



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:44 AM UTC

PDB ID : 7OVB / pdb_00007ovb
EMDB ID : EMD-13083
Title : L. pneumophila Type IV Coupling Complex (T4CC) with density for DotY
N-terminal and middle domains
Authors : Mace, K.; Meir, A.; Lukyanova, N.; Waksman, G.
Deposited on : 2021-06-14
Resolution : 3.61 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

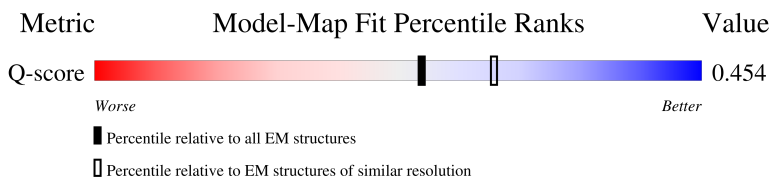
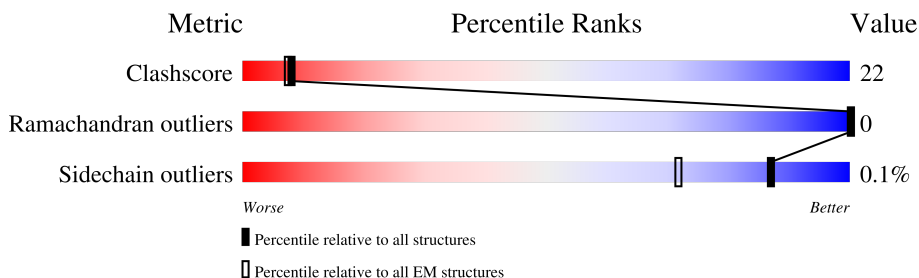
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.61 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	11801 (3.11 - 4.10)

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	783	
2	B	380	
3	C	208	
4	D	294	

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Mol	Chain	Length	Quality of chain
5	E	230	28% 63% 18% • 18%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10854 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 IcmO (DotL).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	473	Total	C	N	O	S	0	0
			3665	2345	619	684	17		

- Molecule 2 is a protein called IcmP (DotM).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	259	Total	C	N	O	S	0	0
			2085	1326	367	377	15		

- Molecule 3 is a protein called IcmJ (DotN).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	202	Total	C	N	O	S	0	0
			1615	1024	277	304	10		

- Molecule 4 is a protein called DotZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	283	Total	C	N	O	S	0	0
			2284	1452	389	441	2		

- Molecule 5 is a protein called DotY.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	188	Total	C	N	O	S	0	0
			1204	742	218	240	4		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Zn	0
			1	1	

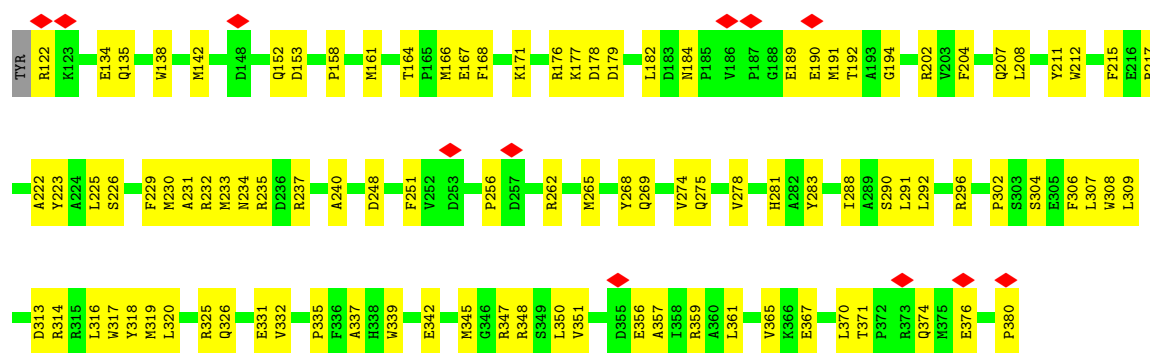
LYS	TYR	ALA	GLY	THR	VAL	ALA	ASN	GLN	GLU	LEU	ILE	GLN	LYS	ASP	PHE	GLN	ASN	ILE	ALA	THR	SER	PRO	TYR	PRO	GLU	GLY	ARG	ASP	VAL	VAL	ASP	ILE	GLN	GLU	THR	THR	GLY	THR	ILE	ILE	ARG	ASP	LEU	SER	ALA	LYS	ILE	SER	ALA	GLU	ARG	GLU	LYS	ALA	ASN	LYS	GLN	LYS	ALA	ALA	GLU	GLU	LEU	THR
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• Molecule 2: IcmP (DotM)

Chain B:  42% 26% 32%

MET	TYR	ILE	GLU	MET	GLN	ALA	GLN	ASN	GLN	GLN	GLN	TYR	LEU	SER	GLY	ASP	THR	ASN	ASP	SER	MET	ALA	PRO	THR	VAL	TRP	ILE	ASP	VAL	ILE	LEU	LEU	PHE	THR	ILE	VAL	THR	MET	ARG	ALA	TYR	PHE	VAL	GLY	ASP	TRP	ALA	LEU	ALA	ARG	TYR	GLN	VAL	ILE	VAL	TYR	ILE	VAL	SER	ILE	LEU	VAL	PHE	THR	THR	GLU	ARG	GLU	LYS	ALA	ASN	ILE	THR	TRP	GLN	ALA	ARG	ASN	LEU	VAL	ASN	THR	LEU	LEU	PHE
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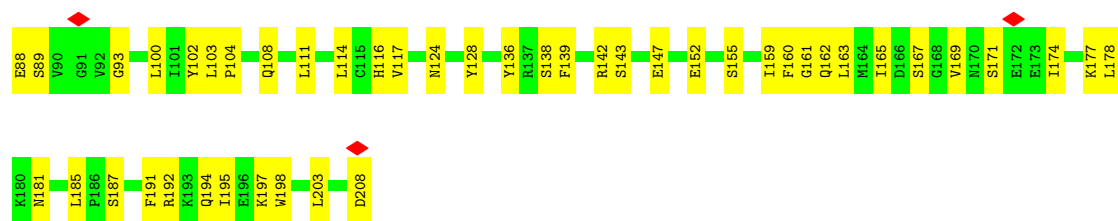
LEU	ASN	ASN	GLN	LEU	LEU	ALA	ASN	GLN	GLN	GLN	TYR	LEU	MET	GLN	SER	THR	LEU	ASP	SER	PRO	ASN	THR	THR	VAL	TRP	ASP	TRP	ILE	GLN	MET	VAL	LEU	LEU	PHE	THR	ILE	VAL	THR	MET	ARG	ALA	TYR	PHE	VAL	GLY	ASP	TRP	ALA	LEU	ALA	ARG	TYR	GLN	VAL	ILE	VAL	CYS	ILE	LEU	VAL	VAL	VAL	THR	THR	ILE	ALA	PHE	VAL	THR	ASN	ILE	THR	TRP	GLN	TYR	ASN	SER	ALA	LEU	VAL	ASN	THR	THR	LEU	LEU	LYS
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• Molecule 3: IcmJ (DotN)

Chain C:  61% 37%

MET	ALA	ASP	ASN	GLN	R7	C8	E9	L10	K11	L12	G17	S18	W19	R20	S23	A24	R25	K26	I27	D28	E29	R30	F31	K32	S33	Y34	E35	Q36	K37	C46	Q47	F48	F51	R54	L55	D58	D65	Y66	T67	N68	L71	S72	N73	C78	F80	Q83
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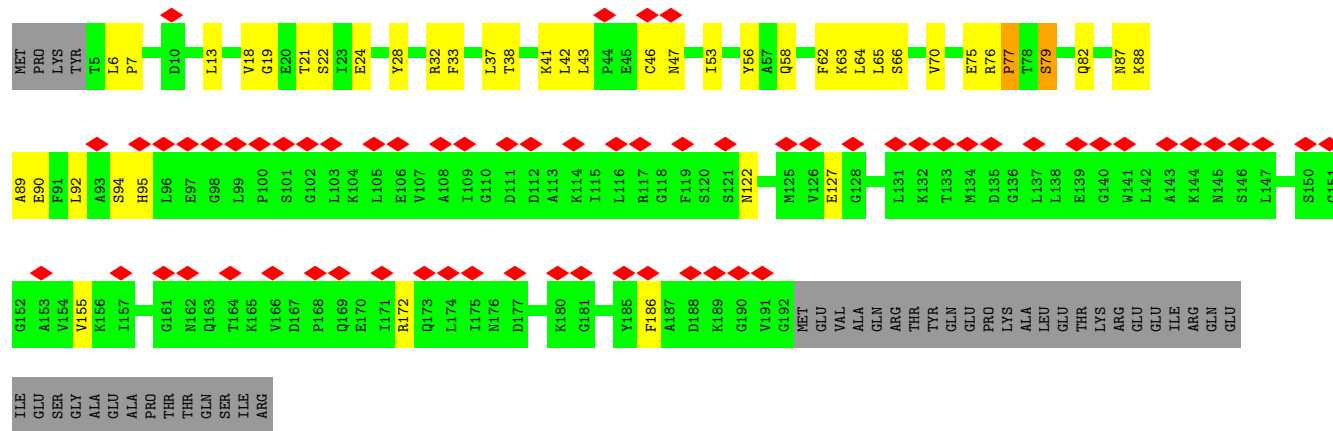


• Molecule 4: DotZ

Chain D:  6% 54% 42%

MET	ASP	GLU	ILE	LYS	ASP	ASP	GLU	LEU	S11	D12	W13	T19	T20	A22	E23	R24	I31	S32	L33	F34	Q35	D36	E37	L38	L39	E40	A41	M42	I43	I44	P45	Y49	R50	H51	Q54	L57	V60	L61	N62	V65	L66	S70	D71	A76	Q77	K78	L79	L80
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183397	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	38.624	Depositor
Minimum map value	-21.045	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	8	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/3727	0.65	0/5031
2	B	0.63	0/2132	0.69	0/2883
3	C	0.66	0/1646	0.69	0/2213
4	D	0.58	0/2318	0.68	0/3131
5	E	0.44	0/1218	0.69	1/1659 (0.1%)
All	All	0.57	0/11041	0.68	1/14917 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	E	77	PRO	N-CA-C	-6.97	100.29	111.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3665	0	3720	211	0
2	B	2085	0	2098	90	0
3	C	1615	0	1578	75	0
4	D	2284	0	2327	105	0
5	E	1204	0	965	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
All	All	10854	0	10688	475	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 22.

