



## Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 10:52 AM JST

PDB ID : 8XCI / pdb\_00008xci  
EMDB ID : EMD-38244  
Title : Open state of central tail fiber of bacteriophage lambda upon binding to LamB  
Authors : Ge, X.F.; Wang, J.W.  
Deposited on : 2023-12-09  
Resolution : 3.57 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

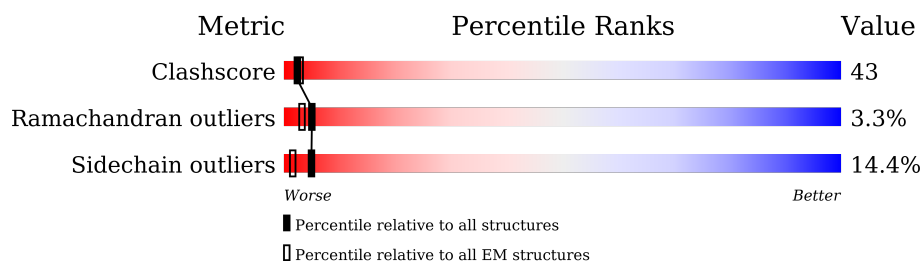
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.57 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	F	1132	 7% 14% 13% 5% • 66%
1	J	1132	 6% 14% 15% • • 66%
1	Z	1132	 13% 16% • • 66%

## 2 Entry composition

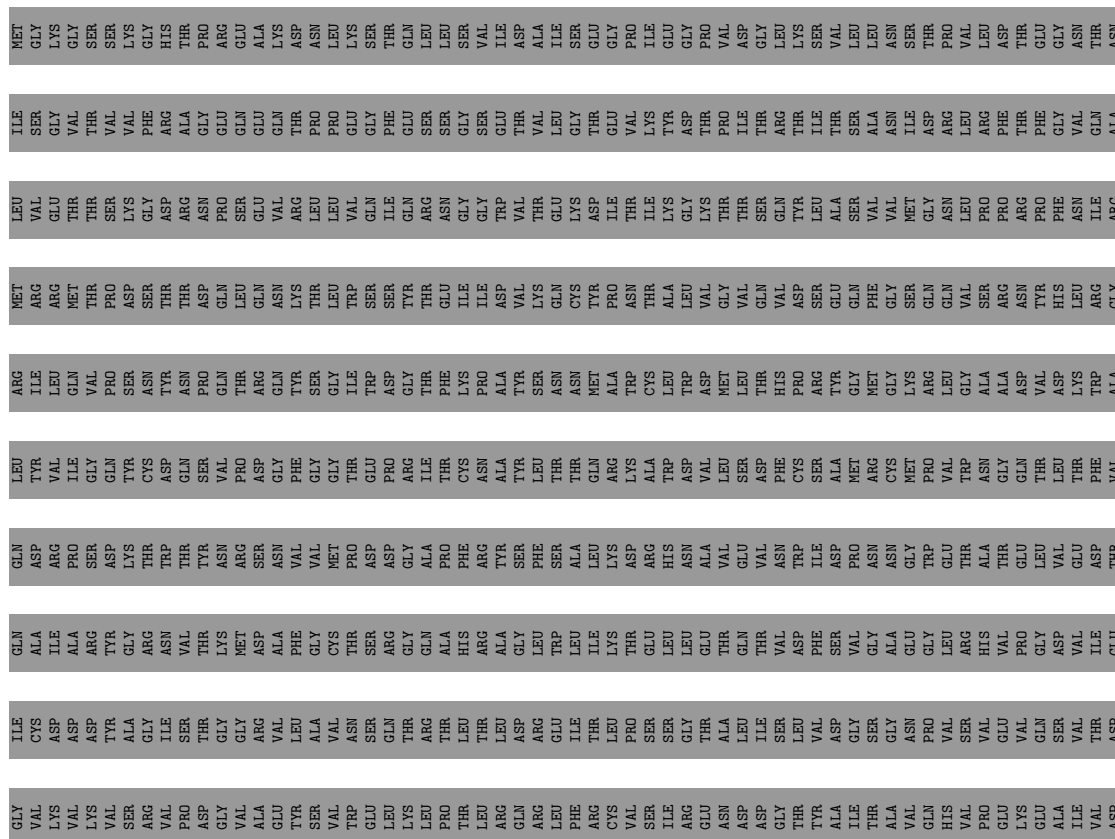
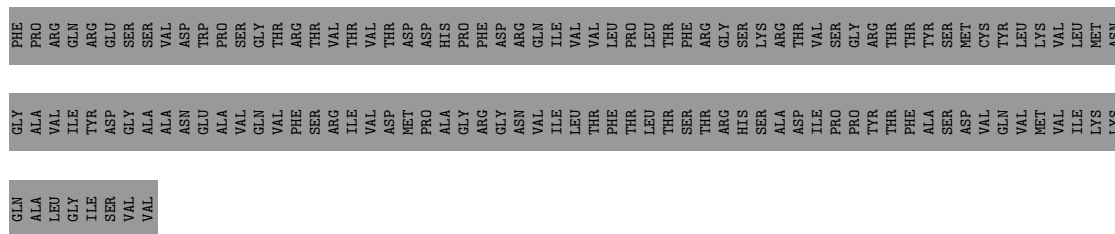
There is only 1 type of molecule in this entry. The entry contains 8842 atoms, of which 0 are hydrogens and 0 are deuteriums.

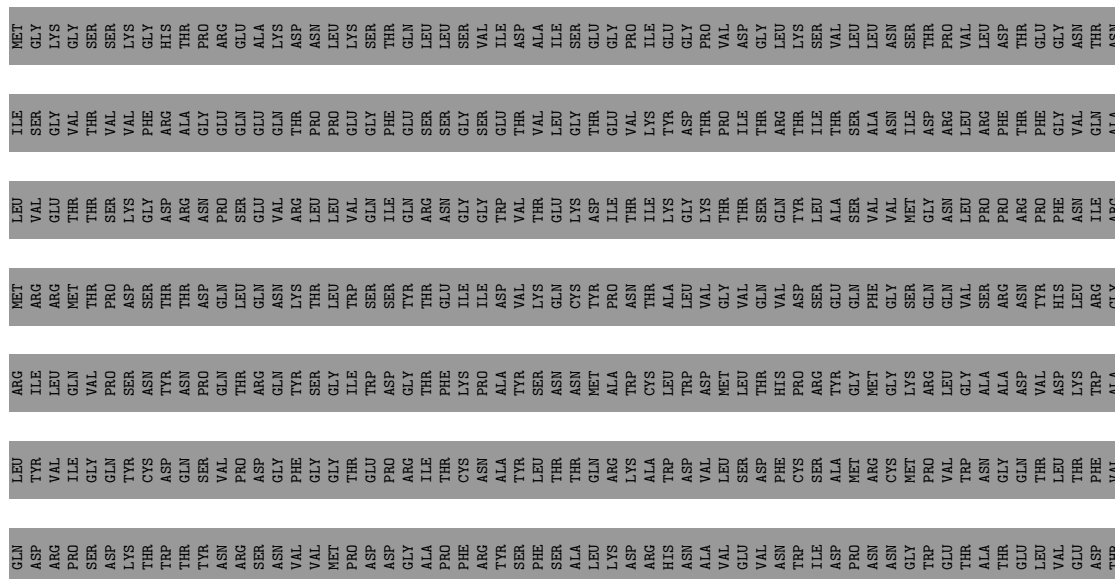
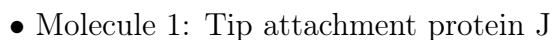
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tip attachment protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	380	Total	C	N	O	S	0	0
			2941	1864	499	573	5		
1	J	380	Total	C	N	O	S	0	0
			2941	1864	499	573	5		
1	Z	383	Total	C	N	O	S	0	0
			2960	1875	503	577	5		









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	358235	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.839	Depositor
Minimum map value	-1.114	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.3	Depositor
Map size ( $\text{\AA}$ )	343.74402, 343.74402, 343.74402	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0742, 1.0742, 1.0742	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	F	1.26	7/3005 (0.2%)	1.59	28/4089 (0.7%)
1	J	1.27	8/3005 (0.3%)	1.71	41/4089 (1.0%)
1	Z	1.28	3/3024 (0.1%)	1.70	42/4115 (1.0%)
All	All	1.27	18/9034 (0.2%)	1.67	111/12293 (0.9%)

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	F	0	3
1	J	0	3
1	Z	0	3
All	All	0	9

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	621	VAL	C-O	7.09	1.31	1.24
1	F	924	PHE	C-O	7.08	1.32	1.24
1	F	938	ILE	C-O	6.58	1.30	1.23
1	Z	667	LEU	C-O	6.43	1.31	1.23
1	F	923	ILE	C-O	6.33	1.30	1.24
1	J	727	PHE	C-O	6.15	1.31	1.24
1	J	731	ALA	C-O	5.91	1.31	1.23
1	J	881	GLY	C-O	5.64	1.31	1.23
1	F	903	ALA	C-O	5.36	1.30	1.24
1	F	896	LEU	C-O	5.36	1.30	1.24
1	J	892	LEU	C-O	5.29	1.29	1.24
1	J	819	LYS	C-O	5.24	1.30	1.24
1	J	803	ALA	C-O	5.22	1.29	1.23
1	J	901	ARG	N-CA	5.20	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	736	ALA	C-O	5.16	1.29	1.24
1	Z	927	ASP	C-O	5.15	1.29	1.23
1	F	928	VAL	N-CA	5.09	1.51	1.46
1	Z	745	GLU	C-O	5.03	1.30	1.24

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	970	SER	CA-C-N	10.16	129.44	121.61
1	J	970	SER	C-N-CA	10.16	129.44	121.61
1	J	895	PHE	CA-C-N	-9.96	108.53	123.07
1	J	895	PHE	C-N-CA	-9.96	108.53	123.07
1	Z	895	PHE	CB-CA-C	-9.75	98.36	111.82
1	J	771	TYR	CA-C-O	-9.50	110.00	121.11
1	J	900	ASN	CA-CB-CG	-8.83	103.77	112.60
1	Z	822	ILE	N-CA-C	-8.83	101.95	110.42
1	J	913	THR	CA-CB-OG1	-8.76	96.46	109.60
1	J	773	ILE	CA-C-N	8.66	134.28	121.72
1	J	773	ILE	C-N-CA	8.66	134.28	121.72
1	F	880	ILE	CA-C-N	8.42	127.99	122.18
1	F	880	ILE	C-N-CA	8.42	127.99	122.18
1	Z	657	THR	CA-CB-OG1	-7.85	97.82	109.60
1	F	947	PHE	CA-C-O	-7.75	113.17	121.38
1	J	772	TRP	CA-C-N	-7.70	113.11	123.12
1	J	772	TRP	C-N-CA	-7.70	113.11	123.12
1	J	895	PHE	CA-C-O	7.65	128.77	120.43
1	Z	916	PHE	CA-CB-CG	7.58	121.38	113.80
1	Z	900	ASN	CB-CA-C	7.57	124.25	109.72
1	Z	956	THR	CA-CB-OG1	-7.54	98.30	109.60
1	Z	783	HIS	CB-CA-C	-7.51	101.58	111.42
1	J	931	LYS	N-CA-C	-7.39	106.19	114.62
1	J	804	VAL	CA-C-O	-7.27	114.44	121.63
1	Z	970	SER	CA-C-N	7.16	128.84	122.47
1	Z	970	SER	C-N-CA	7.16	128.84	122.47
1	J	924	PHE	CA-C-O	-7.02	113.12	120.70
1	J	924	PHE	CA-CB-CG	-7.00	106.81	113.80
1	Z	780	LYS	CB-CA-C	6.91	118.28	108.68
1	J	782	GLY	O-C-N	6.85	128.06	122.51
1	Z	914	PRO	CA-C-O	-6.84	113.62	121.56
1	Z	900	ASN	N-CA-C	-6.69	105.12	113.28
1	F	940	SER	N-CA-C	-6.68	104.83	114.12
1	Z	680	PHE	CA-C-O	-6.60	113.06	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	916	PHE	CB-CA-C	6.59	125.37	110.67
1	Z	682	GLN	CB-CG-CD	6.49	123.64	112.60
1	F	854	ASP	CA-C-N	6.41	129.19	120.54
1	F	854	ASP	C-N-CA	6.41	129.19	120.54
1	Z	904	PHE	CB-CA-C	-6.32	98.37	110.24
1	J	773	ILE	O-C-N	6.29	130.45	123.10
1	F	618	PRO	N-CA-CB	6.25	106.69	103.19
1	Z	682	GLN	CB-CA-C	6.24	122.84	110.42
1	Z	928	VAL	CA-C-O	-6.23	113.38	120.67
1	Z	879	GLY	CA-C-N	6.20	130.23	122.48
1	Z	879	GLY	C-N-CA	6.20	130.23	122.48
1	Z	931	LYS	N-CA-C	-6.17	104.48	111.14
1	J	814	TYR	CA-CB-CG	-6.14	102.85	113.90
1	J	881	GLY	O-C-N	5.82	130.27	122.70
1	F	950	THR	CB-CA-C	5.81	117.49	108.61
1	F	815	LEU	N-CA-C	-5.79	106.84	114.31
1	J	923	ILE	CB-CA-C	5.79	119.73	110.82
1	F	982	CYS	CA-C-N	5.69	129.44	121.02
1	F	982	CYS	C-N-CA	5.69	129.44	121.02
1	F	927	ASP	CB-CA-C	5.68	119.99	109.54
1	Z	809	ASP	CA-CB-CG	5.65	118.25	112.60
1	Z	733	PRO	N-CD-CG	-5.59	94.81	103.20
1	Z	922	GLN	CA-C-O	-5.57	113.18	119.98
1	J	892	LEU	CA-C-N	5.57	131.53	123.13
1	J	892	LEU	C-N-CA	5.57	131.53	123.13
1	J	766	LEU	CA-C-O	-5.56	114.98	120.82
1	Z	897	VAL	O-C-N	5.51	129.04	123.20
1	Z	782	GLY	CA-C-N	5.51	130.20	121.72
1	Z	782	GLY	C-N-CA	5.51	130.20	121.72
1	Z	818	PHE	CA-C-O	-5.50	115.04	120.82
1	Z	919	GLN	CB-CG-CD	5.46	121.87	112.60
1	J	904	PHE	CB-CA-C	5.42	119.18	110.29
1	Z	929	PHE	CB-CA-C	5.41	119.43	110.78
1	J	748	PHE	CB-CA-C	-5.40	100.41	109.48
1	F	621	VAL	O-C-N	5.38	128.85	122.83
1	F	919	GLN	CB-CG-CD	-5.38	103.46	112.60
1	J	811	ALA	N-CA-C	-5.37	106.78	113.55
1	F	915	MET	N-CA-CB	5.34	118.01	110.90
1	Z	826	HIS	CA-C-O	-5.34	115.20	121.07
1	F	955	LEU	CA-C-O	-5.33	115.14	121.16
1	F	939	THR	CA-CB-OG1	-5.31	101.64	109.60
1	Z	672	ARG	CG-CD-NE	5.30	123.67	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	986	GLY	CA-C-N	5.28	130.19	122.85
1	J	986	GLY	C-N-CA	5.28	130.19	122.85
1	J	877	VAL	CA-C-O	-5.27	115.75	121.92
1	F	643	THR	CB-CA-C	5.26	115.99	108.68
1	F	827	LEU	CA-C-N	5.25	125.93	119.99
1	F	827	LEU	C-N-CA	5.25	125.93	119.99
1	J	817	PHE	CB-CA-C	-5.25	102.88	110.96
1	Z	930	LEU	CA-C-O	-5.22	115.09	121.36
1	F	617	THR	CB-CA-C	5.22	116.70	108.88
1	Z	896	LEU	N-CA-CB	-5.22	101.92	110.42
1	F	844	ARG	CG-CD-NE	5.21	123.47	112.00
1	J	812	GLU	N-CA-C	-5.19	105.79	111.82
1	Z	822	ILE	O-C-N	5.19	126.99	121.91
1	J	946	ALA	O-C-N	5.18	127.48	122.09
1	Z	876	TYR	CB-CA-C	-5.18	99.62	111.95
1	J	819	LYS	N-CA-C	-5.15	105.75	111.36
1	J	911	ASN	CA-CB-CG	-5.15	107.45	112.60
1	Z	797	LYS	CB-CA-C	5.13	119.17	109.37
1	F	913	THR	CB-CA-C	5.13	117.72	109.41
1	F	896	LEU	O-C-N	5.12	129.31	123.27
1	F	915	MET	N-CA-C	-5.12	107.70	114.31
1	Z	819	LYS	CA-C-N	5.12	125.66	119.98
1	Z	819	LYS	C-N-CA	5.12	125.66	119.98
1	F	922	GLN	CB-CA-C	-5.11	99.06	109.94
1	J	730	THR	CB-CA-C	5.10	119.26	111.76
1	J	912	GLU	CB-CG-CD	5.09	121.26	112.60
1	F	675	GLU	CA-C-O	-5.07	115.96	121.89
1	J	818	PHE	O-C-N	5.06	128.14	122.22
1	Z	771	TYR	CA-C-O	-5.06	115.60	121.26
1	Z	897	VAL	CA-C-O	-5.04	115.14	120.39
1	Z	791	SER	CA-C-O	-5.04	115.30	121.05
1	J	895	PHE	O-C-N	-5.02	117.60	123.27
1	J	971	GLY	CA-C-O	-5.02	117.20	121.57
1	J	951	PRO	CB-CA-C	-5.01	104.73	111.85
1	F	810	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	713	ALA	Peptide
1	F	929	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	F	934	THR	Peptide
1	J	722	LEU	Peptide
1	J	772	TRP	Peptide
1	J	781	PRO	Peptide
1	Z	878	ALA	Peptide
1	Z	943	ASN	Peptide
1	Z	959	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2941	0	2886	323	0
1	J	2941	0	2885	316	0
1	Z	2960	0	2903	338	0
All	All	8842	0	8674	756	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 43.

