



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:51 PM UTC

PDB ID : 5FJ5 / pdb_00005fj5
EMDB ID : EMD-3185
Title : Structure of the in vitro assembled bacteriophage phi6 polymerase complex
Authors : Ilca, S.; Kotecha, A.; Sun, X.; Poranen, M.P.; Stuart, D.I.; Huiskonen, J.T.
Deposited on : 2015-10-06
Resolution : 4.80 Å(reported)
Based on initial model : 4K7H

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

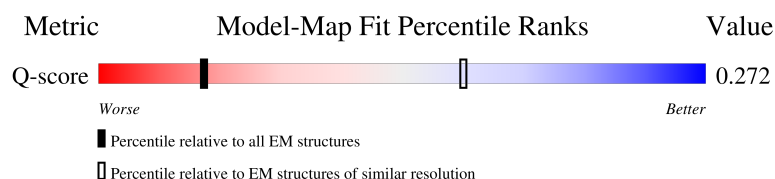
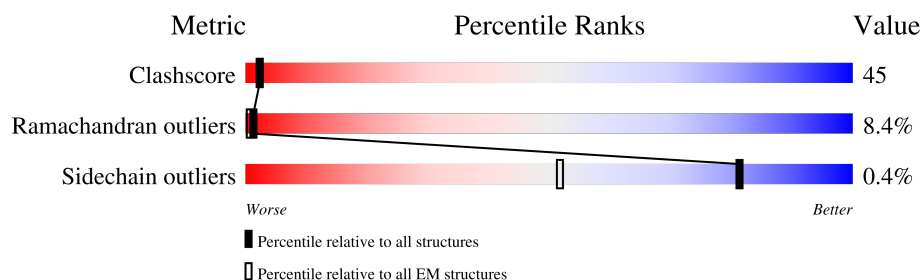
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	1575 (4.30 - 5.30)

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	761	30% 31% 57% 10% .
1	B	761	51% 34% 59% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11840 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 MAJOR INNER PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		
1	B	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		

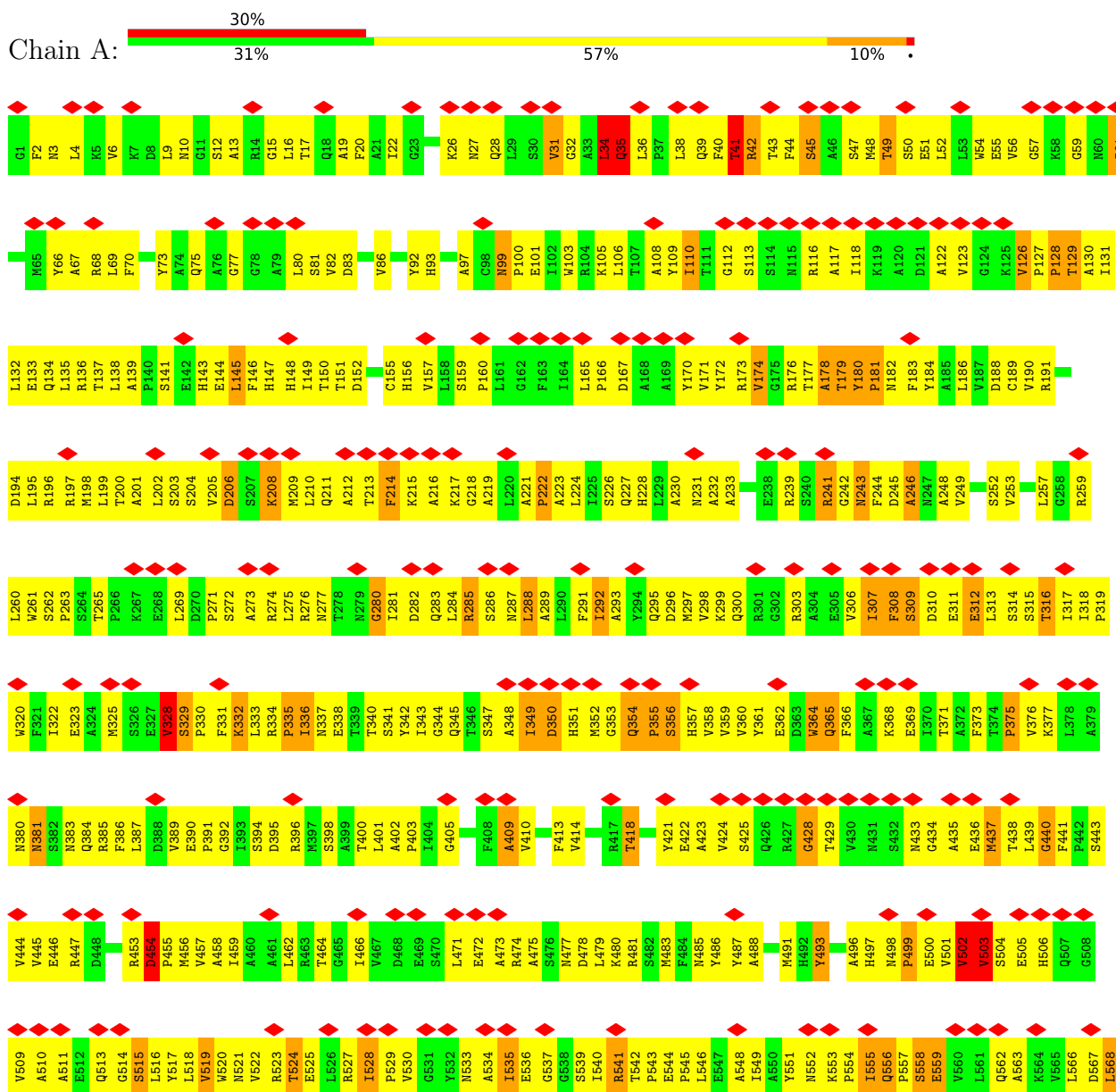
There are 2 discrepancies between the modelled and reference sequences:

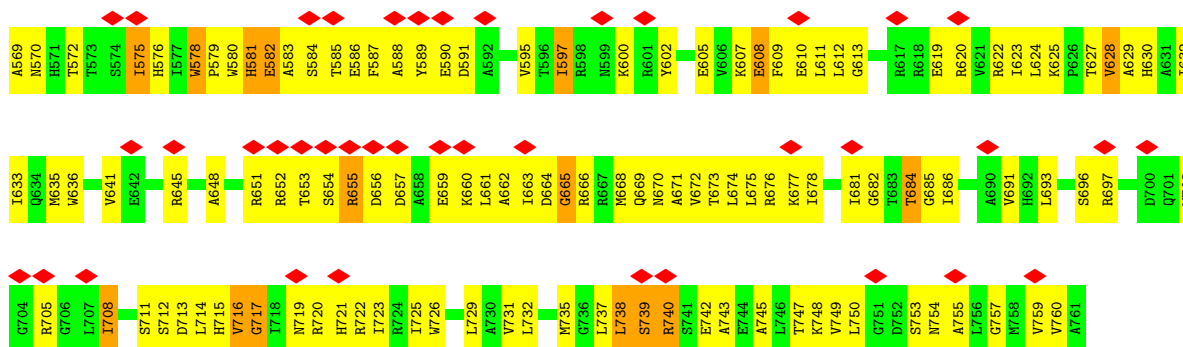
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P11126
B	1	GLY	-	expression tag	UNP P11126

3 Residue-property plots

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

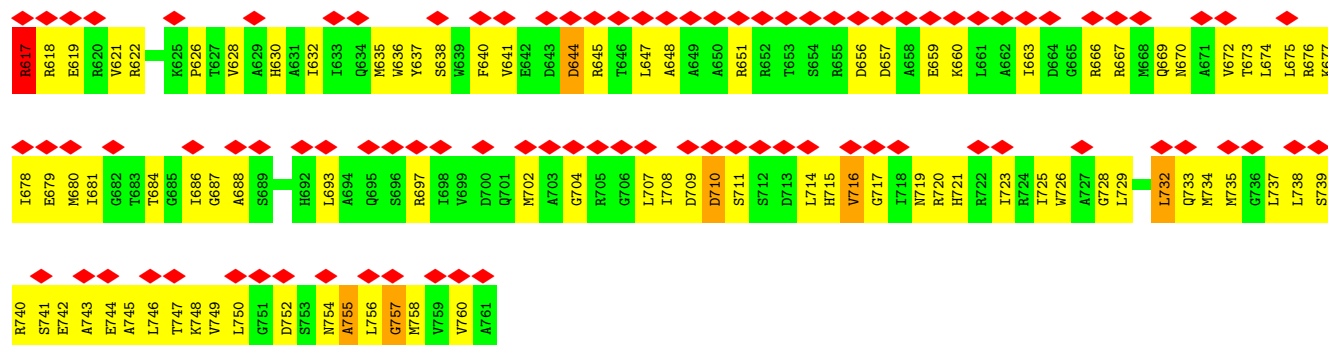
• Molecule 1: MAJOR INNER PROTEIN P1





• Molecule 1: MAJOR INNER PROTEIN P1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	4379	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.049	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	648.0, 648.0, 648.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	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	0.59	0/6040	1.12	44/8206 (0.5%)
1	B	0.53	0/6040	1.11	46/8206 (0.6%)
All	All	0.56	0/12080	1.11	90/16412 (0.5%)

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	5
1	B	0	3
All	All	0	8

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	165	LEU	CA-C-N	18.62	138.94	119.76
1	B	165	LEU	C-N-CA	18.62	138.94	119.76
1	B	126	VAL	CA-C-N	-11.68	108.35	120.38
1	B	126	VAL	C-N-CA	-11.68	108.35	120.38
1	A	179	THR	N-CA-C	10.16	122.36	111.28
1	A	128	PRO	N-CA-C	9.12	125.97	113.65
1	A	128	PRO	CA-C-N	8.46	136.93	121.70
1	A	128	PRO	C-N-CA	8.46	136.93	121.70
1	B	94	GLN	N-CA-C	-8.46	102.94	113.18
1	A	35	GLN	N-CA-C	8.11	120.95	108.30
1	A	502	VAL	CA-C-N	8.05	136.19	121.70
1	A	502	VAL	C-N-CA	8.05	136.19	121.70
1	A	708	ILE	N-CA-C	-7.83	104.93	112.29
1	A	364	TRP	N-CA-C	7.82	120.61	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	PRO	CA-C-O	-7.71	107.83	119.55
1	A	126	VAL	CA-C-N	7.56	128.17	120.38
1	A	126	VAL	C-N-CA	7.56	128.17	120.38
1	B	556	GLN	CA-C-N	7.29	127.21	119.85
1	B	556	GLN	C-N-CA	7.29	127.21	119.85
1	B	32	GLY	N-CA-C	7.24	122.63	114.67
1	A	354	GLN	CA-C-N	-7.17	110.87	119.84
1	A	354	GLN	C-N-CA	-7.17	110.87	119.84
1	A	454	ASP	CA-C-N	7.00	126.97	119.28
1	A	454	ASP	C-N-CA	7.00	126.97	119.28
1	A	265	THR	CA-C-N	6.92	126.90	119.28
1	A	265	THR	C-N-CA	6.92	126.90	119.28
1	B	334	ARG	CA-C-N	6.92	128.49	119.84
1	B	334	ARG	C-N-CA	6.92	128.49	119.84
1	B	735	MET	N-CA-C	-6.90	104.86	113.28
1	B	498	ASN	CA-C-N	6.69	126.64	119.28
1	B	498	ASN	C-N-CA	6.69	126.64	119.28
1	A	418	THR	N-CA-C	-6.66	104.02	111.28
1	A	597	ILE	N-CA-C	-6.54	102.81	110.21
1	B	113	SER	N-CA-C	-6.54	102.84	111.02
1	B	315	SER	N-CA-C	-6.52	105.62	112.93
1	A	655	ARG	CA-C-N	6.45	133.32	121.70
1	A	655	ARG	C-N-CA	6.45	133.32	121.70
1	B	163	PHE	CA-C-N	6.45	133.31	121.70
1	B	163	PHE	C-N-CA	6.45	133.31	121.70
1	A	350	ASP	N-CA-C	6.30	118.09	108.52
1	B	617	ARG	N-CA-C	6.28	124.17	110.80
1	B	166	PRO	N-CA-C	6.27	120.93	111.14
1	A	99	ASN	CA-C-N	6.22	126.13	119.28
1	A	99	ASN	C-N-CA	6.22	126.13	119.28
1	B	318	ILE	CA-C-N	-6.20	112.09	119.84
1	B	318	ILE	C-N-CA	-6.20	112.09	119.84
1	A	493	TYR	N-CA-C	-6.18	105.38	113.17
1	A	541	ARG	N-CA-C	6.12	120.82	113.23
1	A	208	LYS	N-CA-C	-6.07	106.01	113.41
1	B	509	VAL	N-CA-C	-6.06	101.76	109.58
1	A	664	ASP	N-CA-C	-5.99	105.46	112.89
1	A	716	VAL	N-CA-C	5.96	118.21	108.97
1	A	308	PHE	N-CA-C	-5.96	105.87	113.02
1	B	505	GLU	CA-C-N	5.95	132.41	121.70
1	B	505	GLU	C-N-CA	5.95	132.41	121.70
1	A	587	PHE	N-CA-C	5.94	120.19	107.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	607	LYS	CA-C-N	5.93	132.37	121.70
1	B	607	LYS	C-N-CA	5.93	132.37	121.70
1	A	285	ARG	N-CA-C	-5.91	104.91	111.71
1	B	575	ILE	CA-C-N	5.84	132.21	121.70
1	B	575	ILE	C-N-CA	5.84	132.21	121.70
1	B	165	LEU	N-CA-C	-5.73	101.95	110.20
1	A	705	ARG	N-CA-C	-5.68	106.31	113.18
1	B	361	TYR	N-CA-C	5.68	116.06	108.23
1	A	41	THR	N-CA-C	5.53	122.59	110.80
1	A	206	ASP	CB-CA-C	-5.53	110.22	116.63
1	A	524	THR	N-CA-C	5.53	117.58	109.24
1	B	723	ILE	N-CA-C	-5.49	107.45	113.43
1	B	610	GLU	N-CA-C	-5.47	105.87	112.54
1	B	687	GLY	N-CA-C	-5.44	105.81	112.77
1	A	665	GLY	N-CA-C	-5.39	105.96	112.49
1	A	575	ILE	N-CA-C	5.29	116.35	108.46
1	B	35	GLN	N-CA-C	5.29	117.85	109.50
1	B	41	THR	N-CA-C	-5.27	106.72	112.72
1	B	133	GLU	N-CA-C	-5.23	105.76	111.82
1	A	180	TYR	CA-C-N	5.22	126.36	119.84
1	A	180	TYR	C-N-CA	5.22	126.36	119.84
1	B	544	GLU	CA-C-N	5.18	124.98	119.28
1	B	544	GLU	C-N-CA	5.18	124.98	119.28
1	B	741	SER	N-CA-C	-5.18	104.50	111.54
1	B	608	GLU	CA-C-N	5.17	131.01	121.70
1	B	608	GLU	C-N-CA	5.17	131.01	121.70
1	B	273	ALA	N-CA-C	-5.15	106.26	112.54
1	B	128	PRO	N-CA-C	-5.13	106.72	113.65
1	B	757	GLY	N-CA-C	5.10	119.92	113.24
1	A	486	TYR	N-CA-C	-5.09	105.65	111.14
1	B	327	GLU	N-CA-C	-5.09	106.85	113.16
1	A	611	LEU	N-CA-C	-5.04	105.92	111.71
1	A	714	LEU	N-CA-C	-5.02	105.86	112.94
1	B	98	CYS	N-CA-C	-5.02	106.99	113.01

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	VAL	Peptide
1	A	34	LEU	Peptide
1	A	35	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	365	GLN	Peptide
1	A	437	MET	Peptide
1	B	165	LEU	Peptide
1	B	171	VAL	Peptide
1	B	508	GLY	Peptide

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	5920	0	5913	546	0
1	B	5920	0	5913	521	0
All	All	11840	0	11826	1059	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 45.

