



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 09:37 AM UTC

PDB ID : 6WVK / pdb_00006wvk
EMDB ID : EMD-21921
Title : Cryo-EM structure of Bacillus subtilis RNA Polymerase in complex with HelD
Authors : Newing, T.; Tolun, G.; Oakley, A.J.
Deposited on : 2020-05-06
Resolution : 3.36 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

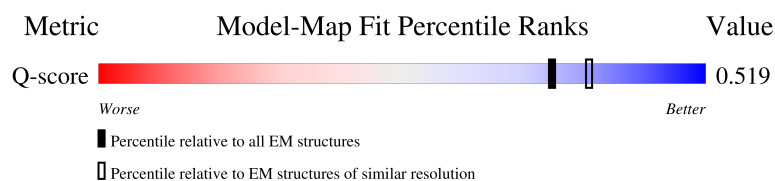
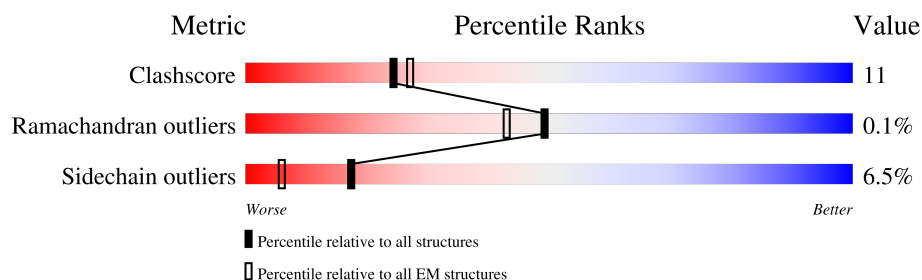
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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	14332 (2.86 - 3.86)

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	314	57% 13% • 29%
1	B	314	55% 15% • 29%
2	C	1193	67% 24% • 8%
3	D	1199	72% 25% ••

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Mol	Chain	Length	Quality of chain
4	E	69	84%14%•
5	F	67	61%28%•9%
6	H	774	65%31%••

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 28227 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	224	Total	C	N	O	0	0
			1691	1069	288	334		
1	B	224	Total	C	N	O	0	0
			1642	1044	279	319		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1099	Total	C	N	O	S	0	0
			8586	5400	1496	1658	32		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1184	Total	C	N	O	S	0	0
			9149	5782	1621	1703	43		

- Molecule 4 is a protein called UPF0356 protein YkzG.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	69	Total	C	N	O	S	0	0
			563	364	89	109	1		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	61	Total	C	N	O	S	0	0
			472	299	80	89	4		

- Molecule 6 is a protein called DNA helicase IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	770	Total	C	N	O	S	0	0
			6121	3902	1058	1130	31		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total	Zn	0
			2	2	

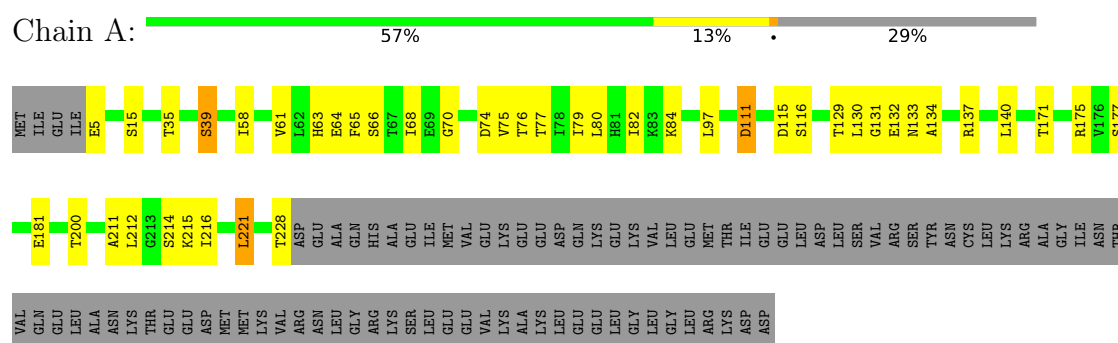
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Mg	0
			1	1	

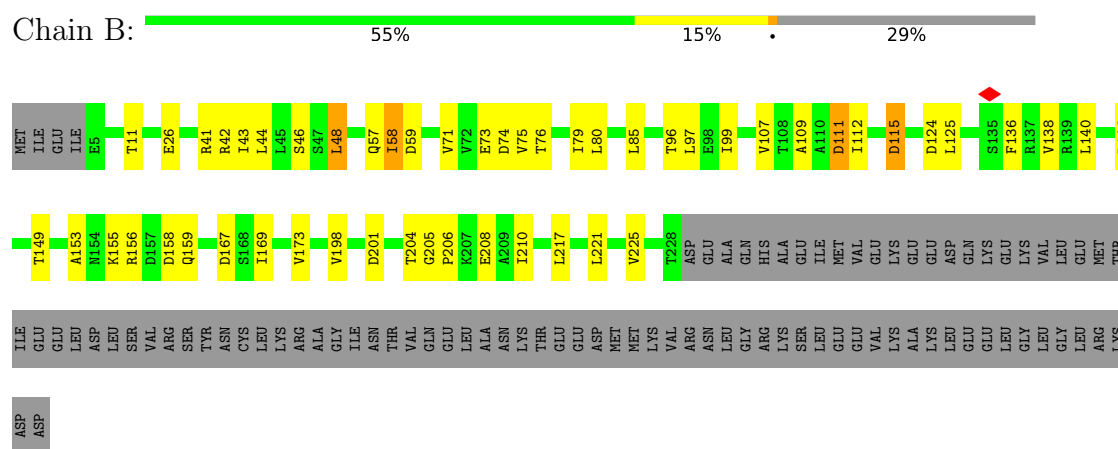
3 Residue-property plots

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.

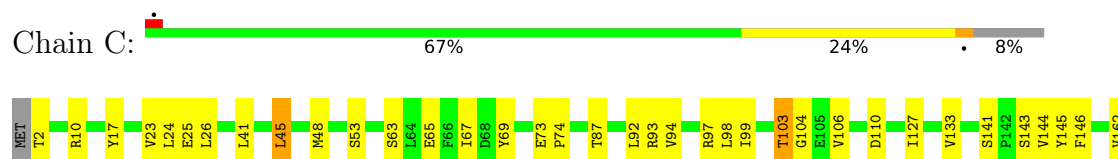
• Molecule 1: DNA-directed RNA polymerase subunit alpha

