



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 02:56 PM UTC

PDB ID : 9ZIT / pdb_00009zit
EMDB ID : EMD-74283
Title : C. elegans PEZO-1 Isoform K
Authors : Bell, B.; Baker, M.L.; Vasquez, V.
Deposited on : 2025-12-04
Resolution : 3.10 Å(reported)
Based on initial model : .

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

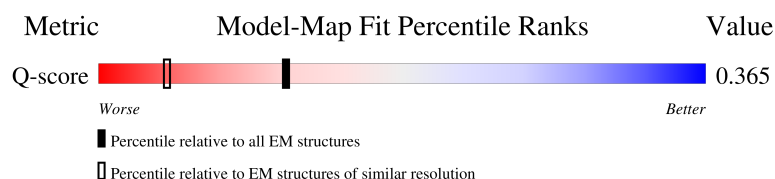
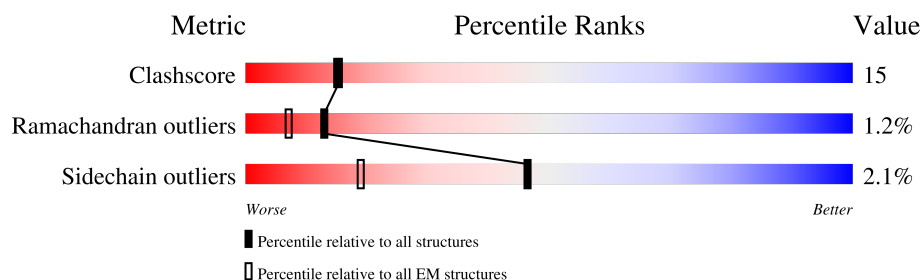
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1686	18% 56% 23% • 19%
1	B	1686	18% 56% 23% • 19%
1	C	1686	18% 55% 23% • 19%

2 Entry composition

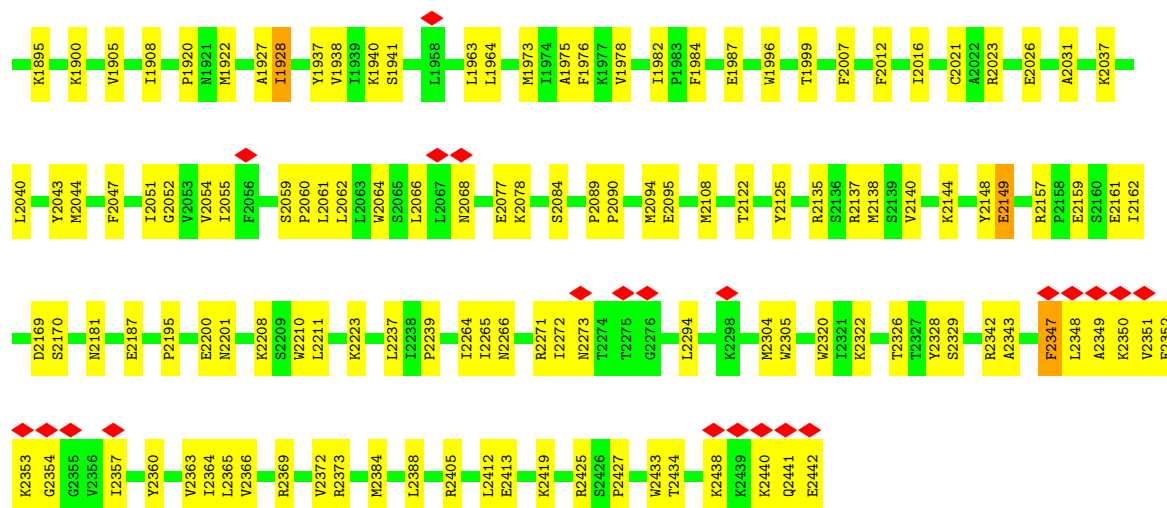
There is only 1 type of molecule in this entry. The entry contains 33087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

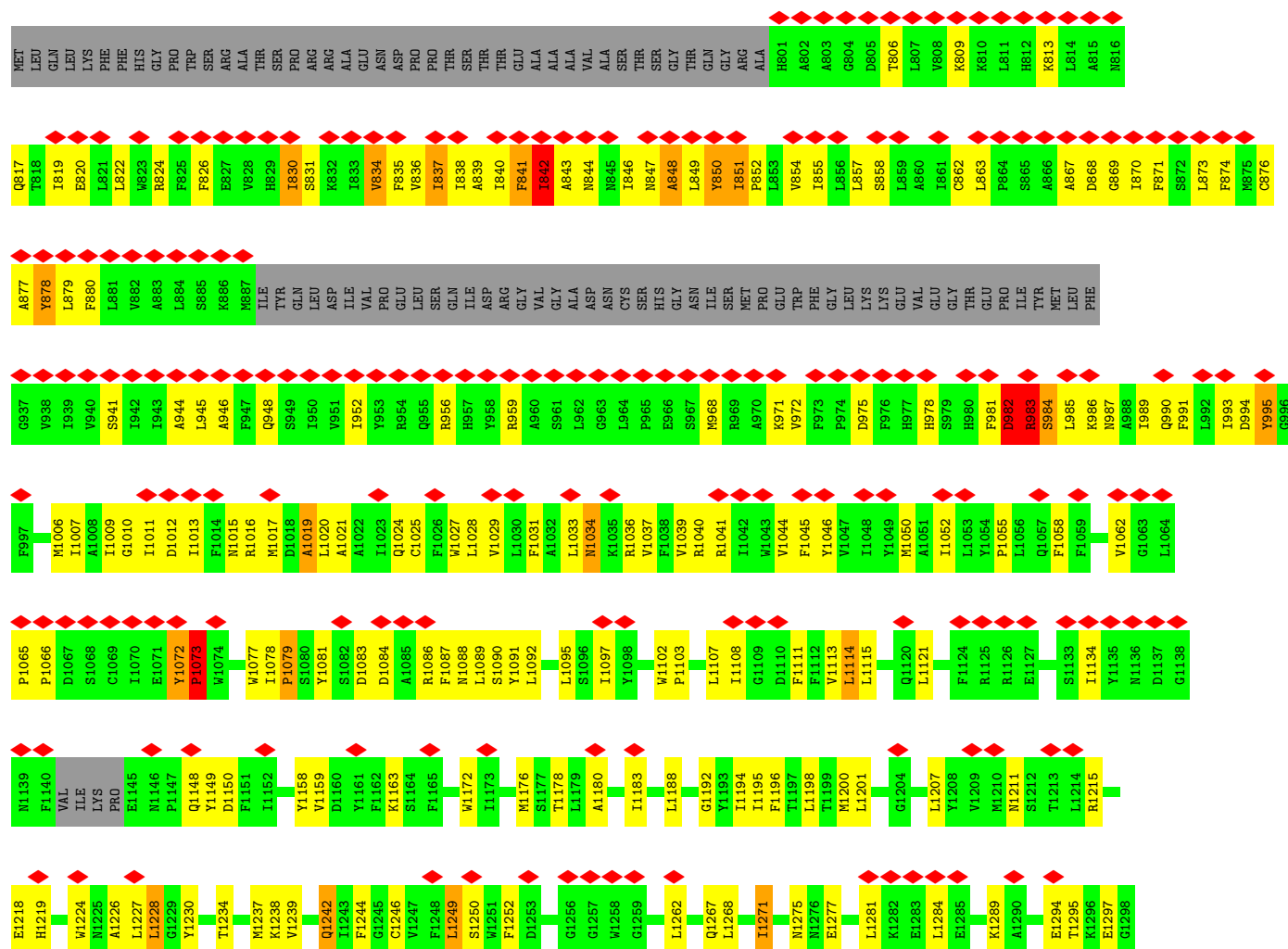
- Molecule 1 is a protein called Piezo-type mechanosensitive ion channel component 1.

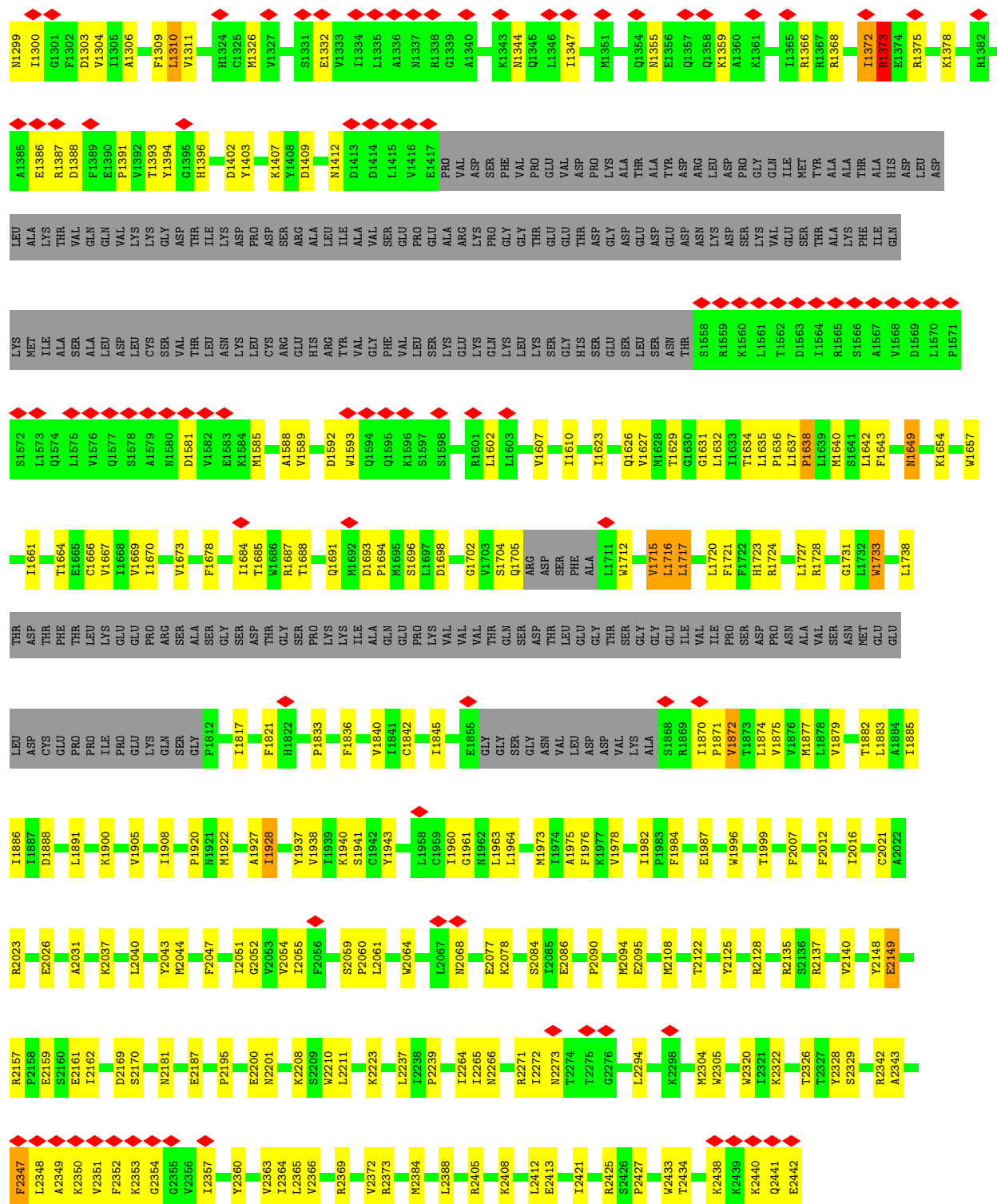
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1359	Total	C	N	O	S	0	0
			11029	7227	1814	1921	67		
1	B	1359	Total	C	N	O	S	0	0
			11029	7227	1814	1921	67		
1	C	1359	Total	C	N	O	S	0	0
			11029	7227	1814	1921	67		





• Molecule 1: Piezo-type mechanosensitive ion channel component 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	158413	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.648	Depositor
Minimum map value	-0.393	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0689	Depositor
Map size (Å)	483.84003, 483.84003, 483.84003	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	0.46	5/11319 (0.0%)	0.71	24/15349 (0.2%)
1	B	0.46	5/11319 (0.0%)	0.71	23/15349 (0.1%)
1	C	0.46	5/11319 (0.0%)	0.71	23/15349 (0.1%)
All	All	0.46	15/33957 (0.0%)	0.71	70/46047 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	6
All	All	0	20

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1073	PRO	N-CD	-10.22	1.33	1.47
1	B	1073	PRO	N-CD	-10.22	1.33	1.47
1	C	1073	PRO	N-CD	-10.18	1.33	1.47
1	A	1079	PRO	N-CD	-9.89	1.33	1.47
1	B	1079	PRO	N-CD	-9.89	1.33	1.47
1	C	1079	PRO	N-CD	-9.88	1.33	1.47
1	C	1638	PRO	N-CD	8.83	1.60	1.47
1	A	1638	PRO	N-CD	8.82	1.60	1.47
1	B	1638	PRO	N-CD	8.82	1.60	1.47
1	C	834	VAL	C-O	-7.43	1.15	1.24
1	A	834	VAL	C-O	-7.42	1.15	1.24
1	B	834	VAL	C-O	-7.40	1.15	1.24
1	C	2347	PHE	C-O	5.16	1.30	1.24
1	B	2347	PHE	C-O	5.14	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2347	PHE	C-O	5.09	1.30	1.24

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	841	PHE	CA-CB-CG	10.10	123.90	113.80
1	A	841	PHE	CA-CB-CG	10.09	123.89	113.80
1	C	841	PHE	CA-CB-CG	10.07	123.87	113.80
1	A	1073	PRO	CA-N-CD	8.77	124.28	112.00
1	C	1073	PRO	CA-N-CD	8.74	124.24	112.00
1	B	1073	PRO	CA-N-CD	8.73	124.23	112.00
1	B	1079	PRO	N-CA-CB	-7.57	95.30	103.25
1	A	1079	PRO	N-CA-CB	-7.56	95.31	103.25
1	C	1079	PRO	N-CA-CB	-7.56	95.31	103.25
1	B	1072	TYR	C-N-CD	-7.52	94.18	125.00
1	C	1072	TYR	C-N-CD	-7.51	94.19	125.00
1	A	1072	TYR	C-N-CD	-7.51	94.20	125.00
1	C	1079	PRO	CA-N-CD	7.03	121.83	112.00
1	B	1079	PRO	CA-N-CD	7.02	121.83	112.00
1	A	1079	PRO	CA-N-CD	7.01	121.82	112.00
1	C	837	ILE	N-CA-C	-7.00	103.47	110.62
1	A	837	ILE	N-CA-C	-6.99	103.49	110.62
1	B	837	ILE	N-CA-C	-6.98	103.50	110.62
1	B	841	PHE	CB-CA-C	6.96	123.79	109.95
1	A	841	PHE	CB-CA-C	6.95	123.78	109.95
1	C	841	PHE	CB-CA-C	6.95	123.77	109.95
1	B	984	SER	CA-C-O	-6.93	113.50	119.18
1	A	984	SER	CA-C-O	-6.89	113.53	119.18
1	B	855	ILE	N-CA-C	-6.85	103.63	110.62
1	C	984	SER	CA-C-O	-6.85	113.56	119.18
1	A	855	ILE	N-CA-C	-6.85	103.64	110.62
1	C	855	ILE	N-CA-C	-6.84	103.65	110.62
1	C	982	ASP	N-CA-C	6.80	119.09	108.96
1	B	982	ASP	N-CA-C	6.80	119.08	108.96
1	A	982	ASP	N-CA-C	6.79	119.08	108.96
1	A	983	ARG	N-CA-CB	-6.77	99.05	110.49
1	B	983	ARG	N-CA-CB	-6.77	99.05	110.49
1	C	983	ARG	N-CA-CB	-6.75	99.08	110.49
1	B	842	ILE	N-CA-C	-6.71	103.98	110.42
1	A	842	ILE	N-CA-C	-6.68	104.01	110.42
1	C	842	ILE	N-CA-C	-6.67	104.02	110.42
1	B	983	ARG	N-CA-C	6.54	124.74	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	983	ARG	N-CA-C	6.53	124.72	110.80
1	C	983	ARG	N-CA-C	6.52	124.69	110.80
1	B	850	TYR	CA-C-O	-6.39	114.11	120.82
1	A	850	TYR	CA-C-O	-6.38	114.12	120.82
1	C	850	TYR	CA-C-O	-6.37	114.13	120.82
1	B	834	VAL	N-CA-CB	6.25	121.55	111.23
1	A	834	VAL	N-CA-CB	6.23	121.52	111.23
1	C	834	VAL	N-CA-CB	6.22	121.49	111.23
1	A	1073	PRO	N-CA-CB	-5.66	97.31	103.25
1	C	1089	LEU	N-CA-C	-5.65	105.12	111.28
1	B	841	PHE	N-CA-C	-5.65	106.34	113.18
1	A	1089	LEU	N-CA-C	-5.63	105.14	111.28
1	B	1089	LEU	N-CA-C	-5.63	105.14	111.28
1	C	1073	PRO	N-CA-CB	-5.62	97.35	103.25
1	A	841	PHE	N-CA-C	-5.62	106.38	113.18
1	B	1073	PRO	N-CA-CB	-5.60	97.37	103.25
1	C	841	PHE	N-CA-C	-5.59	106.42	113.18
1	A	1717	LEU	N-CA-C	-5.34	106.70	113.43
1	C	1717	LEU	N-CA-C	-5.33	106.72	113.43
1	B	1717	LEU	N-CA-C	-5.32	106.73	113.43
1	B	838	ILE	CA-C-O	-5.20	115.66	121.17
1	A	838	ILE	CA-C-O	-5.16	115.70	121.17
1	C	838	ILE	CA-C-O	-5.15	115.71	121.17
1	C	844	ASN	CA-C-O	-5.10	115.47	120.82
1	B	844	ASN	CA-C-O	-5.09	115.47	120.82
1	A	844	ASN	CA-C-O	-5.09	115.48	120.82
1	A	1081	TYR	CA-C-O	-5.02	116.16	121.94
1	B	1246	CYS	CB-CA-C	-5.02	101.34	110.63
1	A	1246	CYS	CB-CA-C	-5.01	101.36	110.63
1	C	1081	TYR	CA-C-O	-5.01	116.17	121.94
1	C	1246	CYS	CB-CA-C	-5.01	101.36	110.63
1	B	1079	PRO	N-CA-C	5.00	122.78	112.47
1	A	1079	PRO	N-CA-C	5.00	122.77	112.47

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1366	ARG	Sidechain
1	A	1373	ARG	Sidechain
1	A	1648	SER	Mainchain
1	A	2342	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2373	ARG	Sidechain
1	A	982	ASP	Mainchain
1	A	983	ARG	Sidechain
1	B	1366	ARG	Sidechain
1	B	1373	ARG	Sidechain
1	B	1648	SER	Mainchain
1	B	2342	ARG	Sidechain
1	B	2373	ARG	Sidechain
1	B	982	ASP	Mainchain
1	B	983	ARG	Sidechain
1	C	1366	ARG	Sidechain
1	C	1373	ARG	Sidechain
1	C	2342	ARG	Sidechain
1	C	2373	ARG	Sidechain
1	C	982	ASP	Mainchain
1	C	983	ARG	Sidechain

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	11029	0	11095	338	0
1	B	11029	0	11095	346	0
1	C	11029	0	11095	354	0
All	All	33087	0	33285	982	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 15.