All (756) 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:F:902:ILE:CD1	1:J:895:PHE:HB2	1.65	1.24
1:Z:905:ILE:HD13	1:Z:912:GLU:O	1.47	1.15
1:F:928:VAL:HG23	1:J:923:ILE:CG2	1.75	1.14
1:F:902:ILE:HD12	1:J:895:PHE:CB	1.80	1.11
1:F:902:ILE:HD12	1:J:895:PHE:HB2	1.19	1.09
1:J:925:MET:HE1	1:Z:925:MET:HE1	1.34	1.05
1:F:928:VAL:CG2	1:J:923:ILE:HG22	1.87	1.03
1:Z:722:LEU:CD1	1:Z:804:VAL:O	2.07	1.02
1:F:923:ILE:HG22	1:Z:928:VAL:HG23	1.39	1.01
1:F:925:MET:HE1	1:J:923:ILE:HG21	1.41	1.01
1:Z:827:LEU:HD22	1:Z:896:LEU:HB3	1.38	1.00
1:F:899:ALA:O	1:Z:906:ASP:HA	1.61	0.99
1:J:746:PHE:HD2	1:J:772:TRP:HB2	1.28	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:722:LEU:HD13	1:Z:804:VAL:O	1.62	0.98
1:J:859:TRP:O	1:J:891:LYS:NZ	1.99	0.96
1:F:955:LEU:HD23	1:F:956:THR:N	1.81	0.95
1:J:720:ILE:HD13	1:J:789:ILE:HD13	1.45	0.95
1:J:960:ALA:O	1:J:962:ILE:HD12	1.69	0.93
1:F:970:SER:O	1:Z:973:LEU:HD23	1.70	0.92
1:J:730:THR:HG23	1:J:773:ILE:HD11	1.50	0.91
1:J:746:PHE:CD2	1:J:772:TRP:HB2	2.06	0.91
1:Z:720:ILE:HG22	1:Z:733:PRO:HB3	1.51	0.91
1:Z:685:LEU:HB2	1:Z:711:ILE:HD13	1.53	0.90
1:J:772:TRP:C	1:J:773:ILE:HD12	1.96	0.90
1:J:766:LEU:HD11	1:J:774:ALA:HB2	1.53	0.90
1:F:928:VAL:HG23	1:J:923:ILE:HG22	0.91	0.88
1:Z:613:VAL:HG11	1:Z:698:TRP:HZ2	1.39	0.87
1:J:628:VAL:HG21	1:J:711:ILE:HD11	1.57	0.87
1:F:884:MET:HE3	1:Z:867:ILE:HD11	1.57	0.86
1:Z:955:LEU:HD13	1:Z:955:LEU:O	1.74	0.86
1:Z:613:VAL:HG11	1:Z:698:TRP:CZ2	2.11	0.86
1:J:914:PRO:HD3	1:Z:819:LYS:HB2	1.59	0.85
1:F:900:ASN:OD1	1:J:893:SER:N	2.10	0.84
1:F:901:ARG:HG2	1:F:919:GLN:HB2	1.59	0.84
1:F:966:VAL:HG12	1:F:966:VAL:O	1.78	0.84
1:F:897:VAL:O	1:Z:904:PHE:HA	1.77	0.84
1:F:618:PRO:HB3	1:F:647:VAL:HG21	1.59	0.84
1:F:657:THR:HG22	1:F:667:LEU:HA	1.60	0.83
1:F:781:PRO:HB3	1:F:809:ASP:HA	1.60	0.83
1:F:624:LEU:HD11	1:F:707:VAL:CG2	2.09	0.83
1:F:917:VAL:HG12	1:F:924:PHE:HD2	1.42	0.83
1:Z:827:LEU:HB3	1:Z:896:LEU:HD23	1.59	0.82
1:Z:776:SER:OG	1:Z:778:ASN:OD1	1.97	0.82
1:Z:905:ILE:HG12	1:Z:914:PRO:HA	1.61	0.82
1:F:814:TYR:CD1	1:Z:924:PHE:CE2	2.68	0.81
1:J:772:TRP:O	1:J:773:ILE:HD12	1.79	0.81
1:F:893:SER:CB	1:Z:878:ALA:HB2	2.10	0.81
1:Z:779:ILE:HG23	1:Z:785:TYR:HE2	1.45	0.81
1:Z:720:ILE:CG2	1:Z:733:PRO:HB3	2.10	0.81
1:F:902:ILE:CD1	1:J:895:PHE:CB	2.45	0.80
1:Z:635:TYR:O	1:Z:683:LEU:HB2	1.80	0.80
1:J:720:ILE:CD1	1:J:789:ILE:HD13	2.11	0.79
1:Z:684:ALA:O	1:Z:688:TYR:OH	2.01	0.79
1:J:863:TRP:CH2	1:J:865:VAL:HG23	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:961:ASP:OD2	1:Z:954:LYS:HD2	1.84	0.78
1:Z:673:THR:OG1	1:Z:674:THR:N	2.13	0.78
1:F:893:SER:OG	1:Z:899:ALA:HA	1.84	0.78
1:Z:955:LEU:O	1:Z:955:LEU:CD1	2.31	0.78
1:J:931:LYS:O	1:J:931:LYS:NZ	2.14	0.78
1:Z:779:ILE:HG23	1:Z:785:TYR:CE2	2.19	0.78
1:F:901:ARG:NH2	1:J:894:GLN:HE22	1.82	0.77
1:J:925:MET:HE1	1:Z:925:MET:CE	2.13	0.77
1:F:937:THR:HG23	1:F:951:PRO:HD3	1.66	0.76
1:F:628:VAL:HG13	1:F:711:ILE:HD12	1.66	0.76
1:Z:978:ILE:HG22	1:Z:980:GLU:O	1.84	0.75
1:F:947:PHE:CD1	1:J:949:LEU:HD22	2.22	0.75
1:J:726:TYR:CZ	1:J:813:GLY:HA3	2.21	0.75
1:Z:721:GLU:OE2	1:Z:732:THR:OG1	2.03	0.74
1:F:728:GLN:HA	1:F:774:ALA:O	1.87	0.74
1:Z:656:LEU:HD23	1:Z:668:VAL:HB	1.68	0.74
1:Z:729:ILE:HD12	1:Z:806:ARG:O	1.88	0.74
1:J:962:ILE:HG22	1:Z:958:LYS:O	1.88	0.74
1:F:720:ILE:HD11	1:F:789:ILE:HD11	1.70	0.74
1:J:972:THR:HG22	1:J:972:THR:O	1.87	0.74
1:F:930:LEU:HD22	1:Z:933:LEU:HD11	1.70	0.74
1:J:973:LEU:H	1:J:973:LEU:HD12	1.51	0.73
1:F:667:LEU:HD11	1:F:670:THR:HG23	1.70	0.73
1:J:920:GLY:C	1:J:922:GLN:H	1.96	0.73
1:Z:933:LEU:O	1:Z:934:THR:OG1	2.04	0.73
1:F:902:ILE:HD11	1:J:895:PHE:HB2	1.68	0.73
1:J:715:ALA:HB3	1:J:735:LEU:HD21	1.69	0.73
1:J:955:LEU:HD23	1:J:956:THR:N	2.04	0.72
1:F:924:PHE:CE1	1:Z:929:PHE:CE2	2.77	0.72
1:Z:905:ILE:HG23	1:Z:913:THR:O	1.89	0.72
1:F:858:LYS:HE2	1:Z:871:LYS:HD3	1.72	0.71
1:J:925:MET:HG2	1:Z:923:ILE:HD13	1.72	0.71
1:J:780:LYS:O	1:J:781:PRO:O	2.08	0.71
1:Z:904:PHE:CE2	1:Z:916:PHE:CD1	2.77	0.71
1:F:884:MET:HE3	1:Z:867:ILE:CD1	2.19	0.71
1:J:730:THR:HG23	1:J:773:ILE:CD1	2.20	0.71
1:J:913:THR:HG23	1:Z:819:LYS:HD2	1.72	0.71
1:Z:722:LEU:HD12	1:Z:804:VAL:O	1.90	0.71
1:J:863:TRP:CH2	1:J:865:VAL:CG2	2.74	0.71
1:J:868:GLU:HG3	1:J:877:VAL:HG23	1.73	0.71
1:F:893:SER:HB2	1:Z:878:ALA:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:685:LEU:HA	1:Z:711:ILE:HG12	1.73	0.71
1:J:717:PRO:HG3	1:J:744:PHE:CE1	2.25	0.70
1:F:914:PRO:HB2	1:J:815:LEU:CD2	2.20	0.70
1:J:781:PRO:HG2	1:Z:929:PHE:CE2	2.26	0.70
1:Z:725:GLY:O	1:Z:808:SER:OG	2.08	0.70
1:Z:788:TYR:HE1	1:Z:802:GLU:HB2	1.56	0.70
1:F:901:ARG:O	1:J:894:GLN:HA	1.92	0.70
1:J:722:LEU:HD12	1:J:722:LEU:N	2.07	0.69
1:J:930:LEU:CD1	1:Z:925:MET:HB2	2.22	0.69
1:F:920:GLY:O	1:F:921:ASN:ND2	2.25	0.69
1:Z:837:LEU:HD21	1:Z:842:ALA:HB3	1.74	0.69
1:F:893:SER:HB3	1:Z:900:ASN:OD1	1.92	0.69
1:F:925:MET:CE	1:J:923:ILE:HG21	2.19	0.69
1:Z:729:ILE:HD11	1:Z:805:GLY:HA3	1.73	0.69
1:F:893:SER:HB2	1:Z:878:ALA:CB	2.22	0.69
1:F:924:PHE:HE1	1:Z:929:PHE:CE2	2.11	0.69
1:J:863:TRP:HB3	1:J:882:LEU:HD21	1.74	0.69
1:Z:720:ILE:HG22	1:Z:733:PRO:CB	2.22	0.69
1:F:884:MET:HE3	1:Z:867:ILE:CG1	2.22	0.68
1:F:914:PRO:HB2	1:J:815:LEU:HD21	1.75	0.68
1:Z:948:SER:C	1:Z:949:LEU:HD12	2.18	0.68
1:F:893:SER:HG	1:Z:899:ALA:HA	1.59	0.68
1:Z:788:TYR:CE1	1:Z:802:GLU:HB2	2.28	0.68
1:J:646:VAL:HG21	1:J:650:VAL:HB	1.75	0.68
1:F:899:ALA:HB1	1:J:893:SER:O	1.94	0.68
1:J:744:PHE:O	1:J:768:THR:HA	1.92	0.68
1:J:867:ILE:CD1	1:Z:882:LEU:CD2	2.72	0.68
1:F:720:ILE:CD1	1:F:789:ILE:HD11	2.23	0.68
1:F:704:PRO:O	1:J:743:GLN:NE2	2.20	0.68
1:F:925:MET:HE1	1:J:923:ILE:CG2	2.21	0.68
1:J:922:GLN:NE2	1:Z:780:LYS:HB3	2.09	0.68
1:J:773:ILE:HD12	1:J:773:ILE:N	2.08	0.67
1:J:939:THR:O	1:Z:934:THR:HG23	1.94	0.67
1:F:982:CYS:SG	1:Z:984:ILE:HG12	2.34	0.66
1:F:827:LEU:HD23	1:F:862:MET:HE1	1.76	0.66
1:Z:636:GLN:HA	1:Z:683:LEU:HD12	1.76	0.66
1:Z:916:PHE:O	1:Z:917:VAL:HG22	1.95	0.66
1:J:920:GLY:O	1:J:922:GLN:N	2.29	0.66
1:J:771:TYR:HD1	1:J:771:TYR:H	1.43	0.66
1:F:905:ILE:HD11	1:J:822:ILE:HD13	1.77	0.66
1:Z:827:LEU:HD21	1:Z:881:GLY:C	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:946:ALA:O	1:J:953:GLY:HA3	1.95	0.65
1:F:845:LEU:HD12	1:F:867:ILE:HD11	1.79	0.65
1:Z:921:ASN:OD1	1:Z:921:ASN:N	2.29	0.65
1:F:906:ASP:OD2	1:J:900:ASN:HA	1.97	0.65
1:J:746:PHE:CD1	1:J:789:ILE:HG22	2.31	0.65
1:J:930:LEU:HD13	1:Z:925:MET:HB2	1.77	0.65
1:Z:895:PHE:CG	1:Z:895:PHE:O	2.43	0.65
1:J:911:ASN:OD1	1:J:912:GLU:N	2.30	0.65
1:F:917:VAL:HG12	1:F:924:PHE:CD2	2.29	0.65
1:J:924:PHE:N	1:J:924:PHE:CD1	2.60	0.65
1:Z:871:LYS:NZ	1:Z:872:ASP:OD2	2.30	0.64
1:J:933:LEU:HD11	1:J:935:ALA:HB2	1.78	0.64
1:J:960:ALA:O	1:J:962:ILE:CD1	2.43	0.64
1:J:726:TYR:OH	1:J:813:GLY:HA3	1.98	0.64
1:J:733:PRO:O	1:J:734:HIS:ND1	2.30	0.64
1:J:880:ILE:HG22	1:J:897:VAL:HA	1.80	0.64
1:F:924:PHE:CE1	1:Z:929:PHE:HE2	2.15	0.64
1:F:958:LYS:O	1:F:959:ASN:HB2	1.97	0.64
1:J:717:PRO:HG3	1:J:744:PHE:CZ	2.33	0.64
1:J:917:VAL:HG11	1:Z:818:PHE:CG	2.33	0.64
1:J:988:LEU:HD23	1:J:989:ARG:N	2.13	0.64
1:Z:897:VAL:HG12	1:Z:897:VAL:O	1.97	0.64
1:F:771:TYR:CE1	1:Z:909:ASN:OD1	2.51	0.64
1:F:814:TYR:CD1	1:Z:924:PHE:HE2	2.16	0.64
1:Z:916:PHE:O	1:Z:917:VAL:CG2	2.46	0.64
1:F:814:TYR:CG	1:Z:924:PHE:HE2	2.17	0.63
1:F:896:LEU:HD12	1:Z:903:ALA:O	1.97	0.63
1:Z:904:PHE:HE2	1:Z:916:PHE:CD1	2.16	0.63
1:Z:903:ALA:HB1	1:Z:914:PRO:HB3	1.81	0.63
1:Z:978:ILE:HD13	1:Z:982:CYS:HB2	1.80	0.63
1:F:722:LEU:HA	1:F:730:THR:O	1.98	0.63
1:F:931:LYS:O	1:F:932:ARG:HB2	1.98	0.63
1:Z:613:VAL:CG1	1:Z:698:TRP:CZ2	2.82	0.62
1:F:876:TYR:HB3	1:J:884:MET:CE	2.29	0.62
1:J:905:ILE:O	1:Z:898:ALA:HA	1.99	0.62
1:Z:918:ALA:CB	1:Z:923:ILE:HG13	2.29	0.62
1:F:618:PRO:HA	1:F:647:VAL:HG11	1.81	0.62
1:F:819:LYS:HD3	1:Z:913:THR:OG1	2.00	0.62
1:F:905:ILE:HD13	1:F:914:PRO:HA	1.80	0.62
1:F:933:LEU:CD1	1:J:930:LEU:HD23	2.29	0.62
1:J:880:ILE:CG2	1:J:897:VAL:HA	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:831:LEU:C	1:Z:832:LEU:HD23	2.25	0.62
1:F:845:LEU:HD11	1:J:849:SER:HB2	1.81	0.62
1:F:882:LEU:HD13	1:Z:880:ILE:HD13	1.82	0.62
1:Z:753:ILE:HD12	1:Z:753:ILE:O	2.00	0.62
1:Z:982:CYS:O	1:Z:982:CYS:SG	2.58	0.62
1:Z:904:PHE:O	1:Z:915:MET:N	2.33	0.61
1:J:814:TYR:O	1:J:817:PHE:HB3	1.99	0.61
1:J:922:GLN:O	1:J:923:ILE:HD12	2.00	0.61
1:F:728:GLN:HB3	1:F:775:ALA:HB2	1.82	0.61
1:F:949:LEU:HD22	1:Z:947:PHE:CD1	2.35	0.61
1:F:978:ILE:HD13	1:J:976:VAL:HG11	1.81	0.61
1:J:906:ASP:OD1	1:J:907:PRO:HD2	2.00	0.61
1:F:922:GLN:C	1:F:923:ILE:HD12	2.26	0.61
1:F:924:PHE:CE1	1:Z:929:PHE:CD2	2.88	0.61
1:F:643:THR:HG22	1:F:646:VAL:H	1.65	0.61
1:F:881:GLY:O	1:F:895:PHE:HA	2.00	0.61
1:F:749:SER:OG	1:F:786:TYR:HB2	2.01	0.61
1:J:773:ILE:CD1	1:J:773:ILE:N	2.64	0.61
1:F:928:VAL:CG1	1:Z:930:LEU:HD13	2.30	0.60
1:J:657:THR:HG22	1:J:667:LEU:HA	1.82	0.60
1:F:902:ILE:CG1	1:J:895:PHE:CB	2.79	0.60
1:F:626:ALA:HB1	1:F:709:PHE:HB3	1.82	0.60
1:F:706:SER:O	1:J:768:THR:OG1	2.19	0.60
1:J:925:MET:CE	1:Z:925:MET:HE1	2.21	0.60
1:Z:636:GLN:HG3	1:Z:679:ARG:HH22	1.65	0.60
1:J:990:ALA:HB3	1:J:993:ILE:HD11	1.84	0.60
1:Z:837:LEU:HD11	1:Z:842:ALA:CB	2.32	0.60
1:F:922:GLN:O	1:F:923:ILE:HD12	2.02	0.60
1:Z:933:LEU:HD12	1:Z:934:THR:H	1.67	0.60
1:F:624:LEU:HD11	1:F:707:VAL:HG21	1.84	0.60
1:Z:683:LEU:HD22	1:Z:688:TYR:CZ	2.37	0.60
1:Z:782:GLY:O	1:Z:783:HIS:ND1	2.35	0.60
1:Z:656:LEU:HD21	1:Z:668:VAL:HG11	1.83	0.59
1:F:955:LEU:HD23	1:F:955:LEU:C	2.27	0.59
1:J:635:TYR:OH	1:J:795:VAL:HG22	2.03	0.59
1:J:880:ILE:HG21	1:J:897:VAL:HG13	1.84	0.59
1:F:746:PHE:HA	1:F:789:ILE:HG22	1.85	0.59
1:Z:656:LEU:CD2	1:Z:668:VAL:CG1	2.80	0.59
1:F:838:THR:HA	1:F:870:THR:HG21	1.84	0.59
1:F:848:PHE:HE2	1:F:850:LYS:HG2	1.65	0.59
1:F:954:LYS:HD2	1:Z:959:ASN:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:786:TYR:HA	1:Z:803:ALA:O	2.02	0.59
1:F:933:LEU:HD12	1:J:930:LEU:HD23	1.83	0.59
1:Z:904:PHE:O	1:Z:914:PRO:HA	2.03	0.59
1:Z:848:PHE:O	1:Z:863:TRP:CD1	2.55	0.59
1:Z:837:LEU:HD11	1:Z:842:ALA:HB1	1.85	0.58
1:F:959:ASN:HB3	1:J:954:LYS:HA	1.85	0.58
1:F:882:LEU:HD11	1:Z:878:ALA:C	2.28	0.58
1:Z:769:ALA:HB3	1:Z:771:TYR:O	2.04	0.58
1:Z:808:SER:O	1:Z:809:ASP:HB3	2.03	0.58
1:Z:656:LEU:O	1:Z:668:VAL:HB	2.04	0.58
1:F:962:ILE:HD12	1:F:962:ILE:N	2.19	0.58
1:Z:756:ILE:HG22	1:Z:800:PHE:HB2	1.84	0.58
1:Z:955:LEU:HD13	1:Z:955:LEU:C	2.28	0.58
1:J:905:ILE:CG2	1:Z:898:ALA:HB2	2.33	0.58
1:Z:636:GLN:HG3	1:Z:679:ARG:NH2	2.19	0.58
1:Z:656:LEU:HD23	1:Z:668:VAL:CB	2.34	0.58
1:Z:685:LEU:HD23	1:Z:685:LEU:H	1.68	0.58
1:Z:744:PHE:N	1:Z:744:PHE:CD2	2.70	0.58
1:Z:916:PHE:C	1:Z:917:VAL:HG23	2.29	0.57
1:F:891:LYS:O	1:Z:876:TYR:CE2	2.57	0.57
1:J:916:PHE:CD1	1:J:916:PHE:C	2.81	0.57
1:Z:720:ILE:HD11	1:Z:803:ALA:HB3	1.86	0.57
1:Z:741:THR:O	1:Z:741:THR:OG1	2.19	0.57
1:Z:949:LEU:HD12	1:Z:949:LEU:N	2.19	0.57
1:J:725:GLY:HA3	1:J:728:GLN:NE2	2.19	0.57
1:J:746:PHE:HD2	1:J:772:TRP:CB	2.11	0.57
1:Z:656:LEU:HD23	1:Z:668:VAL:CG1	2.34	0.57
1:F:901:ARG:HD3	1:F:919:GLN:OE1	2.05	0.57
1:J:938:ILE:HG12	1:Z:933:LEU:HB3	1.86	0.57
1:F:902:ILE:CG2	1:F:904:PHE:HE1	2.16	0.57
1:J:817:PHE:C	1:J:817:PHE:CD2	2.83	0.57
1:F:893:SER:OG	1:Z:878:ALA:HB2	2.04	0.57
1:J:845:LEU:N	1:J:845:LEU:HD12	2.20	0.57
1:Z:827:LEU:CD2	1:Z:896:LEU:HB3	2.26	0.57
1:F:696:ASN:OD1	1:F:700:GLN:N	2.34	0.57
1:F:902:ILE:CG1	1:J:895:PHE:HB2	2.34	0.57
1:J:771:TYR:CD1	1:J:771:TYR:O	2.57	0.57
1:J:837:LEU:HD13	1:J:842:ALA:HB1	1.85	0.57
1:J:851:GLU:HA	1:J:860:ASN:O	2.04	0.57
1:Z:710:ARG:HB2	1:Z:710:ARG:CZ	2.34	0.57
1:F:932:ARG:HG3	1:Z:937:THR:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:744:PHE:HB2	1:J:769:ALA:O	2.03	0.57
1:Z:918:ALA:HB2	1:Z:923:ILE:CG1	2.35	0.57
1:F:837:LEU:HG	1:F:844:ARG:HB2	1.87	0.57
1:F:893:SER:OG	1:Z:899:ALA:CA	2.53	0.57
1:Z:613:VAL:HG12	1:Z:614:ASN:N	2.19	0.57
1:Z:613:VAL:CG1	1:Z:698:TRP:CH2	2.88	0.56
1:F:744:PHE:O	1:F:768:THR:HA	2.05	0.56
1:F:848:PHE:CE2	1:F:850:LYS:HG2	2.38	0.56
1:Z:787:PHE:HB3	1:Z:789:ILE:CD1	2.35	0.56
1:F:647:VAL:HG22	1:F:650:VAL:HB	1.87	0.56
1:F:730:THR:HG23	1:F:773:ILE:HG22	1.86	0.56
1:F:902:ILE:HD12	1:J:895:PHE:N	2.19	0.56
1:F:947:PHE:CG	1:J:949:LEU:HD22	2.41	0.56
1:J:810:ASP:O	1:J:814:TYR:HD2	1.89	0.56
1:F:902:ILE:HG13	1:J:895:PHE:CD2	2.40	0.56
1:J:973:LEU:HD12	1:J:973:LEU:N	2.21	0.56
1:Z:620:ALA:HB2	1:Z:703:ASP:O	2.06	0.56
1:Z:720:ILE:HA	1:Z:733:PRO:HA	1.86	0.56
1:F:836:GLU:HB2	1:F:844:ARG:NH2	2.20	0.56
1:J:766:LEU:HD11	1:J:774:ALA:CB	2.32	0.56
1:J:937:THR:C	1:J:938:ILE:HG13	2.29	0.56
1:F:905:ILE:HD11	1:J:822:ILE:CD1	2.36	0.56
1:J:880:ILE:HG22	1:J:898:ALA:H	1.71	0.56
1:Z:638:LEU:HD11	1:Z:679:ARG:HH21	1.70	0.56
1:J:744:PHE:HB3	1:J:746:PHE:CE1	2.40	0.56
1:J:657:THR:HA	1:J:668:VAL:HG23	1.88	0.55
1:J:771:TYR:CD1	1:J:771:TYR:N	2.74	0.55
1:J:923:ILE:C	1:J:924:PHE:CD1	2.84	0.55
1:Z:907:PRO:HA	1:Z:911:ASN:O	2.06	0.55
1:J:876:TYR:HB2	1:Z:884:MET:HE1	1.88	0.55
1:F:641:TRP:O	1:F:676:THR:HB	2.06	0.55
1:F:882:LEU:HD23	1:Z:865:VAL:HG12	1.89	0.55
1:F:923:ILE:CG2	1:Z:928:VAL:HG23	2.27	0.55
1:F:933:LEU:HD23	1:Z:938:ILE:HG23	1.88	0.55
1:J:920:GLY:C	1:J:922:GLN:N	2.64	0.55
1:Z:916:PHE:C	1:Z:917:VAL:CG2	2.80	0.55
1:F:628:VAL:CG1	1:F:711:ILE:HD12	2.36	0.55
1:J:842:ALA:O	1:J:869:GLN:HA	2.07	0.55
1:F:771:TYR:O	1:Z:909:ASN:ND2	2.38	0.55
1:F:849:SER:HB2	1:Z:845:LEU:HD21	1.88	0.55
1:J:732:THR:HG22	1:J:771:TYR:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:928:VAL:HG11	1:Z:930:LEU:HD13	1.89	0.55
1:J:865:VAL:HG21	1:Z:863:TRP:CZ3	2.42	0.55
1:Z:827:LEU:CB	1:Z:896:LEU:HD23	2.36	0.55
1:F:717:PRO:HG3	1:F:744:PHE:HE2	1.72	0.55
1:F:831:LEU:HD21	1:F:864:ALA:HB1	1.88	0.55
1:F:918:ALA:HA	1:F:922:GLN:O	2.07	0.55
1:F:765:TYR:OH	1:F:873:GLY:O	2.23	0.54
1:F:906:ASP:HB2	1:F:915:MET:HE1	1.89	0.54
1:J:830:GLU:HG2	1:J:848:PHE:CZ	2.42	0.54
1:J:867:ILE:CD1	1:Z:882:LEU:HD21	2.38	0.54
1:Z:781:PRO:HA	1:Z:807:ALA:HB3	1.89	0.54
1:F:641:TRP:HH2	1:F:678:TYR:HB2	1.72	0.54
1:J:746:PHE:HE2	1:J:772:TRP:N	2.05	0.54
1:F:619:PRO:HD3	1:F:647:VAL:CG1	2.38	0.54
1:J:869:GLN:HG3	1:Z:884:MET:SD	2.48	0.54
1:Z:639:ALA:O	1:Z:677:THR:HA	2.07	0.54
1:Z:748:PHE:HD1	1:Z:787:PHE:CE1	2.26	0.54
1:J:722:LEU:O	1:J:724:PRO:HD3	2.08	0.54
1:F:894:GLN:N	1:Z:899:ALA:HB1	2.23	0.54
1:J:843:SER:HB2	1:Z:859:TRP:HE3	1.72	0.54
1:J:922:GLN:OE1	1:Z:781:PRO:HD2	2.08	0.54
1:F:622:GLN:HG3	1:F:644:PRO:HG3	1.90	0.54
1:F:902:ILE:HG13	1:J:895:PHE:CB	2.38	0.54
1:F:966:VAL:O	1:F:966:VAL:CG1	2.47	0.54
1:J:722:LEU:HD22	1:J:805:GLY:HA3	1.89	0.54
1:Z:658:VAL:HG13	1:Z:658:VAL:O	2.08	0.54
1:F:628:VAL:HG12	1:F:794:THR:HG21	1.90	0.54
1:F:893:SER:CB	1:Z:878:ALA:CB	2.81	0.54
1:Z:827:LEU:HD21	1:Z:881:GLY:O	2.07	0.54
1:J:924:PHE:N	1:J:924:PHE:HD1	2.06	0.54
1:Z:847:GLU:HB2	1:Z:865:VAL:HG22	1.90	0.54
1:F:690:LEU:C	1:F:690:LEU:HD13	2.33	0.54
1:F:814:TYR:CG	1:Z:924:PHE:CE2	2.95	0.54
1:Z:711:ILE:HD12	1:Z:711:ILE:C	2.32	0.54
1:Z:827:LEU:HD23	1:Z:831:LEU:HD22	1.90	0.53
1:F:949:LEU:HD22	1:Z:947:PHE:CG	2.43	0.53
1:J:844:ARG:C	1:J:845:LEU:HD12	2.33	0.53
1:J:961:ASP:N	1:J:961:ASP:OD1	2.39	0.53
1:F:619:PRO:HD3	1:F:647:VAL:HG11	1.89	0.53
1:Z:688:TYR:HB2	1:Z:709:PHE:CE1	2.43	0.53
1:J:835:VAL:O	1:J:835:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:880:ILE:O	1:F:880:ILE:HG13	2.09	0.53
1:Z:918:ALA:HB1	1:Z:923:ILE:HG13	1.90	0.53
1:J:730:THR:HG23	1:J:773:ILE:CG1	2.39	0.53
1:J:816:ASP:OD1	1:J:817:PHE:N	2.42	0.53
1:J:849:SER:HB3	1:J:863:TRP:HD1	1.74	0.53
1:F:818:PHE:O	1:F:822:ILE:HG12	2.09	0.53
1:J:718:SER:O	1:J:719:ARG:HG2	2.09	0.53
1:F:900:ASN:HA	1:Z:906:ASP:CG	2.34	0.52
1:F:814:TYR:CE1	1:Z:924:PHE:CE2	2.97	0.52
1:F:902:ILE:HG13	1:J:895:PHE:HD2	1.72	0.52
1:J:695:VAL:HG22	1:J:701:GLN:HG2	1.90	0.52
1:F:931:LYS:O	1:F:932:ARG:CB	2.58	0.52
1:Z:837:LEU:HD13	1:Z:844:ARG:HB2	1.91	0.52
1:F:884:MET:CE	1:Z:867:ILE:HD11	2.36	0.52
1:F:973:LEU:O	1:Z:978:ILE:HA	2.09	0.52
1:J:641:TRP:O	1:J:676:THR:OG1	2.27	0.52
1:J:868:GLU:CG	1:J:877:VAL:HG23	2.38	0.52
1:Z:624:LEU:C	1:Z:624:LEU:HD23	2.34	0.52
1:Z:656:LEU:CD2	1:Z:668:VAL:HG11	2.40	0.52
1:Z:919:GLN:O	1:Z:920:GLY:C	2.51	0.52
1:J:918:ALA:CB	1:J:923:ILE:HD11	2.39	0.52
1:J:790:ARG:CZ	1:J:800:PHE:CZ	2.93	0.52
1:Z:686:GLY:N	1:Z:711:ILE:HD11	2.24	0.52
1:F:901:ARG:NH1	1:J:894:GLN:OE1	2.43	0.52
1:F:970:SER:OG	1:F:971:GLY:N	2.38	0.52
1:F:930:LEU:HB3	1:Z:935:ALA:HB2	1.92	0.52
1:J:826:HIS:C	1:J:862:MET:HE1	2.35	0.52
1:Z:918:ALA:HB2	1:Z:923:ILE:HG13	1.91	0.52
1:J:726:TYR:O	1:J:727:PHE:HB2	2.10	0.51
1:Z:701:GLN:N	1:Z:701:GLN:OE1	2.43	0.51
1:F:913:THR:C	1:F:914:PRO:O	2.51	0.51
1:J:771:TYR:HD1	1:J:771:TYR:N	2.06	0.51
1:J:866:LYS:HG2	1:J:868:GLU:OE1	2.10	0.51
1:F:858:LYS:CE	1:Z:871:LYS:HD3	2.40	0.51
1:F:915:MET:O	1:F:925:MET:HA	2.10	0.51
1:J:720:ILE:HD11	1:J:731:ALA:HB1	1.91	0.51
1:Z:720:ILE:HD11	1:Z:803:ALA:CB	2.40	0.51
1:J:717:PRO:CG	1:J:744:PHE:CE1	2.94	0.51
1:J:810:ASP:O	1:J:814:TYR:CD2	2.63	0.51