All (1059) 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:42:ARG:HD2	1:B:339:THR:H	1.30	0.96
1:A:117:ALA:H	1:A:221:ALA:H	1.10	0.93
1:B:117:ALA:HB1	1:B:221:ALA:HB1	1.50	0.91
1:B:80:LEU:HD12	1:B:81:SER:H	1.36	0.88
1:A:342:TYR:HA	1:A:559:GLU:HG3	1.57	0.86
1:B:259:ARG:HG2	1:B:269:LEU:HG	1.56	0.85
1:A:108:ALA:HA	1:A:112:GLY:HA3	1.59	0.85
1:B:103:TRP:HE1	1:B:230:ALA:H	1.23	0.85
1:B:400:THR:HG21	1:B:686:ILE:HG12	1.59	0.84
1:B:63:PRO:HB3	1:B:199:LEU:HB2	1.60	0.83
1:B:128:PRO:O	1:B:132:LEU:N	2.12	0.83
1:B:172:TYR:HD1	1:B:578:TRP:HB2	1.42	0.83
1:B:254:LEU:HD11	1:B:294:TYR:HA	1.60	0.82
1:B:733:GLN:HG3	1:B:734:MET:HG2	1.62	0.82
1:B:542:THR:HG21	1:B:547:GLU:HB2	1.62	0.82
1:A:502:VAL:HA	1:A:503:VAL:HG12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HG	1:A:436:GLU:HB2	1.60	0.81
1:A:527:ARG:HG3	1:A:529:PRO:HD3	1.61	0.81
1:B:281:ILE:HA	1:B:284:LEU:HB3	1.63	0.80
1:A:44:PHE:HA	1:A:333:LEU:HA	1.64	0.80
1:B:42:ARG:HD3	1:B:337:ASN:H	1.45	0.80
1:A:582:GLU:O	1:A:625:LYS:NZ	2.15	0.80
1:A:715:HIS:HD2	1:A:716:VAL:HG22	1.43	0.80
1:A:16:LEU:HA	1:A:487:TYR:HE1	1.46	0.80
1:B:135:LEU:O	1:B:139:ALA:N	2.15	0.80
1:A:651:ARG:HB2	1:A:663:ILE:HD11	1.63	0.80
1:B:93:HIS:O	1:B:96:THR:OG1	1.99	0.80
1:A:436:GLU:OE2	1:A:439:LEU:N	2.12	0.80
1:A:528:ILE:HG12	1:A:536:GLU:HB3	1.65	0.79
1:A:173:ARG:HB2	1:A:579:PRO:HG2	1.64	0.79
1:B:53:LEU:HD21	1:B:171:VAL:HG23	1.64	0.79
1:B:756:LEU:HG	1:B:757:GLY:H	1.48	0.79
1:A:117:ALA:N	1:A:221:ALA:H	1.81	0.78
1:A:197:ARG:HA	1:A:200:THR:HG22	1.66	0.78
1:B:407:THR:OG1	1:B:680:MET:SD	2.42	0.77
1:A:581:HIS:O	1:A:583:ALA:N	2.17	0.77
1:A:195:LEU:HA	1:A:198:MET:HB3	1.67	0.77
1:B:322:ILE:HG22	1:B:325:MET:HE3	1.67	0.77
1:B:408:PHE:HD1	1:B:413:PHE:HZ	1.33	0.77
1:B:609:PHE:HB3	1:B:611:LEU:H	1.49	0.77
1:B:106:LEU:HD13	1:B:154:VAL:HG21	1.67	0.76
1:A:189:CYS:HB3	1:A:323:GLU:HG3	1.67	0.76
1:B:7:LYS:HD3	1:B:531:GLY:H	1.51	0.76
1:A:176:ARG:HH12	1:A:447:ARG:HA	1.49	0.75
1:B:451:LEU:O	1:B:453:ARG:NH1	2.19	0.75
1:A:387:LEU:HG	1:A:572:THR:HG21	1.66	0.75
1:B:647:LEU:HD23	1:B:667:ARG:HG3	1.67	0.75
1:A:588:ALA:HB1	1:A:589:TYR:HB2	1.67	0.75
1:A:200:THR:HA	1:A:203:SER:HB3	1.67	0.75
1:A:480:LYS:HA	1:A:483:MET:HG2	1.68	0.75
1:B:608:GLU:N	1:B:609:PHE:HB2	2.01	0.75
1:B:575:ILE:HA	1:B:576:HIS:HB2	1.68	0.75
1:A:410:VAL:HA	1:A:413:PHE:HB3	1.66	0.74
1:A:148:HIS:O	1:A:151:THR:OG1	2.04	0.74
1:A:208:LYS:O	1:A:211:GLN:NE2	2.19	0.74
1:B:75:GLN:OE1	1:B:447:ARG:NH2	2.21	0.74
1:A:633:ILE:HD13	1:A:738:LEU:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ASN:ND2	1:B:296:ASP:OD2	2.21	0.74
1:A:134:GLN:O	1:A:137:THR:OG1	2.06	0.74
1:A:347:SER:HA	1:A:358:VAL:HG13	1.70	0.73
1:A:717:GLY:O	1:A:721:HIS:N	2.16	0.73
1:B:95:SER:OG	1:B:99:ASN:ND2	2.21	0.73
1:B:134:GLN:O	1:B:137:THR:OG1	2.06	0.73
1:A:530:VAL:O	1:A:551:TYR:OH	2.07	0.73
1:A:619:GLU:OE2	1:A:620:ARG:NH1	2.21	0.72
1:B:323:GLU:O	1:B:326:SER:OG	2.05	0.72
1:A:359:VAL:HA	1:A:438:THR:HA	1.71	0.72
1:B:14:ARG:HB2	1:B:465:GLY:HA3	1.70	0.72
1:B:46:ALA:HA	1:B:331:PHE:HA	1.71	0.72
1:B:342:TYR:HB3	1:B:559:GLU:HG2	1.72	0.72
1:A:55:GLU:HG3	1:A:171:VAL:HG22	1.70	0.72
1:A:365:GLN:HA	1:A:562:GLN:HB2	1.70	0.72
1:B:348:ALA:HB3	1:B:356:SER:H	1.55	0.72
1:A:352:MET:N	1:A:353:GLY:HA2	2.05	0.72
1:A:533:ASN:HD22	1:A:543:PRO:HD2	1.55	0.72
1:B:152:ASP:O	1:B:156:HIS:N	2.23	0.72
1:B:714:LEU:HB3	1:B:719:ASN:HD22	1.54	0.72
1:A:132:LEU:HD21	1:A:136:ARG:HH21	1.53	0.72
1:B:644:ASP:OD2	1:B:748:LYS:NZ	2.23	0.71
1:A:272:SER:HB2	1:A:275:LEU:HB3	1.72	0.71
1:B:42:ARG:HD2	1:B:339:THR:N	2.05	0.71
1:A:40:PHE:HB2	1:A:288:LEU:HB3	1.73	0.71
1:B:224:LEU:O	1:B:228:HIS:N	2.24	0.71
1:A:630:HIS:HB2	1:A:737:LEU:HD22	1.73	0.71
1:A:334:ARG:HD3	1:A:338:GLU:HB2	1.72	0.71
1:B:677:LYS:HA	1:B:680:MET:HE3	1.72	0.71
1:B:35:GLN:NE2	1:B:504:SER:OG	2.24	0.71
1:A:392:GLY:O	1:A:396:ARG:NH1	2.24	0.70
1:B:231:ASN:O	1:B:234:THR:OG1	2.08	0.70
1:A:172:TYR:CD1	1:A:578:TRP:HB2	2.26	0.70
1:A:73:TYR:O	1:A:77:GLY:N	2.25	0.70
1:B:4:LEU:HD21	1:B:13:ALA:HB3	1.73	0.70
1:B:584:SER:H	1:B:622:ARG:NH1	1.90	0.70
1:A:385:ARG:HD2	1:A:580:TRP:HE1	1.57	0.70
1:A:242:GLY:O	1:A:244:PHE:N	2.24	0.70
1:B:182:ASN:OD1	1:B:183:PHE:N	2.25	0.70
1:A:655:ARG:N	1:A:656:ASP:HB2	2.07	0.69
1:B:163:PHE:HA	1:B:164:ILE:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ALA:H	1:B:536:GLU:HG3	1.57	0.69
1:B:213:THR:O	1:B:215:LYS:N	2.25	0.69
1:A:31:VAL:HG22	1:A:32:GLY:H	1.58	0.69
1:A:453:ARG:NH2	1:A:474:ARG:O	2.26	0.69
1:A:534:ALA:O	1:A:536:GLU:N	2.26	0.69
1:A:739:SER:HG	1:A:742:GLU:CD	2.01	0.69
1:A:40:PHE:HD2	1:A:289:ALA:HA	1.57	0.69
1:A:97:ALA:HA	1:A:103:TRP:HZ2	1.58	0.69
1:A:45:SER:OG	1:A:332:LYS:HB2	1.93	0.68
1:B:46:ALA:O	1:B:334:ARG:NH2	2.27	0.68
1:A:368:LYS:HG2	1:A:402:ALA:HA	1.76	0.68
1:A:126:VAL:HG13	1:A:166:PRO:HD3	1.75	0.67
1:B:678:ILE:HA	1:B:681:ILE:HD12	1.76	0.67
1:A:51:GLU:HA	1:A:174:VAL:HG21	1.75	0.67
1:A:194:ASP:O	1:A:198:MET:N	2.25	0.67
1:A:315:SER:O	1:A:317:ILE:N	2.28	0.67
1:A:580:TRP:HA	1:A:581:HIS:O	1.95	0.67
1:A:712:SER:O	1:A:715:HIS:ND1	2.22	0.67
1:A:739:SER:OG	1:A:740:ARG:N	2.28	0.67
1:A:283:GLN:O	1:A:286:SER:OG	2.09	0.67
1:B:15:GLY:HA3	1:B:462:LEU:HG	1.76	0.67
1:B:10:ASN:HD22	1:B:29:LEU:HD21	1.59	0.66
1:B:337:ASN:OD1	1:B:338:GLU:N	2.28	0.66
1:B:237:PHE:O	1:B:240:SER:OG	2.14	0.66
1:B:334:ARG:HD3	1:B:335:PRO:HD2	1.77	0.66
1:A:179:THR:N	1:A:180:TYR:HA	2.11	0.66
1:A:456:MET:HA	1:A:459:ILE:HD12	1.78	0.66
1:A:521:ASN:O	1:A:539:SER:OG	2.10	0.66
1:A:627:THR:O	1:A:629:ALA:N	2.29	0.66
1:A:112:GLY:HA2	1:A:116:ARG:HD3	1.76	0.66
1:B:667:ARG:NH2	1:B:752:ASP:OD2	2.29	0.66
1:B:30:SER:HB2	1:B:517:TYR:CZ	2.31	0.65
1:A:296:ASP:O	1:A:300:GLN:N	2.19	0.65
1:B:349:ILE:HG13	1:B:351:HIS:H	1.61	0.65
1:B:275:LEU:HB2	1:B:312:GLU:HG2	1.78	0.65
1:A:92:TYR:HE2	1:A:150:THR:HG21	1.62	0.65
1:A:283:GLN:NE2	1:A:286:SER:OG	2.30	0.65
1:A:395:ASP:OD1	1:A:396:ARG:N	2.30	0.65
1:A:505:GLU:HG2	1:A:515:SER:H	1.61	0.65
1:B:274:ARG:HB3	1:B:312:GLU:HG3	1.79	0.65
1:A:306:VAL:O	1:A:308:PHE:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ARG:H	1:A:656:ASP:HB2	1.61	0.65
1:B:170:TYR:HA	1:B:576:HIS:CD2	2.31	0.65
1:A:358:VAL:H	1:A:437:MET:HB3	1.60	0.65
1:A:691:VAL:HG12	1:A:723:ILE:HG12	1.77	0.65
1:B:18:GLN:HE22	1:B:518:LEU:HB2	1.62	0.64
1:A:535:ILE:HD12	1:A:541:ARG:H	1.61	0.64
1:A:729:LEU:HD21	1:A:743:ALA:HB1	1.79	0.64
1:A:501:VAL:HG23	1:A:502:VAL:HG12	1.78	0.64
1:B:125:LYS:HE2	1:B:163:PHE:HB2	1.80	0.64
1:A:45:SER:HB3	1:A:334:ARG:HB2	1.80	0.64
1:B:66:TYR:HD1	1:B:69:LEU:HD12	1.63	0.64
1:B:506:HIS:HB2	1:B:517:TYR:HE2	1.62	0.64
1:A:57:GLY:H	1:A:170:TYR:HB2	1.62	0.64
1:A:315:SER:OG	1:A:316:THR:N	2.30	0.64
1:B:156:HIS:NE2	1:B:206:ASP:OD2	2.16	0.64
1:B:233:ALA:O	1:B:237:PHE:N	2.30	0.64
1:B:606:VAL:HB	1:B:697:ARG:NH2	2.12	0.64
1:A:520:TRP:H	1:A:542:THR:H	1.46	0.64
1:A:602:TYR:CG	1:A:702:MET:HE1	2.32	0.64
1:B:44:PHE:HE2	1:B:181:PRO:HG3	1.63	0.64
1:A:580:TRP:CD2	1:A:581:HIS:HA	2.33	0.64
1:B:420:VAL:HG13	1:B:669:GLN:HE22	1.62	0.64
1:B:132:LEU:HD13	1:B:151:THR:HG22	1.80	0.64
1:A:77:GLY:O	1:A:474:ARG:NH1	2.28	0.64
1:A:358:VAL:N	1:A:437:MET:SD	2.71	0.64
1:A:178:ALA:O	1:A:332:LYS:NZ	2.31	0.63
1:B:83:ASP:HA	1:B:191:ARG:HG2	1.79	0.63
1:B:205:VAL:O	1:B:209:MET:HG2	1.98	0.63
1:A:144:GLU:HG2	1:A:145:LEU:H	1.63	0.63
1:A:554:PRO:O	1:A:556:GLN:N	2.22	0.63
1:B:616:GLN:HG3	1:B:617:ARG:HG2	1.78	0.63
1:A:42:ARG:NH2	1:A:283:GLN:HE21	1.96	0.63
1:B:225:ILE:HA	1:B:228:HIS:HB3	1.79	0.63
1:B:45:SER:OG	1:B:46:ALA:N	2.29	0.63
1:B:449:TYR:HH	1:B:630:HIS:HD1	0.65	0.63
1:B:485:ASN:OD1	1:B:486:TYR:N	2.32	0.63
1:B:593:TYR:HB3	1:B:604:ALA:HB3	1.80	0.63
1:A:597:ILE:HD11	1:A:600:LYS:HE3	1.81	0.63
1:A:498:ASN:HD22	1:A:500:GLU:HG2	1.64	0.63
1:B:312:GLU:O	1:B:315:SER:N	2.24	0.63
1:B:317:ILE:HG12	1:B:320:TRP:CZ2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ILE:HG12	1:B:626:PRO:HG3	1.80	0.63
1:A:4:LEU:H	1:A:436:GLU:HB2	1.64	0.63
1:B:35:GLN:HE21	1:B:502:VAL:HG23	1.64	0.63
1:B:136:ARG:HB2	1:B:147:HIS:NE2	2.14	0.63
1:A:375:PRO:HG3	1:A:622:ARG:HE	1.63	0.62
1:B:77:GLY:HA3	1:B:474:ARG:HH22	1.63	0.62
1:B:608:GLU:HA	1:B:609:PHE:O	1.99	0.62
1:A:10:ASN:HA	1:A:17:THR:HG21	1.81	0.62
1:A:666:ARG:HD3	1:A:669:GLN:NE2	2.14	0.62
1:B:2:PHE:O	1:B:439:LEU:N	2.30	0.62
1:B:153:PHE:HB3	1:B:229:LEU:HD21	1.80	0.62
1:B:635:MET:O	1:B:638:SER:OG	2.10	0.62
1:B:408:PHE:HD1	1:B:413:PHE:CZ	2.16	0.62
1:B:472:GLU:O	1:B:476:SER:N	2.30	0.62
1:A:607:LYS:O	1:A:609:PHE:N	2.32	0.62
1:A:715:HIS:CD2	1:A:716:VAL:HG22	2.31	0.62
1:B:123:VAL:HG23	1:B:164:ILE:HG12	1.80	0.62
1:A:360:VAL:HG22	1:A:438:THR:HG22	1.80	0.62
1:B:16:LEU:HD23	1:B:546:LEU:HD21	1.81	0.62
1:B:132:LEU:HA	1:B:135:LEU:HB2	1.82	0.62
1:A:61:ILE:HD11	1:A:199:LEU:HD21	1.80	0.62
1:A:173:ARG:HD3	1:A:579:PRO:HG2	1.82	0.62
1:A:172:TYR:HD1	1:A:578:TRP:HB2	1.65	0.62
1:B:41:THR:N	1:B:286:SER:OG	2.32	0.62
1:B:128:PRO:HA	1:B:131:ILE:HG22	1.81	0.62
1:B:136:ARG:HB2	1:B:147:HIS:CD2	2.35	0.62
1:B:209:MET:O	1:B:213:THR:OG1	2.09	0.62
1:B:216:ALA:HA	1:B:217:LYS:C	2.25	0.62
1:B:421:TYR:HE2	1:B:427:ARG:HH22	1.47	0.62
1:B:637:TYR:HA	1:B:640:PHE:CD2	2.34	0.62
1:A:40:PHE:CD2	1:A:289:ALA:HA	2.35	0.62
1:B:61:ILE:HG12	1:B:152:ASP:HB2	1.82	0.62
1:A:100:PRO:HA	1:A:103:TRP:HD1	1.63	0.61
1:A:190:VAL:HG12	1:A:323:GLU:HB2	1.81	0.61
1:A:502:VAL:HA	1:A:503:VAL:CG1	2.28	0.61
1:B:481:ARG:HA	1:B:484:PHE:CE2	2.34	0.61
1:A:287:ASN:O	1:A:289:ALA:N	2.33	0.61
1:A:349:ILE:HG13	1:A:350:ASP:H	1.65	0.61
1:A:666:ARG:HG3	1:A:670:ASN:HD21	1.65	0.61
1:A:544:GLU:CD	1:A:546:LEU:H	2.08	0.61
1:B:589:TYR:HB3	1:B:734:MET:HE3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:HIS:NE2	1:B:738:LEU:HA	2.15	0.61
1:A:173:ARG:HE	1:A:566:LEU:HD21	1.65	0.61
1:A:183:PHE:HA	1:A:186:LEU:HD13	1.82	0.61
1:B:153:PHE:CZ	1:B:202:LEU:HB3	2.36	0.61
1:B:745:ALA:O	1:B:748:LYS:HG2	2.01	0.61
1:A:128:PRO:N	1:A:129:THR:HB	2.16	0.61
1:A:505:GLU:HA	1:A:516:LEU:HB3	1.83	0.61
1:A:713:ASP:HA	1:A:715:HIS:CE1	2.36	0.61
1:B:231:ASN:OD1	1:B:232:ALA:N	2.34	0.61
1:A:296:ASP:HA	1:A:299:LYS:HB3	1.82	0.60
1:B:388:ASP:HA	1:B:572:THR:HG21	1.82	0.60
1:A:9:LEU:HA	1:A:12:SER:HB3	1.84	0.60
1:A:127:PRO:HG2	1:A:130:ALA:HB2	1.83	0.60
1:A:176:ARG:NH2	1:A:447:ARG:HD2	2.17	0.60
1:B:75:GLN:HB3	1:B:447:ARG:HH22	1.66	0.60
1:A:135:LEU:HD12	1:A:151:THR:HG22	1.84	0.60
1:A:214:PHE:HA	1:A:215:LYS:O	2.02	0.60
1:A:666:ARG:HA	1:A:669:GLN:HE22	1.65	0.60
1:A:754:ASN:N	1:A:755:ALA:HA	2.16	0.60
1:B:163:PHE:HB3	1:B:164:ILE:HG22	1.84	0.60
1:A:493:TYR:CE2	1:A:549:ILE:HG12	2.36	0.60
1:B:543:PRO:HG2	1:B:544:GLU:HG3	1.83	0.60
1:B:636:TRP:HB3	1:B:640:PHE:CZ	2.37	0.60
1:A:13:ALA:HB1	1:A:16:LEU:HD12	1.83	0.60
1:A:4:LEU:N	1:A:436:GLU:HB2	2.17	0.60
1:B:37:PRO:HA	1:B:502:VAL:HG12	1.84	0.60
1:B:131:ILE:O	1:B:134:GLN:HB3	2.02	0.60
1:B:715:HIS:HB3	1:B:720:ARG:NH2	2.17	0.60
1:B:744:GLU:O	1:B:747:THR:OG1	2.17	0.60
1:A:472:GLU:HB3	1:A:475:ALA:HB3	1.83	0.60
1:B:598:ARG:NH1	1:B:710:ASP:OD1	2.35	0.60
1:A:116:ARG:HB2	1:A:222:PRO:HA	1.83	0.59
1:A:181:PRO:HD3	1:A:485:ASN:HD21	1.67	0.59
1:A:360:VAL:HG13	1:A:438:THR:HG23	1.84	0.59
1:A:671:ALA:O	1:A:674:LEU:HG	2.01	0.59
1:B:583:ALA:N	1:B:584:SER:HA	2.16	0.59
1:A:715:HIS:CD2	1:A:716:VAL:H	2.21	0.59
1:B:521:ASN:HA	1:B:540:ILE:HB	1.84	0.59
1:B:732:LEU:HG	1:B:738:LEU:HD22	1.83	0.59
1:A:660:LYS:O	1:A:663:ILE:HG13	2.02	0.59
1:A:678:ILE:HG21	1:A:725:ILE:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ASP:OD1	1:B:9:LEU:N	2.35	0.59
1:B:597:ILE:O	1:B:602:TYR:OH	2.17	0.59
1:B:288:LEU:O	1:B:291:PHE:HB3	2.03	0.59
1:A:214:PHE:HA	1:A:215:LYS:C	2.28	0.59
1:B:159:SER:OG	1:B:162:GLY:O	2.21	0.59
1:B:312:GLU:C	1:B:315:SER:H	2.10	0.59
1:B:656:ASP:HB3	1:B:659:GLU:HG2	1.84	0.59
1:B:264:SER:HB3	1:B:269:LEU:HD22	1.85	0.59
1:B:279:ASN:O	1:B:281:ILE:N	2.35	0.59
1:B:363:ASP:OD1	1:B:561:LEU:HD22	2.03	0.59
1:B:471:LEU:HB3	1:B:475:ALA:HB3	1.85	0.59
1:A:173:ARG:HB2	1:A:579:PRO:CG	2.33	0.59
1:A:306:VAL:HG12	1:A:309:SER:HA	1.85	0.59
1:B:145:LEU:HD12	1:B:146:PHE:N	2.18	0.59
1:B:332:LYS:HE2	1:B:334:ARG:HH12	1.67	0.59
1:B:478:ASP:OD1	1:B:479:LEU:N	2.36	0.59
1:A:661:LEU:O	1:A:665:GLY:N	2.35	0.58
1:A:144:GLU:O	1:A:146:PHE:N	2.36	0.58
1:A:445:VAL:HG13	1:A:455:PRO:HG3	1.85	0.58
1:A:61:ILE:HG13	1:A:66:TYR:HE2	1.68	0.58
1:A:347:SER:H	1:A:554:PRO:HB3	1.68	0.58
1:A:589:TYR:OH	1:A:740:ARG:NE	2.26	0.58
1:B:479:LEU:O	1:B:482:SER:OG	2.18	0.58
1:A:395:ASP:O	1:A:398:SER:OG	2.14	0.58
1:A:669:GLN:HA	1:A:672:VAL:HB	1.86	0.58
1:B:562:GLN:HG2	1:B:564:LYS:H	1.68	0.58
1:B:746:LEU:HA	1:B:749:VAL:HG22	1.85	0.58
1:A:180:TYR:CE1	1:A:331:PHE:HA	2.38	0.58
1:A:740:ARG:N	1:A:742:GLU:OE1	2.36	0.58
1:B:476:SER:O	1:B:480:LYS:HG2	2.04	0.58
1:A:530:VAL:HG13	1:A:551:TYR:CZ	2.38	0.58
1:A:568:LEU:HD12	1:A:569:ALA:N	2.19	0.58
1:B:407:THR:HG23	1:B:408:PHE:CD2	2.39	0.58
1:B:424:VAL:HG23	1:B:430:VAL:HA	1.85	0.58
1:B:617:ARG:N	1:B:618:ARG:HA	2.18	0.58
1:A:284:LEU:HG	1:A:287:ASN:ND2	2.19	0.58
1:B:170:TYR:HA	1:B:576:HIS:CG	2.39	0.58
1:B:506:HIS:HB2	1:B:517:TYR:CE2	2.39	0.58
1:B:506:HIS:HA	1:B:507:GLN:HB3	1.86	0.58
1:A:47:SER:HB3	1:A:332:LYS:HD3	1.84	0.58
1:A:358:VAL:H	1:A:437:MET:CB	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:SER:HA	1:B:446:GLU:HG2	1.85	0.58
1:B:587:PHE:HB3	1:B:621:VAL:HG23	1.85	0.58
1:A:210:LEU:HD22	1:A:228:HIS:ND1	2.18	0.57
1:A:343:ILE:N	1:A:559:GLU:OE2	2.34	0.57
1:B:182:ASN:H	1:B:185:ALA:HB3	1.69	0.57
1:B:467:VAL:HG13	1:B:469:GLU:HB2	1.86	0.57
1:A:4:LEU:O	1:A:436:GLU:N	2.37	0.57
1:B:194:ASP:OD1	1:B:195:LEU:N	2.36	0.57
1:B:669:GLN:HA	1:B:672:VAL:HG12	1.85	0.57
1:A:661:LEU:HD22	1:B:105:LYS:HD2	1.84	0.57
1:B:75:GLN:OE1	1:B:481:ARG:NH1	2.37	0.57
1:B:560:VAL:O	1:B:561:LEU:HG	2.04	0.57
1:B:324:ALA:HB1	1:B:333:LEU:HB2	1.86	0.57
1:A:97:ALA:HA	1:A:103:TRP:CZ2	2.37	0.57
1:A:375:PRO:HB2	1:A:385:ARG:HD3	1.86	0.57
1:B:610:GLU:C	1:B:612:LEU:H	2.12	0.57
1:A:287:ASN:C	1:A:289:ALA:H	2.13	0.57
1:A:702:MET:HG3	1:A:711:SER:HB3	1.86	0.57
1:A:732:LEU:HG	1:A:738:LEU:HD11	1.86	0.57
1:A:433:ASN:HB3	1:A:434:GLY:CA	2.35	0.57
1:A:200:THR:O	1:A:204:SER:N	2.37	0.57
1:B:607:LYS:HB2	1:B:608:GLU:O	2.05	0.57
1:B:693:LEU:HD23	1:B:697:ARG:HH11	1.70	0.57
1:B:707:LEU:HD12	1:B:708:ILE:HG23	1.86	0.57
1:B:56:VAL:HG23	1:B:170:TYR:HB3	1.86	0.57
1:B:87:ASN:OD1	1:B:88:GLN:N	2.37	0.57
1:B:609:PHE:HB3	1:B:611:LEU:N	2.19	0.57
1:A:67:ALA:HA	1:A:70:PHE:HD2	1.68	0.56
1:A:179:THR:HG21	1:A:488:ALA:HB1	1.87	0.56
1:B:489:ALA:HA	1:B:492:HIS:CE1	2.40	0.56
1:A:354:GLN:NE2	1:A:525:GLU:OE1	2.38	0.56
1:A:400:THR:HG21	1:A:731:VAL:HG21	1.87	0.56
1:B:70:PHE:CE1	1:B:145:LEU:HD13	2.40	0.56
1:A:52:LEU:O	1:A:174:VAL:HG13	2.05	0.56
1:A:342:TYR:O	1:A:362:GLU:HG2	2.05	0.56
1:B:153:PHE:HZ	1:B:202:LEU:HD23	1.70	0.56
1:B:345:GLN:HB2	1:B:554:PRO:HA	1.87	0.56
1:B:377:LYS:HB2	1:B:385:ARG:HG2	1.86	0.56
1:B:586:GLU:O	1:B:622:ARG:NH2	2.38	0.56
1:B:647:LEU:HD21	1:B:663:ILE:HA	1.88	0.56
1:B:199:LEU:HD23	1:B:202:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:PRO:HB2	1:A:559:GLU:HB2	1.87	0.56
1:A:591:ASP:OD2	1:A:726:TRP:NE1	2.38	0.56
1:B:738:LEU:HD23	1:B:742:GLU:HG2	1.86	0.56
1:B:651:ARG:HG2	1:B:663:ILE:HD13	1.88	0.56
1:B:125:LYS:NZ	1:B:158:LEU:O	2.38	0.56
1:B:291:PHE:O	1:B:294:TYR:HB3	2.05	0.56
1:A:422:GLU:OE2	1:B:116:ARG:HB3	2.06	0.56
1:A:473:ALA:O	1:A:477:ASN:ND2	2.39	0.56
