



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:35 AM UTC

PDB ID : 7B5P / pdb_00007b5p
EMDB ID : EMD-12043
Title : AcrB in cycloalkane amphipol
Authors : Higgins, A.J.; Flynn, A.J.; Muench, S.P.
Deposited on : 2020-12-05
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

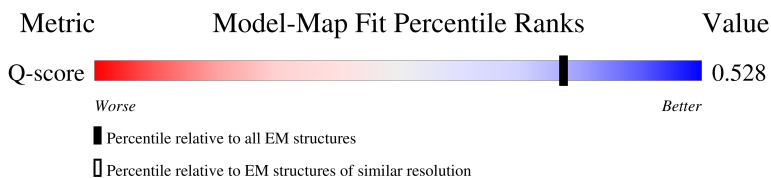
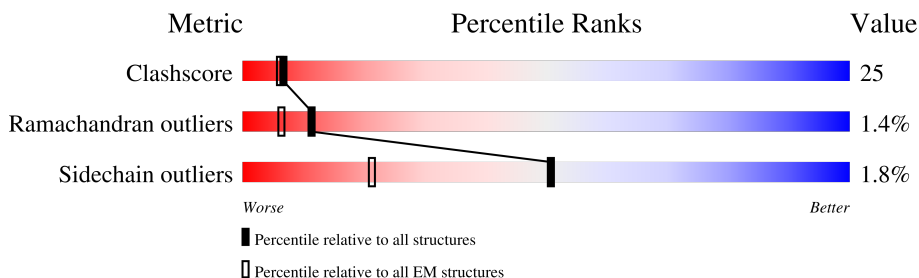
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	1051	
1	B	1051	
1	C	1051	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22527 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1014	Total	C	N	O	S	0	0
			7504	4849	1231	1383	41		
1	C	1014	Total	C	N	O	S	0	0
			7623	4912	1252	1421	38		
1	A	985	Total	C	N	O	S	0	0
			7400	4761	1218	1380	41		

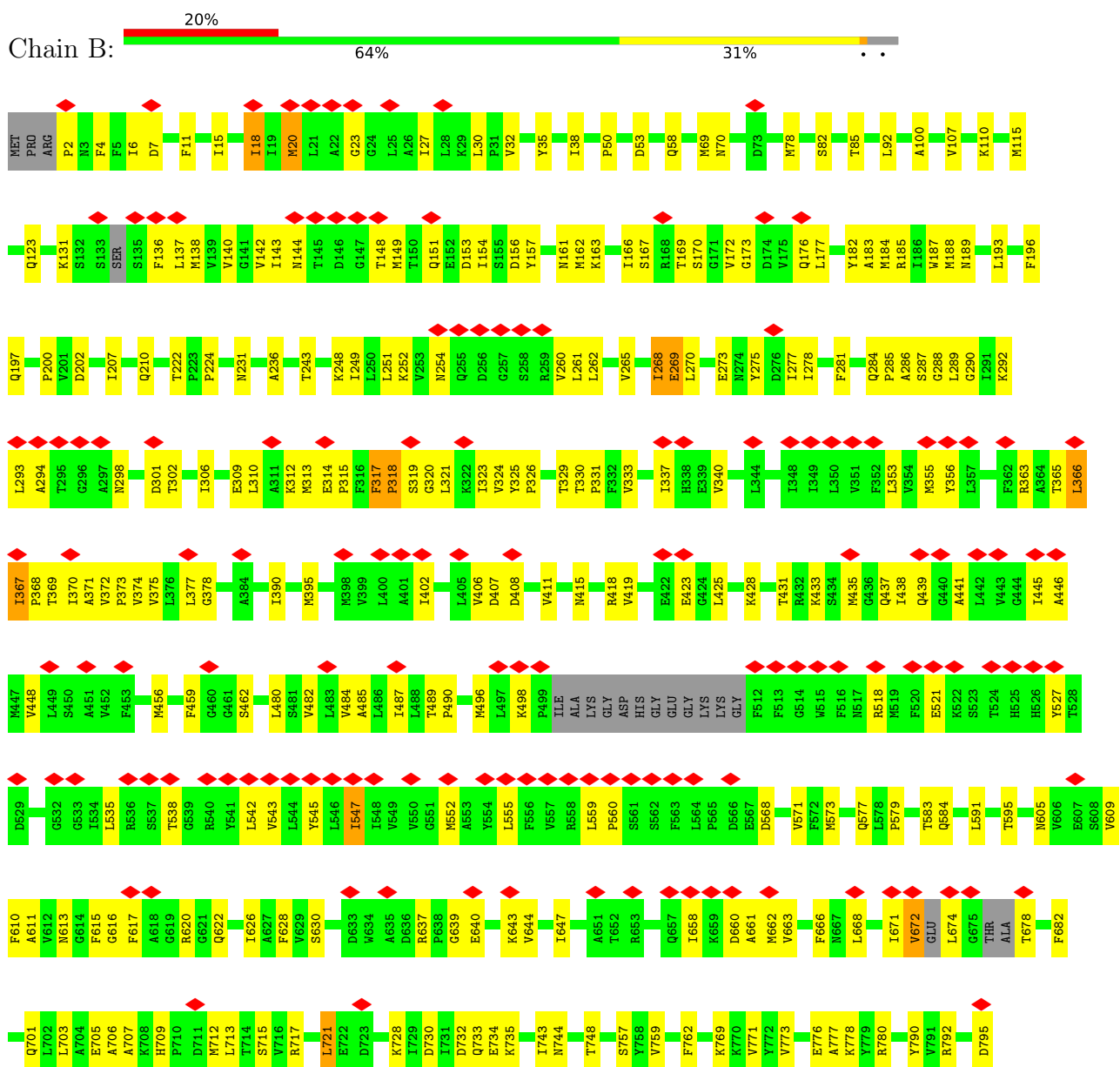
There are 9 discrepancies between the modelled and reference sequences:

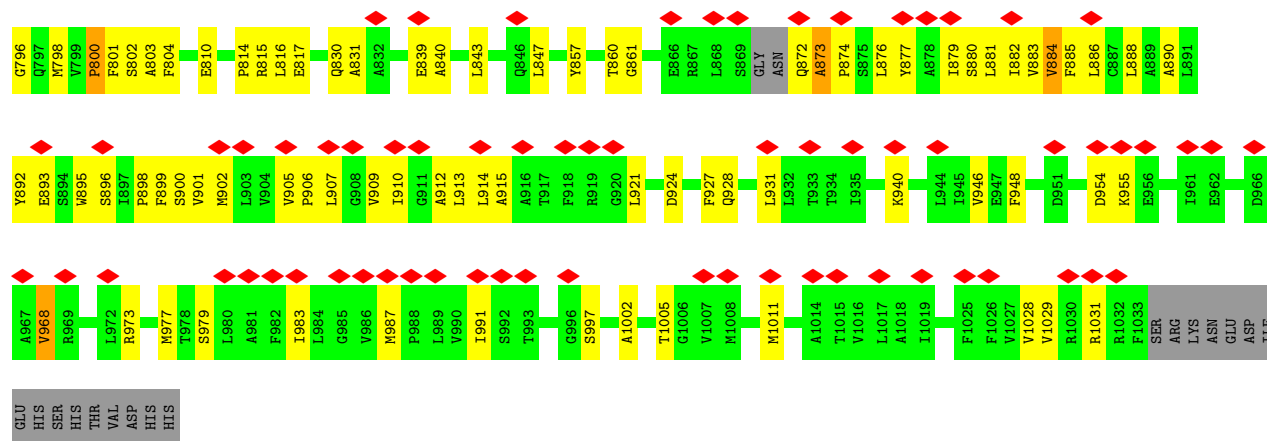
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP E2QH56
B	0	PRO	-	expression tag	UNP E2QH56
B	1	ARG	-	expression tag	UNP E2QH56
C	-1	MET	-	initiating methionine	UNP E2QH56
C	0	PRO	-	expression tag	UNP E2QH56
C	1	ARG	-	expression tag	UNP E2QH56
A	-1	MET	-	initiating methionine	UNP E2QH56
A	0	PRO	-	expression tag	UNP E2QH56
A	1	ARG	-	expression tag	UNP E2QH56

3 Residue-property plots

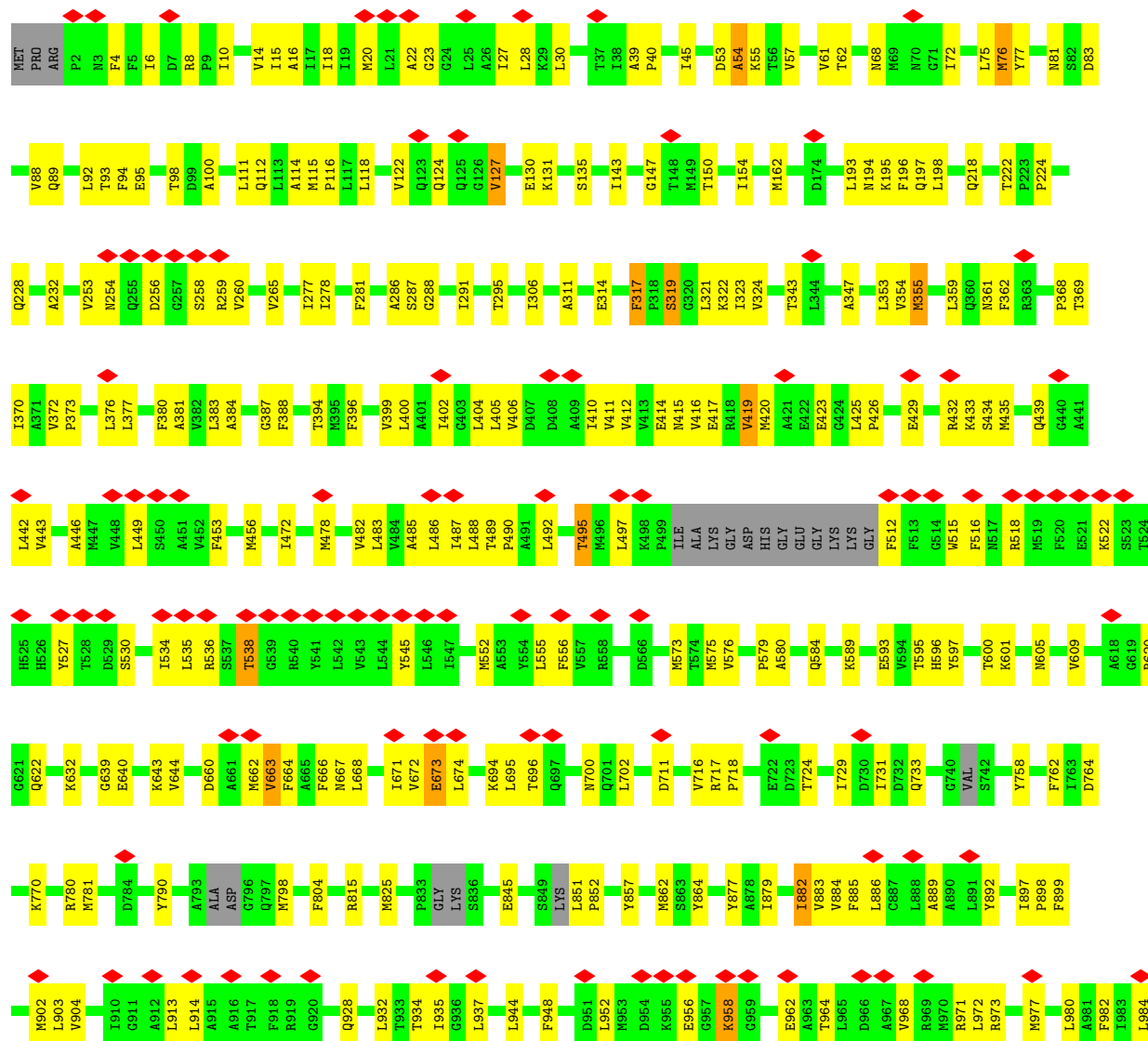
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Efflux pump membrane transporter



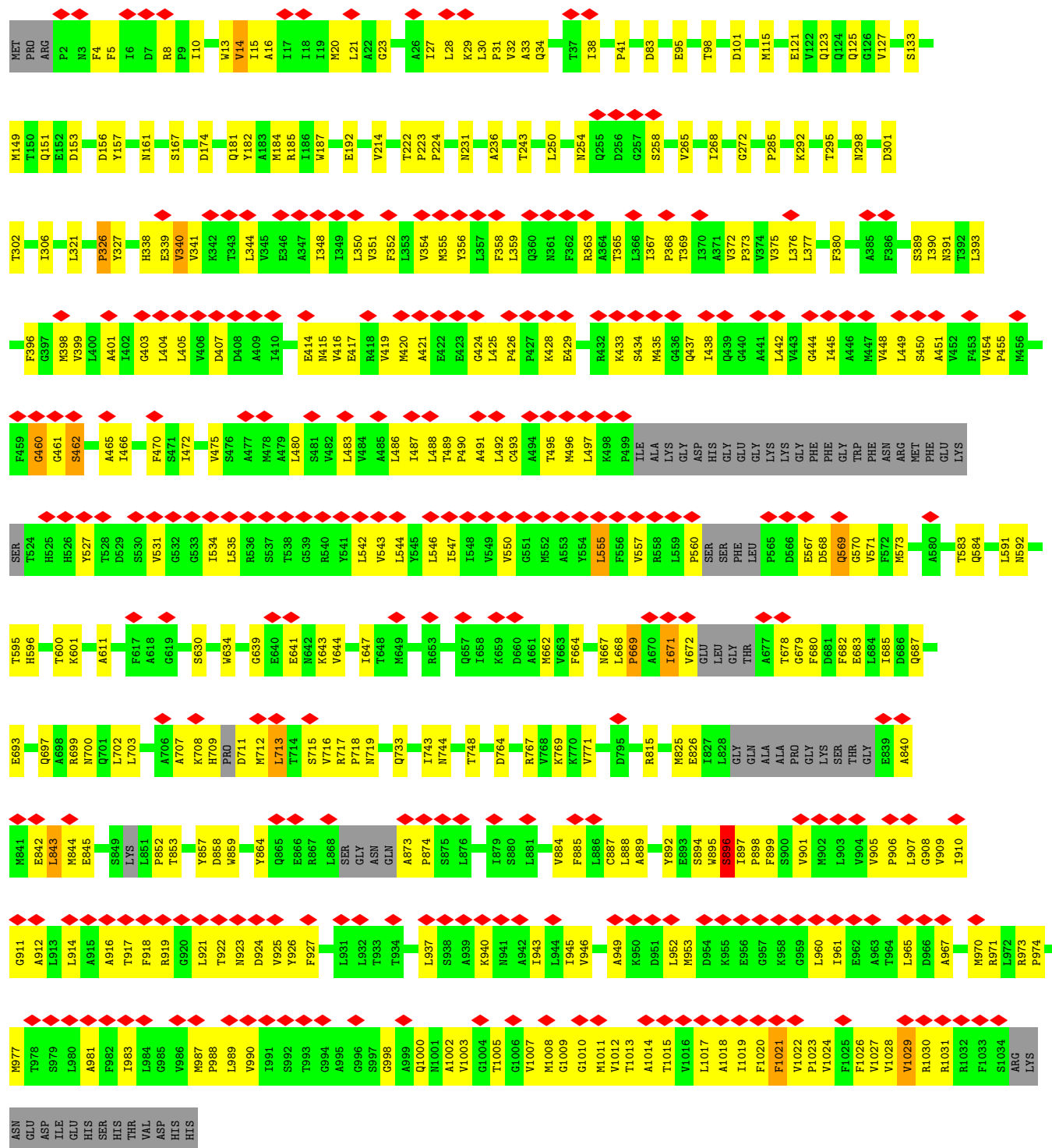


• Molecule 1: Efflux pump membrane transporter





● Molecule 1: Efflux pump membrane transporter



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	100932	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.064	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0224	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.44	0/7528	0.66	2/10230 (0.0%)
1	B	0.38	0/7646	0.65	4/10417 (0.0%)
1	C	0.42	0/7765	0.62	1/10564 (0.0%)
All	All	0.42	0/22939	0.65	7/31211 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	PHE	CA-C-N	6.88	128.44	119.84
1	B	317	PHE	C-N-CA	6.88	128.44	119.84
1	C	265	VAL	N-CA-C	-6.77	106.70	113.20
1	A	1021	PHE	CA-C-N	5.32	125.53	120.43
1	A	1021	PHE	C-N-CA	5.32	125.53	120.43
1	B	367	ILE	CA-C-N	5.05	124.74	119.64
1	B	367	ILE	C-N-CA	5.05	124.74	119.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7400	0	7505	458	0
1	B	7504	0	7503	354	0
1	C	7623	0	7671	329	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22527	0	22679	1115	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 25.

