



Full wwPDB EM Validation Report ⓘ

Nov 5, 2025 – 02:55 PM JST

PDB ID : 9V53 / pdb_00009v53
EMDB ID : EMD-64785
Title : Structure of TolC, YbjP, and AcrABZ complex
Authors : Ge, X.F.; Gu, Z.W.; Wang, J.W.
Deposited on : 2025-05-25
Resolution : 3.39 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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

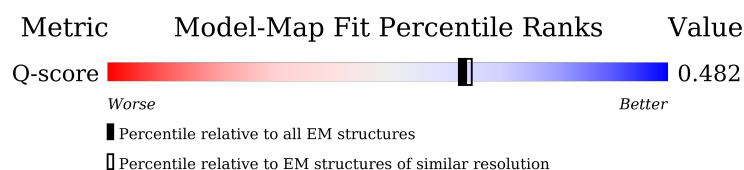
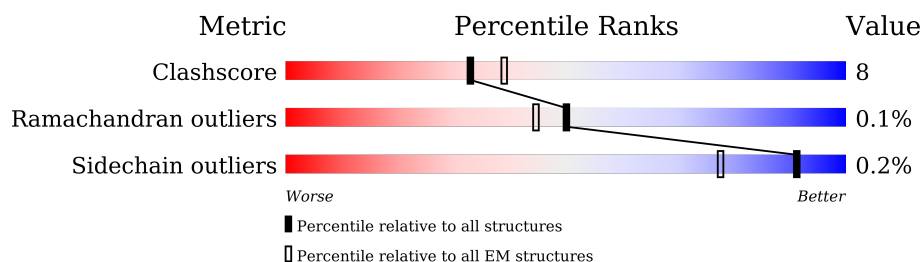
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.39 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14220 (2.89 - 3.89)

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	C1	493	
1	C2	493	
1	C3	493	
2	P1	171	

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Mol	Chain	Length	Quality of chain
2	P2	171	
2	P3	171	
3	A1	397	
3	A2	397	
3	A3	397	
3	a1	397	
3	a2	397	
3	a3	397	
4	BL	1049	
4	BO	1049	
4	BT	1049	
5	ZL	49	
5	ZO	49	
5	ZT	49	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 53464 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 Outer membrane protein TolC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	432	Total	C	N	O	S	0	0
			3331	2054	591	681	5		
1	C2	432	Total	C	N	O	S	0	0
			3331	2054	591	681	5		
1	C3	432	Total	C	N	O	S	0	0
			3331	2054	591	681	5		

- Molecule 2 is a protein called Uncharacterized lipoprotein YbjP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P1	152	Total	C	N	O	S	0	0
			1182	722	218	238	4		
2	P2	152	Total	C	N	O	S	0	0
			1182	722	218	238	4		
2	P3	152	Total	C	N	O	S	0	0
			1182	722	218	238	4		

- Molecule 3 is a protein called Multidrug efflux pump subunit AcrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A1	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		
3	A2	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		
3	A3	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		
3	a2	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		
3	a1	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		
3	a3	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		

- Molecule 4 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BL	1036	Total	C	N	O	S	0	0
			7847	5050	1296	1457	44		
4	BT	1034	Total	C	N	O	S	0	0
			7837	5044	1294	1455	44		
4	BO	1034	Total	C	N	O	S	0	0
			7837	5044	1294	1455	44		

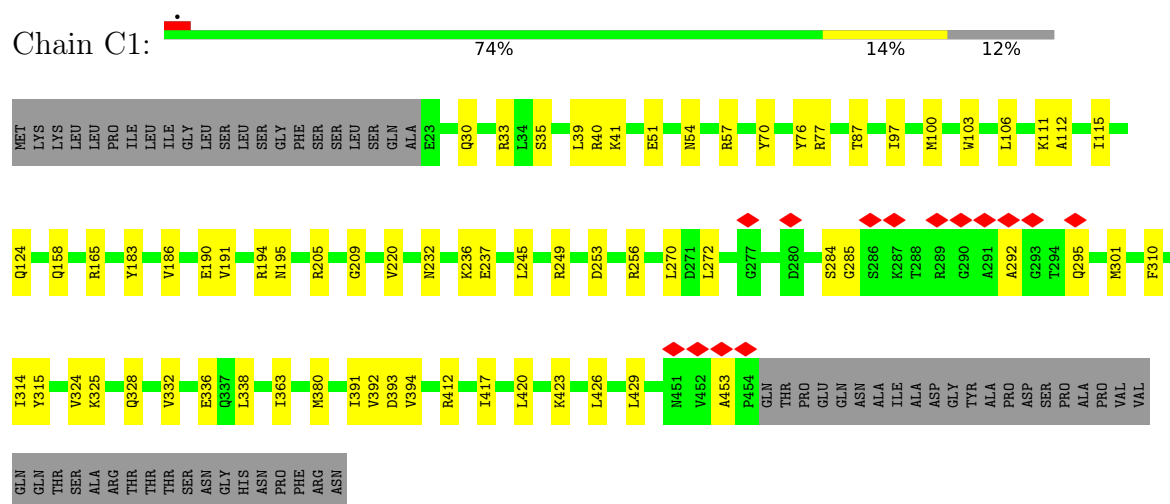
- Molecule 5 is a protein called Multidrug efflux pump accessory protein AcrZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	ZL	39	Total	C	N	O	S	0	0
			294	203	41	47	3		
5	ZT	39	Total	C	N	O	S	0	0
			294	203	41	47	3		
5	ZO	39	Total	C	N	O	S	0	0
			294	203	41	47	3		

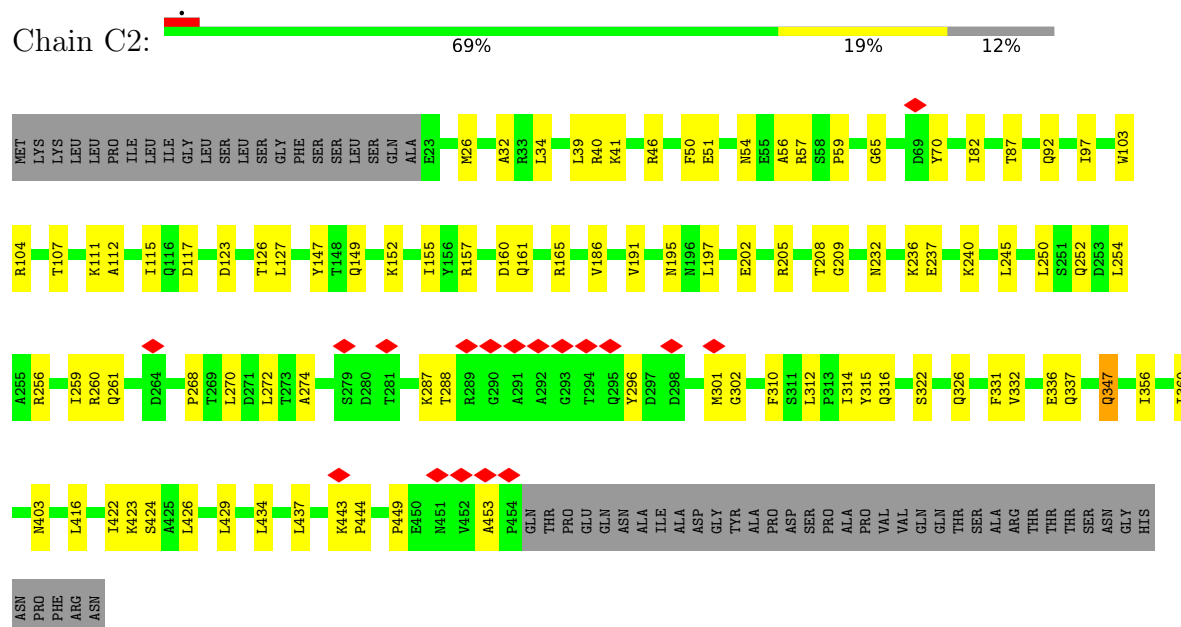
3 Residue-property plots

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.

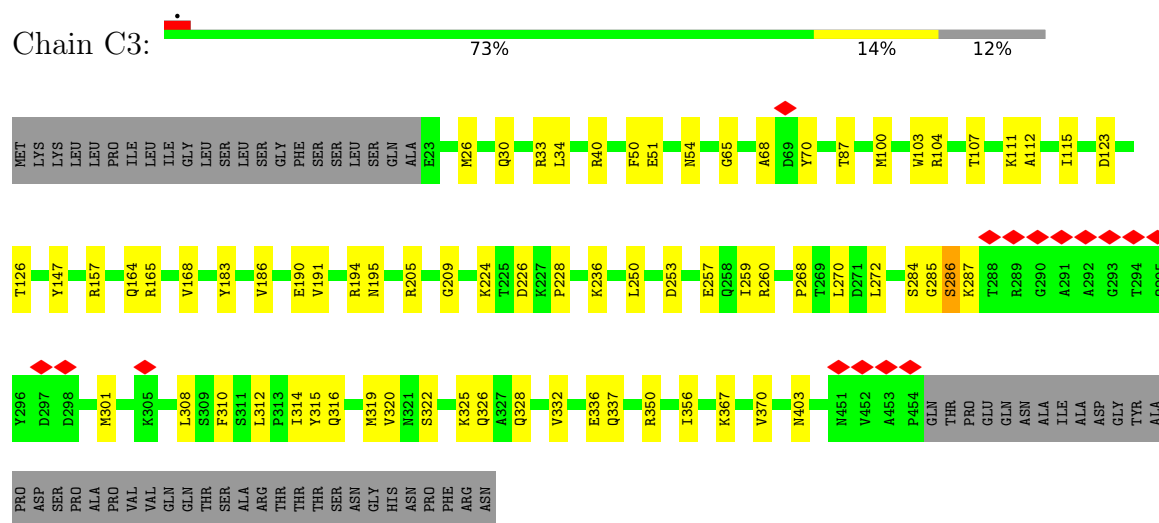
• Molecule 1: Outer membrane protein TolC