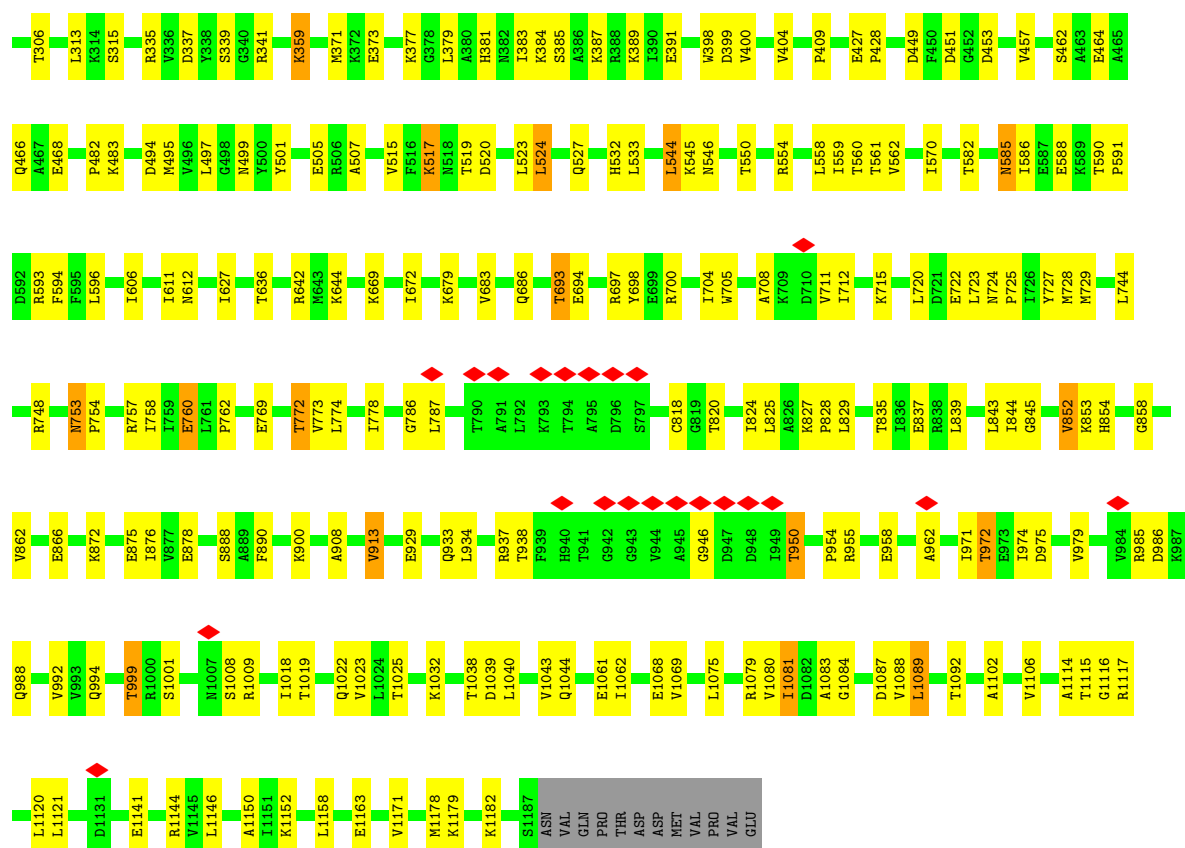


• Molecule 1: DNA-directed RNA polymerase subunit alpha

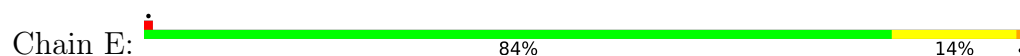


• Molecule 2: DNA-directed RNA polymerase subunit beta

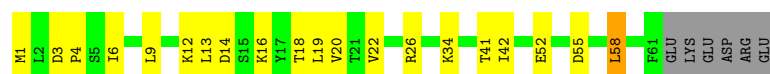




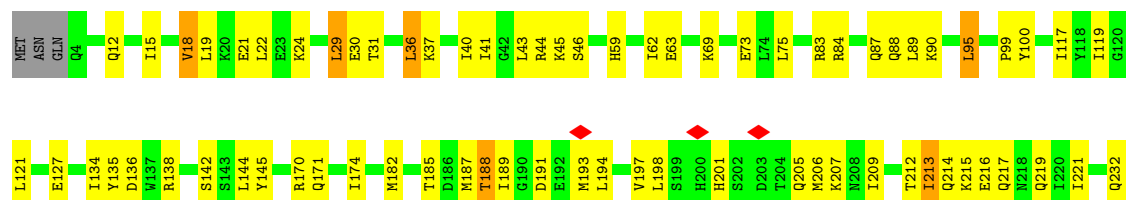
• Molecule 4: UPF0356 protein YkzG

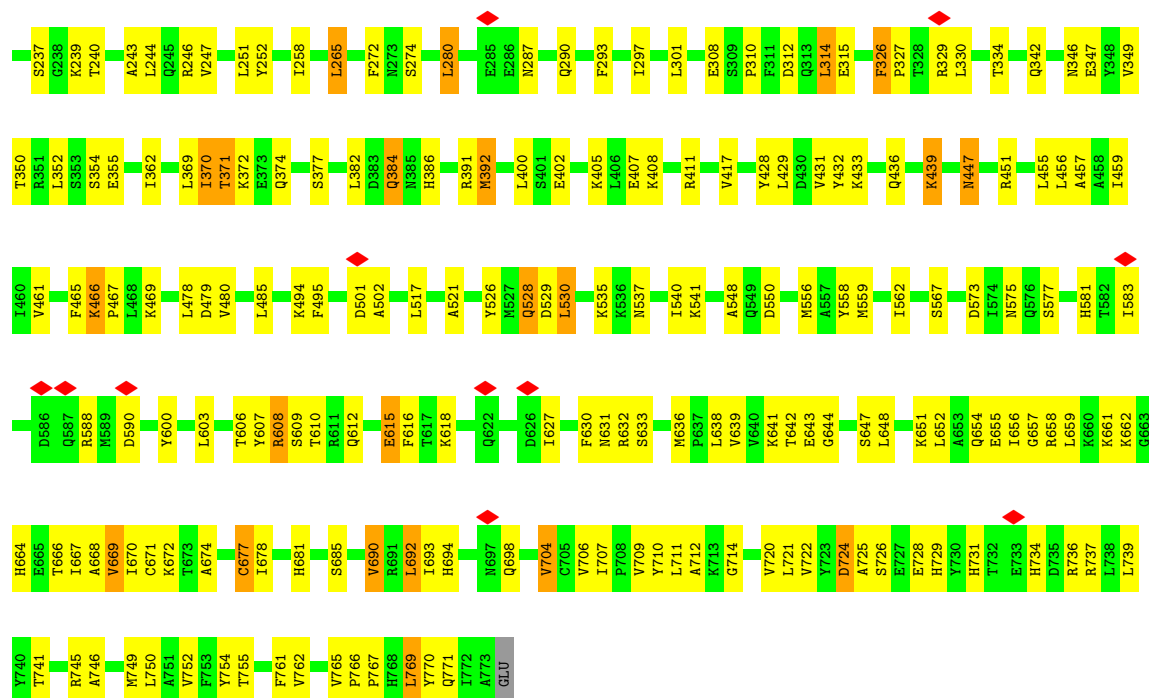


• Molecule 5: DNA-directed RNA polymerase subunit omega



• Molecule 6: DNA helicase IV





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65356	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.6	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	59500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	11.467	Depositor
Minimum map value	-6.290	Depositor
Average map value	0.032	Depositor
Map value standard deviation	0.735	Depositor
Recommended contour level	0.535	Depositor
Map size (Å)	141.95999, 162.95999, 137.76	wwPDB
Map dimensions	164, 194, 169	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.26	0/1717	0.45	0/2340
1	B	0.31	0/1667	0.57	1/2278 (0.0%)
2	C	0.32	1/8738 (0.0%)	0.58	8/11831 (0.1%)
3	D	0.26	0/9300	0.54	4/12577 (0.0%)
4	E	0.22	0/573	0.40	0/771
5	F	0.19	0/477	0.39	0/639
6	H	0.25	0/6252	0.51	0/8445
All	All	0.28	1/28724 (0.0%)	0.54	13/38881 (0.0%)

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
2	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	262	PRO	C-N	-6.71	1.25	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	87	VAL	N-CA-C	-8.66	104.46	112.43
2	C	263	LYS	N-CA-C	-8.35	100.47	111.24
3	D	315	SER	CA-C-O	6.71	121.83	117.94
2	C	263	LYS	N-CA-CB	-6.12	101.08	110.07
3	D	451	ASP	CA-CB-CG	5.95	118.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	263	LYS	CB-CA-C	-5.92	101.09	110.86
3	D	449	ASP	CA-CB-CG	5.91	118.51	112.60
2	C	53	SER	N-CA-CB	-5.55	105.27	111.10
2	C	264	ARG	CA-C-O	-5.24	114.35	120.53
1	B	26	GLU	N-CA-C	5.23	114.32	108.25
2	C	263	LYS	O-C-N	5.11	128.04	122.11
2	C	342	VAL	CA-C-N	5.09	131.06	122.87
2	C	342	VAL	C-N-CA	5.09	131.06	122.87

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	432	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1691	0	1695	22	0
1	B	1642	0	1630	33	0
2	C	8586	0	8466	186	0
3	D	9149	0	9248	187	0
4	E	563	0	547	6	0
5	F	472	0	488	14	0
6	H	6121	0	5939	176	0
7	D	2	0	0	0	0
8	D	1	0	0	0	0
All	All	28227	0	28013	599	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 11.