1:B:567:ASP:OD1	1:B:568:LEU:N	2.34	0.56
1:A:93:HIS:NE2	1:A:202:LEU:HD13	2.21	0.56
1:A:337:ASN:ND2	1:A:496:ALA:HB2	2.21	0.56
1:A:352:MET:HE2	1:A:428:GLY:H	1.71	0.56
1:B:43:THR:HG21	1:B:289:ALA:H	1.70	0.56
1:A:284:LEU:C	1:A:287:ASN:H	2.14	0.55
1:A:558:SER:N	1:A:559:GLU:OE1	2.39	0.55
1:B:43:THR:OG1	1:B:288:LEU:N	2.35	0.55
1:A:274:ARG:HH12	1:A:312:GLU:HG3	1.71	0.55
1:A:344:GLY:N	1:A:361:TYR:O	2.27	0.55
1:A:196:ARG:HD3	1:A:328:VAL:HG12	1.89	0.55
1:B:344:GLY:HA2	1:B:555:ILE:HG13	1.88	0.55
1:B:456:MET:HA	1:B:459:ILE:HD12	1.87	0.55
1:A:435:ALA:N	1:A:437:MET:HE3	2.22	0.55
1:B:42:ARG:HE	1:B:335:PRO:C	2.15	0.55
1:B:640:PHE:CZ	1:B:674:LEU:HD21	2.41	0.55
1:A:291:PHE:HZ	1:A:517:TYR:HA	1.71	0.55
1:A:568:LEU:HD12	1:A:569:ALA:H	1.71	0.55
1:B:93:HIS:CE1	1:B:96:THR:HA	2.41	0.55
1:B:4:LEU:O	1:B:437:MET:N	2.40	0.55
1:B:125:LYS:HZ2	1:B:155:CYS:HA	1.72	0.55
1:A:196:ARG:HH11	1:A:328:VAL:HG12	1.72	0.55
1:A:210:LEU:HG	1:A:213:THR:HA	1.88	0.55
1:A:585:THR:N	1:A:586:GLU:HB2	2.22	0.55
1:B:68:ARG:NH1	1:B:327:GLU:O	2.38	0.55
1:B:272:SER:O	1:B:276:ARG:HG3	2.06	0.55
1:A:505:GLU:OE2	1:A:515:SER:OG	2.15	0.55
1:A:533:ASN:ND2	1:A:543:PRO:HD2	2.21	0.55
1:A:605:GLU:N	1:A:605:GLU:OE1	2.40	0.55
1:B:3:ASN:HB3	1:B:438:THR:HA	1.88	0.55
1:A:42:ARG:NH2	1:A:283:GLN:O	2.40	0.54
1:A:42:ARG:CZ	1:A:283:GLN:HE21	2.20	0.54
1:A:45:SER:HB2	1:A:334:ARG:CZ	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:GLU:HB3	1:A:623:ILE:HG22	1.89	0.54
1:A:693:LEU:O	1:A:697:ARG:HG2	2.08	0.54
1:B:193:SER:HA	1:B:328:VAL:HG11	1.89	0.54
1:B:586:GLU:C	1:B:622:ARG:HE	2.15	0.54
1:B:249:VAL:HG23	1:B:318:ILE:HG23	1.90	0.54
1:B:347:SER:HB3	1:B:355:PRO:HB3	1.88	0.54
1:A:42:ARG:NH2	1:A:286:SER:OG	2.40	0.54
1:B:358:VAL:HG11	1:B:437:MET:SD	2.47	0.54
1:B:666:ARG:O	1:B:669:GLN:HG2	2.07	0.54
1:A:446:GLU:HG3	1:A:627:THR:HB	1.90	0.54
1:B:467:VAL:HG22	1:B:469:GLU:H	1.71	0.54
1:A:22:ILE:HG21	1:A:515:SER:HB2	1.89	0.54
1:A:366:PHE:HE1	1:A:629:ALA:HB2	1.73	0.54
1:B:132:LEU:O	1:B:136:ARG:N	2.40	0.54
1:A:15:GLY:HA2	1:A:20:PHE:CG	2.42	0.54
1:A:127:PRO:C	1:A:129:THR:HB	2.33	0.54
1:A:350:ASP:O	1:A:352:MET:N	2.36	0.54
1:A:558:SER:OG	1:A:559:GLU:N	2.40	0.54
1:B:35:GLN:HB3	1:B:502:VAL:HB	1.88	0.54
1:B:42:ARG:NH1	1:B:339:THR:O	2.40	0.54
1:A:272:SER:HB2	1:A:275:LEU:CB	2.38	0.54
1:B:501:VAL:HG11	1:B:518:LEU:HD13	1.89	0.54
1:B:702:MET:HA	1:B:708:ILE:HD12	1.90	0.54
1:A:349:ILE:HD13	1:A:357:HIS:H	1.71	0.54
1:A:572:THR:HA	1:A:575:ILE:O	2.08	0.54
1:B:100:PRO:HA	1:B:103:TRP:CE3	2.43	0.54
1:A:433:ASN:HB3	1:A:434:GLY:C	2.33	0.53
1:B:354:GLN:HE21	1:B:431:ASN:HB3	1.73	0.53
1:A:144:GLU:HB2	1:A:147:HIS:HB3	1.90	0.53
1:A:165:LEU:N	1:A:166:PRO:HD2	2.23	0.53
1:B:143:HIS:HB2	1:B:146:PHE:CE2	2.43	0.53
1:A:99:ASN:ND2	1:A:101:GLU:OE2	2.41	0.53
1:B:443:SER:O	1:B:446:GLU:HG2	2.08	0.53
1:B:50:SER:H	1:B:176:ARG:HB3	1.74	0.53
1:B:124:GLY:H	1:B:164:ILE:HG21	1.73	0.53
1:A:458:ALA:HB1	1:A:483:MET:HE1	1.91	0.53
1:B:272:SER:O	1:B:276:ARG:N	2.42	0.53
1:B:354:GLN:HE22	1:B:431:ASN:HD22	1.57	0.53
1:B:610:GLU:CD	1:B:614:LEU:H	2.15	0.53
1:A:42:ARG:H	1:A:336:ILE:HD13	1.73	0.53
1:A:383:ASN:O	1:A:385:ARG:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:SER:OG	1:B:395:ASP:N	2.41	0.53
1:B:404:ILE:HG23	1:B:408:PHE:CD2	2.44	0.53
1:B:491:MET:HE1	1:B:545:PRO:HG3	1.91	0.53
1:A:26:LYS:HE3	1:A:509:VAL:HG22	1.91	0.53
1:A:527:ARG:HH11	1:A:528:ILE:H	1.56	0.53
1:B:275:LEU:HD13	1:B:315:SER:HB2	1.91	0.53
1:A:170:TYR:HD1	1:A:576:HIS:CE1	2.27	0.53
1:A:285:ARG:O	1:A:288:LEU:HD13	2.09	0.53
1:A:310:ASP:OD2	1:A:313:LEU:N	2.42	0.53
1:A:435:ALA:H	1:A:437:MET:HE3	1.74	0.53
1:B:42:ARG:HB2	1:B:339:THR:HA	1.91	0.53
1:B:86:VAL:HG21	1:B:191:ARG:HG3	1.90	0.53
1:B:345:GLN:CB	1:B:554:PRO:HA	2.39	0.53
1:A:182:ASN:ND2	1:A:184:TYR:HB2	2.23	0.53
1:B:128:PRO:O	1:B:131:ILE:N	2.42	0.53
1:B:709:ASP:O	1:B:711:SER:N	2.41	0.53
1:B:733:GLN:OE1	1:B:740:ARG:HG3	2.09	0.53
1:A:2:PHE:H	1:A:439:LEU:HD11	1.74	0.53
1:A:44:PHE:HE1	1:A:180:TYR:H	1.57	0.53
1:A:365:GLN:OE1	1:A:563:ALA:HB3	2.09	0.53
1:A:368:LYS:HE2	1:A:402:ALA:HA	1.91	0.53
1:A:702:MET:HB3	1:A:708:ILE:HA	1.91	0.53
1:B:467:VAL:HG22	1:B:469:GLU:N	2.24	0.53
1:B:570:ASN:O	1:B:573:THR:HG22	2.08	0.53
1:B:616:GLN:O	1:B:617:ARG:HB2	2.08	0.53
1:A:143:HIS:CD2	1:A:146:PHE:HE2	2.26	0.52
1:A:585:THR:HB	1:A:586:GLU:HA	1.91	0.52
1:A:641:VAL:O	1:A:645:ARG:HG2	2.08	0.52
1:B:16:LEU:HD13	1:B:462:LEU:HD21	1.91	0.52
1:B:459:ILE:O	1:B:463:ARG:HG3	2.09	0.52
1:B:571:HIS:O	1:B:575:ILE:HG23	2.09	0.52
1:A:34:LEU:HG	1:A:35:GLN:HG3	1.89	0.52
1:A:231:ASN:OD1	1:A:232:ALA:N	2.42	0.52
1:A:630:HIS:N	1:A:737:LEU:HD13	2.24	0.52
1:B:377:LYS:HG3	1:B:384:GLN:O	2.10	0.52
1:B:487:TYR:O	1:B:491:MET:HG2	2.10	0.52
1:A:519:VAL:HG22	1:A:542:THR:N	2.25	0.52
1:A:223:ALA:O	1:A:227:GLN:N	2.34	0.52
1:A:472:GLU:HB3	1:A:475:ALA:CB	2.40	0.52
1:B:80:LEU:CD1	1:B:81:SER:H	2.14	0.52
1:B:133:GLU:OE2	1:B:136:ARG:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:SER:HB2	1:B:223:ALA:HB2	1.90	0.52
1:B:610:GLU:OE2	1:B:614:LEU:N	2.40	0.52
1:A:345:GLN:HG2	1:A:555:ILE:HG12	1.91	0.52
1:A:732:LEU:HD21	1:A:738:LEU:HD21	1.91	0.52
1:A:38:LEU:H	1:A:501:VAL:HG21	1.73	0.52
1:B:42:ARG:HH11	1:B:339:THR:N	2.07	0.52
1:B:378:LEU:HD12	1:B:379:ALA:N	2.24	0.52
1:B:379:ALA:C	1:B:381:ASN:H	2.17	0.52
1:B:400:THR:O	1:B:403:PRO:HD2	2.10	0.52
1:B:575:ILE:HB	1:B:576:HIS:O	2.09	0.52
1:A:524:THR:HG21	1:A:540:ILE:HG12	1.92	0.52
1:B:346:THR:OG1	1:B:359:VAL:HG11	2.10	0.52
1:B:445:VAL:O	1:B:449:TYR:HB3	2.09	0.52
1:B:35:GLN:NE2	1:B:503:VAL:O	2.42	0.52
1:B:585:THR:C	1:B:622:ARG:HB2	2.35	0.52
1:A:713:ASP:HA	1:A:715:HIS:ND1	2.24	0.52
1:B:587:PHE:HA	1:B:622:ARG:HD3	1.92	0.52
1:A:127:PRO:O	1:A:130:ALA:N	2.36	0.51
1:A:159:SER:OG	1:A:160:PRO:HD3	2.09	0.51
1:B:42:ARG:CZ	1:B:334:ARG:HG3	2.39	0.51
1:B:107:THR:HA	1:B:110:ILE:HD12	1.92	0.51
1:B:110:ILE:O	1:B:111:THR:OG1	2.28	0.51
1:B:152:ASP:OD1	1:B:153:PHE:N	2.43	0.51
1:B:408:PHE:CD1	1:B:413:PHE:HZ	2.22	0.51
1:A:100:PRO:HA	1:A:103:TRP:CD1	2.45	0.51
1:A:712:SER:C	1:A:715:HIS:HD1	2.16	0.51
1:B:338:GLU:OE2	1:B:341:SER:N	2.43	0.51
1:B:387:LEU:HD23	1:B:578:TRP:HH2	1.75	0.51
1:A:105:LYS:HE2	1:A:138:LEU:HD11	1.91	0.51
1:A:296:ASP:HB2	1:A:300:GLN:HG2	1.92	0.51
1:B:482:SER:HA	1:B:485:ASN:HD21	1.76	0.51
1:A:32:GLY:H	1:A:541:ARG:HH21	1.59	0.51
1:A:245:ASP:HB2	1:A:248:ALA:HB3	1.93	0.51
1:A:580:TRP:CH2	1:A:622:ARG:HD3	2.45	0.51
1:B:41:THR:C	1:B:43:THR:H	2.17	0.51
1:B:326:SER:HB2	1:B:328:VAL:HG22	1.92	0.51
1:A:39:GLN:HA	1:A:501:VAL:HG11	1.92	0.51
1:A:144:GLU:HG2	1:A:145:LEU:N	2.26	0.51
1:A:157:VAL:O	1:A:160:PRO:HD2	2.10	0.51
1:B:132:LEU:HG	1:B:135:LEU:HB2	1.91	0.51
1:B:198:MET:O	1:B:202:LEU:HD13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:SER:HB3	1:A:306:VAL:HG13	1.93	0.51
1:B:25:LEU:O	1:B:27:ASN:ND2	2.44	0.51
1:B:154:VAL:HA	1:B:229:LEU:HD11	1.92	0.51
1:B:343:ILE:HB	1:B:493:TYR:OH	2.10	0.51
1:B:568:LEU:O	1:B:572:THR:N	2.38	0.51
1:A:103:TRP:O	1:A:226:SER:OG	2.26	0.51
1:A:106:LEU:O	1:A:110:ILE:HG12	2.10	0.51
1:A:720:ARG:HD2	1:A:760:VAL:HG21	1.91	0.51
1:B:100:PRO:HA	1:B:103:TRP:HE3	1.74	0.51
1:B:7:LYS:HA	1:B:531:GLY:HA2	1.93	0.51
1:B:145:LEU:HD12	1:B:146:PHE:H	1.76	0.51
1:A:176:ARG:C	1:A:447:ARG:HH12	2.19	0.51
1:B:363:ASP:OD2	1:B:557:PRO:HB2	2.11	0.51
1:A:196:ARG:O	1:A:197:ARG:NH1	2.40	0.51
1:B:387:LEU:H	1:B:575:ILE:HD11	1.76	0.51
1:A:54:TRP:CZ3	1:A:174:VAL:HG12	2.46	0.50
1:A:261:TRP:CE2	1:A:288:LEU:HG	2.46	0.50
1:A:602:TYR:CD2	1:A:702:MET:HE1	2.46	0.50
1:A:669:GLN:O	1:A:673:THR:N	2.39	0.50
1:B:183:PHE:HB2	1:B:297:MET:HB3	1.92	0.50
1:A:276:ARG:HB2	1:A:281:ILE:HD11	1.93	0.50
1:B:62:ASP:CG	1:B:64:VAL:HG22	2.37	0.50
1:B:114:SER:HB3	1:B:222:PRO:HG2	1.92	0.50
1:B:321:PHE:HA	1:B:325:MET:SD	2.51	0.50
1:A:340:THR:O	1:A:343:ILE:HG22	2.12	0.50
1:A:369:GLU:HA	1:A:398:SER:HB2	1.94	0.50
1:A:387:LEU:H	1:A:572:THR:HG22	1.76	0.50
1:B:4:LEU:H	1:B:437:MET:HB3	1.76	0.50
1:B:16:LEU:HB3	1:B:546:LEU:HD11	1.94	0.50
1:A:409:ALA:O	1:A:413:PHE:N	2.38	0.50
1:B:18:GLN:O	1:B:22:ILE:HG12	2.11	0.50
1:B:584:SER:C	1:B:622:ARG:HG2	2.35	0.50
1:B:413:PHE:HB3	1:B:636:TRP:HZ2	1.76	0.50
1:A:36:LEU:C	1:A:502:VAL:HG11	2.36	0.50
1:A:715:HIS:CG	1:A:716:VAL:H	2.29	0.50
1:B:597:ILE:HG22	1:B:602:TYR:CE2	2.47	0.50
1:A:347:SER:O	1:A:358:VAL:HG22	2.11	0.50
1:A:352:MET:SD	1:A:355:PRO:HD2	2.51	0.50
1:B:352:MET:H	1:B:353:GLY:HA2	1.75	0.50
1:A:366:PHE:HD2	1:A:405:GLY:HA2	1.77	0.50
1:A:497:HIS:HE2	1:A:548:ALA:C	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLU:OE2	1:B:28:GLN:N	2.45	0.50
1:B:71:PHE:O	1:B:75:GLN:HG2	2.12	0.50
1:B:342:TYR:HB3	1:B:559:GLU:CG	2.42	0.50
1:A:502:VAL:HA	1:A:503:VAL:CB	2.42	0.50
1:A:745:ALA:O	1:A:749:VAL:HG23	2.12	0.50
1:B:560:VAL:O	1:B:562:GLN:N	2.45	0.50
1:B:560:VAL:C	1:B:561:LEU:HG	2.36	0.50
1:A:16:LEU:HD11	1:A:462:LEU:HB3	1.94	0.49
1:B:352:MET:H	1:B:353:GLY:CA	2.26	0.49
1:B:58:LYS:HE2	1:B:60:ASN:HD22	1.77	0.49
1:B:666:ARG:HA	1:B:669:GLN:HG2	1.93	0.49
1:A:128:PRO:HG2	1:A:129:THR:OG1	2.13	0.49
1:A:196:ARG:HB3	1:A:197:ARG:NH1	2.27	0.49
1:B:607:LYS:C	1:B:609:PHE:HB2	2.36	0.49
1:A:45:SER:C	1:A:332:LYS:HD2	2.37	0.49
1:A:81:SER:HB2	1:A:188:ASP:OD2	2.12	0.49
1:A:42:ARG:H	1:A:336:ILE:CD1	2.25	0.49
1:A:477:ASN:OD1	1:A:478:ASP:N	2.45	0.49
1:B:45:SER:O	1:B:332:LYS:N	2.45	0.49
1:B:199:LEU:HA	1:B:202:LEU:HB2	1.93	0.49
1:B:209:MET:SD	1:B:228:HIS:HE1	2.35	0.49
1:A:503:VAL:HG21	1:A:517:TYR:C	2.36	0.49
1:A:567:ASP:O	1:A:569:ALA:N	2.45	0.49
1:B:366:PHE:CZ	1:B:405:GLY:HA2	2.47	0.49
1:B:676:ARG:O	1:B:679:GLU:HB3	2.12	0.49
1:A:253:VAL:HG11	1:A:322:ILE:HD13	1.95	0.49
1:B:232:ALA:O	1:B:236:ALA:N	2.43	0.49
1:A:156:HIS:O	1:A:159:SER:OG	2.30	0.49
1:A:585:THR:O	1:A:622:ARG:HG2	2.12	0.49
1:B:379:ALA:O	1:B:381:ASN:N	2.45	0.49
1:B:403:PRO:O	1:B:407:THR:HG22	2.13	0.49
1:A:365:GLN:CA	1:A:562:GLN:HB2	2.41	0.49
1:A:433:ASN:HB3	1:A:434:GLY:HA3	1.95	0.49
1:A:443:SER:O	1:A:447:ARG:HG2	2.11	0.49
1:A:580:TRP:HA	1:A:581:HIS:C	2.36	0.49
1:A:716:VAL:HG21	1:B:386:PHE:CE2	2.48	0.49
1:B:296:ASP:O	1:B:299:LYS:HB3	2.13	0.49
1:B:415:LYS:O	1:B:418:THR:OG1	2.28	0.49
1:A:155:CYS:O	1:A:159:SER:N	2.45	0.49
1:B:42:ARG:HD3	1:B:337:ASN:N	2.21	0.49
1:A:15:GLY:O	1:A:487:TYR:OH	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:MET:HE2	1:A:342:TYR:CZ	2.48	0.48
1:A:396:ARG:HE	1:A:612:LEU:HB3	1.78	0.48
1:B:136:ARG:HE	1:B:147:HIS:CD2	2.31	0.48
1:B:726:TRP:HA	1:B:729:LEU:HD12	1.95	0.48
1:B:737:LEU:HB3	1:B:738:LEU:HD12	1.95	0.48
1:A:209:MET:HE3	1:A:210:LEU:HD12	1.94	0.48
1:A:391:PRO:HA	1:A:394:SER:HB2	1.93	0.48
1:B:30:SER:HB2	1:B:517:TYR:CE2	2.47	0.48
1:B:396:ARG:HD2	1:B:612:LEU:HD13	1.95	0.48
1:A:16:LEU:HA	1:A:487:TYR:CE1	2.36	0.48
1:A:556:GLN:OE1	1:A:557:PRO:HD2	2.13	0.48
1:A:747:THR:HA	1:A:750:LEU:HG	1.96	0.48
1:B:743:ALA:O	1:B:747:THR:N	2.36	0.48
1:A:61:ILE:HG13	1:A:66:TYR:CE2	2.47	0.48
1:A:418:THR:O	1:A:421:TYR:CD1	2.66	0.48
1:A:719:ASN:OD1	1:A:720:ARG:N	2.46	0.48
1:B:30:SER:O	1:B:543:PRO:HG3	2.13	0.48
1:B:41:THR:O	1:B:42:ARG:HG2	2.14	0.48
1:A:729:LEU:O	1:A:732:LEU:HB3	2.14	0.48
1:A:66:TYR:HA	1:A:69:LEU:HD12	1.95	0.48
1:A:283:GLN:C	1:A:286:SER:HG	2.13	0.48
1:A:355:PRO:O	1:A:356:SER:OG	2.28	0.48
1:A:477:ASN:O	1:A:481:ARG:N	2.47	0.48
1:A:516:LEU:O	1:A:516:LEU:HD12	2.13	0.48
1:B:258:GLY:HA2	1:B:261:TRP:HD1	1.78	0.48
1:B:314:SER:OG	1:B:317:ILE:N	2.31	0.48
1:A:696:SER:OG	1:A:697:ARG:NH1	2.47	0.48
1:B:660:LYS:O	1:B:663:ILE:HG13	2.13	0.48
1:A:335:PRO:HB2	1:A:338:GLU:OE2	2.14	0.48
1:A:648:ALA:O	1:A:652:ARG:HG3	2.14	0.48
1:A:754:ASN:HB3	1:A:755:ALA:C	2.39	0.48
1:A:16:LEU:HD21	1:A:462:LEU:HD13	1.96	0.48
1:A:42:ARG:HH21	1:A:286:SER:HG	1.61	0.48
1:A:109:TYR:OH	1:A:130:ALA:HB1	2.14	0.48
1:A:257:LEU:HB3	1:A:261:TRP:CZ2	2.48	0.48
1:B:164:ILE:HG13	1:B:165:LEU:H	1.79	0.48
1:B:254:LEU:HD22	1:B:297:MET:SD	2.54	0.48
1:B:314:SER:HG	1:B:317:ILE:HG13	1.78	0.48
1:B:747:THR:O	1:B:750:LEU:HG	2.13	0.48
1:A:533:ASN:ND2	1:A:542:THR:OG1	2.47	0.47
1:A:665:GLY:HA2	1:A:668:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:VAL:HA	1:A:675:LEU:HD12	1.96	0.47
1:B:132:LEU:HA	1:B:135:LEU:HD13	1.95	0.47
1:B:357:HIS:O	1:B:359:VAL:HG23	2.14	0.47
1:B:510:ALA:HB1	1:B:513:GLN:H	1.79	0.47
1:A:4:LEU:HG	1:A:436:GLU:CB	2.37	0.47
1:A:362:GLU:HB2	1:A:364:TRP:HE1	1.79	0.47
1:B:197:ARG:NH2	1:B:240:SER:HA	2.29	0.47
1:B:288:LEU:O	1:B:292:ILE:HD12	2.14	0.47
1:B:356:SER:HA	1:B:435:ALA:HB1	1.96	0.47
1:B:719:ASN:OD1	1:B:720:ARG:N	2.47	0.47
1:A:334:ARG:HD3	1:A:338:GLU:CB	2.41	0.47
1:B:525:GLU:OE2	1:B:535:ILE:HG12	2.14	0.47
1:A:83:ASP:OD1	1:A:191:ARG:NE	2.47	0.47
1:B:345:GLN:OE1	1:B:360:VAL:HG12	2.14	0.47
1:B:449:TYR:OH	1:B:630:HIS:ND1	2.13	0.47
1:A:375:PRO:CG	1:A:622:ARG:HE	2.26	0.47
1:A:441:PHE:HB2	1:A:444:VAL:HG22	1.96	0.47
1:A:282:ASP:O	1:A:285:ARG:HB3	2.14	0.47
1:A:289:ALA:C	1:A:291:PHE:H	2.22	0.47
1:A:308:PHE:HE2	1:A:318:ILE:HG13	1.80	0.47
1:A:745:ALA:O	1:A:748:LYS:HB3	2.15	0.47
1:B:111:THR:HA	1:B:112:GLY:HA3	1.65	0.47
1:B:725:ILE:O	1:B:729:LEU:HG	2.15	0.47
1:A:80:LEU:HD21	1:A:477:ASN:HD21	1.79	0.47
1:A:212:ALA:H	1:A:218:GLY:C	2.23	0.47
1:A:322:ILE:HG22	1:A:325:MET:HE2	1.95	0.47
1:A:344:GLY:HA2	1:A:557:PRO:HB3	1.96	0.47
1:A:376:VAL:O	1:A:386:PHE:N	2.47	0.47
1:A:580:TRP:CE3	1:A:581:HIS:HA	2.49	0.47
1:A:757:GLY:HA3	1:A:759:VAL:H	1.79	0.47
1:B:145:LEU:O	1:B:149:ILE:HG12	2.14	0.47
1:B:195:LEU:O	1:B:198:MET:HB3	2.14	0.47
1:A:6:VAL:HG11	1:A:530:VAL:HG23	1.96	0.47
1:B:474:ARG:O	1:B:477:ASN:HB3	2.15	0.47
1:A:56:VAL:HG13	1:A:66:TYR:CE1	2.50	0.47
1:A:493:TYR:CZ	1:A:549:ILE:HG12	2.49	0.47
1:B:7:LYS:HD3	1:B:531:GLY:N	2.22	0.47
1:B:54:TRP:CZ3	1:B:65:MET:HG2	2.50	0.47
1:B:125:LYS:NZ	1:B:155:CYS:HA	2.29	0.47
1:B:144:GLU:OE1	1:B:144:GLU:N	2.45	0.47
1:B:619:GLU:N	1:B:619:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:HIS:HE1	1:B:739:SER:HB3	1.80	0.47
1:A:280:GLY:N	1:A:282:ASP:OD1	2.48	0.47
1:A:331:PHE:C	1:A:332:LYS:HG2	2.40	0.47
1:B:9:LEU:HD22	1:B:546:LEU:HD12	1.97	0.47
1:B:136:ARG:HH21	1:B:147:HIS:CG	2.33	0.47
1:A:149:ILE:HA	1:A:152:ASP:OD2	2.15	0.46
1:A:535:ILE:HG13	1:A:540:ILE:HG23	1.96	0.46
1:B:129:THR:HG22	1:B:151:THR:HG21	1.96	0.46
1:B:297:MET:HA	1:B:300:GLN:OE1	2.15	0.46
1:B:414:VAL:O	1:B:418:THR:HG23	2.15	0.46
1:B:449:TYR:HH	1:B:630:HIS:CE1	2.19	0.46
1:B:154:VAL:HG22	1:B:229:LEU:HD13	1.97	0.46
1:B:176:ARG:NH2	1:B:446:GLU:O	2.44	0.46
1:B:317:ILE:HA	1:B:320:TRP:CE2	2.50	0.46
1:B:354:GLN:NE2	1:B:431:ASN:HD22	2.12	0.46
1:B:677:LYS:O	1:B:680:MET:HG2	2.15	0.46
1:A:212:ALA:HB3	1:A:219:ALA:HB3	1.97	0.46
1:A:436:GLU:CD	1:A:438:THR:H	2.23	0.46
1:B:386:PHE:CE1	1:B:576:HIS:N	2.83	0.46
1:B:427:ARG:HB3	1:B:428:GLY:HA3	1.97	0.46
1:B:481:ARG:O	1:B:485:ASN:ND2	2.48	0.46
1:B:577:ILE:HG13	1:B:578:TRP:H	1.80	0.46
1:B:673:THR:O	1:B:677:LYS:HD3	2.14	0.46
1:A:337:ASN:HD21	1:A:496:ALA:HB2	1.80	0.46
1:B:529:PRO:O	1:B:530:VAL:HG13	2.16	0.46
1:B:606:VAL:HB	1:B:697:ARG:CZ	2.46	0.46
1:B:610:GLU:OE1	1:B:610:GLU:N	2.42	0.46
1:B:607:LYS:HB2	1:B:608:GLU:C	2.40	0.46
1:B:648:ALA:HA	1:B:651:ARG:HD3	1.98	0.46
1:B:657:ASP:O	1:B:660:LYS:HB3	2.15	0.46
1:A:282:ASP:OD1	1:A:282:ASP:N	2.48	0.46
1:A:314:SER:HA	1:A:315:SER:C	2.41	0.46
1:A:383:ASN:C	1:A:385:ARG:H	2.22	0.46
1:A:418:THR:O	1:A:421:TYR:HD1	1.99	0.46
1:B:53:LEU:HD22	1:B:571:HIS:ND1	2.30	0.46
1:B:318:ILE:HD12	1:B:318:ILE:H	1.80	0.46