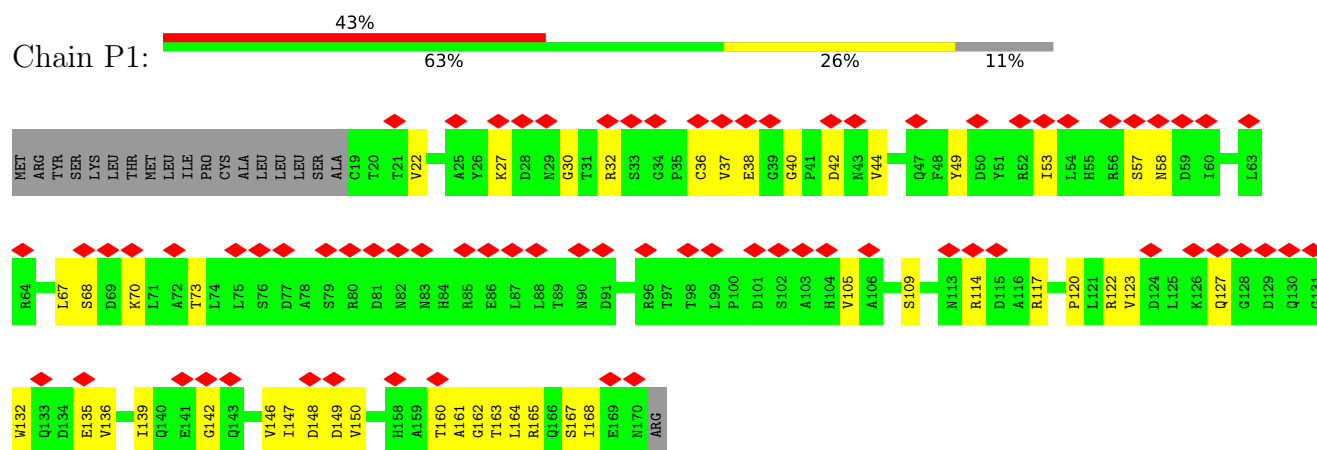
• Molecule 1: Outer membrane protein TolC



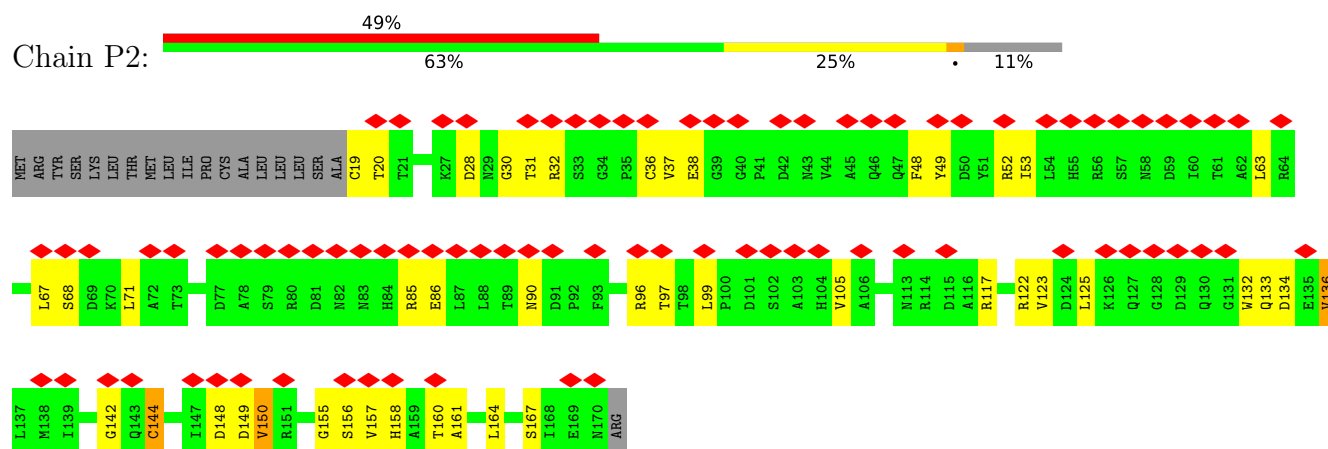
- Molecule 1: Outer membrane protein TolC



- Molecule 2: Uncharacterized lipoprotein YbjP

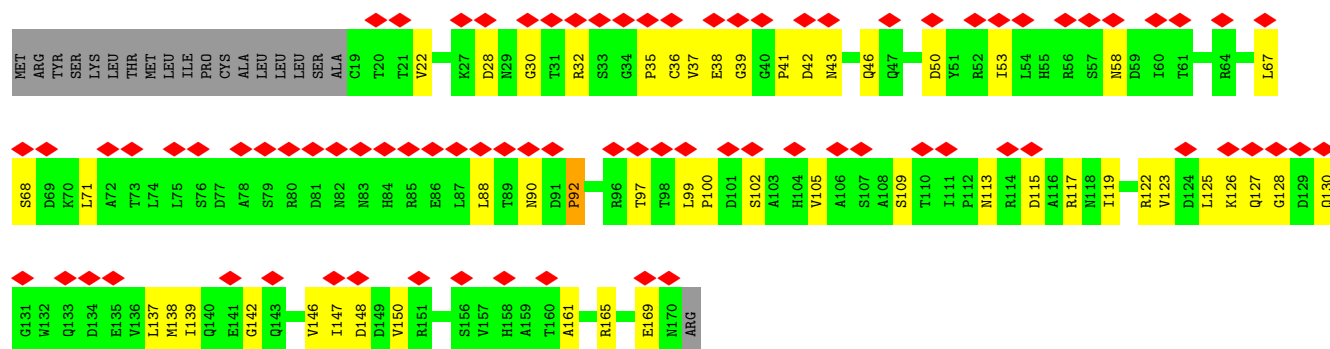


- Molecule 2: Uncharacterized lipoprotein YbjP



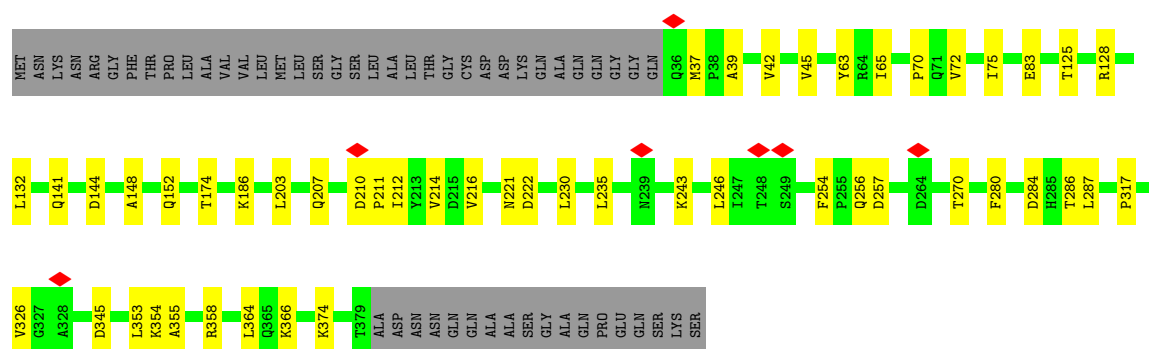
- Molecule 2: Uncharacterized lipoprotein YbjP





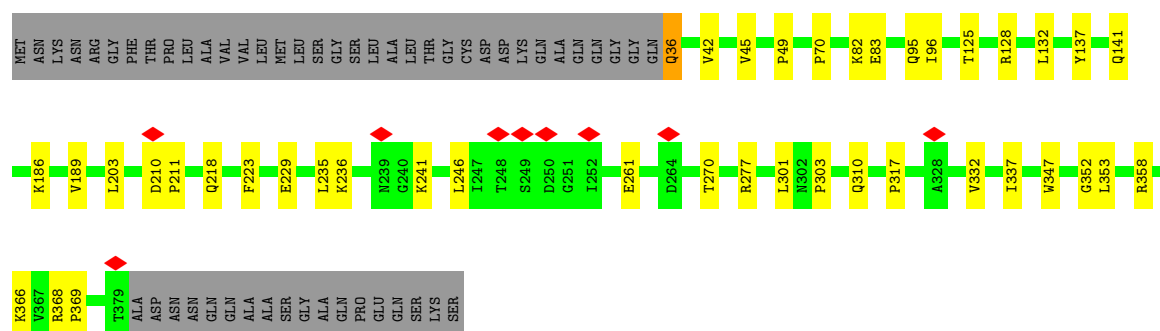
• Molecule 3: Multidrug efflux pump subunit AcrA

Chain A1: 74% 13% 13%



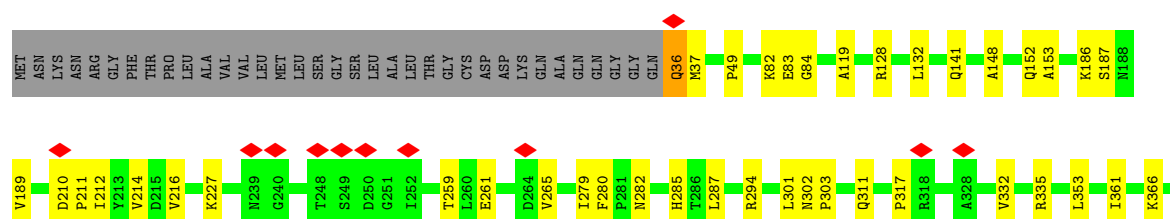
• Molecule 3: Multidrug efflux pump subunit AcrA

