O	1:A:91:THR:HB	2.08	0.52
2:B:128:VAL:CG2	2:B:138:PRO:HB3	2.27	0.52
1:C:175:VAL:HG13	1:C:188:TRP:O	2.09	0.52
3:F:52:HIS:CE1	3:F:80:MET:HE3	2.44	0.52
1:A:172:LEU:C	1:A:174:HIS:H	2.13	0.52
1:A:388:PHE:CD1	1:A:739:ARG:NH2	2.77	0.52
3:F:59:VAL:HG12	3:F:72:SER:HA	1.89	0.52
3:F:78:LYS:HG2	3:F:96:ALA:CB	2.40	0.52
1:A:137:ASP:OD1	1:A:139:ASN:HB2	2.10	0.52
1:C:57:ALA:O	1:C:98:ILE:HG22	2.09	0.52
1:C:106:ASN:ND2	1:C:106:ASN:H	2.04	0.52
1:C:285:TRP:CZ3	1:C:292:GLN:HG3	2.44	0.52
1:C:7:PHE:O	1:C:324:LYS:HD3	2.09	0.52
1:C:172:LEU:C	1:C:174:HIS:H	2.13	0.52
3:F:46:ILE:N	3:F:46:ILE:CD1	2.71	0.52
3:F:188:ASN:HB3	3:F:191:ALA:HB3	1.92	0.52
1:C:137:ASP:OD1	1:C:139:ASN:HB2	2.10	0.52
1:C:145:PRO:O	1:C:146:SER:C	2.48	0.52
1:C:252:LEU:HD13	1:C:285:TRP:CG	2.45	0.52
3:F:233:ILE:H	3:F:233:ILE:CD1	2.10	0.52
1:A:531:LEU:C	1:A:533:ASN:H	2.13	0.52
1:A:742:ILE:H	1:A:742:ILE:HD12	1.73	0.52
2:B:238:ASN:HD22	2:B:240:GLN:N	2.07	0.52
1:C:314:ASP:OD2	1:C:376:TRP:CZ3	2.62	0.52
1:C:22:LEU:CD1	1:C:94:ALA:CB	2.82	0.52
1:C:268:GLN:HA	1:C:373:ALA:HB3	1.88	0.52
1:C:312:ALA:HB1	1:C:315:LEU:HD12	1.92	0.52
3:F:99:SER:O	3:F:100:ALA:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HB	1:A:40:SER:CB	2.40	0.52
1:C:90:SER:O	1:C:91:THR:HB	2.09	0.52
3:F:206:TRP:N	3:F:206:TRP:CD1	2.78	0.52
2:B:117:LEU:HD12	4:B:1340:HOH:O	2.08	0.51
1:C:27:THR:HB	1:C:40:SER:CB	2.40	0.51
1:C:155:GLN:HG3	1:C:194:LYS:HB2	1.93	0.51
1:C:261:LEU:HB2	1:C:277:GLY:HA2	1.92	0.51
3:F:180:ASN:CG	3:F:205:ASP:O	2.49	0.51
3:F:231:CYS:HB3	3:F:248:LEU:HD22	1.92	0.51
1:A:155:GLN:HG3	1:A:194:LYS:HB2	1.92	0.51
1:A:593:TRP:C	1:A:595:PHE:H	2.12	0.51
1:A:688:ILE:HD13	1:A:689:ASN:N	2.25	0.51
1:C:636:LEU:HD12	1:C:688:ILE:HD12	1.93	0.51
1:A:145:PRO:O	1:A:146:SER:C	2.48	0.51
1:A:252:LEU:HD13	1:A:285:TRP:CG	2.45	0.51
1:A:259:GLY:HA3	1:A:278:ARG:HH11	1.74	0.51
1:A:519:VAL:CG1	1:C:599:ALA:HA	2.40	0.51
1:A:649:LEU:HB3	1:A:698:GLN:OE1	2.09	0.51
1:C:129:ASN:C	1:C:131:GLY:H	2.11	0.51
1:A:261:LEU:HB2	1:A:277:GLY:HA2	1.92	0.51
1:A:314:ASP:N	1:A:376:TRP:CZ2	2.72	0.51
1:C:674:LEU:HD21	1:C:705:GLU:HB3	1.91	0.51
3:F:23:ARG:NH1	3:F:68:THR:CG2	2.74	0.51
3:F:123:GLY:HA2	3:F:147:GLY:HA2	1.92	0.51
2:B:255:ASP:CG	2:B:256:VAL:H	2.14	0.51
1:C:70:TRP:HD1	1:C:71:SER:O	1.94	0.51
3:F:85:GLU:O	3:F:86:ASN:HB2	2.11	0.51
1:A:608:ILE:HD13	1:A:611:ARG:NH1	2.24	0.51
2:B:69:ILE:HG22	2:B:70:LEU:N	2.25	0.51
1:C:400:LYS:O	3:F:6:ASN:HA	2.11	0.51
2:B:33:ILE:HB	2:B:49:LEU:HB2	1.92	0.51
1:A:241:ASP:C	1:A:243:ARG:N	2.65	0.51
1:A:584:LEU:H	1:A:584:LEU:CD1	2.22	0.51
1:C:377:TYR:HA	4:C:1513:HOH:O	2.11	0.51
3:F:65:LYS:CD	3:F:110:HIS:HB2	2.40	0.51
3:F:94:VAL:O	3:F:94:VAL:HG13	2.11	0.51
3:F:171:ARG:O	3:F:186:LYS:HA	2.11	0.51
1:A:283:LEU:HD13	1:A:292:GLN:NE2	2.26	0.51
1:A:286:ASN:HB2	1:A:293:LEU:HD11	1.92	0.51
2:B:105:VAL:CG2	2:B:116:LEU:HD21	2.41	0.51
1:C:117:ASN:ND2	1:C:118:ALA:N	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:677:PHE:CD2	1:C:678:ILE:HD12	2.46	0.51
3:F:233:ILE:HG21	3:F:289:TRP:CZ2	2.45	0.51
3:F:259:ARG:HG3	3:F:259:ARG:HH11	1.76	0.51
1:A:524:LYS:HG3	1:A:525:SER:N	2.26	0.51
1:C:241:ASP:C	1:C:243:ARG:N	2.65	0.51
1:C:283:LEU:HD13	1:C:292:GLN:NE2	2.26	0.51
1:C:333:LEU:HG	3:F:100:ALA:HA	1.93	0.51
1:C:430:LEU:HD23	1:C:430:LEU:O	2.11	0.51
1:A:212:LEU:HD13	1:A:227:THR:CG2	2.41	0.50
2:B:95:HIS:CE1	2:B:128:VAL:HG21	2.46	0.50
3:F:92:ILE:HG13	3:F:93:ALA:N	2.26	0.50
1:A:75:LYS:HZ2	1:A:94:ALA:N	2.09	0.50
1:A:274:LEU:HG	1:A:308:PHE:CZ	2.46	0.50
1:A:312:ALA:HB1	1:A:315:LEU:HD12	1.92	0.50
2:B:259:ARG:HG3	2:B:259:ARG:HH11	1.77	0.50
1:A:268:GLN:CB	4:A:2118:HOH:O	2.46	0.50
1:A:608:ILE:HB	1:A:611:ARG:NH1	2.27	0.50
2:B:4:ILE:O	2:B:4:ILE:HG22	2.11	0.50
1:C:271:HIS:O	1:C:272:LEU:HD23	2.12	0.50
3:F:24:MET:CG	3:F:25:ALA:N	2.60	0.50
3:F:27:CYS:HB2	3:F:56:VAL:CG1	2.41	0.50
1:A:70:TRP:HD1	1:A:71:SER:O	1.94	0.50
1:C:519:VAL:C	1:C:521:GLY:N	2.62	0.50
1:A:314:ASP:CB	1:A:376:TRP:CE2	2.95	0.50
1:A:432:ASN:O	1:A:436:VAL:HG23	2.11	0.50
1:C:124:LEU:CG	1:C:125:ALA:H	2.24	0.50
1:C:335:ASN:OD1	3:F:99:SER:HB3	2.11	0.50
3:F:78:LYS:HG2	3:F:96:ALA:HB1	1.94	0.50
1:A:663:ASN:HA	2:B:285:LEU:HD11	1.94	0.50
1:A:731:GLU:HA	1:A:734:LYS:HB3	1.93	0.50
1:C:31:THR:CG2	1:C:32:VAL:N	2.64	0.50
3:F:59:VAL:HA	3:F:71:ALA:O	2.12	0.50
3:F:286:GLU:HG3	3:F:288:LYS:HD2	1.94	0.50
1:A:57:ALA:O	1:A:98:ILE:CG2	2.60	0.50
1:A:664:LYS:HA	1:A:668:GLU:OE1	2.11	0.50
2:B:200:LEU:HD13	2:B:234:TRP:CE3	2.47	0.50
3:F:71:ALA:HB2	3:F:81:ILE:CG2	2.40	0.50
1:A:567:SER:HB3	1:A:570:SER:HB2	1.93	0.50
1:C:274:LEU:HG	1:C:308:PHE:CZ	2.46	0.50
1:C:551:LEU:HD23	1:C:551:LEU:C	2.33	0.50
1:A:11:ALA:HB3	1:A:325:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HG22	1:A:29:SER:N	2.26	0.50
1:A:271:HIS:O	1:A:272:LEU:HD23	2.12	0.50
1:A:402:VAL:HG11	2:B:24:LEU:CD2	2.42	0.50
1:A:505:SER:CB	1:C:589:ASP:HB2	2.37	0.50
1:A:555:VAL:O	1:A:558:ALA:HB3	2.12	0.50
3:F:29:SER:HA	3:F:55:PRO:HB3	1.93	0.50
3:F:63:HIS:ND1	3:F:64:PRO:HD2	2.26	0.50
1:A:72:HIS:HE1	1:A:118:ALA:HA	1.72	0.49
1:A:314:ASP:CG	1:A:376:TRP:CG	2.85	0.49
1:A:15:TRP:HB3	1:A:310:PRO:CD	2.41	0.49
1:A:117:ASN:ND2	1:A:118:ALA:N	2.54	0.49
1:A:314:ASP:OD1	1:A:376:TRP:CG	2.65	0.49
1:A:412:LEU:CD2	1:A:713:THR:HG22	2.38	0.49
1:A:496:THR:HG22	1:A:497:ASN:N	2.27	0.49
1:C:11:ALA:HB3	1:C:325:ILE:HD11	1.93	0.49
1:A:536:LEU:HD23	1:C:537:MET:HE3	1.94	0.49
2:B:112:TYR:CZ	2:B:171:ARG:HG2	2.46	0.49
1:C:601:GLN:HE22	1:C:611:ARG:HD3	1.77	0.49
3:F:10:GLU:CG	3:F:30:ASP:HB3	2.42	0.49
3:F:47:ASP:OD2	3:F:89:TRP:HB2	2.12	0.49
1:C:28:VAL:HG22	1:C:29:SER:N	2.26	0.49
3:F:52:HIS:CG	3:F:80:MET:HE1	2.47	0.49
1:A:115:LYS:O	1:A:124:LEU:HD12	2.13	0.49
1:A:196:VAL:C	1:A:197:ILE:HG13	2.32	0.49
1:A:337:LEU:CD2	2:B:97:VAL:CG1	2.90	0.49
1:C:530:SER:O	1:C:533:ASN:O	2.31	0.49
3:F:131:LYS:HB3	3:F:132:GLU:OE2	2.12	0.49
1:A:15:TRP:HZ3	1:A:307:LYS:O	1.96	0.49
1:A:284:LEU:HD23	1:A:371:LEU:HD11	1.94	0.49
1:A:568:SER:HB2	1:C:511:GLU:OE1	2.13	0.49
1:A:665:THR:HG1	1:A:668:GLU:HG3	1.78	0.49
2:B:148:VAL:O	4:B:1338:HOH:O	2.20	0.49
1:C:196:VAL:C	1:C:197:ILE:HG13	2.32	0.49
1:C:439:ILE:CG2	1:C:659:LEU:HD21	2.39	0.49
1:C:665:THR:HG22	3:F:285:LEU:N	2.27	0.49
1:A:237:ILE:HB	1:A:252:LEU:HB2	1.93	0.49
1:A:268:GLN:HE21	1:A:313:PRO:CG	2.25	0.49
2:B:95:HIS:HE1	2:B:138:PRO:HG3	1.78	0.49
2:B:233:ILE:CD1	2:B:248:LEU:HD13	2.43	0.49
1:C:237:ILE:HB	1:C:252:LEU:HB2	1.93	0.49
1:C:268:GLN:HE21	1:C:313:PRO:CG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:733:VAL:HG12	1:C:737:LYS:HE3	1.95	0.49
3:F:129:GLU:HG2	3:F:130:PHE:N	2.27	0.49
3:F:259:ARG:HB2	3:F:272:SER:HB2	1.95	0.49
1:A:33:ASP:OD1	1:A:37:SER:HB3	2.13	0.49
1:C:15:TRP:HB3	1:C:310:PRO:CD	2.41	0.49
1:C:29:SER:HB2	1:C:82:ASP:OD1	2.13	0.49
1:C:115:LYS:O	1:C:124:LEU:HD12	2.13	0.49
1:C:212:LEU:HD13	1:C:227:THR:CG2	2.41	0.49
1:C:494:ILE:HG23	1:C:495:GLU:N	2.27	0.49
1:A:187:ILE:HB	1:A:197:ILE:HB	1.95	0.49
1:A:430:LEU:O	1:A:430:LEU:HD23	2.13	0.49
1:C:57:ALA:O	1:C:98:ILE:CG2	2.60	0.49
1:A:124:LEU:CG	1:A:125:ALA:N	2.76	0.49
2:B:26:THR:O	2:B:33:ILE:HG23	2.12	0.49
2:B:29:SER:C	2:B:31:LYS:H	2.16	0.49
2:B:63:HIS:CD2	4:B:1334:HOH:O	2.65	0.49
1:C:115:LYS:O	1:C:168:TRP:HZ3	1.96	0.49
1:C:130:ASN:HB3	1:C:132:GLU:HG3	1.95	0.49
1:A:22:LEU:CD1	1:A:94:ALA:CB	2.82	0.48
1:A:31:THR:O	1:A:32:VAL:HG23	2.13	0.48
1:A:130:ASN:HB3	1:A:132:GLU:HG3	1.95	0.48
1:A:203:SER:C	1:A:205:ASN:H	2.17	0.48
1:A:264:ASP:HB2	1:A:307:LYS:HD3	1.94	0.48
1:C:19:LYS:HD2	3:F:206:TRP:NE1	2.27	0.48
1:A:115:LYS:O	1:A:168:TRP:HZ3	1.96	0.48
1:A:420:GLU:CA	1:A:423:LYS:HE2	2.38	0.48
1:A:466:LEU:O	1:A:598:LYS:HE2	2.13	0.48
1:C:15:TRP:HZ3	1:C:307:LYS:O	1.96	0.48
1:C:19:LYS:C	1:C:21:PRO:HD3	2.33	0.48
1:C:75:LYS:HZ1	1:C:94:ALA:CB	2.25	0.48
1:C:154:GLY:O	1:C:155:GLN:CG	2.48	0.48
1:C:325:ILE:N	1:C:325:ILE:CD1	2.76	0.48
3:F:52:HIS:ND1	3:F:74:SER:HB2	2.28	0.48
3:F:75:TYR:C	3:F:77:GLY:H	2.17	0.48
1:A:19:LYS:C	1:A:21:PRO:HD3	2.33	0.48
1:A:151:LEU:CD1	1:A:152:THR:H	2.25	0.48
1:A:325:ILE:N	1:A:325:ILE:CD1	2.76	0.48
1:A:585:VAL:HA	1:A:596:ILE:HG21	1.95	0.48
1:A:593:TRP:C	1:A:595:PHE:N	2.66	0.48
2:B:119:ALA:HB1	2:B:148:VAL:HG12	1.96	0.48
2:B:184:ILE:N	2:B:184:ILE:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:ASP:O	1:C:460:GLU:HB2	2.14	0.48
1:A:124:LEU:CG	1:A:125:ALA:H	2.24	0.48
1:A:331:GLN:HG2	1:A:371:LEU:HD23	1.96	0.48
1:C:203:SER:C	1:C:205:ASN:H	2.16	0.48
1:C:219:PRO:HG3	1:C:266:CYS:O	2.14	0.48
1:C:264:ASP:HB2	1:C:307:LYS:HD3	1.94	0.48
1:C:331:GLN:HG2	1:C:371:LEU:HD23	1.96	0.48
1:A:29:SER:HB2	1:A:82:ASP:OD1	2.13	0.48
1:A:75:LYS:HD2	1:A:91:THR:HG22	1.95	0.48
1:A:86:LEU:HD23	1:A:104:PHE:HB2	1.96	0.48
1:A:514:ILE:HA	1:A:517:ASN:ND2	2.28	0.48
2:B:18:ASP:OD2	2:B:23:ARG:HB3	2.14	0.48
2:B:59:VAL:HA	2:B:71:ALA:O	2.14	0.48
1:C:284:LEU:HD23	1:C:371:LEU:HD11	1.95	0.48
1:C:728:SER:HB3	1:C:737:LYS:NZ	2.29	0.48
3:F:102:VAL:HA	3:F:120:SER:HA	1.96	0.48
3:F:108:ALA:HB3	3:F:115:MET:HB2	1.96	0.48
1:A:365:LYS:HZ3	1:A:371:LEU:HD22	1.77	0.48
1:A:644:VAL:HG11	1:A:684:PHE:CE2	2.48	0.48
2:B:37:GLU:HG2	2:B:46:ILE:CG1	2.44	0.48
2:B:108:ALA:HA	2:B:153:TRP:CD1	2.49	0.48
1:C:664:LYS:N	3:F:285:LEU:CD1	2.53	0.48
3:F:95:HIS:CE1	3:F:128:VAL:HG21	2.48	0.48
1:A:42:LEU:CD2	1:A:98:ILE:HD11	2.44	0.48
2:B:57:TRP:O	2:B:58:ARG:HG2	2.13	0.48
1:C:31:THR:O	1:C:32:VAL:HG23	2.13	0.48
1:C:33:ASP:OD1	1:C:37:SER:HB3	2.13	0.48
1:A:412:LEU:C	1:A:412:LEU:HD23	2.35	0.48
1:C:187:ILE:HB	1:C:197:ILE:HB	1.95	0.48
3:F:24:MET:O	3:F:61:TRP:HZ2	1.97	0.48
3:F:205:ASP:H	3:F:228:ASP:HB3	1.78	0.48
1:C:75:LYS:HD2	1:C:91:THR:HG22	1.95	0.47
3:F:196:LEU:CG	3:F:197:GLU:N	2.77	0.47
1:A:75:LYS:HZ1	1:A:94:ALA:CB	2.25	0.47
1:A:92:ASN:O	1:A:93:GLU:CB	2.62	0.47
2:B:172:LYS:HA	2:B:185:TRP:O	2.13	0.47
1:C:124:LEU:CG	1:C:125:ALA:N	2.76	0.47
1:C:271:HIS:CE1	1:C:288:GLU:OE2	2.67	0.47
1:C:514:ILE:HA	1:C:517:ASN:HD22	1.79	0.47
3:F:82:TRP:N	3:F:82:TRP:CD1	2.82	0.47
1:A:10:THR:O	1:A:11:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ASP:OD1	1:A:429:PRO:HD3	2.14	0.47
1:A:462:LEU:HD13	1:A:637:ALA:HB2	1.97	0.47
1:A:542:ILE:HD11	1:C:573:LEU:HD21	1.96	0.47
2:B:8:HIS:CE1	2:B:34:LYS:HE2	2.48	0.47
2:B:15:ALA:HA	2:B:25:ALA:O	2.14	0.47
2:B:34:LYS:HB3	2:B:36:PHE:HE1	1.80	0.47
2:B:259:ARG:HG3	2:B:259:ARG:NH1	2.30	0.47
1:C:268:GLN:CA	1:C:373:ALA:CB	2.80	0.47
1:C:364:GLU:O	1:C:365:LYS:CB	2.47	0.47
1:C:388:PHE:CE1	1:C:739:ARG:HD3	2.49	0.47
3:F:24:MET:HB3	3:F:36:PHE:HB2	1.96	0.47
3:F:109:PRO:HD2	3:F:112:TYR:CD2	2.49	0.47
3:F:157:THR:HB	3:F:170:SER:OG	2.13	0.47
1:A:7:PHE:HB2	1:A:8:SER:H	1.51	0.47
1:A:114:VAL:HA	1:A:125:ALA:O	2.14	0.47
1:A:219:PRO:HG3	1:A:266:CYS:O	2.13	0.47
2:B:212:TRP:CD2	2:B:222:LEU:HD21	2.49	0.47
1:C:16:SER:HB2	1:C:18:ASP:OD1	2.14	0.47
1:C:186:SER:HB3	1:C:188:TRP:NE1	2.29	0.47
1:C:553:GLU:HG2	1:C:557:ASN:ND2	2.28	0.47
3:F:131:LYS:HD2	3:F:135:THR:O	2.14	0.47
1:A:542:ILE:HD11	1:C:573:LEU:CD2	2.44	0.47
1:A:42:LEU:HD23	1:A:98:ILE:HD11	1.96	0.47