All (475) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PHE:HB3	1:A:297:VAL:HB	1.44	1.00
4:D:101:ARG:NH1	4:D:102:GLU:OE1	2.06	0.88
1:A:219:MET:HB2	1:A:252:MET:HE1	1.55	0.87
1:A:371:VAL:O	1:A:374:ARG:NH2	2.10	0.85
1:A:273:ASN:HB3	1:A:279:ARG:HH12	1.42	0.83
1:A:150:ALA:O	1:A:155:SER:OG	1.96	0.83
1:A:396:LYS:HE2	1:A:444:ALA:H	1.44	0.82
4:D:211:LEU:HA	4:D:214:SER:HB3	1.61	0.82
5:E:58:GLN:O	5:E:62:PHE:HB2	1.79	0.81
4:D:128:LEU:HD13	4:D:239:ARG:HD2	1.66	0.78
2:B:281:HIS:ND1	2:B:342:GLU:OE2	2.18	0.77
1:A:106:THR:OG1	1:A:149:ASN:ND2	2.17	0.77
2:B:207:GLN:NE2	2:B:331:GLU:O	2.18	0.77
1:A:369:ASP:OD1	1:A:373:ASN:ND2	2.19	0.76
1:A:593:PRO:HG2	1:A:598:LEU:HD11	1.68	0.76
1:A:132:PHE:O	1:A:493:MET:N	2.19	0.75
2:B:345:MET:SD	2:B:347:ARG:NH1	2.59	0.75
5:E:90:GLU:O	5:E:94:SER:HB2	1.86	0.75
4:D:104:LEU:HD13	4:D:264:LEU:HD22	1.69	0.74
1:A:175:MET:O	1:A:178:SER:OG	2.04	0.73
1:A:219:MET:HA	1:A:222:GLN:HG2	1.71	0.73
1:A:604:GLN:NE2	3:C:152:GLU:O	2.22	0.72
1:A:263:ALA:HB3	1:A:291:ARG:HH22	1.55	0.72
1:A:273:ASN:O	1:A:279:ARG:NH1	2.23	0.72
1:A:107:PHE:N	1:A:149:ASN:HD21	1.88	0.71
1:A:612:LEU:HD11	3:C:169:VAL:HG11	1.72	0.71
1:A:247:PHE:HB2	1:A:313:TYR:CZ	2.25	0.71
1:A:387:SER:OG	1:A:389:ASP:OD1	2.08	0.69
4:D:208:GLY:HA3	4:D:211:LEU:HB3	1.75	0.69
1:A:222:GLN:HA	1:A:225:VAL:HG22	1.74	0.68
1:A:208:THR:OG1	1:A:364:GLU:OE1	2.08	0.68
3:C:65:ASP:OD2	3:C:67:THR:OG1	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:TRP:CD1	3:C:23:SER:HG	2.12	0.68
4:D:111:LEU:HD13	4:D:257:VAL:HG11	1.75	0.68
1:A:112:ARG:HA	1:A:570:ARG:HH22	1.59	0.67
1:A:617:LEU:HD12	3:C:178:LEU:HD13	1.77	0.67
2:B:166:MET:HE1	2:B:365:VAL:HG23	1.75	0.67
3:C:68:ASN:O	3:C:73:ASN:ND2	2.26	0.67
3:C:203:LEU:HD22	4:D:57:LEU:HD22	1.77	0.67
1:A:291:ARG:NH2	1:A:295:GLU:OE2	2.28	0.66
2:B:230:MET:HE1	2:B:269:GLN:HA	1.78	0.66
1:A:227:LEU:O	1:A:342:GLN:NE2	2.29	0.66
1:A:320:TYR:CD2	1:A:322:LYS:HD2	2.30	0.66
2:B:313:ASP:OD1	2:B:314:ARG:N	2.29	0.66
3:C:19:TRP:NE1	3:C:23:SER:OG	2.28	0.65
3:C:208:ASP:O	4:D:54:GLN:NE2	2.29	0.65
1:A:122:ASN:OD1	1:A:126:ARG:NE	2.30	0.65
3:C:171:SER:HB2	3:C:174:ILE:HG22	1.79	0.65
2:B:351:VAL:HG12	3:C:165:ILE:HD11	1.79	0.65
4:D:91:LYS:HB2	4:D:97:GLY:HA3	1.79	0.65
1:A:256:VAL:HG23	1:A:259:ARG:HH22	1.63	0.65
2:B:189:GLU:OE2	2:B:192:THR:OG1	2.09	0.65
4:D:208:GLY:O	4:D:212:LYS:N	2.30	0.64
1:A:174:SER:HB2	1:A:579:VAL:HG23	1.80	0.64
4:D:34:PRO:HB2	4:D:38:ILE:HG13	1.78	0.64
4:D:13:TRP:HA	4:D:39:LEU:HD11	1.79	0.64
2:B:290:SER:HB2	2:B:339:TRP:HE1	1.62	0.64
1:A:313:TYR:O	1:A:316:THR:HG22	1.98	0.63
5:E:41:LYS:HB2	5:E:43:LEU:HD13	1.81	0.63
2:B:283:TYR:OH	2:B:350:LEU:O	2.07	0.63
1:A:187:LEU:HD12	1:A:378:VAL:O	1.99	0.63
1:A:204:ARG:NH1	1:A:586:GLN:OE1	2.32	0.62
1:A:128:HIS:NE2	1:A:449:ALA:O	2.32	0.62
2:B:337:ALA:HB2	2:B:357:ALA:HB2	1.82	0.62
3:C:54:ARG:HG3	4:D:13:TRP:HH2	1.64	0.62
2:B:251:PHE:HD1	2:B:256:PRO:HG3	1.64	0.62
1:A:181:ARG:NH2	1:A:374:ARG:O	2.32	0.62
5:E:37:LEU:HD22	5:E:46:CYS:HB3	1.82	0.61
1:A:112:ARG:NH1	1:A:568:ARG:HE	1.98	0.61
5:E:65:LEU:O	5:E:87:ASN:ND2	2.33	0.61
1:A:170:ALA:HA	1:A:582:LEU:HD21	1.81	0.61
3:C:19:TRP:CH2	3:C:93:GLY:HA3	2.36	0.61
1:A:227:LEU:HD12	1:A:343:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:SER:OG	3:C:177:LYS:O	2.13	0.61
1:A:407:ALA:HA	1:A:452:PRO:HG2	1.81	0.60
4:D:155:ASN:O	4:D:159:LYS:N	2.26	0.60
3:C:8:CYS:SG	3:C:9:GLU:N	2.74	0.60
1:A:438:ASP:HA	1:A:465:ALA:HB3	1.82	0.60
4:D:198:LYS:HA	4:D:201:GLN:HG2	1.83	0.60
2:B:229:PHE:CZ	2:B:292:LEU:HD12	2.36	0.60
4:D:180:HIS:HB2	4:D:198:LYS:HD3	1.84	0.60
1:A:374:ARG:NH1	1:A:458:LEU:O	2.33	0.59
4:D:95:SER:OG	4:D:96:GLN:N	2.35	0.59
1:A:468:ASP:O	1:A:472:PHE:N	2.35	0.59
4:D:235:GLU:O	4:D:238:ASP:N	2.34	0.59
2:B:306:PHE:HB2	2:B:317:TRP:HZ3	1.68	0.59
4:D:22:ALA:HB1	4:D:42:ILE:HD12	1.84	0.59
2:B:319:MET:SD	2:B:335:PRO:HB2	2.43	0.59
1:A:130:LEU:O	1:A:491:ILE:N	2.36	0.58
2:B:262:ARG:O	2:B:265:MET:N	2.35	0.58
2:B:292:LEU:HD21	2:B:296:ARG:CZ	2.32	0.58
1:A:493:MET:SD	1:A:558:ALA:HB2	2.43	0.58
3:C:19:TRP:HH2	3:C:93:GLY:HA3	1.66	0.58
1:A:560:ILE:HD11	1:A:571:MET:HE2	1.86	0.58
5:E:33:PHE:HB3	5:E:53:ILE:HD11	1.84	0.58
1:A:107:PHE:O	1:A:149:ASN:ND2	2.36	0.58
1:A:371:VAL:HG12	1:A:433:TYR:CE1	2.38	0.57
2:B:217:ARG:HH21	2:B:217:ARG:HG2	1.69	0.57
4:D:158:TYR:HA	4:D:161:THR:HG23	1.85	0.57
2:B:202:ARG:HH12	3:C:27:ILE:HD13	1.69	0.57
5:E:94:SER:HG	5:E:95:HIS:CE1	2.23	0.57
3:C:46:CYS:SG	3:C:78:CYS:N	2.75	0.57
2:B:235:ARG:O	2:B:237:ARG:HG3	2.05	0.57
1:A:150:ALA:HB2	1:A:434:MET:HE3	1.87	0.57
2:B:177:LYS:HD3	2:B:380:PRO:HD3	1.87	0.57
1:A:179:MET:HE3	1:A:179:MET:HA	1.86	0.56
3:C:46:CYS:N	3:C:51:PHE:O	2.32	0.56
4:D:78:LYS:HE2	5:E:28:TYR:CG	2.41	0.56
1:A:128:HIS:HB2	1:A:487:THR:HG22	1.87	0.56
4:D:44:ILE:HG13	4:D:45:PRO:HD2	1.88	0.56
1:A:362:LEU:HD12	2:B:326:GLN:HB2	1.86	0.56
1:A:224:VAL:O	1:A:227:LEU:HB3	2.06	0.56
3:C:55:LEU:O	3:C:198:TRP:NE1	2.28	0.56
1:A:131:ILE:HA	1:A:491:ILE:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLU:HG3	2:B:359:ARG:HH22	1.71	0.56
3:C:25:ARG:HB3	3:C:31:PHE:CG	2.41	0.56
5:E:6:LEU:HD12	5:E:7:PRO:HD2	1.88	0.56
1:A:365:VAL:HG23	1:A:370:VAL:HG21	1.88	0.55
4:D:148:GLU:O	4:D:151:LEU:HB3	2.06	0.55
1:A:283:ILE:HD13	1:A:288:VAL:O	2.06	0.55