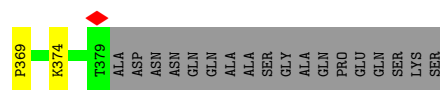
Chain A2: 76% 10% 13%



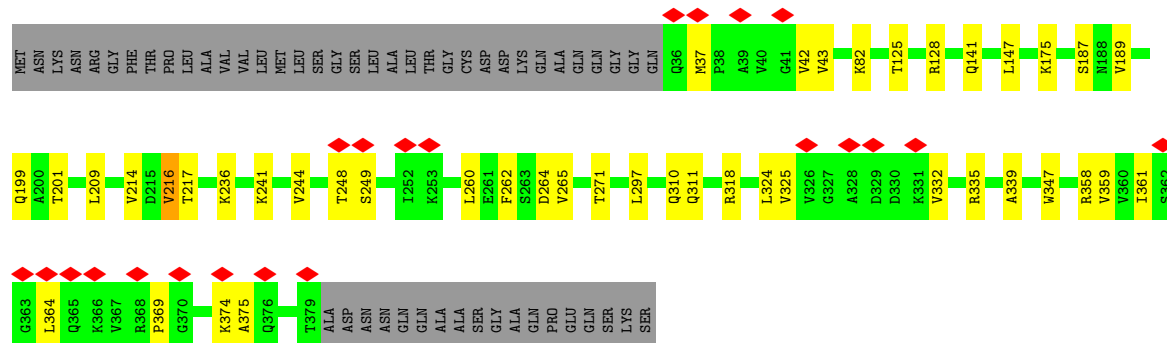
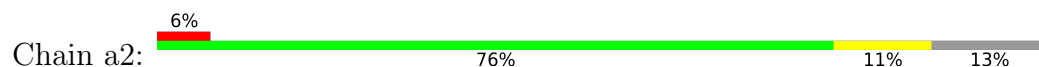
• Molecule 3: Multidrug efflux pump subunit AcrA

Chain A3: 76% 11% 13%

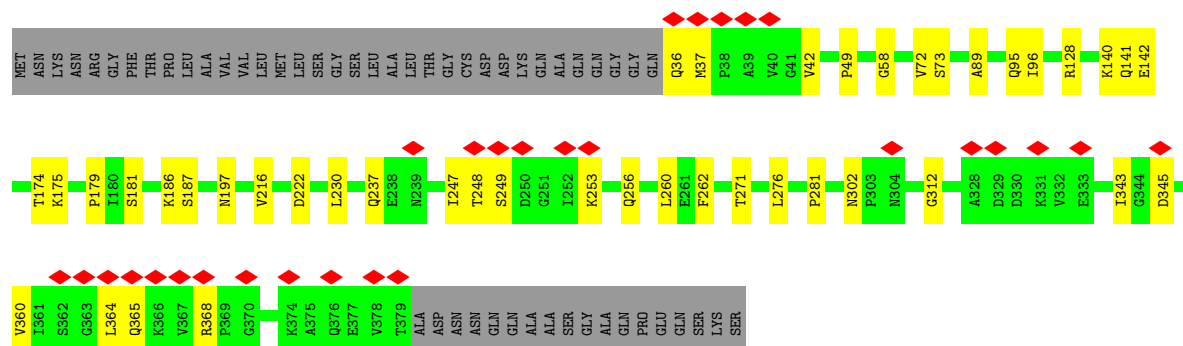
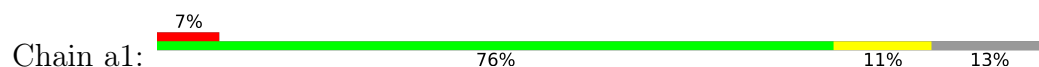




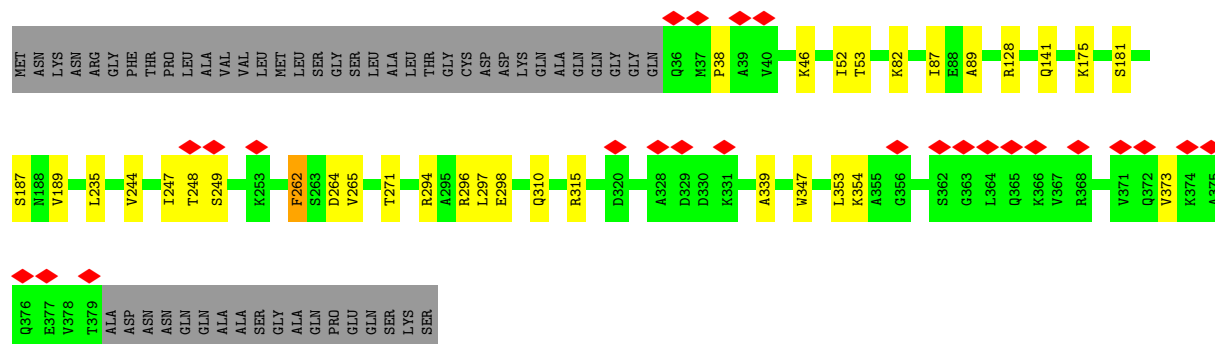
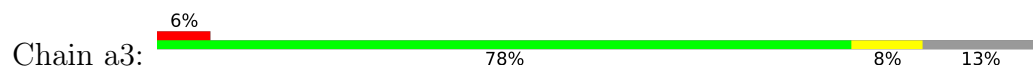
• Molecule 3: Multidrug efflux pump subunit AcrA




• Molecule 3: Multidrug efflux pump subunit AcrA

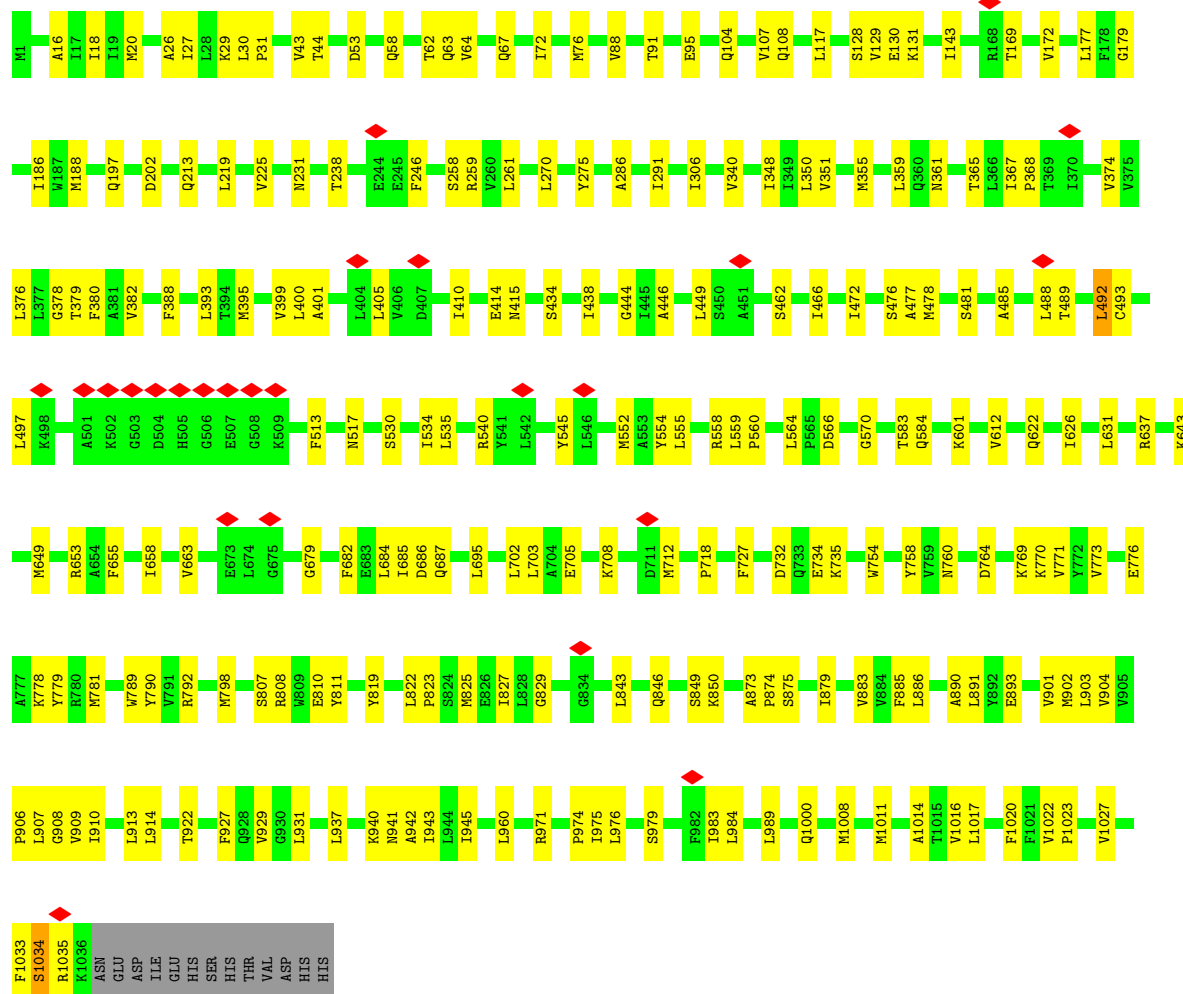


• Molecule 3: Multidrug efflux pump subunit AcrA




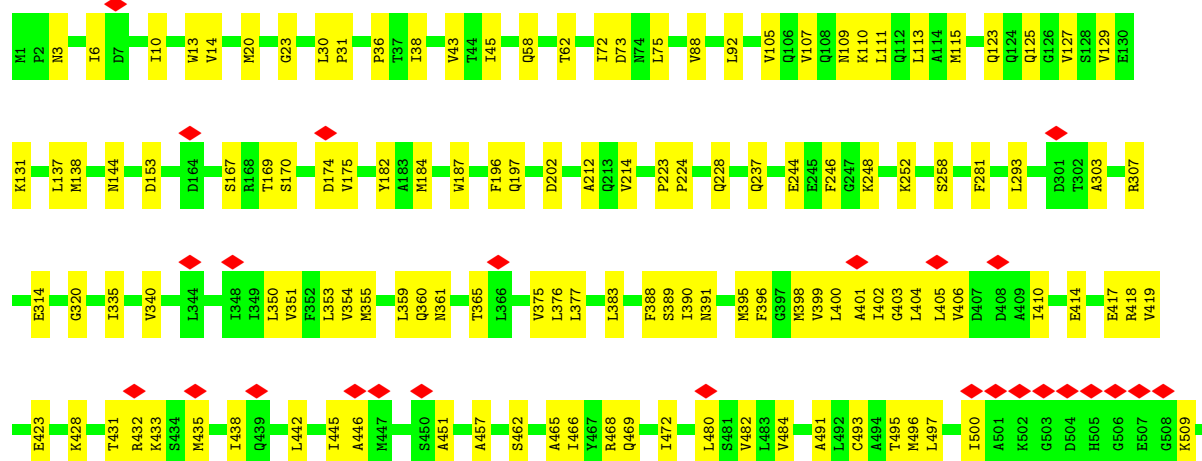
• Molecule 4: Multidrug efflux pump subunit AcrB