1:A:639:GLY:HA2	1:A:688:ILE:CD1	2.35	0.47
3:F:23:ARG:NH1	3:F:68:THR:HG21	2.29	0.47
1:A:15:TRP:CZ3	1:A:317:ALA:N	2.83	0.47
1:A:91:THR:HG22	1:A:91:THR:O	2.14	0.47
1:A:186:SER:HB3	1:A:188:TRP:NE1	2.29	0.47
1:A:271:HIS:CE1	1:A:288:GLU:OE2	2.67	0.47
1:A:336:THR:OG1	2:B:96:ALA:O	2.33	0.47
1:A:392:LEU:CD1	4:A:2219:HOH:O	2.61	0.47
2:B:31:LYS:O	4:B:1321:HOH:O	2.20	0.47
1:C:42:LEU:HD23	1:C:98:ILE:HD11	1.96	0.47
1:C:86:LEU:HD23	1:C:104:PHE:HB2	1.96	0.47
1:C:114:VAL:HA	1:C:125:ALA:O	2.14	0.47
1:C:412:LEU:CD2	1:C:713:THR:HG22	2.45	0.47
1:C:424:THR:O	1:C:425:LYS:CB	2.62	0.47
3:F:31:LYS:HB3	3:F:52:HIS:O	2.15	0.47
3:F:209:ASP:HB2	3:F:258:TRP:O	2.14	0.47
1:A:16:SER:HB2	1:A:18:ASP:OD1	2.14	0.47
1:A:364:GLU:O	1:A:365:LYS:CB	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:LYS:HB3	1:A:668:GLU:HB2	1.96	0.47
2:B:69:ILE:CG2	2:B:70:LEU:N	2.77	0.47
1:C:92:ASN:O	1:C:93:GLU:CB	2.62	0.47
1:C:313:PRO:HG2	4:C:1545:HOH:O	1.83	0.47
1:C:365:LYS:HZ3	1:C:371:LEU:HD22	1.79	0.47
1:C:727:PRO:C	1:C:729:ASP:N	2.67	0.47
1:C:731:GLU:HA	1:C:734:LYS:HB3	1.97	0.47
1:C:739:ARG:CD	3:F:19:TYR:CE2	2.71	0.47
3:F:124:LYS:HG2	3:F:142:ASP:OD1	2.15	0.47
3:F:146:ILE:HB	3:F:178:ALA:HB3	1.96	0.47
1:A:51:ASP:O	1:A:52:SER:C	2.54	0.47
1:A:202:THR:CG2	1:A:209:LYS:HD3	2.45	0.47
1:A:337:LEU:HD21	2:B:140:ILE:HD11	1.97	0.47
1:A:718:LEU:O	1:A:722:PHE:HD1	1.98	0.47
2:B:225:VAL:HG13	2:B:257:LEU:CB	2.43	0.47
1:C:42:LEU:CD2	1:C:98:ILE:HD11	2.44	0.47
1:C:172:LEU:C	1:C:174:HIS:N	2.69	0.47
1:A:572:ILE:CD1	1:C:504:PHE:HE2	2.28	0.47
1:C:312:ALA:O	1:C:314:ASP:N	2.48	0.47
3:F:210:VAL:HG23	3:F:210:VAL:O	2.14	0.47
2:B:72:SER:O	2:B:79:VAL:HG13	2.14	0.46
2:B:121:SER:HA	4:B:1338:HOH:O	2.15	0.46
1:C:10:THR:O	1:C:11:ALA:HB2	2.14	0.46
1:C:386:TRP:HZ3	4:C:1614:HOH:O	1.98	0.46
1:C:641:LEU:HD12	1:C:684:PHE:HE2	1.80	0.46
1:A:172:LEU:C	1:A:174:HIS:N	2.68	0.46
1:A:252:LEU:HD13	1:A:285:TRP:CB	2.45	0.46
1:A:739:ARG:HD2	2:B:19:TYR:CZ	2.50	0.46
2:B:109:PRO:HD2	2:B:112:TYR:CD2	2.50	0.46
2:B:124:LYS:HE2	2:B:142:ASP:OD1	2.15	0.46
1:C:202:THR:CG2	1:C:209:LYS:HD3	2.46	0.46
1:C:314:ASP:OD2	1:C:376:TRP:CH2	2.67	0.46
1:C:439:ILE:HG13	1:C:440:ASP:N	2.27	0.46
2:B:27:CYS:HB2	2:B:56:VAL:CG1	2.45	0.46
1:C:252:LEU:HD13	1:C:285:TRP:CB	2.45	0.46
3:F:99:SER:O	3:F:100:ALA:HB2	2.15	0.46
3:F:118:VAL:HB	3:F:126:SER:OG	2.15	0.46
1:A:68:LEU:HD22	1:A:77:ILE:HG22	1.98	0.46
2:B:93:ALA:HB1	4:B:1344:HOH:O	2.14	0.46
2:B:119:ALA:HB1	2:B:148:VAL:CG1	2.45	0.46
1:C:15:TRP:CZ3	1:C:317:ALA:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:THR:HG22	1:C:91:THR:O	2.14	0.46
1:C:203:SER:C	1:C:205:ASN:N	2.69	0.46
1:C:377:TYR:CA	4:C:1513:HOH:O	2.64	0.46
3:F:69:ILE:CG1	3:F:83:LYS:HG2	2.32	0.46
3:F:152:SER:CB	3:F:211:ALA:HA	2.45	0.46
3:F:226:SER:OG	3:F:227:GLN:N	2.49	0.46
1:A:593:TRP:O	1:A:595:PHE:N	2.48	0.46
2:B:29:SER:O	2:B:31:LYS:HG3	2.14	0.46
2:B:74:SER:CB	2:B:76:ASP:OD1	2.61	0.46
1:C:183:ASN:HA	1:C:211:GLN:HA	1.97	0.46
3:F:40:GLY:O	3:F:41:GLU:CG	2.62	0.46
3:F:75:TYR:O	3:F:77:GLY:N	2.49	0.46
3:F:194:TYR:H	3:F:194:TYR:HD1	1.63	0.46
1:A:608:ILE:CD1	1:A:611:ARG:NH1	2.78	0.46
2:B:117:LEU:HB2	2:B:153:TRP:NE1	2.31	0.46
1:C:45:TRP:CD1	1:C:45:TRP:N	2.84	0.46
1:C:169:ASN:HB3	1:C:172:LEU:O	2.16	0.46
3:F:141:ILE:HD13	3:F:141:ILE:O	2.14	0.46
1:A:68:LEU:HA	1:A:78:ALA:O	2.15	0.46
1:A:169:ASN:HB3	1:A:172:LEU:O	2.16	0.46
1:A:169:ASN:OD1	1:A:172:LEU:HB2	2.16	0.46
1:A:183:ASN:HA	1:A:211:GLN:HA	1.97	0.46
1:A:312:ALA:O	1:A:314:ASP:N	2.48	0.46
1:A:652:PHE:HB3	1:A:653:PRO:CD	2.44	0.46
1:C:68:LEU:HD22	1:C:77:ILE:HG22	1.98	0.46
1:C:458:THR:HG23	1:C:459:GLU:N	2.30	0.46
1:C:674:LEU:O	1:C:678:ILE:HD13	2.15	0.46
3:F:37:GLU:O	3:F:43:HIS:HA	2.15	0.46
1:A:219:PRO:HD3	1:A:265:TRP:CD1	2.51	0.46
2:B:200:LEU:HB3	2:B:234:TRP:CH2	2.50	0.46
1:C:51:ASP:O	1:C:52:SER:C	2.54	0.46
1:C:68:LEU:HA	1:C:78:ALA:O	2.16	0.46
1:C:204:PRO:C	1:C:206:SER:H	2.19	0.46
1:C:212:LEU:HD22	1:C:227:THR:HG22	1.98	0.46
1:A:45:TRP:CD1	1:A:45:TRP:N	2.84	0.46
1:A:663:ASN:CA	2:B:285:LEU:HD11	2.46	0.46
1:C:382:PRO:CB	3:F:278:VAL:HG23	2.46	0.46
1:C:432:ASN:O	1:C:436:VAL:HG23	2.16	0.46
3:F:14:ASP:HB3	3:F:27:CYS:SG	2.55	0.46
1:A:63:SER:HB3	1:A:82:ASP:HB2	1.98	0.46
1:A:259:GLY:HA3	1:A:278:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASP:OD2	1:A:281:THR:HG22	2.16	0.46
1:A:536:LEU:HD23	1:C:537:MET:CE	2.46	0.46
3:F:121:SER:C	3:F:123:GLY:H	2.20	0.46
3:F:200:LEU:HD13	3:F:234:TRP:CE3	2.51	0.46
2:B:127:VAL:HA	4:B:1340:HOH:O	2.15	0.45
1:C:438:VAL:HG23	1:C:443:ASN:ND2	2.30	0.45
3:F:216:VAL:HG12	3:F:216:VAL:O	2.15	0.45
1:A:127:GLY:HA2	1:A:132:GLU:O	2.16	0.45
1:A:162:GLU:HG3	1:A:164:ILE:HG23	1.99	0.45
1:A:441:ASP:HA	4:A:2212:HOH:O	2.15	0.45
2:B:30:ASP:OD1	2:B:30:ASP:C	2.55	0.45
2:B:239:GLU:HG3	4:B:1327:HOH:O	2.16	0.45
1:C:212:LEU:HB3	1:C:227:THR:HG23	1.98	0.45
1:C:268:GLN:HG3	1:C:313:PRO:CB	2.46	0.45
1:C:380:PRO:HG3	3:F:11:MET:HE1	1.93	0.45
1:A:371:LEU:O	1:A:372:GLN:C	2.55	0.45
2:B:284:ASN:HB2	4:B:1352:HOH:O	2.16	0.45
1:C:279:ASP:OD2	1:C:281:THR:HG22	2.15	0.45
3:F:120:SER:O	3:F:148:VAL:HG23	2.16	0.45
3:F:255:ASP:HB2	3:F:275:ASP:HB3	1.98	0.45
3:F:284:ASN:HB3	3:F:290:GLU:CD	2.36	0.45
1:A:337:LEU:HD21	2:B:97:VAL:HG11	1.97	0.45
1:A:564:GLY:HA2	1:A:570:SER:OG	2.16	0.45
1:C:219:PRO:HD3	1:C:265:TRP:CD1	2.51	0.45
1:C:259:GLY:HA3	1:C:278:ARG:NH1	2.31	0.45
1:C:260:ILE:HG23	1:C:261:LEU:N	2.31	0.45
1:C:590:VAL:O	1:C:590:VAL:CG1	2.64	0.45
1:C:596:ILE:O	1:C:600:ILE:HG13	2.16	0.45
1:A:86:LEU:HD21	1:A:104:PHE:HB2	1.99	0.45
1:A:221:ASN:C	1:A:221:ASN:ND2	2.69	0.45
1:A:559:TYR:CE2	1:C:541:VAL:HG21	2.52	0.45
1:C:15:TRP:CH2	1:C:317:ALA:HB2	2.52	0.45
1:C:622:LEU:O	1:C:627:HIS:HB2	2.16	0.45
3:F:46:ILE:CG2	3:F:47:ASP:N	2.66	0.45
1:A:15:TRP:CH2	1:A:317:ALA:HB2	2.52	0.45
1:A:392:LEU:HA	4:A:2219:HOH:O	2.16	0.45
1:A:504:PHE:CZ	1:C:588:LEU:HD13	2.52	0.45
1:A:573:LEU:HD23	1:C:518:LEU:CD1	2.47	0.45
1:A:581:VAL:HG11	1:A:600:ILE:HD13	1.98	0.45
2:B:35:ILE:HG13	2:B:89:TRP:CE2	2.51	0.45
1:C:641:LEU:HD12	1:C:684:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:85:GLU:HG2	3:F:86:ASN:ND2	2.31	0.45
3:F:271:LEU:HD12	3:F:271:LEU:HA	1.57	0.45
1:A:155:GLN:HB2	1:A:195:GLU:HB3	1.99	0.45
1:A:204:PRO:C	1:A:206:SER:H	2.19	0.45
1:A:543:ALA:C	1:A:545:ASP:H	2.19	0.45
1:A:601:GLN:HE22	1:A:611:ARG:HD3	1.82	0.45
1:A:688:ILE:HG12	1:A:689:ASN:H	1.82	0.45
1:C:197:ILE:HG22	1:C:198:HIS:N	2.32	0.45
1:C:221:ASN:C	1:C:221:ASN:ND2	2.69	0.45
1:C:249:LEU:HD23	1:C:249:LEU:C	2.38	0.45
2:B:105:VAL:HG22	2:B:116:LEU:HD11	1.99	0.45
1:C:232:ASP:O	1:C:258:LYS:HA	2.17	0.45
1:C:438:VAL:HG21	1:C:444:GLU:HA	1.97	0.45
1:C:665:THR:CG2	3:F:285:LEU:N	2.80	0.45
1:A:75:LYS:NZ	1:A:94:ALA:CB	2.80	0.45
1:C:5:ALA:N	4:C:2426:HOH:O	2.49	0.45
1:C:169:ASN:OD1	1:C:172:LEU:HB2	2.16	0.45
3:F:196:LEU:CD1	3:F:197:GLU:H	2.30	0.45
3:F:274:GLY:C	3:F:276:ASN:N	2.67	0.45
1:A:289:SER:O	1:A:290:ALA:CB	2.65	0.44
1:A:333:LEU:CD2	4:B:1298:HOH:O	2.13	0.44
1:A:436:VAL:O	1:A:436:VAL:HG12	2.16	0.44
2:B:29:SER:C	2:B:31:LYS:N	2.70	0.44
1:C:66:ASN:HD22	1:C:66:ASN:HA	1.64	0.44
1:C:155:GLN:HB2	1:C:195:GLU:HB3	1.99	0.44
1:C:431:ILE:HD13	1:C:447:TRP:HZ3	1.82	0.44
1:C:727:PRO:O	1:C:729:ASP:N	2.50	0.44
3:F:179:ASP:C	3:F:180:ASN:HD22	2.20	0.44
1:A:5:ALA:N	4:A:1426:HOH:O	2.49	0.44
1:A:212:LEU:HB3	1:A:227:THR:HG23	1.98	0.44
1:A:232:ASP:O	1:A:258:LYS:HA	2.17	0.44
1:A:260:ILE:HG23	1:A:261:LEU:N	2.31	0.44
2:B:30:ASP:OD1	2:B:32:THR:HG23	2.17	0.44
2:B:213:SER:HB2	2:B:262:TRP:CE2	2.53	0.44
1:C:72:HIS:HE1	1:C:118:ALA:HA	1.72	0.44
1:A:75:LYS:HZ1	1:A:94:ALA:N	2.06	0.44
1:A:212:LEU:HD22	1:A:227:THR:HG22	1.98	0.44
1:A:232:ASP:HA	1:A:259:GLY:H	1.83	0.44
1:A:584:LEU:N	1:A:584:LEU:CD1	2.81	0.44
2:B:66:PHE:CD1	2:B:114:PRO:HB3	2.51	0.44
1:C:127:GLY:HA2	1:C:132:GLU:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:SER:O	1:C:290:ALA:CB	2.65	0.44
3:F:38:VAL:HA	3:F:42:THR:O	2.18	0.44
3:F:59:VAL:HG12	3:F:72:SER:CB	2.46	0.44
1:A:88:LEU:CD1	1:A:138:MET:SD	3.06	0.44
1:A:129:ASN:HA	1:A:162:GLU:CB	2.47	0.44
1:A:399:GLY:O	2:B:11:LEU:HD12	2.17	0.44
1:A:423:LYS:HG3	1:A:424:THR:N	2.33	0.44
2:B:74:SER:C	2:B:76:ASP:N	2.71	0.44
1:C:78:ALA:HB3	1:C:114:VAL:CG1	2.45	0.44
1:C:155:GLN:HB3	1:C:195:GLU:HB3	1.99	0.44
1:C:371:LEU:O	1:C:372:GLN:C	2.55	0.44
3:F:52:HIS:ND1	3:F:74:SER:CB	2.81	0.44
1:A:119:LYS:CB	1:A:173:ALA:HB2	2.41	0.44
1:A:242:LEU:N	1:A:242:LEU:HD23	2.33	0.44
1:A:449:LEU:O	1:A:453:LEU:HB2	2.17	0.44
1:A:604:TYR:N	1:A:605:PRO:CD	2.81	0.44
1:A:688:ILE:CG1	1:A:689:ASN:H	2.31	0.44
2:B:4:ILE:HG21	2:B:36:PHE:CE2	2.52	0.44
1:C:232:ASP:HA	1:C:259:GLY:H	1.83	0.44
1:C:242:LEU:N	1:C:242:LEU:HD23	2.33	0.44
3:F:184:ILE:O	3:F:196:LEU:HD12	2.18	0.44
1:A:511:GLU:HG2	1:C:569:LEU:HB2	1.99	0.44
2:B:85:GLU:O	2:B:86:ASN:HB2	2.18	0.44
1:C:27:THR:O	1:C:65:PHE:HB2	2.17	0.44
1:C:63:SER:HB3	1:C:82:ASP:HB2	1.98	0.44
1:C:117:ASN:HD22	1:C:117:ASN:C	2.17	0.44
1:C:162:GLU:HG3	1:C:164:ILE:CG2	2.48	0.44
3:F:63:HIS:HB3	3:F:66:PHE:CE1	2.53	0.44
3:F:72:SER:O	3:F:79:VAL:HA	2.17	0.44
2:B:274:GLY:C	2:B:276:ASN:N	2.69	0.44
1:C:86:LEU:HD21	1:C:104:PHE:HB2	1.99	0.44
1:C:204:PRO:HG2	1:C:208:ILE:O	2.18	0.44
1:A:197:ILE:HG22	1:A:198:HIS:N	2.32	0.44
1:A:379:GLU:HG2	2:B:258:TRP:CZ2	2.53	0.44
1:A:496:THR:CG2	1:A:497:ASN:N	2.81	0.44
2:B:191:ALA:HB1	2:B:193:THR:HG22	1.99	0.44
1:C:20:ILE:O	1:C:20:ILE:CG1	2.65	0.44
1:C:116:PHE:CE1	1:C:124:LEU:HD13	2.53	0.44
1:A:105:SER:C	1:A:107:HIS:N	2.71	0.44
1:A:155:GLN:HB3	1:A:195:GLU:HB3	1.99	0.44
1:A:162:GLU:HG3	1:A:164:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLN:NE2	4:A:2118:HOH:O	2.51	0.44
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.69	0.44
1:A:537:MET:CE	1:C:536:LEU:HD23	2.48	0.44
2:B:63:HIS:CE1	2:B:65:LYS:HB3	2.53	0.44
2:B:181:LEU:CD2	2:B:201:GLU:HG2	2.47	0.44
1:C:151:LEU:CD1	1:C:152:THR:H	2.25	0.44
1:C:162:GLU:HG3	1:C:164:ILE:HG23	1.99	0.44
3:F:259:ARG:HG3	3:F:259:ARG:NH1	2.33	0.44
1:A:24:VAL:CG2	1:A:70:TRP:CZ3	3.01	0.43
1:A:67:ASP:OD2	1:A:113:THR:HG23	2.18	0.43
1:A:232:ASP:HA	1:A:259:GLY:N	2.33	0.43
1:C:42:LEU:O	1:C:42:LEU:HG	2.18	0.43
1:C:313:PRO:HD3	4:C:1546:HOH:O	2.13	0.43
1:C:608:ILE:HD13	1:C:611:ARG:NH1	2.33	0.43
1:A:20:ILE:O	1:A:20:ILE:CG1	2.65	0.43
1:A:27:THR:O	1:A:65:PHE:HB2	2.17	0.43
1:A:42:LEU:O	1:A:42:LEU:HG	2.18	0.43
1:A:116:PHE:CE1	1:A:124:LEU:HD13	2.53	0.43
2:B:14:ASP:HB3	2:B:27:CYS:SG	2.58	0.43
1:C:232:ASP:HA	1:C:259:GLY:N	2.33	0.43
1:C:312:ALA:N	1:C:313:PRO:CD	2.80	0.43
1:C:639:GLY:HA2	1:C:688:ILE:CD1	2.47	0.43
3:F:233:ILE:HG21	3:F:289:TRP:HZ2	1.82	0.43
3:F:240:GLN:O	3:F:241:GLY:C	2.55	0.43
1:A:62:ASP:OD1	1:A:62:ASP:N	2.36	0.43
1:A:249:LEU:HD23	1:A:249:LEU:C	2.38	0.43
1:A:438:VAL:CG2	1:A:439:ILE:N	2.81	0.43
1:A:504:PHE:CE2	1:C:588:LEU:HD13	2.53	0.43
1:C:119:LYS:CB	1:C:173:ALA:HB2	2.41	0.43
1:C:313:PRO:HG2	1:C:376:TRP:NE1	2.34	0.43
1:C:614:MET:HA	1:C:614:MET:HE2	2.01	0.43
3:F:26:THR:O	3:F:33:ILE:HA	2.18	0.43
1:A:429:PRO:HD2	4:A:2159:HOH:O	2.19	0.43