2:B:231:ALA:HB3	2:B:240:ALA:HB2	1.88	0.55
1:A:112:ARG:HG2	1:A:570:ARG:HH12	1.71	0.55
1:A:625:ASN:HB2	1:A:628:ILE:HG12	1.88	0.55
3:C:19:TRP:NE1	3:C:23:SER:HG	2.04	0.55
2:B:134:GLU:HG2	2:B:138:TRP:CD1	2.41	0.55
4:D:181:CYS:SG	4:D:198:LYS:NZ	2.63	0.55
5:E:75:GLU:N	5:E:75:GLU:OE1	2.40	0.55
2:B:176:ARG:N	2:B:194:GLY:O	2.39	0.55
4:D:121:LEU:HD13	4:D:246:GLN:OE1	2.06	0.55
1:A:132:PHE:N	1:A:491:ILE:O	2.40	0.55
1:A:314:LEU:HA	1:A:317:LEU:HD23	1.89	0.55
2:B:178:ASP:OD1	2:B:178:ASP:N	2.36	0.55
1:A:481:ALA:O	1:A:485:ALA:N	2.40	0.54
2:B:248:ASP:OD1	2:B:308:TRP:HD1	1.89	0.54
2:B:275:GLN:HA	2:B:278:VAL:HG12	1.88	0.54
3:C:139:PHE:HB3	3:C:185:LEU:HD22	1.90	0.54
4:D:77:GLN:NE2	5:E:18:VAL:O	2.26	0.54
1:A:591:GLU:HG3	2:B:359:ARG:NH2	2.23	0.54
1:A:625:ASN:OD1	3:C:142:ARG:NE	2.25	0.54
2:B:191:MET:HB3	2:B:370:LEU:O	2.08	0.54
4:D:182:ASP:C	4:D:183:LEU:HD12	2.33	0.54
3:C:114:LEU:O	3:C:114:LEU:HG	2.08	0.53
4:D:51:HIS:CG	4:D:184:VAL:HG11	2.42	0.53
1:A:188:ILE:HA	1:A:206:SER:OG	2.08	0.53
1:A:264:ILE:HB	1:A:291:ARG:HH11	1.73	0.53
3:C:194:GLN:O	3:C:197:LYS:N	2.42	0.53
4:D:66:ILE:HG22	4:D:247:ALA:HB1	1.90	0.53
4:D:155:ASN:ND2	4:D:167:LYS:HD3	2.23	0.53
5:E:62:PHE:CZ	5:E:88:LYS:HA	2.43	0.53
4:D:77:GLN:NE2	5:E:19:GLY:HA2	2.24	0.53
1:A:174:SER:OG	1:A:577:LYS:O	2.12	0.53
5:E:63:LYS:O	5:E:64:LEU:HD22	2.09	0.53
1:A:215:GLY:HA3	1:A:259:ARG:HH12	1.74	0.53
1:A:256:VAL:HG23	1:A:259:ARG:NH2	2.23	0.53
1:A:617:LEU:H	1:A:617:LEU:HD23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:PHE:HB2	2:B:317:TRP:CZ3	2.44	0.53
5:E:92:LEU:HD23	5:E:172:ARG:HA	1.91	0.53
2:B:134:GLU:HG2	2:B:138:TRP:HD1	1.72	0.53
1:A:583:LYS:NZ	2:B:167:GLU:OE1	2.43	0.53
1:A:169:TYR:OH	1:A:584:ILE:HG22	2.09	0.52
1:A:335:GLN:NE2	1:A:339:ILE:HD11	2.25	0.52
3:C:159:ILE:O	3:C:162:GLN:N	2.42	0.52
2:B:158:PRO:O	2:B:314:ARG:NH1	2.42	0.52
3:C:124:ASN:HB2	4:D:60:VAL:CG1	2.39	0.52
5:E:19:GLY:O	5:E:56:TYR:OH	2.27	0.52
1:A:112:ARG:HG2	1:A:570:ARG:NH1	2.24	0.52
1:A:176:VAL:O	1:A:179:MET:N	2.29	0.52
1:A:321:ASN:H	1:A:328:GLN:HB3	1.74	0.52
3:C:80:PHE:O	3:C:83:GLN:NE2	2.43	0.52
3:C:128:TYR:HE2	4:D:24:ARG:HD3	1.74	0.52
5:E:38:THR:HA	5:E:42:LEU:HB2	1.90	0.52
1:A:219:MET:HE2	1:A:252:MET:HE1	1.92	0.52
2:B:356:GLU:OE2	2:B:359:ARG:NH2	2.40	0.52
3:C:54:ARG:HG3	4:D:13:TRP:CH2	2.44	0.52
1:A:147:SER:HB3	1:A:157:PHE:CE2	2.45	0.52
1:A:320:TYR:HD2	1:A:322:LYS:HD2	1.73	0.52
1:A:375:ARG:HD3	2:B:325:ARG:HH11	1.73	0.52
1:A:147:SER:HB3	1:A:157:PHE:CD2	2.45	0.52
1:A:243:ARG:HG2	1:A:339:ILE:HD13	1.92	0.52
1:A:110:ASN:HA	1:A:117:GLU:HA	1.92	0.51
2:B:211:TYR:HE2	3:C:17:GLY:HA3	1.75	0.51
3:C:208:ASP:N	4:D:54:GLN:HE21	2.09	0.51
1:A:252:MET:O	1:A:256:VAL:N	2.35	0.51
2:B:234:ASN:HD22	2:B:268:TYR:HD1	1.58	0.51
2:B:316:LEU:O	2:B:319:MET:N	2.43	0.51
2:B:332:VAL:HG23	2:B:332:VAL:O	2.11	0.51
2:B:223:TYR:CZ	2:B:265:MET:HG2	2.46	0.51
3:C:143:SER:HG	3:C:155:SER:HG	1.58	0.51
1:A:133:GLY:HA3	1:A:493:MET:HB2	1.93	0.51
3:C:19:TRP:CD1	3:C:19:TRP:C	2.89	0.51
1:A:263:ALA:HB3	1:A:291:ARG:NH2	2.23	0.51
2:B:223:TYR:OH	2:B:262:ARG:NH2	2.43	0.51
2:B:318:TYR:C	2:B:332:VAL:HG21	2.36	0.51
4:D:83:TYR:HE1	4:D:268:LEU:HD11	1.76	0.51
1:A:250:ALA:HB1	1:A:310:LEU:HG	1.93	0.51
5:E:90:GLU:O	5:E:94:SER:CB	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:OD1	1:A:270:THR:N	2.35	0.50
5:E:66:SER:HB2	5:E:87:ASN:ND2	2.27	0.50
1:A:628:ILE:HD11	3:C:138:SER:O	2.12	0.50
2:B:184:ASN:HD21	4:D:266:LYS:HE3	1.77	0.50
1:A:179:MET:O	1:A:181:ARG:N	2.41	0.50
1:A:491:ILE:HD13	1:A:571:MET:HE1	1.92	0.50
3:C:10:LEU:HD22	3:C:108:GLN:HG3	1.94	0.50
4:D:167:LYS:O	4:D:170:ILE:HG22	2.11	0.50
1:A:277:LEU:HD11	1:A:314:LEU:HD21	1.94	0.50
1:A:392:SER:HB2	1:A:442:TYR:HB3	1.94	0.50
4:D:104:LEU:O	4:D:107:GLU:N	2.44	0.50
2:B:222:ALA:O	2:B:226:SER:OG	2.27	0.50
1:A:247:PHE:HE1	1:A:280:LEU:HD22	1.77	0.50
2:B:135:GLN:OE1	2:B:142:MET:HG2	2.12	0.50
3:C:25:ARG:HB3	3:C:31:PHE:HB2	1.94	0.50
1:A:182:GLU:OE2	2:B:161:MET:HE3	2.11	0.49
1:A:329:VAL:O	1:A:333:LEU:N	2.32	0.49
4:D:31:ILE:HG23	4:D:31:ILE:O	2.12	0.49
4:D:224:GLN:O	4:D:227:GLU:N	2.45	0.49
1:A:243:ARG:HG3	1:A:313:TYR:OH	2.11	0.49
1:A:583:LYS:HE2	2:B:161:MET:SD	2.52	0.49
4:D:70:SER:O	4:D:70:SER:OG	2.27	0.49
4:D:135:SER:O	4:D:138:LYS:N	2.46	0.49
4:D:81:ILE:O	4:D:85:LEU:HD23	2.13	0.49
4:D:130:ALA:HB2	5:E:70:VAL:HG23	1.95	0.49
3:C:147:GLU:HG2	3:C:152:GLU:HA	1.94	0.49
4:D:65:VAL:HG22	4:D:251:ARG:HH12	1.78	0.49
4:D:31:ILE:HD11	4:D:143:TRP:CZ3	2.47	0.49
4:D:208:GLY:CA	4:D:211:LEU:HB3	2.42	0.49
1:A:117:GLU:HG2	2:B:122:ARG:HB3	1.95	0.49
1:A:382:PRO:HG2	1:A:391:LEU:HB3	1.95	0.48
1:A:258:MET:HE2	1:A:297:VAL:HG11	1.93	0.48
1:A:110:ASN:OD1	1:A:115:GLY:HA2	2.12	0.48
1:A:335:GLN:HE21	1:A:339:ILE:HD11	1.78	0.48
4:D:174:LEU:HA	4:D:199:LEU:HD12	1.95	0.48
4:D:107:GLU:OE2	4:D:260:ARG:NH1	2.46	0.48
3:C:10:LEU:HD11	3:C:48:PHE:HB3	1.95	0.48
5:E:43:LEU:HB2	5:E:46:CYS:SG	2.54	0.48
1:A:125:MET:HE2	1:A:434:MET:HE2	1.95	0.48
4:D:91:LYS:HD3	4:D:97:GLY:C	2.38	0.48
5:E:76:ARG:O	5:E:77:PRO:C	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:MET:SD	1:A:342:GLN:N	2.87	0.48
1:A:371:VAL:HA	1:A:433:TYR:CE2	2.49	0.48
5:E:79:SER:HB2	5:E:82:GLN:OE1	2.13	0.48
1:A:169:TYR:CD1	1:A:187:LEU:HD13	2.48	0.48