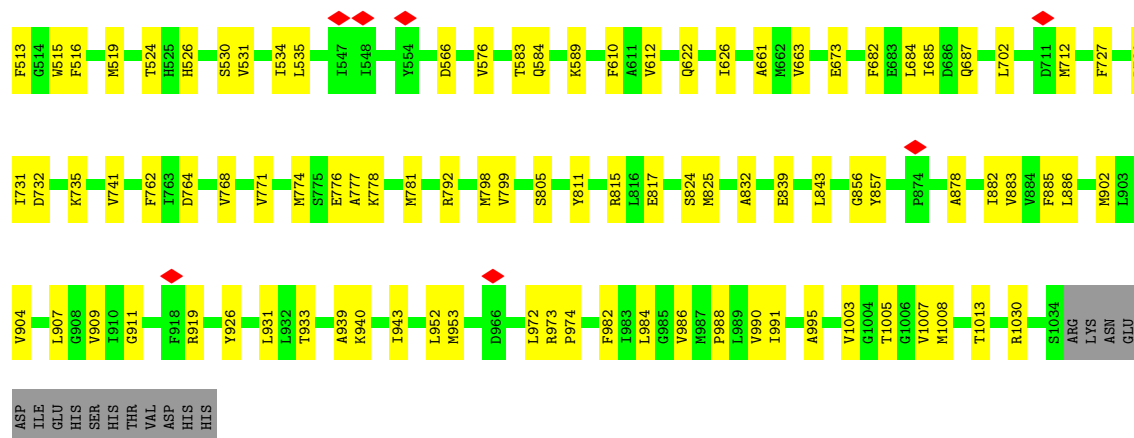
Chain BL:  77% 21%



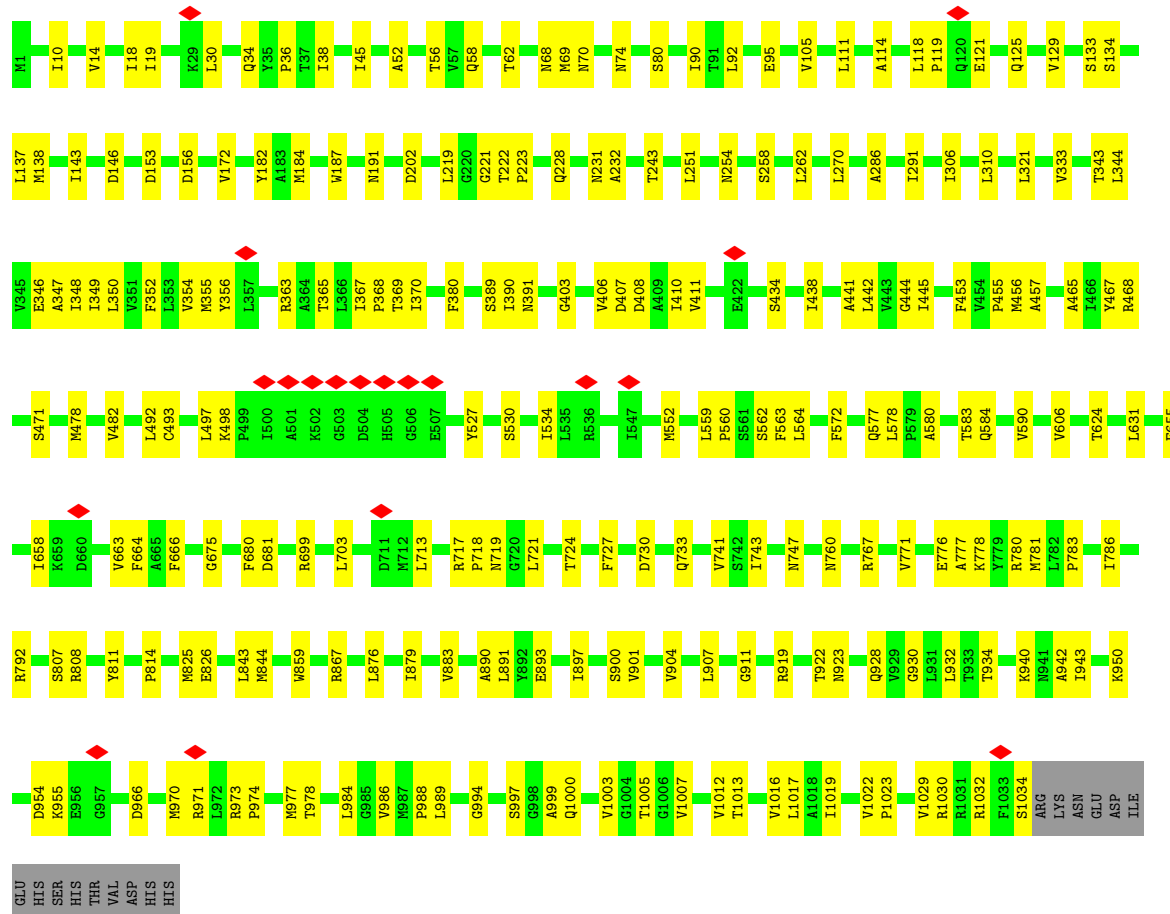
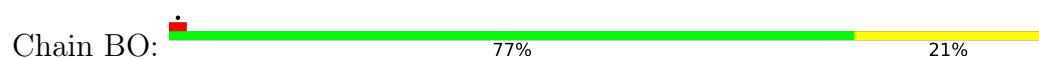
• Molecule 4: Multidrug efflux pump subunit AcrB

Chain BT:  78% 21%

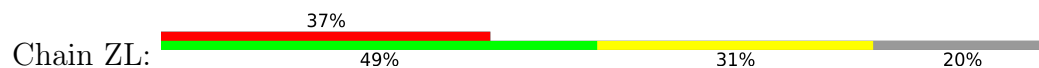


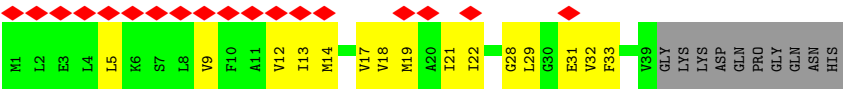


• Molecule 4: Multidrug efflux pump subunit AcrB



• Molecule 5: Multidrug efflux pump accessory protein AcrZ

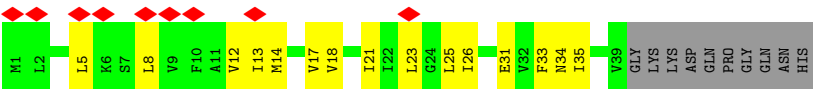




● Molecule 5: Multidrug efflux pump accessory protein AcrZ



● Molecule 5: Multidrug efflux pump accessory protein AcrZ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.495	Depositor
Minimum map value	-0.730	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.29	Depositor
Map size (\AA)	691.2, 691.2, 691.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C1	0.12	0/3373	0.25	0/4584
1	C2	0.12	0/3373	0.25	0/4584
1	C3	0.12	0/3373	0.25	0/4584
2	P1	0.12	0/1204	0.35	0/1640
2	P2	0.14	0/1204	0.37	0/1640
2	P3	0.28	1/1204 (0.1%)	0.55	2/1640 (0.1%)
3	A1	0.10	0/2620	0.25	0/3564
3	A2	0.10	0/2620	0.24	0/3564
3	A3	0.10	0/2620	0.25	0/3564
3	a1	0.10	0/2620	0.24	0/3564
3	a2	0.10	0/2620	0.24	0/3564
3	a3	0.09	0/2620	0.22	0/3564
4	BL	0.11	0/7997	0.27	0/10861
4	BO	0.11	0/7987	0.29	0/10847
4	BT	0.12	0/7987	0.29	0/10847
5	ZL	0.22	0/298	0.53	0/403
5	ZO	0.24	0/298	0.68	0/403
5	ZT	0.16	0/298	0.56	0/403
All	All	0.12	1/54316 (0.0%)	0.29	2/73820 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P3	92	PRO	CG-CD	-6.17	1.29	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P3	92	PRO	CA-N-CD	-11.90	95.34	112.00
2	P3	92	PRO	N-CD-CG	-8.77	90.04	103.20

There are no chirality outliers.

There are no planarity outliers.

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	C1	3331	0	3278	57	0
1	C2	3331	0	3278	70	0
1	C3	3331	0	3278	54	0
2	P1	1182	0	1132	37	0
2	P2	1182	0	1132	37	0
2	P3	1182	0	1132	35	0
3	A1	2587	0	2648	33	0
3	A2	2587	0	2648	31	0
3	A3	2587	0	2648	33	0
3	a1	2587	0	2648	28	0
3	a2	2587	0	2648	32	0
3	a3	2587	0	2648	24	0
4	BL	7847	0	7975	164	0
4	BO	7837	0	7971	163	0
4	BT	7837	0	7971	150	0
5	ZL	294	0	330	13	0
5	ZO	294	0	330	10	0
5	ZT	294	0	330	15	0
All	All	53464	0	54025	883	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 8.