1:A:549:GLU:HA	1:A:552:LYS:HB3	2.01	0.43
2:B:64:PRO:HD2	4:B:1334:HOH:O	2.17	0.43
2:B:238:ASN:ND2	2:B:240:GLN:H	2.15	0.43
1:C:24:VAL:CG2	1:C:70:TRP:CZ3	3.01	0.43
1:C:67:ASP:OD2	1:C:113:THR:HG23	2.18	0.43
1:C:252:LEU:HD13	1:C:285:TRP:CD2	2.53	0.43
1:A:22:LEU:HD21	1:A:95:ASN:ND2	2.33	0.43
1:A:78:ALA:HB3	1:A:114:VAL:CG1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:PRO:HG2	1:A:208:ILE:O	2.18	0.43
1:A:706:PHE:CB	4:A:2200:HOH:O	2.66	0.43
2:B:102:VAL:HG22	4:B:1353:HOH:O	2.14	0.43
2:B:112:TYR:N	2:B:112:TYR:CD1	2.86	0.43
2:B:255:ASP:CG	2:B:256:VAL:N	2.72	0.43
2:B:281:TRP:CD1	2:B:281:TRP:N	2.87	0.43
1:C:412:LEU:HD21	1:C:713:THR:HG22	2.01	0.43
1:C:420:GLU:HA	1:C:423:LYS:HD3	2.01	0.43
1:C:519:VAL:O	1:C:521:GLY:N	2.51	0.43
3:F:224:SER:HB2	3:F:234:TRP:NE1	2.28	0.43
1:A:551:LEU:C	1:A:553:GLU:N	2.71	0.43
1:C:196:VAL:O	1:C:197:ILE:HG13	2.19	0.43
1:C:424:THR:O	1:C:425:LYS:HB3	2.18	0.43
1:A:120:GLN:C	1:A:122:ASN:H	2.22	0.43
1:A:133:ILE:HD11	1:A:163:VAL:CG2	2.41	0.43
1:A:201:TYR:CD2	1:A:238:LEU:HD11	2.54	0.43
1:A:422:LEU:CD2	1:A:721:GLU:HG2	2.49	0.43
1:C:22:LEU:HD21	1:C:95:ASN:ND2	2.33	0.43
1:C:677:PHE:HD2	1:C:678:ILE:HD12	1.83	0.43
3:F:219:ARG:CG	3:F:221:TYR:CE1	3.02	0.43
3:F:233:ILE:HD11	3:F:248:LEU:CD1	2.48	0.43
1:A:203:SER:C	1:A:205:ASN:N	2.69	0.43
1:A:312:ALA:N	1:A:313:PRO:CD	2.80	0.43
1:A:314:ASP:CB	1:A:376:TRP:CZ2	3.02	0.43
2:B:25:ALA:HB2	2:B:61:TRP:HZ2	1.81	0.43
2:B:46:ILE:HG22	2:B:46:ILE:O	2.19	0.43
2:B:107:TRP:CH2	2:B:130:PHE:HE2	2.37	0.43
2:B:227:GLN:HA	2:B:256:VAL:HG13	2.01	0.43
1:C:120:GLN:C	1:C:122:ASN:H	2.22	0.43
1:C:636:LEU:HD12	1:C:688:ILE:CD1	2.48	0.43
3:F:213:SER:OG	3:F:214:PRO:HD2	2.19	0.43
1:A:302:TRP:CD1	1:A:321:PHE:CD1	3.07	0.43
1:A:727:PRO:C	1:A:729:ASP:N	2.69	0.43
2:B:226:SER:HB3	2:B:228:ASP:OD1	2.19	0.43
1:C:78:ALA:CB	1:C:114:VAL:CG1	2.95	0.43
1:C:223:THR:O	1:C:241:ASP:HA	2.19	0.43
1:C:536:LEU:O	1:C:537:MET:C	2.57	0.43
2:B:18:ASP:CG	2:B:23:ARG:HB3	2.39	0.42
1:C:93:GLU:O	1:C:94:ALA:C	2.57	0.42
3:F:39:GLU:HB2	3:F:42:THR:OG1	2.19	0.42
1:A:211:GLN:O	1:A:229:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:TYR:CD2	1:C:238:LEU:HD11	2.54	0.42
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.69	0.42
1:C:664:LYS:C	3:F:285:LEU:HD11	2.38	0.42
1:C:666:ILE:HD13	1:C:666:ILE:HA	1.93	0.42
3:F:3:VAL:HG12	3:F:5:ALA:N	2.34	0.42
3:F:201:GLU:O	3:F:234:TRP:HH2	2.02	0.42
1:A:27:THR:HB	1:A:40:SER:HB2	2.01	0.42
1:A:93:GLU:O	1:A:94:ALA:C	2.57	0.42
1:A:125:ALA:HB2	1:A:168:TRP:CZ3	2.53	0.42
1:A:196:VAL:O	1:A:197:ILE:HG13	2.19	0.42
1:A:204:PRO:HG3	1:A:210:GLN:HG3	2.00	0.42
1:A:299:ARG:HD2	1:A:299:ARG:HA	1.86	0.42
2:B:63:HIS:CD2	2:B:110:HIS:HB3	2.54	0.42
2:B:87:GLY:C	2:B:88:ARG:HG3	2.39	0.42
1:C:314:ASP:CG	1:C:376:TRP:CD2	2.80	0.42
1:C:571:ARG:O	1:C:574:TYR:HB3	2.19	0.42
1:C:590:VAL:HG13	1:C:622:LEU:HD22	1.99	0.42
1:C:661:LYS:C	1:C:663:ASN:N	2.72	0.42
2:B:152:SER:OG	2:B:210:VAL:O	2.33	0.42
1:C:29:SER:OG	1:C:66:ASN:ND2	2.53	0.42
1:C:88:LEU:CD1	1:C:138:MET:SD	3.06	0.42
1:C:105:SER:C	1:C:107:HIS:N	2.71	0.42
1:C:129:ASN:HA	1:C:162:GLU:CB	2.47	0.42
1:C:420:GLU:HA	1:C:423:LYS:CD	2.50	0.42
3:F:62:ALA:HB2	3:F:107:TRP:CE2	2.55	0.42
1:A:223:THR:O	1:A:241:ASP:HA	2.19	0.42
1:A:497:ASN:OD1	1:A:498:PHE:N	2.53	0.42
1:A:608:ILE:HA	1:A:611:ARG:NH1	2.34	0.42
1:C:6:GLU:OE2	1:C:324:LYS:HB2	2.20	0.42
1:C:589:ASP:C	1:C:591:SER:H	2.23	0.42
3:F:250:GLU:C	3:F:251:GLU:OE1	2.58	0.42
1:A:15:TRP:HZ3	1:A:317:ALA:H	1.67	0.42
1:A:70:TRP:C	1:A:71:SER:O	2.55	0.42
1:A:252:LEU:HD13	1:A:285:TRP:CD2	2.53	0.42
1:A:268:GLN:CA	1:A:374:PRO:O	2.63	0.42
1:A:330:LEU:HD12	1:A:330:LEU:HA	1.87	0.42
1:A:540:MET:HB2	1:C:540:MET:HE1	2.01	0.42
1:C:70:TRP:C	1:C:71:SER:O	2.55	0.42
1:C:215:VAL:HA	1:C:226:ALA:O	2.20	0.42
3:F:35:ILE:HG13	3:F:89:TRP:NE1	2.35	0.42
1:A:399:GLY:HA3	2:B:11:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:O	1:A:423:LYS:HG2	2.20	0.42
1:A:694:ILE:HG23	1:A:699:LEU:HD23	2.02	0.42
1:C:9:ARG:HB3	1:C:10:THR:H	1.65	0.42
1:C:211:GLN:O	1:C:229:THR:HA	2.19	0.42
1:C:272:LEU:HD23	1:C:272:LEU:HA	1.81	0.42
1:A:202:THR:O	1:A:202:THR:CG2	2.67	0.42
1:A:237:ILE:N	1:A:237:ILE:HD12	2.35	0.42
1:A:388:PHE:CE2	1:A:716:PHE:HE2	2.37	0.42
1:A:610:GLN:OE1	1:A:610:GLN:HA	2.20	0.42
1:C:133:ILE:HD11	1:C:163:VAL:CG2	2.41	0.42
1:C:204:PRO:HG3	1:C:210:GLN:HG3	2.00	0.42
1:C:302:TRP:CD1	1:C:321:PHE:CD1	3.07	0.42
1:C:379:GLU:HB3	3:F:258:TRP:CZ2	2.54	0.42
1:C:493:GLN:HG3	1:C:494:ILE:N	2.35	0.42
3:F:23:ARG:HD3	3:F:61:TRP:CH2	2.54	0.42
3:F:68:THR:HG22	3:F:89:TRP:CH2	2.54	0.42
3:F:194:TYR:CD1	3:F:194:TYR:N	2.88	0.42
3:F:231:CYS:HB2	3:F:271:LEU:HD21	2.00	0.42
3:F:262:TRP:CE3	3:F:262:TRP:HA	2.55	0.42
1:A:66:ASN:HD22	1:A:66:ASN:HA	1.64	0.42
1:A:261:LEU:N	1:A:277:GLY:HA2	2.35	0.42
1:A:500:PRO:O	1:A:501:GLU:HG2	2.20	0.42
1:A:519:VAL:O	1:A:521:GLY:N	2.52	0.42
2:B:30:ASP:OD1	2:B:32:THR:OG1	2.36	0.42
2:B:213:SER:HB2	2:B:262:TRP:CD2	2.55	0.42
1:C:62:ASP:OD1	1:C:62:ASP:N	2.36	0.42
1:C:202:THR:O	1:C:202:THR:CG2	2.67	0.42
3:F:213:SER:OG	3:F:215:THR:HG22	2.20	0.42
1:A:29:SER:OG	1:A:66:ASN:ND2	2.53	0.42
1:A:152:THR:HA	1:A:153:PRO:HD3	1.81	0.42
1:A:431:ILE:HG21	1:A:451:GLU:HA	2.02	0.42
1:A:447:TRP:O	1:A:451:GLU:N	2.53	0.42
1:A:706:PHE:HB2	4:A:2200:HOH:O	2.19	0.42
2:B:52:HIS:CD2	2:B:56:VAL:HG22	2.55	0.42
1:C:7:PHE:HB2	1:C:8:SER:H	1.51	0.42
1:C:247:THR:HG23	1:C:248:PRO:HD2	2.02	0.42
1:C:438:VAL:HG21	1:C:444:GLU:CA	2.50	0.42
3:F:33:ILE:HD13	3:F:72:SER:HB3	2.02	0.42
3:F:102:VAL:HG22	3:F:120:SER:HB2	2.02	0.42
3:F:105:VAL:HG21	3:F:116:LEU:HD21	2.02	0.42
3:F:232:ILE:HG21	3:F:234:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ALA:CB	1:A:168:TRP:CH2	2.92	0.41
1:A:598:LYS:O	1:A:602:ASN:HB2	2.20	0.41
1:A:644:VAL:HG21	1:A:684:PHE:CZ	2.55	0.41
1:A:733:VAL:HG13	4:A:2255:HOH:O	2.19	0.41
2:B:121:SER:CA	4:B:1338:HOH:O	2.68	0.41
1:C:7:PHE:CD1	1:C:7:PHE:N	2.87	0.41
1:C:31:THR:OG1	1:C:321:PHE:HD2	2.03	0.41
1:C:380:PRO:HG3	3:F:11:MET:HE2	1.96	0.41
1:C:447:TRP:CE3	1:C:450:LEU:HD12	2.55	0.41
3:F:60:ASP:O	3:F:107:TRP:NE1	2.52	0.41
1:A:247:THR:HG23	1:A:248:PRO:HD2	2.02	0.41
1:A:268:GLN:CD	4:A:2118:HOH:O	2.36	0.41
1:A:538:GLU:OE1	1:A:538:GLU:N	2.43	0.41
1:C:261:LEU:N	1:C:277:GLY:HA2	2.35	0.41
1:A:458:THR:CG2	1:A:459:GLU:N	2.81	0.41
1:A:519:VAL:C	1:A:521:GLY:N	2.71	0.41
1:C:187:ILE:HD13	1:C:187:ILE:HA	1.88	0.41
1:C:271:HIS:HB3	1:C:286:ASN:OD1	2.21	0.41
3:F:49:LEU:HD22	3:F:82:TRP:CG	2.55	0.41
3:F:120:SER:OG	3:F:121:SER:N	2.53	0.41
1:A:6:GLU:OE2	1:A:324:LYS:HB2	2.20	0.41
1:A:404:ILE:N	1:A:404:ILE:HD12	2.34	0.41
1:A:563:TYR:C	1:A:565:SER:H	2.24	0.41
2:B:49:LEU:HA	4:B:1355:HOH:O	2.20	0.41
2:B:233:ILE:HD12	2:B:233:ILE:N	2.35	0.41
1:C:27:THR:HB	1:C:40:SER:HB2	2.01	0.41
1:C:252:LEU:HB3	1:C:285:TRP:CE3	2.55	0.41
1:C:572:ILE:HG22	1:C:573:LEU:N	2.35	0.41
1:A:215:VAL:HA	1:A:226:ALA:O	2.20	0.41
1:A:444:GLU:HG2	1:A:448:ASN:ND2	2.36	0.41
2:B:225:VAL:CG2	2:B:271:LEU:HD11	2.50	0.41
1:C:214:VAL:HB	1:C:228:ALA:HB3	2.03	0.41
1:C:331:GLN:NE2	3:F:75:TYR:CZ	2.88	0.41
3:F:112:TYR:HA	3:F:171:ARG:NH2	2.36	0.41
1:A:412:LEU:HD23	1:A:413:GLU:N	2.36	0.41
2:B:4:ILE:N	2:B:4:ILE:CD1	2.83	0.41
2:B:225:VAL:CG1	2:B:257:LEU:O	2.69	0.41
1:C:377:TYR:CD2	3:F:75:TYR:CE1	3.09	0.41
1:A:96:ASN:O	1:A:97:ALA:HB2	2.21	0.41
1:A:229:THR:HG22	1:A:230:GLY:N	2.35	0.41
1:A:396:THR:HB	1:A:398:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LYS:HD3	1:A:580:GLU:OE2	2.20	0.41
1:C:193:LYS:O	1:C:194:LYS:CB	2.65	0.41
1:A:252:LEU:HB3	1:A:285:TRP:CE3	2.55	0.41
2:B:46:ILE:O	2:B:47:ASP:HB2	2.21	0.41
2:B:238:ASN:HB2	4:B:1327:HOH:O	2.20	0.41
1:C:96:ASN:O	1:C:97:ALA:HB2	2.21	0.41
1:C:237:ILE:N	1:C:237:ILE:HD12	2.35	0.41
1:C:497:ASN:CG	1:C:497:ASN:O	2.59	0.41
3:F:58:ARG:HE	3:F:58:ARG:HB2	1.60	0.41
1:A:9:ARG:HA	1:A:324:LYS:HA	2.02	0.41
1:A:31:THR:OG1	1:A:321:PHE:HD2	2.03	0.41
1:A:127:GLY:HA3	1:A:163:VAL:HB	2.03	0.41
1:A:268:GLN:NE2	1:A:313:PRO:CD	2.69	0.41
1:A:271:HIS:HB3	1:A:286:ASN:OD1	2.21	0.41
1:A:329:THR:C	1:A:331:GLN:N	2.73	0.41
1:A:434:ARG:HG3	1:A:447:TRP:CH2	2.55	0.41
1:A:502:GLY:O	1:C:587:ASN:HB3	2.21	0.41
1:A:595:PHE:C	1:A:597:SER:N	2.72	0.41
2:B:16:VAL:HG12	2:B:61:TRP:HD1	1.85	0.41
2:B:282:LYS:HB3	2:B:292:ALA:HB2	2.02	0.41
1:C:41:SER:O	1:C:42:LEU:CB	2.67	0.41
1:C:75:LYS:HZ2	1:C:94:ALA:N	2.17	0.41
1:C:124:LEU:HB2	1:C:138:MET:HE3	2.03	0.41
3:F:4:ILE:N	3:F:4:ILE:CD1	2.84	0.41
3:F:30:ASP:O	3:F:31:LYS:HB2	2.21	0.41
3:F:152:SER:O	3:F:173:PHE:HB2	2.21	0.41
1:C:129:ASN:C	1:C:131:GLY:N	2.74	0.41
1:C:217:TRP:CE3	1:C:225:VAL:HG22	2.56	0.41
1:C:439:ILE:CG1	1:C:440:ASP:H	2.28	0.41
1:A:19:LYS:HD3	1:A:311:GLU:HG3	2.03	0.40
1:A:244:ASN:C	1:A:244:ASN:HD22	2.24	0.40
1:A:428:LYS:CB	1:A:429:PRO:HD3	2.37	0.40
1:A:592:GLN:O	1:A:595:PHE:HB3	2.21	0.40
2:B:17:LEU:HD23	2:B:24:LEU:HA	2.03	0.40
2:B:145:ALA:O	2:B:147:GLY:N	2.50	0.40
1:C:15:TRP:HZ3	1:C:317:ALA:H	1.67	0.40
1:C:127:GLY:HA3	1:C:163:VAL:HB	2.03	0.40
1:C:229:THR:HG22	1:C:230:GLY:N	2.35	0.40
1:A:7:PHE:CD1	1:A:7:PHE:N	2.87	0.40
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.81	0.40
1:A:421:ALA:O	1:A:425:LYS:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ILE:HG13	1:A:440:ASP:H	1.85	0.40
1:C:9:ARG:HA	1:C:324:LYS:HA	2.02	0.40
1:C:289:SER:HG	1:C:291:GLU:HG3	1.87	0.40
1:C:702:LYS:HA	1:C:705:GLU:HB2	2.03	0.40
3:F:59:VAL:HG12	3:F:72:SER:CA	2.50	0.40
1:A:497:ASN:O	1:A:498:PHE:HB3	2.20	0.40
1:C:125:ALA:HB2	1:C:168:TRP:CZ3	2.53	0.40
1:C:438:VAL:HG22	1:C:439:ILE:N	2.36	0.40
1:C:569:LEU:O	1:C:573:LEU:HG	2.21	0.40
3:F:10:GLU:HG3	3:F:30:ASP:CA	2.51	0.40
1:A:83:ASN:O	1:A:84:GLY:C	2.59	0.40
2:B:23:ARG:NH1	2:B:68:THR:CG2	2.83	0.40
2:B:78:LYS:HG2	2:B:96:ALA:CB	2.52	0.40
2:B:87:GLY:O	2:B:88:ARG:HG3	2.21	0.40
2:B:212:TRP:HA	2:B:222:LEU:HD23	2.02	0.40
1:C:314:ASP:N	1:C:376:TRP:HE1	2.20	0.40
3:F:115:MET:HE3	3:F:153:TRP:CZ2	2.56	0.40
1:A:84:GLY:HA2	1:A:111:VAL:HG23	2.03	0.40
1:A:116:PHE:CD1	1:A:124:LEU:HD13	2.57	0.40
1:A:187:ILE:HD13	1:A:187:ILE:HA	1.88	0.40
1:A:217:TRP:CE3	1:A:225:VAL:HG22	2.56	0.40
1:A:218:HIS:CE1	1:A:221:ASN:H	2.40	0.40
1:A:517:ASN:ND2	1:A:529:ASN:ND2	2.63	0.40
1:A:653:PRO:O	1:A:656:GLU:N	2.54	0.40
2:B:17:LEU:HB3	2:B:21:GLY:HA2	2.03	0.40
2:B:69:ILE:HA	2:B:82:TRP:O	2.22	0.40
2:B:143:ALA:O	2:B:144:HIS:CG	2.75	0.40
1:C:113:THR:CG2	1:C:114:VAL:N	2.84	0.40
1:C:400:LYS:HA	3:F:12:ILE:HG13	2.04	0.40
1:C:412:LEU:C	1:C:412:LEU:HD23	2.41	0.40
1:C:592:GLN:NE2	4:C:1629:HOH:O	2.53	0.40
1:C:652:PHE:CE2	1:C:702:LYS:HE2	2.56	0.40
3:F:4:ILE:HG13	3:F:43:HIS:HB3	2.03	0.40
3:F:105:VAL:HG13	3:F:105:VAL:O	2.21	0.40
3:F:247:LEU:C	3:F:249:LYS: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	681/1273 (54%)	518 (76%)	107 (16%)	56 (8%)	1 12
1	C	683/1273 (54%)	532 (78%)	97 (14%)	54 (8%)	1 13
2	B	275/291 (94%)	241 (88%)	30 (11%)	4 (2%)	10 46
3	F	276/291 (95%)	214 (78%)	37 (13%)	25 (9%)	1 11
All	All	1915/3128 (61%)	1505 (79%)	271 (14%)	139 (7%)	2 14