All (982) 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:B:1021:ALA:O	1:B:1025:CYS:SG	2.20	1.00
1:A:1021:ALA:O	1:A:1025:CYS:SG	2.20	0.99
1:C:1021:ALA:O	1:C:1025:CYS:SG	2.20	0.98
1:C:1036:ARG:HB3	1:C:1039:VAL:HG12	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:ARG:HB3	1:A:1039:VAL:HG12	1.50	0.93
1:B:1036:ARG:HB3	1:B:1039:VAL:HG12	1.51	0.91
1:C:2064:TRP:CH2	1:C:2348:LEU:HB3	2.11	0.85
1:B:2064:TRP:CH2	1:B:2348:LEU:HB3	2.11	0.83
1:A:1044:VAL:HG22	1:A:1121:LEU:HD11	1.59	0.83
1:A:2064:TRP:CH2	1:A:2348:LEU:HB3	2.11	0.83
1:C:1044:VAL:HG22	1:C:1121:LEU:HD11	1.59	0.83
1:C:2354:GLY:O	1:C:2357:ILE:HG22	1.79	0.83
1:B:2354:GLY:O	1:B:2357:ILE:HG22	1.79	0.83
1:B:1044:VAL:HG22	1:B:1121:LEU:HD11	1.59	0.82
1:A:2354:GLY:O	1:A:2357:ILE:HG22	1.79	0.81
1:C:1715:VAL:HG12	1:C:1716:LEU:H	1.48	0.79
1:A:879:LEU:HD21	1:A:941:SER:HB3	1.66	0.77
1:C:879:LEU:HD21	1:C:941:SER:HB3	1.66	0.77
1:C:1973:MET:SD	1:C:2021:CYS:SG	2.82	0.77
1:A:1073:PRO:HG2	1:A:1095:LEU:HD11	1.65	0.77
1:A:1973:MET:SD	1:A:2021:CYS:SG	2.82	0.77
1:B:1073:PRO:HG2	1:B:1095:LEU:HD11	1.65	0.77
1:C:1073:PRO:HG2	1:C:1095:LEU:HD11	1.65	0.77
1:A:1715:VAL:HG12	1:A:1716:LEU:H	1.48	0.76
1:B:879:LEU:HD21	1:B:941:SER:HB3	1.66	0.76
1:B:1009:ILE:HG22	1:B:1113:VAL:HG12	1.67	0.76
1:A:1009:ILE:HG22	1:A:1113:VAL:HG12	1.67	0.76
1:B:1715:VAL:HG12	1:B:1716:LEU:H	1.48	0.76
1:C:1009:ILE:HG22	1:C:1113:VAL:HG12	1.67	0.76
1:B:1973:MET:SD	1:B:2021:CYS:SG	2.82	0.75
1:A:2181:ASN:OD1	1:A:2181:ASN:O	2.05	0.75
1:B:2181:ASN:OD1	1:B:2181:ASN:O	2.05	0.75
1:B:2064:TRP:CD1	1:C:1871:PRO:HG2	2.22	0.75
1:A:1871:PRO:HG2	1:C:2064:TRP:CD1	2.22	0.74
1:C:2181:ASN:O	1:C:2181:ASN:OD1	2.05	0.74
1:C:1870:ILE:HG22	1:C:1872:VAL:H	1.52	0.74
1:A:2064:TRP:CD1	1:B:1871:PRO:HG2	2.22	0.74
1:B:1870:ILE:HG22	1:B:1872:VAL:H	1.52	0.74
1:A:1036:ARG:HB3	1:A:1039:VAL:CG1	2.18	0.74
1:B:1211:ASN:CG	1:B:1326:MET:HE3	2.13	0.73
1:C:1211:ASN:CG	1:C:1326:MET:HE3	2.13	0.73
1:A:1870:ILE:HG22	1:A:1872:VAL:H	1.52	0.73
1:C:1036:ARG:HB3	1:C:1039:VAL:CG1	2.18	0.73
1:A:840:ILE:HD12	1:A:1108:ILE:HD11	1.71	0.73
1:B:1036:ARG:HB3	1:B:1039:VAL:CG1	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1211:ASN:OD1	1:B:1326:MET:HE3	1.89	0.72
1:A:1211:ASN:CG	1:A:1326:MET:HE3	2.13	0.72
1:B:840:ILE:HD12	1:B:1108:ILE:HD11	1.71	0.72
1:C:840:ILE:HD12	1:C:1108:ILE:HD11	1.71	0.72
1:A:1200:MET:HE2	1:A:1200:MET:HA	1.71	0.72
1:A:1041:ARG:O	1:A:1045:PHE:CD2	2.43	0.72
1:B:1041:ARG:O	1:B:1045:PHE:CD2	2.43	0.72
1:C:1211:ASN:OD1	1:C:1326:MET:HE3	1.89	0.72
1:B:1148:GLN:O	1:B:1148:GLN:HG3	1.90	0.72
1:A:1211:ASN:OD1	1:A:1326:MET:HE3	1.89	0.71
1:B:1200:MET:HA	1:B:1200:MET:HE2	1.71	0.71
1:C:1041:ARG:O	1:C:1045:PHE:CD2	2.43	0.71
1:B:2140:VAL:HG11	1:C:1688:THR:HG23	1.73	0.71
1:C:1148:GLN:O	1:C:1148:GLN:HG3	1.89	0.71
1:C:826:PHE:O	1:C:830:ILE:HD13	1.91	0.71
1:A:1688:THR:HG23	1:C:2140:VAL:HG11	1.73	0.71
1:A:2140:VAL:HG11	1:B:1688:THR:HG23	1.73	0.71
1:A:826:PHE:O	1:A:830:ILE:HD13	1.90	0.71
1:B:826:PHE:O	1:B:830:ILE:HD13	1.91	0.71
1:B:2200:GLU:O	1:B:2201:ASN:OD1	2.09	0.71
1:A:1888:ASP:HA	1:A:1891:LEU:HD13	1.73	0.70
1:C:1715:VAL:HG12	1:C:1716:LEU:N	2.06	0.70
1:B:1888:ASP:HA	1:B:1891:LEU:HD13	1.73	0.70
1:C:1200:MET:HE2	1:C:1200:MET:HA	1.71	0.70
1:C:2347:PHE:HA	1:C:2350:LYS:HG2	1.73	0.70
1:A:1017:MET:SD	1:A:1239:VAL:HG12	2.32	0.70
1:C:2200:GLU:O	1:C:2201:ASN:OD1	2.09	0.70
1:A:2200:GLU:O	1:A:2201:ASN:OD1	2.09	0.70
1:B:1017:MET:SD	1:B:1239:VAL:HG12	2.32	0.70
1:A:1148:GLN:O	1:A:1148:GLN:HG3	1.90	0.70
1:A:1715:VAL:HG12	1:A:1716:LEU:N	2.06	0.70
1:B:2347:PHE:HA	1:B:2350:LYS:HG2	1.73	0.70
1:C:1888:ASP:HA	1:C:1891:LEU:HD13	1.73	0.70
1:B:1715:VAL:HG12	1:B:1716:LEU:N	2.06	0.69
1:C:1017:MET:SD	1:C:1239:VAL:HG12	2.32	0.69
1:A:2108:MET:HE2	1:A:2149:GLU:HA	1.75	0.69
1:C:2108:MET:HE2	1:C:2149:GLU:HA	1.75	0.69
1:A:2347:PHE:HA	1:A:2350:LYS:HG2	1.73	0.68
1:A:1687:ARG:HH12	1:A:1705:GLN:HB3	1.59	0.68
1:B:2108:MET:HE2	1:B:2149:GLU:HA	1.75	0.68
1:C:1088:ASN:O	1:C:1092:LEU:HG	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1088:ASN:O	1:B:1092:LEU:HG	1.93	0.68
1:B:1006:MET:HE1	1:B:1028:LEU:HD11	1.76	0.68
1:A:1006:MET:HE1	1:A:1028:LEU:HD11	1.76	0.68
1:C:1006:MET:HE1	1:C:1028:LEU:HD11	1.76	0.68
1:C:2161:GLU:HG3	1:C:2162:ILE:HG23	1.77	0.67
1:B:2161:GLU:HG3	1:B:2162:ILE:HG23	1.77	0.67
1:A:1883:LEU:HD21	1:C:2054:VAL:HG22	1.76	0.67
1:A:2161:GLU:HG3	1:A:2162:ILE:HG23	1.77	0.67
1:A:1088:ASN:O	1:A:1092:LEU:HG	1.94	0.67
1:C:1687:ARG:HH12	1:C:1705:GLN:HB3	1.59	0.67
1:A:879:LEU:CD2	1:A:941:SER:HB3	2.25	0.66
1:B:2265:ILE:HA	1:B:2271:ARG:HH12	1.61	0.66
1:A:2054:VAL:HG22	1:B:1883:LEU:HD21	1.76	0.66
1:A:2265:ILE:HA	1:A:2271:ARG:HH12	1.61	0.66
1:C:2265:ILE:HA	1:C:2271:ARG:HH12	1.61	0.66
1:B:879:LEU:CD2	1:B:941:SER:HB3	2.25	0.66
1:A:1872:VAL:CG2	1:A:1875:VAL:HG23	2.26	0.66
1:B:1687:ARG:HH12	1:B:1705:GLN:HB3	1.59	0.66
1:A:1874:LEU:HD12	1:A:1875:VAL:N	2.11	0.66
1:C:1712:TRP:CE3	1:C:1715:VAL:HG21	2.31	0.66
1:A:1368:ARG:O	1:A:1372:ILE:HG22	1.97	0.66
1:B:2054:VAL:HG22	1:C:1883:LEU:HD21	1.77	0.66
1:B:971:LYS:HB3	1:B:978:HIS:CE1	2.32	0.65
1:B:1041:ARG:O	1:B:1045:PHE:HD2	1.80	0.65
1:C:879:LEU:CD2	1:C:941:SER:HB3	2.25	0.65
1:C:971:LYS:HB3	1:C:978:HIS:CE1	2.32	0.65
1:C:1368:ARG:O	1:C:1372:ILE:HG22	1.96	0.65
1:C:1874:LEU:HD12	1:C:1875:VAL:N	2.11	0.65
1:A:1712:TRP:CE3	1:A:1715:VAL:HG21	2.31	0.65
1:B:1872:VAL:CG2	1:B:1875:VAL:HG23	2.26	0.65
1:B:1874:LEU:HD22	1:B:1922:MET:HG2	1.78	0.65
1:B:1712:TRP:CE3	1:B:1715:VAL:HG21	2.31	0.65
1:A:820:GLU:HB3	1:A:824:ARG:HH21	1.61	0.65
1:A:971:LYS:HB3	1:A:978:HIS:CE1	2.32	0.65
1:C:1874:LEU:HD22	1:C:1922:MET:HG2	1.78	0.65
1:A:1833:PRO:HB3	1:A:1963:LEU:HD22	1.80	0.64
1:B:820:GLU:HB3	1:B:824:ARG:HH21	1.61	0.64
1:B:1874:LEU:HD12	1:B:1875:VAL:N	2.11	0.64
1:C:1872:VAL:CG2	1:C:1875:VAL:HG23	2.26	0.64
1:A:1041:ARG:O	1:A:1045:PHE:HD2	1.80	0.64
1:C:1196:PHE:HE2	1:C:1226:ALA:HB1	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1252:PHE:HA	1:C:1262:LEU:HD13	1.80	0.64
1:B:1368:ARG:O	1:B:1372:ILE:HG22	1.96	0.64
1:C:820:GLU:HB3	1:C:824:ARG:HH21	1.61	0.64
1:C:1833:PRO:HB3	1:C:1963:LEU:HD22	1.80	0.64
1:A:1306:ALA:O	1:A:1310:LEU:HD12	1.98	0.64
1:C:1306:ALA:O	1:C:1310:LEU:HD12	1.98	0.64
1:A:1196:PHE:HE2	1:A:1226:ALA:HB1	1.63	0.64
1:A:1252:PHE:HA	1:A:1262:LEU:HD13	1.80	0.64
1:B:1196:PHE:HE2	1:B:1226:ALA:HB1	1.63	0.63
1:A:1874:LEU:HD22	1:A:1922:MET:HG2	1.78	0.63
1:B:1306:ALA:O	1:B:1310:LEU:HD12	1.98	0.63
1:C:1041:ARG:O	1:C:1045:PHE:HD2	1.80	0.63
1:A:1409:ASP:HB3	1:A:1412:ASN:HB2	1.81	0.63
1:B:846:ILE:HG22	1:B:846:ILE:O	1.99	0.63
1:A:867:ALA:O	1:A:868:ASP:C	2.42	0.63
1:B:1252:PHE:HA	1:B:1262:LEU:HD13	1.80	0.63
1:C:1196:PHE:CE2	1:C:1226:ALA:HB1	2.34	0.62
1:C:1409:ASP:HB3	1:C:1412:ASN:HB2	1.81	0.62
1:A:1196:PHE:CE2	1:A:1226:ALA:HB1	2.34	0.62
1:B:1833:PRO:HB3	1:B:1963:LEU:HD22	1.80	0.62
1:B:1409:ASP:HB3	1:B:1412:ASN:HB2	1.81	0.62
1:B:1634:THR:HG23	1:B:1637:LEU:HD12	1.82	0.62
1:A:1634:THR:HG23	1:A:1637:LEU:HD12	1.82	0.62
1:A:846:ILE:HG22	1:A:846:ILE:O	1.99	0.62
1:A:1134:ILE:HD11	1:A:1149:TYR:HB2	1.82	0.61
1:B:1999:THR:HG22	1:B:2405:ARG:HD2	1.82	0.61
1:B:1180:ALA:HA	1:B:1183:ILE:HG12	1.83	0.61
1:B:1196:PHE:CE2	1:B:1226:ALA:HB1	2.34	0.61
1:B:1871:PRO:O	1:B:1872:VAL:HG22	2.01	0.61
1:B:2264:ILE:HD11	1:B:2320:TRP:HH2	1.65	0.61
1:C:846:ILE:O	1:C:846:ILE:HG22	1.99	0.61
1:A:1402:ASP:CG	1:A:1403:TYR:H	2.08	0.61
1:B:867:ALA:O	1:B:868:ASP:C	2.42	0.61
1:B:1134:ILE:HD11	1:B:1149:TYR:HB2	1.82	0.61
1:C:867:ALA:O	1:C:868:ASP:C	2.42	0.61
1:A:2137:ARG:HD3	1:B:1691:GLN:OE1	2.00	0.61
1:C:1402:ASP:CG	1:C:1403:TYR:H	2.08	0.61
1:C:1999:THR:HG22	1:C:2405:ARG:HD2	1.82	0.61
1:C:1134:ILE:HD11	1:C:1149:TYR:HB2	1.82	0.61
1:C:1634:THR:HG23	1:C:1637:LEU:HD12	1.82	0.61
1:C:1871:PRO:O	1:C:1872:VAL:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2363:VAL:HA	1:B:2366:VAL:HG12	1.83	0.61
1:A:848:ALA:HA	1:A:851:ILE:HD12	1.83	0.61
1:A:1691:GLN:OE1	1:C:2137:ARG:HD3	2.00	0.61
1:A:1871:PRO:O	1:A:1872:VAL:HG22	2.01	0.61
1:B:1073:PRO:HB2	1:B:1095:LEU:HD21	1.82	0.61
1:B:2137:ARG:HD3	1:C:1691:GLN:OE1	2.00	0.61
1:C:1073:PRO:HB2	1:C:1095:LEU:HD21	1.83	0.61
1:B:2122:THR:HG22	1:C:1688:THR:HG21	1.83	0.61
1:A:2264:ILE:HD11	1:A:2320:TRP:HH2	1.65	0.61
1:C:2363:VAL:HA	1:C:2366:VAL:HG12	1.83	0.61
1:C:1631:GLY:HA3	1:C:1702:GLY:HA2	1.83	0.60
1:A:1688:THR:HG21	1:C:2122:THR:HG22	1.83	0.60
1:A:2122:THR:HG22	1:B:1688:THR:HG21	1.83	0.60
1:C:2051:ILE:O	1:C:2055:ILE:HG13	2.02	0.60
1:B:848:ALA:HA	1:B:851:ILE:HD12	1.83	0.60
1:B:1012:ASP:OD2	1:B:1113:VAL:HG21	2.02	0.60
1:B:1402:ASP:CG	1:B:1403:TYR:H	2.08	0.60
1:B:1631:GLY:HA3	1:B:1702:GLY:HA2	1.83	0.60
1:C:1188:LEU:HD13	1:C:1268:LEU:HD13	1.84	0.60
1:B:2051:ILE:O	1:B:2055:ILE:HG13	2.01	0.60
1:C:2264:ILE:HD11	1:C:2320:TRP:HH2	1.65	0.60
1:A:1180:ALA:HA	1:A:1183:ILE:HG12	1.83	0.60
1:A:1999:THR:HG22	1:A:2405:ARG:HD2	1.82	0.60
1:C:839:ALA:HA	1:C:842:ILE:HB	1.84	0.59
1:C:848:ALA:HA	1:C:851:ILE:HD12	1.83	0.59
1:A:1029:VAL:O	1:A:1033:LEU:HB2	2.02	0.59
1:A:1012:ASP:OD2	1:A:1113:VAL:HG21	2.02	0.59
1:A:1188:LEU:HD13	1:A:1268:LEU:HD13	1.84	0.59
1:A:2051:ILE:O	1:A:2055:ILE:HG13	2.02	0.59
1:A:2363:VAL:HA	1:A:2366:VAL:HG12	1.83	0.59
1:B:1188:LEU:HD13	1:B:1268:LEU:HD13	1.84	0.59
1:C:1012:ASP:OD2	1:C:1113:VAL:HG21	2.02	0.59
1:A:1073:PRO:HB2	1:A:1095:LEU:HD21	1.83	0.59
1:B:839:ALA:HA	1:B:842:ILE:HB	1.84	0.59
1:B:1227:LEU:O	1:B:1310:LEU:HD22	2.03	0.59
1:A:1227:LEU:O	1:A:1310:LEU:HD22	2.02	0.59
1:C:1180:ALA:HA	1:C:1183:ILE:HG12	1.82	0.58
1:A:2059:SER:OG	1:A:2060:PRO:HD3	2.03	0.58
1:C:2059:SER:OG	1:C:2060:PRO:HD3	2.03	0.58
1:B:1029:VAL:O	1:B:1033:LEU:HB2	2.02	0.58
1:B:2059:SER:OG	1:B:2060:PRO:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ALA:HA	1:A:842:ILE:HB	1.84	0.58
1:A:1631:GLY:HA3	1:A:1702:GLY:HA2	1.83	0.58
1:B:1294:GLU:O	1:B:1295:THR:HG22	2.04	0.58
1:C:1029:VAL:O	1:C:1033:LEU:HB2	2.02	0.58
1:B:2438:LYS:HD2	1:B:2441:GLN:HB3	1.86	0.58
1:C:1227:LEU:O	1:C:1310:LEU:HD22	2.02	0.58
1:A:2438:LYS:HD2	1:A:2441:GLN:HB3	1.86	0.57
1:C:877:ALA:O	1:C:878:TYR:C	2.47	0.57
1:C:1634:THR:O	1:C:1634:THR:HG22	2.05	0.57
1:C:2438:LYS:HD2	1:C:2441:GLN:HB3	1.86	0.57
1:A:1294:GLU:O	1:A:1295:THR:HG22	2.04	0.57
1:B:877:ALA:O	1:B:878:TYR:C	2.48	0.57
1:A:877:ALA:O	1:A:880:PHE:N	2.38	0.57
1:B:1634:THR:HG22	1:B:1634:THR:O	2.05	0.57
1:C:1294:GLU:O	1:C:1295:THR:HG22	2.04	0.56
1:C:1393:THR:HB	1:C:1396:HIS:HB2	1.87	0.56
1:B:1661:ILE:HD11	1:B:1723:HIS:CE1	2.41	0.56
1:C:1661:ILE:HD11	1:C:1723:HIS:CE1	2.41	0.56
1:B:1393:THR:HB	1:B:1396:HIS:HB2	1.87	0.56
1:B:877:ALA:O	1:B:880:PHE:N	2.38	0.56
1:C:877:ALA:O	1:C:880:PHE:N	2.38	0.56
1:A:877:ALA:O	1:A:878:TYR:C	2.48	0.56
1:C:991:PHE:HA	1:C:994:ASP:OD1	2.06	0.56
1:A:991:PHE:HA	1:A:994:ASP:OD1	2.06	0.56
1:A:1024:GLN:HA	1:A:1027:TRP:HB2	1.87	0.56
1:A:1373:ARG:HH22	1:A:2412:LEU:HD23	1.71	0.56
1:B:843:ALA:HB2	1:B:1107:LEU:HD21	1.88	0.56
1:C:2040:LEU:O	1:C:2044:MET:HG3	2.06	0.56
1:A:843:ALA:HB2	1:A:1107:LEU:HD21	1.88	0.56
1:B:1373:ARG:HH22	1:B:2412:LEU:HD23	1.71	0.56
1:A:1073:PRO:CG	1:A:1095:LEU:HD11	2.35	0.55
1:B:1024:GLN:HA	1:B:1027:TRP:HB2	1.87	0.55
1:C:843:ALA:HB2	1:C:1107:LEU:HD21	1.88	0.55
1:A:1393:THR:HB	1:A:1396:HIS:HB2	1.87	0.55
1:A:2040:LEU:O	1:A:2044:MET:HG3	2.06	0.55
1:C:1024:GLN:HA	1:C:1027:TRP:HB2	1.87	0.55
1:A:1589:VAL:HB	1:A:1593:TRP:NE1	2.22	0.55
1:A:1634:THR:HG22	1:A:1634:THR:O	2.05	0.55
1:B:2040:LEU:O	1:B:2044:MET:HG3	2.06	0.55
1:C:1373:ARG:HH22	1:C:2412:LEU:HD23	1.71	0.55
1:A:2169:ASP:OD2	1:B:2159:GLU:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2169:ASP:OD2	1:C:2159:GLU:HG2	2.07	0.55
1:C:876:CYS:HA	1:C:948:GLN:OE1	2.07	0.55
1:C:1009:ILE:HG13	1:C:1010:GLY:N	2.22	0.55
1:A:1661:ILE:HD11	1:A:1723:HIS:CE1	2.41	0.55
1:B:991:PHE:HA	1:B:994:ASP:OD1	2.06	0.55
1:C:1589:VAL:HB	1:C:1593:TRP:NE1	2.22	0.55
1:A:876:CYS:HA	1:A:948:GLN:OE1	2.07	0.55
1:B:876:CYS:HA	1:B:948:GLN:OE1	2.07	0.55
1:A:854:VAL:HG21	1:A:1058:PHE:CD1	2.43	0.54
1:B:1234:THR:O	1:B:1238:LYS:HG2	2.07	0.54
1:C:854:VAL:HG21	1:C:1058:PHE:CD1	2.43	0.54
1:A:1077:TRP:O	1:A:1078:ILE:C	2.50	0.54
1:C:1036:ARG:CB	1:C:1039:VAL:HG12	2.32	0.54
1:C:1372:ILE:HD13	1:C:1375:ARG:HH21	1.72	0.54
1:B:1176:MET:HE3	1:B:1176:MET:HA	1.90	0.54
1:A:1195:ILE:O	1:A:1195:ILE:HD12	2.08	0.54
1:A:2159:GLU:HG2	1:C:2169:ASP:OD2	2.07	0.54
1:B:1077:TRP:O	1:B:1078:ILE:C	2.50	0.54
1:A:1585:MET:HA	1:A:1588:ALA:HB3	1.90	0.54
1:B:1585:MET:HA	1:B:1588:ALA:HB3	1.90	0.54
1:B:1007:ILE:O	1:B:1011:ILE:HG12	2.08	0.54
1:B:1982:ILE:HD12	1:B:1982:ILE:H	1.73	0.54
1:C:1234:THR:O	1:C:1238:LYS:HG2	2.08	0.54
1:C:1007:ILE:O	1:C:1011:ILE:HG12	2.08	0.54
1:C:1195:ILE:HD12	1:C:1195:ILE:O	2.08	0.54
1:B:1009:ILE:HG13	1:B:1010:GLY:N	2.22	0.54
1:B:1705:GLN:HB2	1:B:1712:TRP:HE1	1.73	0.54
1:C:1982:ILE:HD12	1:C:1982:ILE:H	1.73	0.54
1:A:1021:ALA:HB1	1:A:1239:VAL:HG11	1.90	0.53
1:B:854:VAL:HG21	1:B:1058:PHE:CD1	2.43	0.53
1:B:1589:VAL:HB	1:B:1593:TRP:NE1	2.22	0.53
1:C:1891:LEU:HG	1:C:1996:TRP:CE2	2.43	0.53
1:A:1009:ILE:HG13	1:A:1010:GLY:N	2.22	0.53
1:A:1234:THR:O	1:A:1238:LYS:HG2	2.08	0.53
1:A:1891:LEU:HG	1:A:1996:TRP:CE2	2.43	0.53
1:B:1891:LEU:HG	1:B:1996:TRP:CE2	2.43	0.53
1:A:2040:LEU:HD12	1:A:2040:LEU:H	1.74	0.53
1:B:1623:ILE:O	1:B:1627:VAL:HG23	2.09	0.53
1:A:1176:MET:HE3	1:A:1176:MET:HA	1.90	0.53
1:B:1372:ILE:HD13	1:B:1375:ARG:HH21	1.72	0.53
1:A:1623:ILE:O	1:A:1627:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1982:ILE:H	1:A:1982:ILE:HD12	1.73	0.53
1:B:1073:PRO:CG	1:B:1095:LEU:HD11	2.35	0.53
1:B:1271:ILE:CD1	1:B:1297:GLU:HG3	2.39	0.53
1:C:1073:PRO:CG	1:C:1095:LEU:HD11	2.35	0.53
1:A:1007:ILE:O	1:A:1011:ILE:HG12	2.08	0.53
1:B:987:ASN:HA	1:B:990:GLN:HB2	1.91	0.53
1:B:1021:ALA:HB1	1:B:1239:VAL:HG11	1.90	0.53
1:C:2264:ILE:CD1	1:C:2320:TRP:HH2	2.22	0.53
1:A:987:ASN:HA	1:A:990:GLN:HB2	1.91	0.53
1:C:1585:MET:HA	1:C:1588:ALA:HB3	1.90	0.53
1:C:1215:ARG:HD2	1:C:1218:GLU:HB3	1.91	0.53
1:C:1271:ILE:CD1	1:C:1297:GLU:HG3	2.39	0.53
1:C:2326:THR:HG22	1:C:2328:TYR:H	1.74	0.53
1:C:1021:ALA:HB1	1:C:1239:VAL:HG11	1.90	0.52
1:B:1195:ILE:HD12	1:B:1195:ILE:O	2.08	0.52
1:B:2326:THR:HG22	1:B:2328:TYR:H	1.74	0.52
1:A:1006:MET:O	1:A:1006:MET:HE3	2.10	0.52
1:A:1372:ILE:HD13	1:A:1375:ARG:HH21	1.72	0.52
1:A:1705:GLN:HB2	1:A:1712:TRP:HE1	1.73	0.52
1:A:1036:ARG:CB	1:A:1039:VAL:HG12	2.32	0.52
1:A:1627:VAL:HG22	1:A:1937:TYR:CD2	2.45	0.52
1:B:867:ALA:O	1:B:869:GLY:N	2.43	0.52
1:B:1006:MET:HE3	1:B:1006:MET:O	2.10	0.52
1:B:1194:ILE:O	1:B:1198:LEU:HD13	2.10	0.52
1:B:2040:LEU:H	1:B:2040:LEU:HD12	1.74	0.52
1:C:871:PHE:HA	1:C:874:PHE:CD2	2.45	0.52
1:C:1077:TRP:O	1:C:1078:ILE:C	2.51	0.52
1:C:987:ASN:HA	1:C:990:GLN:HB2	1.91	0.52
1:C:1176:MET:HE3	1:C:1176:MET:HA	1.90	0.52
1:C:1705:GLN:HB2	1:C:1712:TRP:HE1	1.73	0.52
1:C:2265:ILE:HA	1:C:2271:ARG:HH22	1.74	0.52
1:A:1194:ILE:O	1:A:1198:LEU:HD13	2.10	0.52
1:C:1006:MET:HE3	1:C:1006:MET:O	2.10	0.52
1:C:1623:ILE:O	1:C:1627:VAL:HG23	2.09	0.52
1:B:2265:ILE:HA	1:B:2271:ARG:HH22	1.74	0.52
1:C:867:ALA:O	1:C:869:GLY:N	2.43	0.52