All (599) 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)
2:C:328:PHE:O	2:C:332:TYR:OH	1.84	0.96
6:H:651:LYS:HE3	6:H:654:GLN:HE22	1.41	0.84
1:B:43:ILE:HD11	1:B:217:LEU:HD13	1.62	0.81
3:D:1084:GLY:HA3	3:D:1114:ALA:HA	1.66	0.76
2:C:317:LYS:HG3	2:C:318:VAL:HG13	1.67	0.74
2:C:272:ARG:NH2	2:C:375:ASN:O	2.21	0.74
6:H:641:LYS:HA	6:H:754:TYR:HE1	1.52	0.74
3:D:170:MET:SD	3:D:282:GLN:NE2	2.60	0.74
6:H:480:VAL:HG21	6:H:528:GLN:HG2	1.70	0.73
3:D:110:ILE:O	3:D:112:SER:N	2.21	0.73
6:H:392:MET:HE1	6:H:478:LEU:HD11	1.70	0.72
3:D:825:LEU:HD23	3:D:827:LYS:HE2	1.71	0.71
4:E:35:THR:HA	4:E:38:LYS:HD2	1.72	0.71
2:C:281:ILE:HD11	2:C:365:GLY:HA3	1.71	0.70
3:D:900:LYS:HG3	3:D:913:VAL:HG23	1.71	0.70
6:H:212:THR:HA	6:H:215:LYS:HE2	1.73	0.70
2:C:400:ASP:O	2:C:406:ASN:ND2	2.25	0.68
2:C:419:GLN:HG2	2:C:461:PHE:HB2	1.75	0.68
6:H:349:VAL:HG11	6:H:530:LEU:HD22	1.75	0.68
1:B:71:VAL:HG12	1:B:73:GLU:H	1.59	0.68
6:H:556:MET:HA	6:H:559:MET:HE3	1.75	0.68
5:F:6:ILE:HA	5:F:9:LEU:HD12	1.77	0.66
6:H:674:ALA:HA	6:H:677:CYS:HB3	1.77	0.66
2:C:827:ARG:HE	2:C:829:ILE:HD13	1.60	0.66
6:H:194:LEU:O	6:H:198:LEU:HG	1.95	0.66
2:C:277:LYS:O	2:C:283:ASN:ND2	2.29	0.66
1:A:175:ARG:HH11	2:C:951:THR:HG23	1.60	0.66
2:C:386:SER:O	2:C:390:ASN:ND2	2.29	0.66
2:C:841:LEU:HD23	2:C:878:ARG:HG3	1.79	0.65
3:D:950:THR:HG21	3:D:954:PRO:HB2	1.79	0.65
1:A:130:LEU:HB3	1:A:134:ALA:HB3	1.78	0.65
2:C:1066:GLY:HA3	2:C:1070:PHE:HB3	1.79	0.65
6:H:720:VAL:HG23	6:H:750:LEU:HD13	1.78	0.65
2:C:811:ARG:HB3	2:C:828:GLY:HA2	1.79	0.64
3:D:686:GLN:OE1	3:D:700:ARG:NH2	2.26	0.64
2:C:23:VAL:HG21	2:C:548:ARG:HH11	1.61	0.64
2:C:143:SER:OG	2:C:144:VAL:N	2.30	0.64
2:C:704:LYS:HD3	2:C:705:GLY:H	1.61	0.64
3:D:950:THR:HB	3:D:955:ARG:HB2	1.79	0.64
6:H:668:ALA:O	6:H:720:VAL:HA	1.98	0.64
3:D:157:ALA:O	3:D:161:LYS:NZ	2.31	0.64
2:C:799:ALA:O	2:C:906:ASN:N	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLU:HG3	4:E:22:SER:HB2	1.80	0.64
1:A:115:ASP:OD1	1:A:116:SER:N	2.28	0.63
2:C:714:LYS:NZ	2:C:726:GLN:O	2.31	0.63
2:C:203:SER:HB3	2:C:206:GLU:HG3	1.81	0.63
2:C:312:ARG:NE	2:C:327:GLY:O	2.31	0.63
6:H:326:PHE:H	6:H:327:PRO:HD3	1.63	0.63
6:H:681:HIS:O	6:H:685:SER:OG	2.11	0.62
6:H:767:PRO:HA	6:H:770:TYR:CZ	2.34	0.62
2:C:1140:MET:HE1	3:D:1146:LEU:HB3	1.82	0.62
2:C:63:SER:HB2	2:C:99:ILE:HB	1.81	0.62
3:D:672:ILE:HD11	3:D:712:ILE:HG12	1.80	0.62
6:H:36:LEU:O	6:H:40:ILE:HG13	1.99	0.62
3:D:278:SER:HA	3:D:281:VAL:HG22	1.81	0.62
3:D:1179:LYS:HA	3:D:1182:LYS:HE2	1.82	0.62
6:H:69:LYS:O	6:H:73:GLU:HG3	2.00	0.62
2:C:434:ARG:NH2	2:C:447:GLN:O	2.32	0.62
3:D:591:PRO:O	3:D:593:ARG:N	2.31	0.62
2:C:291:ALA:HB3	2:C:348:LYS:HG3	1.81	0.62
3:D:1040:LEU:O	3:D:1044:GLN:HG2	1.99	0.62
1:A:80:LEU:O	1:A:84:LYS:NZ	2.26	0.62
2:C:190:LEU:HD12	2:C:191:PRO:HD2	1.82	0.61
2:C:315:LEU:HD12	2:C:316:ASP:H	1.63	0.61
6:H:734:HIS:O	6:H:734:HIS:ND1	2.33	0.61
3:D:66:LYS:O	3:D:66:LYS:HD3	2.00	0.61
3:D:550:THR:O	3:D:554:ARG:HG3	2.00	0.61
6:H:170:ARG:NH1	6:H:182:MET:SD	2.73	0.61
2:C:698:VAL:HG11	2:C:703:VAL:HA	1.81	0.61
3:D:753:ASN:ND2	3:D:754:PRO:O	2.34	0.61
3:D:972:THR:HG21	3:D:1018:ILE:HD12	1.83	0.61
2:C:334:ASN:HA	2:C:342:VAL:O	2.00	0.60
6:H:466:LYS:HG2	6:H:467:PRO:HD3	1.81	0.60
6:H:745:ARG:HA	6:H:745:ARG:NH2	2.16	0.60
2:C:678:HIS:ND1	2:C:697:GLU:OE1	2.35	0.60
2:C:716:VAL:HG23	2:C:724:TYR:HB3	1.82	0.60
2:C:590:ASP:OD1	2:C:605:ARG:NH2	2.35	0.60
6:H:644:GLY:O	6:H:648:LEU:N	2.35	0.60
3:D:1009:ARG:O	3:D:1025:THR:OG1	2.16	0.60
6:H:652:LEU:O	6:H:656:ILE:HG13	2.02	0.60
2:C:737:VAL:HG22	2:C:740:GLU:HG3	1.84	0.60
3:D:120:MET:HG3	3:D:147:LYS:HD3	1.84	0.60
3:D:828:PRO:HD3	3:D:839:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:796:GLU:OE2	2:C:910:ARG:NE	2.35	0.59
6:H:411:ARG:HE	6:H:461:VAL:HG21	1.67	0.59
1:B:204:THR:HB	1:B:208:GLU:HG3	1.84	0.59
2:C:801:ASP:HA	2:C:806:PRO:HA	1.84	0.59
2:C:701:GLN:HB3	2:C:702:LYS:HZ3	1.68	0.59
6:H:501:ASP:OD1	6:H:501:ASP:N	2.35	0.58
3:D:35:ASN:O	3:D:39:LEU:N	2.35	0.58
6:H:206:MET:HB3	6:H:207:LYS:NZ	2.18	0.58
6:H:639:VAL:HG12	6:H:752:VAL:HB	1.85	0.58
3:D:559:ILE:HD11	3:D:596:LEU:HD21	1.85	0.58
3:D:1144:ARG:HH12	6:H:428:TYR:HB3	1.69	0.58
6:H:745:ARG:HA	6:H:745:ARG:HH21	1.69	0.58
2:C:1088:ALA:HA	3:D:468:GLU:OE2	2.03	0.58
2:C:69:TYR:HB3	2:C:94:VAL:HG12	1.86	0.58
2:C:93:ARG:NH2	2:C:110:ASP:O	2.37	0.58
1:B:167:ASP:OD1	1:B:167:ASP:N	2.35	0.58
2:C:291:ALA:HA	2:C:317:LYS:HB2	1.85	0.58
2:C:278:LYS:NZ	2:C:399:ASP:OD2	2.26	0.57
3:D:110:ILE:O	3:D:110:ILE:HG13	2.04	0.57
3:D:189:ASP:O	3:D:193:GLU:HG2	2.03	0.57
6:H:206:MET:HB3	6:H:207:LYS:HZ3	1.69	0.57
6:H:293:PHE:O	6:H:297:ILE:HG13	2.04	0.57
2:C:550:VAL:HG22	2:C:557:VAL:HG22	1.86	0.57
2:C:717:ARG:HG3	2:C:792:ILE:HB	1.85	0.57
3:D:697:ARG:NH2	3:D:760:GLU:OE2	2.37	0.57
3:D:824:ILE:HD11	3:D:890:PHE:HB2	1.85	0.57
3:D:188:VAL:HG21	3:D:217:ARG:HD2	1.86	0.57
2:C:67:ILE:HD11	2:C:97:ARG:HD2	1.87	0.57
2:C:507:HIS:HB3	2:C:510:HIS:CD2	2.40	0.57
1:B:59:ASP:OD1	1:B:59:ASP:N	2.38	0.56
2:C:144:VAL:HG22	2:C:162:VAL:HG22	1.85	0.56
2:C:1027:ASP:OD2	3:D:501:TYR:OH	2.22	0.56
6:H:609:SER:OG	6:H:610:THR:N	2.38	0.56
6:H:674:ALA:O	6:H:678:ILE:HG12	2.04	0.56
2:C:332:TYR:N	2:C:332:TYR:CD1	2.72	0.56
3:D:753:ASN:HD22	3:D:757:ARG:HB3	1.71	0.56
3:D:992:VAL:HG22	3:D:1001:SER:HB3	1.87	0.56
5:F:3:ASP:HB2	5:F:4:PRO:HD3	1.87	0.56
5:F:12:LYS:HE3	5:F:55:ASP:HA	1.87	0.56
6:H:638:LEU:HG	6:H:771:GLN:HB2	1.88	0.56
6:H:709:VAL:O	6:H:712:ALA:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:103:THR:OG1	2:C:104:GLY:N	2.39	0.56
2:C:639:MET:O	2:C:643:MET:HG3	2.06	0.56
3:D:1087:ASP:N	3:D:1087:ASP:OD1	2.36	0.56
6:H:191:ASP:HA	6:H:194:LEU:HG	1.88	0.56
6:H:232:GLN:NE2	6:H:573:ASP:OD1	2.38	0.56
3:D:888:SER:OG	3:D:1068:GLU:OE1	2.24	0.56
6:H:671:CYS:SG	6:H:672:LYS:N	2.79	0.55
6:H:722:VAL:HB	6:H:752:VAL:HA	1.88	0.55
3:D:207:ILE:O	3:D:211:GLU:HG2	2.06	0.55
2:C:472:ASP:H	2:C:482:HIS:HD2	1.54	0.55
3:D:253:ASP:HB3	3:D:313:LEU:HB3	1.89	0.55
2:C:548:ARG:HH21	2:C:557:VAL:HG11	1.71	0.55
3:D:137:THR:O	3:D:146:LYS:NZ	2.38	0.55
6:H:439:LYS:HB3	6:H:451:ARG:HH12	1.71	0.55
2:C:469:GLN:HE21	2:C:482:HIS:HE1	1.53	0.55
3:D:136:VAL:HG12	3:D:168:ALA:HB2	1.87	0.55
6:H:494:LYS:HZ3	6:H:495:PHE:HB3	1.72	0.55
2:C:98:LEU:HB3	2:C:106:VAL:HB	1.88	0.55
3:D:62:CYS:O	3:D:64:LYS:NZ	2.36	0.55
3:D:106:TYR:HB3	3:D:226:MET:HE2	1.88	0.55
3:D:298:ASN:ND2	3:D:313:LEU:O	2.40	0.55
3:D:385:SER:O	3:D:389:LYS:HG3	2.07	0.55
3:D:144:LEU:HD21	3:D:158:TYR:CZ	2.42	0.55
2:C:390:ASN:HB3	2:C:395:VAL:HB	1.89	0.54
6:H:616:PHE:HA	6:H:769:LEU:HD21	1.89	0.54
1:B:169:ILE:HD12	3:D:524:LEU:HD22	1.88	0.54
3:D:725:PRO:O	3:D:729:MET:HG2	2.06	0.54
1:B:74:ASP:OD1	1:B:75:VAL:N	2.37	0.54
4:E:23:LEU:HD21	4:E:67:LEU:HD22	1.87	0.54
6:H:193:MET:HE2	6:H:632:ARG:CB	2.37	0.54
6:H:346:ASN:O	6:H:350:THR:HG23	2.06	0.54
1:A:212:LEU:O	1:A:216:ILE:HG12	2.07	0.54
3:D:872:LYS:O	3:D:876:ILE:HG13	2.06	0.54
6:H:212:THR:O	6:H:216:GLU:HG3	2.08	0.54
2:C:24:LEU:HD13	2:C:561:ILE:HD13	1.88	0.54
2:C:166:ARG:HG2	2:C:266:ASP:HB3	1.90	0.54
2:C:289:ARG:HH21	2:C:318:VAL:HA	1.71	0.54
3:D:184:LEU:HD12	3:D:213:LEU:HG	1.89	0.54
3:D:373:GLU:HG3	3:D:404:VAL:HG22	1.89	0.54
3:D:829:LEU:HB2	3:D:837:GLU:HB2	1.89	0.54
6:H:99:PRO:HD2	6:H:174:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:387:LYS:O	3:D:391:GLU:HG2	2.08	0.53
6:H:201:HIS:O	6:H:205:GLN:HB3	2.07	0.53
6:H:736:ARG:HB3	6:H:761:PHE:CZ	2.43	0.53
2:C:326:ILE:HG23	2:C:329:ARG:CZ	2.39	0.53
2:C:549:ARG:O	2:C:558:THR:OG1	2.22	0.53
3:D:194:GLU:O	3:D:198:SER:OG	2.24	0.53
6:H:631:ASN:OD1	6:H:633:SER:OG	2.27	0.53
2:C:646:GLN:OE1	2:C:1042:HIS:NE2	2.32	0.53
3:D:75:CYS:HB3	3:D:79:GLY:O	2.09	0.53
3:D:1141:GLU:OE2	3:D:1144:ARG:HB2	2.09	0.53
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.72	0.53
6:H:429:LEU:O	6:H:433:LYS:HG2	2.09	0.53
2:C:332:TYR:HB2	2:C:333:PRO:HD3	1.91	0.53
6:H:330:LEU:O	6:H:334:THR:HG23	2.08	0.53
1:B:99:ILE:HB	1:B:112:ILE:HG12	1.90	0.53
3:D:985:ARG:NH2	6:H:290:GLN:OE1	2.42	0.53
6:H:455:LEU:O	6:H:459:ILE:HG13	2.08	0.53
3:D:69:ARG:CD	3:D:69:ARG:H	2.22	0.52
3:D:853:LYS:NZ	3:D:858:GLY:HA2	2.24	0.52
2:C:315:LEU:HD21	2:C:319:LEU:HD22	1.90	0.52
3:D:197:THR:O	3:D:199:GLN:NE2	2.41	0.52
3:D:774:LEU:O	3:D:778:ILE:HG12	2.10	0.52
5:F:13:LEU:HD23	5:F:19:LEU:HD12	1.90	0.52
6:H:447:ASN:O	6:H:451:ARG:HG3	2.09	0.52
2:C:932:LYS:HE2	6:H:63:GLU:OE1	2.09	0.52
3:D:862:VAL:HG13	3:D:866:GLU:HB3	1.92	0.52
6:H:297:ILE:HD13	6:H:521:ALA:HB1	1.92	0.52
6:H:657:GLY:O	6:H:661:LYS:HG3	2.09	0.52
3:D:193:GLU:O	3:D:196:LYS:NZ	2.33	0.52
2:C:377:THR:OG1	2:C:380:ASP:OD2	2.19	0.52
3:D:68:VAL:O	3:D:71:LYS:NZ	2.29	0.52
6:H:658:ARG:HA	6:H:661:LYS:HE3	1.92	0.52
6:H:87:GLN:HE21	6:H:90:LYS:NZ	2.06	0.52
6:H:526:TYR:HE1	6:H:530:LEU:HD12	1.75	0.52
2:C:895:ARG:NH1	2:C:905:VAL:O	2.43	0.52
3:D:103:HIS:CE1	3:D:105:TRP:HB2	2.45	0.52
6:H:667:ILE:O	6:H:704:VAL:HA	2.09	0.52
2:C:729:ILE:HG22	2:C:742:LEU:C	2.35	0.52
3:D:87:VAL:HG22	3:D:90:GLU:HB3	1.91	0.52
3:D:594:PHE:HZ	3:D:612:ASN:HD21	1.58	0.52
6:H:46:SER:O	6:H:46:SER:OG	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:18:THR:O	5:F:22:VAL:HG22	2.10	0.51
3:D:560:THR:OG1	3:D:561:THR:N	2.39	0.51
3:D:42:GLU:OE2	3:D:43:LYS:N	2.42	0.51
1:A:70:GLY:O	1:A:131:GLY:N	2.38	0.51
2:C:296:ASP:HB2	2:C:328:PHE:CE1	2.46	0.51
3:D:214:GLU:HA	3:D:217:ARG:HG2	1.93	0.51
6:H:100:TYR:HD2	6:H:134:ILE:HD12	1.76	0.51
1:A:132:GLU:OE2	2:C:684:ARG:NE	2.43	0.51
2:C:525:ILE:HG22	3:D:786:GLY:HA2	1.92	0.51
2:C:968:ILE:HD11	3:D:744:LEU:HD11	1.92	0.51
3:D:495:MET:O	3:D:499:ASN:ND2	2.41	0.51
2:C:293:THR:OG1	2:C:316:ASP:OD2	2.18	0.51
2:C:440:THR:OG1	2:C:441:ASN:N	2.43	0.51
2:C:592:ILE:HD12	2:C:608:VAL:HG21	1.93	0.51
3:D:124:ALA:O	3:D:128:VAL:HG23	2.10	0.51
2:C:757:ARG:HD3	2:C:786:VAL:HG13	1.92	0.51
2:C:1140:MET:HE2	3:D:1150:ALA:HB2	1.93	0.51
1:B:158:ASP:CG	1:B:159:GLN:H	2.18	0.50
6:H:590:ASP:O	6:H:600:TYR:OH	2.26	0.50
1:B:58:ILE:HG12	1:B:138:VAL:HG13	1.93	0.50
3:D:35:ASN:ND2	3:D:42:GLU:OE1	2.44	0.50
3:D:937:ARG:NH2	6:H:44:ARG:HD3	2.26	0.50
3:D:971:ILE:HA	3:D:1022:GLN:O	2.11	0.50
3:D:73:VAL:HG22	3:D:75:CYS:H	1.75	0.50
6:H:382:LEU:HD13	6:H:391:ARG:HG2	1.93	0.50
2:C:701:GLN:OE1	2:C:702:LYS:NZ	2.33	0.50
6:H:315:GLU:OE2	6:H:315:GLU:N	2.44	0.50
6:H:386:HIS:O	6:H:391:ARG:NH2	2.44	0.50
2:C:523:PRO:HB3	3:D:787:LEU:HD13	1.94	0.50
6:H:643:GLU:HG2	6:H:648:LEU:HD11	1.92	0.50
2:C:556:LYS:NZ	2:C:584:GLU:O	2.43	0.50
3:D:753:ASN:ND2	3:D:757:ARG:HB3	2.27	0.50
2:C:777:MET:HE1	2:C:919:ILE:HG12	1.94	0.49
3:D:962:ALA:HB1	3:D:1032:LYS:NZ	2.27	0.49
6:H:252:TYR:HB2	6:H:280:LEU:HD11	1.93	0.49
6:H:371:THR:OG1	6:H:372:LYS:N	2.45	0.49
1:A:61:VAL:HG13	1:A:66:SER:HB2	1.94	0.49
2:C:45:LEU:HD21	2:C:92:LEU:HD11	1.93	0.49
3:D:708:ALA:O	3:D:712:ILE:HG13	2.12	0.49
1:A:211:ALA:O	1:A:215:LYS:HG3	2.11	0.49
1:B:149:THR:HG23	1:B:153:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:472:ASP:H	2:C:482:HIS:CD2	2.30	0.49
2:C:823:ASN:N	2:C:823:ASN:OD1	2.45	0.49
6:H:41:ILE:HG22	6:H:45:LYS:HE2	1.94	0.49
6:H:100:TYR:CD2	6:H:134:ILE:HD12	2.48	0.49
6:H:643:GLU:HA	6:H:648:LEU:HD11	1.93	0.49
6:H:664:HIS:HB3	6:H:667:ILE:HD11	1.94	0.49
6:H:737:ARG:O	6:H:741:THR:HG22	2.12	0.49
2:C:313:ARG:NH2	2:C:316:ASP:O	2.41	0.49
2:C:1061:GLN:OE1	2:C:1106:ARG:NH1	2.46	0.49
3:D:182:ILE:HG23	3:D:183:ASP:H	1.77	0.49
2:C:312:ARG:HD2	2:C:326:ILE:HG22	1.94	0.49
2:C:328:PHE:CD2	2:C:332:TYR:OH	2.66	0.49
2:C:1063:PRO:HG2	3:D:335:ARG:HB3	1.94	0.49
3:D:221:ASN:HB3	3:D:225:TRP:CZ3	2.48	0.49
3:D:1102:ALA:O	3:D:1106:VAL:HG22	2.13	0.49
2:C:560:ARG:NH2	2:C:562:ASP:OD2	2.46	0.49
1:B:41:ARG:HH12	3:D:527:GLN:HG3	1.78	0.48
2:C:409:LEU:HD21	2:C:486:LEU:HD22	1.95	0.48
2:C:846:VAL:HG22	2:C:872:VAL:N	2.28	0.48
3:D:468:GLU:HG2	5:F:20:VAL:HG11	1.95	0.48
6:H:749:MET:HE3	6:H:749:MET:HA	1.95	0.48
3:D:264:ARG:HH21	3:D:287:MET:HE3	1.77	0.48
6:H:734:HIS:O	6:H:736:ARG:N	2.41	0.48
2:C:328:PHE:CD2	2:C:332:TYR:CZ	3.02	0.48
3:D:283:ASN:OD1	3:D:286:ARG:NH1	2.46	0.48
3:D:853:LYS:HZ3	3:D:858:GLY:HA2	1.79	0.48
2:C:680:GLY:HA2	2:C:696:GLU:HB2	1.96	0.48
6:H:541:LYS:HA	6:H:541:LYS:HD3	1.66	0.48
2:C:1057:SER:OG	2:C:1060:THR:O	2.26	0.48
5:F:16:LYS:O	5:F:20:VAL:HG23	2.13	0.48
6:H:466:LYS:HG2	6:H:467:PRO:CD	2.43	0.48
6:H:526:TYR:CE1	6:H:530:LEU:HD12	2.48	0.48
6:H:529:ASP:OD1	6:H:535:LYS:HB2	2.14	0.48
6:H:736:ARG:HB3	6:H:761:PHE:CE2	2.48	0.48
1:B:76:THR:O	1:B:80:LEU:HD13	2.14	0.48
2:C:536:LYS:HD3	2:C:563:TYR:CE2	2.49	0.48
2:C:999:ASP:O	2:C:1003:THR:HG23	2.13	0.48
2:C:706:ASN:OD1	2:C:706:ASN:N	2.44	0.48
6:H:185:THR:OG1	6:H:187:MET:HG2	2.14	0.48
3:D:1080:VAL:HG12	3:D:1083:ALA:HA	1.95	0.48
3:D:290:GLU:OE1	3:D:301:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:21:GLU:HA	6:H:24:LYS:HE3	1.94	0.48
6:H:29:LEU:HB3	6:H:89:LEU:HD21	1.94	0.48
2:C:241:ARG:NE	2:C:241:ARG:HA	2.29	0.47
3:D:383:ILE:HG13	3:D:384:LYS:HD2	1.96	0.47
3:D:853:LYS:NZ	3:D:854:HIS:O	2.43	0.47
6:H:194:LEU:HA	6:H:197:VAL:HG22	1.96	0.47
6:H:265:LEU:HD22	6:H:272:PHE:CD2	2.48	0.47
3:D:205:ARG:O	3:D:209:ARG:HG3	2.15	0.47
6:H:233:GLY:O	6:H:573:ASP:HB2	2.15	0.47
2:C:1143:LYS:HE2	2:C:1145:LEU:HD11	1.96	0.47
6:H:537:ASN:OD1	6:H:540:ILE:HG12	2.14	0.47
2:C:332:TYR:HB2	2:C:333:PRO:CD	2.44	0.47
2:C:1005:GLU:O	4:E:31:ARG:HG3	2.14	0.47
3:D:483:LYS:HD3	3:D:1062:ILE:HG22	1.95	0.47
3:D:705:TRP:CD2	3:D:762:PRO:HG3	2.49	0.47
3:D:772:THR:HG22	3:D:773:VAL:H	1.80	0.47
3:D:217:ARG:HG3	3:D:217:ARG:HH11	1.79	0.47