1:B:368:LYS:O	1:B:398:SER:OG	2.32	0.46
1:A:210:LEU:HB3	1:A:212:ALA:O	2.16	0.46
1:A:281:ILE:HG22	1:A:319:PRO:HB2	1.98	0.46
1:A:329:SER:HB3	1:A:331:PHE:HB3	1.98	0.46
1:A:349:ILE:HD11	1:A:356:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:ILE:HA	1:A:681:ILE:HG12	1.97	0.46
1:B:18:GLN:OE1	1:B:517:TYR:HB2	2.16	0.46
1:B:164:ILE:HG23	1:B:165:LEU:N	2.31	0.46
1:B:374:THR:N	1:B:387:LEU:O	2.43	0.46
1:A:261:TRP:HE1	1:A:288:LEU:HD11	1.81	0.46
1:A:303:ARG:HB2	1:A:513:GLN:OE1	2.15	0.46
1:B:10:ASN:HB2	1:B:14:ARG:HH11	1.81	0.46
1:B:376:VAL:HG12	1:B:378:LEU:HD23	1.98	0.46
1:B:641:VAL:HG23	1:B:645:ARG:HH12	1.80	0.46
1:B:677:LYS:O	1:B:681:ILE:HG13	2.15	0.46
1:A:328:VAL:HG23	1:A:329:SER:CB	2.46	0.46
1:A:350:ASP:OD1	1:A:350:ASP:N	2.49	0.46
1:A:371:THR:O	1:A:623:ILE:HD12	2.16	0.46
1:A:559:GLU:OE1	1:A:559:GLU:N	2.49	0.46
1:A:666:ARG:O	1:A:670:ASN:ND2	2.49	0.46
1:B:317:ILE:HA	1:B:320:TRP:CD2	2.51	0.46
1:B:590:GLU:HB2	1:B:606:VAL:O	2.16	0.46
1:B:596:THR:HG22	1:B:601:ARG:HD2	1.97	0.46
1:A:3:ASN:HA	1:A:436:GLU:HB3	1.98	0.45
1:A:328:VAL:HG23	1:A:329:SER:HB2	1.97	0.45
1:A:685:GLY:HA2	1:A:686:ILE:HA	1.53	0.45
1:B:63:PRO:HG3	1:B:200:THR:HB	1.98	0.45
1:B:754:ASN:OD1	1:B:755:ALA:N	2.49	0.45
1:A:17:THR:O	1:A:19:ALA:N	2.38	0.45
1:A:410:VAL:CA	1:A:413:PHE:HB3	2.41	0.45
1:B:334:ARG:HA	1:B:335:PRO:HD3	1.80	0.45
1:A:263:PRO:HG3	1:A:504:SER:HA	1.97	0.45
1:A:310:ASP:CG	1:A:311:GLU:H	2.25	0.45
1:A:317:ILE:O	1:A:320:TRP:HB3	2.16	0.45
1:A:662:ALA:HA	1:B:108:ALA:O	2.17	0.45
1:B:10:ASN:ND2	1:B:29:LEU:HD21	2.30	0.45
1:B:413:PHE:HB3	1:B:636:TRP:CZ2	2.51	0.45
1:A:69:LEU:HD22	1:A:172:TYR:HD2	1.80	0.45
1:A:146:PHE:HA	1:A:149:ILE:HB	1.97	0.45
1:A:498:ASN:OD1	1:A:499:PRO:HD2	2.15	0.45
1:A:284:LEU:HA	1:A:287:ASN:CG	2.41	0.45
1:A:298:VAL:HG21	1:A:514:GLY:O	2.17	0.45
1:A:315:SER:O	1:A:319:PRO:HD2	2.16	0.45
1:A:371:THR:HB	1:A:389:VAL:HG23	1.96	0.45
1:A:479:LEU:HB3	1:A:483:MET:HE2	1.98	0.45
1:A:502:VAL:HG23	1:A:503:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:HD12	1:A:568:LEU:HD23	1.98	0.45
1:B:89:PHE:O	1:B:92:TYR:HB3	2.16	0.45
1:A:16:LEU:HD21	1:A:462:LEU:HB3	1.99	0.45
1:A:75:GLN:HE22	1:A:447:ARG:NH2	2.14	0.45
1:A:410:VAL:O	1:A:414:VAL:HG23	2.16	0.45
1:A:428:GLY:HA3	1:A:429:THR:HA	1.59	0.45
1:A:652:ARG:O	1:A:653:THR:OG1	2.30	0.45
1:B:55:GLU:O	1:B:58:LYS:NZ	2.49	0.45
1:B:254:LEU:O	1:B:257:LEU:HB3	2.17	0.45
1:A:201:ALA:HB1	1:A:239:ARG:HD3	1.98	0.45
1:A:209:MET:O	1:A:210:LEU:HB2	2.16	0.45
1:A:503:VAL:HG11	1:A:517:TYR:O	2.16	0.45
1:A:595:VAL:HG12	1:A:597:ILE:HG23	1.99	0.45
1:B:25:LEU:O	1:B:27:ASN:N	2.49	0.45
1:B:42:ARG:HG2	1:B:335:PRO:O	2.17	0.45
1:B:326:SER:CB	1:B:328:VAL:HG22	2.47	0.45
1:A:138:LEU:HB3	1:A:139:ALA:H	1.69	0.45
1:A:498:ASN:C	1:A:500:GLU:H	2.24	0.45
1:A:674:LEU:HA	1:A:677:LYS:NZ	2.32	0.45
1:B:628:VAL:O	1:B:632:ILE:HG22	2.17	0.45
1:A:224:LEU:HA	1:A:227:GLN:HB3	1.99	0.45
1:A:503:VAL:HG22	1:A:504:SER:H	1.81	0.45
1:B:42:ARG:HH11	1:B:339:THR:CA	2.30	0.45
1:B:426:GLN:HA	1:B:427:ARG:HA	1.74	0.45
1:B:497:HIS:HE1	1:B:555:ILE:HD13	1.82	0.45
1:A:211:GLN:O	1:A:218:GLY:HA3	2.18	0.44
1:B:143:HIS:HB3	1:B:145:LEU:HG	1.98	0.44
1:B:321:PHE:CE1	1:B:325:MET:HG3	2.52	0.44
1:B:346:THR:OG1	1:B:359:VAL:HG21	2.17	0.44
1:A:435:ALA:C	1:A:437:MET:HG3	2.42	0.44
1:B:125:LYS:HB2	1:B:163:PHE:HB3	1.98	0.44
1:B:437:MET:HE2	1:B:546:LEU:HB3	1.99	0.44
1:B:454:ASP:O	1:B:457:VAL:HG22	2.17	0.44
1:A:313:LEU:HB3	1:A:314:SER:HB3	1.99	0.44
1:A:366:PHE:O	1:A:368:LYS:HD2	2.17	0.44
1:A:500:GLU:HB3	1:A:521:ASN:H	1.83	0.44
1:B:125:LYS:HB3	1:B:165:LEU:O	2.18	0.44
1:B:609:PHE:HA	1:B:616:GLN:OE1	2.18	0.44
1:A:51:GLU:CA	1:A:174:VAL:HG21	2.44	0.44
1:A:57:GLY:N	1:A:170:TYR:HB2	2.30	0.44
1:A:271:PRO:HA	1:A:276:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:VAL:O	1:A:753:SER:OG	2.35	0.44
1:B:122:ALA:H	1:B:163:PHE:HE1	1.64	0.44
1:B:125:LYS:HE2	1:B:163:PHE:CB	2.47	0.44
1:A:55:GLU:N	1:A:55:GLU:OE1	2.51	0.44
1:A:719:ASN:O	1:A:722:ARG:HB3	2.18	0.44
1:B:61:ILE:HD13	1:B:156:HIS:HB3	1.99	0.44
1:B:274:ARG:CB	1:B:312:GLU:HG3	2.46	0.44
1:B:332:LYS:HE2	1:B:334:ARG:NH1	2.30	0.44
1:A:66:TYR:HD1	1:A:69:LEU:HD12	1.83	0.44
1:A:423:ALA:HA	1:A:424:VAL:HA	1.48	0.44
1:B:233:ALA:HA	1:B:236:ALA:HB3	1.98	0.44
1:B:280:GLY:HA2	1:B:283:GLN:HE22	1.83	0.44
1:B:292:ILE:HG21	1:B:488:ALA:HB2	1.98	0.44
1:B:577:ILE:HG13	1:B:578:TRP:N	2.33	0.44
1:A:366:PHE:CD2	1:A:405:GLY:HA2	2.52	0.44
1:A:549:ILE:HA	1:A:552:ASN:HB2	2.00	0.44
1:A:590:GLU:OE1	1:A:607:LYS:HD3	2.18	0.44
1:B:56:VAL:O	1:B:170:TYR:N	2.50	0.44
1:B:106:LEU:O	1:B:109:TYR:HB3	2.17	0.44
1:A:260:LEU:HD11	1:A:285:ARG:HH12	1.82	0.44
1:A:337:ASN:O	1:A:341:SER:N	2.50	0.44
1:A:610:GLU:C	1:A:613:GLY:H	2.26	0.44
1:B:172:TYR:CE1	1:B:579:PRO:HG2	2.51	0.44
1:B:225:ILE:O	1:B:228:HIS:HB3	2.18	0.44
1:B:228:HIS:CD2	1:B:228:HIS:C	2.95	0.44
1:B:387:LEU:HD23	1:B:578:TRP:CH2	2.53	0.44
1:A:56:VAL:HB	1:A:170:TYR:HB2	2.00	0.44
1:A:199:LEU:HD23	1:A:203:SER:HB2	1.99	0.44
1:A:385:ARG:HD2	1:A:580:TRP:NE1	2.29	0.44
1:A:737:LEU:O	1:A:738:LEU:HG	2.18	0.44
1:B:14:ARG:CZ	1:B:26:LYS:HA	2.48	0.44
1:B:321:PHE:CD1	1:B:325:MET:HG3	2.53	0.44
1:B:656:ASP:HB3	1:B:659:GLU:CG	2.48	0.44
1:A:116:ARG:HA	1:A:118:ILE:H	1.82	0.43
1:A:348:ALA:O	1:A:349:ILE:HG22	2.18	0.43
1:B:9:LEU:HD12	1:B:10:ASN:N	2.33	0.43
1:B:251:SER:O	1:B:254:LEU:HB3	2.18	0.43
1:B:610:GLU:HG2	1:B:612:LEU:N	2.33	0.43
1:B:675:LEU:HD21	1:B:757:GLY:O	2.18	0.43
1:A:293:ALA:O	1:A:297:MET:HB2	2.19	0.43
1:A:402:ALA:HB3	1:A:403:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ASP:O	1:A:457:VAL:HG12	2.18	0.43
1:B:66:TYR:CD1	1:B:69:LEU:HD12	2.49	0.43
1:A:68:ARG:CZ	1:A:330:PRO:HG3	2.49	0.43
1:A:389:VAL:HG13	1:A:391:PRO:HD3	1.99	0.43
1:A:655:ARG:H	1:A:656:ASP:CB	2.30	0.43
1:B:62:ASP:HB3	1:B:65:MET:HE2	2.00	0.43
1:B:228:HIS:O	1:B:230:ALA:N	2.51	0.43
1:B:349:ILE:HD12	1:B:353:GLY:HA3	2.00	0.43
1:A:259:ARG:O	1:A:262:SER:OG	2.23	0.43
1:A:359:VAL:HG22	1:A:437:MET:O	2.19	0.43
1:A:590:GLU:OE2	1:A:607:LYS:HA	2.18	0.43
1:A:682:GLY:O	1:A:684:THR:N	2.51	0.43
1:B:133:GLU:O	1:B:136:ARG:HB3	2.18	0.43
1:B:209:MET:HG3	1:B:228:HIS:CE1	2.54	0.43
1:B:230:ALA:HB1	1:B:233:ALA:HB3	2.00	0.43
1:A:501:VAL:C	1:A:519:VAL:HG12	2.43	0.43
1:B:41:THR:C	1:B:43:THR:N	2.77	0.43
1:B:225:ILE:O	1:B:229:LEU:N	2.23	0.43
1:B:234:THR:O	1:B:237:PHE:HB3	2.17	0.43
1:B:313:LEU:HD12	1:B:313:LEU:O	2.18	0.43
1:B:681:ILE:HG21	1:B:728:GLY:HA2	1.99	0.43
1:A:59:GLY:HA3	1:A:155:CYS:HB3	2.00	0.43
1:A:204:SER:O	1:A:206:ASP:N	2.52	0.43
1:A:221:ALA:HB1	1:A:224:LEU:HB3	1.99	0.43
1:A:362:GLU:OE1	1:A:443:SER:OG	2.35	0.43
1:A:424:VAL:HG12	1:A:425:SER:O	2.18	0.43
1:B:604:ALA:HB1	1:B:697:ARG:NH2	2.32	0.43
1:A:49:THR:OG1	1:A:50:SER:N	2.44	0.43
1:A:349:ILE:HD12	1:A:349:ILE:HA	1.79	0.43
1:A:674:LEU:HA	1:A:677:LYS:HG2	2.00	0.43
1:B:510:ALA:HB3	1:B:511:ALA:C	2.44	0.43
1:B:675:LEU:O	1:B:678:ILE:HG13	2.19	0.43
1:A:241:ARG:HG3	1:A:243:ASN:H	1.84	0.43
1:A:329:SER:C	1:A:331:PHE:H	2.27	0.43
1:A:345:GLN:HE22	1:A:549:ILE:HG23	1.83	0.43
1:A:368:LYS:HE2	1:A:402:ALA:O	2.18	0.43
1:A:369:GLU:HA	1:A:398:SER:CB	2.49	0.43
1:A:436:GLU:C	1:A:438:THR:H	2.26	0.43
1:A:544:GLU:HG2	1:A:545:PRO:HD2	2.01	0.43
1:A:602:TYR:CD1	1:A:702:MET:HE1	2.53	0.43
1:A:715:HIS:HB2	1:A:716:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:ASN:H	1:A:755:ALA:HA	1.82	0.43
1:B:521:ASN:OD1	1:B:539:SER:HB3	2.18	0.43
1:B:721:HIS:CD2	1:B:757:GLY:HA2	2.54	0.43
1:B:732:LEU:HD13	1:B:743:ALA:HB2	2.00	0.43
1:A:177:THR:HA	1:A:447:ARG:HH22	1.83	0.43
1:A:368:LYS:HA	1:A:401:LEU:HD23	2.01	0.43
1:B:2:PHE:N	1:B:439:LEU:O	2.50	0.43
1:B:160:PRO:HG3	1:B:210:LEU:HD22	2.00	0.43
1:B:314:SER:C	1:B:316:THR:H	2.27	0.43
1:B:604:ALA:HB1	1:B:697:ARG:HH21	1.83	0.43
1:A:54:TRP:CH2	1:A:174:VAL:HG12	2.54	0.43
1:A:176:ARG:NH1	1:A:447:ARG:HA	2.26	0.43
1:A:566:LEU:CD1	1:A:568:LEU:HB3	2.49	0.43
1:B:3:ASN:HA	1:B:437:MET:O	2.19	0.43
1:B:153:PHE:CZ	1:B:202:LEU:HD23	2.51	0.43
1:B:359:VAL:HG22	1:B:418:THR:HG22	2.00	0.43
1:B:360:VAL:HG23	1:B:439:LEU:HB3	2.00	0.43
1:B:376:VAL:N	1:B:386:PHE:O	2.50	0.43
1:A:41:THR:OG1	1:A:42:ARG:N	2.51	0.42
1:A:182:ASN:HD21	1:A:184:TYR:HD2	1.67	0.42
1:A:536:GLU:N	1:A:536:GLU:OE1	2.40	0.42
1:A:628:VAL:O	1:A:632:ILE:HD12	2.19	0.42
1:A:666:ARG:HA	1:A:669:GLN:NE2	2.31	0.42
1:A:732:LEU:O	1:A:735:MET:HB3	2.18	0.42
1:B:13:ALA:HA	1:B:463:ARG:O	2.19	0.42
1:B:423:ALA:O	1:B:430:VAL:HG22	2.19	0.42
1:A:80:LEU:HA	1:A:81:SER:HA	1.78	0.42
1:A:520:TRP:CH2	1:A:545:PRO:HG3	2.54	0.42
1:A:716:VAL:HG21	1:B:386:PHE:CD2	2.54	0.42
1:B:257:LEU:HG	1:B:261:TRP:HE1	1.84	0.42
1:B:316:THR:HG22	1:B:320:TRP:CD1	2.53	0.42
1:B:675:LEU:HD21	1:B:758:MET:N	2.34	0.42
1:A:630:HIS:HD2	1:A:633:ILE:HD11	1.83	0.42
1:B:716:VAL:C	1:B:720:ARG:HH12	2.27	0.42
1:A:246:ALA:O	1:A:249:VAL:HG22	2.19	0.42
1:A:292:ILE:HD11	1:A:491:MET:HG3	2.02	0.42
1:A:523:ARG:HA	1:A:539:SER:HB2	2.01	0.42
1:A:739:SER:OG	1:A:742:GLU:OE1	2.32	0.42
1:B:130:ALA:O	1:B:133:GLU:HB3	2.20	0.42
1:B:345:GLN:O	1:B:554:PRO:HB3	2.20	0.42
1:B:606:VAL:HG22	1:B:607:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:ARG:C	1:B:619:GLU:HB3	2.43	0.42
1:A:2:PHE:HE2	1:A:4:LEU:HD23	1.85	0.42
1:A:43:THR:HA	1:A:289:ALA:CB	2.50	0.42
1:A:259:ARG:HG3	1:A:269:LEU:HD13	2.01	0.42
1:A:291:PHE:O	1:A:292:ILE:HB	2.19	0.42
1:B:40:PHE:CZ	1:B:495:VAL:HG13	2.54	0.42
1:A:383:ASN:C	1:A:385:ARG:N	2.76	0.42
1:A:474:ARG:HA	1:A:474:ARG:HD3	1.82	0.42
1:A:498:ASN:ND2	1:A:500:GLU:HG2	2.33	0.42
1:A:510:ALA:HA	1:A:511:ALA:HA	1.72	0.42
1:B:43:THR:HG21	1:B:289:ALA:N	2.34	0.42
1:B:518:LEU:O	1:B:543:PRO:HA	2.19	0.42
1:A:608:GLU:HG3	1:A:609:PHE:N	2.35	0.42
1:A:676:ARG:NH1	1:B:165:LEU:HD23	2.34	0.42
1:B:254:LEU:HD22	1:B:297:MET:HE2	2.02	0.42
1:B:684:THR:O	1:B:688:ALA:N	2.51	0.42
1:A:331:PHE:O	1:A:332:LYS:HG2	2.19	0.42
1:A:373:PHE:CE1	1:A:387:LEU:HD22	2.54	0.42
1:B:2:PHE:CZ	1:B:463:ARG:HG2	2.55	0.42
1:B:19:ALA:HB1	1:B:24:GLU:HB3	2.02	0.42
1:B:494:ALA:HB2	1:B:549:ILE:HD11	2.02	0.42
1:A:41:THR:HG23	1:A:286:SER:O	2.20	0.42
1:A:82:VAL:O	1:A:86:VAL:HG23	2.19	0.42
1:A:101:GLU:OE1	1:A:101:GLU:N	2.49	0.42
1:A:133:GLU:O	1:A:137:THR:HG23	2.20	0.42
1:A:292:ILE:HA	1:A:295:GLN:CG	2.50	0.42
1:A:377:LYS:HD2	1:A:380:ASN:HA	2.01	0.42
1:A:629:ALA:HA	1:A:632:ILE:HD13	2.02	0.42
1:B:257:LEU:HG	1:B:261:TRP:NE1	2.34	0.42
1:B:387:LEU:HD11	1:B:568:LEU:HD13	2.02	0.42
1:B:522:VAL:HB	1:B:540:ILE:HD11	2.02	0.42
1:B:546:LEU:O	1:B:549:ILE:HB	2.19	0.42
1:B:610:GLU:CG	1:B:614:LEU:H	2.33	0.42
1:A:117:ALA:H	1:A:221:ALA:N	1.94	0.41
1:A:181:PRO:HB2	1:A:182:ASN:H	1.43	0.41
1:A:356:SER:C	1:A:437:MET:HE2	2.45	0.41
1:A:386:PHE:HE1	1:A:576:HIS:H	1.68	0.41
1:A:413:PHE:CZ	1:A:636:TRP:HA	2.54	0.41
1:B:19:ALA:HB1	1:B:24:GLU:CB	2.50	0.41
1:B:43:THR:HG21	1:B:289:ALA:HB3	2.02	0.41
1:B:194:ASP:OD1	1:B:194:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:GLU:HG3	1:B:614:LEU:H	1.85	0.41
1:B:640:PHE:HA	1:B:670:ASN:HD21	1.85	0.41
1:B:757:GLY:N	1:B:758:MET:HA	2.35	0.41
1:A:358:VAL:N	1:A:437:MET:HB3	2.31	0.41
1:A:590:GLU:CD	1:A:607:LYS:HD3	2.44	0.41
1:A:753:SER:HA	1:A:754:ASN:HA	1.85	0.41
1:B:313:LEU:HA	1:B:314:SER:HA	1.32	0.41
1:B:384:GLN:HA	1:B:577:ILE:HG21	2.01	0.41
1:A:38:LEU:HD23	1:A:39:GLN:O	2.19	0.41
1:A:230:ALA:HA	1:A:233:ALA:HB3	2.03	0.41
1:A:349:ILE:HG21	1:A:354:GLN:O	2.20	0.41
1:A:708:ILE:O	1:A:711:SER:OG	2.22	0.41
1:B:401:LEU:O	1:B:405:GLY:N	2.53	0.41
1:A:144:GLU:O	1:A:145:LEU:C	2.63	0.41
1:A:349:ILE:HG13	1:A:353:GLY:O	2.21	0.41
1:A:553:LYS:O	1:A:555:ILE:HG23	2.20	0.41
1:B:118:ILE:H	1:B:222:PRO:HD2	1.85	0.41
1:B:284:LEU:HA	1:B:287:ASN:HD22	1.86	0.41
1:B:410:VAL:HA	1:B:413:PHE:HD2	1.85	0.41
1:B:522:VAL:O	1:B:540:ILE:HG13	2.20	0.41
1:A:281:ILE:O	1:A:284:LEU:HB2	2.21	0.41
1:A:307:ILE:C	1:A:309:SER:H	2.27	0.41
1:A:366:PHE:CE1	1:A:629:ALA:HB2	2.54	0.41
1:B:59:GLY:C	1:B:61:ILE:HD12	2.45	0.41
1:B:198:MET:HG3	1:B:202:LEU:HD22	2.02	0.41
1:B:289:ALA:HA	1:B:292:ILE:HD13	2.02	0.41
1:B:637:TYR:O	1:B:641:VAL:HG22	2.20	0.41
1:A:44:PHE:HE1	1:A:180:TYR:N	2.18	0.41
1:A:128:PRO:O	1:A:131:ILE:HB	2.21	0.41
1:A:128:PRO:HD3	1:A:166:PRO:HB2	2.03	0.41
1:A:241:ARG:C	1:A:243:ASN:H	2.28	0.41
1:A:357:HIS:HA	1:A:437:MET:HG2	2.02	0.41
1:A:657:ASP:O	1:A:660:LYS:HG2	2.20	0.41
1:B:13:ALA:HB1	1:B:462:LEU:HD23	2.03	0.41
1:B:62:ASP:HB3	1:B:65:MET:HG3	2.03	0.41
1:B:669:GLN:O	1:B:672:VAL:HG12	2.21	0.41
1:B:43:THR:HG22	1:B:44:PHE:O	2.21	0.41
1:B:92:TYR:OH	1:B:150:THR:HG21	2.21	0.41
1:B:132:LEU:HD23	1:B:147:HIS:NE2	2.35	0.41
1:B:267:LYS:HA	1:B:270:ASP:CG	2.45	0.41
1:B:383:ASN:O	1:B:577:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:ARG:H	1:B:428:GLY:HA3	1.86	0.41
1:A:173:ARG:HH11	1:A:579:PRO:HG2	1.86	0.41
1:A:186:LEU:O	1:A:190:VAL:HG13	2.21	0.41
1:A:257:LEU:O	1:A:260:LEU:HB3	2.21	0.41
1:A:334:ARG:HG3	1:A:335:PRO:HD2	2.03	0.41
1:A:349:ILE:CD1	1:A:356:SER:HB2	2.51	0.41
1:A:521:ASN:HA	1:A:540:ILE:O	2.21	0.41
1:A:659:GLU:O	1:A:662:ALA:HB3	2.20	0.41
1:B:35:GLN:HE21	1:B:502:VAL:CG2	2.32	0.41
1:B:171:VAL:HG12	1:B:576:HIS:HB3	2.03	0.41
1:B:342:TYR:HA	1:B:558:SER:H	1.86	0.41
1:B:505:GLU:HB2	1:B:506:HIS:O	2.20	0.41
1:B:674:LEU:HA	1:B:674:LEU:HD23	1.82	0.41
1:B:676:ARG:HA	1:B:679:GLU:OE1	2.21	0.41
1:A:17:THR:C	1:A:19:ALA:H	2.23	0.41
1:A:27:ASN:OD1	1:A:28:GLN:N	2.54	0.41
1:A:216:ALA:HA	1:A:217:LYS:HA	1.72	0.41
1:A:436:GLU:O	1:A:438:THR:N	2.54	0.41
1:A:657:ASP:HA	1:A:660:LYS:HE3	2.03	0.41
1:B:135:LEU:HG	1:B:138:LEU:HD12	2.02	0.41
1:B:162:GLY:HA2	1:B:163:PHE:C	2.46	0.41
1:B:210:LEU:HD12	1:B:211:GLN:N	2.36	0.41
1:A:141:SER:HB3	1:A:144:GLU:HA	2.03	0.41
1:A:440:GLY:O	1:A:635:MET:HE3	2.20	0.41
1:A:506:HIS:CD2	1:A:517:TYR:CE2	3.09	0.41
1:B:68:ARG:NH1	1:B:328:VAL:O	2.54	0.41
1:B:132:LEU:CA	1:B:135:LEU:HB2	2.49	0.41
1:B:141:SER:CB	1:B:147:HIS:HB2	2.50	0.41
1:B:173:ARG:CZ	1:B:578:TRP:HE1	2.34	0.41
1:B:272:SER:C	1:B:276:ARG:HG3	2.46	0.41
1:B:451:LEU:HG	1:B:453:ARG:CZ	2.51	0.41
1:B:510:ALA:N	1:B:511:ALA:HA	2.35	0.41
1:A:306:VAL:C	1:A:307:ILE:HG13	2.45	0.40
1:A:674:LEU:O	1:A:678:ILE:HG13	2.22	0.40
1:B:303:ARG:HB2	1:B:305:GLU:OE2	2.20	0.40
1:B:519:VAL:HG12	1:B:543:PRO:HA	2.03	0.40
1:A:517:TYR:HD1	1:A:518:LEU:H	1.69	0.40
1:B:103:TRP:HH2	1:B:234:THR:HG21	1.86	0.40
1:B:493:TYR:O	1:B:496:ALA:HB3	2.22	0.40
1:B:747:THR:HA	1:B:750:LEU:HG	2.02	0.40
1:A:3:ASN:HA	1:A:436:GLU:CB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ASN:N	1:A:381:ASN:OD1	2.54	0.40
1:A:464:THR:HG23	1:A:466:ILE:HG13	2.04	0.40
1:A:567:ASP:OD2	1:A:570:ASN:ND2	2.31	0.40
1:A:674:LEU:O	1:A:675:LEU:C	2.64	0.40
1:B:6:VAL:HG12	1:B:435:ALA:N	2.36	0.40
1:B:118:ILE:O	1:B:120:ALA:N	2.54	0.40
1:B:321:PHE:CZ	1:B:326:SER:HB3	2.57	0.40
1:B:501:VAL:HG22	1:B:520:TRP:CD1	2.56	0.40
1:A:361:TYR:CD1	1:A:414:VAL:HG21	2.57	0.40
1:A:666:ARG:HD3	1:A:669:GLN:HE22	1.87	0.40
1:B:497:HIS:HE1	1:B:555:ILE:CD1	2.35	0.40
1:A:156:HIS:C	1:A:159:SER:HG	2.26	0.40
1:A:361:TYR:CG	1:A:414:VAL:HG21	2.56	0.40
1:A:389:VAL:HG22	1:A:390:GLU:N	2.37	0.40
1:A:425:SER:CB	1:B:116:ARG:HE	2.35	0.40
1:A:716:VAL:HG11	1:B:386:PHE:CD2	2.56	0.40
1:B:230:ALA:O	1:B:234:THR:HG23	2.22	0.40
1:B:610:GLU:C	1:B:612:LEU:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	759/761 (100%)	593 (78%)	92 (12%)	74 (10%)	0	8
1	B	759/761 (100%)	597 (79%)	108 (14%)	54 (7%)	1	11
All	All	1518/1522 (100%)	1190 (78%)	200 (13%)	128 (8%)	1	9