1:A:1271:ILE:CD1	1:A:1297:GLU:HG3	2.39	0.52
1:A:2326:THR:HG22	1:A:2328:TYR:H	1.74	0.52
1:C:1627:VAL:HG22	1:C:1937:TYR:CD2	2.45	0.52
1:C:2040:LEU:HD12	1:C:2040:LEU:H	1.74	0.52
1:A:2264:ILE:CD1	1:A:2320:TRP:HH2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2265:ILE:HA	1:A:2271:ARG:HH22	1.74	0.52
1:B:1036:ARG:CB	1:B:1039:VAL:HG12	2.32	0.52
1:C:1194:ILE:O	1:C:1198:LEU:HD13	2.10	0.52
1:A:1215:ARG:HD2	1:A:1218:GLU:HB3	1.91	0.51
1:C:1627:VAL:HG22	1:C:1937:TYR:HD2	1.75	0.51
1:A:871:PHE:HA	1:A:874:PHE:CD2	2.45	0.51
1:B:871:PHE:HA	1:B:874:PHE:CD2	2.45	0.51
1:B:1627:VAL:HG22	1:B:1937:TYR:HD2	1.75	0.51
1:B:1627:VAL:HG22	1:B:1937:TYR:CD2	2.45	0.51
1:B:2264:ILE:CD1	1:B:2320:TRP:HH2	2.22	0.51
1:A:867:ALA:O	1:A:869:GLY:N	2.43	0.51
1:B:2200:GLU:O	1:B:2201:ASN:CG	2.54	0.51
1:A:2200:GLU:O	1:A:2201:ASN:CG	2.54	0.51
1:B:1011:ILE:HD12	1:B:1304:VAL:HB	1.92	0.51
1:B:1871:PRO:C	1:B:1872:VAL:HG22	2.36	0.51
1:B:1215:ARG:HD2	1:B:1218:GLU:HB3	1.91	0.51
1:C:1111:PHE:HA	1:C:1114:LEU:HD23	1.93	0.51
1:A:1211:ASN:CG	1:A:1326:MET:CE	2.83	0.51
1:A:1011:ILE:HD12	1:A:1304:VAL:HB	1.92	0.51
1:C:1667:VAL:HA	1:C:1670:ILE:HG22	1.93	0.51
1:A:1372:ILE:HD12	1:A:1372:ILE:O	2.11	0.51
1:C:834:VAL:O	1:C:835:PHE:C	2.53	0.51
1:A:1871:PRO:C	1:A:1872:VAL:HG22	2.36	0.50
1:A:1978:VAL:O	1:A:1982:ILE:HD12	2.12	0.50
1:B:1211:ASN:CG	1:B:1326:MET:CE	2.83	0.50
1:A:1102:TRP:HE3	1:A:1103:PRO:HD2	1.76	0.50
1:A:1667:VAL:HA	1:A:1670:ILE:HG22	1.93	0.50
1:A:1627:VAL:HG22	1:A:1937:TYR:HD2	1.75	0.50
1:B:1006:MET:CE	1:B:1028:LEU:HD11	2.40	0.50
1:C:2200:GLU:O	1:C:2201:ASN:CG	2.54	0.50
1:A:2304:MET:HE1	1:C:2169:ASP:OD2	2.11	0.50
1:B:1581:ASP:C	1:B:1585:MET:HE2	2.37	0.50
1:C:982:ASP:H	1:C:987:ASN:ND2	2.10	0.50
1:B:2064:TRP:CZ3	1:B:2348:LEU:HD12	2.47	0.50
1:C:1011:ILE:HD12	1:C:1304:VAL:HB	1.92	0.50
1:C:1871:PRO:C	1:C:1872:VAL:HG22	2.36	0.50
1:B:834:VAL:O	1:B:835:PHE:C	2.54	0.50
1:B:1654:LYS:HA	1:B:1657:TRP:HD1	1.77	0.50
1:C:1299:ASN:HB2	1:C:1303:ASP:HB2	1.94	0.50
1:A:1111:PHE:HA	1:A:1114:LEU:HD23	1.93	0.50
1:B:1037:VAL:HG13	1:B:1040:ARG:HE	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:ASP:H	1:A:987:ASN:ND2	2.10	0.50
1:A:1037:VAL:HG13	1:A:1040:ARG:HE	1.77	0.50
1:A:2064:TRP:CH2	1:A:2348:LEU:CB	2.92	0.50
1:B:1978:VAL:O	1:B:1982:ILE:HD12	2.12	0.50
1:C:1006:MET:CE	1:C:1028:LEU:HD11	2.40	0.50
1:C:1581:ASP:C	1:C:1585:MET:HE2	2.37	0.50
1:A:857:LEU:HD22	1:A:857:LEU:O	2.12	0.50
1:A:2094:MET:HE3	1:A:2157:ARG:HB2	1.94	0.50
1:A:2169:ASP:OD2	1:B:2304:MET:HE1	2.12	0.50
1:B:1102:TRP:HE3	1:B:1103:PRO:HD2	1.76	0.50
1:C:1037:VAL:HG13	1:C:1040:ARG:HE	1.77	0.50
1:C:1927:ALA:O	1:C:1928:ILE:HB	2.11	0.50
1:A:2064:TRP:CZ3	1:A:2348:LEU:HD12	2.47	0.49
1:B:1017:MET:HG3	1:B:1017:MET:O	2.12	0.49
1:C:1111:PHE:O	1:C:1115:LEU:HG	2.12	0.49
1:A:1006:MET:CE	1:A:1028:LEU:HD11	2.40	0.49
1:A:1017:MET:O	1:A:1017:MET:HG3	2.12	0.49
1:A:1581:ASP:C	1:A:1585:MET:HE2	2.37	0.49
1:B:1667:VAL:HA	1:B:1670:ILE:HG22	1.93	0.49
1:C:1978:VAL:O	1:C:1982:ILE:HD12	2.12	0.49
1:B:1228:LEU:HD11	1:B:1311:VAL:HG12	1.94	0.49
1:B:1882:THR:HA	1:B:1885:ILE:HG12	1.94	0.49
1:B:1927:ALA:O	1:B:1928:ILE:HB	2.12	0.49
1:C:1102:TRP:HE3	1:C:1103:PRO:HD2	1.76	0.49
1:B:1372:ILE:O	1:B:1372:ILE:HD12	2.11	0.49
1:C:1134:ILE:CD1	1:C:1149:TYR:HB2	2.43	0.49
1:C:1211:ASN:CG	1:C:1326:MET:CE	2.83	0.49
1:A:1111:PHE:O	1:A:1115:LEU:HG	2.12	0.49
1:B:857:LEU:HD22	1:B:857:LEU:O	2.12	0.49
1:B:982:ASP:H	1:B:987:ASN:ND2	2.10	0.49
1:B:1072:TYR:O	1:B:1073:PRO:C	2.55	0.49
1:C:1017:MET:O	1:C:1017:MET:HG3	2.12	0.49
1:C:1654:LYS:HA	1:C:1657:TRP:HD1	1.77	0.49
1:A:834:VAL:O	1:A:835:PHE:C	2.54	0.49
1:A:1715:VAL:O	1:A:1716:LEU:C	2.56	0.49
1:B:2094:MET:HE3	1:B:2157:ARG:HB2	1.94	0.49
1:C:2064:TRP:CZ3	1:C:2348:LEU:HD12	2.47	0.49
1:A:819:ILE:HA	1:A:822:LEU:HD12	1.95	0.49
1:A:1927:ALA:O	1:A:1928:ILE:HB	2.12	0.49
1:A:1299:ASN:HB2	1:A:1303:ASP:HB2	1.94	0.49
1:B:981:PHE:HB3	1:B:991:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2169:ASP:OD2	1:C:2304:MET:HE1	2.12	0.49
1:C:857:LEU:O	1:C:857:LEU:HD22	2.12	0.49
1:C:1372:ILE:HD12	1:C:1372:ILE:O	2.11	0.49
1:C:2094:MET:HE3	1:C:2157:ARG:HB2	1.94	0.49
1:A:2135:ARG:CZ	1:A:2266:ASN:HD22	2.26	0.49
1:B:2108:MET:HE3	1:B:2148:TYR:O	2.13	0.49
1:A:981:PHE:HB3	1:A:991:PHE:HE2	1.77	0.49
1:A:1654:LYS:HA	1:A:1657:TRP:HD1	1.77	0.49
1:A:1874:LEU:HD12	1:A:1874:LEU:C	2.38	0.49
1:A:1882:THR:HA	1:A:1885:ILE:HG12	1.94	0.49
1:A:2125:TYR:CE1	1:B:1289:LYS:HE2	2.48	0.49
1:B:1034:ASN:HD21	1:B:1039:VAL:HG21	1.78	0.49
1:B:2125:TYR:CE1	1:C:1289:LYS:HE2	2.48	0.49
1:C:1050:MET:HA	1:C:1050:MET:HE2	1.95	0.49
1:A:851:ILE:HB	1:A:852:PRO:HD3	1.95	0.48
1:A:1134:ILE:CD1	1:A:1149:TYR:HB2	2.43	0.48
1:A:2108:MET:HE3	1:A:2148:TYR:O	2.13	0.48
1:B:1134:ILE:CD1	1:B:1149:TYR:HB2	2.43	0.48
1:B:1874:LEU:HA	1:B:1877:MET:HE2	1.95	0.48
1:C:2043:TYR:O	1:C:2047:PHE:HB2	2.14	0.48
1:A:989:ILE:O	1:A:993:ILE:HG12	2.13	0.48
1:A:1192:GLY:O	1:A:1196:PHE:HB2	2.13	0.48
1:A:2438:LYS:HE3	1:A:2442:GLU:HB2	1.95	0.48
1:B:1111:PHE:HA	1:B:1114:LEU:HD23	1.93	0.48
1:B:1192:GLY:O	1:B:1196:PHE:HB2	2.13	0.48
1:B:2223:LYS:HA	1:B:2223:LYS:HD3	1.66	0.48
1:C:989:ILE:O	1:C:993:ILE:HG12	2.13	0.48
1:C:1072:TYR:O	1:C:1073:PRO:C	2.55	0.48
1:C:851:ILE:HB	1:C:852:PRO:HD3	1.95	0.48
1:C:1015:ASN:HB3	1:C:1300:ILE:HD13	1.95	0.48
1:C:1034:ASN:HD21	1:C:1039:VAL:HG21	1.78	0.48
1:C:1178:THR:HG21	1:C:1309:PHE:HD2	1.79	0.48
1:C:1632:LEU:HA	1:C:1635:LEU:HB2	1.96	0.48
1:C:1684:ILE:HG23	1:C:1685:THR:N	2.28	0.48
1:C:1882:THR:HA	1:C:1885:ILE:HG12	1.94	0.48
1:A:1228:LEU:HD11	1:A:1311:VAL:HG12	1.94	0.48
1:B:1111:PHE:O	1:B:1115:LEU:HG	2.12	0.48
1:B:1715:VAL:O	1:B:1716:LEU:C	2.56	0.48
1:B:2135:ARG:CZ	1:B:2266:ASN:HD22	2.26	0.48
1:C:1192:GLY:O	1:C:1196:PHE:HB2	2.13	0.48
1:C:1715:VAL:O	1:C:1716:LEU:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:ASN:HB3	1:A:1300:ILE:HD13	1.95	0.48
1:A:1072:TYR:O	1:A:1073:PRO:C	2.55	0.48
1:A:1289:LYS:HE2	1:C:2125:TYR:CE1	2.48	0.48
1:A:1632:LEU:HA	1:A:1635:LEU:HB2	1.96	0.48
1:B:989:ILE:O	1:B:993:ILE:HG12	2.13	0.48
1:B:1111:PHE:CE1	1:B:1115:LEU:HD21	2.49	0.48
1:B:1874:LEU:HD12	1:B:1874:LEU:C	2.38	0.48
1:C:1228:LEU:HD11	1:C:1311:VAL:HG12	1.94	0.48
1:C:1874:LEU:HA	1:C:1877:MET:HE2	1.96	0.48
1:C:2135:ARG:CZ	1:C:2266:ASN:HD22	2.26	0.48
1:A:945:LEU:HD12	1:A:946:ALA:N	2.29	0.48
1:A:1654:LYS:HE3	1:A:1738:LEU:HB2	1.96	0.48
1:C:1111:PHE:CE1	1:C:1115:LEU:HD21	2.49	0.48
1:A:1111:PHE:CE1	1:A:1115:LEU:HD21	2.49	0.48
1:A:1871:PRO:HG2	1:C:2064:TRP:NE1	2.29	0.48
1:B:1028:LEU:HD13	1:B:1028:LEU:HA	1.68	0.48
1:B:1299:ASN:HB2	1:B:1303:ASP:HB2	1.94	0.48
1:C:1224:TRP:O	1:C:1228:LEU:HB2	2.14	0.48
1:C:2108:MET:HE3	1:C:2148:TYR:O	2.13	0.48
1:A:1684:ILE:HG23	1:A:1685:THR:N	2.29	0.48
1:A:1874:LEU:HA	1:A:1877:MET:HE2	1.95	0.48
1:A:2031:ALA:O	1:B:1393:THR:HA	2.14	0.48
1:A:2043:TYR:O	1:A:2047:PHE:HB2	2.13	0.48
1:C:1874:LEU:HD12	1:C:1874:LEU:C	2.38	0.48
1:A:1178:THR:HG21	1:A:1309:PHE:HD2	1.79	0.48
1:B:851:ILE:HB	1:B:852:PRO:HD3	1.95	0.48
1:B:1306:ALA:C	1:B:1310:LEU:HD12	2.39	0.48
1:B:1684:ILE:HG23	1:B:1685:THR:N	2.29	0.48
1:B:2043:TYR:O	1:B:2047:PHE:HB2	2.14	0.48
1:C:834:VAL:O	1:C:837:ILE:HG22	2.14	0.48
1:C:1306:ALA:C	1:C:1310:LEU:HD12	2.39	0.48
1:C:2347:PHE:HA	1:C:2350:LYS:CG	2.44	0.48
1:A:1306:ALA:C	1:A:1310:LEU:HD12	2.39	0.47
1:A:2384:MET:HE2	1:A:2427:PRO:HB3	1.96	0.47
1:B:819:ILE:HA	1:B:822:LEU:HD12	1.95	0.47
1:B:2438:LYS:HE3	1:B:2442:GLU:HB2	1.95	0.47
1:C:1344:ASN:O	1:C:1347:ILE:HG13	2.14	0.47
1:C:1402:ASP:CG	1:C:1403:TYR:N	2.72	0.47
1:C:1874:LEU:HD22	1:C:1922:MET:CG	2.44	0.47
1:C:2384:MET:HE2	1:C:2427:PRO:HB3	1.96	0.47
1:C:2438:LYS:HE3	1:C:2442:GLU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1872:VAL:HG23	1:A:1875:VAL:HG23	1.96	0.47
1:B:842:ILE:HD11	1:B:854:VAL:HG12	1.96	0.47
1:B:1178:THR:HG21	1:B:1309:PHE:HD2	1.79	0.47
1:B:1632:LEU:HA	1:B:1635:LEU:HB2	1.96	0.47
1:B:2064:TRP:NE1	1:C:1871:PRO:HG2	2.29	0.47
1:B:2384:MET:HE2	1:B:2427:PRO:HB3	1.96	0.47
1:C:945:LEU:HD12	1:C:946:ALA:N	2.29	0.47
1:A:834:VAL:O	1:A:837:ILE:HG22	2.14	0.47
1:A:879:LEU:HD21	1:A:941:SER:CB	2.41	0.47
1:A:1344:ASN:O	1:A:1347:ILE:HG13	2.14	0.47
1:A:1632:LEU:HD23	1:A:1632:LEU:O	2.14	0.47
1:A:2264:ILE:HD11	1:A:2320:TRP:CH2	2.48	0.47
1:B:1632:LEU:O	1:B:1632:LEU:HD23	2.14	0.47
1:C:819:ILE:HA	1:C:822:LEU:HD12	1.95	0.47
1:C:842:ILE:HD11	1:C:854:VAL:HG12	1.95	0.47
1:C:981:PHE:HB3	1:C:991:PHE:HE2	1.77	0.47
1:A:1050:MET:HA	1:A:1050:MET:HE2	1.95	0.47
1:B:1015:ASN:HB3	1:B:1300:ILE:HD13	1.95	0.47
1:B:1050:MET:HE2	1:B:1050:MET:HA	1.95	0.47
1:C:851:ILE:HG12	1:C:1062:VAL:HG21	1.96	0.47
1:A:1281:LEU:HD21	1:A:1284:LEU:HD13	1.97	0.47
1:A:1874:LEU:HD22	1:A:1922:MET:CG	2.44	0.47
1:B:1378:LYS:HD2	1:B:1378:LYS:O	2.14	0.47
1:B:2031:ALA:O	1:C:1393:THR:HA	2.14	0.47
1:A:880:PHE:HB2	1:A:945:LEU:HD21	1.97	0.47
1:A:1016:ARG:NH1	1:A:1016:ARG:HA	2.30	0.47
1:A:1378:LYS:HD2	1:A:1378:LYS:O	2.14	0.47
1:A:1627:VAL:HG21	1:A:1938:VAL:HG22	1.97	0.47
1:B:1083:ASP:O	1:B:1086:ARG:HG2	2.14	0.47
1:B:1402:ASP:CG	1:B:1403:TYR:N	2.72	0.47
1:B:2440:LYS:HE3	1:C:1396:HIS:NE2	2.30	0.47
1:C:1083:ASP:O	1:C:1086:ARG:HG2	2.14	0.47
1:C:1281:LEU:HD21	1:C:1284:LEU:HD13	1.96	0.47
1:C:1355:ASN:O	1:C:1359:LYS:HG2	2.14	0.47
1:C:1871:PRO:O	1:C:1872:VAL:CG2	2.63	0.47
1:A:851:ILE:CG1	1:A:1062:VAL:HG21	2.44	0.47
1:A:1034:ASN:HD21	1:A:1039:VAL:HG21	1.78	0.47
1:A:1224:TRP:O	1:A:1228:LEU:HB2	2.14	0.47
1:A:1355:ASN:O	1:A:1359:LYS:HG2	2.14	0.47
1:A:2064:TRP:NE1	1:B:1871:PRO:HG2	2.29	0.47
1:A:2440:LYS:HE3	1:B:1396:HIS:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:851:ILE:HG12	1:B:1062:VAL:HG21	1.96	0.47
1:B:1016:ARG:NH1	1:B:1016:ARG:HA	2.30	0.47
1:C:848:ALA:O	1:C:849:LEU:C	2.58	0.47
1:C:1627:VAL:HG21	1:C:1938:VAL:HG22	1.97	0.47
1:A:842:ILE:HD11	1:A:854:VAL:HG12	1.95	0.47
1:A:1871:PRO:O	1:A:1872:VAL:CG2	2.63	0.47
1:A:1987:GLU:OE1	1:C:2372:VAL:HG12	2.14	0.47
1:B:1224:TRP:O	1:B:1228:LEU:HB2	2.14	0.47
1:B:1654:LYS:HE3	1:B:1738:LEU:HB2	1.96	0.47
1:B:2170:SER:OG	1:C:2161:GLU:HA	2.15	0.47
1:B:2372:VAL:HG12	1:C:1987:GLU:OE1	2.14	0.47
1:A:1201:LEU:HD21	1:A:1724:ARG:NH2	2.30	0.47
1:A:2161:GLU:HA	1:C:2170:SER:OG	2.14	0.47
1:B:851:ILE:CG1	1:B:1062:VAL:HG21	2.44	0.47
1:B:1281:LEU:HD21	1:B:1284:LEU:HD13	1.96	0.47
1:B:1344:ASN:O	1:B:1347:ILE:HG13	2.14	0.47
1:C:851:ILE:CG1	1:C:1062:VAL:HG21	2.44	0.47
1:C:880:PHE:HB2	1:C:945:LEU:HD21	1.97	0.47
1:C:1378:LYS:HD2	1:C:1378:LYS:O	2.14	0.47
1:A:1083:ASP:O	1:A:1086:ARG:HG2	2.14	0.47
1:A:1393:THR:HA	1:C:2031:ALA:O	2.14	0.47
1:A:1396:HIS:NE2	1:C:2440:LYS:HE3	2.30	0.47
1:B:880:PHE:HB2	1:B:945:LEU:HD21	1.97	0.47
1:B:945:LEU:HD12	1:B:946:ALA:N	2.29	0.47
1:B:1201:LEU:HD21	1:B:1724:ARG:NH2	2.30	0.47
1:B:1872:VAL:HG23	1:B:1875:VAL:HG23	1.96	0.47
1:C:1669:VAL:O	1:C:1673:VAL:HG23	2.15	0.47
1:C:2237:LEU:HD23	1:C:2239:PRO:HD3	1.96	0.47
1:A:1239:VAL:O	1:A:1242:GLN:HG3	2.15	0.46
1:A:2372:VAL:HG12	1:B:1987:GLU:OE1	2.14	0.46
1:B:806:THR:O	1:B:809:LYS:HG2	2.15	0.46
1:B:834:VAL:O	1:B:837:ILE:HG22	2.14	0.46
1:B:985:LEU:HG	1:B:986:LYS:H	1.80	0.46
1:B:1669:VAL:O	1:B:1673:VAL:HG23	2.15	0.46
1:C:985:LEU:HG	1:C:986:LYS:H	1.80	0.46
1:C:1016:ARG:HA	1:C:1016:ARG:NH1	2.30	0.46
1:C:1239:VAL:O	1:C:1242:GLN:HG3	2.15	0.46
1:A:851:ILE:HG12	1:A:1062:VAL:HG21	1.96	0.46
1:A:1669:VAL:O	1:A:1673:VAL:HG23	2.15	0.46
1:B:1627:VAL:HG21	1:B:1938:VAL:HG22	1.97	0.46
1:C:826:PHE:O	1:C:830:ILE:CD1	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1715:VAL:CG1	1:C:1716:LEU:N	2.78	0.46
1:A:1188:LEU:HD22	1:A:1268:LEU:HD13	1.97	0.46
1:A:2170:SER:OG	1:B:2161:GLU:HA	2.15	0.46
1:B:1148:GLN:O	1:B:1148:GLN:CG	2.61	0.46
1:B:1188:LEU:HD22	1:B:1268:LEU:HD13	1.97	0.46
1:C:1188:LEU:HD22	1:C:1268:LEU:HD13	1.97	0.46
1:C:1391:PRO:HD2	1:C:1396:HIS:CD2	2.50	0.46
1:C:1666:CYS:O	1:C:1670:ILE:HG22	2.15	0.46
1:A:1391:PRO:HD2	1:A:1396:HIS:CD2	2.50	0.46
1:B:1172:TRP:HZ2	1:B:1727:LEU:HB3	1.80	0.46
1:B:1355:ASN:O	1:B:1359:LYS:HG2	2.14	0.46
1:B:2237:LEU:HD23	1:B:2239:PRO:HD3	1.96	0.46
1:C:870:ILE:HG22	1:C:874:PHE:CZ	2.51	0.46
1:C:1632:LEU:HD23	1:C:1632:LEU:O	2.14	0.46
1:C:1654:LYS:HE3	1:C:1738:LEU:HB2	1.96	0.46
1:A:806:THR:O	1:A:809:LYS:HG2	2.15	0.46
1:A:870:ILE:HG22	1:A:874:PHE:CZ	2.51	0.46
1:A:1172:TRP:HZ2	1:A:1727:LEU:HB3	1.80	0.46
1:A:1267:GLN:HG3	1:A:1678:PHE:HB3	1.98	0.46
1:C:1172:TRP:HZ2	1:C:1727:LEU:HB3	1.80	0.46
1:A:848:ALA:O	1:A:849:LEU:C	2.58	0.46
1:A:1019:ALA:O	1:A:1020:LEU:C	2.59	0.46
1:B:1249:LEU:O	1:B:1250:SER:C	2.59	0.46
1:A:1666:CYS:O	1:A:1670:ILE:HG22	2.15	0.46
1:A:2237:LEU:HD23	1:A:2239:PRO:HD3	1.97	0.46
1:B:842:ILE:HG13	1:B:850:TYR:CD1	2.51	0.46
1:C:806:THR:O	1:C:809:LYS:HG2	2.15	0.46
1:C:1629:THR:HG21	1:C:1634:THR:HB	1.98	0.46
1:A:1629:THR:HG21	1:A:1634:THR:HB	1.98	0.46
1:A:1900:LYS:HD2	1:A:1900:LYS:HA	1.71	0.46
1:A:2067:LEU:HD23	1:A:2067:LEU:HA	1.84	0.46
1:B:2064:TRP:CH2	1:B:2348:LEU:CB	2.92	0.46
1:B:2294:LEU:HD12	1:B:2305:TRP:NE1	2.31	0.46
1:B:2347:PHE:HA	1:B:2350:LYS:CG	2.44	0.46
1:A:842:ILE:HG13	1:A:850:TYR:CD1	2.51	0.46
1:B:2322:LYS:HB3	1:B:2322:LYS:HE3	1.79	0.46
1:C:1900:LYS:HA	1:C:1900:LYS:HD2	1.70	0.46
1:A:985:LEU:HG	1:A:986:LYS:H	1.80	0.45
1:B:870:ILE:HG22	1:B:874:PHE:CZ	2.51	0.45
1:B:1871:PRO:O	1:B:1872:VAL:CG2	2.63	0.45
1:B:2187:GLU:OE1	1:B:2211:LEU:CD2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1019:ALA:O	1:C:1020:LEU:C	2.59	0.45
1:C:2064:TRP:CH2	1:C:2348:LEU:CB	2.92	0.45
1:B:1036:ARG:HB2	1:B:1036:ARG:NH1	2.32	0.45
1:B:1239:VAL:O	1:B:1242:GLN:HG3	2.15	0.45
1:B:1900:LYS:HD2	1:B:1900:LYS:HA	1.70	0.45
1:C:2264:ILE:HD11	1:C:2320:TRP:CH2	2.48	0.45
1:B:1391:PRO:HD2	1:B:1396:HIS:CD2	2.50	0.45
1:B:2064:TRP:HD1	1:C:1871:PRO:HG2	1.78	0.45
1:C:842:ILE:HG13	1:C:850:TYR:CD1	2.51	0.45
1:C:1201:LEU:HD21	1:C:1724:ARG:NH2	2.30	0.45
1:C:1833:PRO:HG2	1:C:1963:LEU:HD13	1.99	0.45
1:C:1872:VAL:HG23	1:C:1875:VAL:HG23	1.96	0.45
1:A:1009:ILE:HG13	1:A:1010:GLY:H	1.82	0.45
1:B:1666:CYS:O	1:B:1670:ILE:HG22	2.15	0.45
1:C:813:LYS:O	1:C:817:GLN:HG3	2.17	0.45
1:C:995:TYR:HD1	1:C:995:TYR:HA	1.63	0.45
1:C:1987:GLU:HA	1:C:2007:PHE:HE1	1.82	0.45
1:A:2187:GLU:OE1	1:A:2211:LEU:CD2	2.64	0.45
1:C:1028:LEU:HA	1:C:1028:LEU:HD13	1.68	0.45
1:C:1249:LEU:O	1:C:1250:SER:C	2.59	0.45
1:A:826:PHE:O	1:A:830:ILE:CD1	2.62	0.45
1:A:2294:LEU:HD12	1:A:2305:TRP:NE1	2.31	0.45
1:B:1874:LEU:HD22	1:B:1922:MET:CG	2.43	0.45
1:C:1183:ILE:HD12	1:C:1194:ILE:HG12	1.99	0.45
1:C:2052:GLY:HA2	1:C:2055:ILE:HD11	1.98	0.45
1:C:2187:GLU:OE1	1:C:2211:LEU:CD2	2.64	0.45
1:A:1626:GLN:HG3	1:A:1638:PRO:HG3	1.98	0.45
1:A:1833:PRO:HG2	1:A:1963:LEU:HD13	1.99	0.45
1:A:2326:THR:HG21	1:A:2329:SER:OG	2.17	0.45
1:B:952:ILE:HG22	1:B:956:ARG:HE	1.82	0.45
1:B:1629:THR:HG21	1:B:1634:THR:HB	1.98	0.45
1:B:2064:TRP:HZ3	1:B:2348:LEU:HD12	1.82	0.45
1:A:2351:VAL:HG12	1:A:2352:PHE:N	2.32	0.45
1:B:848:ALA:O	1:B:849:LEU:C	2.58	0.45
1:B:1013:ILE:HG13	1:B:1024:GLN:NE2	2.32	0.45
1:B:1183:ILE:HD12	1:B:1194:ILE:HG12	1.99	0.45
1:B:2326:THR:HG21	1:B:2329:SER:OG	2.17	0.45
1:B:2351:VAL:HG12	1:B:2352:PHE:N	2.32	0.45