All (1115) 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:A:393:LEU:HD22	1:A:470:PHE:CE2	1.44	1.49
1:A:679:GLY:HA2	1:A:712:MET:CE	1.38	1.49
1:C:489:THR:CG2	1:C:490:PRO:HD3	1.53	1.36
1:A:897:ILE:CG2	1:A:898:PRO:HD3	1.57	1.35
1:A:892:TYR:OH	1:A:943:ILE:HG23	1.28	1.32
1:A:907:LEU:HD11	1:A:1017:LEU:CD2	1.60	1.28
1:A:960:LEU:CD1	1:A:1030:ARG:HG2	1.62	1.27
1:B:144:ASN:ND2	1:B:154:ILE:HD11	1.48	1.27
1:A:393:LEU:CD2	1:A:470:PHE:CZ	2.20	1.25
1:A:393:LEU:HD22	1:A:470:PHE:CZ	1.73	1.22
1:C:439:GLN:O	1:C:443:VAL:HG23	1.41	1.18
1:A:960:LEU:HD11	1:A:1030:ARG:CG	1.74	1.17
1:B:197:GLN:HA	1:B:798:MET:HE3	1.25	1.17
1:A:393:LEU:CD2	1:A:470:PHE:CE2	2.30	1.14
1:C:355:MET:SD	1:C:410:ILE:CD1	2.38	1.11
1:A:425:LEU:HD12	1:A:426:PRO:CD	1.79	1.11
1:B:149:MET:HE1	1:B:321:LEU:HD11	1.26	1.10
1:A:425:LEU:HD21	1:A:429:GLU:HB3	1.29	1.10
1:A:908:GLY:CA	1:A:1014:ALA:HB2	1.81	1.10
1:A:897:ILE:HG22	1:A:898:PRO:HD3	1.12	1.10
1:A:350:LEU:O	1:A:354:VAL:HG23	1.53	1.09
1:A:393:LEU:HD23	1:A:470:PHE:HZ	1.17	1.09
1:A:679:GLY:CA	1:A:712:MET:CE	2.31	1.08
1:A:425:LEU:CD1	1:A:426:PRO:HD2	1.83	1.08
1:C:899:PHE:O	1:C:903:LEU:HD13	1.51	1.08
1:A:415:ASN:HD22	1:A:438:ILE:CD1	1.66	1.08
1:C:68:ASN:HD22	1:C:114:ALA:HB2	1.15	1.07
1:A:907:LEU:CD1	1:A:1017:LEU:CD2	2.33	1.07
1:C:489:THR:HG22	1:C:490:PRO:HD3	1.16	1.07
1:C:489:THR:HG23	1:C:490:PRO:HD3	1.34	1.06
1:C:664:PHE:CZ	1:C:717:ARG:HD3	1.91	1.06
1:A:679:GLY:HA2	1:A:712:MET:HE3	1.36	1.05
1:C:355:MET:SD	1:C:410:ILE:HD11	1.96	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:VAL:HG21	1:C:984:LEU:HD12	1.35	1.04
1:A:425:LEU:HD12	1:A:426:PRO:HD2	1.33	1.03
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.38	1.03
1:B:197:GLN:HA	1:B:798:MET:CE	1.88	1.03
1:A:679:GLY:HA2	1:A:712:MET:HE2	1.06	1.03
1:A:415:ASN:ND2	1:A:438:ILE:CD1	2.22	1.02
1:C:317:PHE:CD2	1:C:321:LEU:HD22	1.93	1.02
1:C:354:VAL:HG21	1:C:984:LEU:CD1	1.88	1.02
1:B:873:ALA:H	1:B:874:PRO:HD2	1.27	0.99
1:A:961:ILE:HD11	1:A:1031:ARG:NH2	1.77	0.99
1:C:489:THR:CG2	1:C:490:PRO:CD	2.40	0.99
1:B:162:MET:CE	1:B:317:PHE:HZ	1.74	0.99
1:B:149:MET:CE	1:B:321:LEU:HD11	1.92	0.98
1:C:355:MET:SD	1:C:410:ILE:HD12	2.03	0.98
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.44	0.97
1:A:897:ILE:HG23	1:A:898:PRO:HD3	1.45	0.97
1:A:897:ILE:CG2	1:A:898:PRO:CD	2.43	0.97
1:A:393:LEU:HB3	1:A:470:PHE:CE2	2.00	0.97
1:C:40:PRO:HD2	1:C:674:LEU:HD23	1.45	0.96
1:A:679:GLY:CA	1:A:712:MET:HE2	1.94	0.96
1:B:189:ASN:O	1:B:193:LEU:HD13	1.65	0.96
1:A:960:LEU:HD11	1:A:1030:ARG:HG2	0.97	0.96
1:A:355:MET:HE2	1:A:365:THR:HA	1.49	0.95
1:C:354:VAL:CG2	1:C:984:LEU:CD1	2.45	0.95
1:C:731:ILE:HD11	1:C:804:PHE:HD1	1.31	0.95
1:A:907:LEU:HD11	1:A:1017:LEU:HD23	1.46	0.95
1:C:664:PHE:CE2	1:C:717:ARG:HD3	2.01	0.95
1:C:404:LEU:HD22	1:C:449:LEU:HD21	1.49	0.94
1:A:393:LEU:CD2	1:A:470:PHE:HZ	1.66	0.94
1:B:355:MET:SD	1:B:368:PRO:HG2	2.08	0.94
1:A:393:LEU:HA	1:A:470:PHE:CZ	2.02	0.94
1:A:911:GLY:HA3	1:A:1009:GLY:O	1.66	0.93
1:A:897:ILE:HG22	1:A:898:PRO:CD	1.98	0.92
1:A:717:ARG:HB2	1:A:718:PRO:HD2	1.51	0.92
1:B:733:GLN:OE1	1:B:743:ILE:HD11	1.68	0.92
1:C:952:LEU:O	1:C:956:GLU:HB3	1.70	0.92
1:C:68:ASN:ND2	1:C:114:ALA:HB2	1.84	0.92
1:A:404:LEU:HD23	1:A:937:LEU:HD13	1.51	0.92
1:A:873:ALA:HB3	1:A:874:PRO:CD	1.99	0.92
1:C:489:THR:HG23	1:C:490:PRO:CD	1.99	0.92
1:A:30:LEU:HG	1:A:31:PRO:HD2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:GLY:HA3	1:A:1014:ALA:HB2	1.50	0.91
1:A:156:ASP:CG	1:A:182:TYR:CE2	2.49	0.91
1:A:960:LEU:CD1	1:A:1030:ARG:CG	2.37	0.91
1:A:983:ILE:HD11	1:A:1011:MET:HB2	1.52	0.91
1:A:425:LEU:HD21	1:A:429:GLU:CB	2.01	0.90
1:A:699:ARG:HD3	1:A:825:MET:SD	2.11	0.90
1:A:926:TYR:HB3	1:A:1003:VAL:HG13	1.53	0.90
1:A:857:TYR:O	1:A:858:ASP:OD1	1.89	0.90
1:A:845:GLU:CD	1:A:845:GLU:O	2.15	0.90
1:B:571:VAL:HG23	1:B:668:LEU:HD11	1.51	0.89
1:A:393:LEU:CB	1:A:470:PHE:CZ	2.55	0.89
1:A:907:LEU:CD1	1:A:1017:LEU:HD23	1.99	0.89
1:B:162:MET:CE	1:B:317:PHE:CZ	2.55	0.89
1:B:197:GLN:CA	1:B:798:MET:HE3	2.03	0.89
1:C:731:ILE:HD11	1:C:804:PHE:CD1	2.08	0.89
1:A:907:LEU:HD11	1:A:1017:LEU:HD21	1.50	0.89
1:A:30:LEU:HD22	1:A:390:ILE:HG12	1.53	0.88
1:A:425:LEU:HD12	1:A:426:PRO:HD3	1.55	0.88
1:A:546:LEU:O	1:A:550:VAL:HG23	1.74	0.88
1:A:892:TYR:HH	1:A:943:ILE:HG23	1.34	0.88
1:C:439:GLN:O	1:C:443:VAL:CG2	2.20	0.88
1:C:731:ILE:CD1	1:C:804:PHE:HD1	1.85	0.88
1:A:907:LEU:CD1	1:A:1017:LEU:HD21	2.00	0.88
1:A:907:LEU:CD2	1:A:1018:ALA:HA	2.04	0.87
1:A:156:ASP:CG	1:A:182:TYR:CD2	2.52	0.87
1:C:449:LEU:HB3	1:C:478:MET:HE2	1.56	0.87
1:C:851:LEU:HB3	1:C:852:PRO:HD2	1.56	0.87
1:C:194:ASN:ND2	1:C:790:TYR:CD2	2.43	0.87
1:A:907:LEU:HD21	1:A:1018:ALA:HA	1.54	0.87
1:C:354:VAL:CG2	1:C:984:LEU:HD12	2.04	0.86
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.58	0.86
1:C:958:LYS:HZ1	1:C:962:GLU:HG3	1.39	0.86
1:A:967:ALA:HA	1:A:970:MET:HE2	1.59	0.85
1:B:144:ASN:CG	1:B:154:ILE:HD11	2.01	0.85
1:B:892:TYR:O	1:B:893:GLU:HG2	1.74	0.85
1:B:873:ALA:H	1:B:874:PRO:CD	1.89	0.85
1:C:277:ILE:HD11	1:C:620:ARG:HH22	1.40	0.85
1:C:928:GLN:O	1:C:932:LEU:HD13	1.75	0.85
1:A:907:LEU:HD11	1:A:1017:LEU:CG	2.05	0.84
1:A:393:LEU:CA	1:A:470:PHE:CZ	2.60	0.84
1:C:396:PHE:O	1:C:400:LEU:HD13	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:CD2	1:A:390:ILE:HG12	2.08	0.83
1:B:248:LYS:C	1:B:261:LEU:HD22	2.02	0.83
1:A:535:LEU:CD2	1:A:965:LEU:HD21	2.07	0.83
1:B:661:ALA:O	1:B:663:VAL:HG23	1.78	0.83
1:A:892:TYR:CB	1:A:897:ILE:HG21	2.08	0.83
1:B:151:GLN:NE2	1:B:285:PRO:HB3	1.93	0.83
1:A:393:LEU:HB3	1:A:470:PHE:CZ	2.12	0.83
1:C:605:ASN:O	1:C:632:LYS:HG3	1.78	0.82
1:A:492:LEU:HD11	1:A:496:MET:HE2	1.58	0.82
1:A:888:LEU:CD1	1:A:901:VAL:HG11	2.09	0.82
1:C:354:VAL:CG2	1:C:984:LEU:HD13	2.09	0.82
1:A:907:LEU:HD23	1:A:1018:ALA:HB2	1.61	0.82
1:A:268:ILE:HD12	1:A:268:ILE:H	1.43	0.82
1:B:184:MET:HE3	1:B:268:ILE:CG2	2.09	0.82
1:B:184:MET:HE3	1:B:268:ILE:HG21	1.61	0.82
1:C:937:LEU:CD2	1:C:1011:MET:SD	2.68	0.82
1:B:136:PHE:HE2	1:B:176:GLN:HG2	1.45	0.82
1:A:907:LEU:HD21	1:A:1018:ALA:CA	2.10	0.82
1:C:30:LEU:HD21	1:C:384:ALA:HB2	1.62	0.82
1:C:30:LEU:HD21	1:C:384:ALA:CB	2.10	0.81
1:C:899:PHE:O	1:C:903:LEU:CD1	2.28	0.81
1:B:149:MET:HB3	1:B:153:ASP:HB2	1.60	0.81
1:C:10:ILE:HD12	1:A:895:TRP:NE1	1.95	0.81
1:C:731:ILE:HD12	1:C:804:PHE:O	1.79	0.81
1:A:415:ASN:ND2	1:A:438:ILE:HD11	1.93	0.81
1:B:873:ALA:N	1:B:874:PRO:HD2	1.96	0.81
1:C:595:THR:HG23	1:C:609:VAL:HG21	1.63	0.81
1:A:351:VAL:O	1:A:355:MET:HG2	1.80	0.81
1:C:406:VAL:O	1:C:410:ILE:HG12	1.80	0.81
1:A:38:ILE:HD11	1:A:671:ILE:HG21	1.62	0.81
1:C:162:MET:HE1	1:C:317:PHE:CE1	2.15	0.81
1:B:162:MET:HE1	1:B:317:PHE:HZ	1.46	0.80
1:A:448:VAL:HG12	1:A:887:CYS:HB3	1.62	0.80
1:C:194:ASN:ND2	1:C:790:TYR:CE2	2.49	0.80
1:A:34:GLN:O	1:A:391:ASN:HB2	1.81	0.80
1:A:352:PHE:HD1	1:A:369:THR:HG1	1.29	0.80
1:A:905:VAL:O	1:A:909:VAL:HG23	1.81	0.80
1:B:15:ILE:HD11	1:B:487:ILE:HG21	1.65	0.79
1:B:366:LEU:HA	1:B:369:THR:HG22	1.63	0.79
1:C:664:PHE:CE2	1:C:717:ARG:CD	2.64	0.79
1:C:717:ARG:HB2	1:C:718:PRO:HD2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:MET:N	1:C:116:PRO:CD	2.47	0.78
1:A:671:ILE:HG22	1:A:672:VAL:N	1.98	0.78
1:C:664:PHE:HZ	1:C:717:ARG:HD3	1.47	0.78
1:A:892:TYR:OH	1:A:943:ILE:CG2	2.23	0.78
1:A:892:TYR:HB3	1:A:897:ILE:HG21	1.66	0.78
1:B:197:GLN:CA	1:B:798:MET:CE	2.59	0.78
1:B:709:HIS:HB3	1:B:712:MET:HE3	1.65	0.78
1:C:579:PRO:HG2	1:C:660:ASP:OD1	1.84	0.78
1:A:393:LEU:HD22	1:A:470:PHE:HE2	1.02	0.78
1:B:790:TYR:HA	1:B:800:PRO:HA	1.65	0.78
1:C:579:PRO:CG	1:C:660:ASP:OD1	2.31	0.78
1:A:924:ASP:OD2	1:A:1002:ALA:HB1	1.84	0.77
1:A:393:LEU:HD23	1:A:470:PHE:CZ	2.02	0.77
1:B:895:TRP:CZ2	1:A:10:ILE:CD1	2.68	0.77
1:A:843:LEU:H	1:A:843:LEU:CD1	1.96	0.77
1:A:555:LEU:HD21	1:A:914:LEU:HD23	1.67	0.77
1:C:420:MET:HG3	1:C:425:LEU:O	1.85	0.77
1:B:197:GLN:HG3	1:B:798:MET:HE3	1.65	0.76
1:A:678:THR:O	1:A:712:MET:HE2	1.85	0.76
1:A:961:ILE:HD11	1:A:1031:ARG:HH21	1.50	0.76
1:A:38:ILE:CD1	1:A:671:ILE:HG21	2.15	0.76
1:C:75:LEU:O	1:C:77:TYR:N	2.19	0.76
1:A:907:LEU:HD23	1:A:1018:ALA:CB	2.16	0.76
1:B:900:SER:HB3	1:B:1029:VAL:HG11	1.68	0.75
1:A:5:PHE:CE2	1:A:487:ILE:CG2	2.69	0.75
1:A:591:LEU:HD12	1:A:611:ALA:HB1	1.68	0.75
1:B:571:VAL:HG23	1:B:668:LEU:CD1	2.16	0.75
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.20	0.74
1:B:559:LEU:HD12	1:B:560:PRO:HD2	1.69	0.74
1:C:429:GLU:HA	1:C:432:ARG:HD2	1.67	0.74
1:A:685:ILE:HD13	1:A:858:ASP:OD2	1.87	0.74
1:B:431:THR:O	1:B:435:MET:HG2	1.87	0.74
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.69	0.74
1:A:535:LEU:HD21	1:A:965:LEU:HD21	1.66	0.74
1:A:699:ARG:HH12	1:A:718:PRO:HG3	1.52	0.74
1:A:393:LEU:CD2	1:A:470:PHE:HE2	1.88	0.74
1:A:415:ASN:HD22	1:A:438:ILE:HD12	1.52	0.74
1:A:888:LEU:CD1	1:A:901:VAL:CG1	2.65	0.74
1:B:151:GLN:OE1	1:B:151:GLN:N	2.19	0.74
1:B:924:ASP:O	1:B:928:GLN:HG3	1.87	0.74
1:A:960:LEU:HD21	1:A:1027:VAL:HG12	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:LEU:HD23	1:B:721:LEU:N	2.01	0.74
1:C:958:LYS:NZ	1:C:962:GLU:CG	2.51	0.74
1:C:958:LYS:HZ2	1:C:962:GLU:HG2	1.52	0.73
1:A:393:LEU:CB	1:A:470:PHE:CE2	2.70	0.73
1:A:460:GLY:O	1:A:462:SER:N	2.21	0.73
1:B:137:LEU:HD11	1:B:293:LEU:HB2	1.68	0.73
1:A:542:LEU:HD12	1:A:542:LEU:O	1.87	0.73
1:A:32:VAL:HG22	1:A:390:ILE:HD11	1.69	0.73
1:A:600:THR:HG23	1:A:601:LYS:N	2.03	0.73
1:A:702:LEU:C	1:A:702:LEU:HD23	2.14	0.73
1:A:1008:MET:O	1:A:1012:VAL:HG23	1.88	0.73
1:B:366:LEU:C	1:B:366:LEU:HD12	2.15	0.72
1:C:731:ILE:CD1	1:C:804:PHE:O	2.37	0.72
1:A:888:LEU:HD13	1:A:901:VAL:CG1	2.20	0.72
1:A:393:LEU:O	1:A:470:PHE:CE1	2.43	0.72
1:B:162:MET:HE3	1:B:317:PHE:CZ	2.23	0.72
1:A:919:ARG:NH1	1:A:1005:THR:CG2	2.53	0.72
1:C:112:GLN:HE21	1:C:115:MET:HE1	1.55	0.72
1:A:596:HIS:O	1:A:600:THR:HG22	1.89	0.72
1:C:937:LEU:HD21	1:C:1011:MET:SD	2.30	0.72
1:A:156:ASP:OD1	1:A:182:TYR:CD2	2.42	0.72
1:A:454:VAL:N	1:A:455:PRO:CD	2.53	0.71
1:C:115:MET:N	1:C:116:PRO:HD2	2.06	0.71