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	49	ALA
1	A	74	ASN
1	A	110	SER
1	A	143	GLU
1	A	146	SER
1	A	147	ASN
1	A	159	SER
1	A	203	SER
1	A	242	LEU
1	A	290	ALA
1	A	301	ASN
1	A	313	PRO
1	A	335	ASN
1	A	336	THR
1	A	365	LYS
1	A	369	PHE
1	A	497	ASN
2	B	131	LYS
1	C	33	ASP
1	C	49	ALA
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	110	SER
1	C	143	GLU
1	C	146	SER
1	C	147	ASN
1	C	159	SER
1	C	203	SER
1	C	242	LEU
1	C	290	ALA
1	C	301	ASN
1	C	313	PRO
1	C	335	ASN
1	C	336	THR
1	C	365	LYS
1	C	369	PHE
1	C	715	ASN
3	F	76	ASP
3	F	100	ALA
3	F	131	LYS
1	A	10	THR
1	A	84	GLY
1	A	105	SER
1	A	160	VAL
1	A	194	LYS
1	A	238	LEU
1	A	266	CYS
1	A	322	ASP
1	A	332	ASN
1	A	337	LEU
1	A	388	PHE
1	A	425	LYS
1	A	518	LEU
2	B	135	THR
1	C	10	THR
1	C	84	GLY
1	C	105	SER
1	C	160	VAL
1	C	194	LYS
1	C	238	LEU
1	C	266	CYS
1	C	322	ASP
1	C	332	ASN
1	C	337	LEU