1:C:1013:ILE:HG13	1:C:1024:GLN:NE2	2.32	0.45
1:C:2052:GLY:O	1:C:2055:ILE:HD12	2.17	0.45
1:C:2294:LEU:HD12	1:C:2305:TRP:NE1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2326:THR:HG21	1:C:2329:SER:OG	2.17	0.45
1:C:2354:GLY:O	1:C:2357:ILE:CG2	2.60	0.45
1:B:813:LYS:O	1:B:817:GLN:HG3	2.17	0.45
1:B:2061:LEU:HD23	1:B:2061:LEU:HA	1.82	0.45
1:C:1267:GLN:HG3	1:C:1678:PHE:HB3	1.98	0.45
1:A:1036:ARG:NH1	1:A:1036:ARG:HB2	2.32	0.45
1:A:1249:LEU:O	1:A:1250:SER:C	2.59	0.45
1:A:2052:GLY:HA2	1:A:2055:ILE:HD11	1.98	0.45
1:A:2108:MET:CE	1:A:2149:GLU:HA	2.45	0.45
1:B:1009:ILE:HG13	1:B:1010:GLY:H	1.82	0.45
1:B:1019:ALA:O	1:B:1020:LEU:C	2.59	0.45
1:B:1267:GLN:HG3	1:B:1678:PHE:HB3	1.98	0.45
1:C:1842:CYS:HA	1:C:1845:ILE:HG22	1.98	0.45
1:C:1940:LYS:HB3	1:C:1940:LYS:HE2	1.85	0.45
1:C:2064:TRP:HZ3	1:C:2348:LEU:HD12	1.82	0.45
1:A:952:ILE:HG22	1:A:956:ARG:HE	1.82	0.44
1:A:1817:ILE:HD12	1:A:1821:PHE:HB2	1.99	0.44
1:A:2347:PHE:HA	1:A:2350:LYS:CG	2.44	0.44
1:B:826:PHE:O	1:B:830:ILE:CD1	2.62	0.44
1:C:952:ILE:HG22	1:C:956:ARG:HE	1.82	0.44
1:C:1207:LEU:HD13	1:C:1219:HIS:CE1	2.53	0.44
1:A:2052:GLY:O	1:A:2055:ILE:HD12	2.17	0.44
1:B:956:ARG:HA	1:B:959:ARG:HD2	1.99	0.44
1:C:1733:TRP:HA	1:C:1733:TRP:CE3	2.52	0.44
1:C:1882:THR:O	1:C:1886:ILE:HG13	2.17	0.44
1:A:840:ILE:CD1	1:A:1108:ILE:HD11	2.45	0.44
1:A:1013:ILE:HG13	1:A:1024:GLN:NE2	2.32	0.44
1:A:1183:ILE:HD12	1:A:1194:ILE:HG12	1.99	0.44
1:A:1987:GLU:HA	1:A:2007:PHE:HE1	1.81	0.44
1:B:1207:LEU:HD13	1:B:1219:HIS:CE1	2.53	0.44
1:B:1882:THR:O	1:B:1886:ILE:HG13	2.17	0.44
1:B:1987:GLU:HA	1:B:2007:PHE:HE1	1.81	0.44
1:C:840:ILE:CD1	1:C:1108:ILE:HD11	2.45	0.44
1:C:956:ARG:HA	1:C:959:ARG:HD2	1.99	0.44
1:A:857:LEU:HD12	1:A:1111:PHE:HE1	1.82	0.44
1:A:1842:CYS:HA	1:A:1845:ILE:HG22	1.98	0.44
1:B:1817:ILE:HD12	1:B:1821:PHE:HB2	1.99	0.44
1:B:2052:GLY:O	1:B:2055:ILE:HD12	2.17	0.44
1:C:2351:VAL:HG12	1:C:2352:PHE:N	2.32	0.44
1:A:813:LYS:O	1:A:817:GLN:HG3	2.17	0.44
1:A:983:ARG:O	1:A:984:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1623:ILE:HD13	1:A:1941:SER:HB3	2.00	0.44
1:A:2064:TRP:HZ3	1:A:2348:LEU:HD12	1.82	0.44
1:B:1623:ILE:HD13	1:B:1941:SER:HB3	2.00	0.44
1:B:1626:GLN:HG3	1:B:1638:PRO:HG3	1.98	0.44
1:C:1036:ARG:NH1	1:C:1036:ARG:HB2	2.32	0.44
1:C:2322:LYS:HB3	1:C:2322:LYS:HE3	1.79	0.44
1:A:1084:ASP:HA	1:A:1087:PHE:HB3	2.00	0.44
1:A:2061:LEU:HD23	1:A:2061:LEU:HA	1.82	0.44
1:B:1277:GLU:O	1:B:1277:GLU:HG3	2.18	0.44
1:B:1833:PRO:HG2	1:B:1963:LEU:HD13	1.99	0.44
1:B:2441:GLN:HG3	1:C:1388:ASP:HA	2.00	0.44
1:C:2084:SER:HB3	1:C:2090:PRO:HA	1.99	0.44
1:A:1871:PRO:HG2	1:C:2064:TRP:HD1	1.78	0.44
1:A:1984:PHE:CZ	1:C:2372:VAL:HG21	2.53	0.44
1:A:2264:ILE:CD1	1:A:2320:TRP:CH2	3.01	0.44
1:A:2438:LYS:HD2	1:A:2438:LYS:HA	1.81	0.44
1:B:879:LEU:HD21	1:B:941:SER:CB	2.41	0.44
1:B:1084:ASP:HA	1:B:1087:PHE:HB3	2.00	0.44
1:B:1589:VAL:HA	1:B:1592:ASP:OD1	2.18	0.44
1:B:1842:CYS:HA	1:B:1845:ILE:HG22	1.98	0.44
1:B:2388:LEU:HB3	1:B:2434:THR:HG21	2.00	0.44
1:C:983:ARG:O	1:C:984:SER:HB3	2.18	0.44
1:C:1031:PHE:CD1	1:C:1031:PHE:C	2.96	0.44
1:C:1084:ASP:HA	1:C:1087:PHE:HB3	2.00	0.44
1:C:1623:ILE:HD13	1:C:1941:SER:HB3	2.00	0.44
1:C:2061:LEU:HD23	1:C:2061:LEU:HA	1.82	0.44
1:A:956:ARG:HA	1:A:959:ARG:HD2	1.99	0.44
1:A:2068:ASN:HD22	1:B:1870:ILE:HG23	1.83	0.44
1:A:2354:GLY:O	1:A:2357:ILE:CG2	2.60	0.44
1:B:1252:PHE:CD1	1:B:1252:PHE:N	2.86	0.44
1:B:1372:ILE:HD13	1:B:1375:ARG:NH2	2.33	0.44
1:B:2052:GLY:HA2	1:B:2055:ILE:HD11	1.98	0.44
1:C:1626:GLN:HG3	1:C:1638:PRO:HG3	1.98	0.44
1:C:1817:ILE:HD12	1:C:1821:PHE:HB2	1.99	0.44
1:C:2208:LYS:HG2	1:C:2210:TRP:CZ2	2.53	0.44
1:A:1402:ASP:CG	1:A:1403:TYR:N	2.72	0.43
1:A:1733:TRP:CE3	1:A:1733:TRP:HA	2.52	0.43
1:B:2208:LYS:HG2	1:B:2210:TRP:CZ2	2.53	0.43
1:B:2264:ILE:HD11	1:B:2320:TRP:CH2	2.48	0.43
1:C:2078:LYS:HD2	1:C:2095:GLU:OE2	2.18	0.43
1:C:2388:LEU:HB3	1:C:2434:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1388:ASP:HA	1:C:2441:GLN:HG3	2.00	0.43
1:A:1589:VAL:HA	1:A:1592:ASP:OD1	2.18	0.43
1:A:2078:LYS:HD2	1:A:2095:GLU:OE2	2.18	0.43
1:B:1031:PHE:CD1	1:B:1031:PHE:C	2.96	0.43
1:B:1733:TRP:HA	1:B:1733:TRP:CE3	2.52	0.43
1:C:1629:THR:O	1:C:1928:ILE:HD11	2.18	0.43
1:A:1031:PHE:CD1	1:A:1031:PHE:C	2.96	0.43
1:A:1207:LEU:HD13	1:A:1219:HIS:CE1	2.53	0.43
1:A:1882:THR:O	1:A:1886:ILE:HG13	2.17	0.43
1:B:2264:ILE:CD1	1:B:2320:TRP:CH2	3.01	0.43
1:B:983:ARG:O	1:B:984:SER:HB3	2.18	0.43
1:B:2084:SER:HB3	1:B:2090:PRO:HA	1.99	0.43
1:C:1009:ILE:HG13	1:C:1010:GLY:H	1.82	0.43
1:A:837:ILE:HA	1:A:840:ILE:HG22	2.01	0.43
1:A:1252:PHE:CD1	1:A:1252:PHE:N	2.86	0.43
1:A:1629:THR:O	1:A:1928:ILE:HD11	2.18	0.43
1:A:1870:ILE:HG23	1:C:2068:ASN:HD22	1.83	0.43
1:B:2365:LEU:HD11	1:B:2369:ARG:HD2	2.00	0.43
1:A:1642:LEU:HD13	1:A:1908:ILE:HD13	2.00	0.43
1:A:2208:LYS:HG2	1:A:2210:TRP:CZ2	2.53	0.43
1:A:2441:GLN:HG3	1:B:1388:ASP:HA	2.00	0.43
1:B:1629:THR:O	1:B:1928:ILE:HD11	2.18	0.43
1:B:1728:ARG:HH11	1:B:1731:GLY:HA3	1.83	0.43
1:C:1183:ILE:HG23	1:C:1194:ILE:HG12	2.01	0.43
1:C:1277:GLU:HG3	1:C:1277:GLU:O	2.18	0.43
1:C:1694:PRO:HB2	1:C:1920:PRO:HB3	2.00	0.43
1:C:2264:ILE:CD1	1:C:2320:TRP:CH2	3.01	0.43
1:A:1372:ILE:HD13	1:A:1375:ARG:NH2	2.33	0.43
1:A:1694:PRO:HB2	1:A:1920:PRO:HB3	2.00	0.43
1:A:2084:SER:HB3	1:A:2090:PRO:HA	1.99	0.43
1:C:857:LEU:HD12	1:C:1111:PHE:HE1	1.82	0.43
1:A:2372:VAL:HG21	1:B:1984:PHE:CZ	2.53	0.43
1:B:1593:TRP:CD2	1:B:1602:LEU:HD13	2.54	0.43
1:B:2384:MET:HA	1:C:2425:ARG:HG2	2.01	0.43
1:A:1183:ILE:HG23	1:A:1194:ILE:HG12	2.01	0.43
1:A:1394:TYR:CD2	1:C:2037:LYS:NZ	2.85	0.43
1:A:1728:ARG:HH11	1:A:1731:GLY:HA3	1.83	0.43
1:A:2365:LEU:HD11	1:A:2369:ARG:HD2	2.00	0.43
1:B:1178:THR:HB	1:B:1306:ALA:HA	2.01	0.43
1:B:1877:MET:HE2	1:B:1877:MET:HB2	1.90	0.43
1:B:1940:LYS:HB3	1:B:1940:LYS:HE2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2372:VAL:HG21	1:C:1984:PHE:CZ	2.53	0.43
1:C:1252:PHE:CD1	1:C:1252:PHE:N	2.86	0.43
1:C:1593:TRP:CD2	1:C:1602:LEU:HD13	2.54	0.43
1:C:1728:ARG:HH11	1:C:1731:GLY:HA3	1.83	0.43
1:A:1636:PRO:O	1:A:1640:MET:HB2	2.19	0.43
1:A:2388:LEU:HB3	1:A:2434:THR:HG21	2.00	0.43
1:B:857:LEU:HD12	1:B:1111:PHE:HE1	1.83	0.43
1:B:1636:PRO:O	1:B:1640:MET:HB2	2.18	0.43
1:B:2068:ASN:HD22	1:C:1870:ILE:HG23	1.83	0.43
1:C:879:LEU:HD21	1:C:941:SER:CB	2.41	0.43
1:C:1372:ILE:HD13	1:C:1375:ARG:NH2	2.33	0.43
1:C:1589:VAL:HA	1:C:1592:ASP:OD1	2.18	0.43
1:C:1836:PHE:O	1:C:1840:VAL:HG23	2.19	0.43
1:A:1349:LYS:HD3	1:A:1349:LYS:HA	1.83	0.42
1:A:2384:MET:HA	1:B:2425:ARG:HG2	2.00	0.42
1:A:2421:ILE:HD13	1:A:2421:ILE:HA	1.87	0.42
1:B:1973:MET:CE	1:B:2021:CYS:SG	3.07	0.42
1:C:1041:ARG:HA	1:C:1044:VAL:HG23	2.01	0.42
1:C:1636:PRO:O	1:C:1640:MET:HB2	2.18	0.42
1:A:1180:ALA:O	1:A:1183:ILE:HB	2.19	0.42
1:A:1593:TRP:CD2	1:A:1602:LEU:HD13	2.54	0.42
1:A:2064:TRP:HD1	1:B:1871:PRO:HG2	1.78	0.42
1:C:1178:THR:HB	1:C:1306:ALA:HA	2.01	0.42
1:A:1643:PHE:HE1	1:A:1905:VAL:HG22	1.84	0.42
1:B:1643:PHE:HE1	1:B:1905:VAL:HG22	1.84	0.42
1:C:837:ILE:HA	1:C:840:ILE:HG22	2.01	0.42
1:C:2360:TYR:CE1	1:C:2364:ILE:HD11	2.55	0.42
1:C:2421:ILE:HD13	1:C:2421:ILE:HA	1.87	0.42
1:A:1041:ARG:HA	1:A:1044:VAL:HG23	2.01	0.42
1:B:1180:ALA:O	1:B:1183:ILE:HB	2.19	0.42
1:B:2419:LYS:HE2	1:B:2419:LYS:HB3	1.91	0.42
1:C:1643:PHE:HE1	1:C:1905:VAL:HG22	1.84	0.42
1:A:1973:MET:CE	1:A:2021:CYS:SG	3.07	0.42
1:A:2425:ARG:HG2	1:C:2384:MET:HA	2.00	0.42
1:B:837:ILE:HA	1:B:840:ILE:HG22	2.01	0.42
1:B:1180:ALA:HB1	1:B:1720:LEU:HD22	2.02	0.42
1:B:1642:LEU:HD13	1:B:1908:ILE:HD13	2.00	0.42
1:C:1693:ASP:OD1	1:C:1696:SER:HB3	2.20	0.42
1:C:2347:PHE:O	1:C:2351:VAL:HG23	2.19	0.42
1:A:1836:PHE:O	1:A:1840:VAL:HG23	2.19	0.42
1:B:831:SER:HA	1:B:834:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1687:ARG:O	1:B:1691:GLN:HG3	2.20	0.42
1:B:1693:ASP:OD1	1:B:1696:SER:HB3	2.20	0.42
1:B:2089:PRO:HA	1:B:2090:PRO:HD3	1.95	0.42
1:C:2408:LYS:HA	1:C:2408:LYS:HD3	1.79	0.42
1:A:1180:ALA:HB1	1:A:1720:LEU:HD22	2.02	0.42
1:A:2360:TYR:CE1	1:A:2364:ILE:HD11	2.55	0.42
1:B:1041:ARG:HA	1:B:1044:VAL:HG23	2.01	0.42
1:B:2347:PHE:O	1:B:2351:VAL:HG23	2.19	0.42
1:B:2363:VAL:O	1:B:2364:ILE:C	2.63	0.42
1:C:1973:MET:CE	1:C:2021:CYS:SG	3.07	0.42
1:C:2108:MET:CE	1:C:2149:GLU:HA	2.45	0.42
1:A:1693:ASP:OD1	1:A:1696:SER:HB3	2.20	0.42
1:A:2303:LYS:HE3	1:A:2303:LYS:HB2	1.71	0.42
1:B:1183:ILE:HG23	1:B:1194:ILE:HG12	2.01	0.42
1:C:1180:ALA:O	1:C:1183:ILE:HB	2.19	0.42
1:C:1642:LEU:HD13	1:C:1908:ILE:HD13	2.00	0.42
1:C:2365:LEU:HD11	1:C:2369:ARG:HD2	2.00	0.42
1:A:2347:PHE:O	1:A:2351:VAL:HG23	2.19	0.42
1:B:2078:LYS:HD2	1:B:2095:GLU:OE2	2.19	0.42
1:B:2360:TYR:CE1	1:B:2364:ILE:HD11	2.55	0.42
1:C:834:VAL:HG13	1:C:835:PHE:N	2.35	0.42
1:C:1717:LEU:HG	1:C:1721:PHE:HE2	1.85	0.42
1:A:1158:TYR:CD2	1:A:1159:VAL:HG23	2.55	0.42
1:A:1698:ASP:HB3	1:A:1704:SER:HB2	2.02	0.42
1:A:1717:LEU:HG	1:A:1721:PHE:HE2	1.85	0.42
1:B:1694:PRO:HB2	1:B:1920:PRO:HB3	2.00	0.42
1:B:1717:LEU:HG	1:B:1721:PHE:HE2	1.85	0.42
1:B:1836:PHE:O	1:B:1840:VAL:HG23	2.19	0.42
1:B:2023:ARG:O	1:B:2026:GLU:HG3	2.20	0.42
1:C:1180:ALA:HB1	1:C:1720:LEU:HD22	2.02	0.42
1:A:831:SER:HA	1:A:834:VAL:HG12	2.01	0.41
1:A:1277:GLU:O	1:A:1277:GLU:HG3	2.18	0.41
1:B:1158:TYR:CD2	1:B:1159:VAL:HG23	2.55	0.41
1:C:2077:GLU:OE1	1:C:2195:PRO:HG3	2.20	0.41
1:A:1237:MET:O	1:A:1238:LYS:C	2.63	0.41
1:A:1343:LYS:HA	1:A:1343:LYS:HD2	1.88	0.41
1:B:834:VAL:HG13	1:B:835:PHE:N	2.35	0.41
1:B:2144:LYS:HA	1:B:2144:LYS:HD3	1.92	0.41
1:C:831:SER:HA	1:C:834:VAL:HG12	2.01	0.41
1:C:1687:ARG:O	1:C:1691:GLN:HG3	2.20	0.41
1:C:1964:LEU:HD22	1:C:1975:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1964:LEU:HD22	1:A:1975:ALA:HB1	2.02	0.41
1:A:2023:ARG:O	1:A:2026:GLU:HG3	2.20	0.41
1:B:1698:ASP:HB3	1:B:1704:SER:HB2	2.02	0.41
1:B:1817:ILE:CD1	1:B:1821:PHE:HD2	2.33	0.41
1:B:2108:MET:CE	1:B:2149:GLU:HA	2.45	0.41
1:C:1688:THR:HA	1:C:1691:GLN:OE1	2.20	0.41
1:A:1178:THR:HB	1:A:1306:ALA:HA	2.01	0.41
1:A:1687:ARG:O	1:A:1691:GLN:HG3	2.20	0.41
1:A:1817:ILE:CD1	1:A:1821:PHE:HD2	2.33	0.41
1:B:1964:LEU:HD22	1:B:1975:ALA:HB1	2.02	0.41
1:B:2012:PHE:O	1:B:2016:ILE:HG12	2.21	0.41
1:B:2349:ALA:O	1:B:2350:LYS:C	2.64	0.41
1:C:873:LEU:HD13	1:C:873:LEU:HA	1.89	0.41
1:A:2322:LYS:HB3	1:A:2322:LYS:HE3	1.79	0.41
1:A:2353:LYS:O	1:A:2354:GLY:C	2.64	0.41
1:B:1237:MET:O	1:B:1238:LYS:C	2.63	0.41
1:B:1244:PHE:CZ	1:B:1249:LEU:HB3	2.56	0.41
1:B:1634:THR:O	1:B:1634:THR:CG2	2.69	0.41
1:C:873:LEU:O	1:C:876:CYS:HB2	2.21	0.41
1:C:1237:MET:O	1:C:1238:LYS:C	2.63	0.41
1:A:834:VAL:HG13	1:A:835:PHE:N	2.35	0.41
1:A:1148:GLN:OE1	1:A:1150:ASP:OD2	2.39	0.41
1:B:824:ARG:HH12	1:B:972:VAL:HG21	1.85	0.41
1:C:824:ARG:HH12	1:C:972:VAL:HG21	1.85	0.41
1:C:1012:ASP:HA	1:C:1015:ASN:ND2	2.36	0.41
1:A:1688:THR:HA	1:A:1691:GLN:OE1	2.20	0.41
1:A:2223:LYS:HD3	1:A:2223:LYS:HA	1.66	0.41
1:B:1040:ARG:O	1:B:1044:VAL:HG23	2.21	0.41
1:B:1895:LYS:HA	1:B:1895:LYS:HD3	1.97	0.41
1:C:1148:GLN:OE1	1:C:1150:ASP:OD2	2.39	0.41
1:C:1158:TYR:CE2	1:C:1159:VAL:HG23	2.56	0.41
1:C:1407:LYS:HE2	1:C:1407:LYS:HB3	1.82	0.41
1:C:2349:ALA:O	1:C:2350:LYS:C	2.64	0.41
1:C:2438:LYS:HD2	1:C:2438:LYS:HA	1.81	0.41
1:A:2077:GLU:OE1	1:A:2195:PRO:HG3	2.20	0.41
1:B:995:TYR:HD1	1:B:995:TYR:HA	1.63	0.41
1:B:1027:TRP:CZ2	1:B:1046:TYR:HB3	2.56	0.41
1:B:1052:ILE:O	1:B:1055:PRO:HD2	2.21	0.41
1:B:1077:TRP:O	1:B:1077:TRP:CG	2.74	0.41
1:B:2037:LYS:NZ	1:C:1394:TYR:CD2	2.85	0.41
1:C:858:SER:O	1:C:862:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1052:ILE:O	1:C:1055:PRO:HD2	2.21	0.41
1:C:2128:ARG:HE	1:C:2128:ARG:HB2	1.76	0.41
1:A:847:ASN:OD1	1:A:848:ALA:N	2.54	0.41
1:A:1077:TRP:O	1:A:1077:TRP:CG	2.74	0.41
1:A:1158:TYR:CE2	1:A:1159:VAL:HG23	2.56	0.41
1:A:1879:VAL:HA	1:A:1882:THR:HG22	2.03	0.41
1:B:1012:ASP:HA	1:B:1015:ASN:ND2	2.36	0.41
1:B:1715:VAL:CG1	1:B:1716:LEU:N	2.78	0.41
1:B:2077:GLU:OE1	1:B:2195:PRO:HG3	2.20	0.41
1:B:2138:MET:HE2	1:B:2138:MET:HB3	1.95	0.41
1:B:2353:LYS:O	1:B:2354:GLY:C	2.64	0.41
1:C:1040:ARG:O	1:C:1044:VAL:HG23	2.21	0.41
1:C:1244:PHE:CZ	1:C:1249:LEU:HB3	2.56	0.41
1:C:1661:ILE:HD12	1:C:1661:ILE:HA	1.89	0.41
1:C:1698:ASP:HB3	1:C:1704:SER:HB2	2.02	0.41
1:C:1879:VAL:HA	1:C:1882:THR:HG22	2.03	0.41
1:C:2012:PHE:O	1:C:2016:ILE:HG12	2.21	0.41
1:C:2353:LYS:O	1:C:2354:GLY:C	2.64	0.41
1:A:1065:PRO:O	1:A:1066:PRO:C	2.64	0.41
1:B:1373:ARG:HH12	1:B:2412:LEU:HD23	1.86	0.41
1:B:1386:GLU:O	1:B:1387:ARG:HG2	2.21	0.41
1:B:2438:LYS:HD2	1:B:2438:LYS:HA	1.81	0.41
1:A:1052:ILE:O	1:A:1055:PRO:HD2	2.21	0.40
1:A:2408:LYS:HA	1:A:2408:LYS:HD3	1.79	0.40
1:B:873:LEU:O	1:B:876:CYS:HB2	2.21	0.40
1:B:1349:LYS:HA	1:B:1349:LYS:HD3	1.84	0.40
1:B:1626:GLN:HA	1:B:1629:THR:HG22	2.03	0.40
1:C:847:ASN:OD1	1:C:848:ALA:N	2.54	0.40
1:C:941:SER:HA	1:C:944:ALA:HB3	2.03	0.40
1:C:1163:LYS:HD3	1:C:1163:LYS:HA	1.80	0.40
1:C:1268:LEU:C	1:C:1268:LEU:HD12	2.46	0.40
1:C:1386:GLU:O	1:C:1387:ARG:HG2	2.21	0.40
1:C:1664:THR:O	1:C:1667:VAL:HG12	2.21	0.40
1:A:834:VAL:O	1:A:836:VAL:N	2.55	0.40
1:A:873:LEU:O	1:A:876:CYS:HB2	2.21	0.40
1:B:847:ASN:OD1	1:B:848:ALA:N	2.54	0.40
1:B:941:SER:HA	1:B:944:ALA:HB3	2.03	0.40
1:B:1064:LEU:HD21	1:B:1068:SER:OG	2.21	0.40
1:B:1156:LYS:HB3	1:B:1161:TYR:CD1	2.57	0.40
1:B:1268:LEU:HD12	1:B:1268:LEU:C	2.46	0.40
1:B:1688:THR:HA	1:B:1691:GLN:OE1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2062:LEU:CD1	1:B:2066:LEU:HD12	2.52	0.40
1:C:1158:TYR:CD2	1:C:1159:VAL:HG23	2.55	0.40
1:C:1607:VAL:O	1:C:1610:ILE:HG22	2.21	0.40
1:C:1654:LYS:HA	1:C:1657:TRP:CD1	2.56	0.40
1:C:2023:ARG:O	1:C:2026:GLU:HG3	2.20	0.40
1:A:1016:ARG:HA	1:A:1016:ARG:CZ	2.51	0.40
1:A:2012:PHE:O	1:A:2016:ILE:HG12	2.21	0.40
1:A:2349:ALA:O	1:A:2350:LYS:C	2.64	0.40
1:B:1607:VAL:O	1:B:1610:ILE:HG22	2.21	0.40
1:C:1027:TRP:CZ2	1:C:1046:TYR:HB3	2.56	0.40
1:C:1817:ILE:CD1	1:C:1821:PHE:HD2	2.33	0.40
1:C:1960:ILE:HG13	1:C:1961:GLY:H	1.87	0.40
1:C:2363:VAL:O	1:C:2364:ILE:C	2.63	0.40
1:A:867:ALA:O	1:A:870:ILE:N	2.53	0.40
1:A:941:SER:HA	1:A:944:ALA:HB3	2.03	0.40
1:A:1156:LYS:H	1:A:1156:LYS:HG3	1.77	0.40
1:A:1244:PHE:CZ	1:A:1249:LEU:HB3	2.56	0.40
1:A:1377:GLN:C	1:A:1377:GLN:OE1	2.65	0.40
1:A:1960:ILE:HG13	1:A:1961:GLY:H	1.87	0.40
1:C:975:ASP:HA	1:C:978:HIS:HD1	1.86	0.40
1:C:1090:SER:O	1:C:1091:TYR:C	2.65	0.40
1:C:1727:LEU:HD13	1:C:1727:LEU:HA	1.94	0.40
1:C:1940:LYS:O	1:C:1943:TYR:HB3	2.22	0.40
1:C:2223:LYS:HD3	1:C:2223:LYS:HA	1.66	0.40
1:A:1156:LYS:HB3	1:A:1161:TYR:CD1	2.57	0.40
1:A:1188:LEU:HD22	1:A:1268:LEU:CD1	2.52	0.40
1:A:1293:VAL:HG13	1:A:1295:THR:H	1.87	0.40
1:B:1585:MET:O	1:B:1589:VAL:HG13	2.22	0.40
1:B:1879:VAL:HA	1:B:1882:THR:HG22	2.03	0.40
1:B:2077:GLU:OE2	1:B:2077:GLU:N	2.55	0.40
1:C:834:VAL:O	1:C:836:VAL:N	2.55	0.40
1:C:1016:ARG:HA	1:C:1016:ARG:CZ	2.51	0.40
1:C:1065:PRO:O	1:C:1066:PRO:C	2.64	0.40
1:C:1626:GLN:HA	1:C:1629:THR:HG22	2.03	0.40
1:C:2077:GLU:OE2	1:C:2077:GLU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1345/1686 (80%)	1208 (90%)	121 (9%)	16 (1%)	10	37
1	B	1345/1686 (80%)	1207 (90%)	122 (9%)	16 (1%)	10	37
1	C	1345/1686 (80%)	1208 (90%)	121 (9%)	16 (1%)	10	37
All	All	4035/5058 (80%)	3623 (90%)	364 (9%)	48 (1%)	13	37