1:Z:669:SER:OG	1:Z:670:THR:N	2.44	0.51
1:Z:895:PHE:O	1:Z:895:PHE:CD2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:962:ILE:HD13	1:Z:966:VAL:HG22	1.93	0.51
1:Z:650:VAL:HG12	1:Z:650:VAL:O	2.11	0.51
1:F:928:VAL:HG22	1:F:929:PHE:N	2.26	0.51
1:F:985:ASN:OD1	1:F:985:ASN:N	2.43	0.51
1:J:781:PRO:HA	1:J:807:ALA:HB3	1.93	0.51
1:J:810:ASP:OD1	1:J:811:ALA:N	2.43	0.51
1:Z:982:CYS:SG	1:Z:984:ILE:HD11	2.51	0.51
1:F:791:SER:O	1:F:797:LYS:HA	2.11	0.51
1:J:922:GLN:OE1	1:J:924:PHE:CZ	2.64	0.51
1:Z:919:GLN:HE22	1:Z:922:GLN:HB2	1.75	0.51
1:F:729:ILE:HG23	1:F:774:ALA:HB3	1.93	0.51
1:F:900:ASN:OD1	1:J:892:LEU:HG	2.10	0.51
1:F:960:ALA:O	1:Z:966:VAL:HA	2.11	0.51
1:F:980:GLU:C	1:Z:986:GLY:HA3	2.35	0.51
1:J:712:ALA:C	1:J:795:VAL:HG11	2.35	0.51
1:J:925:MET:SD	1:Z:925:MET:CE	2.99	0.51
1:F:978:ILE:HD13	1:J:976:VAL:CG1	2.41	0.50
1:Z:853:LYS:HE3	1:Z:859:TRP:CD1	2.45	0.50
1:Z:933:LEU:O	1:Z:934:THR:CB	2.58	0.50
1:F:619:PRO:HG3	1:F:645:LYS:HG2	1.92	0.50
1:F:851:GLU:HB2	1:Z:845:LEU:HD23	1.93	0.50
1:F:906:ASP:OD2	1:J:900:ASN:O	2.28	0.50
1:J:843:SER:HB2	1:Z:859:TRP:CE3	2.46	0.50
1:J:928:VAL:HG23	1:J:930:LEU:CD2	2.42	0.50
1:Z:904:PHE:HB2	1:Z:915:MET:HE2	1.93	0.50
1:F:917:VAL:HG11	1:J:818:PHE:CD2	2.47	0.50
1:J:628:VAL:HG21	1:J:711:ILE:CD1	2.35	0.50
1:J:902:ILE:C	1:J:902:ILE:HD12	2.36	0.50
1:F:624:LEU:HD11	1:F:707:VAL:CB	2.42	0.50
1:J:854:ASP:OD2	1:J:860:ASN:ND2	2.45	0.50
1:F:726:TYR:HD1	1:F:810:ASP:HA	1.77	0.50
1:F:863:TRP:CD2	1:Z:865:VAL:HG21	2.47	0.50
1:J:739:ASP:OD1	1:J:741:THR:HG22	2.11	0.50
1:J:880:ILE:HD13	1:J:895:PHE:CZ	2.47	0.50
1:J:925:MET:SD	1:Z:925:MET:HE2	2.52	0.50
1:J:955:LEU:HD23	1:J:956:THR:O	2.11	0.50
1:F:618:PRO:HD3	1:F:696:ASN:HB3	1.94	0.50
1:F:902:ILE:CG1	1:J:895:PHE:HB3	2.41	0.50
1:Z:861:ALA:O	1:Z:883:SER:HB2	2.11	0.50
1:F:924:PHE:HE1	1:Z:929:PHE:CD2	2.29	0.50
1:Z:780:LYS:CB	1:Z:780:LYS:NZ	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:790:ARG:HD3	1:F:800:PHE:CE1	2.47	0.50
1:F:917:VAL:CG1	1:F:924:PHE:HD2	2.18	0.50
1:Z:722:LEU:HD23	1:Z:731:ALA:HA	1.94	0.50
1:Z:837:LEU:CD2	1:Z:842:ALA:HB3	2.42	0.50
1:J:845:LEU:HD21	1:Z:861:ALA:HB1	1.94	0.50
1:J:778:ASN:O	1:J:780:LYS:HG3	2.12	0.49
1:Z:618:PRO:O	1:Z:702:GLY:HA3	2.12	0.49
1:Z:802:GLU:CG	1:Z:803:ALA:N	2.73	0.49
1:Z:831:LEU:O	1:Z:832:LEU:HD23	2.11	0.49
1:J:729:ILE:HG21	1:J:787:PHE:HE2	1.77	0.49
1:J:926:ASN:OD1	1:Z:921:ASN:HB3	2.13	0.49
1:Z:647:VAL:H	1:Z:650:VAL:HG23	1.78	0.49
1:Z:846:GLU:HB3	1:Z:866:LYS:O	2.11	0.49
1:Z:884:MET:HG3	1:Z:884:MET:O	2.13	0.49
1:J:816:ASP:OD1	1:J:816:ASP:C	2.54	0.49
1:Z:845:LEU:O	1:Z:845:LEU:HG	2.12	0.49
1:F:893:SER:CB	1:Z:900:ASN:OD1	2.58	0.49
1:J:689:ARG:NH2	1:J:706:SER:O	2.46	0.49
1:J:759:VAL:HG13	1:J:763:THR:HG21	1.94	0.49
1:F:689:ARG:NH1	1:F:689:ARG:HB2	2.28	0.49
1:F:876:TYR:HB3	1:J:884:MET:HE1	1.93	0.49
1:F:933:LEU:HD21	1:F:935:ALA:CB	2.43	0.49
1:J:635:TYR:CE1	1:J:711:ILE:HD13	2.48	0.49
1:Z:773:ILE:HD12	1:Z:773:ILE:O	2.13	0.49
1:F:621:VAL:CG2	1:F:705:ALA:HB3	2.43	0.49
1:J:880:ILE:HD13	1:J:895:PHE:CE1	2.47	0.49
1:F:746:PHE:O	1:F:766:LEU:HB2	2.13	0.49
1:J:742:VAL:HG12	1:J:793:ASN:HB3	1.95	0.48
1:J:938:ILE:HG12	1:Z:933:LEU:CB	2.42	0.48
1:J:978:ILE:HG23	1:Z:974:SER:O	2.13	0.48
1:Z:625:THR:HG22	1:Z:640:ARG:O	2.13	0.48
1:F:902:ILE:HG22	1:F:904:PHE:HE1	1.78	0.48
1:F:913:THR:O	1:F:914:PRO:O	2.30	0.48
1:Z:717:PRO:O	1:Z:801:VAL:HG21	2.13	0.48
1:F:759:VAL:O	1:F:763:THR:OG1	2.30	0.48
1:F:842:ALA:HA	1:J:859:TRP:CZ3	2.48	0.48
1:F:978:ILE:CD1	1:J:976:VAL:HG11	2.43	0.48
1:J:938:ILE:HG12	1:Z:933:LEU:HD23	1.94	0.48
1:F:733:PRO:HG3	1:F:744:PHE:CE1	2.48	0.48
1:J:918:ALA:HB2	1:J:923:ILE:HD11	1.95	0.48
1:Z:767:GLY:HA3	1:Z:772:TRP:CH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:816:ASP:OD1	1:Z:816:ASP:N	2.46	0.48
1:F:905:ILE:HG22	1:F:906:ASP:N	2.29	0.48
1:F:926:ASN:HB3	1:J:921:ASN:O	2.14	0.48
1:F:955:LEU:C	1:F:955:LEU:CD2	2.87	0.48
1:J:758:GLN:OE1	1:J:758:GLN:N	2.46	0.48
1:J:932:ARG:HB2	1:Z:927:ASP:CG	2.38	0.48
1:F:777:ILE:HD13	1:F:829:LYS:HG2	1.94	0.48
1:F:936:PRO:O	1:F:951:PRO:HG3	2.14	0.48
1:F:725:GLY:N	1:F:808:SER:HB3	2.28	0.48
1:F:897:VAL:O	1:Z:904:PHE:CA	2.58	0.48
1:J:722:LEU:N	1:J:722:LEU:CD1	2.76	0.48
1:J:724:PRO:HB3	1:J:806:ARG:O	2.14	0.48
1:Z:624:LEU:HD23	1:Z:625:THR:N	2.29	0.48
1:Z:725:GLY:C	1:Z:808:SER:HG	2.18	0.48
1:Z:730:THR:HG23	1:Z:773:ILE:HG22	1.96	0.48
1:F:675:GLU:OE2	1:F:678:TYR:HD1	1.96	0.48
1:F:928:VAL:HG12	1:Z:930:LEU:HD13	1.95	0.48
1:J:867:ILE:HD11	1:Z:882:LEU:CD2	2.42	0.48
1:Z:918:ALA:CB	1:Z:923:ILE:CG1	2.92	0.48
1:F:821:LYS:HE3	1:Z:901:ARG:HH22	1.78	0.47
1:F:914:PRO:CB	1:J:815:LEU:CD2	2.90	0.47
1:F:930:LEU:O	1:Z:811:ALA:CB	2.61	0.47
1:J:937:THR:O	1:J:938:ILE:HG13	2.14	0.47
1:F:884:MET:CE	1:Z:867:ILE:CG1	2.92	0.47
1:Z:711:ILE:C	1:Z:711:ILE:CD1	2.87	0.47
1:Z:753:ILE:HG13	1:Z:788:TYR:CE2	2.49	0.47
1:F:882:LEU:HD23	1:Z:865:VAL:CG1	2.45	0.47
1:F:884:MET:HA	1:F:892:LEU:O	2.14	0.47
1:J:959:ASN:HB2	1:Z:954:LYS:HA	1.96	0.47
1:F:902:ILE:HD12	1:J:895:PHE:CA	2.43	0.47
1:F:946:ALA:O	1:J:953:GLY:CA	2.60	0.47
1:Z:717:PRO:HG3	1:Z:789:ILE:HG22	1.96	0.47
1:F:980:GLU:HA	1:Z:986:GLY:HA3	1.96	0.47
1:F:987:THR:OG1	1:F:989:ARG:NH2	2.47	0.47
1:F:619:PRO:HB2	1:F:644:PRO:HG2	1.96	0.47
1:Z:683:LEU:CD2	1:Z:688:TYR:CZ	2.97	0.47
1:Z:919:GLN:NE2	1:Z:922:GLN:HB2	2.29	0.47
1:F:624:LEU:HD11	1:F:707:VAL:HB	1.97	0.47
1:F:746:PHE:CD2	1:F:772:TRP:HB3	2.49	0.47
1:F:756:ILE:HD12	1:F:757:ARG:N	2.30	0.47
1:J:770:LEU:HD23	1:J:770:LEU:HA	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:626:ALA:HB2	1:F:707:VAL:CG1	2.45	0.47
1:F:656:LEU:HD21	1:F:688:TYR:HB3	1.95	0.47
1:F:812:GLU:O	1:F:816:ASP:HB2	2.14	0.47
1:F:827:LEU:CD2	1:F:881:GLY:HA3	2.45	0.47
1:J:635:TYR:OH	1:J:795:VAL:HA	2.13	0.47
1:F:900:ASN:O	1:F:919:GLN:HG3	2.15	0.47
1:F:904:PHE:CD1	1:F:904:PHE:N	2.83	0.47
1:J:721:GLU:C	1:J:722:LEU:HD12	2.40	0.47
1:J:880:ILE:HB	1:J:897:VAL:HA	1.97	0.47
1:J:913:THR:HG23	1:Z:819:LYS:CD	2.43	0.47
1:F:643:THR:CG2	1:F:646:VAL:H	2.27	0.47
1:F:832:LEU:HD22	1:Z:912:GLU:HG3	1.97	0.47
1:F:904:PHE:CD1	1:F:916:PHE:HD2	2.33	0.47
1:J:745:GLU:HG2	1:J:768:THR:HG22	1.97	0.47
1:J:919:GLN:O	1:J:920:GLY:O	2.33	0.47
1:F:619:PRO:CG	1:F:645:LYS:HG2	2.44	0.46
1:F:790:ARG:HD2	1:F:797:LYS:HB3	1.97	0.46
1:F:863:TRP:CD1	1:Z:847:GLU:OE1	2.68	0.46
1:F:927:ASP:OD2	1:F:927:ASP:C	2.59	0.46
1:J:933:LEU:HD12	1:J:934:THR:H	1.79	0.46
1:Z:753:ILE:HD13	1:Z:755:ASP:O	2.15	0.46
1:F:928:VAL:HG11	1:Z:930:LEU:CD1	2.46	0.46
1:Z:725:GLY:HA3	1:Z:728:GLN:CG	2.45	0.46
1:F:869:GLN:HE22	1:F:871:LYS:HB2	1.80	0.46
1:J:861:ALA:O	1:J:883:SER:OG	2.31	0.46
1:F:776:SER:N	1:F:779:ILE:HD12	2.30	0.46
1:J:653:LEU:O	1:J:692:VAL:HA	2.14	0.46
1:Z:849:SER:HB3	1:Z:863:TRP:HD1	1.80	0.46
1:F:888:GLU:HA	1:F:888:GLU:OE1	2.14	0.46
1:J:812:GLU:OE1	1:Z:931:LYS:NZ	2.47	0.46
1:F:858:LYS:NZ	1:Z:841:ASN:OD1	2.45	0.46
1:J:869:GLN:OE1	1:Z:884:MET:HE2	2.16	0.46
1:J:880:ILE:HG22	1:J:898:ALA:N	2.31	0.46
1:Z:735:LEU:HD23	1:Z:736:ALA:N	2.31	0.46
1:Z:892:LEU:C	1:Z:893:SER:O	2.59	0.46
1:F:722:LEU:CD1	1:F:729:ILE:HD11	2.45	0.46
1:F:814:TYR:CE1	1:Z:924:PHE:CZ	3.04	0.46
1:F:928:VAL:CG2	1:J:923:ILE:CG2	2.68	0.46
1:J:665:GLU:CD	1:J:689:ARG:HG3	2.41	0.46
1:J:962:ILE:HG12	1:Z:960:ALA:HB2	1.98	0.46
1:F:847:GLU:OE2	1:J:847:GLU:OE2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:756:ILE:HD11	1:J:802:GLU:OE2	2.16	0.46
1:F:933:LEU:HD11	1:J:930:LEU:HD23	1.98	0.46
1:J:636:GLN:HA	1:J:680:PHE:O	2.15	0.46
1:J:745:GLU:HA	1:J:768:THR:HG22	1.97	0.46
1:F:720:ILE:HD13	1:F:733:PRO:HA	1.99	0.45
1:J:716:ALA:O	1:J:717:PRO:C	2.58	0.45
1:F:733:PRO:O	1:F:734:HIS:ND1	2.48	0.45
1:F:884:MET:HB3	1:F:893:SER:HA	1.97	0.45
1:F:776:SER:OG	1:F:777:ILE:N	2.49	0.45
1:F:902:ILE:CG2	1:F:904:PHE:CE1	2.98	0.45
1:J:918:ALA:CB	1:J:923:ILE:CD1	2.93	0.45
1:F:728:GLN:CB	1:F:775:ALA:HB2	2.46	0.45
1:F:757:ARG:HH11	1:F:758:GLN:HB3	1.80	0.45
1:F:821:LYS:HE3	1:Z:901:ARG:NH2	2.31	0.45
1:F:880:ILE:O	1:F:880:ILE:CG1	2.65	0.45
1:J:905:ILE:HG22	1:Z:898:ALA:HB2	1.97	0.45
1:F:899:ALA:O	1:Z:907:PRO:HD2	2.16	0.45
1:F:932:ARG:CG	1:Z:937:THR:HB	2.46	0.45
1:J:917:VAL:HG21	1:Z:818:PHE:CD2	2.51	0.45
1:Z:624:LEU:C	1:Z:624:LEU:CD2	2.89	0.45
1:Z:785:TYR:O	1:Z:805:GLY:N	2.50	0.45
1:F:901:ARG:NH2	1:J:894:GLN:NE2	2.59	0.45
1:F:750:GLU:H	1:F:750:GLU:CD	2.23	0.45
1:Z:955:LEU:CD1	1:Z:957:ALA:HB2	2.47	0.45
1:J:714:PRO:HB3	1:J:742:VAL:HG11	1.99	0.45
1:J:863:TRP:CZ3	1:J:865:VAL:HG23	2.51	0.45
1:J:880:ILE:HD12	1:J:881:GLY:N	2.32	0.45
1:Z:905:ILE:HG21	1:Z:912:GLU:C	2.42	0.45
1:Z:934:THR:HG22	1:Z:934:THR:O	2.17	0.45
1:F:901:ARG:CD	1:F:919:GLN:OE1	2.64	0.45
1:J:747:TRP:CE3	1:J:765:TYR:HA	2.52	0.45
1:Z:637:VAL:HG13	1:Z:637:VAL:O	2.17	0.45
1:F:924:PHE:CD1	1:Z:929:PHE:HD2	2.35	0.45
1:J:755:ASP:OD2	1:J:757:ARG:NH2	2.50	0.45
1:J:845:LEU:N	1:J:845:LEU:CD1	2.80	0.45
1:Z:691:THR:HG22	1:Z:706:SER:OG	2.16	0.45
1:Z:849:SER:HB3	1:Z:863:TRP:CD1	2.52	0.45
1:F:726:TYR:HE2	1:F:820:GLY:HA3	1.83	0.44
1:F:757:ARG:NH1	1:F:758:GLN:HB3	2.32	0.44
1:J:917:VAL:HB	1:Z:818:PHE:CE2	2.53	0.44
1:F:624:LEU:HD11	1:F:707:VAL:HG23	1.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:934:THR:HG21	1:J:929:PHE:CE2	2.53	0.44
1:J:832:LEU:O	1:J:834:LYS:N	2.49	0.44
1:J:880:ILE:CB	1:J:897:VAL:HA	2.47	0.44
1:J:913:THR:CG2	1:Z:819:LYS:CD	2.95	0.44
1:Z:790:ARG:HB3	1:Z:800:PHE:CD1	2.53	0.44
1:Z:802:GLU:HG2	1:Z:803:ALA:N	2.31	0.44
1:J:746:PHE:CD2	1:J:772:TRP:CD1	3.05	0.44
1:Z:939:THR:HG22	1:Z:941:GLY:H	1.82	0.44
1:F:905:ILE:HD13	1:F:914:PRO:CA	2.45	0.44
1:F:954:LYS:HD2	1:Z:959:ASN:O	2.17	0.44
1:J:720:ILE:HB	1:J:789:ILE:CD1	2.48	0.44
1:F:706:SER:OG	1:J:768:THR:OG1	2.17	0.44
1:J:884:MET:HE2	1:J:891:LYS:HB2	1.99	0.44
1:Z:720:ILE:O	1:Z:720:ILE:HG13	2.17	0.44
1:F:990:ALA:HB2	1:J:984:ILE:HD12	2.00	0.44
1:J:621:VAL:HG13	1:J:641:TRP:HB2	2.00	0.44
1:F:636:GLN:HG3	1:F:681:THR:HA	1.98	0.44
1:F:656:LEU:HD22	1:F:657:THR:N	2.33	0.44
1:J:916:PHE:C	1:J:916:PHE:HD1	2.23	0.44
1:Z:790:ARG:HD2	1:Z:797:LYS:HB3	2.00	0.44
1:Z:904:PHE:O	1:Z:914:PRO:CA	2.65	0.44
1:F:819:LYS:HG3	1:Z:913:THR:HA	1.99	0.43
1:F:893:SER:HG	1:Z:899:ALA:CA	2.30	0.43
1:J:958:LYS:O	1:J:959:ASN:OD1	2.36	0.43
1:J:966:VAL:O	1:J:966:VAL:HG12	2.18	0.43
1:F:877:VAL:HG22	1:F:878:ALA:N	2.33	0.43
1:F:880:ILE:HG22	1:F:897:VAL:HG13	1.99	0.43
1:F:884:MET:HE3	1:Z:867:ILE:HG13	1.97	0.43
1:J:844:ARG:O	1:J:844:ARG:HG3	2.18	0.43
1:Z:632:SER:O	1:Z:632:SER:OG	2.27	0.43
1:F:733:PRO:HG3	1:F:744:PHE:CD1	2.53	0.43
1:F:679:ARG:HD2	1:F:680:PHE:C	2.43	0.43
1:F:827:LEU:HD22	1:F:881:GLY:HA3	2.00	0.43
1:J:739:ASP:OD1	1:J:740:PRO:HD2	2.19	0.43
1:J:867:ILE:HD13	1:Z:882:LEU:CD2	2.48	0.43
1:J:925:MET:CE	1:Z:925:MET:CE	2.87	0.43
1:J:970:SER:HB3	1:Z:965:SER:HA	2.00	0.43
1:J:962:ILE:HG22	1:Z:958:LYS:C	2.41	0.43
1:Z:638:LEU:HD11	1:Z:679:ARG:NH2	2.32	0.43
1:F:893:SER:OG	1:Z:878:ALA:CB	2.66	0.43
1:J:918:ALA:HB2	1:J:923:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:962:ILE:HG21	1:Z:960:ALA:HB2	2.00	0.43
1:Z:746:PHE:CD2	1:Z:789:ILE:HG13	2.54	0.43
1:F:899:ALA:N	1:Z:905:ILE:O	2.40	0.43
1:J:737:VAL:HG13	1:J:737:VAL:O	2.19	0.43
1:F:845:LEU:HA	1:F:867:ILE:HD13	2.01	0.43
1:F:917:VAL:HG11	1:J:818:PHE:CG	2.53	0.43
1:J:750:GLU:N	1:J:750:GLU:OE1	2.52	0.43
1:J:822:ILE:HG23	1:J:896:LEU:HD11	2.01	0.43
1:J:932:ARG:HG3	1:J:932:ARG:HH11	1.84	0.43
1:Z:933:LEU:HD12	1:Z:934:THR:N	2.31	0.43
1:F:901:ARG:HG2	1:F:919:GLN:CB	2.37	0.43
1:F:914:PRO:HG3	1:J:822:ILE:HD12	2.01	0.43
1:Z:928:VAL:HG22	1:Z:930:LEU:HD23	2.01	0.43
1:F:902:ILE:HD12	1:J:895:PHE:H	1.80	0.43
1:F:950:THR:OG1	1:F:952:ASP:OD1	2.28	0.43
1:J:739:ASP:OD2	1:J:742:VAL:HG13	2.18	0.43
1:J:943:ASN:HB2	1:J:944:PRO:HD3	2.01	0.43
1:F:904:PHE:O	1:F:914:PRO:HA	2.18	0.42
1:F:946:ALA:CB	1:J:951:PRO:O	2.67	0.42
1:Z:831:LEU:HA	1:Z:866:LYS:HD3	2.01	0.42
1:F:884:MET:HE2	1:F:893:SER:HB2	2.01	0.42
1:F:976:VAL:HG12	1:F:977:THR:N	2.34	0.42
1:J:962:ILE:HD12	1:J:962:ILE:H	1.83	0.42
1:Z:837:LEU:CG	1:Z:842:ALA:HB3	2.49	0.42
1:F:745:GLU:OE2	1:F:790:ARG:NH2	2.45	0.42
1:F:830:GLU:O	1:F:866:LYS:HE2	2.20	0.42
1:F:845:LEU:CD1	1:J:849:SER:HB2	2.49	0.42
1:J:722:LEU:HD23	1:J:729:ILE:CG2	2.49	0.42
1:Z:836:GLU:HB2	1:Z:844:ARG:CZ	2.49	0.42
1:J:744:PHE:O	1:J:768:THR:CA	2.62	0.42
1:Z:896:LEU:C	1:Z:896:LEU:HD12	2.44	0.42
1:Z:945:PRO:HB3	1:Z:948:SER:HG	1.85	0.42
1:Z:945:PRO:HB3	1:Z:948:SER:OG	2.19	0.42
1:F:683:LEU:HD12	1:F:683:LEU:HA	1.90	0.42
1:F:832:LEU:CD2	1:Z:912:GLU:HG3	2.49	0.42
1:F:882:LEU:HD21	1:Z:878:ALA:O	2.19	0.42
1:F:884:MET:SD	1:Z:869:GLN:OE1	2.78	0.42
1:F:895:PHE:CE1	1:Z:880:ILE:HG12	2.54	0.42
1:F:924:PHE:CE1	1:Z:929:PHE:HD2	2.36	0.42
1:F:925:MET:CE	1:J:923:ILE:CG2	2.92	0.42
1:F:938:ILE:HG22	1:F:939:THR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:903:ALA:HB2	1:J:917:VAL:HG13	2.00	0.42
1:F:621:VAL:HG23	1:F:705:ALA:HB3	2.01	0.42
1:F:809:ASP:O	1:F:810:ASP:OD1	2.36	0.42
1:J:910:GLY:O	1:J:912:GLU:OE1	2.38	0.42
1:J:913:THR:HG22	1:Z:819:LYS:HD3	2.02	0.42
1:Z:722:LEU:HD21	1:Z:731:ALA:HB2	2.01	0.42
1:J:962:ILE:HG12	1:Z:960:ALA:CB	2.49	0.42
1:F:842:ALA:HA	1:J:859:TRP:CE3	2.55	0.42
1:F:903:ALA:CB	1:F:917:VAL:HG23	2.49	0.42
1:F:913:THR:CA	1:J:819:LYS:HD3	2.49	0.42
1:F:914:PRO:HG2	1:J:815:LEU:HD23	2.01	0.42
1:F:983:THR:C	1:F:984:ILE:HD12	2.44	0.42
1:J:727:PHE:HE1	1:J:780:LYS:HA	1.84	0.42
1:J:913:THR:HA	1:Z:819:LYS:HB2	2.01	0.42
1:Z:615:GLY:HA2	1:Z:698:TRP:CZ3	2.54	0.42
1:Z:746:PHE:CD1	1:Z:746:PHE:N	2.88	0.42
1:Z:771:TYR:N	1:Z:771:TYR:CD1	2.88	0.42
1:F:946:ALA:HB1	1:J:951:PRO:O	2.20	0.42
1:J:691:THR:HG23	1:J:706:SER:HB3	2.02	0.42
1:J:915:MET:O	1:Z:923:ILE:HD11	2.20	0.42
1:Z:695:VAL:HG12	1:Z:701:GLN:HG3	2.01	0.42
1:Z:826:HIS:CE1	1:Z:852:TRP:CZ2	3.08	0.42
1:F:902:ILE:O	1:F:903:ALA:HB2	2.20	0.41
1:F:967:ASN:OD1	1:F:967:ASN:C	2.63	0.41
1:J:680:PHE:CE1	1:J:690:LEU:HD11	2.55	0.41
1:J:720:ILE:HD13	1:J:789:ILE:HG21	2.02	0.41
1:Z:683:LEU:HD22	1:Z:688:TYR:CE2	2.55	0.41
1:Z:832:LEU:HD23	1:Z:832:LEU:N	2.35	0.41
1:F:722:LEU:HD12	1:F:729:ILE:HD11	2.02	0.41
1:F:895:PHE:CE1	1:Z:880:ILE:CG1	3.03	0.41
1:J:980:GLU:CD	1:J:981:ASN:H	2.29	0.41
1:Z:928:VAL:CG2	1:Z:930:LEU:HD23	2.50	0.41
1:F:930:LEU:O	1:Z:811:ALA:HB2	2.21	0.41
1:J:972:THR:O	1:J:972:THR:CG2	2.54	0.41
1:Z:916:PHE:HA	1:Z:924:PHE:O	2.19	0.41
1:F:683:LEU:HD11	1:F:688:TYR:CE2	2.55	0.41
1:J:843:SER:HA	1:J:868:GLU:O	2.21	0.41
1:F:832:LEU:HD13	1:Z:912:GLU:CD	2.46	0.41
1:F:882:LEU:HD12	1:F:894:GLN:O	2.20	0.41
1:Z:962:ILE:HG22	1:Z:964:GLY:O	2.20	0.41
1:F:871:LYS:O	1:F:874:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:989:ARG:HB2	1:J:983:THR:HA	2.02	0.41
1:J:634:GLU:OE1	1:J:634:GLU:HA	2.20	0.41
1:J:928:VAL:HG23	1:J:930:LEU:HD22	2.01	0.41
1:F:827:LEU:HD23	1:F:862:MET:CE	2.47	0.41
1:J:696:ASN:HD21	1:J:700:GLN:HB3	1.86	0.41
1:J:766:LEU:HA	1:J:766:LEU:HD23	1.85	0.41
1:J:916:PHE:HD1	1:J:916:PHE:O	2.03	0.41
1:Z:719:ARG:NH2	1:Z:734:HIS:ND1	2.68	0.41
1:F:966:VAL:HG23	1:Z:968:ALA:HB1	2.02	0.41
1:J:729:ILE:O	1:J:773:ILE:HG23	2.21	0.41
1:J:742:VAL:HG23	1:J:742:VAL:O	2.20	0.41
1:J:902:ILE:HG13	1:J:918:ALA:HB3	2.02	0.41
1:J:922:GLN:HG3	1:Z:780:LYS:HE2	2.02	0.41
1:J:962:ILE:CG2	1:Z:958:LYS:C	2.93	0.41
1:F:832:LEU:HD13	1:Z:912:GLU:OE1	2.21	0.41
1:F:891:LYS:O	1:Z:876:TYR:HE2	2.01	0.41
1:F:900:ASN:ND2	1:J:893:SER:OG	2.54	0.41
1:F:993:ILE:CD1	1:J:988:LEU:HD22	2.51	0.41
1:J:657:THR:HG22	1:J:667:LEU:HD12	2.02	0.41
1:J:747:TRP:CH2	1:J:765:TYR:CG	3.09	0.41
1:F:626:ALA:HB2	1:F:707:VAL:HG12	2.02	0.41
1:F:641:TRP:CH2	1:F:678:TYR:HB2	2.55	0.41
1:F:993:ILE:HD13	1:J:988:LEU:HD22	2.03	0.41
1:J:747:TRP:HB2	1:J:788:TYR:HB2	2.02	0.41
1:Z:655:ARG:HA	1:Z:670:THR:HA	2.02	0.41
1:Z:905:ILE:HG12	1:Z:914:PRO:CA	2.40	0.41
1:J:746:PHE:CD2	1:J:772:TRP:HD1	2.40	0.40
1:J:817:PHE:CD2	1:J:818:PHE:N	2.89	0.40
1:J:863:TRP:HH2	1:J:865:VAL:CG2	2.33	0.40
1:Z:793:ASN:OD1	1:Z:795:VAL:HG22	2.21	0.40
1:Z:815:LEU:HD13	1:Z:815:LEU:HA	1.65	0.40
1:F:914:PRO:CG	1:J:815:LEU:CD2	2.99	0.40
1:F:721:GLU:HB2	1:F:732:THR:OG1	2.21	0.40
1:F:814:TYR:HD1	1:F:814:TYR:O	2.04	0.40
1:F:905:ILE:HB	1:J:898:ALA:HB2	2.02	0.40
1:F:912:GLU:O	1:J:819:LYS:HG3	2.20	0.40
1:J:756:ILE:O	1:J:759:VAL:HG23	2.21	0.40
1:J:788:TYR:HA	1:J:801:VAL:O	2.21	0.40
1:Z:860:ASN:OD1	1:Z:886:ASP:N	2.54	0.40
1:Z:884:MET:HE3	1:Z:884:MET:HB2	1.89	0.40
1:Z:903:ALA:HB1	1:Z:914:PRO:CB	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:882:LEU:HD11	1:Z:878:ALA:CB	2.51	0.40
1:F:932:ARG:CD	1:Z:937:THR:HG21	2.52	0.40
1:J:672:ARG:NH1	1:J:672:ARG:O	2.54	0.40
1:F:882:LEU:CD2	1:Z:865:VAL:HG12	2.51	0.40
1:Z:833:GLU:O	1:Z:833:GLU:HG2	2.22	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	F	378/1132 (33%)	311 (82%)	50 (13%)	17 (4%)	2	18
1	J	378/1132 (33%)	317 (84%)	53 (14%)	8 (2%)	5	33
1	Z	381/1132 (34%)	311 (82%)	57 (15%)	13 (3%)	3	25
All	All	1137/3396 (34%)	939 (83%)	160 (14%)	38 (3%)	5	25