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	41	THR
1	A	129	THR
1	A	145	LEU
1	A	174	VAL
1	A	222	PRO
1	A	243	ASN
1	A	288	LEU
1	A	292	ILE
1	A	307	ILE
1	A	349	ILE
1	A	503	VAL
1	A	535	ILE
1	A	568	LEU
1	A	581	HIS
1	A	582	GLU
1	A	608	GLU
1	A	684	THR
1	A	738	LEU
1	B	27	ASN
1	B	31	VAL
1	B	126	VAL
1	B	127	PRO
1	B	164	ILE
1	B	280	GLY
1	B	335	PRO
1	B	337	ASN
1	B	359	VAL
1	B	424	VAL
1	B	582	GLU
1	A	45	SER
1	A	61	ILE
1	A	110	ILE
1	A	122	ALA
1	A	181	PRO
1	A	241	ARG
1	A	277	ASN
1	A	309	SER
1	A	316	THR
1	A	332	LYS
1	A	355	PRO
1	A	356	SER
1	A	381	ASN

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Mol	Chain	Res	Type
1	A	502	VAL
1	A	522	VAL
1	A	537	GLY
1	A	555	ILE
1	A	558	SER
1	A	559	GLU
1	A	717	GLY
1	A	740	ARG
1	B	43	THR
1	B	44	PHE
1	B	48	MET
1	B	61	ILE
1	B	80	LEU
1	B	129	THR
1	B	229	LEU
1	B	342	TYR
1	B	388	ASP
1	B	394	SER
1	B	421	TYR
1	B	565	VAL
1	B	583	ALA
1	B	605	GLU
1	B	609	PHE
1	B	717	GLY
1	B	732	LEU
1	A	34	LEU
1	A	167	ASP
1	A	205	VAL
1	A	214	PHE
1	A	335	PRO
1	A	351	HIS
1	A	384	GLN
1	A	409	ALA
1	A	584	SER
1	A	654	SER
1	A	739	SER
1	B	216	ALA
1	B	710	ASP
1	B	755	ALA
1	B	760	VAL
1	A	49	THR
1	A	113	SER