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	848	ALA
1	A	983	ARG
1	A	1073	PRO
1	A	1079	PRO
1	A	1716	LEU
1	A	1872	VAL
1	B	848	ALA
1	B	983	ARG
1	B	1073	PRO
1	B	1079	PRO
1	B	1716	LEU
1	B	1872	VAL
1	C	848	ALA
1	C	983	ARG
1	C	1073	PRO
1	C	1079	PRO
1	C	1716	LEU
1	C	1872	VAL
1	A	1271	ILE
1	B	1271	ILE
1	C	1271	ILE
1	A	1019	ALA
1	A	1097	ILE
1	A	2272	ILE

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Mol	Chain	Res	Type
1	A	2343	ALA
1	B	1019	ALA
1	B	1097	ILE
1	B	2272	ILE
1	B	2343	ALA
1	C	1019	ALA
1	C	1097	ILE
1	C	2272	ILE
1	C	2343	ALA
1	A	1649	ASN
1	A	1715	VAL
1	B	1649	ASN
1	B	1715	VAL
1	C	1649	ASN
1	C	1715	VAL
1	A	830	ILE
1	A	1928	ILE
1	B	830	ILE
1	B	1928	ILE
1	C	830	ILE
1	C	1928	ILE
1	A	851	ILE
1	B	851	ILE
1	C	851	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1203/1482 (81%)	1178 (98%)	25 (2%)	47	71
1	B	1203/1482 (81%)	1179 (98%)	24 (2%)	48	72
1	C	1203/1482 (81%)	1177 (98%)	26 (2%)	45	71
All	All	3609/4446 (81%)	3534 (98%)	75 (2%)	46	71