All (883) 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)
3:A2:36:GLN:HE21	3:A2:36:GLN:N	1.57	1.01
3:A3:36:GLN:HE21	3:A3:36:GLN:N	1.62	0.98
1:C2:259:ILE:HD11	1:C2:331:PHE:HB2	1.61	0.82
3:A2:36:GLN:N	3:A2:36:GLN:NE2	2.27	0.81
3:A3:36:GLN:N	3:A3:36:GLN:NE2	2.30	0.79
4:BL:449:LEU:HB2	4:BL:478:MET:HE1	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P3:41:PRO:HB3	2:P3:138:MET:HG3	1.66	0.75
2:P3:138:MET:HE1	2:P3:147:ILE:HD13	1.69	0.75
5:ZO:23:LEU:HA	5:ZO:26:ILE:HD12	1.70	0.73
4:BO:356:TYR:HA	4:BO:365:THR:HG21	1.71	0.73
3:A3:49:PRO:HB3	3:A3:303:PRO:HG3	1.69	0.72
4:BO:911:GLY:H	4:BO:1013:THR:HG21	1.55	0.72
4:BT:167:SER:O	4:BO:70:ASN:ND2	2.23	0.71
5:ZO:17:VAL:O	5:ZO:21:ILE:HD12	1.90	0.71
1:C1:40:ARG:HB2	1:C2:336:GLU:HG3	1.73	0.71
1:C3:236:LYS:HB2	2:P3:161:ALA:HB1	1.72	0.70
4:BO:876:LEU:HD21	4:BO:932:LEU:HD11	1.72	0.70
3:a2:43:VAL:HG22	3:a2:361:ILE:HD11	1.74	0.69
1:C1:40:ARG:HH22	2:P2:117:ARG:HG3	1.57	0.69
4:BL:415:ASN:OD1	4:BL:971:ARG:NH2	2.26	0.69
3:a1:271:THR:HG21	4:BL:258:SER:HB2	1.75	0.69
1:C1:253:ASP:OD1	2:P1:122:ARG:NH2	2.27	0.68
4:BL:552:MET:HE1	4:BL:910:ILE:HA	1.75	0.68
2:P2:86:GLU:N	2:P2:86:GLU:OE2	2.25	0.68
1:C2:424:SER:HB2	1:C2:429:LEU:HD22	1.77	0.67
1:C2:46:ARG:NH1	1:C2:117:ASP:OD2	2.28	0.67
3:A2:337:ILE:HG21	3:A2:353:LEU:HD23	1.77	0.67
1:C2:256:ARG:HA	1:C2:259:ILE:HD12	1.77	0.67
4:BT:10:ILE:HD11	4:BO:893:GLU:HA	1.76	0.67
4:BT:732:ASP:HB3	4:BT:735:LYS:HB2	1.77	0.67
2:P1:70:LYS:HE2	2:P1:165:ARG:HH12	1.59	0.66
1:C2:252:GLN:OE1	2:P2:122:ARG:NH1	2.28	0.66
4:BT:988:PRO:HA	4:BT:991:ILE:HG22	1.77	0.66
4:BO:989:LEU:HD22	4:BO:1000:GLN:HB3	1.77	0.66
2:P2:30:GLY:HA2	2:P2:142:GLY:HA2	1.78	0.66
4:BT:435:MET:HE3	4:BT:435:MET:HA	1.77	0.66
4:BT:446:ALA:HB2	4:BT:482:VAL:HG11	1.78	0.66
4:BL:67:GLN:OE1	4:BO:767:ARG:NH1	2.28	0.65
2:P3:39:GLY:O	2:P3:43:ASN:ND2	2.29	0.65
4:BT:878:ALA:O	4:BT:882:ILE:HG13	1.97	0.65
4:BT:919:ARG:HD3	4:BT:1005:THR:HG21	1.79	0.65
1:C1:314:ILE:HG22	1:C1:315:TYR:H	1.59	0.65
4:BL:446:ALA:HA	4:BL:478:MET:HE2	1.78	0.65
4:BO:1030:ARG:HH12	4:BO:1034:SER:HA	1.60	0.65
4:BT:314:GLU:N	4:BT:314:GLU:OE1	2.28	0.65
5:ZT:17:VAL:O	5:ZT:21:ILE:HD12	1.97	0.65
1:C2:314:ILE:HG22	1:C2:315:TYR:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:ZT:21:ILE:O	5:ZT:25:LEU:HD22	1.97	0.64
1:C2:149:GLN:HG3	1:C2:453:ALA:HB1	1.78	0.64
3:A2:337:ILE:HG22	3:A2:352:GLY:HA3	1.79	0.64
4:BL:622:GLN:OE1	4:BO:231:ASN:ND2	2.30	0.64
4:BO:897:ILE:HD11	4:BO:950:LYS:HG2	1.79	0.64
2:P1:147:ILE:HD12	2:P1:148:ASP:H	1.62	0.64
1:C2:232:ASN:HB3	2:P2:161:ALA:HB3	1.78	0.64
3:a1:256:GLN:HG2	3:a1:281:PRO:HG2	1.79	0.64
2:P3:119:ILE:HB	2:P3:138:MET:HB2	1.78	0.64
2:P1:27:LYS:HA	2:P1:114:ARG:HH21	1.63	0.63
1:C1:256:ARG:HH12	2:P1:122:ARG:HH21	1.45	0.63
4:BT:30:LEU:HD12	4:BT:31:PRO:HD2	1.81	0.63
2:P1:30:GLY:HA2	2:P1:142:GLY:HA2	1.79	0.63
5:ZT:8:LEU:O	5:ZT:12:VAL:HG23	1.99	0.63
1:C1:30:GLN:OE1	1:C1:33:ARG:NH2	2.32	0.63
5:ZL:17:VAL:O	5:ZL:21:ILE:HG23	1.99	0.63
4:BT:228:GLN:NE2	4:BO:781:MET:SD	2.71	0.63
3:A1:366:LYS:NZ	4:BL:658:ILE:O	2.32	0.63
4:BL:554:TYR:OH	4:BL:558:ARG:NH1	2.32	0.63
1:C1:51:GLU:OE2	1:C1:54:ASN:ND2	2.32	0.62
4:BL:960:LEU:HD21	4:BL:1027:VAL:HG13	1.80	0.62
4:BT:62:THR:HB	4:BT:88:VAL:HG21	1.81	0.62
5:ZT:9:VAL:O	5:ZT:13:ILE:HG12	1.98	0.62
1:C1:191:VAL:O	1:C1:195:ASN:ND2	2.31	0.62
1:C3:191:VAL:O	1:C3:195:ASN:ND2	2.31	0.62
1:C3:30:GLN:OE1	1:C3:33:ARG:NH2	2.32	0.62
2:P2:96:ARG:NH1	2:P2:155:GLY:O	2.32	0.62
3:a2:318:ARG:NH2	4:BT:153:ASP:OD1	2.33	0.62
4:BL:808:ARG:NH2	4:BL:810:GLU:OE2	2.32	0.62
4:BT:244:GLU:OE1	4:BT:248:LYS:NZ	2.33	0.62
2:P1:32:ARG:NH1	2:P1:68:SER:O	2.33	0.62
4:BL:20:MET:HE2	4:BL:374:VAL:HG22	1.80	0.62
4:BL:552:MET:HA	4:BL:552:MET:HE2	1.80	0.62
4:BO:444:GLY:HA2	4:BO:891:LEU:HD21	1.82	0.62
3:A3:301:LEU:HD12	3:A3:303:PRO:HD3	1.80	0.61
4:BT:445:ILE:HG12	4:BT:940:LYS:HD3	1.81	0.61
4:BO:478:MET:O	4:BO:482:VAL:HG23	2.00	0.61
4:BL:213:GLN:HE22	4:BL:238:THR:HG22	1.64	0.61
4:BT:340:VAL:HG21	4:BT:395:MET:HB3	1.83	0.61
1:C1:57:ARG:HA	1:C1:106:LEU:HD21	1.82	0.61
3:a2:325:VAL:HG21	3:a2:335:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:202:ASP:OD2	4:BL:792:ARG:NH2	2.34	0.61
4:BL:893:GLU:HA	4:BO:10:ILE:HD11	1.82	0.61
2:P3:139:ILE:HG13	2:P3:146:VAL:HB	1.82	0.61
3:A1:210:ASP:HB3	3:A1:211:PRO:HD3	1.83	0.60
4:BO:730:ASP:OD2	4:BO:808:ARG:NH1	2.27	0.60
1:C2:40:ARG:HH12	2:P3:117:ARG:HD3	1.65	0.60
4:BT:3:ASN:HA	4:BT:6:ILE:HD12	1.82	0.60
4:BT:184:MET:HB3	4:BT:771:VAL:HG12	1.84	0.60
1:C2:65:GLY:HA2	1:C3:314:ILE:HG12	1.83	0.60
1:C2:256:ARG:HH12	1:C2:260:ARG:HG3	1.66	0.60
1:C1:190:GLU:OE2	1:C1:194:ARG:NH2	2.35	0.60
3:A3:366:LYS:NZ	4:BO:658:ILE:O	2.30	0.60
1:C2:165:ARG:HG2	3:A2:132:LEU:HD21	1.83	0.60
4:BO:776:GLU:O	4:BO:778:LYS:N	2.35	0.60
4:BL:367:ILE:HG12	4:BL:492:LEU:HB3	1.84	0.60
4:BL:405:LEU:HD22	4:BL:481:SER:HB3	1.84	0.60
4:BL:545:TYR:OH	4:BL:903:LEU:O	2.18	0.60
4:BT:396:PHE:HE2	4:BT:1003:VAL:HG21	1.66	0.60
2:P3:42:ASP:N	2:P3:42:ASP:OD1	2.34	0.60
4:BL:18:ILE:HG13	4:BT:886:LEU:HD23	1.84	0.60
5:ZL:18:VAL:O	5:ZL:22:ILE:HG12	2.02	0.59
4:BO:1032:ARG:O	4:BO:1032:ARG:NH1	2.34	0.59
1:C1:39:LEU:HD11	1:C1:124:GLN:HG2	1.83	0.59
4:BT:712:MET:HE1	4:BT:839:GLU:HG2	1.85	0.59