3:D:258:TYR:O	3:D:262:ILE:HG13	2.15	0.47
3:D:929:GLU:O	3:D:933:GLN:HG2	2.14	0.47
6:H:411:ARG:HG3	6:H:411:ARG:HH11	1.80	0.47
2:C:48:MET:HE1	2:C:420:PHE:HB3	1.96	0.47
3:D:184:LEU:O	3:D:188:VAL:HG23	2.15	0.47
6:H:720:VAL:HG22	6:H:746:ALA:HB2	1.96	0.47
2:C:146:PHE:HB3	2:C:391:LEU:HD11	1.96	0.47
2:C:242:PRO:HG2	2:C:244:GLU:OE2	2.14	0.47
2:C:693:ARG:HG3	2:C:695:TYR:HD2	1.80	0.47
2:C:714:LYS:HD2	2:C:714:LYS:HA	1.63	0.47
2:C:917:ARG:HH11	2:C:1043:MET:HE2	1.79	0.47
3:D:64:LYS:HE2	3:D:64:LYS:HB2	1.79	0.47
3:D:188:VAL:HG22	3:D:213:LEU:HB3	1.97	0.47
3:D:693:THR:OG1	3:D:694:GLU:N	2.48	0.47
3:D:698:TYR:OH	3:D:758:ILE:O	2.32	0.47
6:H:494:LYS:NZ	6:H:495:PHE:HB3	2.28	0.47
1:B:44:LEU:HD22	1:B:173:VAL:HG21	1.96	0.47
5:F:26:ARG:HD3	5:F:58:LEU:HD21	1.97	0.47
6:H:258:ILE:HG21	6:H:541:LYS:HG3	1.97	0.47
1:A:61:VAL:HG11	1:A:75:VAL:HG21	1.96	0.47
1:B:221:LEU:O	1:B:225:VAL:HG23	2.15	0.47
2:C:23:VAL:HG21	2:C:548:ARG:NH1	2.28	0.47
2:C:25:GLU:H	2:C:25:GLU:CD	2.23	0.47
2:C:289:ARG:HG3	2:C:289:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:679:LYS:HD3	3:D:704:ILE:HD12	1.95	0.47
6:H:121:LEU:HD12	6:H:138:ARG:HH22	1.80	0.47
6:H:191:ASP:O	6:H:194:LEU:HG	2.15	0.46
6:H:736:ARG:O	6:H:739:LEU:HG	2.14	0.46
2:C:832:ILE:HD12	2:C:832:ILE:H	1.80	0.46
3:D:934:LEU:O	3:D:938:THR:HG23	2.15	0.46
6:H:15:ILE:O	6:H:18:VAL:HG12	2.15	0.46
6:H:362:ILE:HG13	6:H:370:ILE:HG13	1.97	0.46
2:C:10:ARG:NH2	2:C:735:GLU:O	2.49	0.46
2:C:26:LEU:HD11	2:C:665:VAL:HG21	1.97	0.46
3:D:720:LEU:HD13	3:D:727:TYR:HB2	1.97	0.46
6:H:407:GLU:HA	6:H:465:PHE:CE2	2.49	0.46
1:B:206:PRO:O	1:B:210:ILE:HG13	2.15	0.46
2:C:94:VAL:O	2:C:110:ASP:HA	2.15	0.46
6:H:761:PHE:O	6:H:765:VAL:HG23	2.16	0.46
2:C:259:PHE:HB3	2:C:376:ILE:HD11	1.96	0.46
6:H:615:GLU:HA	6:H:618:LYS:HG2	1.97	0.46
2:C:98:LEU:HD22	2:C:445:PRO:HD3	1.96	0.46
2:C:744:ASP:OD2	2:C:750:LEU:N	2.49	0.46
3:D:48:CYS:SG	3:D:51:ILE:HG22	2.55	0.46
3:D:50:ARG:HA	3:D:80:VAL:HG23	1.96	0.46
3:D:234:ILE:HG13	3:D:235:PRO:HD2	1.96	0.46
6:H:658:ARG:O	6:H:662:LYS:HG2	2.15	0.46
3:D:862:VAL:HG22	3:D:872:LYS:HD2	1.97	0.46
3:D:1178:MET:O	3:D:1182:LYS:HG2	2.16	0.46
6:H:478:LEU:HA	6:H:478:LEU:HD12	1.68	0.46
1:B:42:ARG:O	1:B:46:SER:OG	2.27	0.46
6:H:342:GLN:NE2	6:H:526:TYR:OH	2.27	0.46
1:A:221:LEU:HD21	1:B:217:LEU:HD23	1.98	0.46
1:B:155:LYS:HD3	1:B:156:ARG:N	2.31	0.46
2:C:548:ARG:NH2	2:C:557:VAL:HG11	2.31	0.46
5:F:41:THR:OG1	5:F:42:ILE:N	2.49	0.46
2:C:183:ARG:HH11	2:C:183:ARG:HG2	1.81	0.45
3:D:18:ASP:N	3:D:18:ASP:OD1	2.46	0.45
6:H:209:ILE:O	6:H:213:ILE:HG23	2.17	0.45
3:D:123:ARG:O	3:D:127:GLU:HG3	2.16	0.45
3:D:264:ARG:NE	3:D:287:MET:HB3	2.31	0.45
6:H:618:LYS:NZ	6:H:627:ILE:O	2.27	0.45
6:H:681:HIS:NE2	6:H:690:VAL:O	2.36	0.45
2:C:41:LEU:O	2:C:69:TYR:OH	2.30	0.45
2:C:575:ALA:HB3	2:C:611:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:999:THR:O	3:D:999:THR:OG1	2.31	0.45
3:D:1089:LEU:O	3:D:1092:THR:HG22	2.16	0.45
6:H:59:HIS:HA	6:H:62:ILE:HD12	1.98	0.45
6:H:251:LEU:HD23	6:H:251:LEU:HA	1.81	0.45
6:H:607:TYR:CD1	6:H:630:PHE:HB2	2.52	0.45
3:D:843:LEU:O	3:D:845:GLY:N	2.49	0.45
6:H:724:ASP:HA	6:H:755:THR:HG23	1.98	0.45
2:C:691:TRP:CZ2	2:C:709:LYS:HD3	2.51	0.45
3:D:1081:ILE:O	3:D:1115:THR:OG1	2.28	0.45
6:H:608:ARG:HD3	6:H:608:ARG:HA	1.67	0.45
6:H:726:SER:HB3	6:H:729:HIS:CD2	2.52	0.45
2:C:188:ARG:HB2	2:C:239:ARG:NH1	2.31	0.45
3:D:669:LYS:NZ	3:D:769:GLU:OE1	2.47	0.45
3:D:774:LEU:HD23	3:D:774:LEU:HA	1.72	0.45
6:H:22:LEU:HD21	6:H:95:LEU:HB3	1.99	0.45
6:H:431:VAL:HG13	6:H:455:LEU:HD23	1.99	0.45
1:A:132:GLU:HG2	1:A:133:ASN:N	2.32	0.45
3:D:67:ARG:HA	3:D:69:ARG:HD3	1.97	0.45
1:B:205:GLY:O	1:B:208:GLU:HG2	2.17	0.45
3:D:875:GLU:HA	3:D:878:GLU:CD	2.42	0.45
6:H:308:GLU:HG3	6:H:312:ASP:HB2	1.99	0.45
6:H:670:ILE:HG22	6:H:721:LEU:O	2.17	0.45
2:C:274:LYS:HD2	2:C:274:LYS:HA	1.75	0.45
2:C:800:ARG:HG3	2:C:904:GLY:O	2.17	0.45
3:D:173:GLU:O	3:D:177:LYS:HG2	2.17	0.45
6:H:136:ASP:OD1	6:H:138:ARG:NH1	2.50	0.45
6:H:217:GLN:O	6:H:221:ILE:HG13	2.16	0.45
2:C:895:ARG:HH11	2:C:901:LEU:HG	1.81	0.44
2:C:989:SER:O	2:C:989:SER:OG	2.34	0.44
3:D:337:ASP:OD1	3:D:337:ASP:N	2.47	0.44
2:C:279:LEU:HD23	2:C:387:TYR:HD2	1.82	0.44
2:C:376:ILE:HD12	2:C:381:ILE:HD11	1.98	0.44
3:D:159:LEU:HD12	3:D:159:LEU:HA	1.81	0.44
3:D:985:ARG:HA	3:D:985:ARG:NE	2.32	0.44
1:A:63:HIS:CE1	1:A:65:PHE:HB2	2.52	0.44
2:C:774:ALA:HB1	2:C:936:SER:OG	2.17	0.44
3:D:453:ASP:OD1	3:D:453:ASP:N	2.50	0.44
3:D:464:GLU:O	3:D:468:GLU:HG3	2.17	0.44
3:D:507:ALA:HB2	3:D:611:ILE:HD11	1.99	0.44
3:D:1144:ARG:HG2	3:D:1144:ARG:HH11	1.82	0.44
6:H:669:VAL:HG13	6:H:706:VAL:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLN:HG3	1:B:57:GLN:O	2.18	0.44
1:B:111:ASP:OD1	1:B:111:ASP:N	2.50	0.44
3:D:482:PRO:HB3	3:D:908:ALA:HB2	2.00	0.44
3:D:711:VAL:O	3:D:715:LYS:HG3	2.17	0.44
6:H:43:LEU:HB3	6:H:75:LEU:HD13	2.00	0.44
6:H:329:ARG:HD2	6:H:502:ALA:HB1	1.98	0.44
2:C:565:THR:HG22	2:C:566:ALA:H	1.81	0.44
2:C:370:GLU:O	2:C:373:ILE:HG12	2.17	0.44
3:D:872:LYS:O	3:D:875:GLU:HG2	2.17	0.44
6:H:87:GLN:HE21	6:H:90:LYS:HZ2	1.64	0.44
1:B:96:THR:C	1:B:97:LEU:HD12	2.42	0.44
2:C:547:TYR:CE1	2:C:574:VAL:HG11	2.53	0.44
2:C:766:TRP:CH2	2:C:939:LEU:HD21	2.53	0.44
3:D:1117:ARG:HH11	3:D:1117:ARG:HG3	1.81	0.44
6:H:117:ILE:HG23	6:H:135:TYR:CD2	2.53	0.44
6:H:145:TYR:OH	6:H:171:GLN:HG2	2.18	0.44
6:H:681:HIS:CG	6:H:692:LEU:HB3	2.53	0.44
6:H:728:GLU:HA	6:H:731:HIS:CE1	2.53	0.44
2:C:257:SER:HA	2:C:261:ASP:OD2	2.17	0.44
3:D:1040:LEU:HD11	3:D:1075:LEU:HD22	1.99	0.44
6:H:188:THR:O	6:H:189:ILE:HG13	2.18	0.44
1:A:35:THR:O	1:A:39:SER:OG	2.33	0.44
2:C:627:PRO:HA	2:C:660:THR:HG22	1.99	0.44
6:H:37:LYS:O	6:H:41:ILE:HG13	2.18	0.44
6:H:213:ILE:HG13	6:H:214:GLN:N	2.32	0.43
6:H:246:ARG:HG3	6:H:246:ARG:HH11	1.83	0.43
2:C:924:LYS:HD2	2:C:932:LYS:HD2	2.00	0.43
3:D:497:LEU:HD11	3:D:729:MET:HB3	1.99	0.43
3:D:722:GLU:C	3:D:724:ASN:H	2.26	0.43
2:C:73:GLU:HG2	2:C:74:PRO:HD2	2.00	0.43
2:C:223:LYS:O	2:C:223:LYS:HD3	2.18	0.43
6:H:352:LEU:HD23	6:H:352:LEU:HA	1.79	0.43
2:C:803:LYS:HE3	2:C:804:LEU:HG	1.99	0.43
3:D:377:LYS:NZ	3:D:400:VAL:HG12	2.33	0.43
5:F:34:LYS:HD2	5:F:34:LYS:N	2.33	0.43
5:F:42:ILE:HB	5:F:52:GLU:OE1	2.19	0.43
6:H:84:ARG:O	6:H:88:GLN:HG3	2.19	0.43
2:C:296:ASP:HB2	2:C:328:PHE:HE1	1.83	0.43
2:C:672:ALA:O	2:C:726:GLN:NE2	2.52	0.43
3:D:544:LEU:O	3:D:546:ASN:N	2.51	0.43
6:H:402:GLU:HA	6:H:405:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:366:ASN:OD1	2:C:366:ASN:N	2.43	0.43
3:D:371:MET:HE1	3:D:387:LYS:HG2	2.00	0.43
2:C:842:LEU:HD21	2:C:879:VAL:HG22	2.00	0.43
3:D:359:LYS:HG2	3:D:398:TRP:CZ3	2.54	0.43
6:H:310:PRO:O	6:H:314:LEU:HD23	2.19	0.43
2:C:2:THR:HG21	2:C:999:ASP:OD1	2.19	0.43
2:C:434:ARG:HB3	2:C:448:LEU:HD23	2.01	0.43
2:C:811:ARG:HB3	2:C:828:GLY:CA	2.47	0.43
6:H:237:SER:HA	6:H:606:THR:HA	2.01	0.43
6:H:616:PHE:CE1	6:H:765:VAL:HG11	2.54	0.43
3:D:1163:GLU:OE1	3:D:1163:GLU:N	2.50	0.43
6:H:240:THR:O	6:H:244:LEU:HG	2.17	0.43
6:H:766:PRO:HA	6:H:767:PRO:HD3	1.91	0.43
1:A:214:SER:HB2	1:B:225:VAL:HG22	2.00	0.42
2:C:693:ARG:HA	2:C:693:ARG:HD3	1.88	0.42
3:D:177:LYS:HA	3:D:177:LYS:HD3	1.89	0.42
6:H:119:ILE:HG12	6:H:142:SER:HB2	2.01	0.42
6:H:432:TYR:O	6:H:436:GLN:HG2	2.17	0.42
6:H:485:LEU:HD23	6:H:485:LEU:HA	1.84	0.42
2:C:551:ASP:HB2	2:C:558:THR:HG23	2.01	0.42
3:D:852:VAL:HG12	3:D:853:LYS:H	1.83	0.42
6:H:636:MET:HE2	6:H:771:GLN:HE21	1.83	0.42
6:H:714:GLY:HA2	6:H:745:ARG:HH11	1.84	0.42
2:C:894:ASN:OD1	2:C:895:ARG:N	2.52	0.42
3:D:16:SER:O	3:D:20:ILE:HG13	2.19	0.42
3:D:157:ALA:HA	3:D:160:ASP:OD2	2.19	0.42
3:D:462:SER:O	3:D:466:GLN:HG3	2.19	0.42
6:H:693:ILE:HG13	6:H:698:GLN:CD	2.45	0.42
2:C:427:MET:HE3	2:C:427:MET:HB3	1.89	0.42
2:C:556:LYS:HE3	2:C:556:LYS:HB2	1.74	0.42
2:C:997:GLU:HA	2:C:1000:VAL:HG22	2.01	0.42
3:D:189:ASP:HA	3:D:192:LYS:HZ2	1.84	0.42
6:H:30:GLU:HG3	6:H:31:THR:N	2.34	0.42
6:H:494:LYS:HG3	6:H:495:PHE:N	2.34	0.42
1:A:58:ILE:HG21	1:A:68:ILE:HD11	2.01	0.42
2:C:141:SER:O	2:C:145:TYR:OH	2.34	0.42
2:C:580:ARG:HB3	2:C:588:ILE:HD12	2.01	0.42
3:D:191:LEU:HD21	3:D:209:ARG:NH1	2.35	0.42
3:D:339:SER:HA	3:D:457:VAL:O	2.19	0.42
2:C:701:GLN:HB3	2:C:702:LYS:NZ	2.33	0.42
3:D:65:TYR:HA	3:D:67:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:570:ILE:O	3:D:642:ARG:NH1	2.43	0.42
3:D:582:THR:O	3:D:586:ILE:HG13	2.19	0.42
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.85	0.42
2:C:686:GLU:HG2	2:C:688:LYS:H	1.84	0.42
2:C:729:ILE:HG22	2:C:742:LEU:O	2.20	0.42
5:F:41:THR:OG1	5:F:52:GLU:OE2	2.36	0.42
6:H:37:LYS:HB3	6:H:37:LYS:HE3	1.65	0.42
1:A:137:ARG:NH1	1:A:137:ARG:HB2	2.35	0.42
2:C:320:PRO:C	2:C:322:LEU:HD12	2.45	0.42
2:C:1058:LEU:HD23	2:C:1058:LEU:HA	1.92	0.42
3:D:66:LYS:O	3:D:69:ARG:NH2	2.52	0.42
3:D:409:PRO:HG3	5:F:1:MET:HE1	2.00	0.42
6:H:354:SER:C	6:H:355:GLU:HG3	2.44	0.42
6:H:548:ALA:C	6:H:550:ASP:H	2.28	0.42
6:H:670:ILE:HD12	6:H:707:ILE:O	2.19	0.42
1:B:124:ASP:OD1	1:B:124:ASP:N	2.45	0.42
3:D:1039:ASP:O	3:D:1043:VAL:HG23	2.20	0.42
4:E:62:GLU:O	4:E:63:ASN:ND2	2.53	0.42
6:H:354:SER:HA	6:H:384:GLN:NE2	2.35	0.42
2:C:798:GLU:OE2	2:C:800:ARG:NH1	2.49	0.42
3:D:986:ASP:HB2	3:D:988:GLN:HG3	2.02	0.42
2:C:294:LEU:HB3	2:C:328:PHE:CD2	2.55	0.41
3:D:256:ASP:O	3:D:260:ARG:HD3	2.20	0.41
3:D:1079:ARG:O	3:D:1116:GLY:HA2	2.20	0.41
6:H:655:GLU:HB3	6:H:659:LEU:HD13	2.01	0.41
1:B:109:ALA:HB2	1:B:125:LEU:HB3	2.02	0.41
2:C:197:ARG:NH2	2:C:202:GLY:O	2.52	0.41
2:C:556:LYS:NZ	2:C:584:GLU:HB3	2.36	0.41
2:C:584:GLU:N	2:C:584:GLU:OE1	2.53	0.41
5:F:13:LEU:HD12	5:F:14:ASP:H	1.84	0.41
6:H:19:LEU:HD23	6:H:19:LEU:HA	1.87	0.41
1:B:48:LEU:O	1:B:146:ARG:HA	2.20	0.41
3:D:156:ARG:HA	3:D:156:ARG:NE	2.35	0.41
3:D:532:HIS:CG	3:D:533:LEU:N	2.89	0.41
1:A:64:GLU:HG2	1:A:76:THR:HG22	2.01	0.41
1:B:115:ASP:OD1	1:B:115:ASP:N	2.49	0.41
3:D:98:ALA:HB1	3:D:272:LEU:HD21	2.03	0.41
3:D:156:ARG:HA	3:D:156:ARG:CZ	2.51	0.41
6:H:457:ALA:O	6:H:461:VAL:HG13	2.20	0.41
1:A:111:ASP:OD1	1:A:111:ASP:N	2.53	0.41
1:B:85:LEU:HD12	1:B:85:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:VAL:HG21	1:B:136:PHE:CD2	2.55	0.41
2:C:235:GLU:O	2:C:238:GLU:HG3	2.20	0.41
2:C:847:THR:HG23	2:C:873:ARG:NH1	2.36	0.41
6:H:142:SER:C	6:H:144:LEU:H	2.28	0.41
6:H:583:ILE:HG21	6:H:588:ARG:CZ	2.50	0.41
6:H:641:LYS:O	6:H:643:GLU:N	2.54	0.41
2:C:837:LYS:HB2	2:C:837:LYS:HE2	1.71	0.41
3:D:818:CYS:SG	3:D:820:THR:OG1	2.62	0.41
3:D:1144:ARG:HH12	6:H:428:TYR:CB	2.32	0.41
6:H:233:GLY:O	6:H:239:LYS:NZ	2.53	0.41
2:C:17:TYR:OH	2:C:1003:THR:HG21	2.20	0.41
2:C:87:THR:HG23	2:C:127:ILE:HD13	2.03	0.41
3:D:87:VAL:C	3:D:89:ARG:H	2.29	0.41
3:D:523:LEU:HD23	3:D:523:LEU:HA	1.81	0.41
3:D:585:ASN:HD22	3:D:585:ASN:C	2.29	0.41
3:D:683:VAL:HG22	3:D:700:ARG:HH21	1.85	0.41
6:H:370:ILE:HG22	6:H:374:GLN:NE2	2.35	0.41
6:H:666:THR:O	6:H:667:ILE:HD13	2.21	0.41
1:A:97:LEU:HB2	1:A:140:LEU:HB2	2.03	0.41
2:C:281:ILE:HG22	2:C:285:LEU:HD12	2.02	0.41
2:C:422:ILE:HD13	2:C:422:ILE:HA	1.87	0.41
2:C:813:ILE:H	2:C:813:ILE:HD12	1.85	0.41
3:D:946:GLY:HA2	6:H:83:ARG:HD3	2.02	0.41
6:H:326:PHE:H	6:H:327:PRO:CD	2.32	0.41
1:A:64:GLU:HG3	1:A:79:ILE:HD12	2.02	0.41
2:C:234:LEU:HD21	2:C:248:VAL:HA	2.03	0.41
2:C:848:PRO:O	2:C:873:ARG:NH2	2.54	0.41
3:D:51:ILE:HG23	3:D:52:PHE:H	1.86	0.41
3:D:69:ARG:H	3:D:69:ARG:HD2	1.86	0.41
4:E:25:ILE:HG13	4:E:67:LEU:HD23	2.03	0.41
6:H:297:ILE:HG23	6:H:301:LEU:HD13	2.03	0.41
6:H:347:GLU:OE2	6:H:350:THR:OG1	2.38	0.41
6:H:694:HIS:N	6:H:698:GLN:OE1	2.44	0.41
6:H:725:ALA:HB3	6:H:754:TYR:HA	2.03	0.41
1:B:80:LEU:HG	3:D:517:LYS:HB3	2.03	0.41
2:C:252:LYS:HA	2:C:252:LYS:HD2	1.90	0.41
2:C:294:LEU:O	2:C:313:ARG:HB3	2.21	0.41
3:D:297:ASP:OD1	3:D:300:ARG:HB2	2.21	0.41
3:D:427:GLU:HA	3:D:428:PRO:HD3	1.95	0.41
3:D:495:MET:SD	3:D:644:LYS:HG3	2.61	0.41
2:C:223:LYS:HD3	2:C:223:LYS:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:704:LYS:HD3	2:C:705:GLY:N	2.33	0.40
2:C:886:ILE:HG22	2:C:914:VAL:HG13	2.03	0.40
3:D:644:LYS:HB3	3:D:644:LYS:HE2	1.93	0.40
6:H:187:MET:SD	6:H:213:ILE:HD11	2.60	0.40
6:H:243:ALA:O	6:H:247:VAL:HG23	2.21	0.40
6:H:558:TYR:O	6:H:562:ILE:HG12	2.21	0.40
6:H:642:THR:O	6:H:648:LEU:HD21	2.20	0.40
6:H:710:TYR:HD2	6:H:711:LEU:HD23	1.86	0.40
3:D:1120:LEU:O	3:D:1121:LEU:HD23	2.21	0.40
6:H:215:LYS:O	6:H:219:GLN:HG2	2.21	0.40
1:B:75:VAL:O	1:B:79:ILE:HG12	2.22	0.40
2:C:267:LEU:HD23	2:C:267:LEU:HA	1.90	0.40
2:C:580:ARG:HH11	2:C:580:ARG:HG2	1.85	0.40
3:D:86:LYS:HE3	3:D:86:LYS:HA	2.03	0.40
3:D:289:GLN:O	3:D:289:GLN:NE2	2.54	0.40
3:D:505:GLU:HB3	3:D:611:ILE:HG23	2.03	0.40
6:H:456:LEU:HD23	6:H:456:LEU:HA	1.89	0.40
6:H:647:SER:O	6:H:651:LYS:HG2	2.22	0.40
2:C:321:TYR:O	2:C:323:GLU:HG2	2.21	0.40
2:C:329:ARG:HE	2:C:329:ARG:HB2	1.47	0.40
2:C:65:GLU:O	2:C:97:ARG:HG2	2.21	0.40
2:C:837:LYS:HB3	2:C:838:ASP:H	1.79	0.40
2:C:927:GLY:HA3	2:C:931:ASN:HD22	1.87	0.40
3:D:723:LEU:HA	3:D:728:MET:HE2	2.03	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	214/314 (68%)	209 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	222/314 (71%)	208 (94%)	14 (6%)	0	100	100
2	C	1091/1193 (92%)	987 (90%)	102 (9%)	2 (0%)	43	70
3	D	1182/1199 (99%)	1087 (92%)	93 (8%)	2 (0%)	43	70
4	E	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
5	F	59/67 (88%)	53 (90%)	6 (10%)	0	100	100
6	H	768/774 (99%)	692 (90%)	75 (10%)	1 (0%)	48	76
All	All	3603/3930 (92%)	3300 (92%)	298 (8%)	5 (0%)	49	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	80	VAL
6	H	326	PHE
2	C	332	TYR
3	D	1038	THR
2	C	962	VAL