1:A:907:LEU:CD2	1:A:1018:ALA:CA	2.67	0.71
1:C:399:VAL:HG13	1:C:400:LEU:HD12	1.72	0.71
1:C:597:TYR:CD1	1:C:601:LYS:HD2	2.24	0.71
1:A:568:ASP:O	1:A:570:GLY:N	2.23	0.71
1:C:790:TYR:HB3	1:C:798:MET:HB3	1.73	0.71
1:C:404:LEU:HD21	1:C:937:LEU:HD12	1.72	0.71
1:A:897:ILE:HG23	1:A:898:PRO:CD	2.16	0.71
1:B:801:PHE:C	1:B:803:ALA:H	1.98	0.71
1:C:419:VAL:HG22	1:C:433:LYS:HZ1	1.56	0.71
1:C:489:THR:HG22	1:C:490:PRO:CD	2.07	0.71
1:A:843:LEU:H	1:A:843:LEU:HD12	1.53	0.71
1:B:35:TYR:CD1	1:B:671:ILE:HD11	2.25	0.70
1:B:701:GLN:O	1:B:705:GLU:CB	2.39	0.70
1:B:909:VAL:O	1:B:913:LEU:HG	1.91	0.70
1:A:678:THR:O	1:A:712:MET:CE	2.39	0.70
1:B:157:TYR:CE2	1:B:318:PRO:HG2	2.27	0.70
1:B:314:GLU:N	1:B:315:PRO:CD	2.53	0.70
1:A:404:LEU:CD2	1:A:937:LEU:HD13	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ILE:CD1	1:B:289:LEU:CD1	2.70	0.70
1:A:892:TYR:HB2	1:A:897:ILE:HG21	1.73	0.70
1:B:678:THR:HG22	1:B:830:GLN:HB2	1.73	0.70
1:B:419:VAL:CG1	1:B:433:LYS:HE3	2.22	0.70
1:C:904:VAL:HG22	1:C:1025:PHE:CE1	2.27	0.70
1:A:23:GLY:O	1:A:27:ILE:HG13	1.92	0.70
1:B:210:GLN:HG3	1:C:733:GLN:HE22	1.56	0.70
1:C:958:LYS:NZ	1:C:962:GLU:HG3	2.07	0.70
1:C:1025:PHE:HA	1:C:1028:VAL:HG12	1.72	0.70
1:A:535:LEU:HD23	1:A:965:LEU:HD21	1.74	0.70
1:A:702:LEU:HD23	1:A:702:LEU:O	1.91	0.70
1:A:888:LEU:HD11	1:A:901:VAL:HG11	1.73	0.69
1:A:911:GLY:CA	1:A:1009:GLY:O	2.38	0.69
1:B:896:SER:HA	1:B:899:PHE:HD2	1.56	0.69
1:C:317:PHE:CE2	1:C:321:LEU:HD22	2.26	0.69
1:B:538:THR:O	1:B:542:LEU:HD13	1.92	0.69
1:A:184:MET:SD	1:A:243:THR:HG22	2.31	0.69
1:A:466:ILE:HG22	1:A:466:ILE:O	1.91	0.69
1:A:568:ASP:OD2	1:A:634:TRP:CD1	2.45	0.69
1:C:162:MET:HE1	1:C:317:PHE:CZ	2.28	0.69
1:B:366:LEU:CA	1:B:369:THR:HG22	2.22	0.69
1:C:347:ALA:HB1	1:C:402:ILE:HD11	1.75	0.69
1:B:182:TYR:HB3	1:B:270:LEU:HD11	1.74	0.69
1:A:5:PHE:CE2	1:A:487:ILE:HG23	2.28	0.69
1:A:703:LEU:HD11	1:A:718:PRO:HD3	1.73	0.69
1:A:960:LEU:HD12	1:A:1030:ARG:HG2	1.69	0.69
1:C:115:MET:H	1:C:116:PRO:CD	2.03	0.68
1:C:347:ALA:HB1	1:C:402:ILE:CD1	2.23	0.68
1:A:32:VAL:HG22	1:A:390:ILE:CD1	2.23	0.68
1:A:355:MET:CE	1:A:365:THR:HA	2.20	0.68
1:A:919:ARG:NH1	1:A:1005:THR:HG21	2.09	0.68
1:C:885:PHE:HD2	1:C:902:MET:HG3	1.58	0.68
1:B:733:GLN:OE1	1:B:743:ILE:CD1	2.42	0.68
1:A:372:VAL:HG23	1:A:405:LEU:CD2	2.23	0.68
1:A:568:ASP:C	1:A:570:GLY:H	2.01	0.68
1:A:679:GLY:CA	1:A:712:MET:HE3	2.15	0.68
1:A:961:ILE:HD11	1:A:1031:ARG:HH22	1.59	0.68
1:B:15:ILE:O	1:B:18:ILE:HG13	1.94	0.68
1:B:366:LEU:HA	1:B:369:THR:CG2	2.23	0.68
1:A:535:LEU:HD12	1:A:535:LEU:O	1.94	0.68
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:PHE:CE1	1:B:876:LEU:HD12	2.29	0.67
1:B:895:TRP:CE2	1:A:10:ILE:CD1	2.77	0.67
1:C:446:ALA:CB	1:C:482:VAL:CG2	2.71	0.67
1:A:30:LEU:HD21	1:A:390:ILE:N	2.09	0.67
1:A:907:LEU:HD11	1:A:1017:LEU:HG	1.74	0.67
1:B:196:PHE:HD2	1:B:260:VAL:HG11	1.59	0.67
1:C:419:VAL:HG22	1:C:433:LYS:NZ	2.10	0.67
1:B:366:LEU:C	1:B:369:THR:HG22	2.19	0.67
1:A:438:ILE:HG22	1:A:438:ILE:O	1.94	0.67
1:A:680:PHE:O	1:A:680:PHE:CD1	2.47	0.67
1:B:905:VAL:N	1:B:906:PRO:HD2	2.09	0.67
1:B:189:ASN:C	1:B:193:LEU:HD13	2.20	0.67
1:C:111:LEU:HD21	1:C:127:VAL:HG11	1.74	0.67
1:C:197:GLN:CG	1:C:798:MET:HE1	2.25	0.67
1:C:372:VAL:HG12	1:C:405:LEU:HD11	1.76	0.67
1:C:952:LEU:O	1:C:956:GLU:CB	2.43	0.67
1:B:815:ARG:NH2	1:B:817:GLU:OE2	2.28	0.67
1:C:317:PHE:CG	1:C:321:LEU:HD22	2.30	0.67
1:A:843:LEU:HD12	1:A:843:LEU:N	2.09	0.67
1:B:552:MET:HG3	1:B:910:ILE:HD13	1.76	0.66
1:B:892:TYR:O	1:B:893:GLU:CG	2.43	0.66
1:C:347:ALA:CB	1:C:402:ILE:CD1	2.73	0.66
1:A:873:ALA:CB	1:A:874:PRO:CD	2.71	0.66
1:B:616:GLY:HA2	1:B:626:ILE:HG12	1.78	0.66
1:A:908:GLY:HA3	1:A:1014:ALA:CB	2.25	0.66
1:C:30:LEU:HD21	1:C:384:ALA:CA	2.25	0.66
1:B:367:ILE:N	1:B:368:PRO:CD	2.59	0.66
1:B:896:SER:HA	1:B:899:PHE:CD2	2.30	0.66
1:C:53:ASP:OD1	1:C:53:ASP:O	2.14	0.66
1:A:29:LYS:HZ3	1:A:29:LYS:HB2	1.61	0.66
1:A:1011:MET:O	1:A:1015:THR:HG23	1.96	0.66
1:B:166:ILE:CD1	1:B:289:LEU:HD13	2.24	0.66
1:A:372:VAL:HG23	1:A:405:LEU:HD23	1.78	0.66
1:A:712:MET:O	1:A:712:MET:HG3	1.96	0.66
1:A:905:VAL:N	1:A:906:PRO:CD	2.58	0.66
1:B:20:MET:HG2	1:B:377:LEU:HD12	1.78	0.66
1:B:375:VAL:CG2	1:B:484:VAL:HG11	2.26	0.66
1:A:38:ILE:HD11	1:A:671:ILE:HG13	1.78	0.66
1:C:228:GLN:OE1	1:C:228:GLN:HA	1.96	0.65
1:A:671:ILE:HG22	1:A:672:VAL:H	1.60	0.65
1:A:974:PRO:HA	1:A:977:MET:HG2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:ILE:HG23	1:A:1008:MET:HE2	1.78	0.65
1:B:169:THR:HG21	1:B:306:ILE:CD1	2.26	0.65
1:A:5:PHE:O	1:A:491:ALA:HB2	1.96	0.65
1:A:699:ARG:NH1	1:A:718:PRO:HG3	2.12	0.65
1:B:435:MET:CE	1:B:490:PRO:CG	2.75	0.65
1:B:136:PHE:CE2	1:B:176:GLN:HG2	2.31	0.65
1:C:277:ILE:HD11	1:C:620:ARG:NH2	2.11	0.65
1:C:904:VAL:HG12	1:C:904:VAL:O	1.97	0.65
1:A:493:CYS:HA	1:A:497:LEU:HD23	1.79	0.65
1:C:197:GLN:HG2	1:C:798:MET:HE1	1.77	0.65
1:A:268:ILE:HD12	1:A:268:ILE:N	2.11	0.65
1:A:912:ALA:HB1	1:A:927:PHE:CE1	2.32	0.65
1:B:163:LYS:HE3	1:B:177:LEU:HD22	1.77	0.64
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.33	0.64
1:A:31:PRO:O	1:A:389:SER:HB2	1.96	0.64
1:A:888:LEU:HD13	1:A:901:VAL:HG11	1.77	0.64
1:B:895:TRP:NE1	1:A:10:ILE:HD11	2.12	0.64
1:B:185:ARG:NH2	1:B:273:GLU:O	2.29	0.64
1:A:396:PHE:HA	1:A:399:VAL:HG12	1.80	0.64
1:C:904:VAL:CG2	1:C:1025:PHE:HE1	2.11	0.64
1:A:953:MET:O	1:A:953:MET:HG3	1.98	0.64
1:B:801:PHE:O	1:B:803:ALA:N	2.30	0.64
1:C:904:VAL:HG21	1:C:1022:VAL:HG12	1.79	0.64
1:A:535:LEU:CD2	1:A:965:LEU:CD2	2.76	0.64
1:A:842:GLU:O	1:A:844:MET:CE	2.46	0.64
1:B:639:GLY:O	1:B:643:LYS:HE2	1.98	0.63
1:C:162:MET:CE	1:C:317:PHE:HE1	2.10	0.63
1:A:415:ASN:ND2	1:A:438:ILE:HD13	2.12	0.63
1:B:314:GLU:N	1:B:315:PRO:HD2	2.13	0.63
1:B:438:ILE:O	1:B:438:ILE:HG13	1.97	0.63
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.80	0.63
1:C:419:VAL:CG2	1:C:433:LYS:NZ	2.61	0.63
1:C:483:LEU:HD12	1:C:487:ILE:CD1	2.28	0.63
1:A:555:LEU:HD21	1:A:914:LEU:CD2	2.28	0.63
1:B:202:ASP:CG	1:B:792:ARG:NH2	2.57	0.63
1:A:569:GLN:NE2	1:A:669:PRO:O	2.32	0.63
1:B:137:LEU:HD21	1:B:293:LEU:HB2	1.79	0.63
1:A:842:GLU:O	1:A:844:MET:HE3	1.98	0.63
1:A:425:LEU:CG	1:A:426:PRO:HD2	2.29	0.63
1:B:892:TYR:C	1:B:893:GLU:HG2	2.24	0.63
1:B:907:LEU:HD12	1:B:907:LEU:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:TYR:HE1	1:B:907:LEU:HD11	1.62	0.63
1:C:162:MET:HE1	1:C:317:PHE:HE1	1.61	0.63
1:C:446:ALA:HA	1:C:478:MET:HE3	1.79	0.63
1:A:888:LEU:HD11	1:A:901:VAL:CG1	2.27	0.63
1:B:222:THR:HA	1:B:224:PRO:HD3	1.79	0.63
1:C:596:HIS:O	1:C:600:THR:HG22	1.99	0.62
1:C:958:LYS:NZ	1:C:962:GLU:HG2	2.11	0.62
1:B:366:LEU:HD11	1:B:496:MET:SD	2.39	0.62
1:C:483:LEU:CD1	1:C:487:ILE:CD1	2.77	0.62
1:C:664:PHE:CZ	1:C:717:ARG:CD	2.76	0.62
1:B:166:ILE:HD12	1:B:289:LEU:CD1	2.30	0.62
1:C:317:PHE:CE2	1:C:321:LEU:CD2	2.83	0.62
1:A:535:LEU:HD23	1:A:965:LEU:CD2	2.30	0.62
1:A:393:LEU:CG	1:A:470:PHE:CE2	2.83	0.62
1:B:907:LEU:CD1	1:B:907:LEU:H	2.13	0.62
1:A:417:GLU:O	1:A:421:ALA:CB	2.48	0.62
1:C:729:ILE:HG23	1:C:729:ILE:O	2.00	0.62
1:A:873:ALA:CB	1:A:874:PRO:HD3	2.21	0.62
1:A:557:VAL:HG12	1:A:557:VAL:O	2.00	0.61
1:B:142:VAL:HG12	1:B:142:VAL:O	2.00	0.61
1:A:926:TYR:HB3	1:A:1003:VAL:CG1	2.28	0.61
1:C:193:LEU:HD13	1:C:198:LEU:O	2.00	0.61
1:A:181:GLN:HE21	1:A:769:LYS:HE2	1.65	0.61
1:A:693:GLU:O	1:A:697:GLN:HG3	1.99	0.61
1:B:202:ASP:OD1	1:B:792:ARG:NH2	2.33	0.61
1:B:248:LYS:O	1:B:261:LEU:HD22	2.00	0.61
1:C:30:LEU:HD21	1:C:384:ALA:HA	1.82	0.61
1:C:904:VAL:CG2	1:C:1025:PHE:CE1	2.83	0.61
1:A:567:GLU:OE1	1:A:567:GLU:HA	1.99	0.61
1:B:637:ARG:O	1:B:637:ARG:HG3	2.01	0.61
1:A:662:MET:HE3	1:A:664:PHE:HE2	1.66	0.61
1:A:668:LEU:N	1:A:668:LEU:HD12	2.15	0.61
1:A:700:ASN:HA	1:A:703:LEU:HB2	1.83	0.61
1:B:243:THR:HG23	1:B:268:ILE:HG21	1.83	0.61
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.80	0.61
1:A:121:GLU:N	1:A:121:GLU:OE1	2.33	0.61
1:C:195:LYS:HE3	1:C:196:PHE:HE1	1.64	0.61
1:B:15:ILE:HA	1:B:18:ILE:HG12	1.80	0.61
1:C:446:ALA:HA	1:C:478:MET:CE	2.31	0.61
1:A:30:LEU:CG	1:A:31:PRO:HD2	2.30	0.61
1:A:153:ASP:HA	1:A:182:TYR:OH	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:898:PRO:O	1:C:902:MET:HG2	2.01	0.60
1:A:1007:VAL:O	1:A:1011:MET:HG2	2.01	0.60
1:C:355:MET:CE	1:C:410:ILE:HD12	2.30	0.60
1:C:485:ALA:O	1:C:489:THR:HG21	2.01	0.60
1:A:185:ARG:NH2	1:A:272:GLY:O	2.35	0.60
1:A:492:LEU:CD1	1:A:496:MET:HE2	2.31	0.60
1:A:905:VAL:N	1:A:906:PRO:HD2	2.15	0.60
1:B:166:ILE:O	1:B:169:THR:HG22	2.00	0.60
1:A:568:ASP:HA	1:A:644:VAL:CG2	2.31	0.60
1:B:166:ILE:HD13	1:B:289:LEU:HD13	1.81	0.60
1:C:111:LEU:HD21	1:C:127:VAL:CG1	2.30	0.60
1:C:426:PRO:HG2	1:C:429:GLU:HB3	1.83	0.60
1:C:664:PHE:HE2	1:C:717:ARG:CD	2.12	0.60
1:A:907:LEU:HD12	1:A:1017:LEU:CD2	2.30	0.60
1:B:622:GLN:OE1	1:A:231:ASN:ND2	2.34	0.60
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.82	0.60
1:C:879:ILE:O	1:C:883:VAL:HG23	2.01	0.60
1:B:189:ASN:O	1:B:193:LEU:CD1	2.46	0.60
1:C:317:PHE:CD2	1:C:321:LEU:CD2	2.78	0.60
1:A:32:VAL:HG22	1:A:390:ILE:CG1	2.32	0.60
1:A:393:LEU:HA	1:A:470:PHE:HZ	1.60	0.60
1:C:948:PHE:HB2	1:C:971:ARG:NH1	2.16	0.59
1:A:845:GLU:O	1:A:845:GLU:OE1	2.19	0.59
1:B:210:GLN:HG3	1:C:733:GLN:NE2	2.17	0.59
1:A:30:LEU:HD21	1:A:390:ILE:H	1.65	0.59
1:B:678:THR:HG22	1:B:678:THR:O	2.01	0.59
1:A:20:MET:HG2	1:A:377:LEU:HD12	1.83	0.59
1:A:415:ASN:HD22	1:A:438:ILE:HD13	1.61	0.59
1:C:404:LEU:HD21	1:C:937:LEU:CD1	2.32	0.59
1:C:671:ILE:O	1:C:671:ILE:HG13	2.01	0.59
1:A:38:ILE:HD12	1:A:38:ILE:O	2.03	0.59
1:A:445:ILE:HG21	1:A:940:LYS:NZ	2.18	0.59
1:A:713:LEU:HG	1:A:843:LEU:HD21	1.83	0.59
1:C:731:ILE:CD1	1:C:804:PHE:CD1	2.75	0.59
1:A:680:PHE:HZ	1:A:716:VAL:CG2	2.14	0.59
1:A:960:LEU:CD1	1:A:1030:ARG:HG3	2.33	0.59
1:B:197:GLN:CG	1:B:798:MET:HE3	2.32	0.59
1:B:780:ARG:O	1:B:780:ARG:HG3	2.02	0.59
1:C:53:ASP:C	1:C:55:LYS:H	2.11	0.59
1:C:483:LEU:CD1	1:C:487:ILE:HD11	2.32	0.59
1:A:442:LEU:HD11	1:A:486:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:ND2	1:B:149:MET:HB2	2.17	0.59
1:B:882:ILE:O	1:B:886:LEU:HD23	2.03	0.59