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	713	ALA
1	J	920	GLY
1	Z	651	SER
1	Z	893	SER
1	Z	934	THR
1	F	926	ASN
1	F	932	ARG
1	F	946	ALA
1	F	959	ASN
1	J	781	PRO
1	Z	809	ASP
1	Z	967	ASN

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Mol	Chain	Res	Type
1	Z	969	ASN
1	F	646	VAL
1	F	812	GLU
1	F	948	SER
1	J	962	ILE
1	Z	648	LYS
1	Z	894	GLN
1	Z	944	PRO
1	F	769	ALA
1	F	809	ASP
1	F	862	MET
1	F	991	GLU
1	J	838	THR
1	J	921	ASN
1	Z	650	VAL
1	F	714	PRO
1	F	944	PRO
1	J	723	THR
1	F	712	ALA
1	J	833	GLU
1	Z	943	ASN
1	F	813	GLY
1	F	914	PRO
1	Z	644	PRO
1	Z	945	PRO
1	J	984	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	F	312/958 (33%)	268 (86%)	44 (14%)	3	17
1	J	312/958 (33%)	268 (86%)	44 (14%)	3	17
1	Z	314/958 (33%)	267 (85%)	47 (15%)	2	15
All	All	938/2874 (33%)	803 (86%)	135 (14%)	5	16