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	184/273 (67%)	171 (93%)	13 (7%)	13	39
1	B	172/273 (63%)	164 (95%)	8 (5%)	23	50
2	C	928/1026 (90%)	872 (94%)	56 (6%)	17	44
3	D	972/1027 (95%)	904 (93%)	68 (7%)	14	40
4	E	60/65 (92%)	57 (95%)	3 (5%)	22	49
5	F	52/61 (85%)	51 (98%)	1 (2%)	50	66
6	H	634/682 (93%)	588 (93%)	46 (7%)	13	39
All	All	3002/3407 (88%)	2807 (94%)	195 (6%)	17	42

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	15	SER
1	A	39	SER
1	A	74	ASP
1	A	77	THR
1	A	82	ILE
1	A	111	ASP
1	A	129	THR
1	A	171	THR
1	A	177	SER
1	A	200	THR
1	A	221	LEU
1	A	228	THR
1	B	11	THR
1	B	48	LEU
1	B	58	ILE
1	B	111	ASP
1	B	115	ASP
1	B	140	LEU
1	B	198	VAL
1	B	201	ASP
2	C	45	LEU
2	C	103	THR
2	C	133	VAL
2	C	170	LEU
2	C	171	GLU
2	C	178	ASP
2	C	240	LEU
2	C	255	LEU
2	C	264	ARG
2	C	269	ASN
2	C	270	VAL
2	C	275	ILE
2	C	294	LEU
2	C	312	ARG
2	C	333	PRO
2	C	343	THR
2	C	384	SER
2	C	444	THR
2	C	470	PHE
2	C	471	MET
2	C	519	THR
2	C	529	ASN