1:A:448:VAL:HG23	1:A:449:LEU:HD12	1.85	0.59
1:A:568:ASP:OD2	1:A:634:TRP:HD1	1.84	0.59
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.85	0.59
1:B:419:VAL:HG13	1:B:433:LYS:HE3	1.84	0.59
1:A:414:GLU:OE1	1:A:973:ARG:HG3	2.03	0.59
1:B:100:ALA:HB1	1:B:131:LYS:HD3	1.85	0.59
1:B:287:SER:OG	1:B:288:GLY:N	2.34	0.58
1:A:924:ASP:OD2	1:A:1002:ALA:CB	2.51	0.58
1:B:485:ALA:O	1:B:489:THR:OG1	2.20	0.58
1:B:53:ASP:OD1	1:B:53:ASP:N	2.37	0.58
1:B:184:MET:HB3	1:B:771:VAL:HG22	1.85	0.58
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.85	0.58
1:B:886:LEU:HD12	1:A:14:VAL:HG22	1.85	0.58
1:C:10:ILE:CD1	1:A:895:TRP:NE1	2.66	0.58
1:B:435:MET:CE	1:B:490:PRO:HG3	2.34	0.58
1:A:685:ILE:CD1	1:A:858:ASP:OD2	2.52	0.58
1:B:579:PRO:HG3	1:B:660:ASP:OD2	2.03	0.58
1:C:317:PHE:CZ	1:C:323:ILE:HD11	2.37	0.58
1:B:706:ALA:CB	1:B:847:LEU:HD21	2.34	0.58
1:A:912:ALA:HB1	1:A:927:PHE:CZ	2.38	0.58
1:A:600:THR:HG23	1:A:601:LYS:H	1.67	0.58
1:B:188:MET:HE1	1:B:200:PRO:HB3	1.86	0.58
1:B:415:ASN:OD1	1:B:418:ARG:NH2	2.29	0.58
1:C:368:PRO:CB	1:C:410:ILE:HD13	2.33	0.58
1:A:917:THR:O	1:A:917:THR:HG22	2.04	0.58
1:B:207:ILE:HG23	1:B:759:VAL:HG11	1.86	0.57
1:A:897:ILE:N	1:A:898:PRO:HD2	2.18	0.57
1:A:911:GLY:HA3	1:A:1009:GLY:C	2.28	0.57
1:B:366:LEU:O	1:B:369:THR:HG22	2.04	0.57
1:B:885:PHE:HD1	1:B:886:LEU:HD22	1.69	0.57
1:A:393:LEU:HA	1:A:470:PHE:CE1	2.40	0.57
1:A:897:ILE:N	1:A:898:PRO:CD	2.67	0.57
1:A:339:GLU:OE1	1:A:339:GLU:HA	2.03	0.57
1:B:435:MET:HE2	1:B:490:PRO:CG	2.35	0.57
1:B:441:ALA:O	1:B:445:ILE:HG12	2.04	0.57
1:C:383:LEU:HD21	1:C:394:THR:HG21	1.87	0.57
1:A:960:LEU:C	1:A:960:LEU:HD23	2.30	0.57
1:B:419:VAL:HG11	1:B:433:LYS:HE3	1.86	0.57
1:C:287:SER:OG	1:C:288:GLY:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:THR:HG22	1:B:584:GLN:H	1.68	0.57
1:C:443:VAL:HG12	1:C:443:VAL:O	2.04	0.57
1:A:32:VAL:CG2	1:A:390:ILE:HD11	2.35	0.57
1:A:425:LEU:CD2	1:A:429:GLU:CB	2.80	0.57
1:A:907:LEU:CD2	1:A:1018:ALA:CB	2.83	0.57
1:B:4:PHE:HE2	1:B:11:PHE:CE2	2.23	0.57
1:B:728:LYS:HB2	1:B:810:GLU:OE2	2.04	0.57
1:C:483:LEU:HD13	1:C:487:ILE:HD11	1.85	0.57
1:A:544:LEU:HA	1:A:547:ILE:HD12	1.85	0.57
1:B:2:PRO:HD3	1:B:439:GLN:HE22	1.70	0.57
1:B:423:GLU:OE1	1:B:433:LYS:HE2	2.05	0.57
1:C:355:MET:HE1	1:C:410:ILE:HD12	1.87	0.57
1:A:156:ASP:CB	1:A:182:TYR:CE2	2.87	0.57
1:B:2:PRO:HD3	1:B:439:GLN:NE2	2.20	0.56
1:A:568:ASP:HA	1:A:644:VAL:HG21	1.86	0.56
1:A:884:VAL:O	1:A:888:LEU:HG	2.04	0.56
1:B:895:TRP:CZ2	1:A:10:ILE:HD13	2.38	0.56
1:A:268:ILE:H	1:A:268:ILE:CD1	2.18	0.56
1:A:662:MET:HE3	1:A:664:PHE:CE2	2.39	0.56
1:B:251:LEU:HD11	1:B:262:LEU:HD23	1.86	0.56
1:B:757:SER:HB3	1:B:773:VAL:HG22	1.88	0.56
1:C:40:PRO:HD2	1:C:674:LEU:CD2	2.27	0.56
1:A:921:LEU:CD1	1:A:1005:THR:OG1	2.53	0.56
1:A:1019:ILE:HG13	1:A:1020:PHE:N	2.19	0.56
1:B:58:GLN:HE21	1:B:816:LEU:HB2	1.69	0.56
1:B:185:ARG:HG2	1:B:187:TRP:CZ2	2.40	0.56
1:A:892:TYR:HB2	1:A:897:ILE:CG2	2.35	0.56
1:B:909:VAL:O	1:B:909:VAL:HG12	2.04	0.56
1:C:347:ALA:CB	1:C:402:ILE:HD11	2.35	0.56
1:C:575:MET:HE1	1:C:717:ARG:NH1	2.20	0.56
1:B:197:GLN:HG3	1:B:798:MET:CE	2.34	0.56
1:B:355:MET:SD	1:B:368:PRO:CG	2.91	0.56
1:C:135:SER:OG	1:C:672:VAL:HB	2.05	0.56
1:A:5:PHE:CZ	1:A:487:ILE:HG23	2.41	0.56
1:A:115:MET:O	1:A:123:GLN:NE2	2.38	0.56
1:B:591:LEU:HD12	1:B:611:ALA:HB1	1.88	0.56
1:A:910:ILE:HB	1:A:1013:THR:HG21	1.87	0.56
1:B:162:MET:HE1	1:B:317:PHE:CZ	2.34	0.56
1:C:486:LEU:O	1:C:486:LEU:HG	2.05	0.56
1:B:552:MET:HB2	1:B:910:ILE:HD11	1.87	0.56
1:A:717:ARG:HB2	1:A:718:PRO:CD	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:HB3	1:B:153:ASP:CB	2.34	0.55
1:C:758:TYR:CE1	1:C:770:LYS:HG2	2.41	0.55
1:A:156:ASP:OD2	1:A:182:TYR:CE2	2.58	0.55
1:A:600:THR:CG2	1:A:601:LYS:N	2.69	0.55
1:B:210:GLN:O	1:B:210:GLN:HG2	2.06	0.55
1:C:6:ILE:HG22	1:C:6:ILE:O	2.07	0.55
1:C:419:VAL:HG13	1:C:433:LYS:NZ	2.20	0.55
1:C:903:LEU:N	1:C:903:LEU:HD12	2.20	0.55
1:B:907:LEU:N	1:B:907:LEU:CD1	2.70	0.55
1:C:23:GLY:HA3	1:C:377:LEU:O	2.07	0.55
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.39	0.55
1:B:197:GLN:CB	1:B:798:MET:HE3	2.36	0.55
1:A:435:MET:HG2	1:A:490:PRO:HG3	1.88	0.55
1:A:1021:PHE:O	1:A:1024:VAL:N	2.39	0.55
1:B:310:LEU:HD12	1:B:323:ILE:HD13	1.89	0.55
1:A:32:VAL:HG22	1:A:390:ILE:HG13	1.88	0.55
1:A:358:PHE:HD2	1:A:977:MET:HB3	1.72	0.55
1:A:438:ILE:O	1:A:438:ILE:CG2	2.54	0.55
1:A:583:THR:HG22	1:A:584:GLN:H	1.71	0.55
1:B:713:LEU:HD11	1:B:843:LEU:HD23	1.88	0.55
1:A:393:LEU:CG	1:A:470:PHE:CZ	2.89	0.55
1:B:275:TYR:HD2	1:A:223:PRO:HD3	1.71	0.55
1:A:466:ILE:O	1:A:466:ILE:CG2	2.55	0.55
1:B:85:THR:HG21	1:B:620:ARG:O	2.07	0.55
1:C:419:VAL:CG1	1:C:433:LYS:NZ	2.70	0.55
1:A:644:VAL:HG21	1:A:667:ASN:ND2	2.22	0.55
1:B:143:ILE:HD12	1:B:284:GLN:OE1	2.07	0.54
1:B:157:TYR:CE1	1:B:161:ASN:ND2	2.74	0.54
1:B:144:ASN:HD22	1:B:154:ILE:HD11	1.59	0.54
1:C:10:ILE:CD1	1:A:895:TRP:CE2	2.90	0.54
1:C:253:VAL:HG23	1:C:259:ARG:HG2	1.89	0.54
1:A:417:GLU:O	1:A:421:ALA:HB2	2.07	0.54
1:C:419:VAL:CG2	1:C:433:LYS:HZ1	2.20	0.54
1:A:149:MET:HE1	1:A:321:LEU:HD12	1.89	0.54
1:B:423:GLU:HB3	1:B:425:LEU:HD13	1.89	0.54
1:C:53:ASP:O	1:C:53:ASP:CG	2.48	0.54
1:C:311:ALA:HA	1:C:314:GLU:HG3	1.88	0.54
1:A:843:LEU:CD1	1:A:843:LEU:N	2.65	0.54
1:B:356:TYR:HA	1:B:365:THR:HG21	1.90	0.54
1:B:610:PHE:HB3	1:B:628:PHE:HB2	1.89	0.54
1:B:671:ILE:HG22	1:B:672:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:882:ILE:O	1:C:886:LEU:HG	2.07	0.54
1:A:416:VAL:HG22	1:A:434:SER:OG	2.07	0.54
1:A:567:GLU:OE2	1:A:998:GLY:N	2.41	0.54
1:B:69:MET:HE1	1:B:107:VAL:HG13	1.89	0.54
1:B:249:ILE:O	1:B:261:LEU:HD23	2.08	0.54
1:B:435:MET:HE2	1:B:490:PRO:HG2	1.89	0.54
1:C:885:PHE:CD1	1:C:885:PHE:C	2.86	0.54
1:A:5:PHE:O	1:A:491:ALA:CB	2.55	0.54
1:A:668:LEU:N	1:A:668:LEU:CD1	2.71	0.54
1:B:640:GLU:OE2	1:B:640:GLU:HA	2.06	0.54
1:C:716:VAL:HG23	1:C:716:VAL:O	2.08	0.54
1:C:958:LYS:HZ1	1:C:962:GLU:CG	2.09	0.54
1:B:169:THR:HG21	1:B:306:ILE:HD11	1.88	0.54
1:C:600:THR:HG23	1:C:601:LYS:HG3	1.90	0.54
1:C:702:LEU:HD12	1:C:851:LEU:HD11	1.89	0.54
1:B:78:MET:HE2	1:B:92:LEU:HD21	1.89	0.54
1:B:370:ILE:HG13	1:B:370:ILE:O	2.06	0.54
1:B:448:VAL:HG23	1:B:884:VAL:HG22	1.90	0.53
1:B:706:ALA:HB2	1:B:847:LEU:HD21	1.89	0.53
1:C:405:LEU:C	1:C:405:LEU:HD12	2.34	0.53
1:A:30:LEU:HD22	1:A:390:ILE:CG1	2.31	0.53
1:B:552:MET:HG3	1:B:910:ILE:CD1	2.38	0.53
1:C:399:VAL:HG13	1:C:400:LEU:CD1	2.38	0.53
1:A:27:ILE:O	1:A:27:ILE:HG22	2.07	0.53
1:A:302:THR:O	1:A:306:ILE:HG12	2.09	0.53
1:B:149:MET:CE	1:B:321:LEU:CD1	2.77	0.53
1:B:197:GLN:HA	1:B:798:MET:HE1	1.85	0.53
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.89	0.53
1:C:8:ARG:O	1:C:8:ARG:HG3	2.09	0.53
1:A:352:PHE:HD1	1:A:369:THR:OG1	1.91	0.53
1:A:355:MET:HE2	1:A:365:THR:CA	2.32	0.53
1:A:445:ILE:HG21	1:A:940:LYS:HZ3	1.74	0.53
1:A:174:ASP:HB3	1:A:292:LYS:HD2	1.91	0.53
1:A:907:LEU:CD2	1:A:1018:ALA:HB2	2.33	0.53
1:A:709:HIS:C	1:A:709:HIS:CD2	2.86	0.53
1:B:137:LEU:HD11	1:B:293:LEU:CB	2.38	0.53
1:B:277:ILE:CD1	1:B:615:PHE:HB2	2.39	0.53
1:B:703:LEU:C	1:B:705:GLU:H	2.15	0.53
1:C:928:GLN:O	1:C:932:LEU:CD1	2.52	0.53
1:A:680:PHE:HZ	1:A:716:VAL:HG21	1.74	0.53
1:B:795:ASP:OD1	1:B:796:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HG	1:A:429:GLU:HB2	1.89	0.53
1:B:157:TYR:CE2	1:B:318:PRO:CG	2.91	0.53
1:B:568:ASP:HA	1:B:644:VAL:HG21	1.91	0.53
1:B:872:GLN:O	1:B:872:GLN:HG3	2.08	0.53
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.39	0.53
1:A:699:ARG:HH11	1:A:718:PRO:HB3	1.73	0.53
1:C:22:ALA:O	1:C:381:ALA:HB2	2.08	0.53
1:A:560:PRO:C	1:A:923:ASN:OD1	2.52	0.53
1:B:193:LEU:HD12	1:B:265:VAL:HB	1.91	0.52
1:B:721:LEU:HB2	1:B:814:PRO:HG2	1.89	0.52
1:C:935:ILE:HG22	1:C:935:ILE:O	2.09	0.52
1:B:143:ILE:HG21	1:B:281:PHE:HB3	1.91	0.52
1:C:281:PHE:CZ	1:C:324:VAL:HG11	2.44	0.52
1:C:347:ALA:HB3	1:C:402:ILE:CD1	2.39	0.52
1:A:184:MET:HB3	1:A:771:VAL:HG22	1.91	0.52
1:C:317:PHE:HE2	1:C:323:ILE:HG12	1.75	0.52
1:A:416:VAL:O	1:A:420:MET:N	2.40	0.52
1:A:425:LEU:CG	1:A:429:GLU:HB2	2.40	0.52
1:B:197:GLN:CB	1:B:798:MET:CE	2.88	0.52
1:C:695:LEU:HB2	1:C:825:MET:HE1	1.91	0.52
1:C:664:PHE:CE2	1:C:717:ARG:HD2	2.44	0.52
1:A:425:LEU:CD1	1:A:426:PRO:CD	2.55	0.52
1:B:407:ASP:O	1:B:411:VAL:HG23	2.10	0.52
1:A:393:LEU:HD11	1:A:466:ILE:HG23	1.92	0.52
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.10	0.52
1:B:879:ILE:HG23	1:A:21:LEU:HD11	1.92	0.52
1:B:901:VAL:HG12	1:B:946:VAL:HG21	1.92	0.52
1:C:16:ALA:O	1:C:20:MET:HG3	2.10	0.52
1:A:454:VAL:N	1:A:455:PRO:HD3	2.25	0.51
1:C:415:ASN:OD1	1:C:434:SER:HB2	2.10	0.51
1:C:489:THR:HG23	1:C:490:PRO:N	2.23	0.51
1:A:896:SER:H	1:A:898:PRO:HD2	1.75	0.51
1:B:713:LEU:CD1	1:B:843:LEU:HD23	2.40	0.51
1:C:419:VAL:HG13	1:C:433:LYS:HZ1	1.74	0.51
1:A:703:LEU:CD1	1:A:718:PRO:HD3	2.38	0.51
1:A:38:ILE:HG22	1:A:465:ALA:HB3	1.92	0.51
1:B:314:GLU:H	1:B:315:PRO:CD	2.24	0.51
1:B:744:ASN:O	1:B:748:THR:HG22	2.10	0.51
1:B:1011:MET:HE3	1:B:1011:MET:HA	1.93	0.51
1:C:530:SER:O	1:C:534:ILE:HD12	2.10	0.51
1:A:367:ILE:HG12	1:A:492:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:SER:HA	1:A:899:PHE:HD2	1.75	0.51
1:C:671:ILE:CG1	1:C:862:MET:SD	2.99	0.51
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.11	0.51
1:B:243:THR:HG23	1:B:268:ILE:CG2	2.40	0.51
1:B:913:LEU:HD23	1:B:927:PHE:HZ	1.76	0.51
1:A:222:THR:HA	1:A:224:PRO:HD3	1.92	0.51
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.92	0.50
1:B:157:TYR:O	1:B:161:ASN:HB2	2.12	0.50
1:B:800:PRO:O	1:B:804:PHE:CE2	2.63	0.50
1:B:898:PRO:O	1:B:902:MET:HG2	2.12	0.50
1:C:412:VAL:O	1:C:416:VAL:HG23	2.11	0.50
1:C:877:TYR:HE1	1:C:932:LEU:CD1	2.24	0.50
1:A:919:ARG:NH1	1:A:1005:THR:HG22	2.26	0.50
1:B:32:VAL:HG22	1:B:390:ILE:HB	1.91	0.50
1:C:115:MET:O	1:C:122:VAL:HG22	2.10	0.50
1:C:903:LEU:CD1	1:C:903:LEU:N	2.75	0.50
1:A:907:LEU:HD12	1:A:1017:LEU:HD21	1.90	0.50
1:C:944:LEU:O	1:C:971:ARG:NH1	2.38	0.50
1:C:53:ASP:O	1:C:55:LYS:N	2.45	0.50
1:C:671:ILE:HD12	1:C:674:LEU:HG	1.93	0.50