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	841	PHE
1	A	842	ILE
1	A	863	LEU
1	A	878	TYR
1	A	983	ARG
1	A	995	TYR
1	A	1034	ASN
1	A	1114	LEU
1	A	1228	LEU
1	A	1230	TYR
1	A	1232	LEU
1	A	1242	GLN
1	A	1249	LEU
1	A	1275	ASN
1	A	1310	LEU
1	A	1332	GLU
1	A	1372	ILE
1	A	1373	ARG
1	A	1649	ASN
1	A	1733	TRP
1	A	1976	PHE
1	A	2149	GLU
1	A	2273	ASN
1	A	2413	GLU
1	A	2433	TRP
1	B	841	PHE
1	B	842	ILE
1	B	863	LEU
1	B	878	TYR
1	B	983	ARG
1	B	995	TYR
1	B	1034	ASN
1	B	1114	LEU
1	B	1228	LEU
1	B	1230	TYR
1	B	1242	GLN
1	B	1249	LEU
1	B	1275	ASN
1	B	1310	LEU
1	B	1332	GLU
1	B	1372	ILE
1	B	1373	ARG
1	B	1649	ASN

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Mol	Chain	Res	Type
1	B	1733	TRP
1	B	1976	PHE
1	B	2149	GLU
1	B	2273	ASN
1	B	2413	GLU
1	B	2433	TRP
1	C	841	PHE
1	C	842	ILE
1	C	863	LEU
1	C	878	TYR
1	C	968	MET
1	C	983	ARG
1	C	995	TYR
1	C	1034	ASN
1	C	1114	LEU
1	C	1228	LEU
1	C	1230	TYR
1	C	1242	GLN
1	C	1249	LEU
1	C	1275	ASN
1	C	1310	LEU
1	C	1332	GLU
1	C	1372	ILE
1	C	1373	ARG
1	C	1649	ASN
1	C	1733	TRP
1	C	1976	PHE
1	C	2086	GLU
1	C	2149	GLU
1	C	2273	ASN
1	C	2413	GLU
1	C	2433	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2015	HIS
1	B	2301	ASN
1	C	2015	HIS
1	C	2301	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 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.

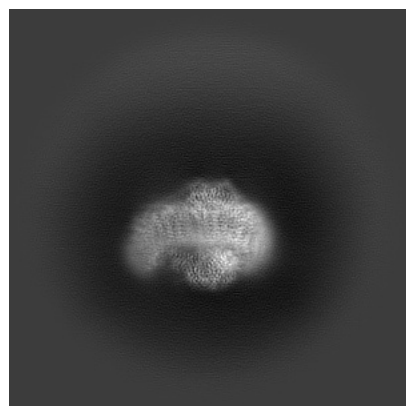
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74283. These allow visual inspection of the internal detail of the map and identification of artifacts.

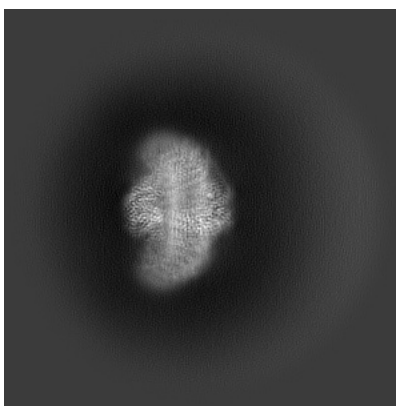
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

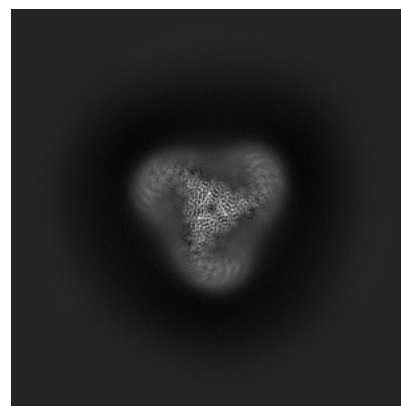
6.1.1 Primary map



X

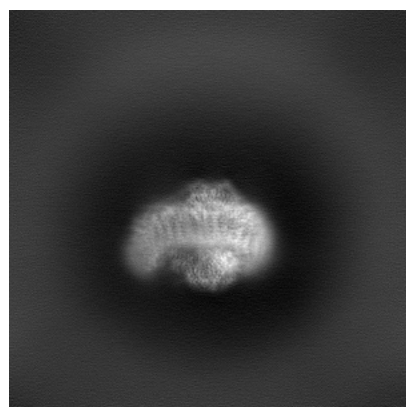


Y

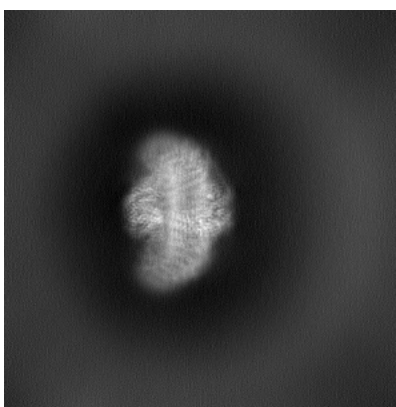


Z

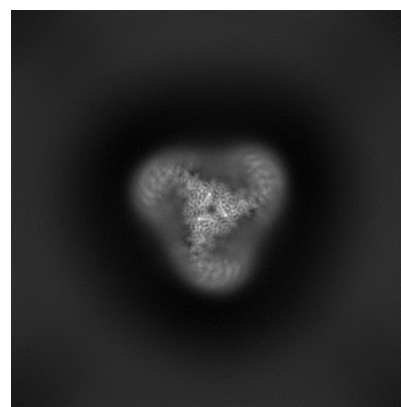
6.1.2 Raw map



X



Y

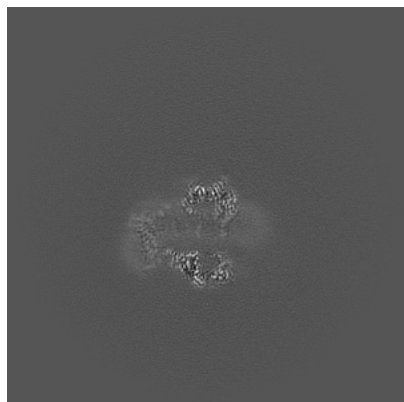


Z

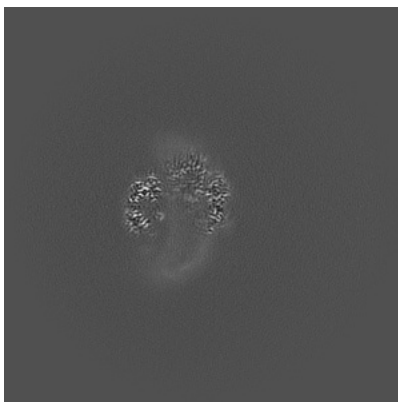
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