4:BL:379:THR:HG22	4:BL:477:ALA:HA	1.84	0.59
4:BT:115:MET:O	4:BT:123:GLN:NE2	2.34	0.59
4:BO:445:ILE:HG23	4:BO:940:LYS:HG3	1.83	0.59
4:BO:577:GLN:HG2	4:BO:624:THR:HG22	1.84	0.59
4:BO:343:THR:HG23	4:BO:988:PRO:HB2	1.83	0.59
4:BO:919:ARG:HD3	4:BO:1005:THR:HG21	1.85	0.59
5:ZO:8:LEU:O	5:ZO:12:VAL:HG23	2.02	0.59
1:C2:32:ALA:HB2	1:C2:208:THR:HG22	1.83	0.59
3:a2:310:GLN:NE2	3:a2:311:GLN:OE1	2.35	0.59
4:BO:467:TYR:OH	4:BO:928:GLN:OE1	2.20	0.59
1:C2:205:ARG:NH2	2:P3:169:GLU:OE2	2.36	0.59
1:C3:253:ASP:OD1	2:P3:122:ARG:NH2	2.35	0.59
1:C2:155:ILE:HG13	1:C2:186:VAL:HG21	1.85	0.59
2:P2:136:VAL:HG23	2:P2:150:VAL:HG22	1.85	0.59
3:a2:324:LEU:HD12	3:a2:364:LEU:HD22	1.85	0.59
4:BL:62:THR:HB	4:BL:88:VAL:HG21	1.84	0.59
1:C2:152:LYS:HA	1:C2:186:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P1:32:ARG:NE	2:P1:36:CYS:SG	2.73	0.58
3:a3:244:VAL:HG22	3:a3:297:LEU:HD12	1.84	0.58
4:BL:979:SER:HA	4:BL:1011:MET:HE2	1.85	0.58
4:BT:197:GLN:HA	4:BT:798:MET:HE3	1.85	0.58
4:BL:291:ILE:HD13	4:BL:306:ILE:HD13	1.86	0.58
4:BT:414:GLU:HG2	4:BT:974:PRO:HG3	1.85	0.58
1:C2:51:GLU:HG2	1:C3:325:LYS:HB3	1.84	0.58
1:C2:191:VAL:O	1:C2:195:ASN:ND2	2.36	0.58
4:BL:30:LEU:HD12	4:BL:31:PRO:HD2	1.85	0.58
4:BL:104:GLN:OE1	4:BL:131:LYS:NZ	2.32	0.58
4:BO:153:ASP:OD1	4:BO:182:TYR:OH	2.19	0.58
4:BT:687:GLN:HE22	4:BT:856:GLY:HA3	1.68	0.58
3:A1:243:LYS:NZ	3:A1:257:ASP:OD2	2.37	0.58
1:C3:34:LEU:O	1:C3:40:ARG:NH1	2.36	0.58
3:A1:128:ARG:NH1	3:a1:141:GLN:OE1	2.34	0.58
4:BT:495:THR:HG23	4:BT:496:MET:HG3	1.86	0.58
2:P3:30:GLY:HA2	2:P3:142:GLY:HA2	1.84	0.57
1:C1:237:GLU:HG2	1:C1:426:LEU:HD21	1.86	0.57
2:P3:138:MET:HE2	2:P3:138:MET:HA	1.87	0.57
3:A1:42:VAL:HG11	3:A1:358:ARG:HB3	1.87	0.57
3:A1:212:ILE:HG21	3:A1:287:LEU:HD11	1.86	0.57
4:BL:43:VAL:HG11	4:BL:107:VAL:HG21	1.87	0.57
1:C3:26:MET:HA	1:C3:26:MET:HE3	1.85	0.57
3:A3:128:ARG:NH1	3:a3:141:GLN:OE1	2.38	0.57
5:ZL:5:LEU:O	5:ZL:9:VAL:HG12	2.04	0.57
2:P2:49:TYR:O	2:P2:53:ILE:HG12	2.04	0.57
4:BO:719:ASN:ND2	4:BO:826:GLU:OE1	2.36	0.57
1:C3:314:ILE:HG22	1:C3:315:TYR:H	1.69	0.57
4:BL:684:LEU:HD11	4:BL:702:LEU:HD23	1.87	0.57
4:BT:986:VAL:HG11	4:BT:1007:VAL:HG11	1.85	0.57
1:C1:77:ARG:NH2	1:C2:301:MET:O	2.37	0.57
2:P2:28:ASP:N	2:P2:28:ASP:OD1	2.37	0.57
4:BT:224:PRO:HA	4:BO:781:MET:HE1	1.86	0.57
4:BL:400:LEU:HD23	4:BL:929:VAL:HG12	1.87	0.56
1:C1:100:MET:HA	1:C1:103:TRP:HD1	1.69	0.56
4:BT:815:ARG:NH1	4:BT:817:GLU:OE2	2.38	0.56
1:C2:40:ARG:HB2	1:C3:336:GLU:HG3	1.87	0.56
2:P2:96:ARG:NH1	2:P2:156:SER:OG	2.38	0.56
1:C1:270:LEU:HD13	1:C1:310:PHE:HB2	1.88	0.56
4:BO:74:ASN:HB3	4:BO:95:GLU:HB3	1.88	0.56
4:BO:251:LEU:HD11	4:BO:262:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:340:VAL:HG11	4:BL:395:MET:HB3	1.88	0.56
4:BL:886:LEU:HD12	4:BO:18:ILE:HG13	1.88	0.56
3:a2:248:THR:HG22	3:a2:249:SER:H	1.70	0.56
4:BL:560:PRO:HG2	4:BL:922:THR:HG22	1.88	0.56
1:C1:57:ARG:HB2	1:C1:106:LEU:HD11	1.86	0.56
2:P1:105:VAL:HG12	2:P1:123:VAL:HG22	1.87	0.56
2:P3:105:VAL:HA	2:P3:123:VAL:HA	1.86	0.56
3:A2:218:GLN:HG2	3:A2:223:PHE:HB2	1.88	0.56
4:BL:350:LEU:HD11	4:BL:984:LEU:HD13	1.88	0.56
4:BL:58:GLN:HA	4:BL:62:THR:HG22	1.87	0.56
4:BT:137:LEU:HD23	4:BT:138:MET:HB3	1.88	0.56
4:BT:576:VAL:HG22	4:BT:663:VAL:HG22	1.88	0.56
4:BT:768:VAL:HG21	4:BO:119:PRO:HG3	1.88	0.56
1:C1:97:ILE:HD11	1:C1:272:LEU:HD23	1.87	0.55
4:BT:75:LEU:HD11	4:BT:92:LEU:HD23	1.88	0.55
1:C2:92:GLN:NE2	1:C2:274:ALA:O	2.39	0.55
3:a1:230:LEU:HD11	3:a1:237:GLN:HB2	1.87	0.55
4:BT:926:TYR:HB3	4:BT:1003:VAL:HG23	1.89	0.55
4:BO:655:PHE:HB3	4:BO:663:VAL:HG13	1.86	0.55
3:A3:83:GLU:HG2	3:A3:186:LYS:HA	1.86	0.55
4:BL:1016:VAL:HG12	4:BL:1017:LEU:HD23	1.88	0.55
4:BO:202:ASP:OD2	4:BO:792:ARG:NH2	2.39	0.55
4:BO:455:PRO:HG3	4:BO:883:VAL:HG11	1.89	0.55
3:A2:317:PRO:HA	4:BT:811:TYR:HB2	1.89	0.55
4:BO:1012:VAL:O	4:BO:1016:VAL:HG22	2.06	0.55
1:C2:34:LEU:O	1:C2:40:ARG:NH1	2.40	0.55
4:BT:531:VAL:HA	4:BT:534:ILE:HG12	1.89	0.55
4:BO:478:MET:HE3	4:BO:478:MET:HA	1.87	0.55
2:P3:71:LEU:HD11	2:P3:148:ASP:HA	1.89	0.55
4:BO:900:SER:HB3	4:BO:1029:VAL:HG11	1.88	0.55
4:BT:214:VAL:HG11	4:BO:747:ASN:HB3	1.89	0.55
1:C2:443:LYS:HD2	1:C2:444:PRO:HD2	1.88	0.54
4:BO:350:LEU:HD22	4:BO:984:LEU:HD12	1.88	0.54
4:BO:572:PHE:HE1	4:BO:631:LEU:HD21	1.72	0.54
1:C3:259:ILE:HD11	1:C3:328:GLN:HA	1.89	0.54
2:P2:52:ARG:HH21	2:P2:99:LEU:HD21	1.72	0.54
4:BT:990:VAL:HG21	4:BT:1008:MET:HG3	1.88	0.54
4:BL:908:GLY:HA2	4:BL:1014:ALA:HB2	1.88	0.54
1:C2:288:THR:HA	1:C2:296:TYR:HD2	1.72	0.54
1:C3:328:GLN:NE2	2:P3:109:SER:O	2.40	0.54
3:a2:332:VAL:HG23	3:a2:369:PRO:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:655:PHE:HB3	4:BL:663:VAL:HG13	1.89	0.54
4:BL:879:ILE:O	4:BL:883:VAL:HG22	2.08	0.54
4:BL:906:PRO:HA	4:BL:909:VAL:HG22	1.88	0.54
4:BT:350:LEU:HD11	4:BT:984:LEU:HB3	1.88	0.54
4:BO:121:GLU:OE2	4:BO:125:GLN:NE2	2.41	0.54
4:BO:407:ASP:OD1	4:BO:408:ASP:N	2.40	0.54
3:A2:83:GLU:HG2	3:A2:186:LYS:HA	1.88	0.54
4:BT:105:VAL:HG21	4:BO:105:VAL:HG13	1.88	0.54
3:A1:317:PRO:HA	4:BL:811:TYR:HB2	1.88	0.54
4:BO:562:SER:OG	4:BO:563:PHE:N	2.40	0.54
4:BT:359:LEU:HD22	4:BT:417:GLU:HG2	1.90	0.54
1:C1:236:LYS:HB2	2:P1:161:ALA:HB1	1.91	0.53
1:C3:70:TYR:HD1	1:C3:87:THR:HG22	1.73	0.53