1:C:980:LEU:O	1:C:984:LEU:HB2	2.11	0.50
1:B:390:ILE:HG23	1:B:395:MET:SD	2.51	0.50
1:C:419:VAL:HG13	1:C:433:LYS:CE	2.42	0.50
1:C:442:LEU:C	1:C:442:LEU:HD12	2.37	0.50
1:A:30:LEU:HG	1:A:31:PRO:CD	2.34	0.50
1:A:415:ASN:O	1:A:419:VAL:HG23	2.11	0.50
1:A:416:VAL:O	1:A:420:MET:CB	2.60	0.50
1:A:643:LYS:O	1:A:647:ILE:HG12	2.11	0.50
1:A:889:ALA:HA	1:A:898:PRO:HG3	1.94	0.50
1:B:138:MET:HE3	1:B:325:TYR:HD2	1.76	0.50
1:C:81:ASN:HD22	1:C:815:ARG:NH2	2.09	0.50
1:A:13:TRP:CZ2	1:A:492:LEU:HD13	2.47	0.50
1:A:919:ARG:HH11	1:A:1005:THR:CG2	2.24	0.50
1:B:224:PRO:HA	1:C:781:MET:HE1	1.94	0.50
1:C:575:MET:HG2	1:C:666:PHE:HE2	1.77	0.50
1:A:350:LEU:O	1:A:354:VAL:CG2	2.43	0.50
1:A:937:LEU:HD23	1:A:1011:MET:HE1	1.94	0.50
1:B:895:TRP:CE2	1:A:10:ILE:HD11	2.45	0.49
1:B:157:TYR:CZ	1:B:161:ASN:ND2	2.80	0.49
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.13	0.49
1:C:370:ILE:O	1:C:373:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:556:PHE:HD1	1:C:913:LEU:HD11	1.78	0.49
1:A:5:PHE:HE2	1:A:15:ILE:HD12	1.76	0.49
1:A:429:GLU:OE2	1:A:429:GLU:N	2.43	0.49
1:A:702:LEU:C	1:A:702:LEU:CD2	2.85	0.49
1:A:719:ASN:ND2	1:A:826:GLU:OE2	2.41	0.49
1:B:144:ASN:HA	1:B:320:GLY:O	2.12	0.49
1:C:904:VAL:HG22	1:C:1025:PHE:CZ	2.47	0.49
1:A:450:SER:O	1:A:454:VAL:HG23	2.12	0.49
1:B:518:ARG:HA	1:B:521:GLU:HG2	1.93	0.49
1:A:493:CYS:O	1:A:497:LEU:HB2	2.12	0.49
1:B:312:LYS:O	1:B:312:LYS:HG2	2.12	0.49
1:C:423:GLU:OE1	1:C:433:LYS:HE2	2.13	0.49
1:C:937:LEU:HD23	1:C:937:LEU:O	2.13	0.49
1:A:156:ASP:CB	1:A:182:TYR:CZ	2.95	0.49
1:A:363:ARG:HD2	1:A:496:MET:HB3	1.94	0.49
1:C:118:LEU:HD23	1:C:118:LEU:N	2.27	0.49
1:A:83:ASP:HB3	1:A:815:ARG:HG2	1.94	0.49
1:A:367:ILE:HG23	1:A:492:LEU:HD23	1.94	0.49
1:A:907:LEU:HD21	1:A:1018:ALA:N	2.26	0.49
1:B:166:ILE:HD12	1:B:289:LEU:HD13	1.94	0.49
1:C:195:LYS:HG2	1:C:196:PHE:CD1	2.48	0.49
1:A:671:ILE:CG2	1:A:672:VAL:H	2.22	0.49
1:C:429:GLU:O	1:C:429:GLU:HG3	2.12	0.49
1:A:401:ALA:O	1:A:405:LEU:HB2	2.12	0.49
1:A:894:SER:HB2	1:A:897:ILE:CG2	2.43	0.49
1:A:923:ASN:OD1	1:A:923:ASN:N	2.45	0.49
1:C:904:VAL:O	1:C:904:VAL:CG1	2.61	0.49
1:A:744:ASN:O	1:A:748:THR:HG22	2.12	0.49
1:B:730:ASP:OD1	1:B:730:ASP:N	2.44	0.48
1:C:256:ASP:OD1	1:C:256:ASP:N	2.45	0.48
1:B:115:MET:O	1:B:123:GLN:NE2	2.46	0.48
1:B:197:GLN:CA	1:B:798:MET:HE1	2.39	0.48
1:C:162:MET:CE	1:C:317:PHE:CE1	2.87	0.48
1:C:369:THR:O	1:C:372:VAL:HG22	2.12	0.48
1:A:375:VAL:HB	1:A:405:LEU:HD11	1.96	0.48
1:B:173:GLY:N	1:B:292:LYS:O	2.44	0.48
1:C:72:ILE:HG21	1:C:94:PHE:HE1	1.78	0.48
1:C:423:GLU:HG2	1:C:425:LEU:HG	1.95	0.48
1:C:483:LEU:HD13	1:C:487:ILE:CD1	2.43	0.48
1:C:595:THR:HG23	1:C:609:VAL:CG2	2.38	0.48
1:B:302:THR:O	1:B:306:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:SER:O	1:B:1029:VAL:HG21	2.14	0.48
1:C:115:MET:H	1:C:116:PRO:HD3	1.77	0.48
1:C:851:LEU:HB3	1:C:852:PRO:CD	2.38	0.48
1:A:926:TYR:CB	1:A:1003:VAL:HG13	2.35	0.48
1:B:2:PRO:HG3	1:B:439:GLN:OE1	2.13	0.48
1:B:661:ALA:O	1:B:663:VAL:N	2.46	0.48
1:B:1028:VAL:HA	1:B:1031:ARG:HG3	1.96	0.48
1:C:579:PRO:HG2	1:C:660:ASP:CG	2.38	0.48
1:A:38:ILE:HD12	1:A:671:ILE:HG21	1.95	0.48
1:B:35:TYR:CG	1:B:671:ILE:HD11	2.48	0.48
1:B:895:TRP:CE2	1:A:10:ILE:HD12	2.48	0.48
1:C:483:LEU:HD12	1:C:487:ILE:HD12	1.94	0.48
1:B:568:ASP:CG	1:B:644:VAL:HG13	2.39	0.48
1:C:39:ALA:CB	1:C:673:GLU:CB	2.92	0.48
1:C:72:ILE:HD12	1:C:72:ILE:H	1.78	0.48
1:A:600:THR:CG2	1:A:601:LYS:H	2.26	0.48
1:A:842:GLU:HA	1:A:842:GLU:OE1	2.14	0.48
1:A:961:ILE:O	1:A:961:ILE:HG22	2.14	0.48
1:C:354:VAL:HG22	1:C:984:LEU:CD1	2.40	0.48
1:A:544:LEU:HA	1:A:547:ILE:CD1	2.44	0.48
1:B:330:THR:N	1:B:331:PRO:HD2	2.28	0.48
1:C:10:ILE:HG23	1:A:895:TRP:HE1	1.79	0.48
1:B:202:ASP:CG	1:B:792:ARG:HH21	2.21	0.47
1:A:5:PHE:CD2	1:A:487:ILE:CG2	2.97	0.47
1:A:356:TYR:O	1:A:359:LEU:O	2.32	0.47
1:A:685:ILE:HG22	1:A:687:GLN:HG2	1.96	0.47
1:A:926:TYR:O	1:A:1003:VAL:HG12	2.14	0.47
1:C:376:LEU:O	1:C:380:PHE:CD2	2.67	0.47
1:C:483:LEU:CD1	1:C:487:ILE:HD12	2.44	0.47
1:A:896:SER:HA	1:A:899:PHE:CD2	2.49	0.47
1:B:792:ARG:HB3	1:B:798:MET:SD	2.54	0.47
1:C:671:ILE:CD1	1:C:674:LEU:HD21	2.44	0.47
1:A:340:VAL:HG22	1:A:396:PHE:CE1	2.48	0.47
1:A:571:VAL:HG23	1:A:630:SER:HA	1.96	0.47
1:B:715:SER:O	1:B:717:ARG:NH1	2.47	0.47
1:B:905:VAL:H	1:B:906:PRO:HD2	1.78	0.47
1:A:149:MET:HE1	1:A:321:LEU:CD1	2.44	0.47
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.95	0.47
1:A:888:LEU:HD13	1:A:901:VAL:HB	1.95	0.47
1:B:70:ASN:HB2	1:A:167:SER:HB3	1.95	0.47
1:B:703:LEU:C	1:B:705:GLU:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ALA:HB1	1:C:131:LYS:HD3	1.97	0.47
1:C:396:PHE:HA	1:C:399:VAL:HG12	1.96	0.47
1:C:667:ASN:OD1	1:C:668:LEU:N	2.46	0.47
1:C:987:MET:O	1:C:991:ILE:HG12	2.15	0.47
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.45	0.47
1:A:911:GLY:CA	1:A:1009:GLY:C	2.88	0.47
1:B:366:LEU:C	1:B:366:LEU:CD1	2.85	0.47
1:B:378:GLY:HA3	1:B:480:LEU:HD21	1.97	0.47
1:B:435:MET:CE	1:B:490:PRO:HG2	2.43	0.47
1:C:115:MET:H	1:C:116:PRO:HD2	1.71	0.47
1:A:491:ALA:O	1:A:495:THR:HG23	2.14	0.47
1:B:915:ALA:HB1	1:B:1005:THR:HG22	1.97	0.47
1:C:414:GLU:OE2	1:C:973:ARG:HD2	2.15	0.47
1:C:579:PRO:CD	1:C:660:ASP:OD1	2.63	0.47
1:B:231:ASN:ND2	1:C:622:GLN:OE1	2.48	0.47
1:B:987:MET:HG3	1:B:991:ILE:HD11	1.96	0.47
1:C:45:ILE:O	1:C:89:GLN:HA	2.15	0.47
1:C:194:ASN:CG	1:C:790:TYR:CD2	2.93	0.47
1:C:453:PHE:HD1	1:C:456:MET:HE2	1.81	0.47
1:C:589:LYS:O	1:C:593:GLU:HG3	2.15	0.47
1:A:680:PHE:CZ	1:A:716:VAL:HG22	2.49	0.47
1:B:169:THR:HG22	1:B:172:VAL:HG21	1.97	0.46
1:B:268:ILE:HG22	1:B:269:GLU:N	2.30	0.46
1:B:438:ILE:CG2	1:B:948:PHE:CE1	2.98	0.46
1:A:888:LEU:HD13	1:A:901:VAL:CB	2.45	0.46
1:B:184:MET:HB2	1:B:762:PHE:CE1	2.50	0.46
1:B:518:ARG:HB2	1:B:518:ARG:NH1	2.30	0.46
1:B:839:GLU:HA	1:B:839:GLU:OE1	2.13	0.46
1:A:254:ASN:HB2	1:A:258:SER:HB3	1.97	0.46
1:A:425:LEU:CG	1:A:426:PRO:CD	2.93	0.46
1:A:433:LYS:O	1:A:437:GLN:HG2	2.15	0.46
1:B:182:TYR:O	1:B:769:LYS:HG3	2.15	0.46
1:C:150:THR:O	1:C:154:ILE:HG13	2.16	0.46
1:A:682:PHE:HD1	1:A:859:TRP:CZ3	2.33	0.46
1:A:639:GLY:O	1:A:643:LYS:HE2	2.16	0.46
1:B:156:ASP:OD2	1:B:182:TYR:CD2	2.68	0.46
1:B:890:ALA:HB2	1:A:14:VAL:HG11	1.98	0.46
1:B:921:LEU:HD13	1:B:1002:ALA:HA	1.98	0.46
1:C:254:ASN:ND2	1:C:258:SER:OG	2.38	0.46
1:C:442:LEU:HD12	1:C:443:VAL:N	2.30	0.46
1:C:576:VAL:HG22	1:C:663:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.98	0.46
1:A:380:PHE:CE1	1:A:398:MET:HE1	2.51	0.46
1:A:892:TYR:CB	1:A:897:ILE:CG2	2.87	0.46
1:A:909:VAL:HG12	1:A:909:VAL:O	2.16	0.46
1:B:873:ALA:N	1:B:874:PRO:CD	2.52	0.46
1:C:671:ILE:HG13	1:C:862:MET:SD	2.56	0.46
1:A:151:GLN:HG3	1:A:285:PRO:HB3	1.98	0.46
1:A:943:ILE:HA	1:A:946:VAL:HG12	1.98	0.46
1:A:989:LEU:HD22	1:A:1000:GLN:HB2	1.96	0.46
1:B:375:VAL:HG12	1:B:375:VAL:O	2.15	0.46
1:C:76:MET:HB3	1:C:93:THR:O	2.16	0.46
1:C:76:MET:HE2	1:C:864:TYR:CE2	2.51	0.46
1:A:472:ILE:HA	1:A:475:VAL:HG12	1.97	0.46
1:A:711:ASP:N	1:A:840:ALA:HB2	2.31	0.46
1:B:278:ILE:CG1	1:B:613:ASN:HB3	2.46	0.46
1:B:881:LEU:HD23	1:B:881:LEU:HA	1.81	0.46
1:C:317:PHE:CE2	1:C:323:ILE:HD11	2.50	0.46
1:C:417:GLU:OE1	1:C:420:MET:HE2	2.16	0.46
1:A:451:ALA:O	1:A:455:PRO:HG2	2.16	0.46
1:A:568:ASP:C	1:A:570:GLY:N	2.67	0.46
1:A:685:ILE:HD13	1:A:858:ASP:CG	2.40	0.46
1:C:485:ALA:O	1:C:489:THR:CG2	2.64	0.46
1:A:393:LEU:CA	1:A:470:PHE:CE1	2.99	0.46
1:A:483:LEU:O	1:A:487:ILE:HG12	2.16	0.46
1:B:58:GLN:NE2	1:B:82:SER:HB2	2.31	0.46
1:B:196:PHE:CD2	1:B:260:VAL:HG11	2.46	0.46
1:B:275:TYR:CD2	1:A:223:PRO:HD3	2.49	0.46
1:C:600:THR:HG23	1:C:601:LYS:N	2.30	0.46
1:C:964:THR:O	1:C:968:VAL:HG22	2.16	0.46
1:A:560:PRO:C	1:A:922:THR:HB	2.41	0.46
1:A:952:LEU:HD11	1:A:970:MET:HE1	1.97	0.46
1:B:30:LEU:HD23	1:B:390:ILE:HG13	1.97	0.45
1:B:148:THR:HG22	1:B:149:MET:N	2.30	0.45
1:C:512:PHE:CD1	1:C:512:PHE:C	2.94	0.45
1:A:354:VAL:HG11	1:A:981:ALA:HB2	1.98	0.45
1:A:842:GLU:O	1:A:844:MET:HE2	2.15	0.45
1:B:4:PHE:HE2	1:B:11:PHE:HE2	1.62	0.45
1:B:905:VAL:N	1:B:906:PRO:CD	2.79	0.45
1:C:62:THR:OG1	1:C:88:VAL:HG21	2.17	0.45
1:A:460:GLY:C	1:A:462:SER:N	2.75	0.45
1:B:38:ILE:HG22	1:B:462:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:VAL:N	1:B:373:PRO:CD	2.79	0.45
1:C:937:LEU:HD22	1:C:1011:MET:SD	2.56	0.45
1:A:340:VAL:CG2	1:A:396:PHE:CE1	3.00	0.45
1:A:407:ASP:OD2	1:A:940:LYS:HG2	2.15	0.45
1:B:197:GLN:C	1:B:798:MET:HE1	2.40	0.45
1:B:912:ALA:HB3	1:B:931:LEU:HD11	1.99	0.45
1:C:368:PRO:HB2	1:C:410:ILE:CD1	2.46	0.45
1:A:121:GLU:O	1:A:125:GLN:HG2	2.17	0.45
1:B:210:GLN:NE2	1:C:733:GLN:OE1	2.50	0.45
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.98	0.45
1:C:321:LEU:HD23	1:C:322:LYS:N	2.31	0.45
1:C:435:MET:HE2	1:C:490:PRO:HG3	1.97	0.45
1:C:359:LEU:C	1:C:361:ASN:H	2.25	0.45
1:A:685:ILE:HD11	1:A:858:ASP:HB2	1.97	0.45
1:B:329:THR:O	1:B:333:VAL:HG23	2.17	0.45
1:A:21:LEU:HD23	1:A:21:LEU:C	2.42	0.45
1:A:149:MET:HB3	1:A:153:ASP:HB2	1.98	0.45
1:A:344:LEU:HD21	1:A:376:LEU:HD23	1.99	0.45
1:A:460:GLY:C	1:A:462:SER:H	2.19	0.45
1:A:583:THR:HG22	1:A:584:GLN:N	2.32	0.45
1:B:138:MET:HE2	1:B:140:VAL:HG22	1.98	0.45
1:C:193:LEU:C	1:C:193:LEU:HD12	2.42	0.45
1:B:446:ALA:HB2	1:B:482:VAL:HG11	1.99	0.45
1:C:538:THR:HG22	1:C:1024:VAL:HG13	1.99	0.45
1:A:298:ASN:HB3	1:A:301:ASP:OD1	2.16	0.45
1:A:444:GLY:O	1:A:448:VAL:HG13	2.17	0.45
1:B:23:GLY:O	1:B:27:ILE:HG13	2.17	0.44
1:B:136:PHE:CG	1:B:290:GLY:O	2.70	0.44
1:B:605:ASN:ND2	1:B:647:ILE:HD11	2.32	0.44
1:C:527:TYR:CE2	1:C:972:LEU:HD12	2.52	0.44
1:C:973:ARG:HG2	1:C:977:MET:SD	2.56	0.44
1:A:489:THR:OG1	1:A:490:PRO:HD3	2.17	0.44
1:A:543:VAL:HA	1:A:546:LEU:HD12	1.97	0.44
1:A:709:HIS:CD2	1:A:709:HIS:O	2.70	0.44
1:B:252:LYS:CE	1:B:254:ASN:HD21	2.29	0.44
1:B:340:VAL:HG11	1:B:395:MET:HB3	1.99	0.44
1:B:371:ALA:C	1:B:374:VAL:HG12	2.42	0.44
1:B:538:THR:O	1:B:542:LEU:CD1	2.62	0.44
1:C:512:PHE:CD1	1:C:512:PHE:O	2.70	0.44
1:C:535:LEU:HB2	1:C:536:ARG:NH1	2.32	0.44
1:C:573:MET:HE3	1:C:573:MET:HB2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.99	0.44