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Mol	Chain	Res	Type
2	C	533	SER
2	C	560	ARG
2	C	573	VAL
2	C	591	SER
2	C	599	GLU
2	C	605	ARG
2	C	607	ARG
2	C	611	MET
2	C	623	THR
2	C	682	VAL
2	C	698	VAL
2	C	703	VAL
2	C	706	ASN
2	C	736	VAL
2	C	737	VAL
2	C	740	GLU
2	C	818	GLU
2	C	823	ASN
2	C	879	VAL
2	C	907	GLN
2	C	949	ASP
2	C	951	THR
2	C	973	GLU
2	C	974	LEU
2	C	991	VAL
2	C	1010	SER
2	C	1017	LEU
2	C	1030	VAL
2	C	1046	ASP
2	C	1062	GLN
2	C	1103	VAL
2	C	1114	VAL
2	C	1143	LYS
2	C	1145	LEU
3	D	4	VAL
3	D	11	ASN
3	D	25	PHE
3	D	28	VAL
3	D	48	CYS
3	D	60	CYS
3	D	73	VAL
3	D	80	VAL

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Mol	Chain	Res	Type
3	D	90	GLU
3	D	91	ARG
3	D	92	MET
3	D	166	PHE
3	D	173	GLU
3	D	184	LEU
3	D	221	ASN
3	D	256	ASP
3	D	267	ARG
3	D	274	LEU
3	D	306	THR
3	D	341	ARG
3	D	359	LYS
3	D	379	LEU
3	D	381	HIS
3	D	399	ASP
3	D	494	ASP
3	D	515	VAL
3	D	517	LYS
3	D	519	THR
3	D	520	ASP
3	D	524	LEU
3	D	544	LEU
3	D	545	LYS
3	D	558	LEU
3	D	562	VAL
3	D	585	ASN
3	D	588	GLU
3	D	590	THR
3	D	606	ILE
3	D	627	ILE
3	D	636	THR
3	D	693	THR
3	D	748	ARG
3	D	753	ASN
3	D	760	GLU
3	D	772	THR
3	D	835	THR
3	D	844	ILE
3	D	852	VAL
3	D	913	VAL
3	D	950	THR

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Mol	Chain	Res	Type
3	D	958	GLU
3	D	972	THR
3	D	974	ILE
3	D	975	ASP
3	D	979	VAL
3	D	994	GLN
3	D	999	THR
3	D	1008	SER
3	D	1019	THR
3	D	1023	VAL
3	D	1061	GLU
3	D	1069	VAL
3	D	1081	ILE
3	D	1088	VAL
3	D	1089	LEU
3	D	1152	LYS
3	D	1158	LEU
3	D	1171	VAL
4	E	12	ASP
4	E	20	THR
4	E	63	ASN
5	F	58	LEU
6	H	12	GLN
6	H	18	VAL
6	H	29	LEU
6	H	36	LEU
6	H	95	LEU
6	H	127	GLU
6	H	188	THR
6	H	213	ILE
6	H	265	LEU
6	H	274	SER
6	H	280	LEU
6	H	287	ASN
6	H	314	LEU
6	H	369	LEU
6	H	370	ILE
6	H	371	THR
6	H	377	SER
6	H	384	GLN
6	H	392	MET
6	H	400	LEU

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Mol	Chain	Res	Type
6	H	408	LYS
6	H	417	VAL
6	H	439	LYS
6	H	447	ASN
6	H	466	LYS
6	H	469	LYS
6	H	479	ASP
6	H	517	LEU
6	H	528	GLN
6	H	530	LEU
6	H	567	SER
6	H	575	ASN
6	H	577	SER
6	H	581	HIS
6	H	603	LEU
6	H	608	ARG
6	H	612	GLN
6	H	615	GLU
6	H	669	VAL
6	H	677	CYS
6	H	690	VAL
6	H	692	LEU
6	H	704	VAL
6	H	724	ASP
6	H	762	VAL
6	H	769	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
2	C	33	GLN
2	C	287	ASN
2	C	345	GLN
2	C	390	ASN
2	C	469	GLN
2	C	510	HIS
2	C	635	ASN
2	C	642	ASN
2	C	726	GLN
2	C	970	GLN
2	C	1062	GLN

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Mol	Chain	Res	Type
2	C	1118	ASN
3	D	35	ASN
3	D	381	HIS
3	D	413	ASN
3	D	753	ASN
3	D	781	HIS
3	D	933	GLN
4	E	60	GLN
5	F	44	HIS
6	H	71	GLN
6	H	87	GLN
6	H	93	HIS
6	H	294	GLN
6	H	342	GLN
6	H	575	ASN
6	H	771	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

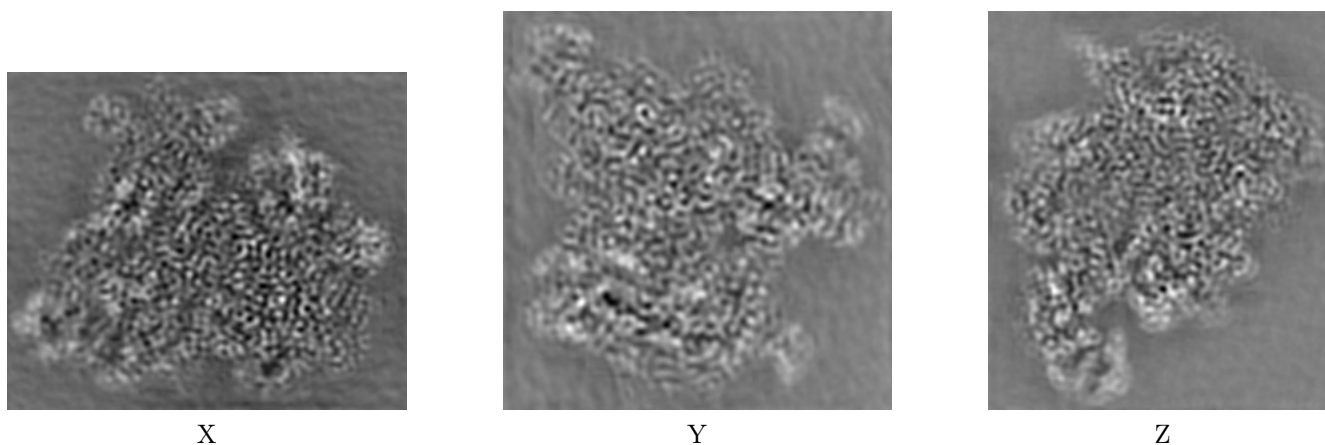
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21921. 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](#)