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Mol	Chain	Res	Type
1	C	425	LYS
3	F	30	ASP
3	F	41	GLU
3	F	133	ASN
3	F	241	GLY
3	F	254	PRO
3	F	256	VAL
3	F	273	GLY
1	A	16	SER
1	A	52	SER
1	A	60	GLN
1	A	93	GLU
1	A	121	ASP
1	A	153	PRO
1	A	204	PRO
1	A	299	ARG
1	A	363	LYS
1	A	520	SER
1	A	728	SER
2	B	190	ASP
1	C	16	SER
1	C	52	SER
1	C	60	GLN
1	C	93	GLU
1	C	121	ASP
1	C	153	PRO
1	C	204	PRO
1	C	299	ARG
1	C	363	LYS
1	C	439	ILE
1	C	552	LYS
1	C	728	SER
3	F	40	GLY
3	F	47	ASP
3	F	101	SER
3	F	145	ALA
3	F	240	GLN
3	F	291	PRO
1	A	91	THR
1	A	148	TYR
1	A	302	TRP
1	A	368	VAL

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Mol	Chain	Res	Type
1	A	439	ILE
1	A	498	PHE
1	A	561	ALA
2	B	202	GLY
1	C	91	THR
1	C	148	TYR
1	C	302	TRP
1	C	368	VAL
1	C	407	PRO
3	F	46	ILE
3	F	218	LEU
3	F	267	ASN
3	F	274	GLY
1	A	9	ARG
1	A	94	ALA
1	A	109	SER
1	A	207	GLY
1	A	548	ASN
1	A	653	PRO
1	C	9	ARG
1	C	94	ALA
1	C	109	SER
1	C	207	GLY
1	C	520	SER
1	C	662	ASP
3	F	51	GLY
3	F	170	SER
3	F	187	TYR
3	F	21	GLY
3	F	287	GLY
1	A	287	PRO
1	C	287	PRO
1	C	494	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	608/1113 (55%)	562 (92%)	46 (8%)	13	37
1	C	610/1113 (55%)	562 (92%)	48 (8%)	12	35
2	B	237/247 (96%)	232 (98%)	5 (2%)	53	72
3	F	238/247 (96%)	218 (92%)	20 (8%)	11	33
All	All	1693/2720 (62%)	1574 (93%)	119 (7%)	19	40