1:A:338:HIS:O	1:A:338:HIS:CG	2.70	0.44
1:A:699:ARG:CD	1:A:825:MET:SD	2.95	0.44
1:C:362:PHE:O	1:C:362:PHE:CD1	2.70	0.44
1:A:326:PRO:O	1:A:327:TYR:C	2.60	0.44
1:A:568:ASP:HA	1:A:644:VAL:HG22	1.99	0.44
1:B:459:PHE:CE1	1:B:876:LEU:CD1	2.99	0.44
1:C:20:MET:O	1:C:377:LEU:HD23	2.18	0.44
1:C:57:VAL:HG13	1:C:61:VAL:CG1	2.48	0.44
1:C:449:LEU:HD23	1:C:478:MET:CE	2.47	0.44
1:C:1022:VAL:HA	1:C:1025:PHE:CE1	2.52	0.44
1:A:905:VAL:O	1:A:909:VAL:CG2	2.57	0.44
1:B:143:ILE:CG2	1:B:281:PHE:HB3	2.48	0.44
1:B:909:VAL:O	1:B:909:VAL:CG1	2.66	0.44
1:C:515:TRP:O	1:C:515:TRP:CD1	2.70	0.44
1:A:764:ASP:HB3	1:A:769:LYS:HD2	2.00	0.44
1:A:894:SER:HB2	1:A:897:ILE:HG22	2.00	0.44
1:B:375:VAL:HG21	1:B:484:VAL:HG11	2.00	0.44
1:A:918:PHE:HD2	1:A:919:ARG:HG3	1.83	0.44
1:B:2:PRO:O	1:B:6:ILE:HG12	2.17	0.44
1:B:137:LEU:HD11	1:B:293:LEU:CA	2.47	0.44
1:B:252:LYS:HE3	1:B:254:ASN:ND2	2.33	0.44
1:B:277:ILE:HD12	1:B:615:PHE:HB2	1.98	0.44
1:B:2:PRO:CG	1:B:439:GLN:OE1	2.65	0.44
1:B:527:TYR:HE1	1:B:968:VAL:CG1	2.31	0.44
1:B:615:PHE:CD2	1:B:615:PHE:O	2.70	0.44
1:C:195:LYS:HG2	1:C:196:PHE:CE1	2.53	0.44
1:C:419:VAL:HG13	1:C:419:VAL:O	2.18	0.44
1:A:27:ILE:HD11	1:A:380:PHE:CD2	2.53	0.44
1:A:38:ILE:HD11	1:A:671:ILE:CG2	2.40	0.44
1:A:157:TYR:CE1	1:A:161:ASN:ND2	2.81	0.44
1:A:683:GLU:OE2	1:A:826:GLU:HG3	2.18	0.44
1:C:420:MET:CG	1:C:425:LEU:O	2.63	0.44
1:C:892:TYR:HD2	1:C:897:ILE:HG21	1.82	0.44
1:A:363:ARG:HA	1:A:363:ARG:HD3	1.74	0.44
1:A:372:VAL:CG1	1:A:373:PRO:HD3	2.48	0.44
1:A:527:TYR:O	1:A:527:TYR:CD1	2.70	0.44
1:A:338:HIS:O	1:A:338:HIS:CD2	2.71	0.43
1:B:298:ASN:OD1	1:B:301:ASP:HB2	2.18	0.43
1:B:801:PHE:C	1:B:803:ALA:N	2.63	0.43
1:C:4:PHE:O	1:C:4:PHE:CD1	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD12	1:A:895:TRP:CD1	2.52	0.43
1:C:355:MET:HE2	1:C:355:MET:HB3	1.79	0.43
1:A:425:LEU:HG	1:A:426:PRO:HD2	1.97	0.43
1:A:703:LEU:HD23	1:A:703:LEU:HA	1.78	0.43
1:B:196:PHE:CD2	1:B:260:VAL:CG1	3.01	0.43
1:A:29:LYS:HB2	1:A:29:LYS:NZ	2.27	0.43
1:A:350:LEU:C	1:A:354:VAL:HG23	2.36	0.43
1:B:144:ASN:ND2	1:B:154:ILE:CD1	2.44	0.43
1:B:435:MET:HE1	1:B:490:PRO:HG3	2.01	0.43
1:B:790:TYR:CG	1:B:800:PRO:HB3	2.53	0.43
1:C:515:TRP:O	1:C:515:TRP:CG	2.70	0.43
1:B:535:LEU:HD23	1:B:535:LEU:HA	1.90	0.43
1:B:877:TYR:HA	1:B:880:SER:HB3	2.00	0.43
1:B:151:GLN:H	1:B:151:GLN:CD	2.17	0.43
1:B:924:ASP:O	1:B:928:GLN:CG	2.62	0.43
1:B:979:SER:O	1:B:983:ILE:HG12	2.17	0.43
1:C:368:PRO:CB	1:C:410:ILE:CD1	2.95	0.43
1:C:711:ASP:OD1	1:C:711:ASP:N	2.43	0.43
1:A:95:GLU:O	1:A:98:THR:HG23	2.19	0.43
1:A:896:SER:O	1:A:1029:VAL:HG11	2.18	0.43
1:A:1024:VAL:O	1:A:1028:VAL:HG23	2.18	0.43
1:B:895:TRP:CZ2	1:A:10:ILE:HD12	2.52	0.43
1:A:214:VAL:HB	1:A:236:ALA:HB3	2.00	0.43
1:A:403:GLY:O	1:A:407:ASP:HB2	2.18	0.43
1:B:552:MET:CB	1:B:910:ILE:HD11	2.48	0.43
1:A:185:ARG:HG2	1:A:187:TRP:CZ2	2.53	0.43
1:A:641:GLU:OE1	1:A:641:GLU:N	2.44	0.43
1:B:169:THR:HG21	1:B:306:ILE:HD13	1.97	0.43
1:B:196:PHE:HD2	1:B:260:VAL:CG1	2.29	0.43
1:B:547:ILE:HD13	1:B:547:ILE:N	2.34	0.43
1:C:6:ILE:O	1:C:6:ILE:CG2	2.66	0.43
1:C:95:GLU:O	1:C:98:THR:HG23	2.19	0.43
1:C:162:MET:HE2	1:C:162:MET:HB3	1.74	0.43
1:C:319:SER:O	1:C:319:SER:OG	2.32	0.43
1:C:696:THR:O	1:C:700:ASN:HB2	2.18	0.43
1:C:935:ILE:O	1:C:935:ILE:CG2	2.66	0.43
1:A:919:ARG:HH11	1:A:1005:THR:HG22	1.84	0.43
1:B:367:ILE:N	1:B:368:PRO:HD3	2.32	0.42
1:B:973:ARG:O	1:B:977:MET:HB2	2.19	0.42
1:C:30:LEU:CD2	1:C:384:ALA:HA	2.49	0.42
1:C:717:ARG:HB2	1:C:718:PRO:CD	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:HA	1:A:555:LEU:HD12	1.79	0.42
1:A:894:SER:HB2	1:A:897:ILE:HB	2.00	0.42
1:B:353:LEU:HD23	1:B:353:LEU:HA	1.77	0.42
1:B:571:VAL:HG12	1:B:630:SER:HA	2.01	0.42
1:B:860:THR:OG1	1:B:861:GLY:N	2.52	0.42
1:C:81:ASN:HD22	1:C:815:ARG:HH21	1.67	0.42
1:C:442:LEU:HD12	1:C:443:VAL:CG2	2.49	0.42
1:C:488:LEU:HG	1:C:492:LEU:HD13	2.00	0.42
1:C:497:LEU:HD12	1:C:497:LEU:HA	1.83	0.42
1:C:885:PHE:CD2	1:C:902:MET:HG3	2.45	0.42
1:C:54:ALA:HB2	1:C:83:ASP:C	2.44	0.42
1:B:69:MET:HE3	1:B:92:LEU:HD11	2.01	0.42
1:B:182:TYR:CD2	1:B:270:LEU:HD21	2.55	0.42
1:B:595:THR:HG23	1:B:609:VAL:HG11	2.01	0.42
1:C:75:LEU:CD1	1:C:92:LEU:HD23	2.49	0.42
1:A:733:GLN:OE1	1:A:743:ILE:HD12	2.20	0.42
1:B:518:ARG:HA	1:B:521:GLU:CD	2.45	0.42
1:C:545:TYR:CD1	1:C:545:TYR:C	2.97	0.42
1:C:674:LEU:HD12	1:C:674:LEU:C	2.44	0.42
1:C:762:PHE:CE2	1:C:764:ASP:HB2	2.55	0.42
1:C:982:PHE:HD2	1:C:1011:MET:HG2	1.84	0.42
1:B:277:ILE:HD11	1:B:615:PHE:HB2	2.01	0.42
1:B:309:GLU:O	1:B:313:MET:HG3	2.19	0.42
1:B:428:LYS:HB2	1:B:428:LYS:HE3	1.77	0.42
1:B:431:THR:O	1:B:435:MET:CG	2.62	0.42
1:B:888:LEU:HD13	1:B:901:VAL:HG21	2.02	0.42
1:C:845:GLU:HG2	1:C:857:TYR:OH	2.20	0.42
1:A:4:PHE:CZ	1:A:8:ARG:NH1	2.88	0.42
1:A:5:PHE:CD2	1:A:487:ILE:HG23	2.55	0.42
1:B:317:PHE:HA	1:B:318:PRO:HD3	1.79	0.42
1:C:222:THR:HA	1:C:224:PRO:HD3	2.02	0.42
1:B:183:ALA:HB2	1:B:273:GLU:HG2	2.01	0.42
1:B:456:MET:HG2	1:B:877:TYR:OH	2.20	0.42
1:B:831:ALA:HB2	1:B:840:ALA:CB	2.50	0.42
1:C:372:VAL:CG2	1:C:373:PRO:HD3	2.50	0.42
1:C:555:LEU:HD11	1:C:914:LEU:HD13	2.01	0.42
1:B:249:ILE:O	1:B:261:LEU:CD2	2.68	0.42
1:B:678:THR:CG2	1:B:831:ALA:H	2.32	0.42
1:C:76:MET:HE2	1:C:864:TYR:HE2	1.84	0.42
1:C:596:HIS:O	1:C:600:THR:CG2	2.65	0.42
1:C:889:ALA:HB2	1:C:898:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:ILE:O	1:A:961:ILE:CG2	2.67	0.42
1:B:363:ARG:HG3	1:B:498:LYS:HG3	2.02	0.42
1:C:780:ARG:O	1:C:780:ARG:HG2	2.19	0.42
1:C:884:VAL:HG13	1:C:885:PHE:N	2.35	0.42
1:A:101:ASP:OD1	1:A:101:ASP:N	2.50	0.42
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	2.02	0.42
1:B:527:TYR:O	1:B:527:TYR:CG	2.71	0.41
1:B:732:ASP:CG	1:B:735:LYS:HG3	2.44	0.41
1:B:776:GLU:C	1:B:778:LYS:H	2.28	0.41
1:B:987:MET:O	1:B:991:ILE:HD12	2.19	0.41
1:C:419:VAL:CG2	1:C:433:LYS:HZ2	2.32	0.41
1:C:552:MET:HE2	1:C:552:MET:HB3	1.87	0.41
1:A:925:VAL:O	1:A:925:VAL:HG12	2.19	0.41
1:B:734:GLU:HG3	1:A:250:LEU:HD22	2.01	0.41
1:C:278:ILE:HD12	1:C:584:GLN:NE2	2.35	0.41
1:C:368:PRO:HB2	1:C:410:ILE:HD11	2.02	0.41
1:C:426:PRO:HG2	1:C:429:GLU:CB	2.50	0.41
1:C:512:PHE:O	1:C:512:PHE:CG	2.72	0.41
1:C:904:VAL:CG2	1:C:1022:VAL:HG12	2.49	0.41
1:A:16:ALA:HB2	1:A:488:LEU:HD12	2.02	0.41
1:A:987:MET:N	1:A:988:PRO:HD2	2.35	0.41
1:C:446:ALA:HB1	1:C:482:VAL:CG2	2.49	0.41
1:C:518:ARG:O	1:C:522:LYS:HG3	2.21	0.41
1:A:960:LEU:HD12	1:A:1030:ARG:CG	2.39	0.41
1:A:971:ARG:C	1:A:974:PRO:HD2	2.45	0.41
1:B:169:THR:CG2	1:B:172:VAL:HG11	2.49	0.41
1:B:666:PHE:CD1	1:B:666:PHE:O	2.73	0.41
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.55	0.41
1:A:712:MET:HB3	1:A:843:LEU:CD1	2.50	0.41
1:B:438:ILE:HG22	1:B:948:PHE:CE1	2.56	0.41
1:C:1024:VAL:O	1:C:1028:VAL:HG12	2.21	0.41
1:A:33:ALA:O	1:A:391:ASN:HA	2.20	0.41
1:A:348:ILE:HG12	1:A:372:VAL:HG11	2.02	0.41
1:A:573:MET:CE	1:A:668:LEU:HD11	2.50	0.41
1:A:712:MET:O	1:A:712:MET:CG	2.68	0.41
1:B:70:ASN:OD1	1:B:70:ASN:O	2.38	0.41
1:B:337:ILE:CD1	1:B:395:MET:HG3	2.50	0.41
1:C:597:TYR:HD1	1:C:601:LYS:HD2	1.83	0.41
1:C:640:GLU:HA	1:C:643:LYS:HG2	2.03	0.41
1:C:729:ILE:O	1:C:729:ILE:CG2	2.68	0.41
1:C:1025:PHE:HA	1:C:1028:VAL:CG1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PRO:HG2	1:A:389:SER:HB3	2.02	0.41
1:A:680:PHE:CZ	1:A:716:VAL:CG2	3.00	0.41
1:A:864:TYR:CD1	1:A:864:TYR:C	2.98	0.41
1:B:721:LEU:N	1:B:721:LEU:CD2	2.73	0.41
1:A:375:VAL:CB	1:A:405:LEU:HD11	2.51	0.41
1:A:375:VAL:HG13	1:A:480:LEU:HB2	2.03	0.41
1:A:919:ARG:HH12	1:A:990:VAL:HG13	1.84	0.41
1:B:7:ASP:OD1	1:B:7:ASP:N	2.48	0.41
1:B:577:GLN:O	1:B:661:ALA:HA	2.20	0.41
1:C:353:LEU:HD23	1:C:353:LEU:HA	1.80	0.41
1:A:945:ILE:HD11	1:A:1022:VAL:HG11	2.01	0.41
1:A:949:ALA:HB1	1:A:1026:PHE:CE2	2.55	0.41
1:B:144:ASN:HB2	1:B:320:GLY:O	2.21	0.41
1:B:176:GLN:HG3	1:B:290:GLY:HA3	2.02	0.41
1:B:555:LEU:CD1	1:B:914:LEU:HD23	2.51	0.41
1:B:678:THR:HG22	1:B:831:ALA:H	1.85	0.41
1:B:707:ALA:C	1:B:709:HIS:N	2.79	0.41
1:B:886:LEU:CD1	1:A:14:VAL:HG22	2.49	0.41
1:C:130:GLU:N	1:C:130:GLU:OE1	2.54	0.41
1:A:30:LEU:HD23	1:A:31:PRO:N	2.36	0.41
1:A:181:GLN:HE22	1:A:767:ARG:HE	1.68	0.41
1:A:192:GLU:HB3	1:A:265:VAL:HG12	2.02	0.41
1:A:592:ASN:HA	1:A:595:THR:HG22	2.00	0.41
1:A:699:ARG:NH1	1:A:718:PRO:HB3	2.36	0.41
1:A:885:PHE:CD1	1:A:885:PHE:C	2.99	0.41
1:B:907:LEU:HD12	1:B:907:LEU:H	1.75	0.41
1:C:317:PHE:HD1	1:C:317:PHE:HA	1.76	0.41
1:A:911:GLY:HA3	1:A:1010:GLY:HA2	2.03	0.41
1:B:138:MET:CE	1:B:325:TYR:CD2	3.04	0.40
1:B:169:THR:HG23	1:B:172:VAL:HG13	2.04	0.40
1:B:367:ILE:CB	1:B:368:PRO:HD3	2.48	0.40
1:B:445:ILE:HA	1:B:448:VAL:HG12	2.03	0.40
1:B:954:ASP:OD1	1:B:955:LYS:N	2.55	0.40
1:C:639:GLY:O	1:C:643:LYS:HE2	2.21	0.40
1:C:1012:VAL:O	1:C:1016:VAL:HG22	2.21	0.40
1:A:960:LEU:CD2	1:A:1027:VAL:HG12	2.43	0.40
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.81	0.40
1:B:248:LYS:O	1:B:261:LEU:CD2	2.67	0.40
1:C:196:PHE:HD2	1:C:260:VAL:HG21	1.86	0.40
1:C:376:LEU:O	1:C:380:PHE:HD2	2.02	0.40
1:C:694:LYS:O	1:C:695:LEU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LYS:HA	1:A:601:LYS:HD3	1.84	0.40
1:B:252:LYS:HE2	1:B:252:LYS:HB3	1.96	0.40
1:B:402:ILE:O	1:B:406:VAL:HG22	2.20	0.40
1:C:218:GLN:HB2	1:C:232:ALA:O	2.21	0.40
1:C:609:VAL:HG23	1:C:609:VAL:O	2.22	0.40
1:C:958:LYS:HE3	1:C:958:LYS:HB3	1.36	0.40
1:A:156:ASP:HB2	1:A:182:TYR:CZ	2.56	0.40
1:A:454:VAL:N	1:A:455:PRO:HD2	2.35	0.40
1:B:573:MET:HE2	1:B:573:MET:HB3	1.83	0.40
1:C:354:VAL:HG21	1:C:984:LEU:HD13	1.74	0.40
1:C:1030:ARG:HA	1:C:1030:ARG:HD3	1.81	0.40
1:A:916:ALA:HB2	1:A:927:PHE:CE1	2.56	0.40
1:B:188:MET:HE3	1:B:193:LEU:HD21	2.04	0.40
1:C:388:PHE:CD2	1:C:472:ILE:HG21	2.57	0.40
1:C:662:MET:CA	1:C:662:MET:HE3	2.52	0.40
1:A:905:VAL:H	1:A:906:PRO:CD	2.35	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	969/1051 (92%)	881 (91%)	70 (7%)	18 (2%)	6	33
1	B	1002/1051 (95%)	896 (89%)	92 (9%)	14 (1%)	9	39
1	C	1002/1051 (95%)	888 (89%)	104 (10%)	10 (1%)	12	45
All	All	2973/3153 (94%)	2665 (90%)	266 (9%)	42 (1%)	11	39