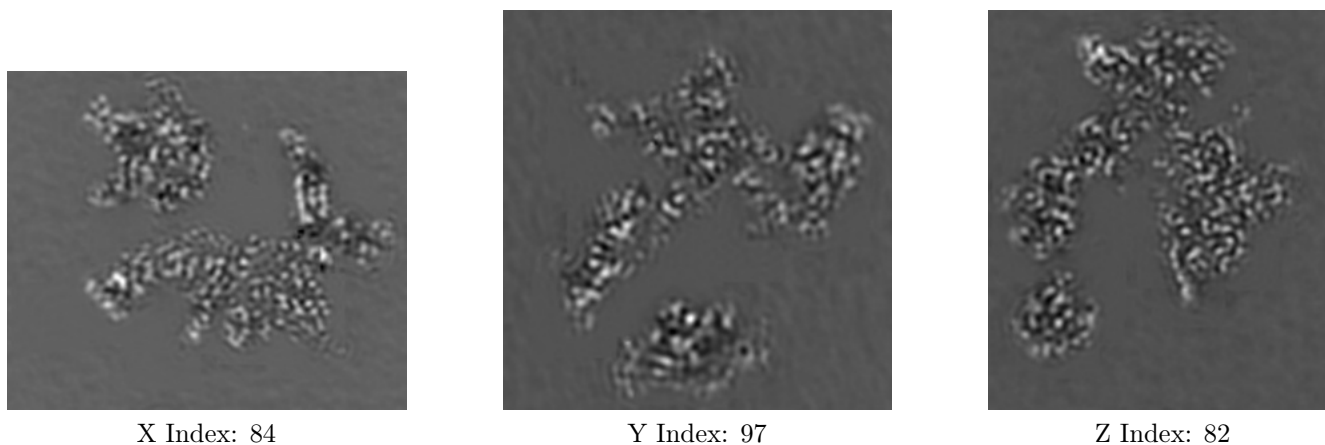
6.1.1 Primary map



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

6.2 Central slices [i](#)

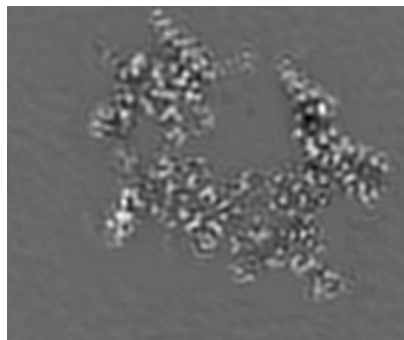
6.2.1 Primary map



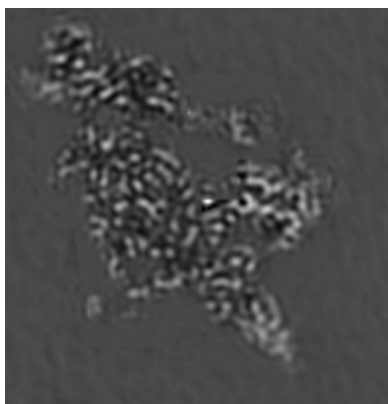
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

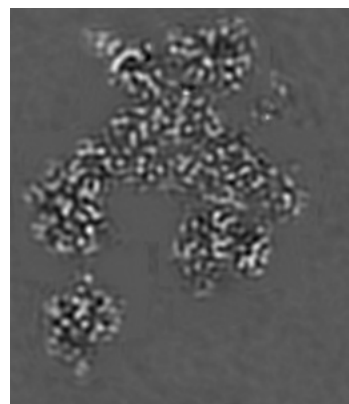
6.3.1 Primary map



X Index: 89



Y Index: 141

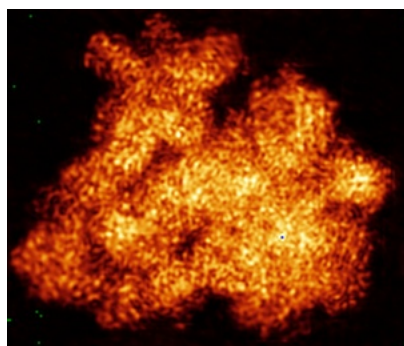


Z Index: 77

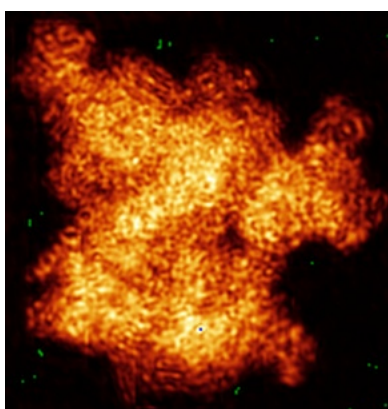
The images above show the largest variance slices of the map in three orthogonal directions.

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

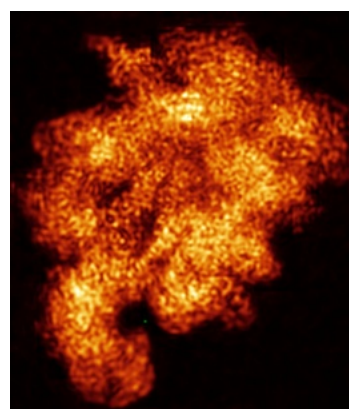
6.4.1 Primary map



X



Y

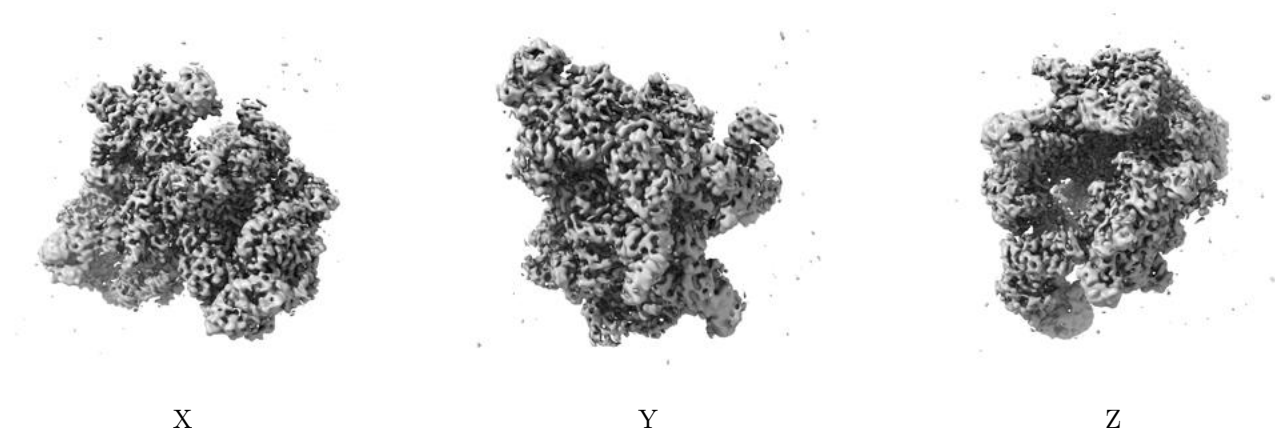


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.535. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

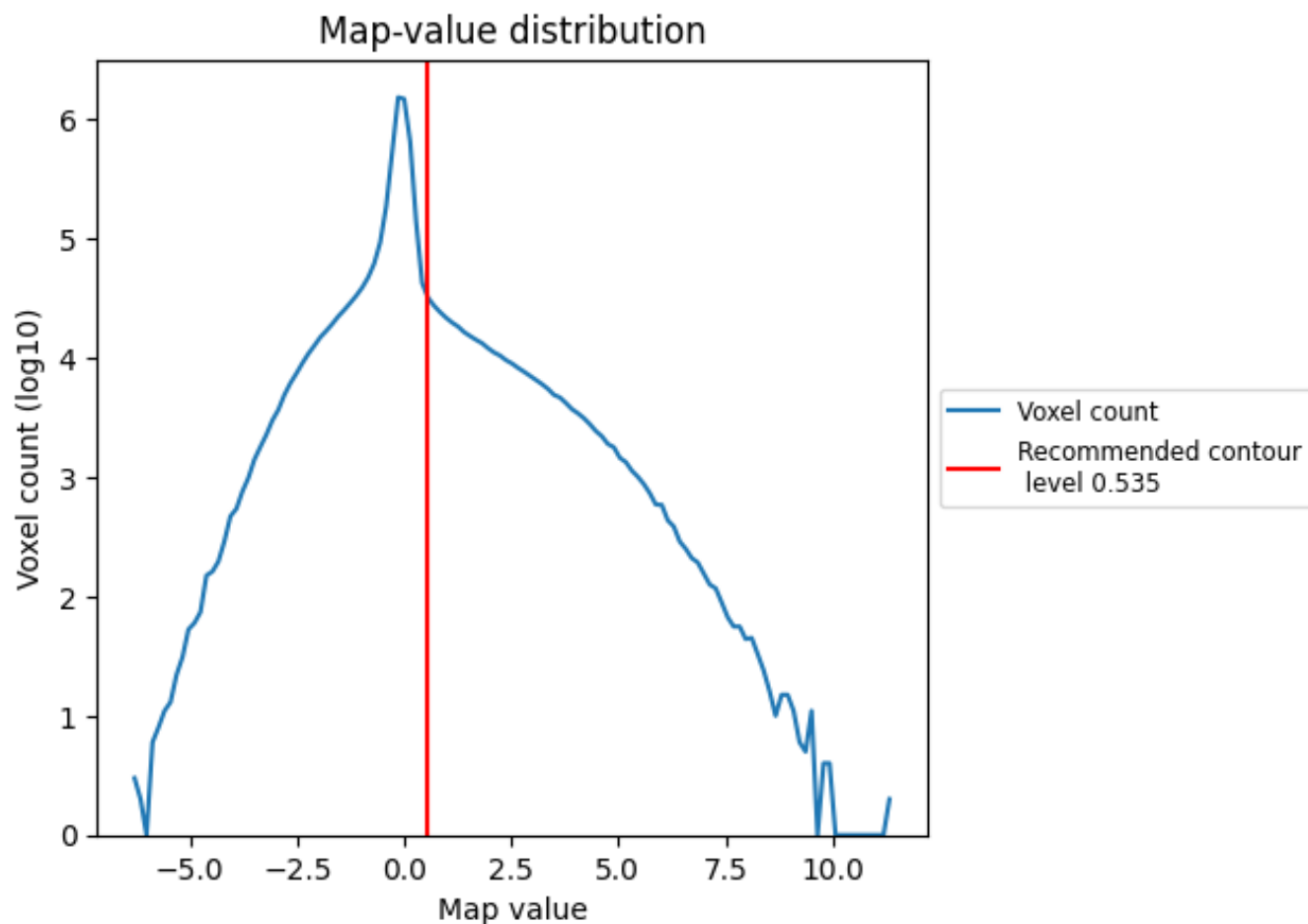
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