1:A:406:MET:HE1	1:A:460:PHE:CD2	2.49	0.48
1:A:107:PHE:N	1:A:149:ASN:ND2	2.58	0.48
1:A:250:ALA:CB	1:A:310:LEU:HG	2.43	0.48
1:A:219:MET:O	1:A:223:LEU:N	2.26	0.47
4:D:109:GLN:O	4:D:112:VAL:HG12	2.12	0.47
4:D:165:ILE:HG12	4:D:203:LEU:HD13	1.96	0.47
1:A:243:ARG:HB3	1:A:339:ILE:HD13	1.96	0.47
1:A:252:MET:HE2	1:A:252:MET:HB3	1.59	0.47
2:B:166:MET:O	2:B:168:PHE:N	2.47	0.47
3:C:124:ASN:HB2	4:D:60:VAL:HG11	1.96	0.47
4:D:248:LYS:HE2	4:D:292:GLY:O	2.14	0.47
5:E:63:LYS:C	5:E:64:LEU:HD22	2.39	0.47
1:A:382:PRO:HG3	1:A:391:LEU:HD22	1.96	0.47
1:A:436:ILE:C	1:A:437:LEU:HD12	2.40	0.47
1:A:190:PHE:CE1	1:A:357:ILE:HG21	2.49	0.47
1:A:388:PRO:O	1:A:392:SER:HB3	2.15	0.47
1:A:392:SER:OG	1:A:442:TYR:O	2.32	0.47
2:B:204:PHE:HE2	2:B:357:ALA:O	1.97	0.47
1:A:172:VAL:O	1:A:175:MET:N	2.43	0.47
1:A:277:LEU:HD13	1:A:336:HIS:NE2	2.30	0.47
3:C:19:TRP:HD1	3:C:19:TRP:O	1.98	0.47
4:D:250:PHE:O	4:D:254:PHE:HD2	1.96	0.47
1:A:112:ARG:HH11	1:A:113:LYS:HZ1	1.62	0.47
1:A:222:GLN:HB2	1:A:400:SER:OG	2.14	0.47
3:C:19:TRP:O	3:C:20:ARG:C	2.57	0.47
3:C:29:GLU:O	3:C:33:SER:N	2.29	0.47
3:C:88:GLU:HA	3:C:161:GLY:HA3	1.97	0.47
4:D:37:GLU:O	4:D:40:GLU:N	2.47	0.47
4:D:177:ALA:HB1	4:D:195:LEU:HG	1.96	0.47
1:A:258:MET:HE3	1:A:262:GLY:HA3	1.96	0.47
1:A:432:PRO:HA	1:A:459:GLY:O	2.14	0.47
3:C:103:LEU:HD12	3:C:103:LEU:O	2.15	0.47
1:A:581:GLN:OE1	1:A:581:GLN:N	2.48	0.47
1:A:131:ILE:HG22	1:A:491:ILE:HD12	1.97	0.46
2:B:168:PHE:O	2:B:171:LYS:N	2.48	0.46
4:D:91:LYS:HD3	4:D:97:GLY:O	2.16	0.46
4:D:277:GLN:HG3	4:D:281:ASN:ND2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HA	1:A:168:LEU:HD12	1.58	0.46
3:C:25:ARG:HB3	3:C:31:PHE:CB	2.45	0.46
3:C:160:PHE:HE2	3:C:179:PHE:CE1	2.34	0.46
1:A:583:LYS:HE3	2:B:164:THR:HG23	1.98	0.46
1:A:190:PHE:HE1	1:A:357:ILE:HG21	1.80	0.46
1:A:196:ASP:OD1	1:A:197:ILE:HG12	2.15	0.46
1:A:291:ARG:NE	1:A:295:GLU:OE1	2.48	0.46
1:A:219:MET:HB2	1:A:252:MET:CE	2.37	0.46
1:A:269:ASN:ND2	1:A:351:ALA:HB1	2.30	0.46
1:A:106:THR:C	1:A:149:ASN:HD21	2.23	0.46
1:A:281:GLU:O	1:A:284:VAL:N	2.44	0.46
2:B:179:ASP:N	2:B:179:ASP:OD1	2.49	0.45
2:B:233:MET:HB3	2:B:233:MET:HE2	1.71	0.45
4:D:132:SER:HA	4:D:236:PHE:CZ	2.52	0.45
3:C:30:ARG:HD3	3:C:30:ARG:HA	1.70	0.45
5:E:155:VAL:HA	5:E:186:PHE:O	2.16	0.45
1:A:220:LEU:HD23	1:A:249:GLU:HG2	1.97	0.45
1:A:305:LEU:O	1:A:305:LEU:HD23	2.17	0.45
3:C:58:ASP:OD1	3:C:58:ASP:N	2.47	0.45
4:D:180:HIS:C	4:D:198:LYS:HZ2	2.23	0.45
2:B:215:PHE:HB3	2:B:265:MET:HE2	1.98	0.45
3:C:136:TYR:OH	3:C:187:SER:HA	2.17	0.45
4:D:78:LYS:HG2	5:E:28:TYR:CD2	2.52	0.45
1:A:131:ILE:HG22	1:A:491:ILE:HB	1.99	0.45
2:B:202:ARG:NH1	3:C:27:ILE:HD13	2.32	0.45
1:A:191:MET:HE3	1:A:380:LEU:HB3	1.98	0.45
4:D:230:ASN:O	4:D:234:ASP:N	2.50	0.45
1:A:197:ILE:HG21	1:A:356:HIS:HB3	1.99	0.45
1:A:618:SER:OG	3:C:177:LYS:HG2	2.17	0.45
4:D:114:LEU:HA	4:D:114:LEU:HD23	1.56	0.45
1:A:227:LEU:HB2	1:A:343:LEU:HD21	1.99	0.45
3:C:19:TRP:HZ3	3:C:89:SER:O	2.00	0.45
3:C:124:ASN:ND2	4:D:21:THR:OG1	2.50	0.45
4:D:83:TYR:HD2	4:D:84:LEU:HD23	1.81	0.45
1:A:252:MET:O	1:A:256:VAL:HG12	2.16	0.44
1:A:299:ILE:O	1:A:299:ILE:HG22	2.17	0.44
1:A:337:GLY:O	1:A:341:MET:HB3	2.17	0.44
5:E:24:GLU:OE1	5:E:24:GLU:N	2.34	0.44
4:D:19:THR:O	4:D:23:GLU:HB2	2.18	0.44
4:D:57:LEU:HA	4:D:57:LEU:HD23	1.66	0.44
1:A:471:ALA:HA	1:A:474:LYS:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:MET:C	2:B:168:PHE:N	2.74	0.44
3:C:12:LEU:H	3:C:12:LEU:HD12	1.82	0.44
4:D:125:GLN:HA	4:D:243:LEU:HD21	1.99	0.44
4:D:161:THR:OG1	4:D:163:SER:O	2.36	0.44
4:D:233:LEU:O	4:D:233:LEU:HD23	2.18	0.44
1:A:562:PHE:HD2	1:A:564:SER:H	1.65	0.44
2:B:232:ARG:HA	2:B:232:ARG:HD3	1.73	0.44
4:D:61:LEU:HD12	4:D:61:LEU:HA	1.65	0.44
1:A:188:ILE:HG22	1:A:207:ASN:O	2.17	0.44
2:B:166:MET:HE2	2:B:166:MET:HA	2.00	0.44
2:B:307:LEU:HD23	2:B:307:LEU:HA	1.74	0.44
2:B:318:TYR:O	2:B:332:VAL:HG21	2.18	0.44
1:A:264:ILE:HB	1:A:291:ARG:NH1	2.33	0.44
1:A:269:ASN:ND2	1:A:272:ARG:HH11	2.15	0.44
2:B:166:MET:CE	2:B:365:VAL:HG23	2.44	0.44
1:A:106:THR:HG23	1:A:120:PHE:HB2	2.00	0.44
1:A:580:LYS:HB2	1:A:581:GLN:OE1	2.17	0.44
4:D:37:GLU:O	4:D:41:ALA:N	2.46	0.44
4:D:258:ILE:HD12	4:D:258:ILE:HA	1.85	0.44
1:A:124:ASP:O	1:A:127:THR:N	2.51	0.44
2:B:166:MET:C	2:B:168:PHE:H	2.25	0.44
2:B:182:LEU:HD11	4:D:285:LEU:O	2.18	0.44
2:B:248:ASP:OD1	2:B:308:TRP:CD1	2.69	0.44
1:A:118:LEU:HD13	1:A:567:VAL:HG11	1.99	0.44
1:A:176:VAL:O	1:A:178:SER:N	2.51	0.44
1:A:267:ASP:CG	1:A:269:ASN:H	2.25	0.43
2:B:212:TRP:CH2	2:B:278:VAL:HG22	2.53	0.43
2:B:230:MET:HE3	2:B:274:VAL:HG11	2.00	0.43
5:E:21:THR:OG1	5:E:22:SER:N	2.50	0.43
2:B:229:PHE:O	2:B:233:MET:HG3	2.19	0.43
3:C:102:TYR:CE1	3:C:181:ASN:ND2	2.86	0.43
4:D:76:ALA:HA	4:D:258:ILE:HD13	2.00	0.43
5:E:43:LEU:O	5:E:47:ASN:N	2.45	0.43
1:A:289:PHE:CD2	1:A:299:ILE:HD11	2.53	0.43
1:A:325:LYS:HD2	1:A:328:GLN:NE2	2.33	0.43
4:D:178:PHE:HE2	4:D:195:LEU:HD11	1.82	0.43
5:E:122:ASN:HA	5:E:127:GLU:CB	2.48	0.43
1:A:367:PHE:O	1:A:371:VAL:HG22	2.18	0.43
2:B:152:GLN:HG2	2:B:153:ASP:H	1.84	0.43
4:D:227:GLU:C	4:D:229:LEU:N	2.77	0.43
1:A:190:PHE:HE1	1:A:357:ILE:HG13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD21	1:A:271:ILE:HD11	2.00	0.43
1:A:303:PRO:O	1:A:306:VAL:HG12	2.19	0.43