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	617	THR
1	F	623	HIS
1	F	624	LEU
1	F	656	LEU
1	F	679	ARG
1	F	687	ASN
1	F	723	THR
1	F	732	THR
1	F	770	LEU
1	F	789	ILE
1	F	797	LYS
1	F	815	LEU
1	F	821	LYS
1	F	836	GLU
1	F	837	LEU
1	F	838	THR
1	F	839	GLU
1	F	844	ARG
1	F	847	GLU
1	F	849	SER
1	F	865	VAL
1	F	882	LEU
1	F	892	LEU
1	F	893	SER
1	F	897	VAL
1	F	900	ASN
1	F	902	ILE
1	F	913	THR
1	F	915	MET
1	F	917	VAL
1	F	921	ASN
1	F	923	ILE
1	F	927	ASP
1	F	937	THR
1	F	943	ASN
1	F	954	LYS
1	F	955	LEU
1	F	962	ILE
1	F	970	SER
1	F	972	THR
1	F	982	CYS
1	F	985	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	987	THR
1	F	993	ILE
1	J	628	VAL
1	J	634	GLU
1	J	654	LEU
1	J	672	ARG
1	J	677	THR
1	J	683	LEU
1	J	685	LEU
1	J	687	ASN
1	J	720	ILE
1	J	721	GLU
1	J	748	PHE
1	J	762	SER
1	J	772	TRP
1	J	773	ILE
1	J	780	LYS
1	J	784	ASP
1	J	815	LEU
1	J	819	LYS
1	J	822	ILE
1	J	839	GLU
1	J	844	ARG
1	J	845	LEU
1	J	874	LYS
1	J	880	ILE
1	J	882	LEU
1	J	894	GLN
1	J	896	LEU
1	J	902	ILE
1	J	905	ILE
1	J	913	THR
1	J	917	VAL
1	J	921	ASN
1	J	923	ILE
1	J	925	MET
1	J	928	VAL
1	J	940	SER
1	J	949	LEU
1	J	950	THR
1	J	955	LEU
1	J	961	ASP