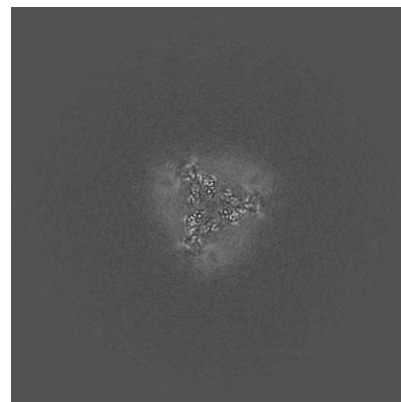
6.2.1 Primary map



X Index: 224

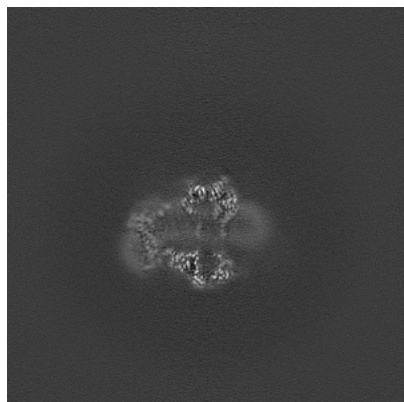


Y Index: 224

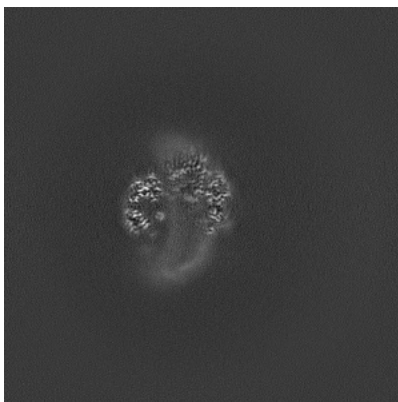


Z Index: 224

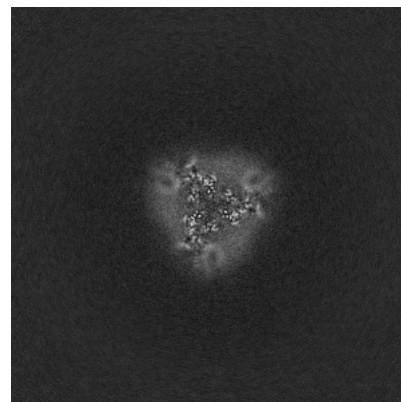
6.2.2 Raw map



X Index: 224



Y Index: 224

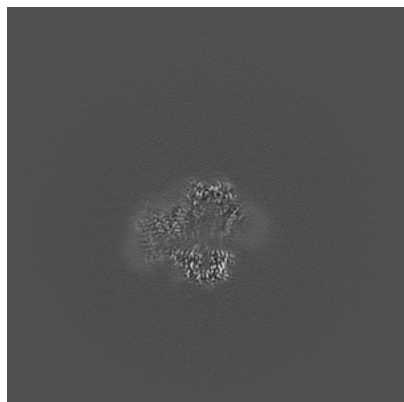


Z Index: 224

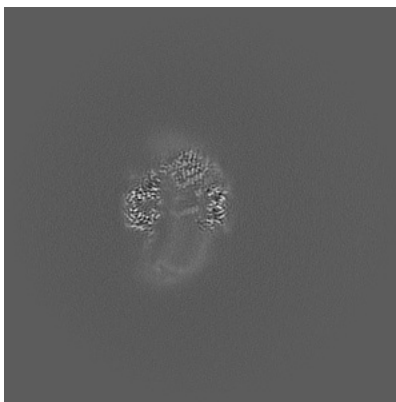
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

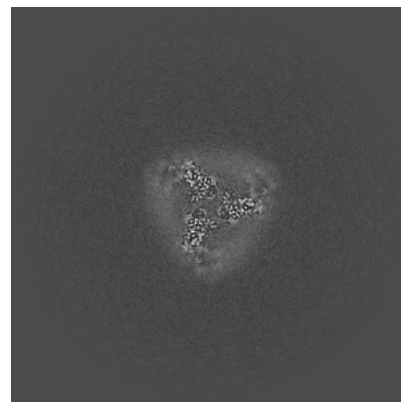
6.3.1 Primary map



X Index: 214

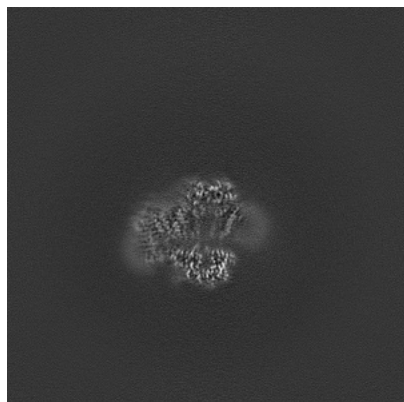


Y Index: 230

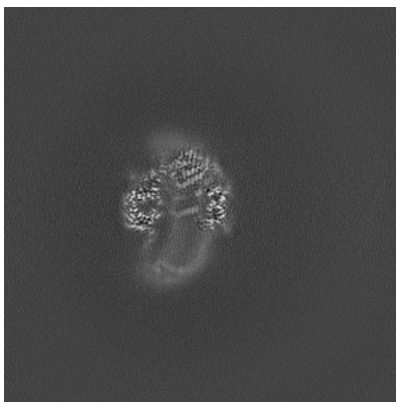


Z Index: 220

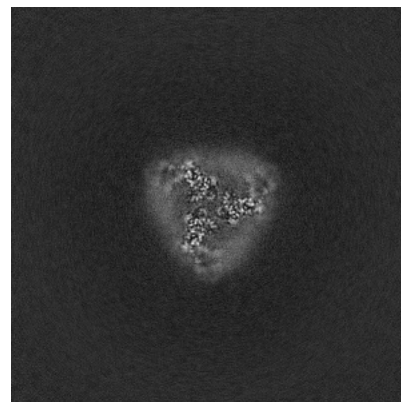
6.3.2 Raw map



X Index: 214



Y Index: 230

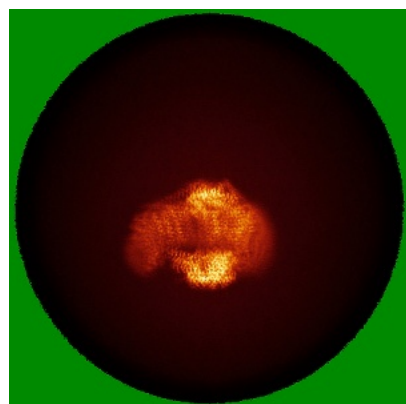


Z Index: 220

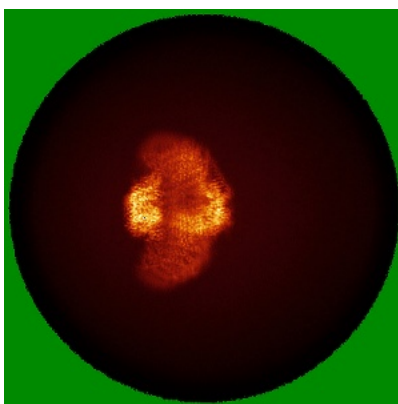
The images above show the largest variance slices of the map in three orthogonal directions.

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

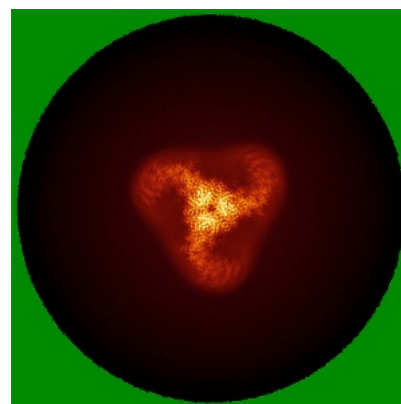
6.4.1 Primary map



X

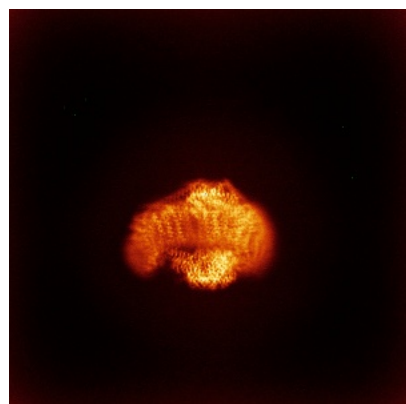


Y

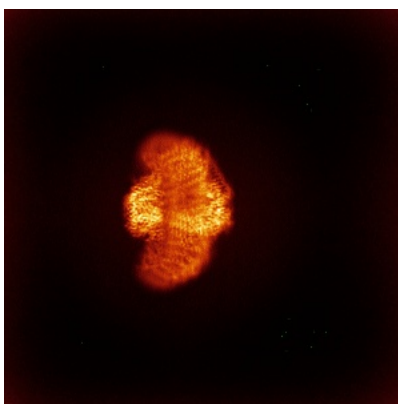


Z

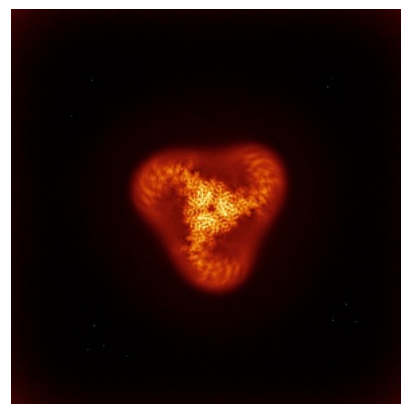
6.4.2 Raw map



X



Y

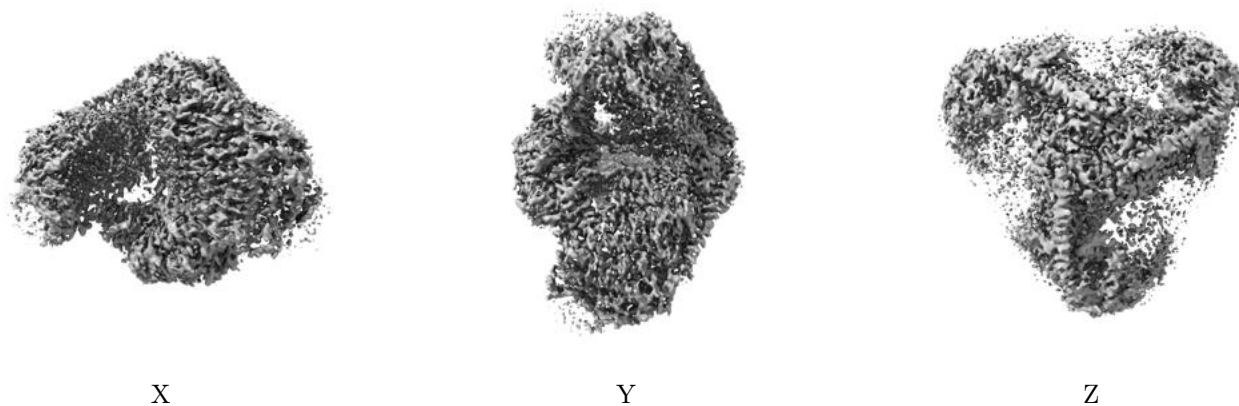


Z

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

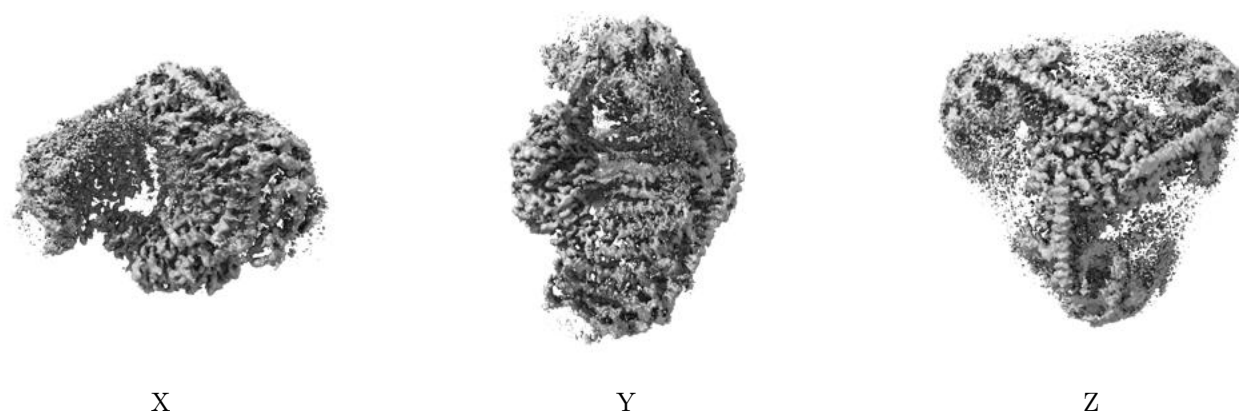
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0689. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

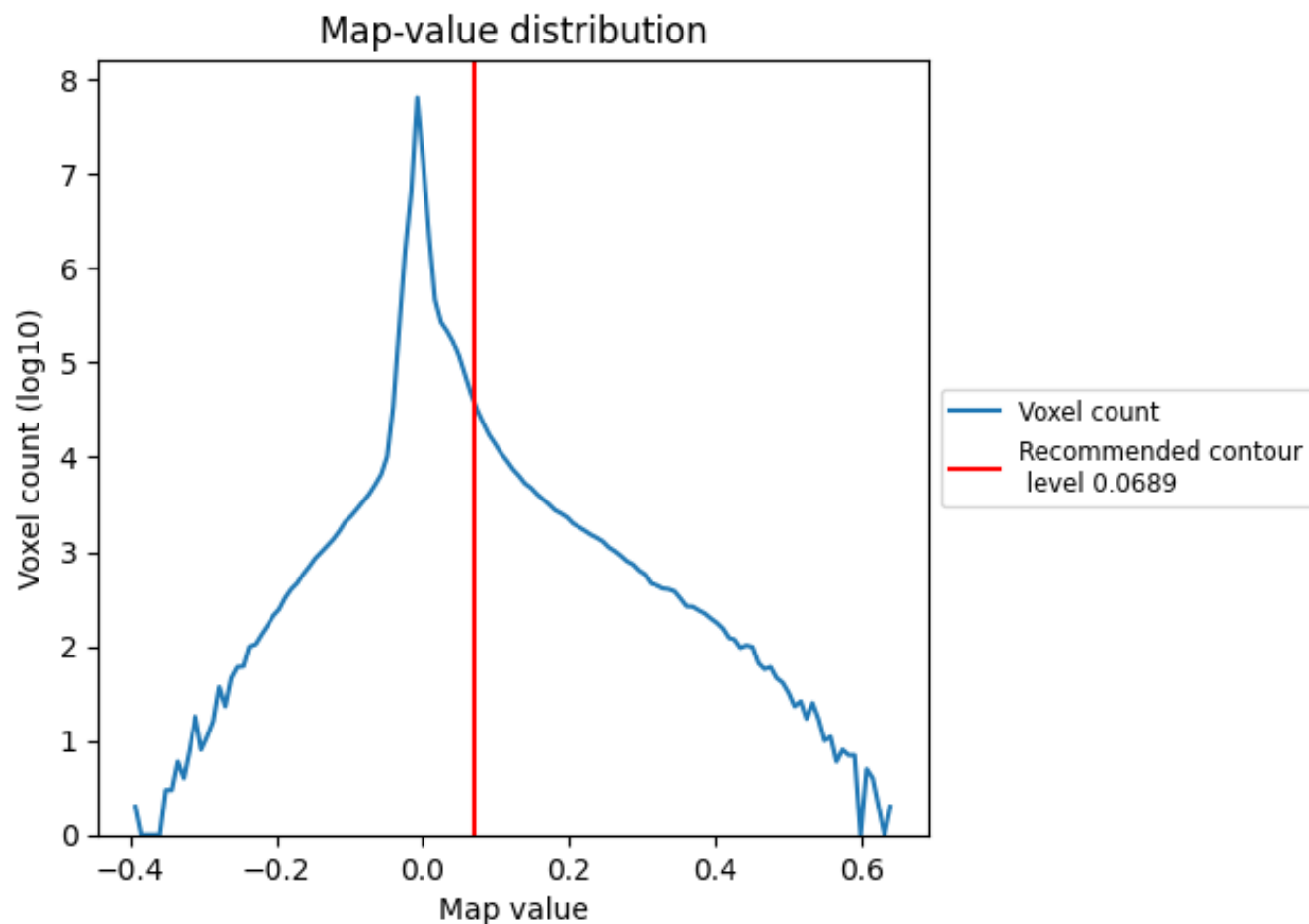
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

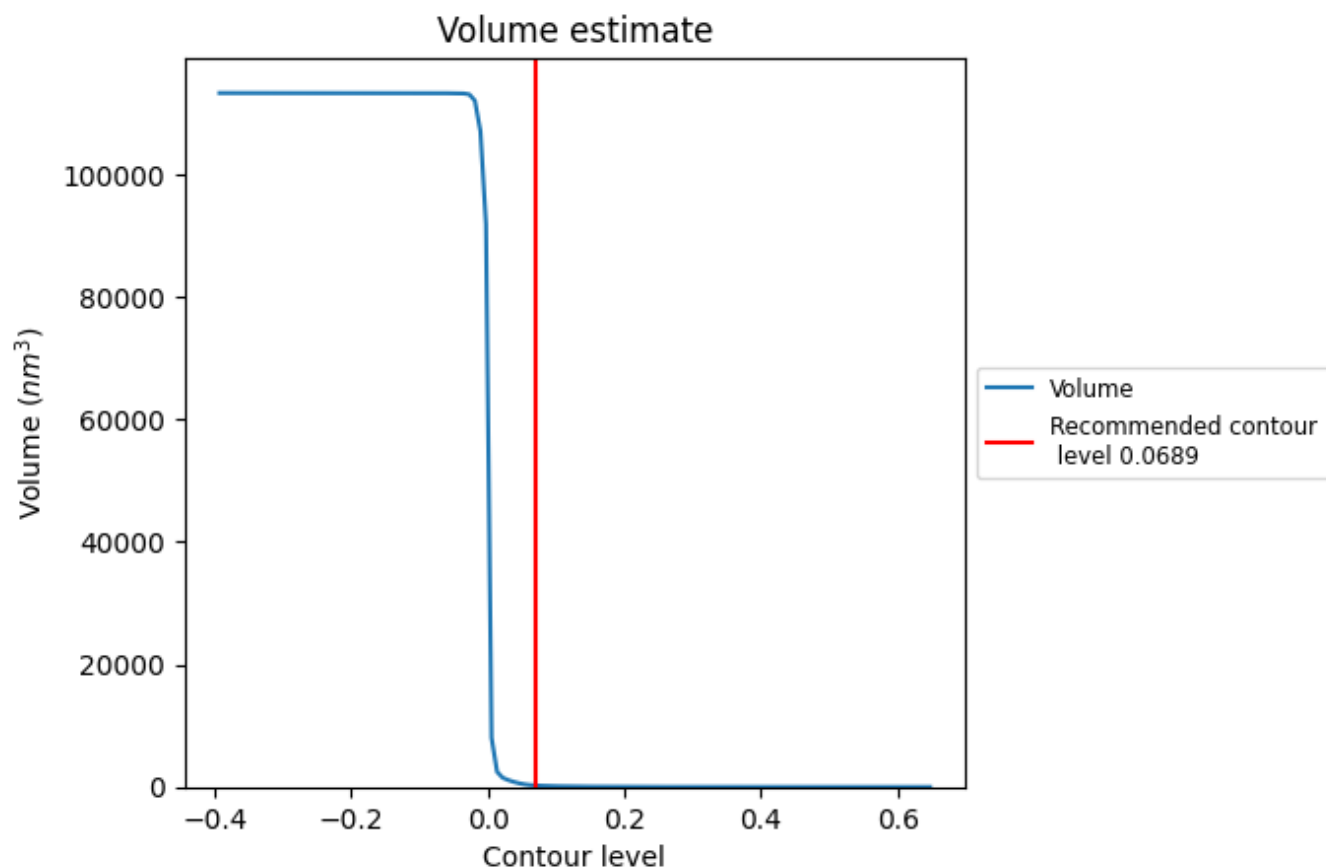
This section contains the results of statistical analysis of the map.