2:B:309:LEU:HD21	2:B:316:LEU:HG	2.01	0.43
3:C:191:PHE:O	3:C:195:ILE:HG12	2.19	0.43
4:D:49:TYR:HD1	4:D:179:ILE:HD11	1.82	0.43
2:B:251:PHE:HB2	2:B:256:PRO:HB3	2.01	0.43
1:A:434:MET:HE2	1:A:434:MET:HB3	1.74	0.43
3:C:20:ARG:CZ	3:C:20:ARG:HB3	2.49	0.43
3:C:192:ARG:NH2	4:D:71:ASP:OD2	2.51	0.43
4:D:155:ASN:O	4:D:158:TYR:N	2.45	0.43
4:D:166:LYS:HE3	4:D:166:LYS:HB3	1.73	0.43
4:D:178:PHE:CE2	4:D:195:LEU:HD11	2.53	0.43
1:A:179:MET:O	1:A:181:ARG:HG2	2.18	0.43
1:A:280:LEU:O	1:A:283:ILE:HB	2.19	0.43
2:B:292:LEU:HD21	2:B:296:ARG:NH2	2.34	0.43
1:A:119:TRP:O	1:A:120:PHE:CD1	2.72	0.43
1:A:179:MET:C	1:A:181:ARG:H	2.26	0.43
2:B:361:LEU:HD12	2:B:361:LEU:HA	1.85	0.43
1:A:494:LYS:HE2	1:A:494:LYS:HB2	1.82	0.43
2:B:135:GLN:OE1	2:B:142:MET:HE3	2.19	0.42
3:C:37:LYS:HD2	3:C:71:LEU:HD21	2.00	0.42
4:D:252:THR:O	4:D:255:TYR:N	2.52	0.42
1:A:169:TYR:CD1	1:A:187:LEU:HD22	2.54	0.42
1:A:365:VAL:O	1:A:365:VAL:HG13	2.19	0.42
1:A:385:GLU:N	1:A:385:GLU:OE1	2.52	0.42
1:A:628:ILE:HD12	3:C:139:PHE:CE1	2.54	0.42
5:E:32:ARG:HG2	5:E:32:ARG:HH11	1.84	0.42
5:E:37:LEU:HD13	5:E:46:CYS:HB3	2.00	0.42
1:A:131:ILE:HD11	1:A:143:LEU:HD21	2.00	0.42
1:A:257:TYR:OH	1:A:302:ILE:HD12	2.19	0.42
1:A:321:ASN:HB2	1:A:328:GLN:HB3	2.02	0.42
4:D:121:LEU:HA	4:D:121:LEU:HD12	1.72	0.42
5:E:33:PHE:HB3	5:E:53:ILE:CD1	2.49	0.42
1:A:176:VAL:O	1:A:177:ARG:C	2.63	0.42
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.67	0.42
2:B:192:THR:C	2:B:370:LEU:HD12	2.44	0.42
3:C:100:LEU:HD23	3:C:100:LEU:HA	1.74	0.42
4:D:33:LEU:HD11	4:D:171:ARG:NH1	2.34	0.42
4:D:104:LEU:HD12	4:D:104:LEU:HA	1.80	0.42
1:A:169:TYR:CE1	1:A:187:LEU:HD22	2.54	0.42
1:A:455:ALA:HB1	1:A:458:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:VAL:HA	3:C:117:VAL:HG11	2.01	0.42
4:D:62:ASN:HD21	4:D:244:SER:HB2	1.85	0.42
2:B:225:LEU:HA	2:B:225:LEU:HD23	1.74	0.42
4:D:125:GLN:O	4:D:128:LEU:N	2.52	0.42
1:A:188:ILE:O	1:A:188:ILE:HG13	2.18	0.42
1:A:263:ALA:N	1:A:291:ARG:HH12	2.18	0.42
1:A:321:ASN:OD1	1:A:327:LYS:HB3	2.20	0.42
4:D:155:ASN:HB2	4:D:167:LYS:HE3	2.00	0.42
4:D:215:ILE:HG13	4:D:216:LEU:N	2.33	0.42
1:A:220:LEU:H	1:A:220:LEU:HD12	1.85	0.42
1:A:283:ILE:O	1:A:287:LYS:HA	2.20	0.42
1:A:484:GLY:O	1:A:490:LYS:NZ	2.50	0.42
1:A:604:GLN:HB3	3:C:163:LEU:HD11	2.01	0.42
1:A:406:MET:HE1	1:A:460:PHE:CE2	2.55	0.42
1:A:621:LYS:HB2	1:A:621:LYS:HE3	1.82	0.42
2:B:365:VAL:C	2:B:367:GLU:H	2.28	0.42
5:E:41:LYS:HE2	5:E:41:LYS:HB3	1.89	0.42
1:A:402:LEU:HD21	1:A:460:PHE:HZ	1.84	0.42
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.81	0.42
4:D:135:SER:CB	4:D:232:LYS:HD3	2.50	0.42
1:A:122:ASN:ND2	1:A:432:PRO:HD3	2.35	0.41
1:A:181:ARG:HE	1:A:181:ARG:HB2	1.69	0.41
3:C:111:LEU:HA	3:C:111:LEU:HD12	1.86	0.41
4:D:51:HIS:ND1	4:D:184:VAL:HG11	2.35	0.41
4:D:23:GLU:CD	4:D:38:ILE:HD13	2.45	0.41
4:D:44:ILE:HG21	4:D:179:ILE:O	2.20	0.41
2:B:306:PHE:CE2	2:B:320:LEU:HD13	2.54	0.41
3:C:55:LEU:HD23	3:C:55:LEU:HA	1.77	0.41
4:D:259:LEU:HD12	4:D:259:LEU:HA	1.81	0.41
1:A:181:ARG:HH21	1:A:184:ASP:CG	2.27	0.41
3:C:68:ASN:O	3:C:68:ASN:OD1	2.38	0.41
4:D:91:LYS:HD2	4:D:101:ARG:HD3	2.02	0.41
4:D:111:LEU:HA	4:D:111:LEU:HD12	1.76	0.41
1:A:280:LEU:HD11	1:A:310:LEU:HD13	2.02	0.41
2:B:371:THR:OG1	2:B:374:GLN:HG2	2.21	0.41
3:C:31:PHE:O	3:C:35:GLU:HB2	2.20	0.41
1:A:110:ASN:O	1:A:569:ALA:HB1	2.20	0.41
1:A:112:ARG:HH22	1:A:568:ARG:HH21	1.69	0.41
1:A:124:ASP:O	1:A:127:THR:OG1	2.20	0.41
1:A:126:ARG:NH2	1:A:429:ALA:O	2.54	0.41
1:A:222:GLN:HG3	1:A:223:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:TRP:O	2:B:317:TRP:CG	2.74	0.41
2:B:347:ARG:HG2	2:B:348:ARG:O	2.21	0.41
2:B:351:VAL:HG11	3:C:162:GLN:OE1	2.21	0.41
3:C:80:PHE:CE2	3:C:116:HIS:CE1	3.09	0.41
4:D:211:LEU:O	4:D:215:ILE:HG12	2.20	0.41
5:E:88:LYS:O	5:E:89:ALA:C	2.63	0.41
4:D:168:ASN:OD1	4:D:169:ALA:N	2.54	0.41
1:A:174:SER:OG	1:A:174:SER:O	2.38	0.41
3:C:104:PRO:HB3	3:C:181:ASN:CG	2.46	0.41
4:D:79:LEU:HD23	4:D:79:LEU:HA	1.84	0.41
4:D:231:THR:HA	4:D:234:ASP:HB2	2.02	0.41
1:A:186:LEU:HD22	1:A:365:VAL:HB	2.02	0.41
1:A:390:GLU:C	1:A:391:LEU:HD23	2.45	0.41
2:B:376:GLU:H	2:B:376:GLU:HG3	1.75	0.41
5:E:13:LEU:HD23	5:E:13:LEU:HA	1.81	0.41
5:E:18:VAL:O	5:E:18:VAL:HG22	2.19	0.41
1:A:278:GLN:HG2	1:A:279:ARG:N	2.36	0.41
1:A:308:ASP:N	1:A:309:PRO:HD2	2.36	0.41
1:A:122:ASN:O	1:A:126:ARG:HG3	2.21	0.40
1:A:405:MET:HE3	1:A:405:MET:HB2	1.78	0.40
2:B:302:PRO:C	2:B:304:SER:H	2.28	0.40
3:C:208:ASP:H	4:D:54:GLN:HE21	1.69	0.40
4:D:80:LEU:HA	4:D:80:LEU:HD23	1.75	0.40
1:A:562:PHE:HB3	1:A:565:LYS:O	2.20	0.40
2:B:222:ALA:HB1	2:B:288:ILE:CD1	2.50	0.40
2:B:189:GLU:O	2:B:190:GLU:HG2	2.21	0.40
3:C:19:TRP:C	3:C:19:TRP:HD1	2.28	0.40
1:A:112:ARG:HA	1:A:570:ARG:NH2	2.33	0.40
1:A:251:LEU:O	1:A:255:LEU:N	2.49	0.40
1:A:289:PHE:N	1:A:297:VAL:O	2.43	0.40
1:A:560:ILE:HG23	1:A:560:ILE:HD12	1.84	0.40
1:A:609:GLN:OE1	3:C:167:SER:OG	2.35	0.40
2:B:208:LEU:HD23	2:B:208:LEU:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/783 (59%)	426 (92%)	39 (8%)	0	100	100
2	B	257/380 (68%)	225 (88%)	32 (12%)	0	100	100
3	C	200/208 (96%)	177 (88%)	23 (12%)	0	100	100
4	D	281/294 (96%)	247 (88%)	34 (12%)	0	100	100
5	E	186/230 (81%)	153 (82%)	33 (18%)	0	100	100
All	All	1389/1895 (73%)	1228 (88%)	161 (12%)	0	100	100