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	802	SER

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Mol	Chain	Res	Type
1	C	76	MET
1	C	319	SER
1	A	569	GLN
1	A	669	PRO
1	A	671	ILE
1	B	617	PHE
1	B	662	MET
1	C	54	ALA
1	C	147	GLY
1	A	461	GLY
1	A	708	LYS
1	A	843	LEU
1	A	896	SER
1	B	236	ALA
1	B	268	ILE
1	B	777	ALA
1	B	800	PRO
1	A	460	GLY
1	A	852	PRO
1	A	853	THR
1	B	170	SER
1	B	294	ALA
1	B	318	PRO
1	B	319	SER
1	C	295	THR
1	C	516	PHE
1	C	673	GLU
1	A	133	SER
1	A	534	ILE
1	B	50	PRO
1	B	269	GLU
1	C	387	GLY
1	C	495	THR
1	A	707	ALA
1	A	713	LEU
1	A	715	SER
1	B	873	ALA
1	C	124	GLN
1	A	462	SER
1	A	424	GLY
1	A	326	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	785/857 (92%)	775 (99%)	10 (1%)	61	78
1	B	775/857 (90%)	760 (98%)	15 (2%)	50	73
1	C	804/857 (94%)	787 (98%)	17 (2%)	47	71
All	All	2364/2571 (92%)	2322 (98%)	42 (2%)	51	74

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	ILE
1	B	20	MET
1	B	167	SER
1	B	366	LEU
1	B	437	GLN
1	B	543	VAL
1	B	547	ILE
1	B	658	ILE
1	B	672	VAL
1	B	674	LEU
1	B	721	LEU
1	B	883	VAL
1	B	884	VAL
1	B	968	VAL
1	B	997	SER
1	C	14	VAL
1	C	15	ILE
1	C	18	ILE
1	C	27	ILE
1	C	28	LEU
1	C	127	VAL
1	C	317	PHE
1	C	355	MET
1	C	411	VAL
1	C	419	VAL
1	C	495	THR

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Mol	Chain	Res	Type
1	C	538	THR
1	C	644	VAL
1	C	663	VAL
1	C	882	ILE
1	C	934	THR
1	C	958	LYS
1	A	14	VAL
1	A	28	LEU
1	A	127	VAL
1	A	340	VAL
1	A	341	VAL
1	A	428	LYS
1	A	531	VAL
1	A	555	LEU
1	A	896	SER
1	A	1029	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	58	GLN
1	B	81	ASN
1	B	231	ASN
1	B	657	GLN
1	B	700	ASN
1	B	923	ASN
1	C	68	ASN
1	C	81	ASN
1	C	151	GLN
1	C	161	ASN
1	C	231	ASN
1	C	517	ASN
1	C	584	GLN
1	C	700	ASN
1	C	719	ASN
1	C	744	ASN
1	C	1001	ASN
1	A	176	GLN
1	A	181	GLN
1	A	254	ASN
1	A	415	ASN
1	A	577	GLN

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Mol	Chain	Res	Type
1	A	700	ASN
1	A	709	HIS
1	A	865	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

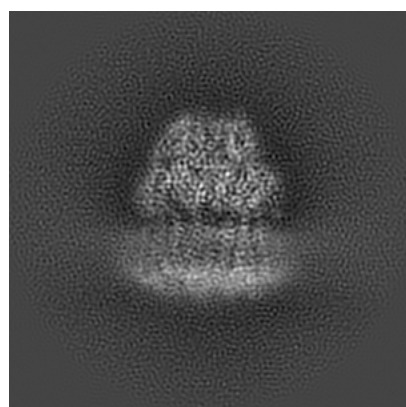
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12043. These allow visual inspection of the internal detail of the map and identification of artifacts.

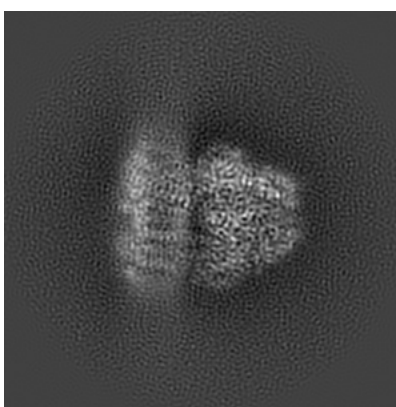
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

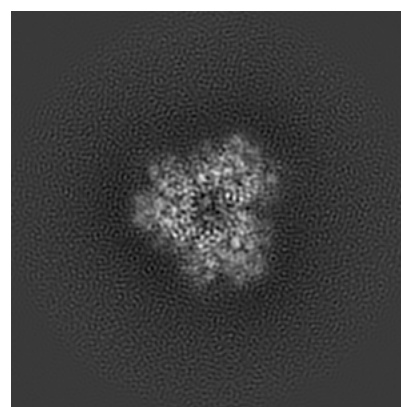
6.1.1 Primary map



X



Y

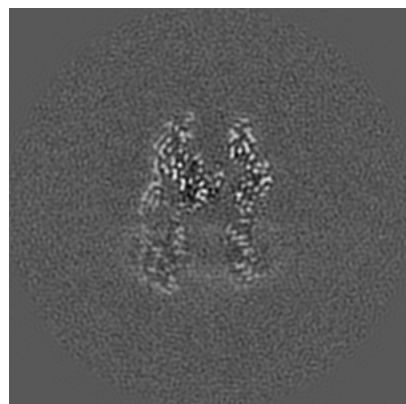


Z

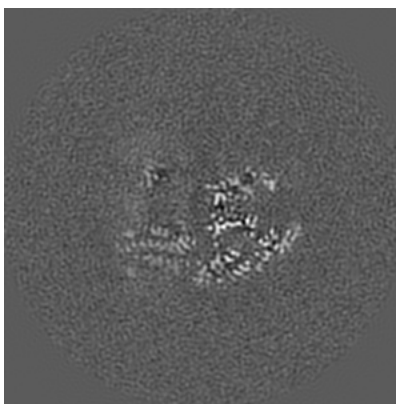
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

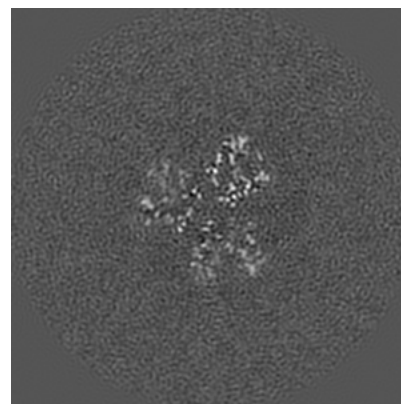
6.2.1 Primary map



X Index: 128



Y Index: 128

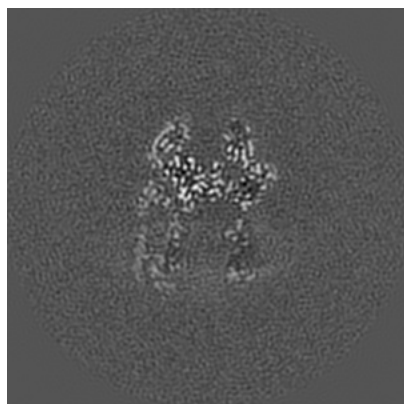


Z Index: 128

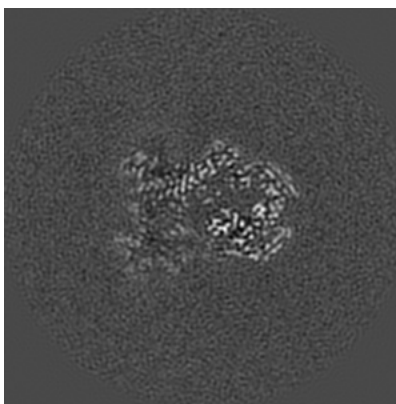
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

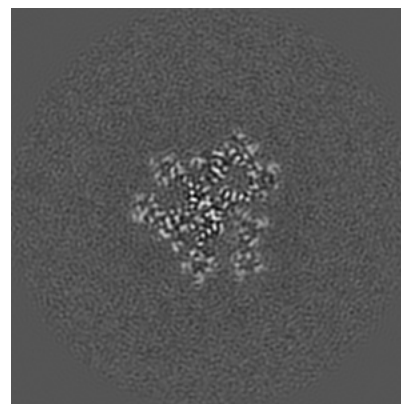
6.3.1 Primary map



X Index: 126



Y Index: 142

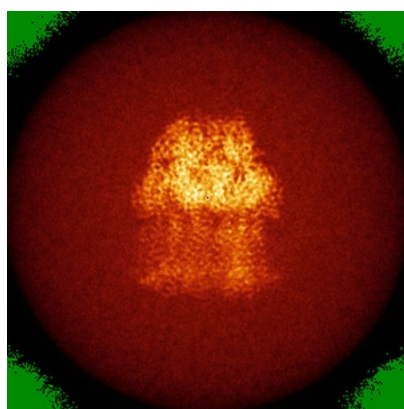


Z Index: 138

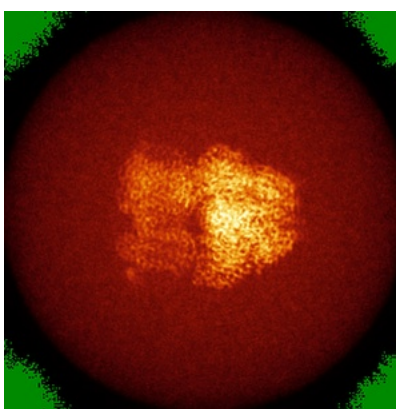
The images above show the largest variance slices of the map in three orthogonal directions.

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

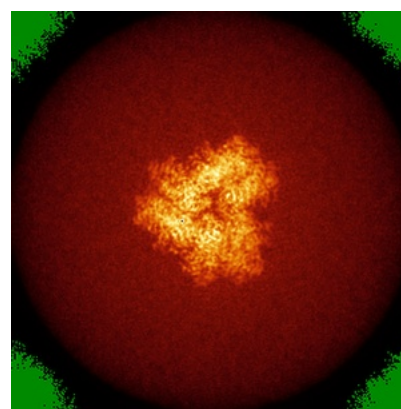
6.4.1 Primary map



X



Y

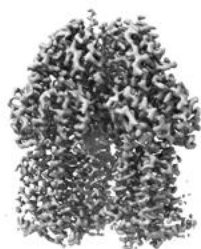


Z

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

6.5 Orthogonal surface views [i](#)

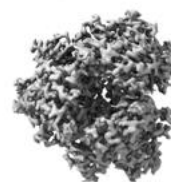
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0224. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

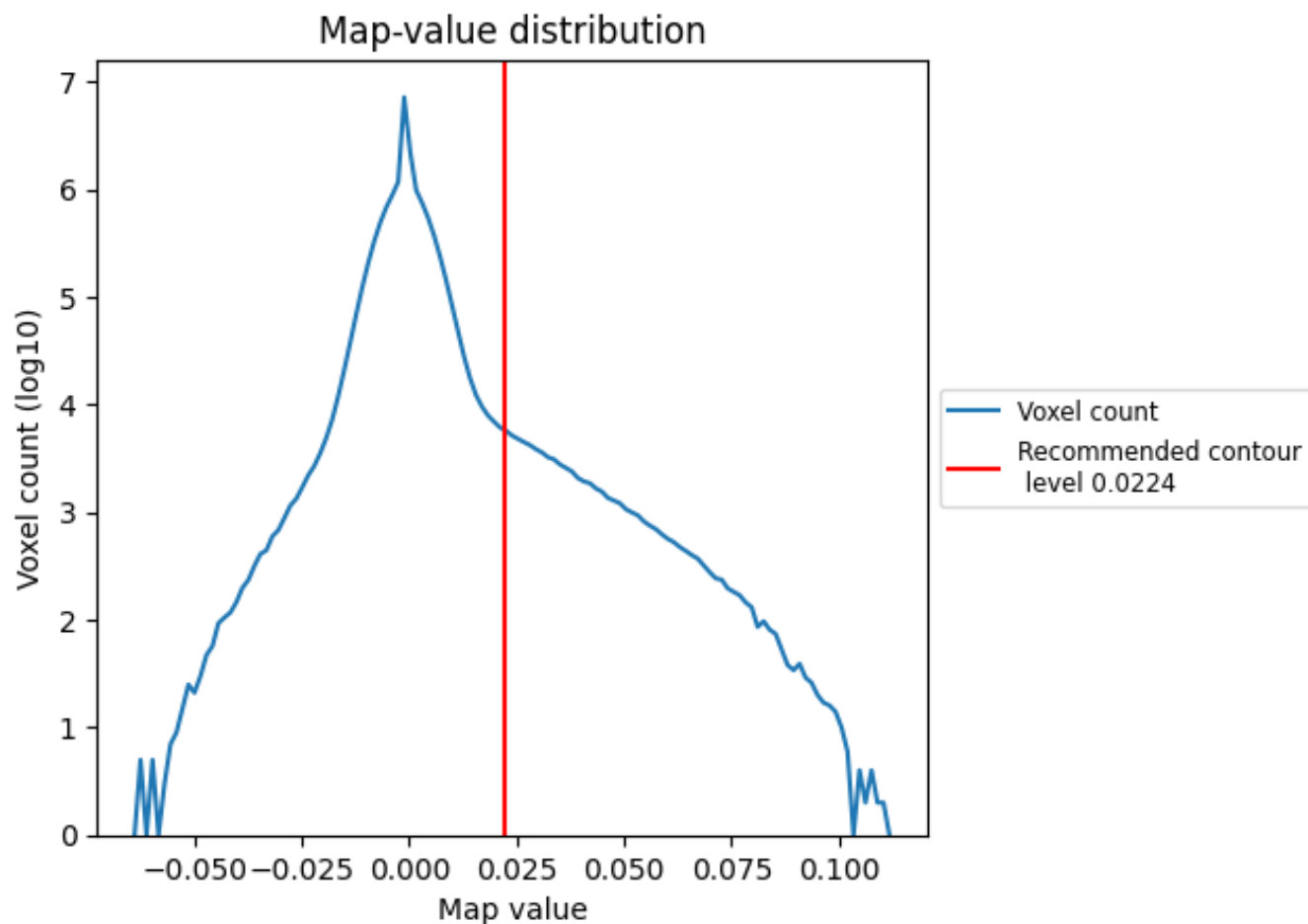
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