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	15	TRP
1	A	18	ASP
1	A	20	ILE
1	A	33	ASP
1	A	51	ASP
1	A	61	VAL
1	A	62	ASP
1	A	66	ASN
1	A	73	ASN
1	A	74	ASN
1	A	99	ASN
1	A	104	PHE
1	A	106	ASN
1	A	117	ASN
1	A	130	ASN
1	A	136	TRP
1	A	147	ASN
1	A	156	SER
1	A	168	TRP
1	A	169	ASN
1	A	170	GLN
1	A	183	ASN
1	A	198	HIS
1	A	204	PRO
1	A	216	GLU
1	A	221	ASN
1	A	232	ASP
1	A	244	ASN
1	A	253	ASN
1	A	261	LEU
1	A	266	CYS
1	A	268	GLN

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Mol	Chain	Res	Type
1	A	281	THR
1	A	304	PHE
1	A	327	VAL
1	A	334	THR
1	A	430	LEU
1	A	509	ASN
1	A	534	ASP
1	A	537	MET
1	A	545	ASP
1	A	657	ASP
1	A	688	ILE
1	A	703	PHE
1	A	720	THR
2	B	92	ILE
2	B	180	ASN
2	B	204	SER
2	B	225	VAL
2	B	238	ASN
1	C	7	PHE
1	C	15	TRP
1	C	18	ASP
1	C	20	ILE
1	C	33	ASP
1	C	51	ASP
1	C	61	VAL
1	C	62	ASP
1	C	66	ASN
1	C	73	ASN
1	C	74	ASN
1	C	99	ASN
1	C	104	PHE
1	C	106	ASN
1	C	117	ASN
1	C	130	ASN
1	C	136	TRP
1	C	147	ASN
1	C	156	SER
1	C	168	TRP
1	C	169	ASN
1	C	170	GLN
1	C	183	ASN
1	C	198	HIS

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Mol	Chain	Res	Type
1	C	204	PRO
1	C	216	GLU
1	C	221	ASN
1	C	232	ASP
1	C	244	ASN
1	C	253	ASN
1	C	261	LEU
1	C	266	CYS
1	C	268	GLN
1	C	281	THR
1	C	304	PHE
1	C	327	VAL
1	C	334	THR
1	C	377	TYR
1	C	381	SER
1	C	408	LYS
1	C	413	GLU
1	C	432	ASN
1	C	509	ASN
1	C	510	ILE
1	C	534	ASP
1	C	538	GLU
1	C	545	ASP
1	C	629	GLN
3	F	33	ILE
3	F	66	PHE
3	F	81	ILE
3	F	82	TRP
3	F	122	ASP
3	F	129	GLU
3	F	133	ASN
3	F	141	ILE
3	F	180	ASN
3	F	199	THR
3	F	200	LEU
3	F	205	ASP
3	F	206	TRP
3	F	225	VAL
3	F	233	ILE
3	F	237	ASP
3	F	247	LEU
3	F	255	ASP

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Mol	Chain	Res	Type
3	F	261	SER
3	F	286	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	72	HIS
1	A	73	ASN
1	A	74	ASN
1	A	95	ASN
1	A	96	ASN
1	A	99	ASN
1	A	106	ASN
1	A	117	ASN
1	A	129	ASN
1	A	130	ASN
1	A	139	ASN
1	A	147	ASN
1	A	221	ASN
1	A	244	ASN
1	A	246	ASN
1	A	250	GLN
1	A	268	GLN
1	A	292	GLN
1	A	370	HIS
1	A	433	GLN
1	A	443	ASN
1	A	448	ASN
1	A	509	ASN
1	A	517	ASN
1	A	592	GLN
1	A	601	GLN
2	B	95	HIS
2	B	103	ASN
2	B	149	ASN
2	B	180	ASN
2	B	238	ASN
2	B	240	GLN
2	B	276	ASN
1	C	66	ASN
1	C	72	HIS

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Mol	Chain	Res	Type
1	C	73	ASN
1	C	74	ASN
1	C	95	ASN
1	C	96	ASN
1	C	99	ASN
1	C	106	ASN
1	C	117	ASN
1	C	129	ASN
1	C	130	ASN
1	C	139	ASN
1	C	147	ASN
1	C	221	ASN
1	C	244	ASN
1	C	246	ASN
1	C	250	GLN
1	C	268	GLN
1	C	292	GLN
1	C	443	ASN
1	C	448	ASN
1	C	493	GLN
1	C	509	ASN
1	C	517	ASN
1	C	557	ASN
1	C	592	GLN
1	C	601	GLN
1	C	606	ASN
1	C	670	HIS
1	C	686	ASN
3	F	86	ASN
3	F	149	ASN
3	F	180	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)

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

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	372:GLN	C	373:ALA	N	16.58
1	C	372:GLN	C	373:ALA	N	16.33

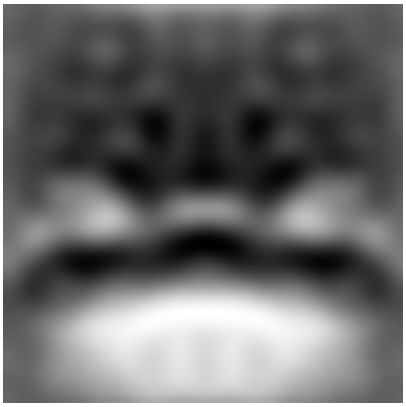
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2430. These allow visual inspection of the internal detail of the map and identification of artifacts.