There are no Ramachandran outliers to report.

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	397/676 (59%)	397 (100%)	0	100	100
2	B	222/332 (67%)	222 (100%)	0	100	100
3	C	173/179 (97%)	173 (100%)	0	100	100
4	D	256/269 (95%)	256 (100%)	0	100	100
5	E	81/192 (42%)	80 (99%)	1 (1%)	63	70
All	All	1129/1648 (68%)	1128 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	79	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
2	B	321	ASN
3	C	116	HIS
4	D	12	GLN
4	D	54	GLN
4	D	67	GLN
5	E	87	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](#)

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

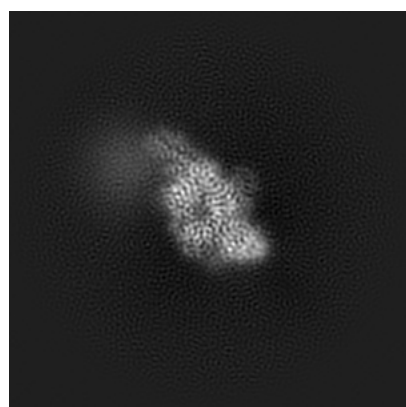
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13083. These allow visual inspection of the internal detail of the map and identification of artifacts.

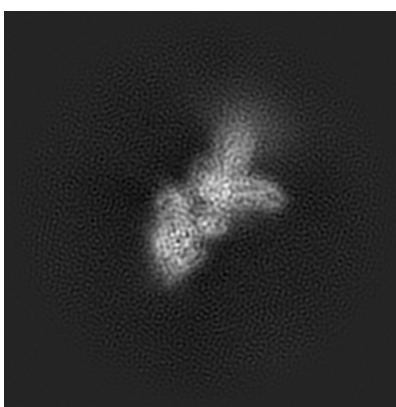
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

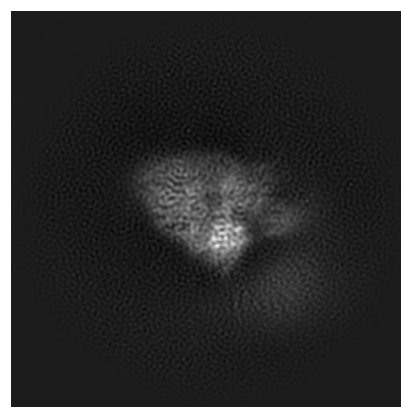
6.1.1 Primary map



X



Y

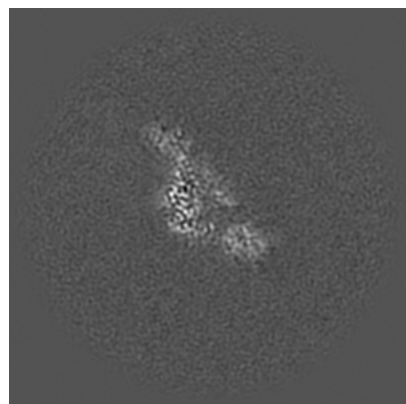


Z

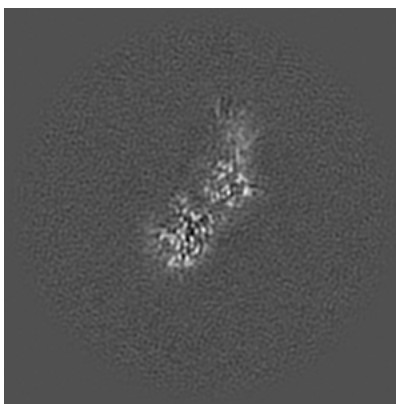
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

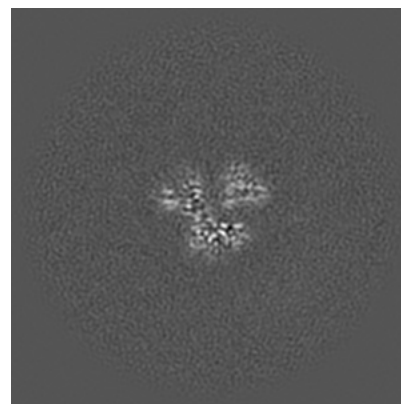
6.2.1 Primary map



X Index: 150



Y Index: 150

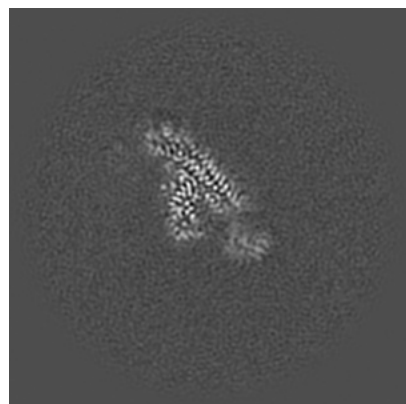


Z Index: 150

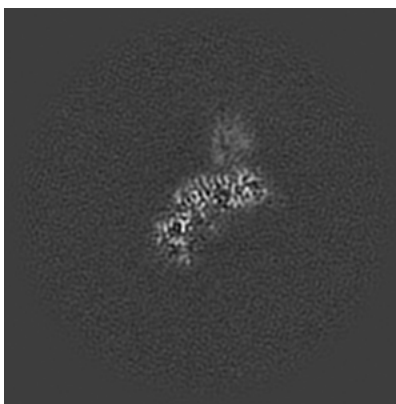
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

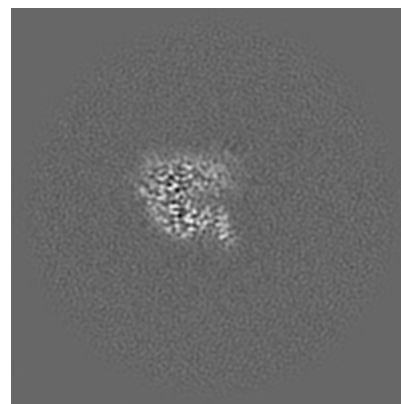
6.3.1 Primary map



X Index: 161



Y Index: 137

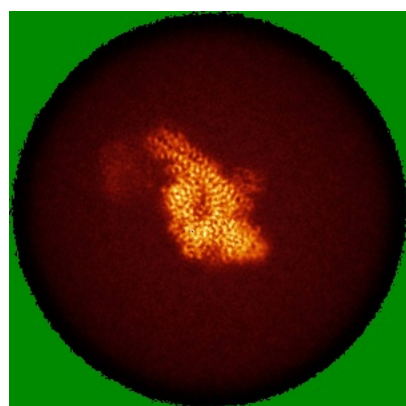


Z Index: 130

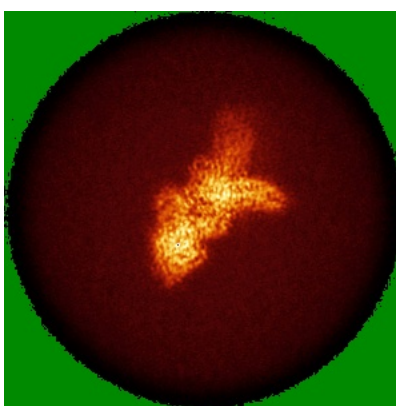
The images above show the largest variance slices of the map in three orthogonal directions.

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

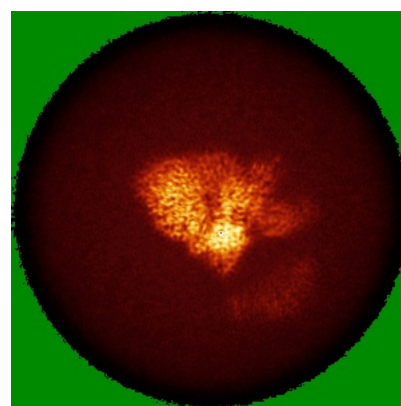
6.4.1 Primary map



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 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