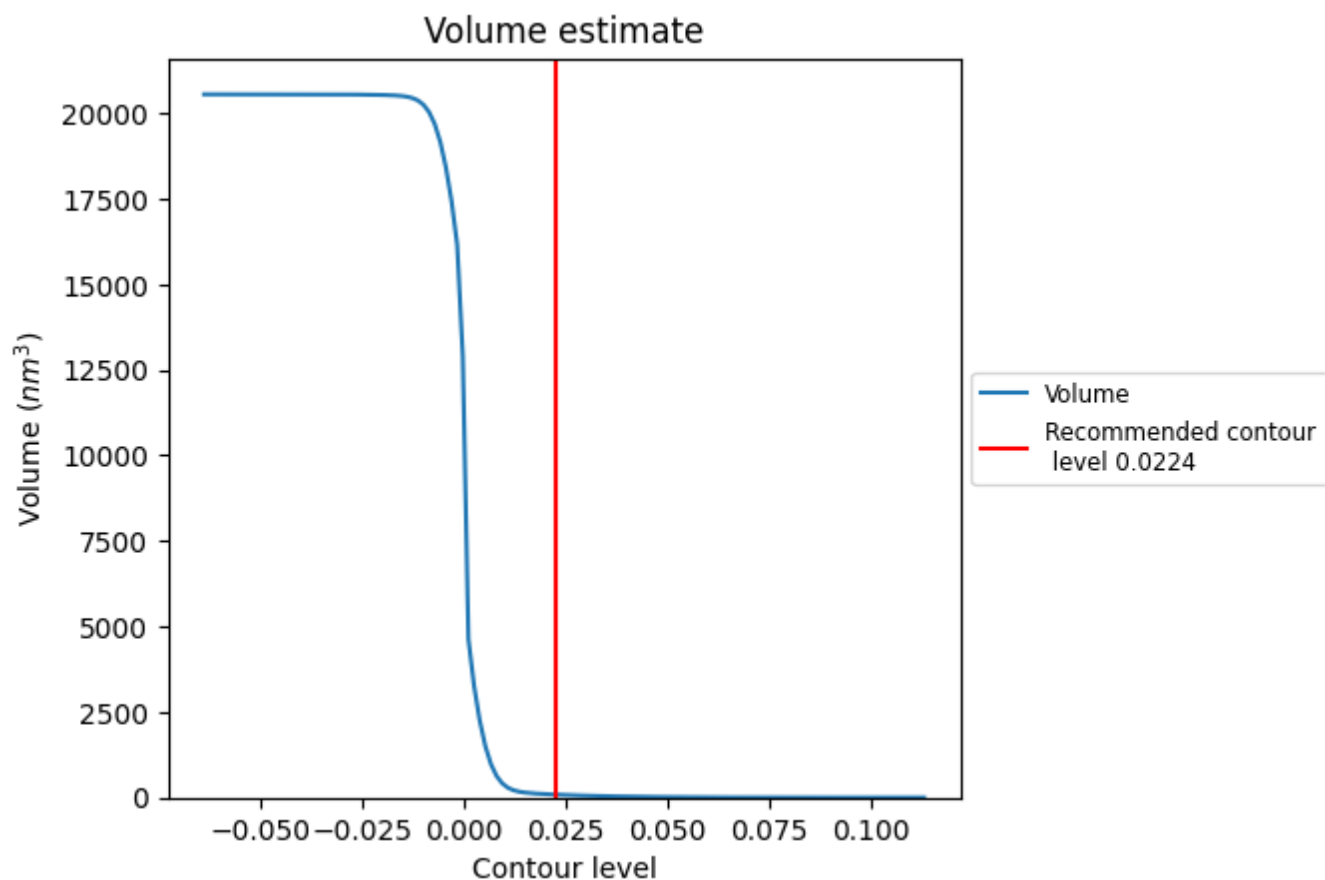
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

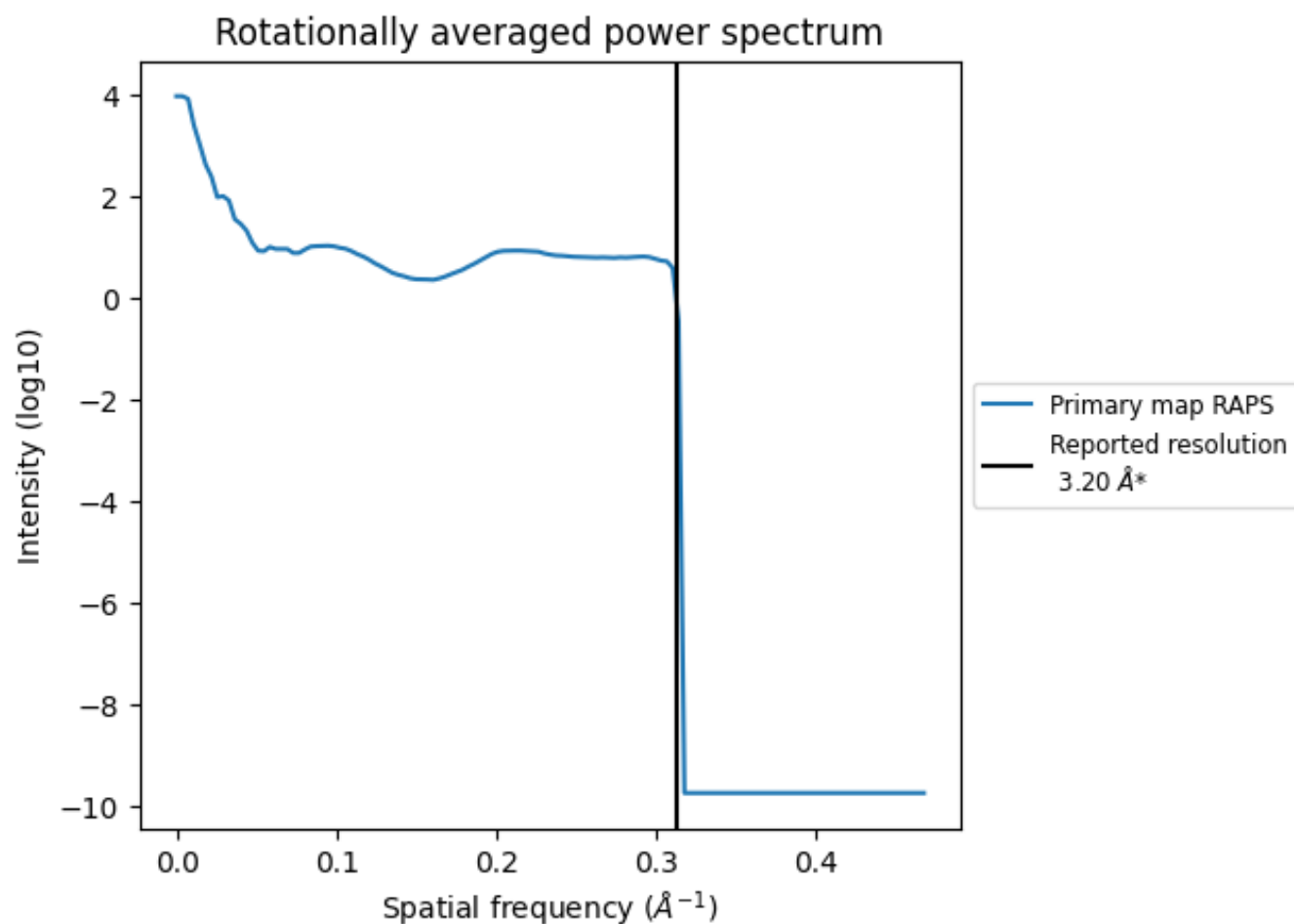
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm³; this corresponds to an approximate mass of 78 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

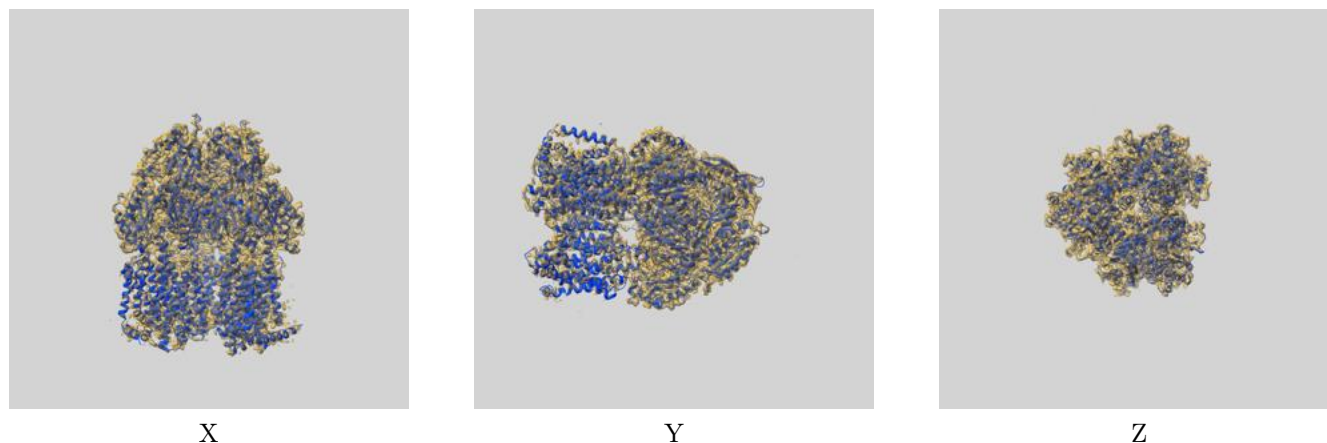
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

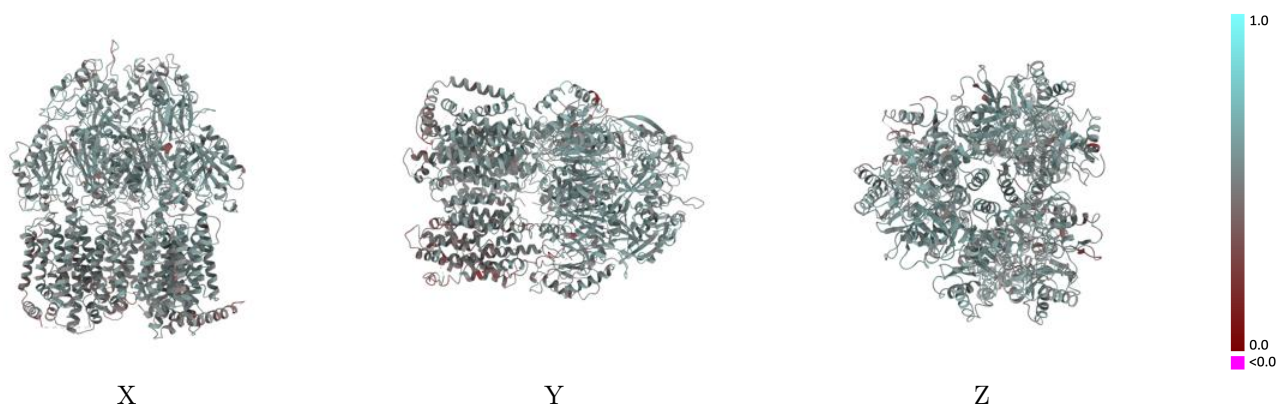
This section contains information regarding the fit between EMDB map EMD-12043 and PDB model 7B5P. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



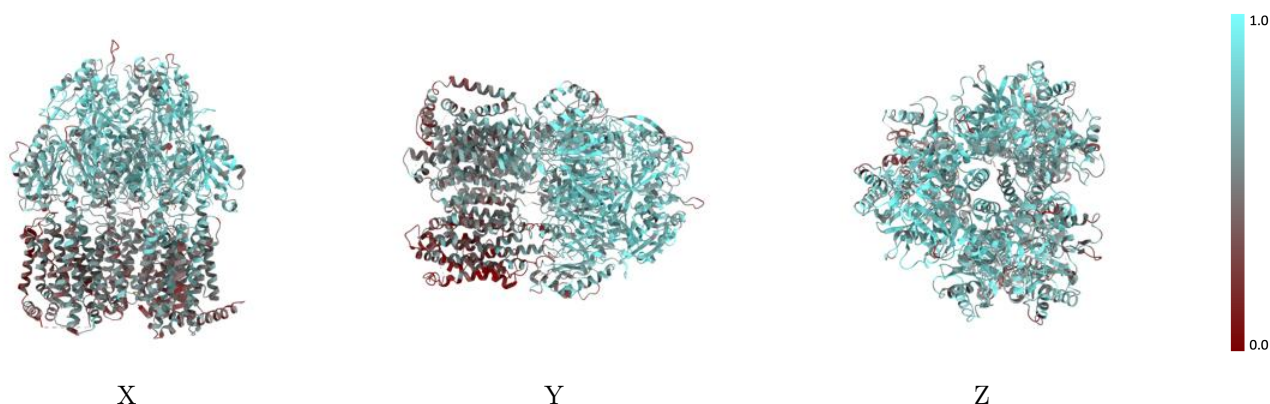
The images above show the 3D surface view of the map at the recommended contour level 0.0224 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



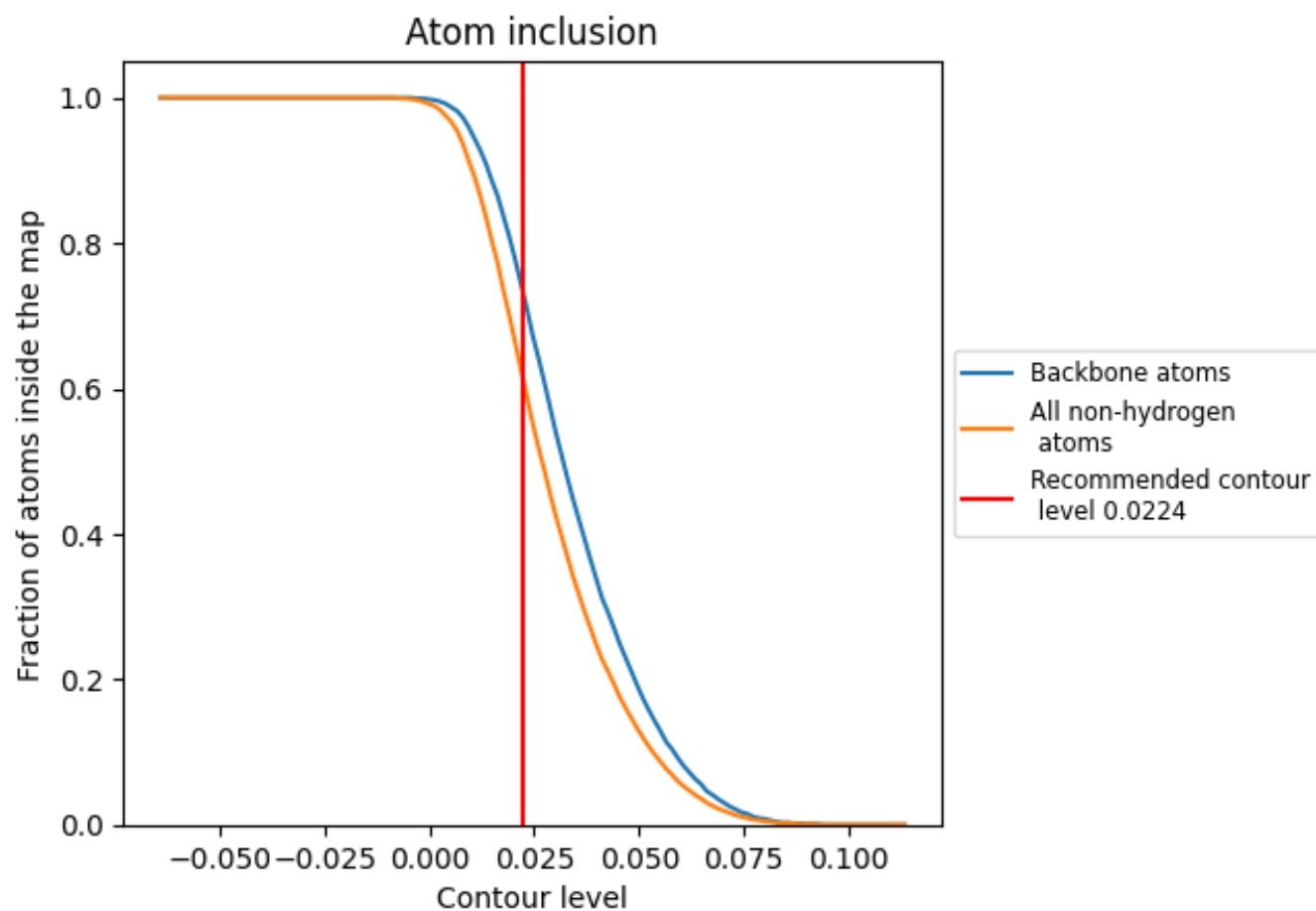
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0224).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0224) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6130	0.5280
A	0.5910	0.5160
B	0.5970	0.5270
C	0.6500	0.5400