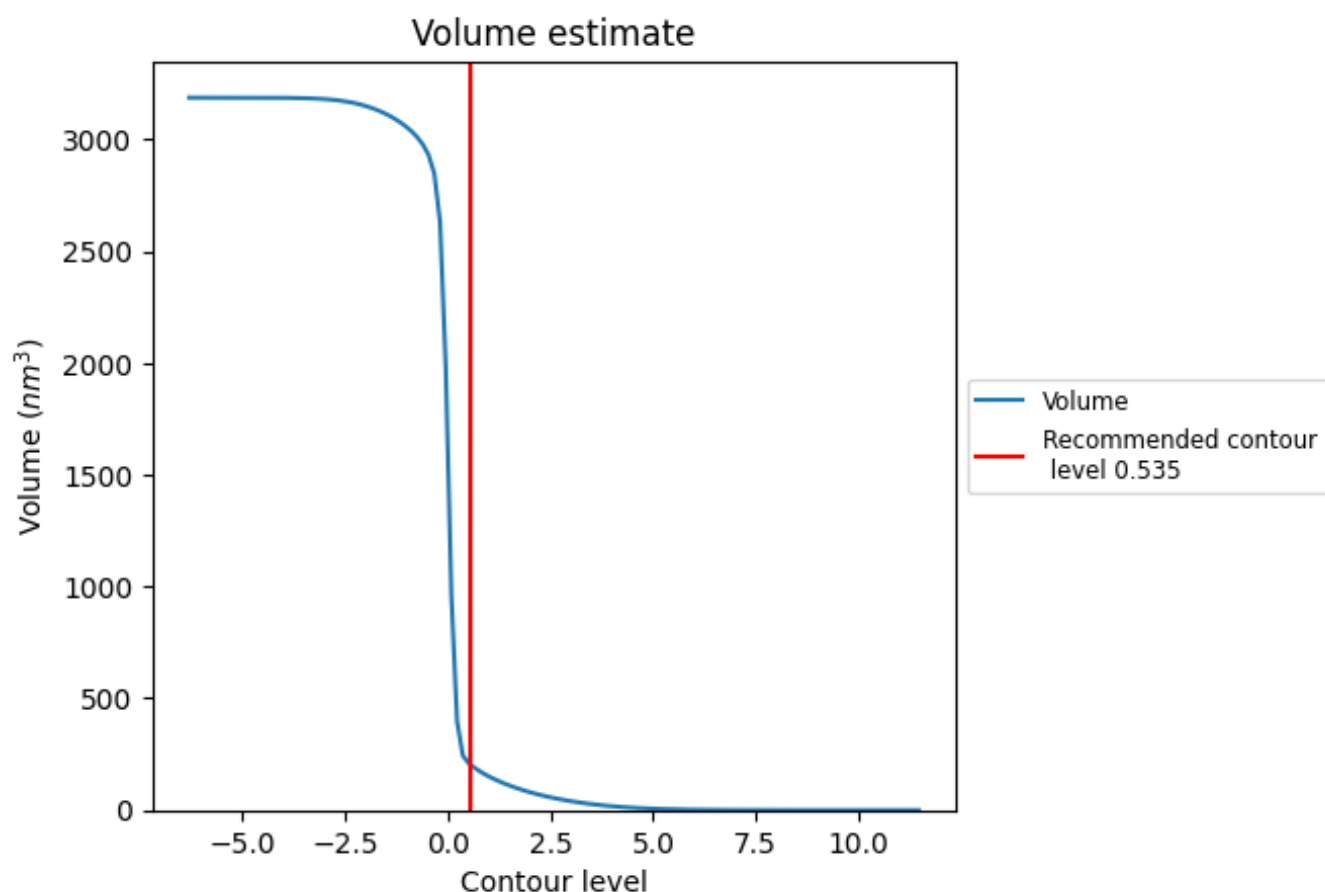
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm^3 ; this corresponds to an approximate mass of 187 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

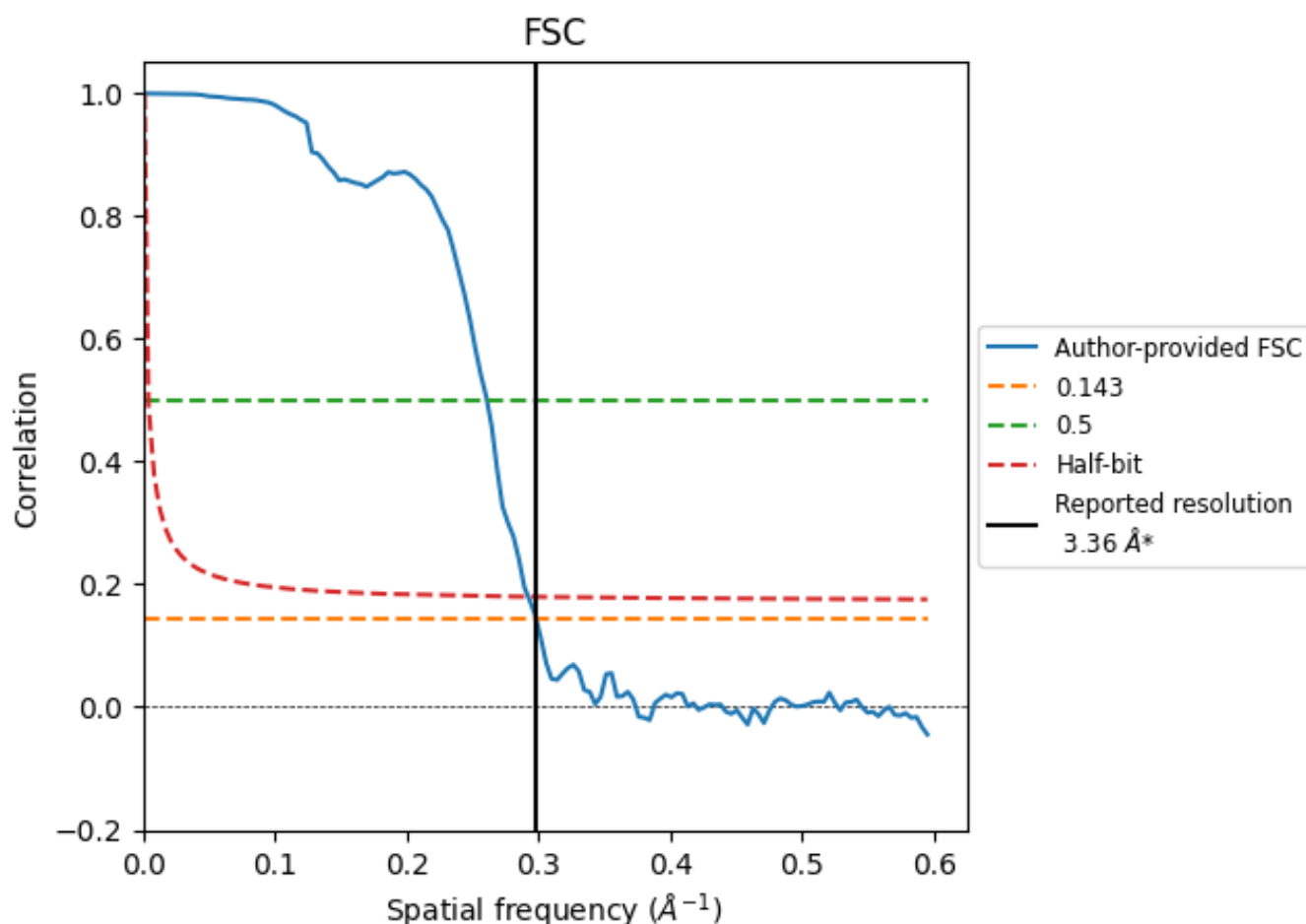
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.298 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.35	3.83	3.42
Unmasked-calculated*	-	-	-

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

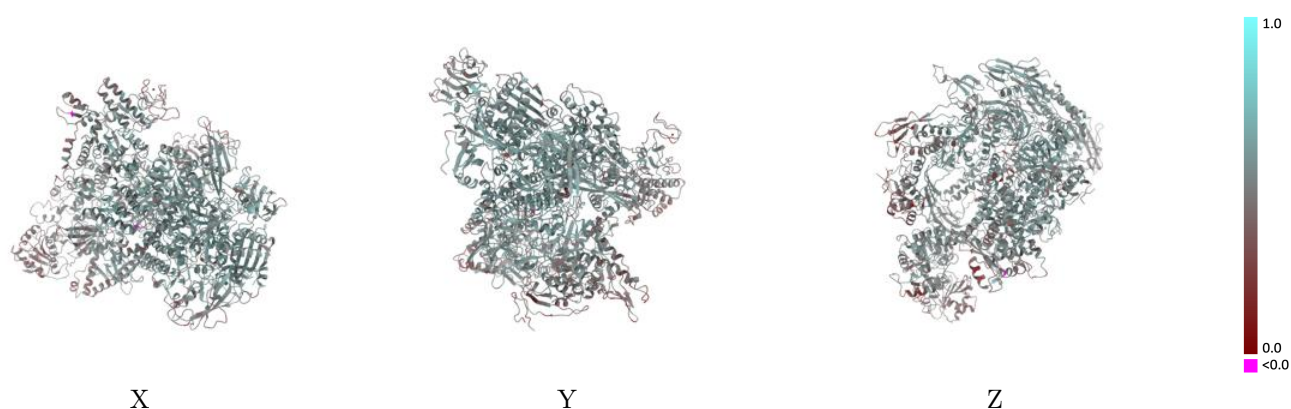
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21921 and PDB model 6WVK. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

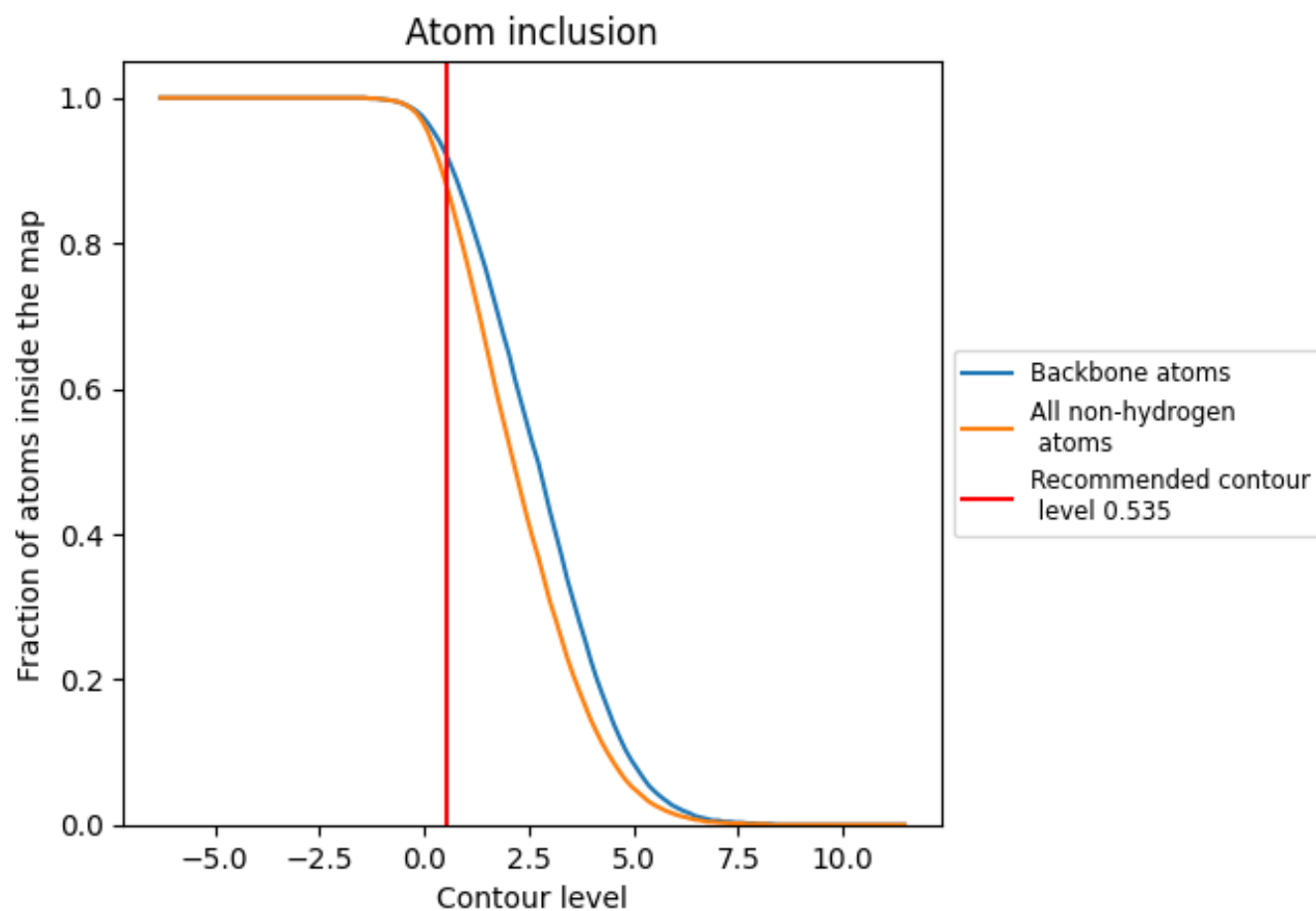


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.535) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.5190
A	0.9060	0.5550
B	0.8780	0.5130
C	0.8760	0.5200
D	0.8830	0.5310
E	0.8900	0.5630
F	0.8650	0.5370
H	0.8720	0.4840

1.0

0.0

<0.0