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Mol	Chain	Res	Type
1	A	178	ALA
1	A	273	ALA
1	A	312	GLU
1	A	375	PRO
1	A	556	GLN
1	B	157	VAL
1	B	254	LEU
1	B	363	ASP
1	B	378	LEU
1	B	506	HIS
1	B	527	ARG
1	B	530	VAL
1	B	603	THR
1	B	617	ARG
1	B	644	ASP
1	A	42	ARG
1	A	123	VAL
1	A	328	VAL
1	A	454	ASP
1	A	499	PRO
1	A	515	SER
1	A	624	LEU
1	A	628	VAL
1	B	34	LEU
1	B	214	PHE
1	B	277	ASN
1	B	454	ASP
1	B	704	GLY
1	A	246	ALA
1	A	329	SER
1	A	471	LEU
1	A	578	TRP
1	B	305	GLU
1	B	568	LEU
1	A	336	ILE
1	A	440	GLY
1	A	428	GLY
1	B	162	GLY
1	B	222	PRO
1	A	280	GLY
1	B	322	ILE
1	B	716	VAL

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Mol	Chain	Res	Type
1	B	118	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	629/629 (100%)	626 (100%)	3 (0%)	81	82
1	B	629/629 (100%)	627 (100%)	2 (0%)	86	84
All	All	1258/1258 (100%)	1253 (100%)	5 (0%)	81	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	VAL
1	A	519	VAL
1	A	528	ILE
1	B	292	ILE
1	B	530	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	337	ASN
1	A	345	GLN
1	A	485	ASN
1	A	492	HIS
1	A	506	HIS
1	A	670	ASN
1	A	692	HIS
1	A	695	GLN
1	A	701	GLN
1	B	27	ASN
1	B	35	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	72	GLN
1	B	93	HIS
1	B	99	ASN
1	B	228	HIS
1	B	431	ASN
1	B	492	HIS
1	B	497	HIS
1	B	507	GLN
1	B	634	GLN
1	B	669	GLN
1	B	670	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.