4:BO:133:SER:OG	4:BO:134:SER:N	2.42	0.53
1:C2:202:GLU:OE1	1:C3:350:ARG:NH1	2.41	0.53
1:C3:284:SER:OG	1:C3:285:GLY:N	2.41	0.53
4:BL:231:ASN:ND2	4:BT:622:GLN:OE1	2.39	0.53
2:P3:113:ASN:HD21	2:P3:115:ASP:HB2	1.73	0.53
2:P3:28:ASP:OD1	2:P3:28:ASP:N	2.37	0.53
4:BL:177:LEU:HG	4:BL:179:GLY:H	1.73	0.53
4:BL:1034:SER:OG	4:BL:1035:ARG:N	2.42	0.53
4:BT:457:ALA:O	4:BT:468:ARG:NH1	2.41	0.53
1:C1:301:MET:HE2	1:C1:301:MET:HA	1.90	0.53
3:A1:230:LEU:HA	3:A1:235:LEU:HB2	1.90	0.53
3:A3:317:PRO:HA	4:BO:811:TYR:HB2	1.90	0.53
3:a3:247:ILE:HD11	3:a3:296:ARG:HH12	1.74	0.53
4:BL:776:GLU:HG3	4:BL:778:LYS:HG2	1.90	0.53
4:BT:395:MET:O	4:BT:399:VAL:HG13	2.09	0.53
1:C2:160:ASP:OD2	3:A2:137:TYR:OH	2.25	0.53
4:BT:153:ASP:OD1	4:BT:182:TYR:OH	2.25	0.53
4:BL:225:VAL:H	4:BT:781:MET:HE3	1.74	0.53
4:BT:38:ILE:HG22	4:BT:462:SER:HB3	1.91	0.53
4:BO:346:GLU:HA	4:BO:349:ILE:HG22	1.91	0.53
4:BL:776:GLU:HB3	4:BL:779:TYR:HD2	1.73	0.53
4:BT:530:SER:O	4:BT:534:ILE:HG23	2.09	0.53
3:A3:294:ARG:NH1	4:BO:191:ASN:OD1	2.42	0.52
4:BT:451:ALA:HB1	4:BT:883:VAL:HG12	1.91	0.52
4:BT:491:ALA:O	4:BT:495:THR:HG22	2.08	0.52
2:P1:42:ASP:OD1	2:P1:42:ASP:N	2.40	0.52
4:BO:527:TYR:OH	4:BO:1019:ILE:O	2.25	0.52
4:BO:971:ARG:HH22	4:BO:974:PRO:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:ZL:14:MET:O	5:ZL:18:VAL:HG23	2.09	0.52
3:A2:125:THR:OG1	3:a2:141:GLN:NE2	2.42	0.52
4:BL:545:TYR:HE1	4:BL:907:LEU:HD21	1.75	0.52
4:BT:72:ILE:HD11	4:BT:110:LYS:HG3	1.92	0.52
2:P2:160:THR:HG21	2:P2:167:SER:HB3	1.91	0.52
4:BL:275:TYR:HB2	4:BO:223:PRO:HD3	1.91	0.52
5:ZT:3:GLU:HA	5:ZT:6:LYS:HG2	1.92	0.52
1:C1:40:ARG:HH12	2:P2:117:ARG:HG3	1.75	0.52
3:A1:70:PRO:HD3	3:A1:203:LEU:HD13	1.91	0.52
3:A3:210:ASP:HB3	3:A3:211:PRO:HD3	1.92	0.52
4:BL:444:GLY:HA3	4:BL:891:LEU:HD22	1.91	0.52
4:BT:196:PHE:O	4:BT:252:LYS:NZ	2.42	0.52
4:BL:983:ILE:HG23	4:BL:1008:MET:SD	2.50	0.52
4:BO:713:LEU:HD13	4:BO:843:LEU:HD23	1.91	0.52
2:P2:90:ASN:HD22	2:P2:97:THR:HB	1.74	0.52
2:P3:127:GLN:HG3	2:P3:128:GLY:H	1.75	0.52
3:A3:187:SER:OG	3:A3:189:VAL:O	2.27	0.52
4:BT:20:MET:HG2	4:BT:377:LEU:HD12	1.92	0.52
2:P1:57:SER:O	2:P1:58:ASN:ND2	2.43	0.51
4:BL:395:MET:O	4:BL:399:VAL:HG13	2.09	0.51
2:P1:49:TYR:CE2	2:P1:123:VAL:HG11	2.45	0.51
4:BO:34:GLN:HB2	4:BO:333:VAL:HG22	1.92	0.51
1:C2:115:ILE:HG22	1:C2:250:LEU:HB3	1.92	0.51
3:a2:217:THR:HG21	4:BT:258:SER:HA	1.92	0.51
4:BL:355:MET:HG2	4:BL:365:THR:HA	1.92	0.51
4:BL:764:ASP:OD2	4:BL:769:LYS:NZ	2.31	0.51
4:BT:712:MET:HA	4:BT:832:ALA:HB2	1.92	0.51
4:BO:733:GLN:HG2	4:BO:743:ILE:HD12	1.93	0.51
1:C2:54:ASN:OD1	1:C2:57:ARG:NH2	2.43	0.51
2:P1:70:LYS:HE2	2:P1:165:ARG:HH22	1.74	0.51
3:a2:262:PHE:CG	3:a2:262:PHE:O	2.62	0.51
4:BL:72:ILE:HD13	4:BL:107:VAL:HG12	1.92	0.51
4:BT:115:MET:HE1	4:BT:127:VAL:HG22	1.93	0.51
4:BO:456:MET:HG2	4:BO:471:SER:HB2	1.92	0.51
1:C2:50:PHE:HB3	2:P3:22:VAL:HG12	1.93	0.51
3:A2:189:VAL:HG21	3:A2:203:LEU:HD22	1.93	0.51
3:A3:37:MET:HA	3:A3:37:MET:HE2	1.92	0.51
4:BT:223:PRO:HG2	4:BO:780:ARG:HH22	1.76	0.51
4:BL:703:LEU:HD11	4:BL:718:PRO:HG3	1.93	0.51
4:BT:187:TRP:HA	4:BT:774:MET:O	2.10	0.51
4:BT:401:ALA:O	4:BT:405:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BT:953:MET:HE1	4:BT:1030:ARG:HE	1.76	0.51
4:BL:44:THR:HG22	4:BL:91:THR:HG23	1.93	0.51
4:BL:76:MET:HE2	4:BL:95:GLU:HA	1.92	0.51
5:ZO:14:MET:O	5:ZO:18:VAL:HG23	2.10	0.51
2:P2:31:THR:HG22	2:P2:31:THR:O	2.11	0.51
4:BL:695:LEU:HG	4:BL:825:MET:HG3	1.91	0.51
5:ZL:29:LEU:HA	5:ZL:32:VAL:HG12	1.93	0.51
4:BT:335:ILE:HD13	4:BT:995:ALA:HB1	1.93	0.51
4:BT:465:ALA:O	4:BT:469:GLN:HG2	2.11	0.51
4:BO:370:ILE:HD11	4:BO:492:LEU:HD11	1.92	0.51
1:C3:190:GLU:OE2	1:C3:194:ARG:NH2	2.41	0.50
4:BL:534:ILE:HD13	5:ZL:33:PHE:HE1	1.76	0.50
1:C2:236:LYS:HE2	2:P2:157:VAL:HG21	1.92	0.50
4:BL:559:LEU:HD12	4:BL:560:PRO:HD2	1.93	0.50
4:BT:137:LEU:HD12	4:BT:293:LEU:HB2	1.92	0.50
5:ZT:28:GLY:O	5:ZT:32:VAL:HG12	2.11	0.50
4:BO:583:THR:OG1	4:BO:584:GLN:N	2.45	0.50
1:C1:310:PHE:HD2	1:C3:68:ALA:HB3	1.76	0.50
1:C2:82:ILE:HD11	1:C2:287:LYS:HD3	1.92	0.50
3:a1:95:GLN:NE2	3:a1:96:ILE:O	2.44	0.50
4:BO:184:MET:HE1	4:BO:243:THR:HG22	1.92	0.50
1:C1:380:MET:HE3	1:C1:393:ASP:HB3	1.94	0.50
1:C3:301:MET:HE2	1:C3:301:MET:HA	1.92	0.50
4:BT:353:LEU:HD21	5:ZT:15:VAL:HG11	1.94	0.50
1:C3:228:PRO:HG3	1:C3:356:ILE:HG21	1.93	0.50
4:BO:441:ALA:O	4:BO:445:ILE:HD12	2.11	0.50
4:BO:681:ASP:OD1	4:BO:681:ASP:N	2.42	0.50
5:ZL:19:MET:HE2	5:ZL:19:MET:HA	1.93	0.50
4:BT:414:GLU:OE2	4:BT:973:ARG:NE	2.43	0.50
4:BO:363:ARG:HD2	4:BO:498:LYS:HZ2	1.77	0.50
3:A2:128:ARG:NH1	3:a2:141:GLN:OE1	2.44	0.50
3:a3:294:ARG:NH2	4:BL:734:GLU:OE2	2.35	0.50
5:ZO:21:ILE:O	5:ZO:25:LEU:HD22	2.12	0.50
2:P2:123:VAL:O	2:P2:133:GLN:HA	2.12	0.49
3:A3:335:ARG:HH21	3:A3:353:LEU:HA	1.76	0.49
3:a3:264:ASP:OD1	3:a3:265:VAL:N	2.44	0.49
4:BL:622:GLN:HE22	4:BO:221:GLY:HA2	1.77	0.49
1:C3:112:ALA:O	1:C3:115:ILE:HG12	2.13	0.49
4:BL:378:GLY:O	4:BL:382:VAL:HG12	2.12	0.49
4:BL:393:LEU:HD13	4:BL:466:ILE:HG23	1.95	0.49
4:BO:219:LEU:HD12	4:BO:232:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P1:148:ASP:OD1	2:P1:149:ASP:N	2.45	0.49
2:P3:88:LEU:HD12	2:P3:92:PRO:HG3	1.95	0.49
3:A2:95:GLN:NE2	3:A2:96:ILE:O	2.45	0.49
3:a1:89:ALA:N	3:a1:181:SER:OG	2.46	0.49