*Continued on next page...*

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Mol	Chain	Res	Type
1	J	962	ILE
1	J	973	LEU
1	J	983	THR
1	J	994	VAL
1	Z	621	VAL
1	Z	627	GLU
1	Z	632	SER
1	Z	635	TYR
1	Z	645	LYS
1	Z	646	VAL
1	Z	656	LEU
1	Z	661	ASP
1	Z	682	GLN
1	Z	695	VAL
1	Z	703	ASP
1	Z	711	ILE
1	Z	771	TYR
1	Z	777	ILE
1	Z	780	LYS
1	Z	791	SER
1	Z	792	VAL
1	Z	804	VAL
1	Z	812	GLU
1	Z	815	LEU
1	Z	822	ILE
1	Z	832	LEU
1	Z	837	LEU
1	Z	839	GLU
1	Z	844	ARG
1	Z	845	LEU
1	Z	851	GLU
1	Z	867	ILE
1	Z	877	VAL
1	Z	880	ILE
1	Z	897	VAL
1	Z	902	ILE
1	Z	904	PHE
1	Z	916	PHE
1	Z	921	ASN
1	Z	929	PHE
1	Z	931	LYS
1	Z	933	LEU

*Continued on next page...*

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Mol	Chain	Res	Type
1	Z	939	THR
1	Z	945	PRO
1	Z	948	SER
1	Z	958	LYS
1	Z	961	ASP
1	Z	972	THR
1	Z	976	VAL
1	Z	982	CYS
1	Z	994	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	700	GLN
1	F	728	GLN
1	F	860	ASN
1	F	921	ASN
1	F	926	ASN
1	F	943	ASN
1	F	981	ASN
1	J	981	ASN
1	Z	700	GLN
1	Z	909	ASN
1	Z	919	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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

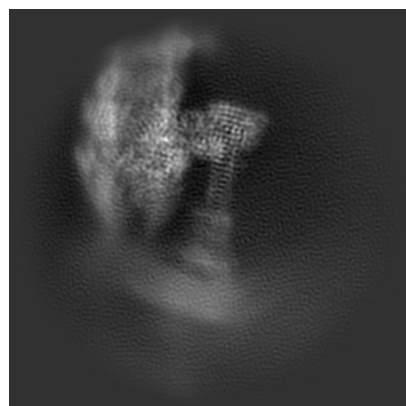
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38244. These allow visual inspection of the internal detail of the map and identification of artifacts.

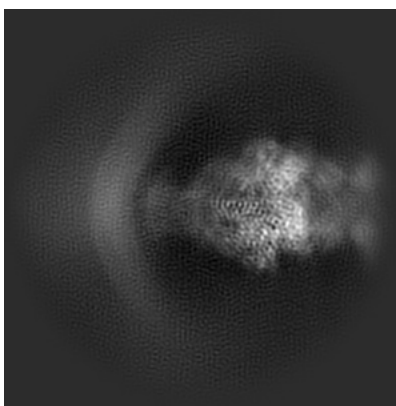
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

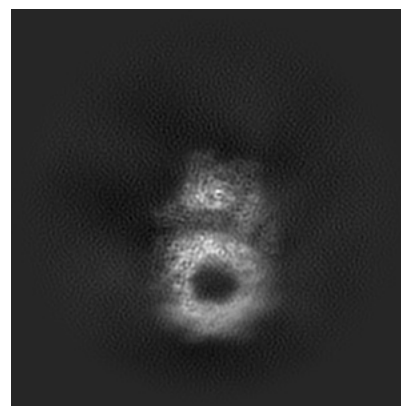
#### 6.1.1 Primary map



X

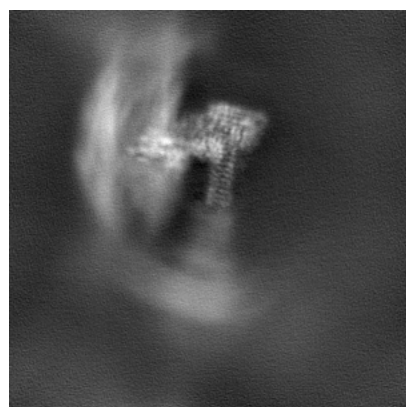


Y

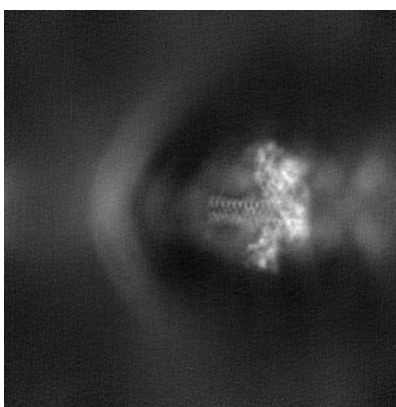


Z

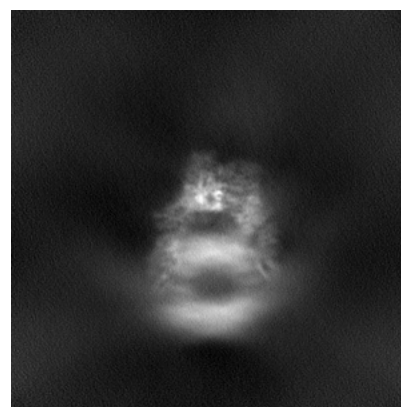
#### 6.1.2 Raw map



X



Y

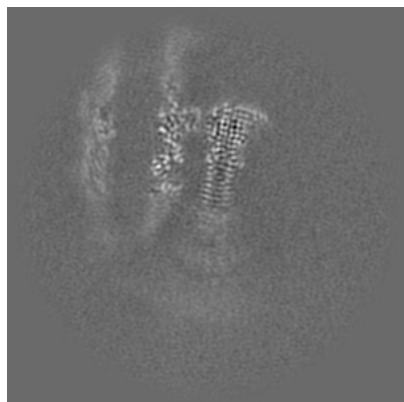


Z

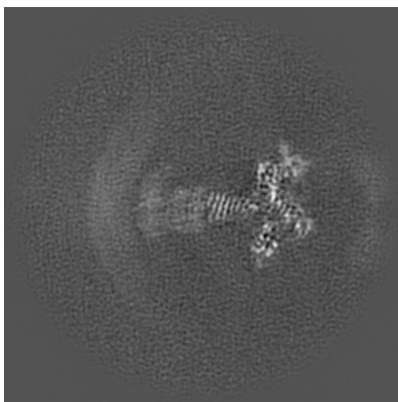
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