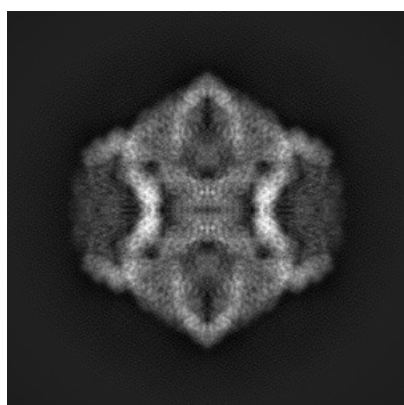
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3185. These allow visual inspection of the internal detail of the map and identification of artifacts.

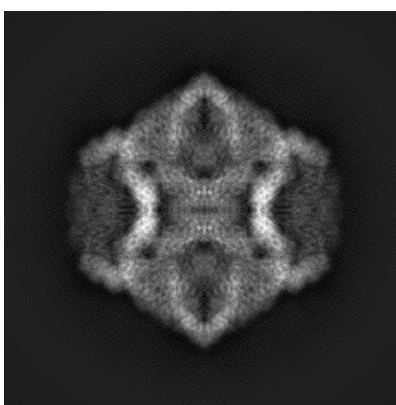
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

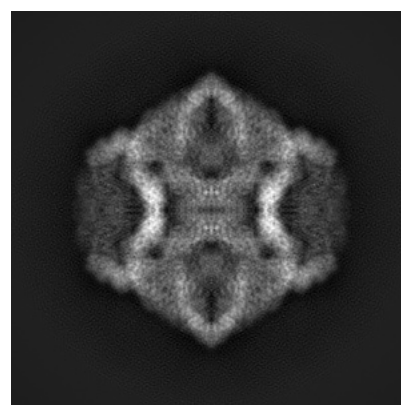
6.1.1 Primary map



X



Y

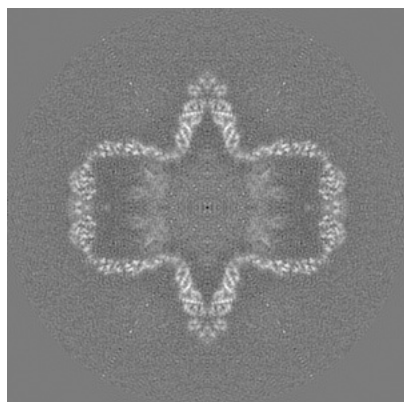


Z

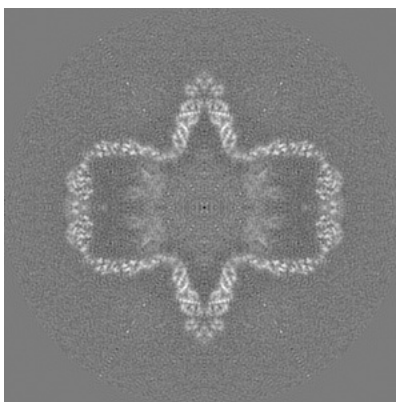
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

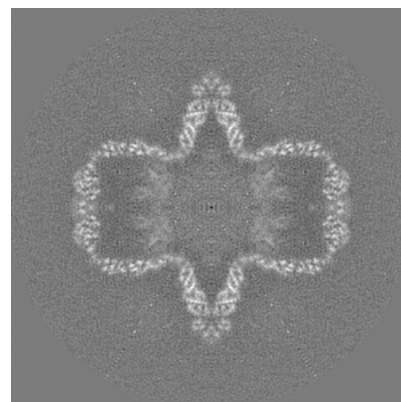
6.2.1 Primary map



X Index: 240



Y Index: 240

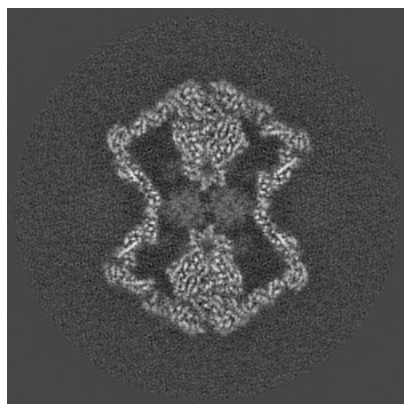


Z Index: 240

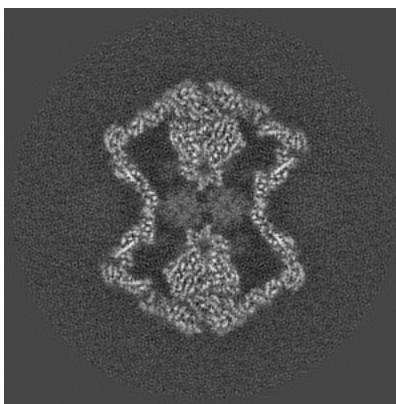
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

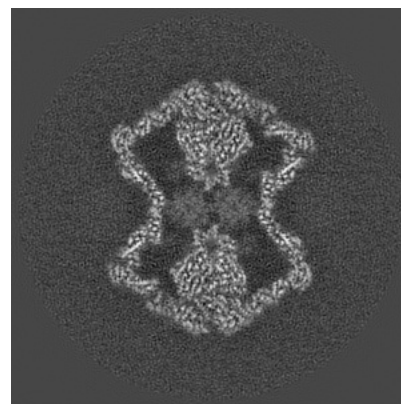
6.3.1 Primary map



X Index: 309



Y Index: 309

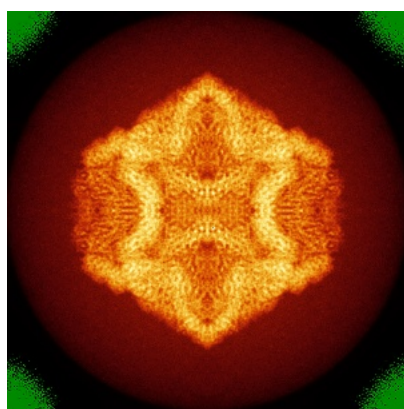


Z Index: 309

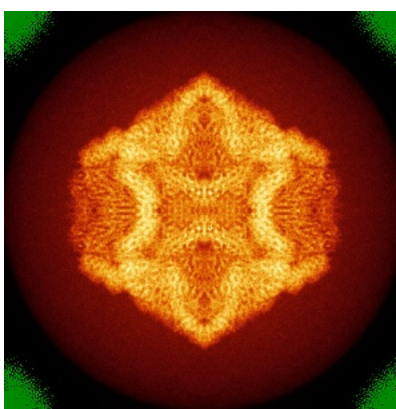
The images above show the largest variance slices of the map in three orthogonal directions.

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

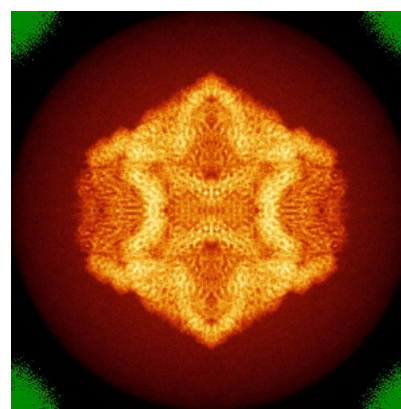
6.4.1 Primary map



X



Y



Z

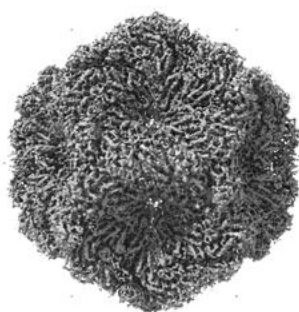
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

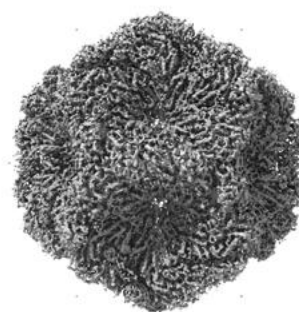
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

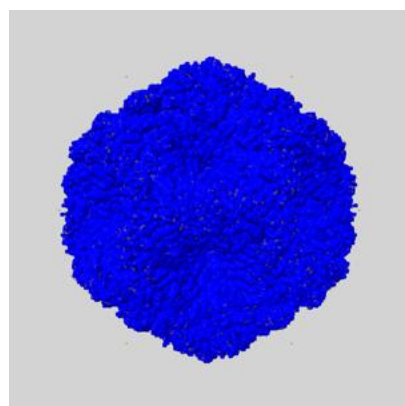
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

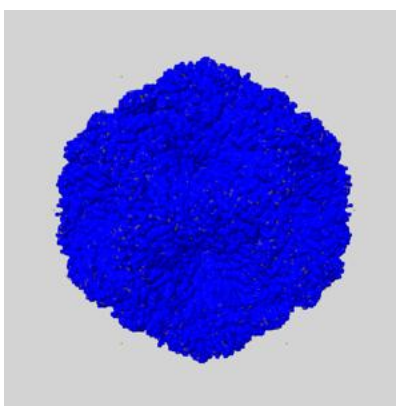
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

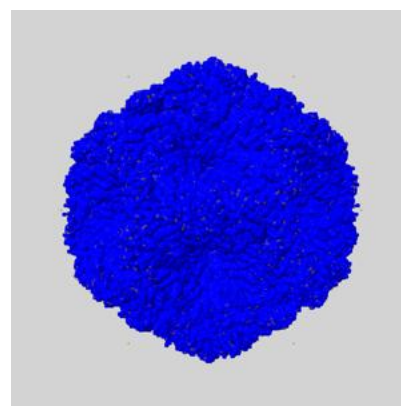
6.6.1 emd_3185_msk_1.map [i](#)



X



Y

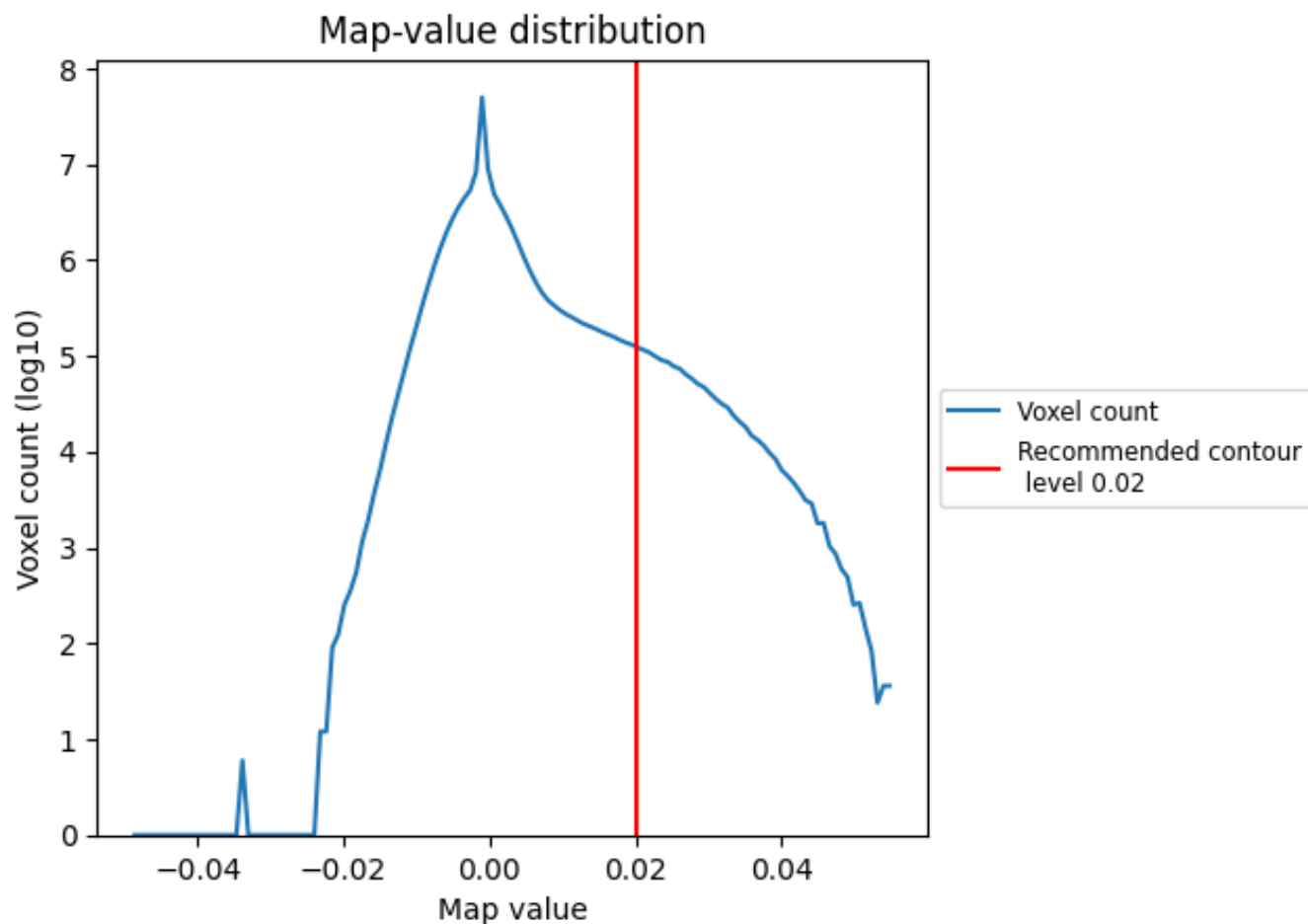


Z

7 Map analysis [i](#)

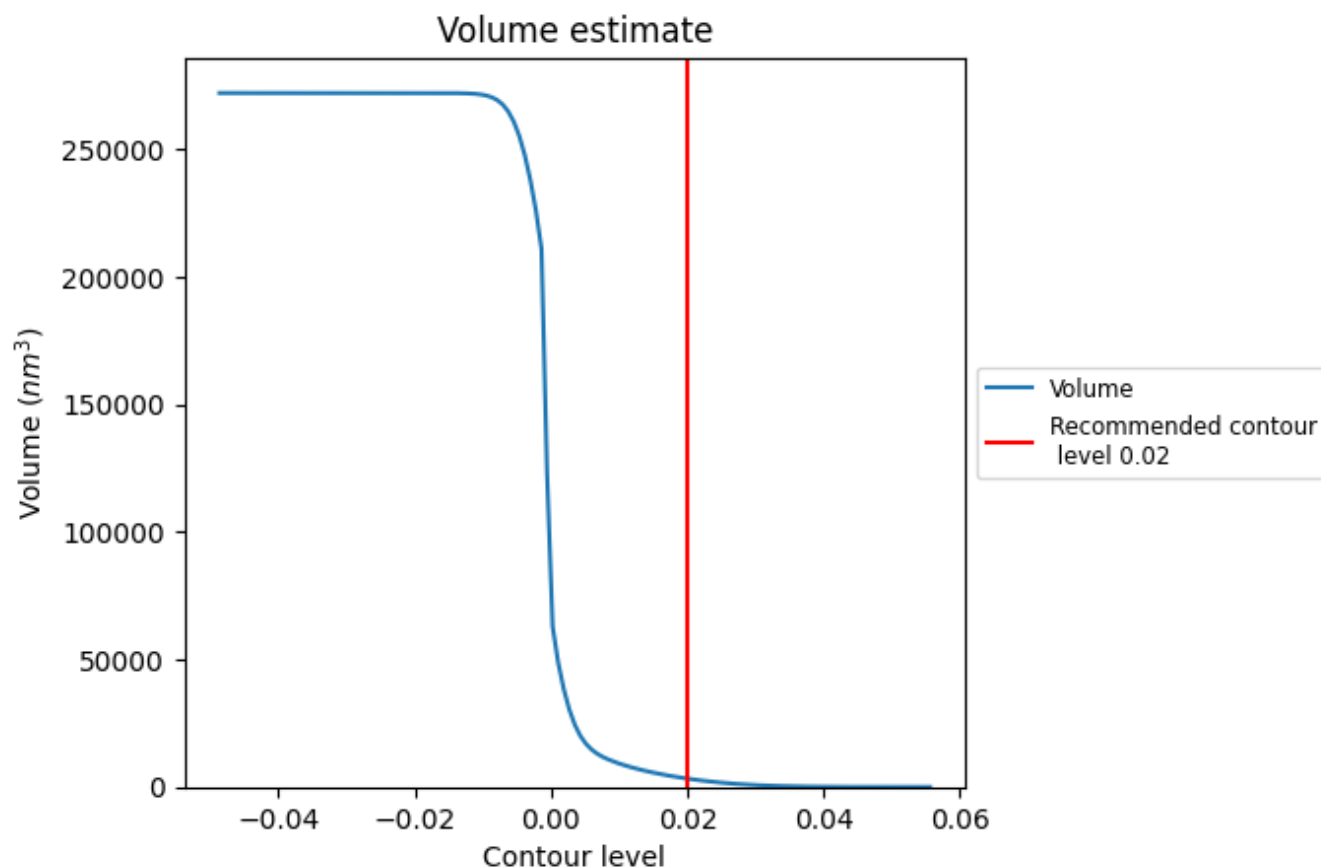
This section contains the results of statistical analysis of the map.

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.