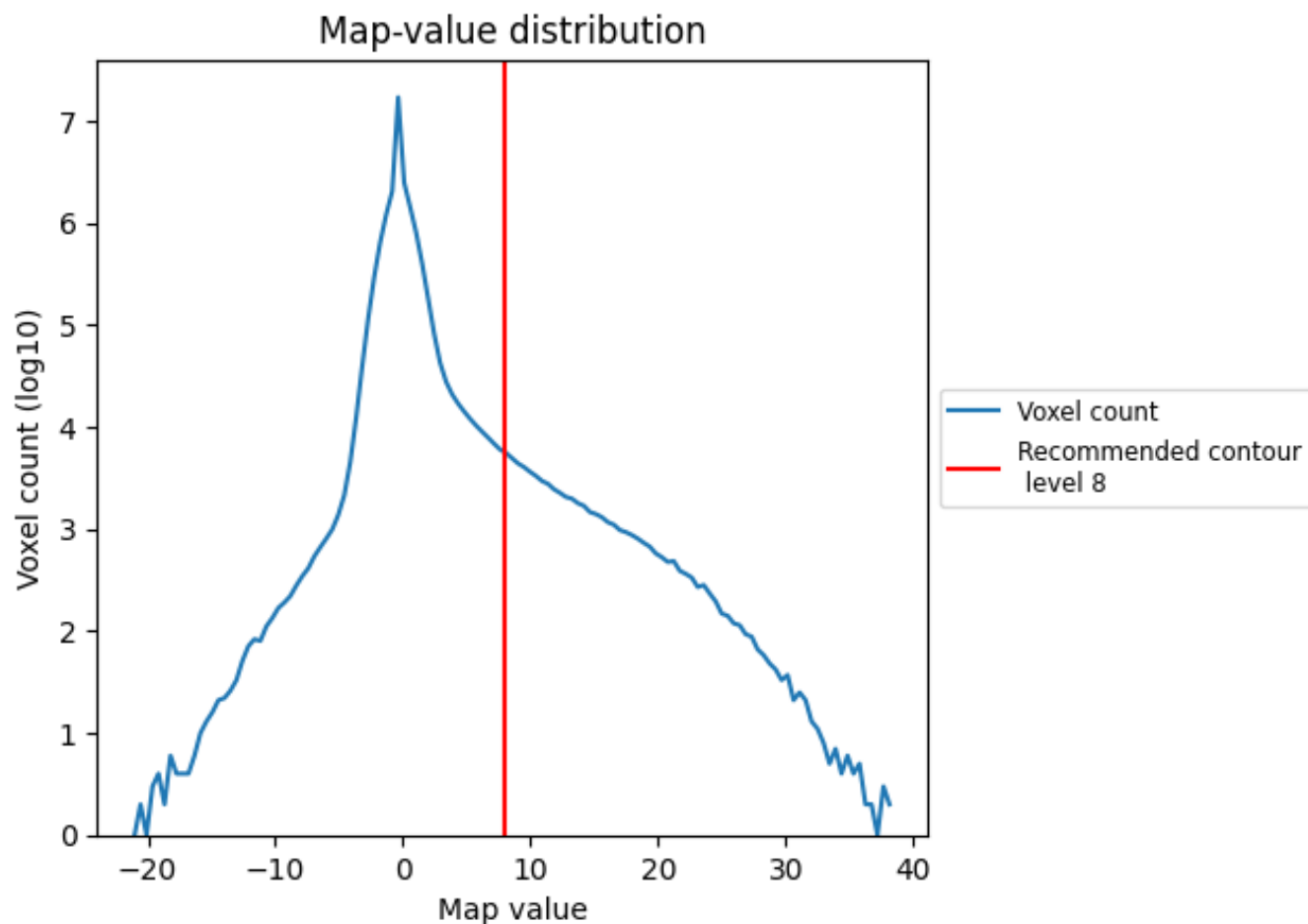
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

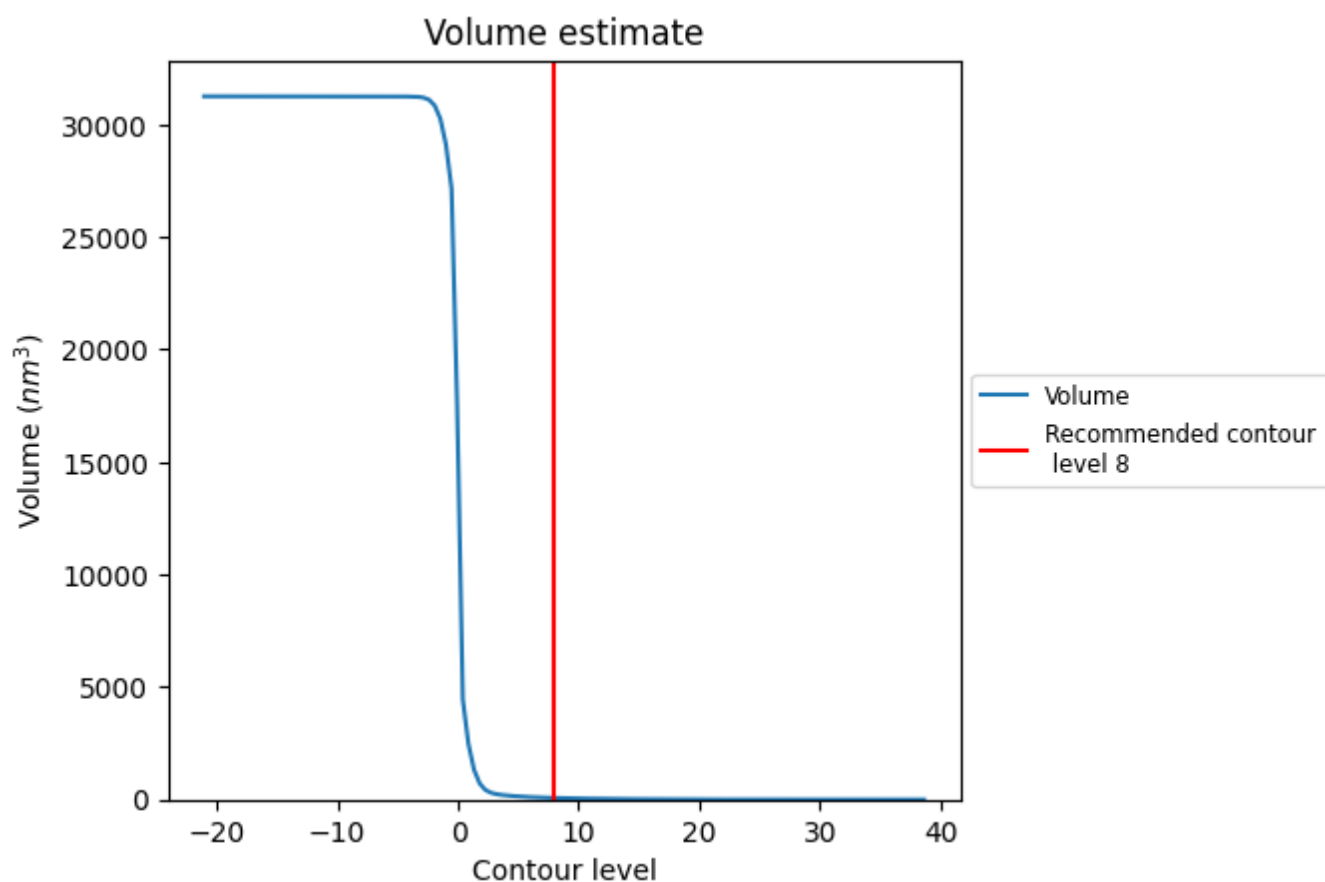
This section contains the results of statistical analysis of the map.

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.

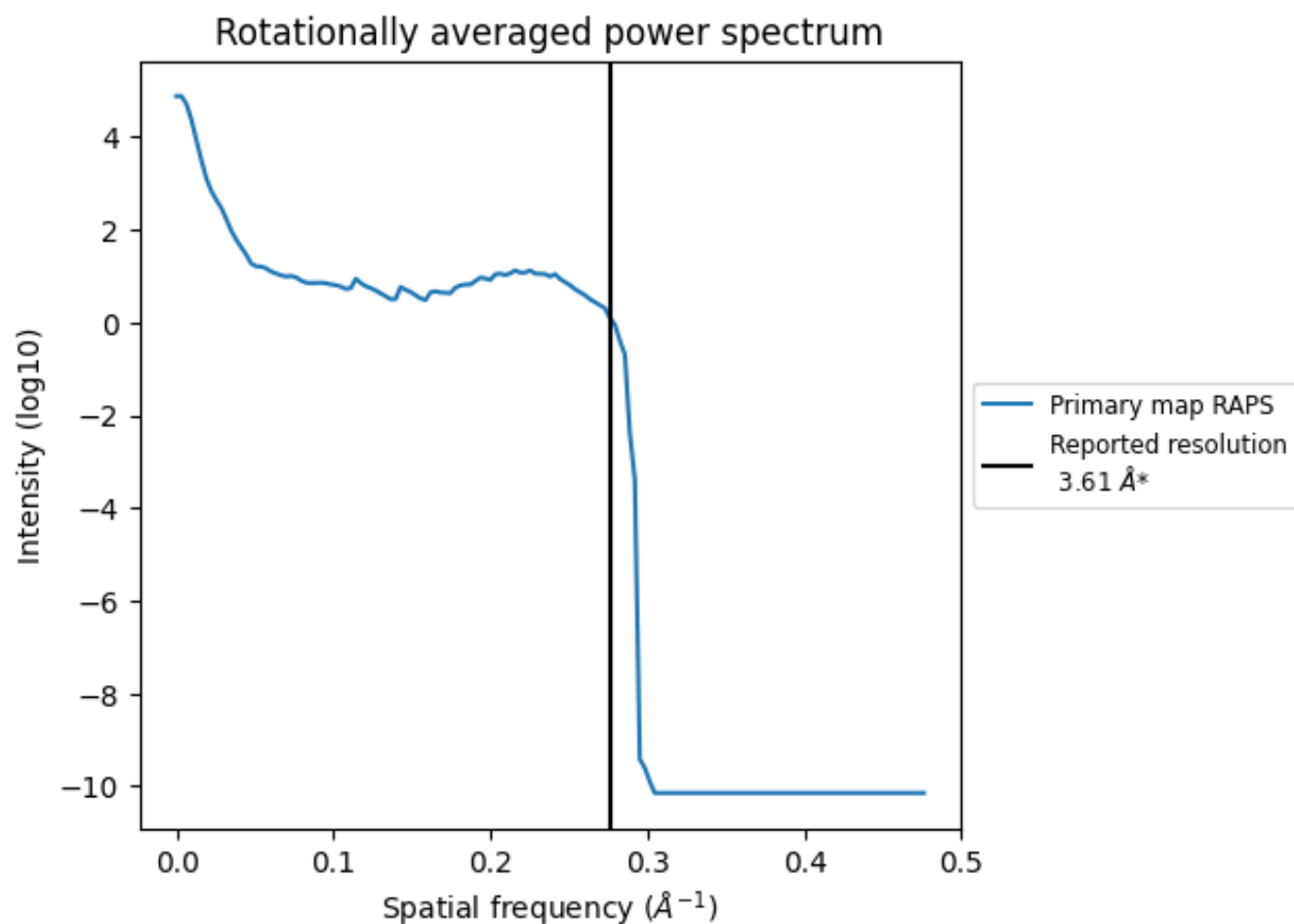
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm³; this corresponds to an approximate mass of 64 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 0.277 Å⁻¹