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.

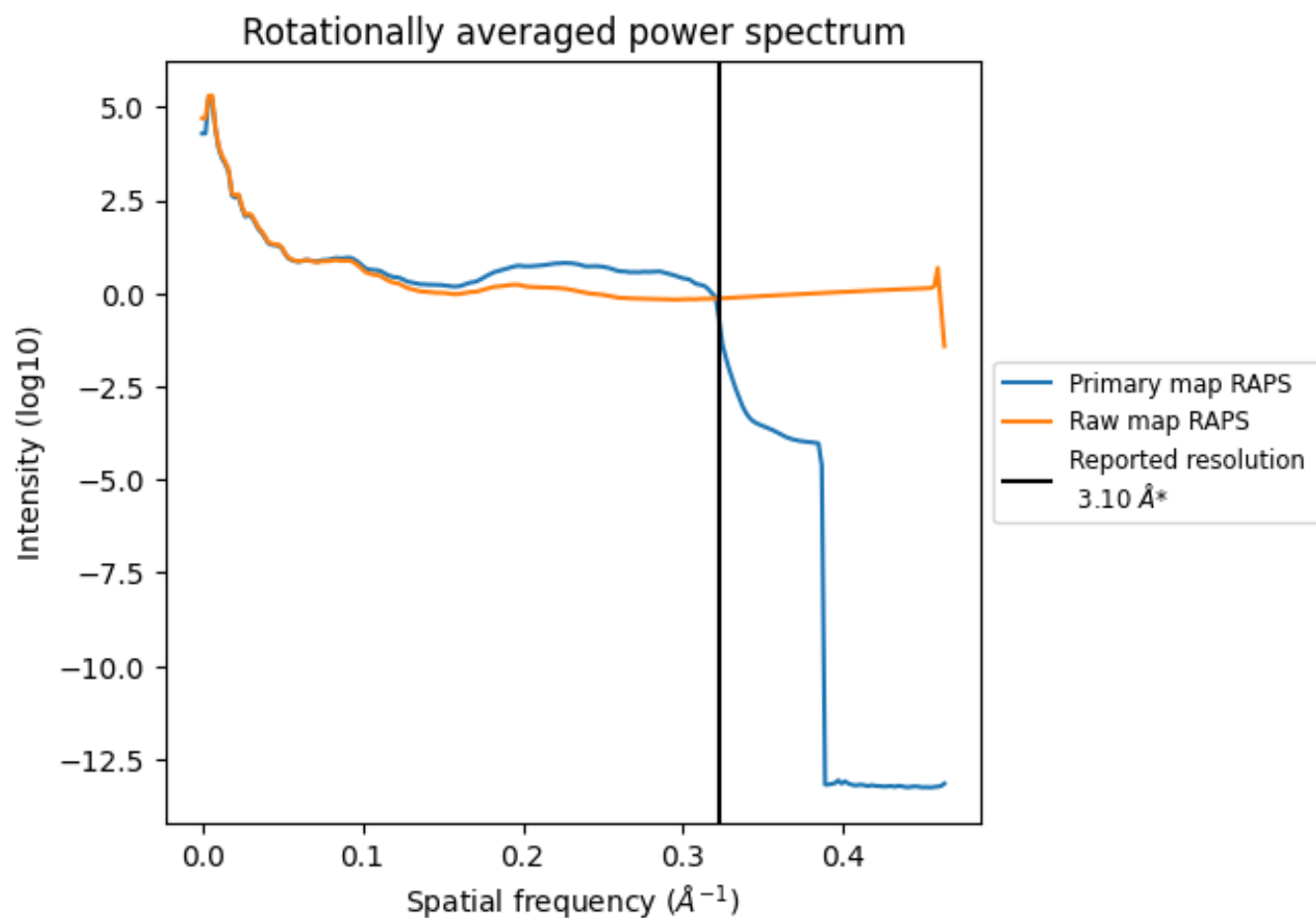
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 250 nm^3 ; this corresponds to an approximate mass of 226 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 ⓘ

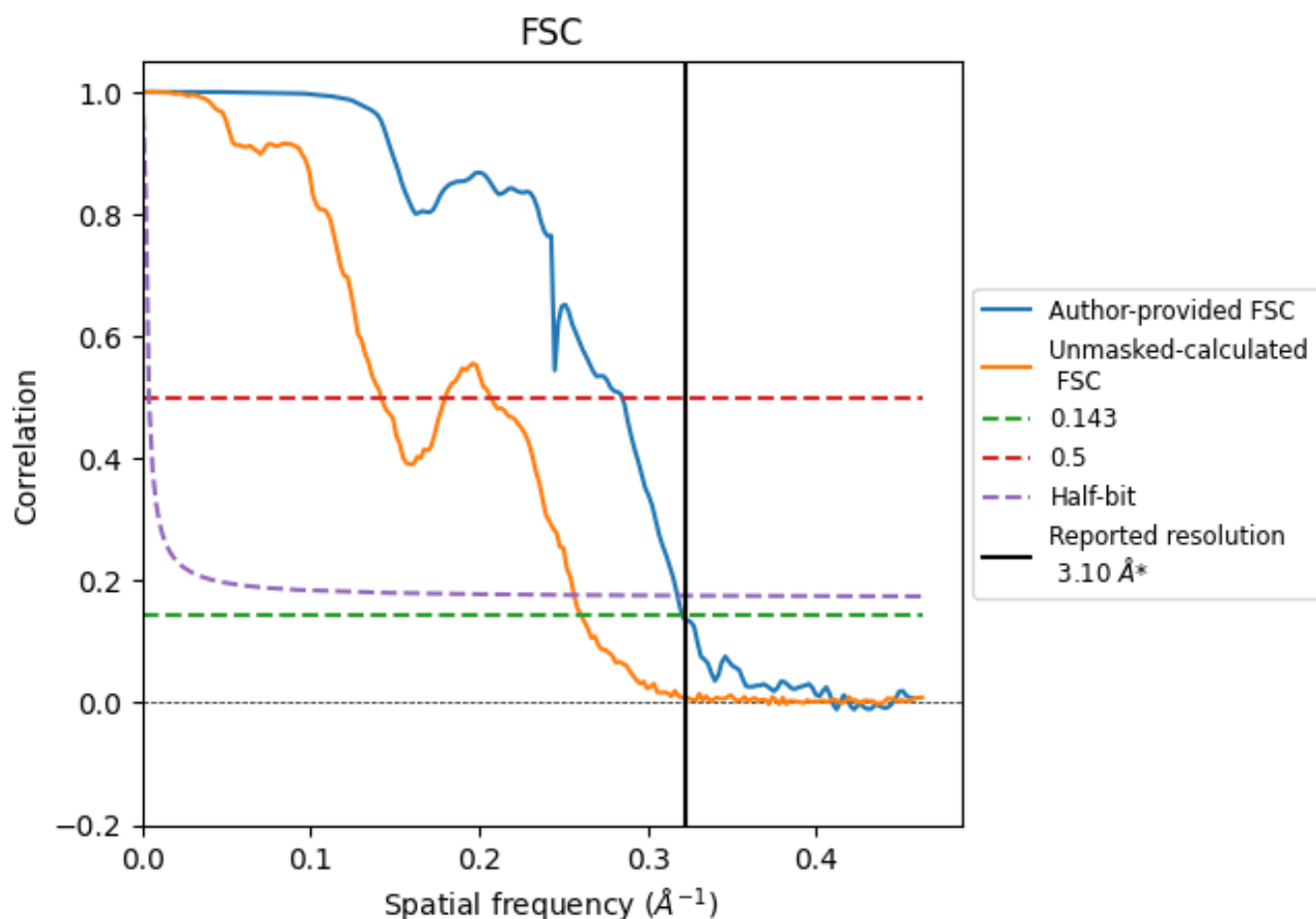


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

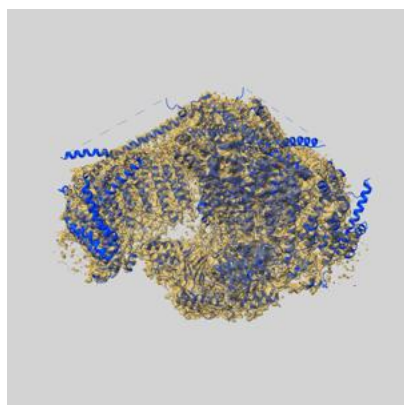
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.51	3.15
Unmasked-calculated*	3.84	7.05	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 3.1 by more than 10 %

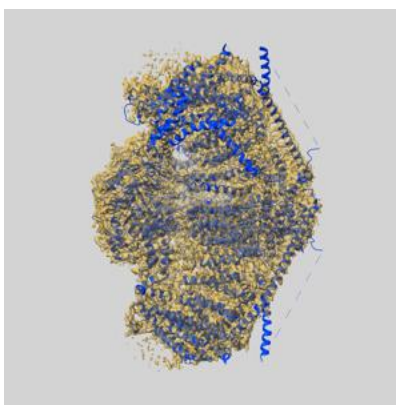
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74283 and PDB model 9ZIT. Per-residue inclusion information can be found in section [3](#) on page [4](#).

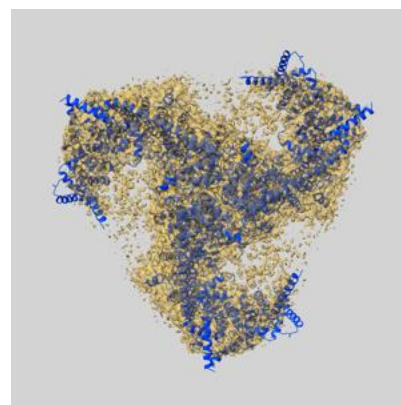
9.1 Map-model overlay [i](#)



X



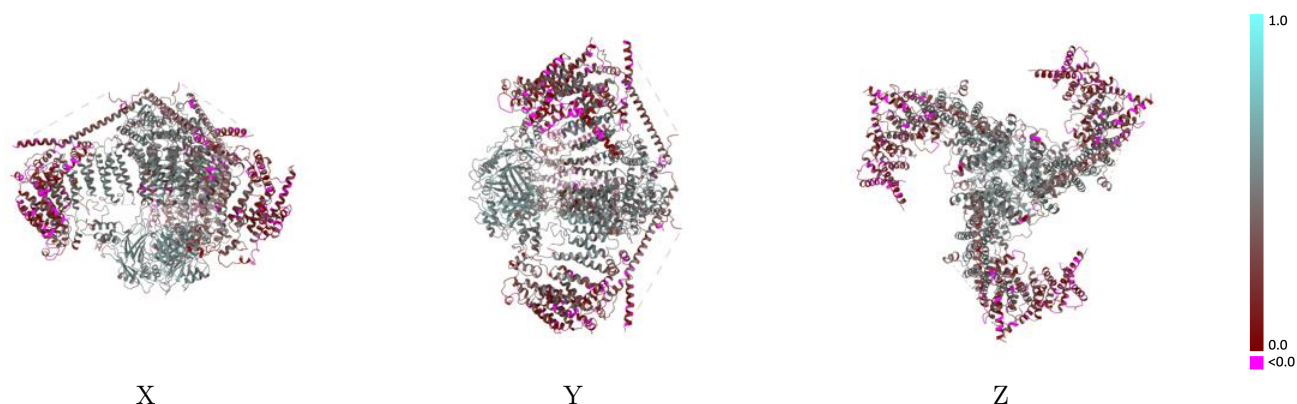
Y



Z

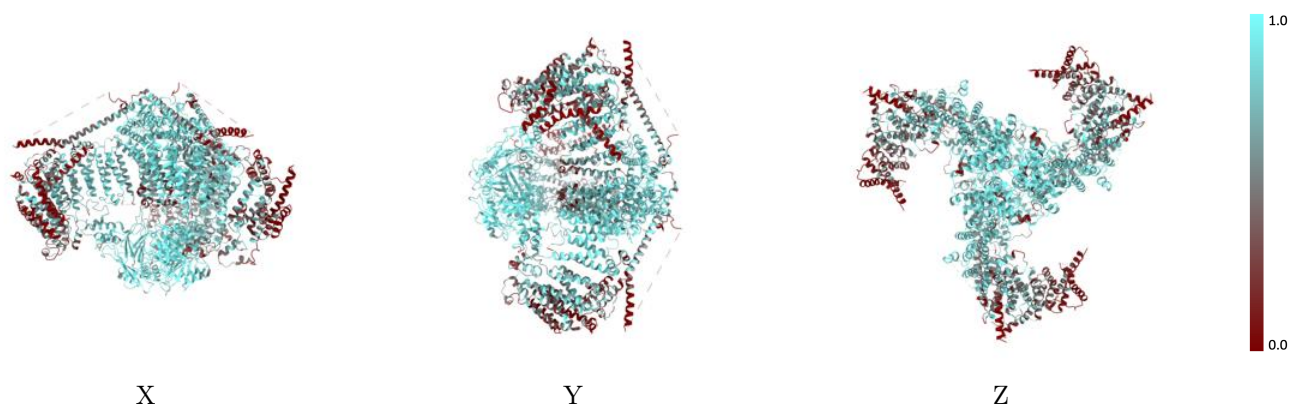
The images above show the 3D surface view of the map at the recommended contour level 0.0689 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



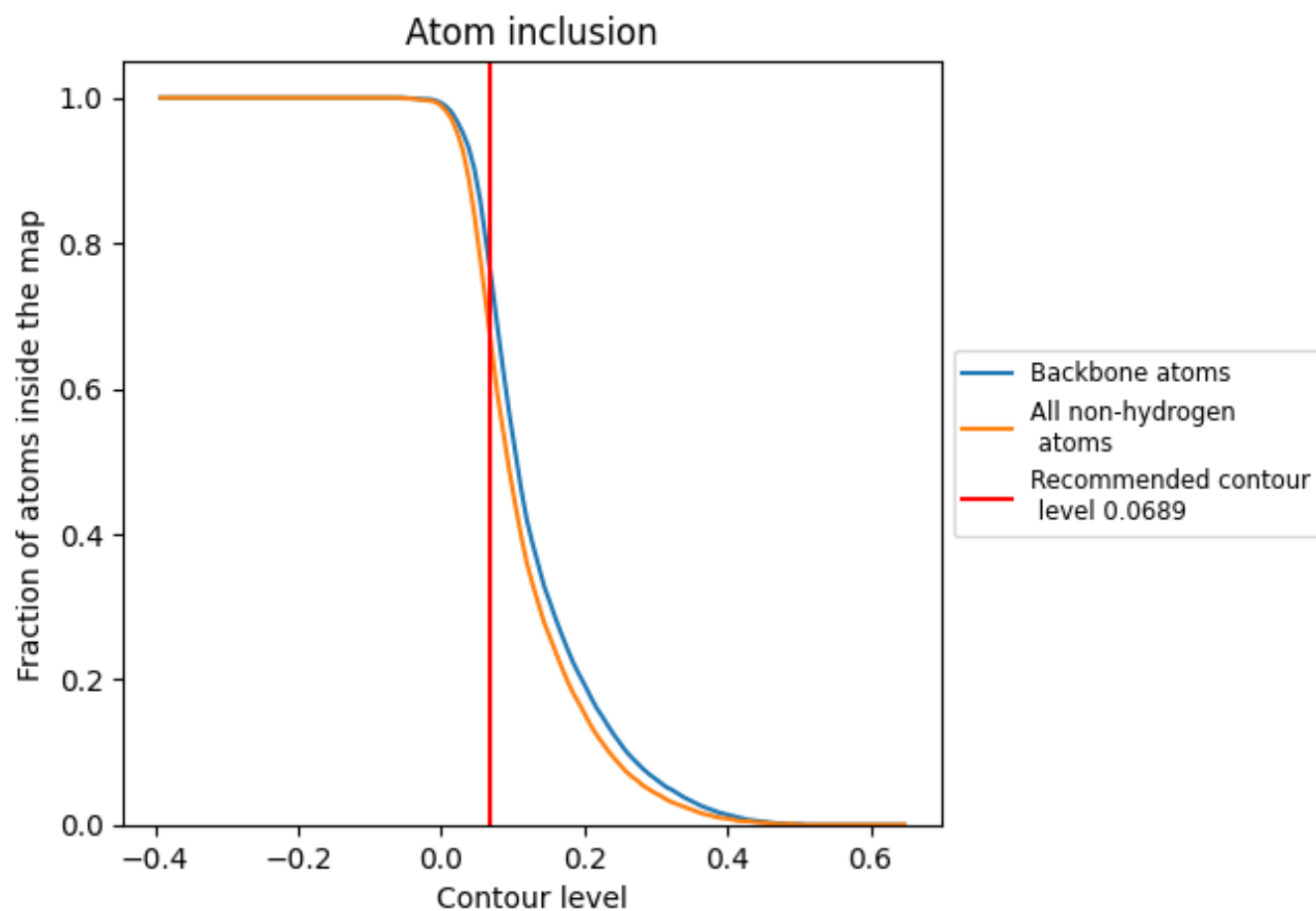
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0689).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 66% 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 (0.0689) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6650	0.3650
A	0.6650	0.3650
B	0.6650	0.3650
C	0.6630	0.3630