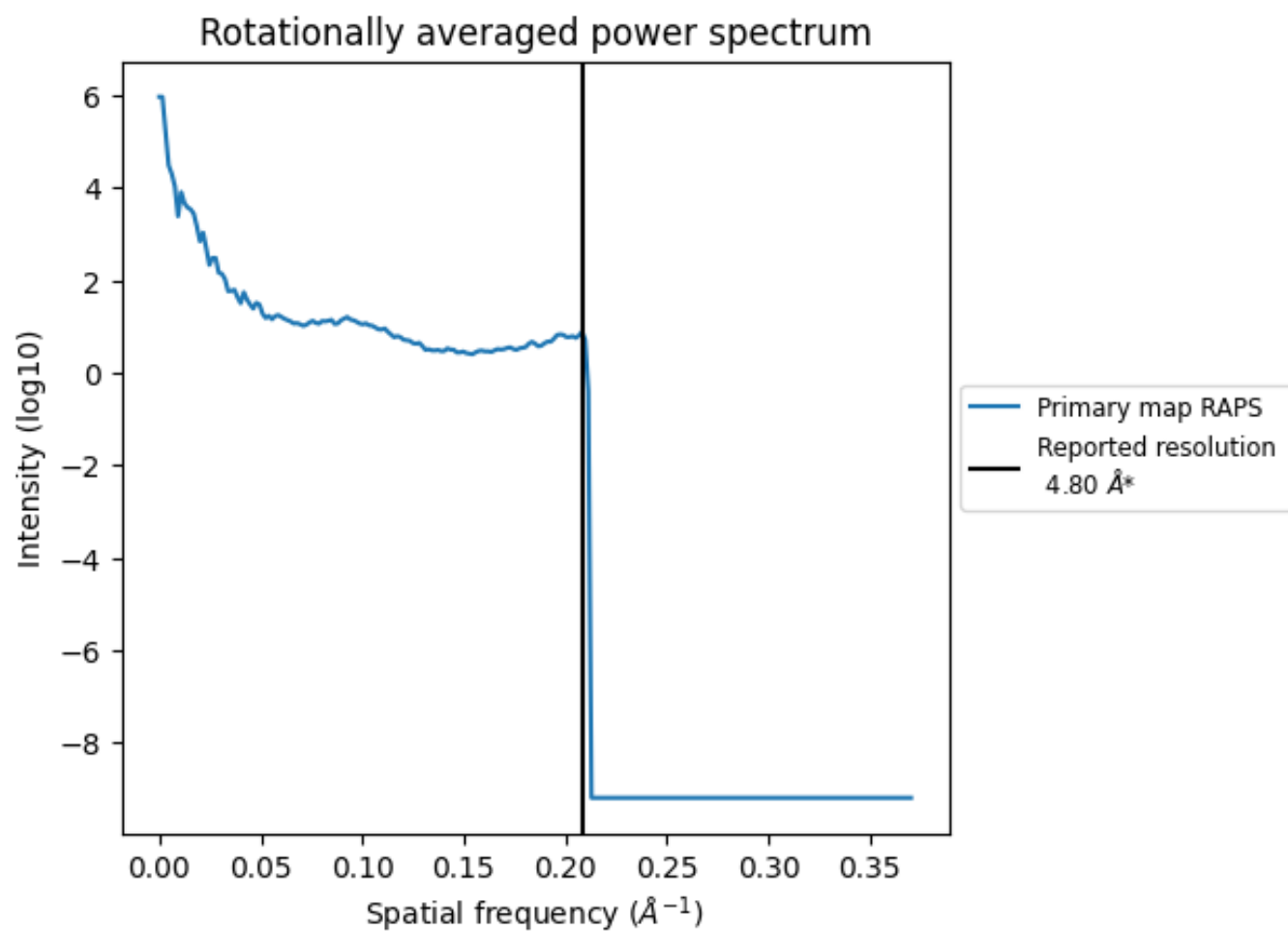
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3274 nm³; this corresponds to an approximate mass of 2957 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 ⓘ

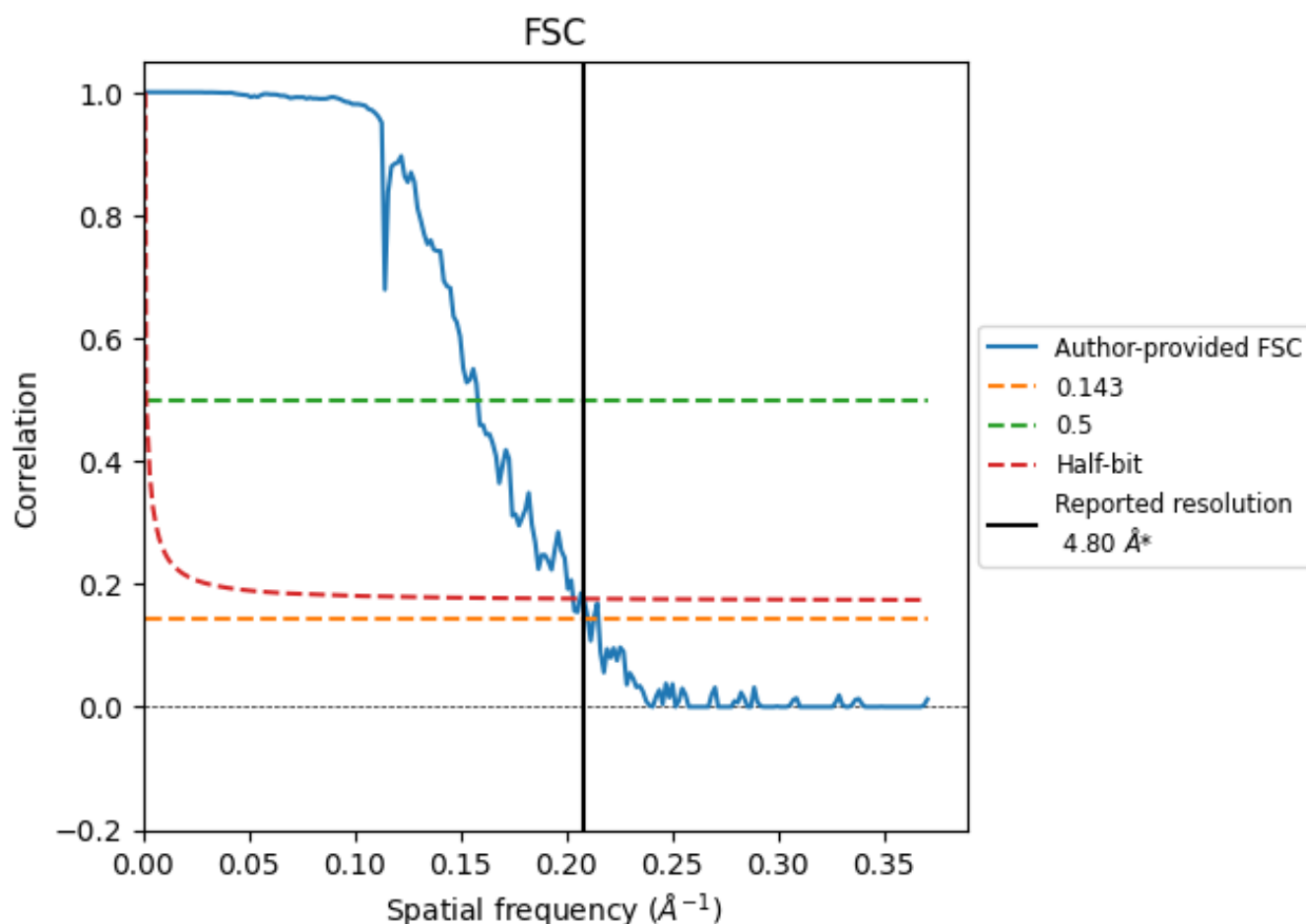


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	4.76	6.33	4.92
Unmasked-calculated*	-	-	-

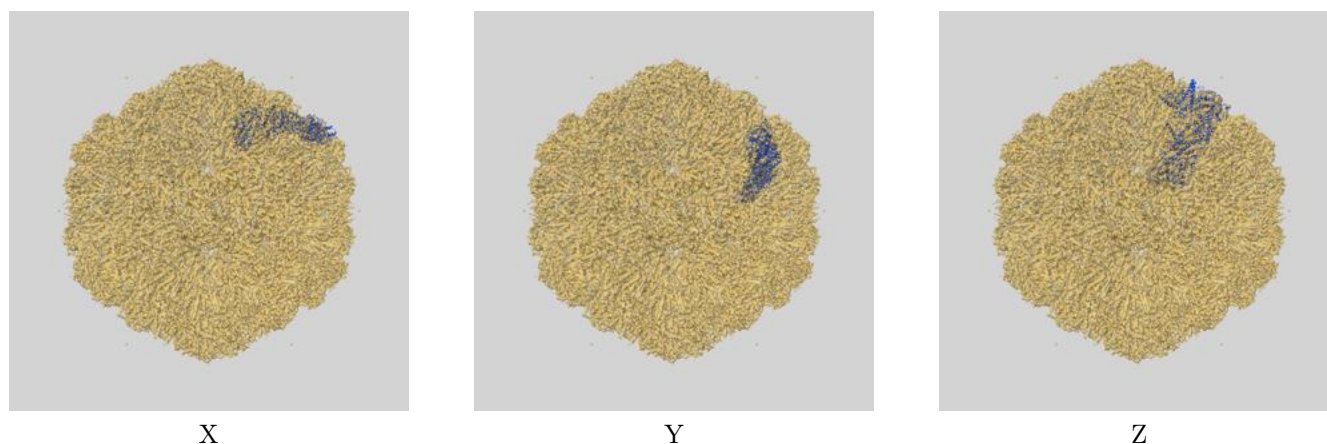
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

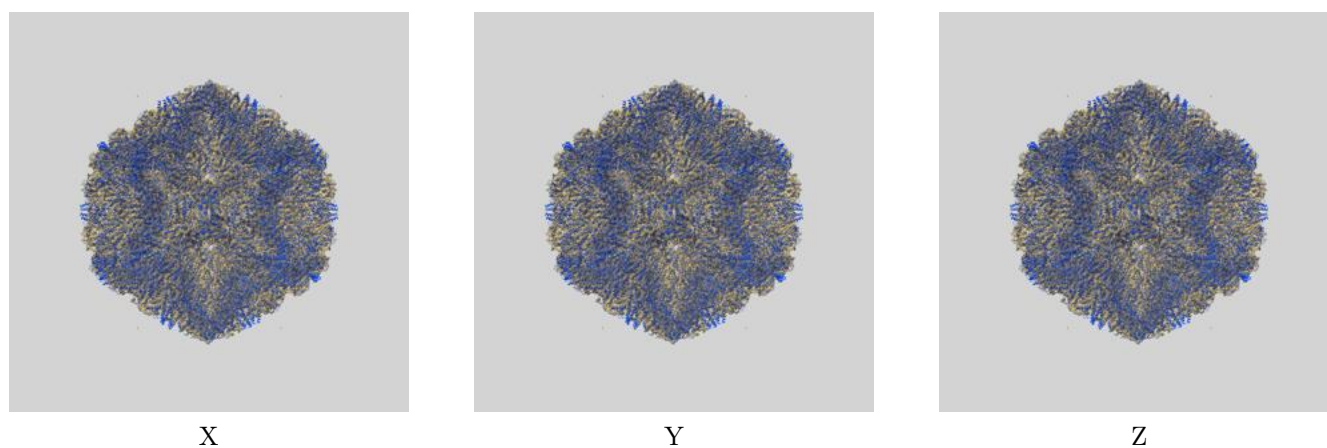
This section contains information regarding the fit between EMDB map EMD-3185 and PDB model 5FJ5. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

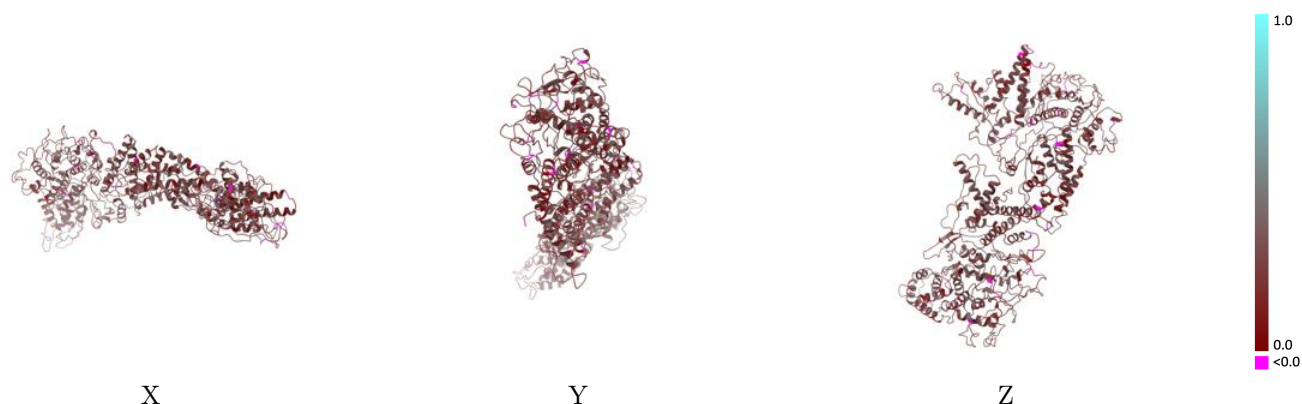


9.1.2 Map-model assembly overlay [i](#)



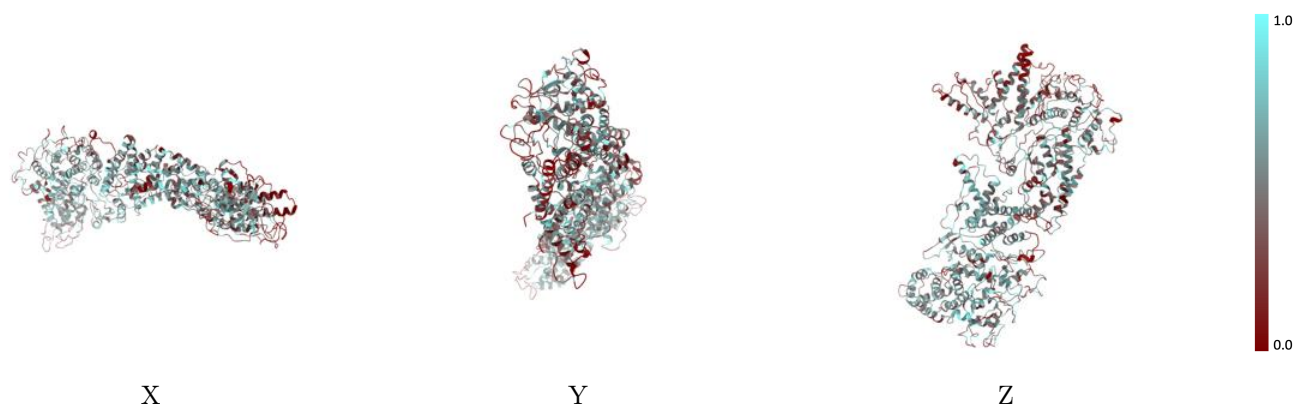
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



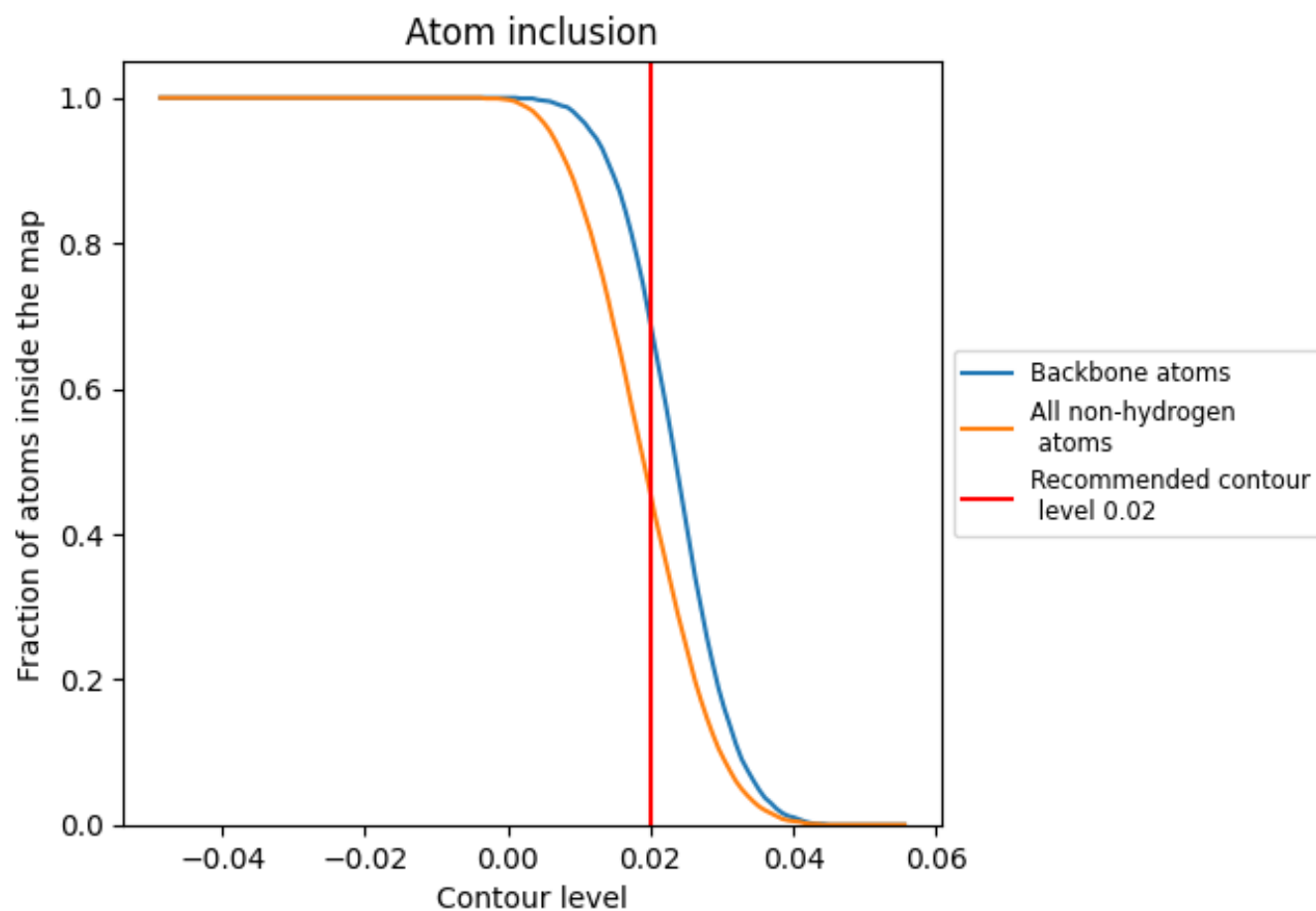
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 46% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4570	0.2720
A	0.5100	0.2860
B	0.4040	0.2590