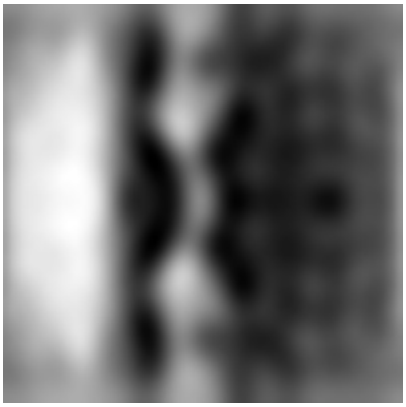
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

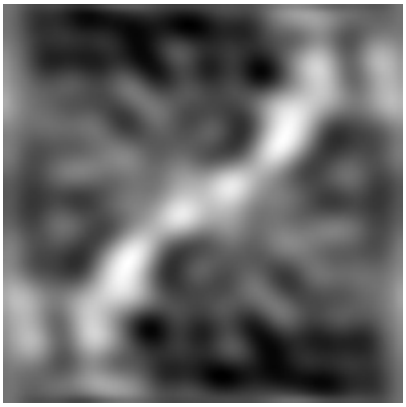
6.1.1 Primary map



X



Y

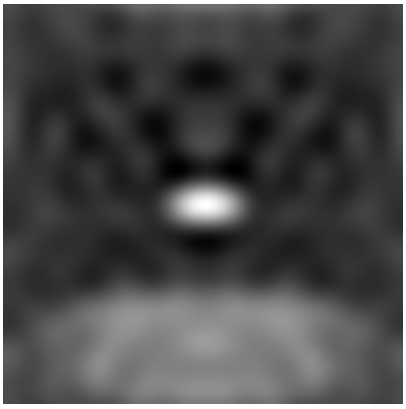


Z

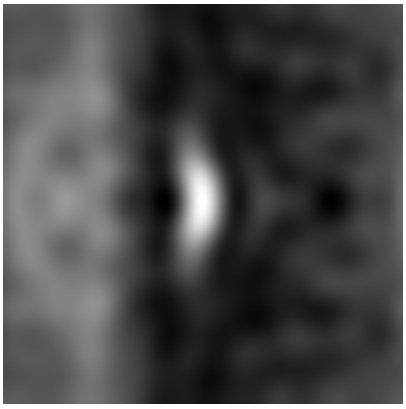
The images above show the map projected in three orthogonal directions.

6.2 Central slices

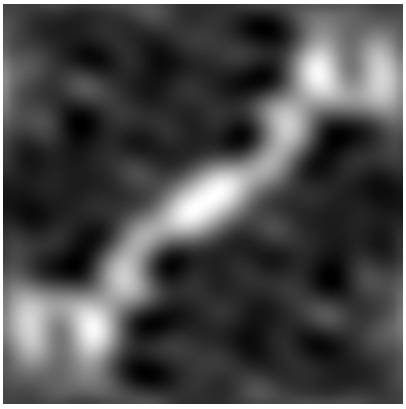
6.2.1 Primary map



X Index: 36



Y Index: 36

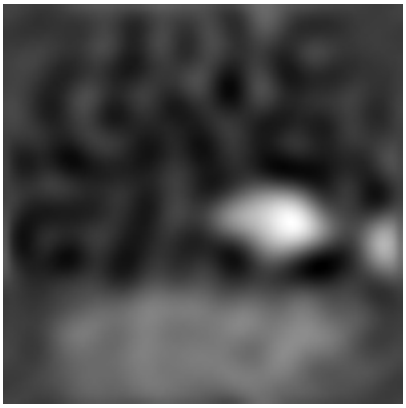


Z Index: 36

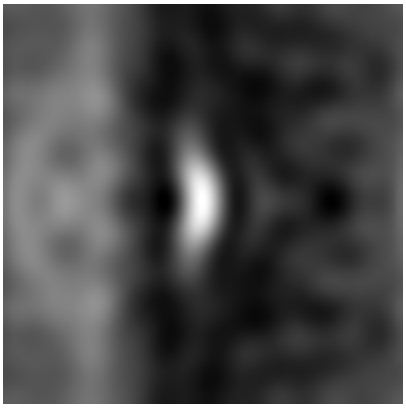
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

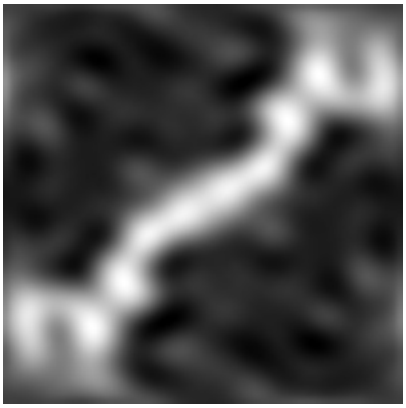
6.3.1 Primary map



X Index: 50



Y Index: 36

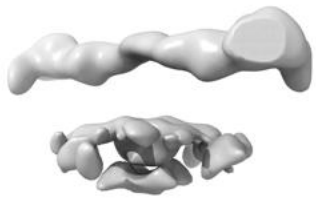


Z Index: 34

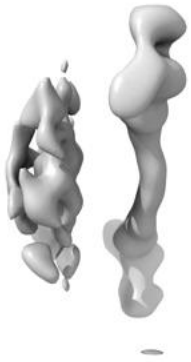
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

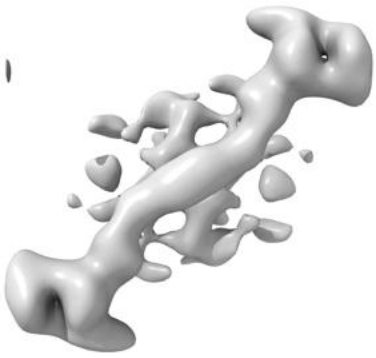
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

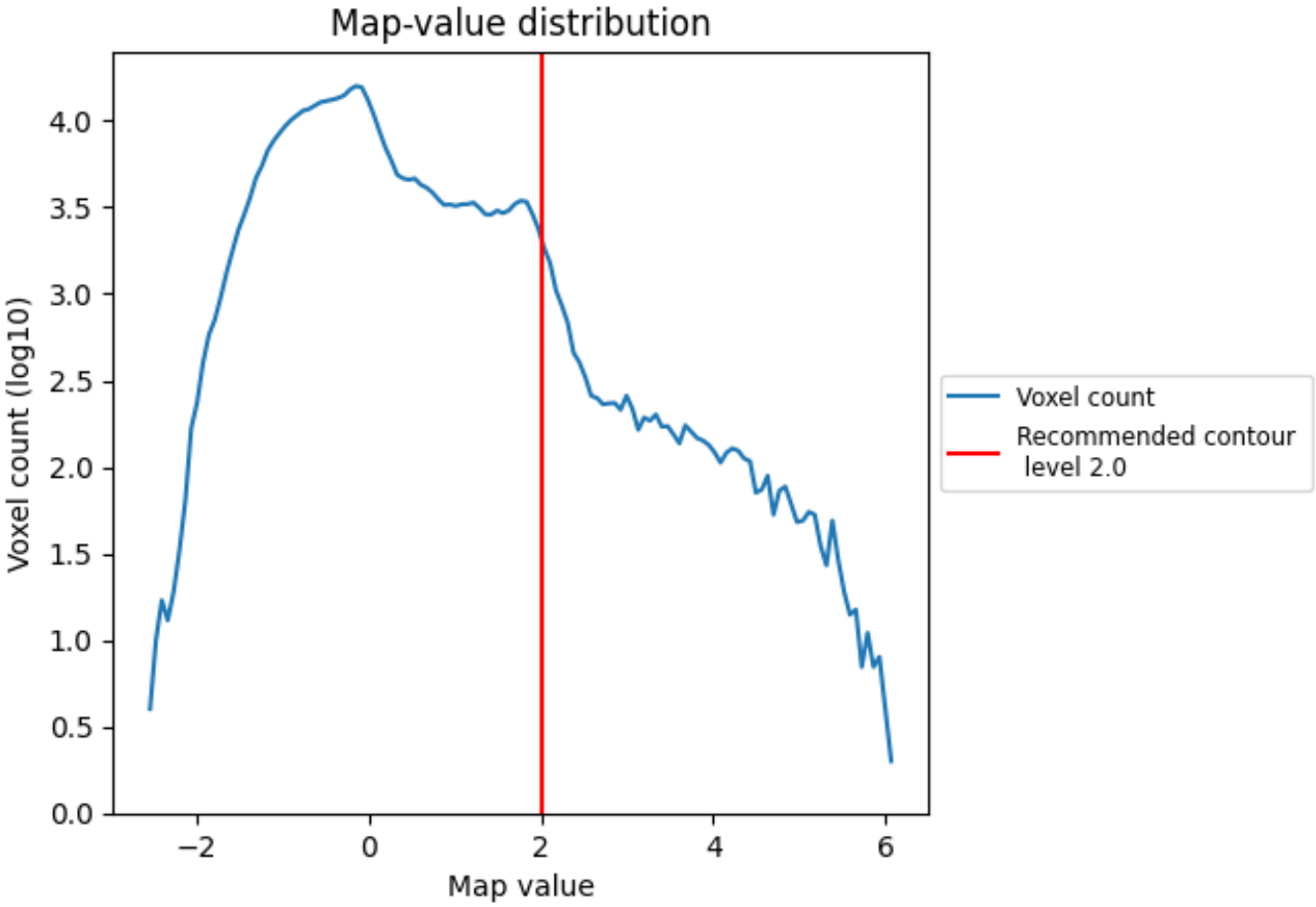
6.5 Mask visualisation (i)

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

7 Map analysis

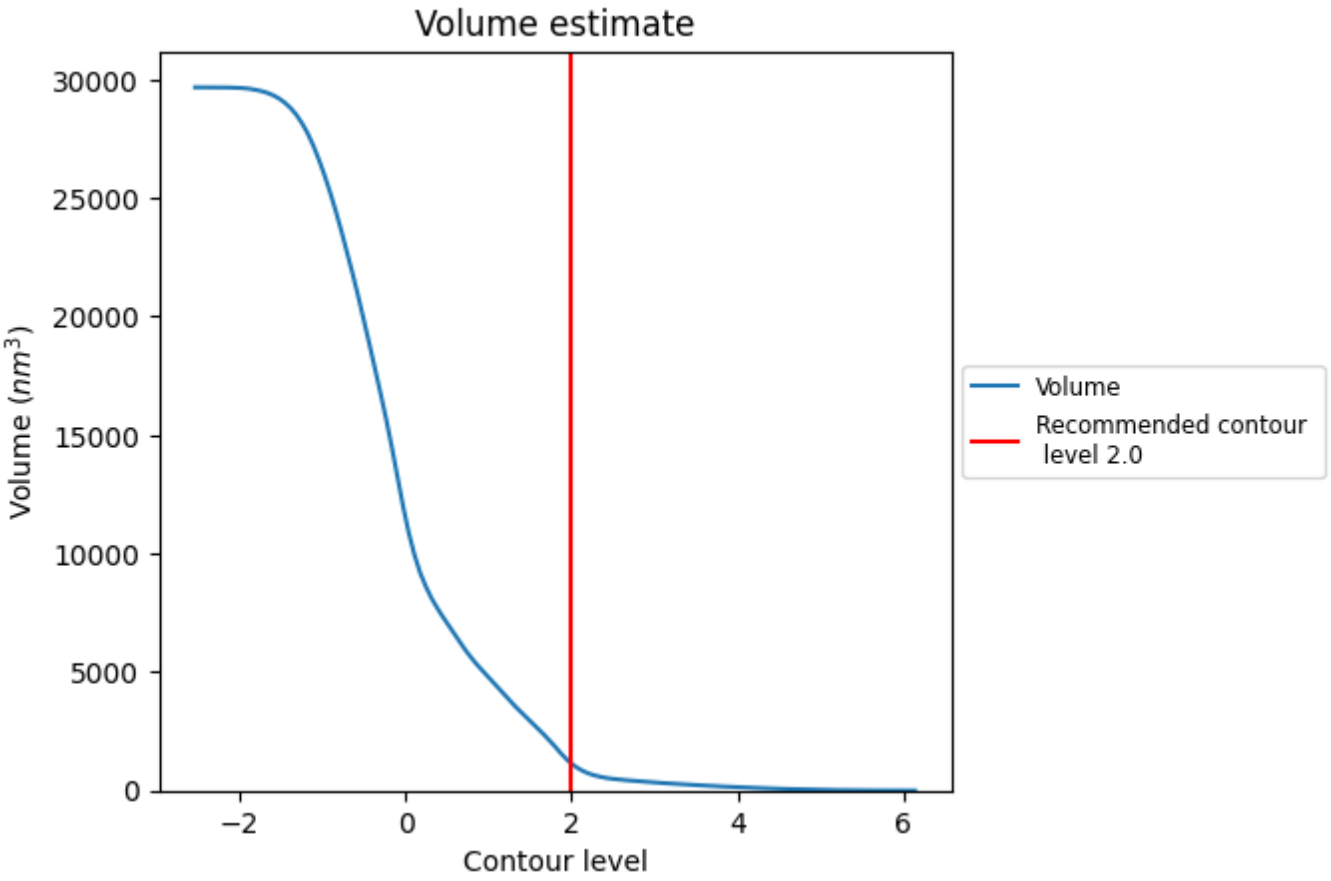
This section contains the results of statistical analysis of the map.