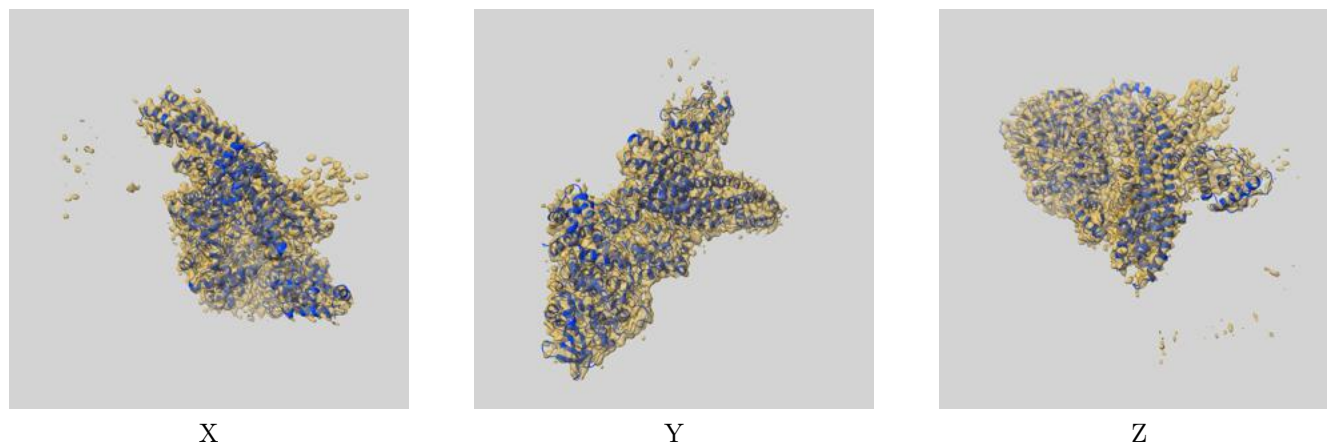
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

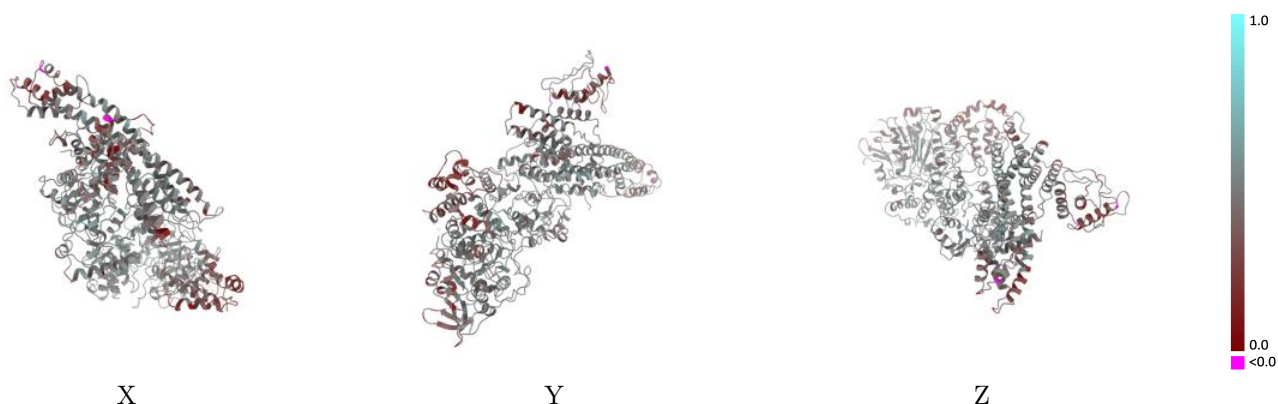
This section contains information regarding the fit between EMDB map EMD-13083 and PDB model 7OVB. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



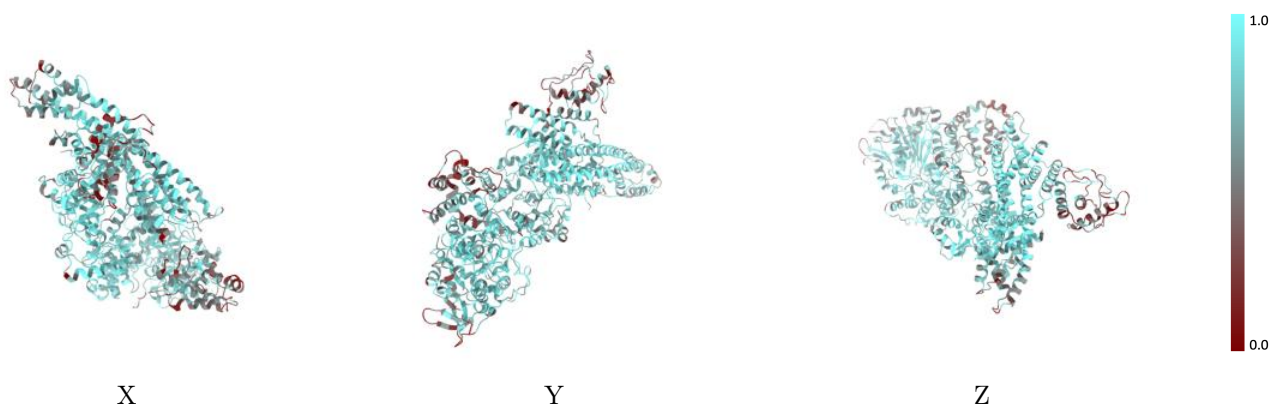
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



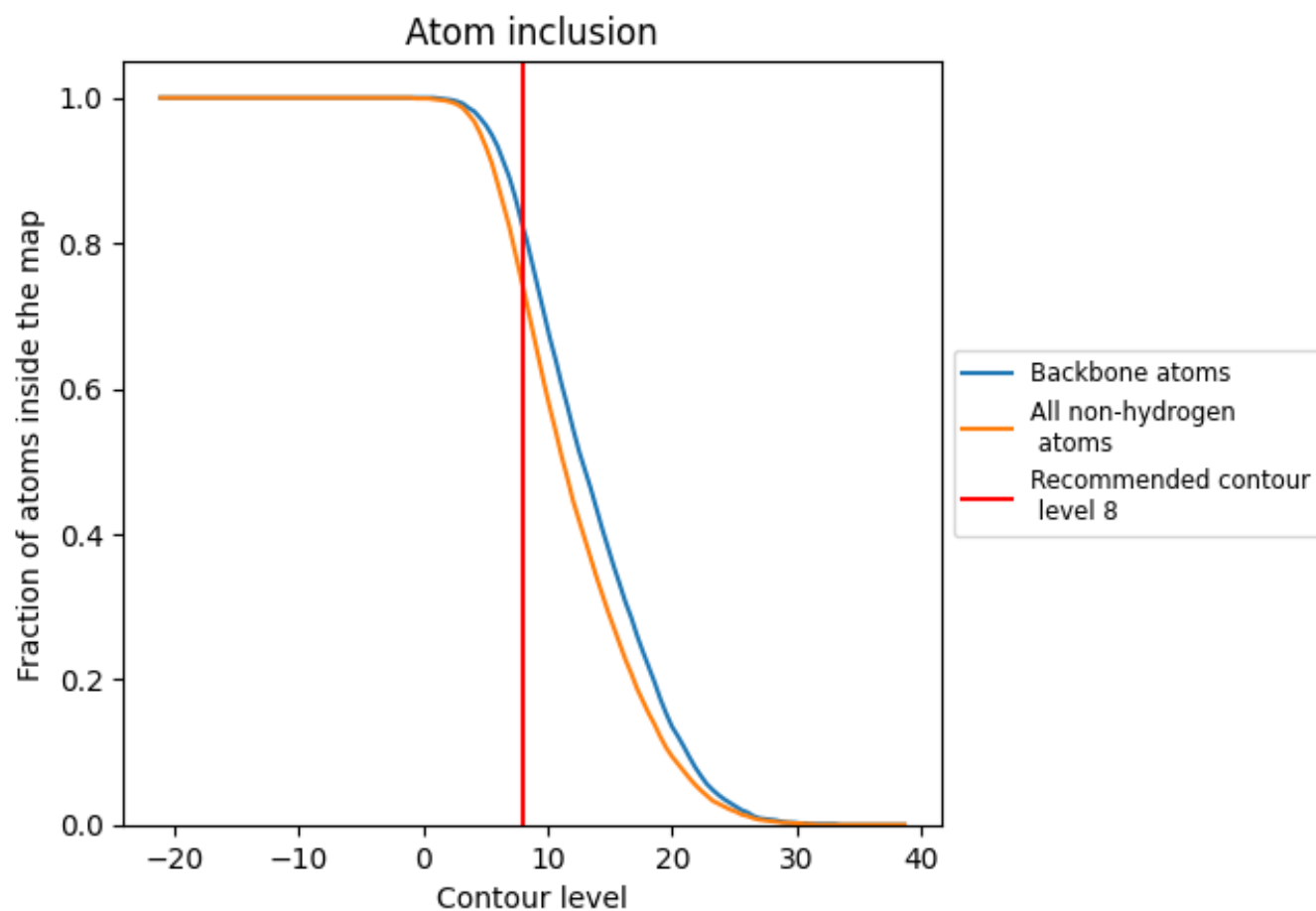
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 74% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7410	0.4540
A	0.6820	0.4290
B	0.7960	0.4870
C	0.8560	0.5030
D	0.7780	0.4510
E	0.6010	0.4170