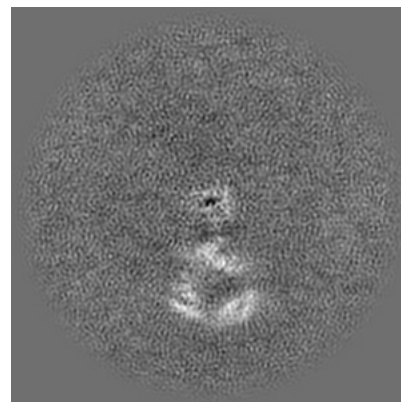
### 6.2.1 Primary map



X Index: 160

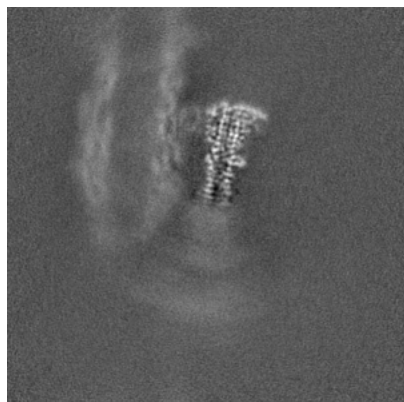


Y Index: 160

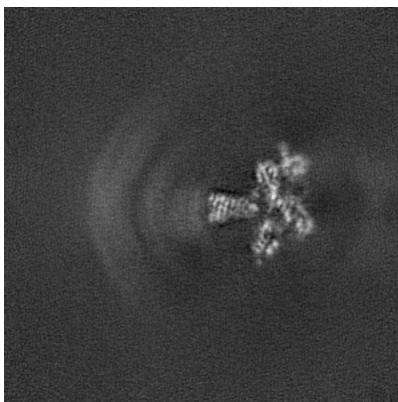


Z Index: 160

### 6.2.2 Raw map



X Index: 160



Y Index: 160



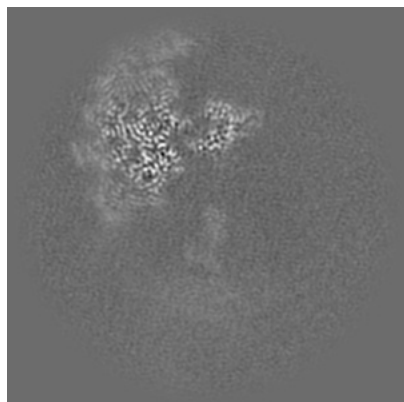
Z Index: 160

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

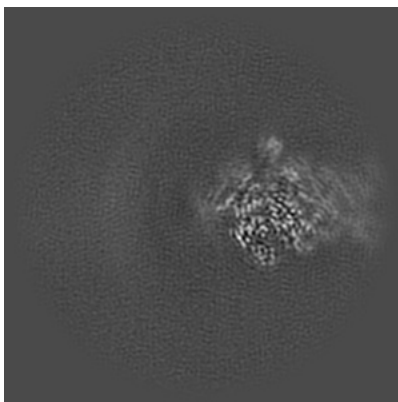


## 6.3 Largest variance slices [i](#)

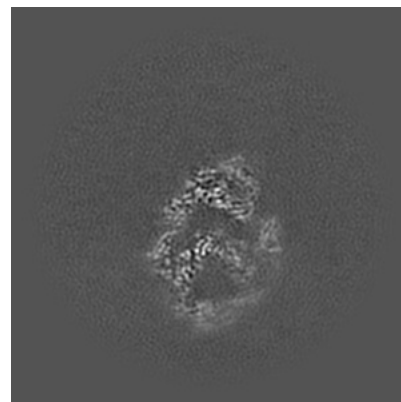
### 6.3.1 Primary map



X Index: 141

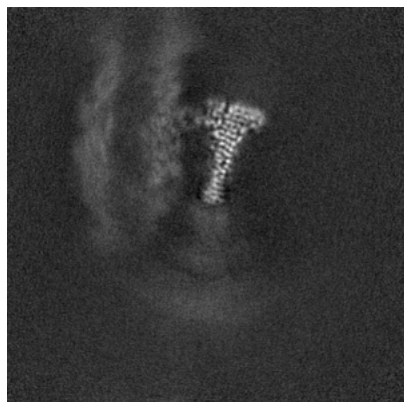


Y Index: 126

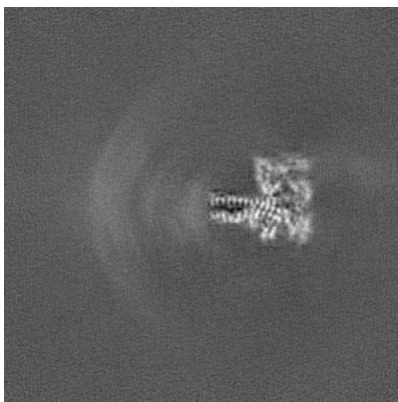


Z Index: 215

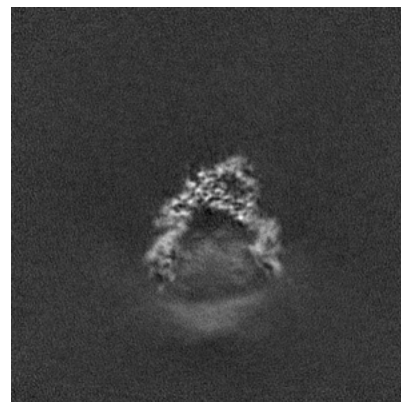
### 6.3.2 Raw map



X Index: 151



Y Index: 168

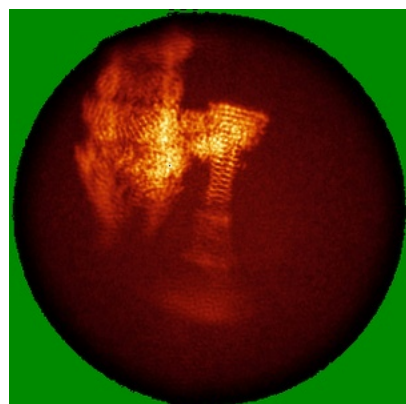


Z Index: 214

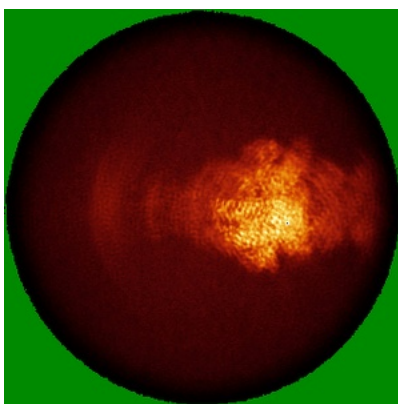
The images above show the largest variance slices of the map in three orthogonal directions.

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

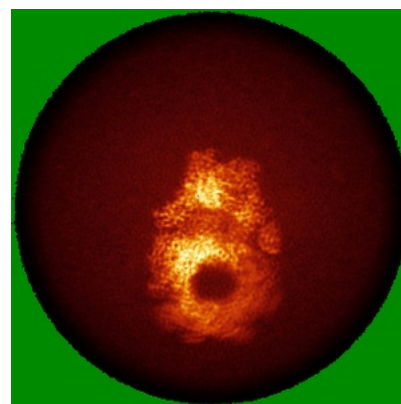
### 6.4.1 Primary map



X

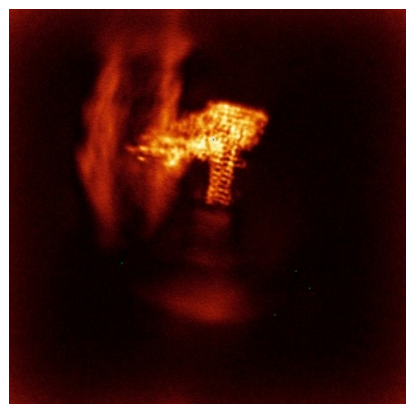


Y

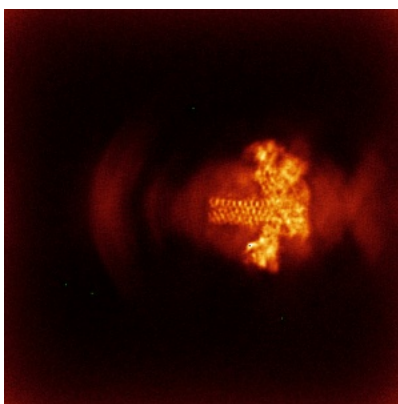


Z

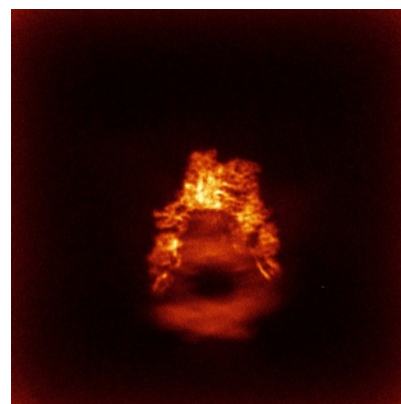
### 6.4.2 Raw map



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.

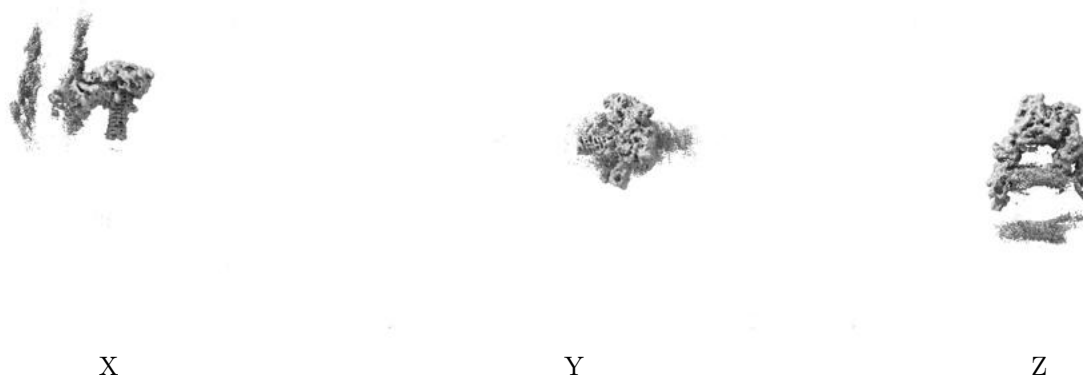
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

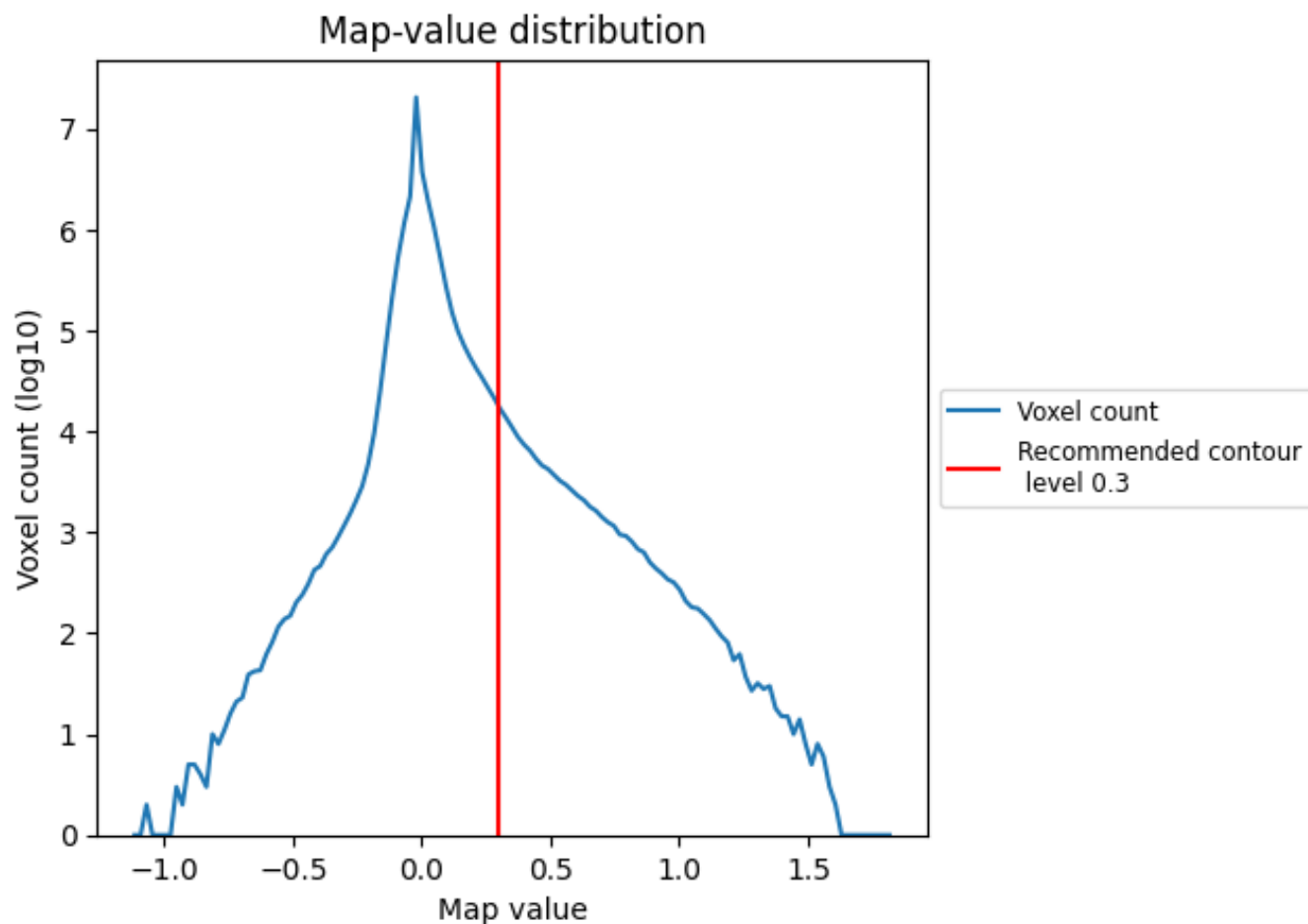
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

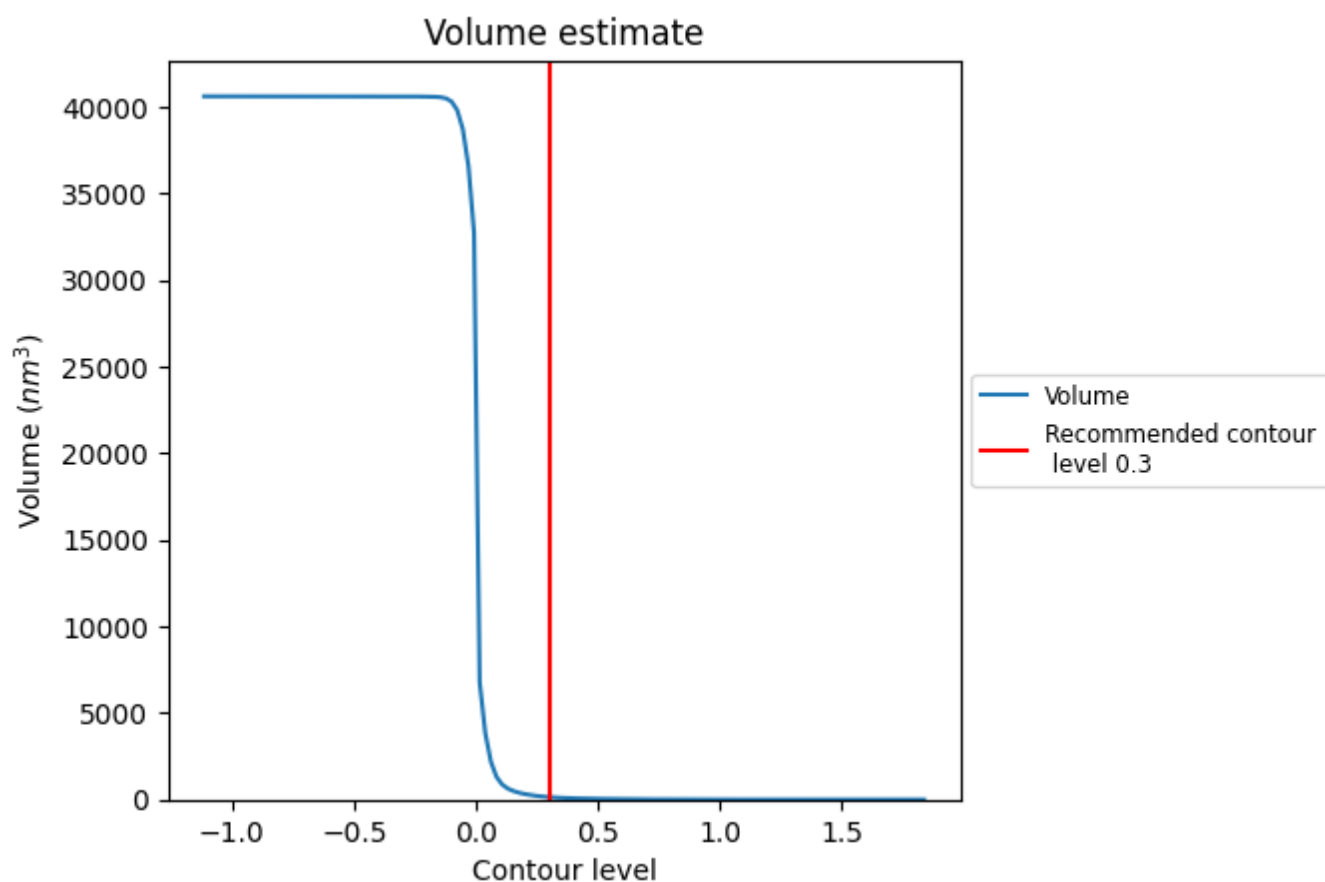
This section contains the results of statistical analysis of the map.