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.

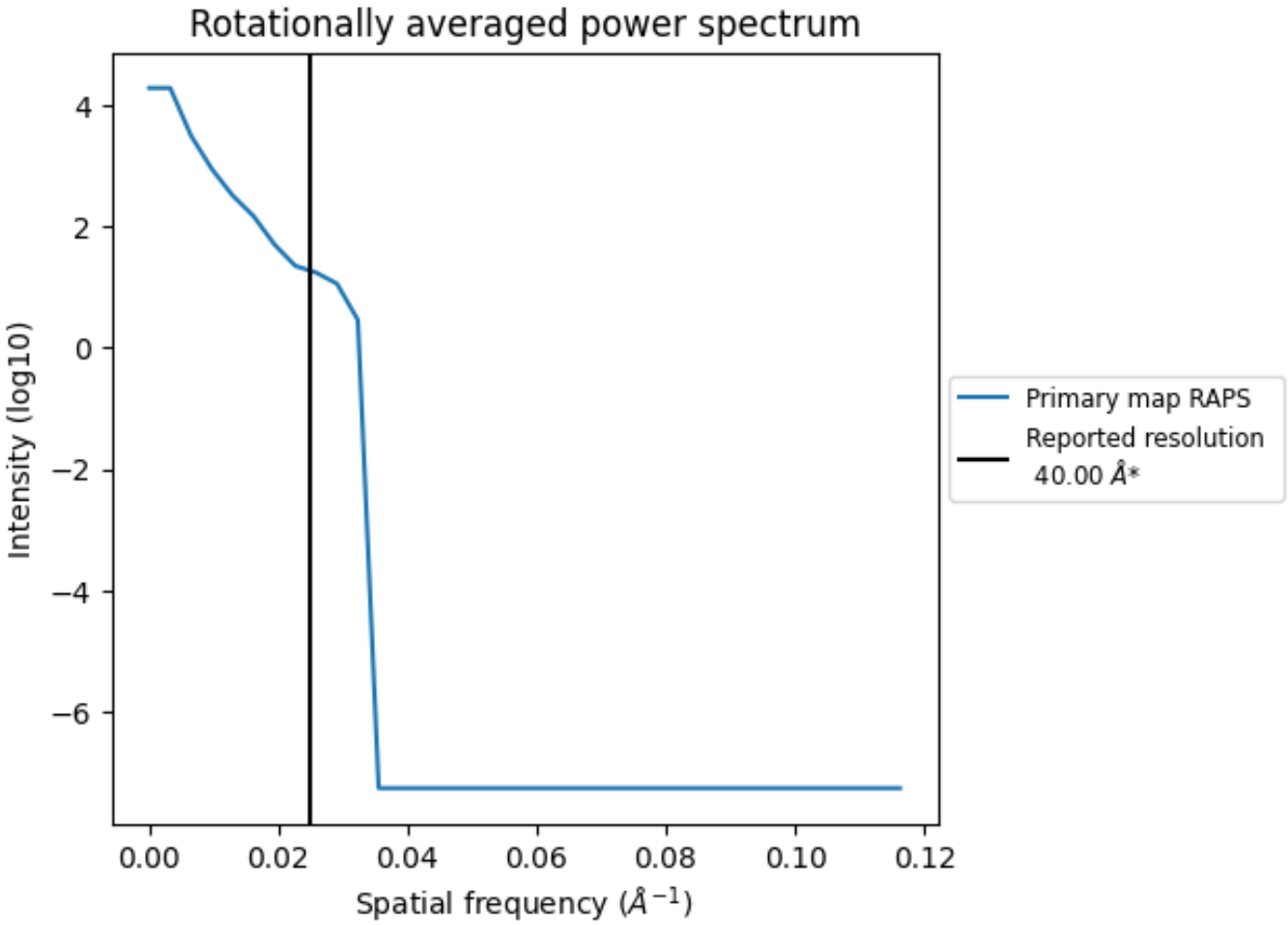
7.2 Volume estimate



The volume at the recommended contour level is 1130 nm^3; this corresponds to an approximate mass of 1021 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 0.025 Å^{-1}

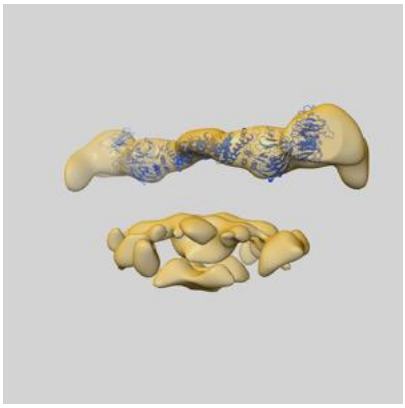
8 Fourier-Shell correlation (i)

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

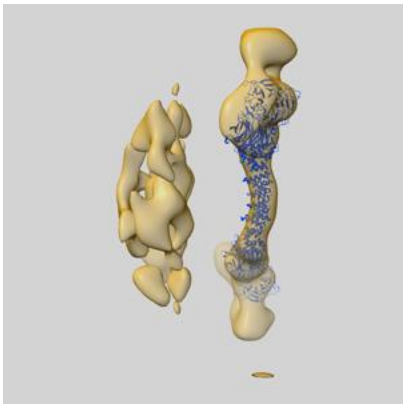
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2430 and PDB model 4BZJ. Per-residue inclusion information can be found in section 3 on page 5.

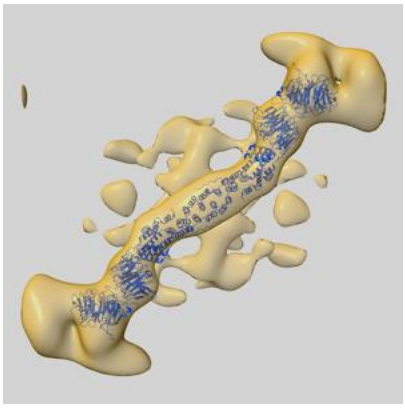
9.1 Map-model overlay



X



Y



Z

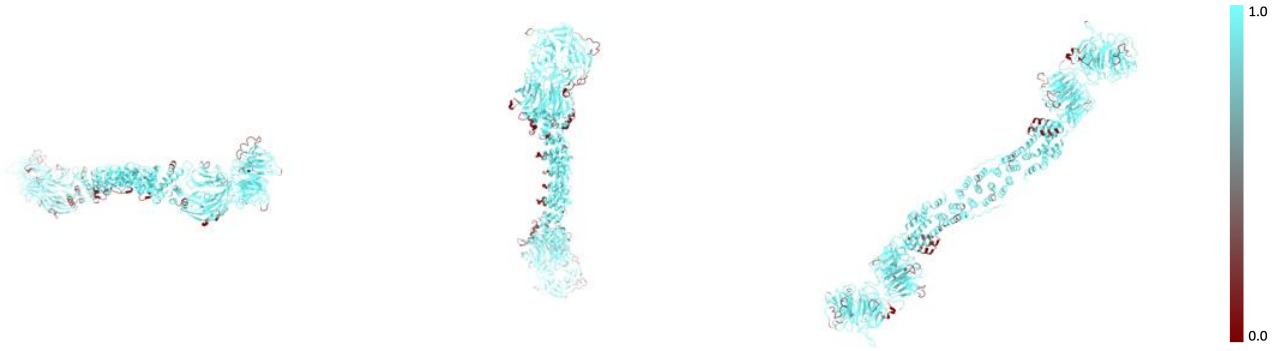
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

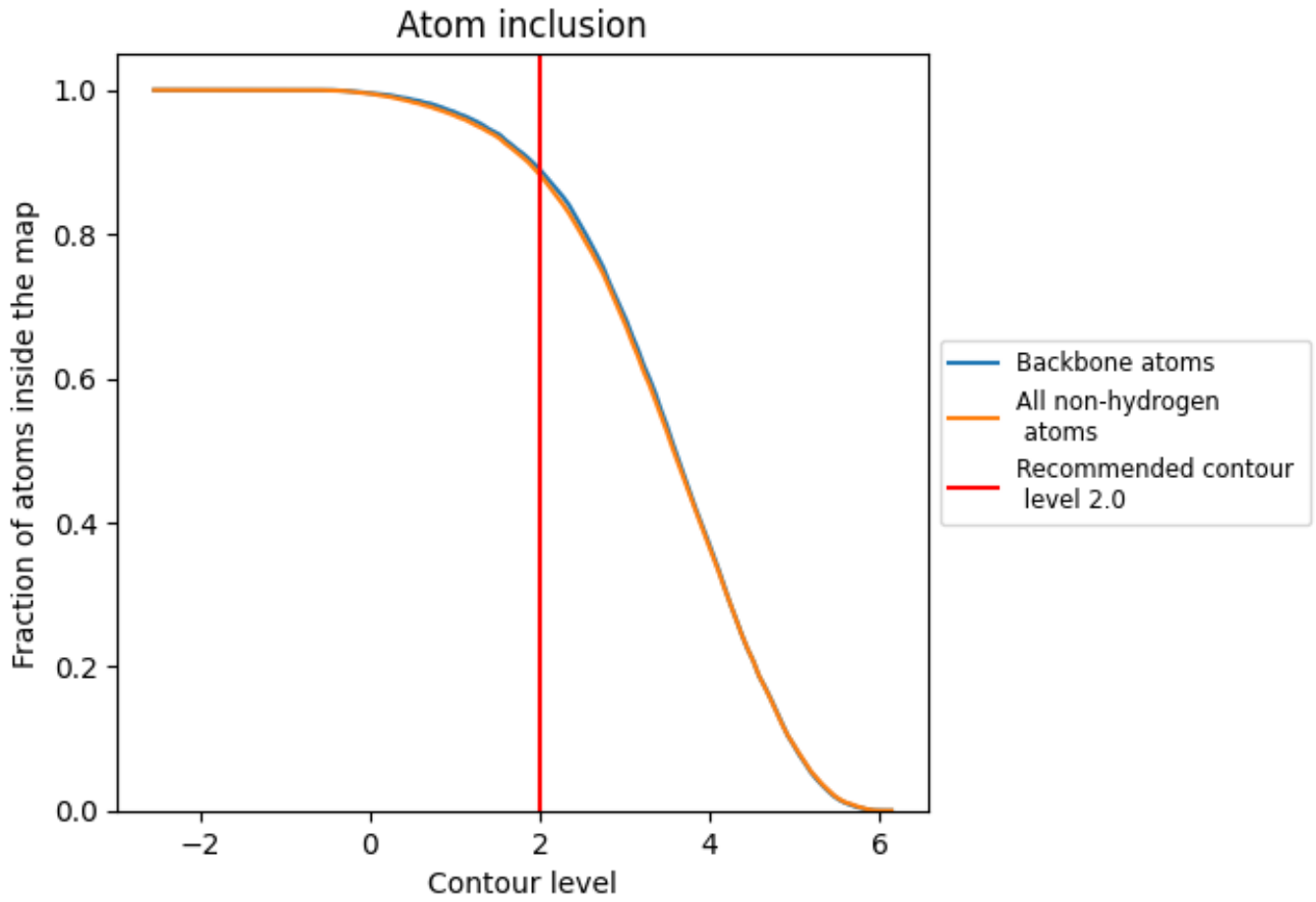
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8826	0.0520
A	0.8627	0.0520
B	0.8967	0.0500
C	0.8907	0.0540
F	0.8966	0.0530