### 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.

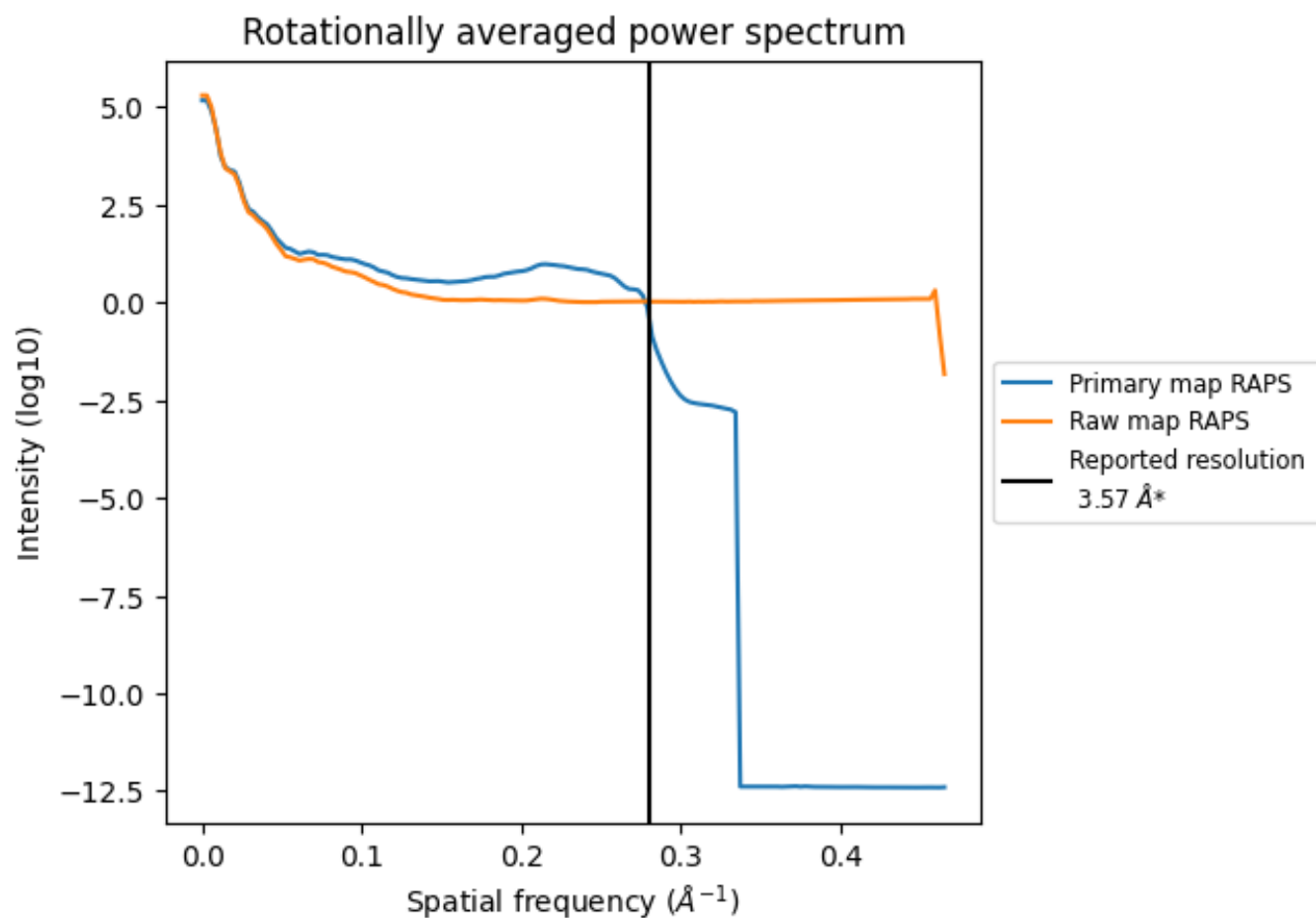
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm<sup>3</sup>; this corresponds to an approximate mass of 128 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 ⓘ

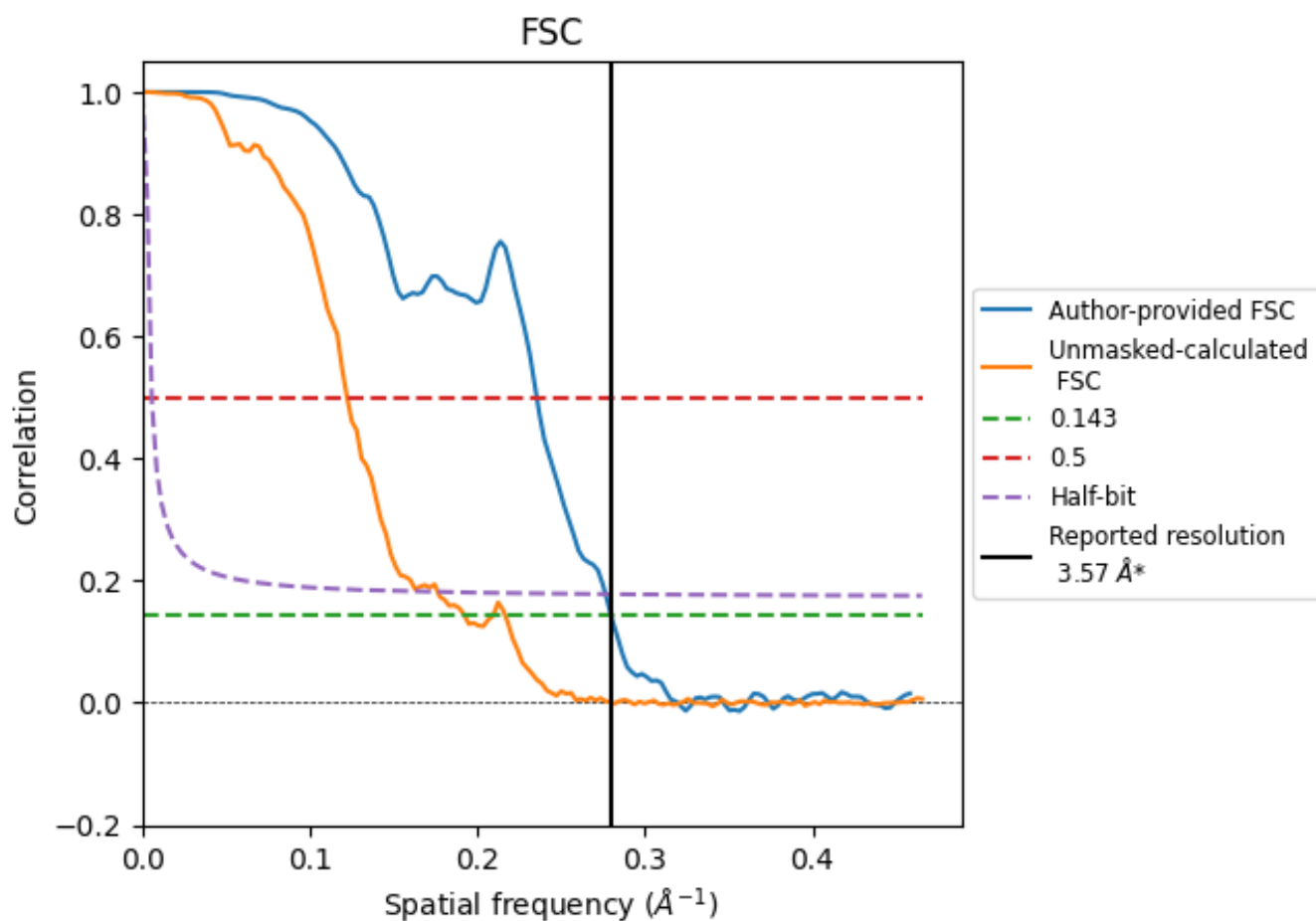


\*Reported resolution corresponds to spatial frequency of 0.280  $\text{\AA}^{-1}$

## 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 0.280  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	4.25	3.62
Unmasked-calculated*	5.20	8.18	5.67

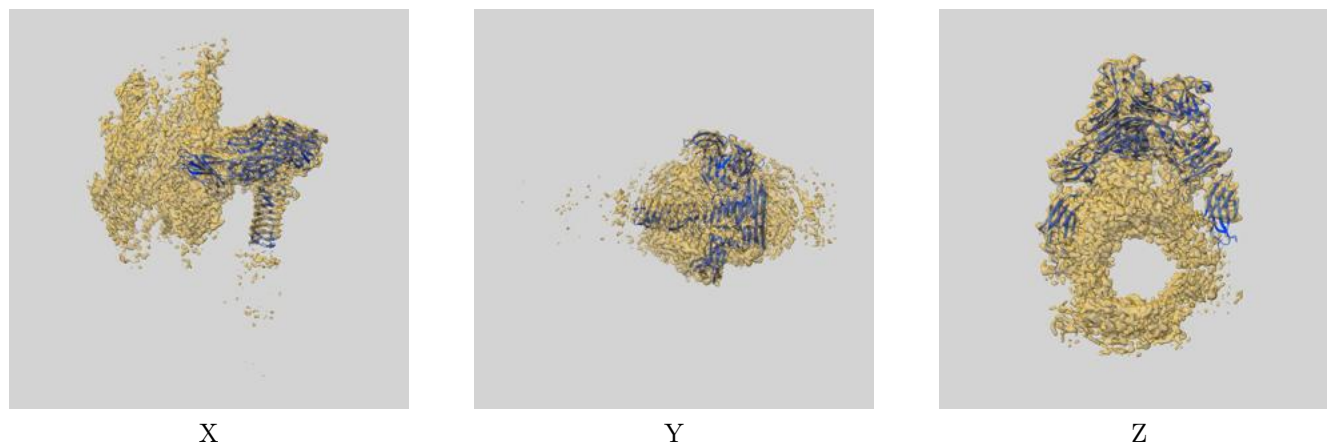
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.20 differs from the reported value 3.57 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38244 and PDB model 8XCI. 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 0.3 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](#)



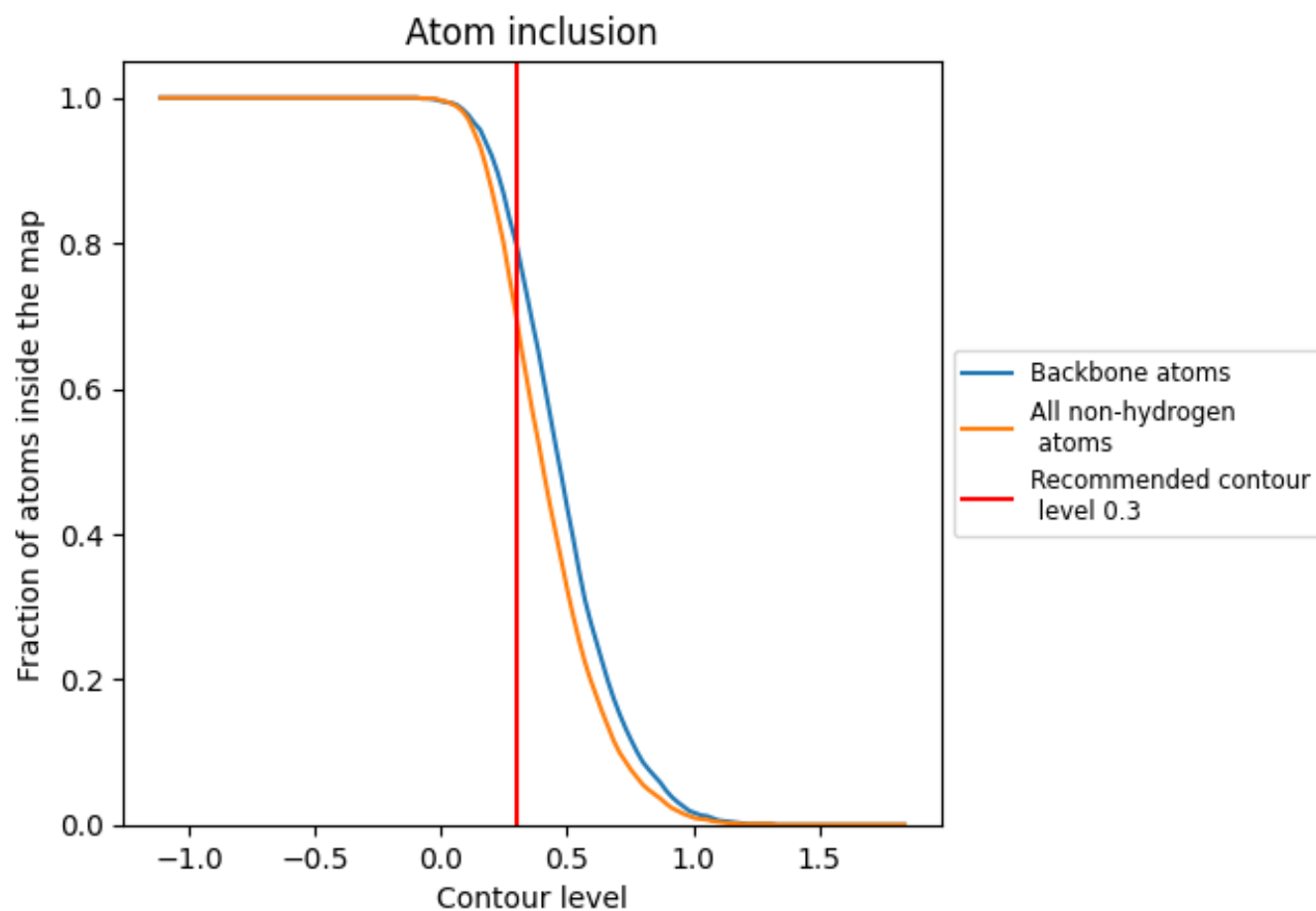
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 70% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6950	<div></div> 0.4240
F	<div></div> 0.6530	<div></div> 0.4030
J	<div></div> 0.6650	<div></div> 0.4090
Z	<div></div> 0.7680	<div></div> 0.4610