4:BL:63:GLN:O	4:BL:67:GLN:HG3	2.12	0.49
4:BT:375:VAL:HG13	4:BT:480:LEU:HB3	1.94	0.49
1:C1:332:VAL:O	1:C1:336:GLU:HG2	2.12	0.49
2:P1:163:THR:O	2:P1:167:SER:OG	2.26	0.49
3:a2:214:VAL:HG12	3:a2:216:VAL:HG23	1.94	0.49
4:BL:679:GLY:HA3	4:BL:829:GLY:O	2.13	0.49
4:BT:401:ALA:HA	4:BT:404:LEU:HG	1.94	0.49
4:BO:559:LEU:HD12	4:BO:560:PRO:HD2	1.94	0.49
1:C3:50:PHE:HB3	2:P1:22:VAL:HG12	1.94	0.49
4:BL:108:GLN:HG3	4:BL:129:VAL:HG11	1.95	0.49
4:BT:712:MET:SD	4:BT:843:LEU:HD13	2.53	0.49
4:BL:197:GLN:HA	4:BL:798:MET:HE2	1.94	0.49
1:C1:292:ALA:HB1	1:C1:295:GLN:HG3	1.95	0.49
1:C3:104:ARG:HH22	1:C3:260:ARG:HE	1.60	0.49
4:BL:682:PHE:HB3	4:BL:827:ILE:HG12	1.94	0.49
4:BL:754:TRP:HE1	4:BL:789:TRP:CD1	2.30	0.49
4:BL:904:VAL:HG11	4:BL:942:ALA:HB2	1.94	0.49
1:C1:57:ARG:HH22	2:P2:20:THR:HG23	1.77	0.49
1:C3:322:SER:O	1:C3:326:GLN:HG3	2.13	0.49
4:BT:281:PHE:HD1	4:BT:610:PHE:HD1	1.60	0.49
4:BO:156:ASP:HB2	4:BO:182:TYR:CD1	2.48	0.49
4:BO:457:ALA:HB1	4:BO:468:ARG:HG2	1.95	0.49
4:BO:727:PHE:CZ	4:BO:807:SER:HB2	2.48	0.49
3:a2:187:SER:OG	3:a2:189:VAL:O	2.25	0.48
4:BT:212:ALA:O	4:BT:237:GLN:NE2	2.46	0.48
1:C3:165:ARG:HG2	3:A3:132:LEU:HD21	1.95	0.48
4:BL:552:MET:SD	4:BL:909:VAL:HG23	2.53	0.48
4:BO:69:MET:HE1	4:BO:111:LEU:HA	1.94	0.48
4:BO:901:VAL:HG21	4:BO:943:ILE:HD13	1.95	0.48
5:ZO:31:GLU:O	5:ZO:35:ILE:HG22	2.12	0.48
1:C2:123:ASP:HA	1:C2:126:THR:HG22	1.95	0.48
2:P1:117:ARG:HH21	2:P1:139:ILE:HB	1.78	0.48
3:a2:82:LYS:HB2	3:a2:82:LYS:HE3	1.69	0.48
4:BL:781:MET:HE3	4:BO:228:GLN:HG3	1.95	0.48
4:BT:909:VAL:HG22	4:BT:931:LEU:HD11	1.95	0.48
3:A1:37:MET:HG3	3:A1:374:LYS:HD2	1.94	0.48
3:a2:264:ASP:OD1	3:a2:265:VAL:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a3:339:ALA:HB1	3:a3:347:TRP:HB3	1.94	0.48
4:BT:355:MET:HB3	4:BT:365:THR:HG22	1.95	0.48
4:BT:516:PHE:HA	4:BT:519:MET:HE3	1.95	0.48
4:BT:776:GLU:O	4:BT:778:LYS:N	2.46	0.48
5:ZO:5:LEU:H	5:ZO:5:LEU:HD12	1.76	0.48
4:BO:493:CYS:HB2	4:BO:497:LEU:HD12	1.94	0.48
4:BO:721:LEU:HD12	4:BO:814:PRO:HB2	1.95	0.48
1:C3:270:LEU:HD13	1:C3:310:PHE:HB2	1.94	0.48
3:a3:248:THR:HG22	3:a3:249:SER:H	1.79	0.48
4:BT:383:LEU:HG	4:BT:388:PHE:HB2	1.95	0.48
4:BT:682:PHE:CE1	4:BT:857:TYR:HB2	2.48	0.48
4:BO:187:TRP:HB3	4:BO:776:GLU:HB2	1.95	0.48
3:a2:199:GLN:NE2	3:a2:201:THR:O	2.45	0.48
4:BT:73:ASP:OD1	4:BT:73:ASP:N	2.47	0.48
4:BT:885:PHE:HB2	4:BT:902:MET:HE1	1.95	0.48
4:BO:389:SER:O	4:BO:391:ASN:ND2	2.43	0.48
3:A2:277:ARG:HH22	3:a1:186:LYS:HE2	1.79	0.48
3:A3:141:GLN:OE1	3:a2:128:ARG:NH1	2.41	0.48
4:BL:379:THR:CG2	4:BL:477:ALA:HA	2.43	0.48
4:BT:911:GLY:HA3	4:BT:1013:THR:OG1	2.14	0.48
3:A2:241:LYS:HE3	3:A2:261:GLU:HG2	1.95	0.48
3:a2:42:VAL:HG21	3:a2:358:ARG:HG2	1.96	0.48
4:BL:355:MET:HE1	4:BL:410:ILE:HG12	1.96	0.48
4:BT:400:LEU:HD11	4:BT:933:THR:HG21	1.96	0.48
1:C1:205:ARG:O	1:C1:209:GLY:N	2.46	0.48
3:a1:142:GLU:OE1	3:a1:142:GLU:N	2.45	0.48
4:BL:446:ALA:HA	4:BL:478:MET:CE	2.42	0.48
1:C1:338:LEU:HD23	2:P1:120:PRO:HG2	1.96	0.47
2:P2:105:VAL:HG12	2:P2:123:VAL:HB	1.96	0.47
4:BO:344:LEU:O	4:BO:348:ILE:HG23	2.15	0.47
3:A3:259:THR:HG22	3:A3:279:ILE:HG22	1.96	0.47
4:BO:930:GLY:O	4:BO:934:THR:HG23	2.14	0.47
2:P1:40:GLY:O	2:P1:44:VAL:N	2.34	0.47
2:P3:90:ASN:ND2	2:P3:97:THR:OG1	2.34	0.47
4:BL:259:ARG:HH21	4:BL:261:LEU:HD11	1.79	0.47
4:BL:434:SER:O	4:BL:438:ILE:HG12	2.14	0.47
4:BL:945:ILE:HD11	4:BL:975:ILE:HD11	1.95	0.47
4:BO:45:ILE:HG12	4:BO:129:VAL:HG22	1.95	0.47
4:BO:970:MET:HE3	4:BO:971:ARG:HD3	1.96	0.47
3:a2:271:THR:HG21	4:BT:258:SER:HB2	1.97	0.47
4:BL:128:SER:OG	4:BL:130:GLU:OE1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BT:43:VAL:HG11	4:BT:107:VAL:HG21	1.96	0.47
4:BT:45:ILE:HG12	4:BT:129:VAL:HG12	1.96	0.47
1:C3:286:SER:OG	1:C3:287:LYS:N	2.48	0.47
3:A1:75:ILE:HD11	3:a1:179:PRO:HB3	1.97	0.47
4:BL:219:LEU:O	4:BL:231:ASN:HA	2.15	0.47
4:BL:348:ILE:O	4:BL:351:VAL:HG12	2.14	0.47
4:BT:14:VAL:HG11	4:BO:890:ALA:HB2	1.96	0.47
1:C2:39:LEU:HD22	1:C2:127:LEU:HD23	1.96	0.47
2:P2:67:LEU:HD13	2:P2:71:LEU:HB3	1.95	0.47
3:a3:82:LYS:HE3	3:a3:82:LYS:HB2	1.64	0.47
4:BL:414:GLU:CD	4:BL:974:PRO:HG3	2.39	0.47
4:BL:927:PHE:O	4:BL:931:LEU:HD23	2.15	0.47
1:C2:112:ALA:O	1:C2:115:ILE:HG12	2.15	0.47
2:P3:67:LEU:HB3	2:P3:71:LEU:HB2	1.97	0.47
2:P3:100:PRO:HG3	2:P3:125:LEU:HD23	1.95	0.47
3:A2:332:VAL:HG23	3:A2:369:PRO:HA	1.96	0.47
4:BO:354:VAL:HG13	4:BO:355:MET:CE	2.44	0.47
4:BO:534:ILE:HD11	5:ZO:33:PHE:HB3	1.97	0.47
4:BO:578:LEU:HD11	4:BO:590:VAL:HG21	1.97	0.47
3:a2:244:VAL:HG22	3:a2:297:LEU:HG	1.97	0.47
1:C1:220:VAL:HG12	1:C1:412:ARG:HH12	1.80	0.47
5:ZL:9:VAL:HA	5:ZL:12:VAL:HG22	1.97	0.47
4:BO:347:ALA:HB2	4:BO:988:PRO:HG2	1.97	0.47
3:a1:72:VAL:HG21	3:a1:174:THR:HG22	1.97	0.46
4:BO:68:ASN:CG	4:BO:114:ALA:HB2	2.39	0.46
4:BO:69:MET:HB3	4:BO:92:LEU:HD21	1.97	0.46
1:C2:356:ILE:HG13	1:C2:422:ILE:HD12	1.97	0.46
2:P1:127:GLN:HB2	2:P1:132:TRP:HH2	1.81	0.46
3:A2:42:VAL:HG11	3:A2:358:ARG:HB3	1.97	0.46
3:a3:38:PRO:HG2	3:a3:373:VAL:HG22	1.97	0.46
4:BL:219:LEU:HD11	4:BT:727:PHE:CD2	2.50	0.46
4:BL:513:PHE:O	4:BL:517:ASN:ND2	2.49	0.46
4:BO:403:GLY:HA2	4:BO:406:VAL:HG22	1.97	0.46
4:BL:367:ILE:HD13	4:BL:493:CYS:HB3	1.96	0.46
4:BL:686:ASP:HB3	4:BL:823:PRO:HG2	1.98	0.46
4:BT:361:ASN:O	4:BT:365:THR:HG23	2.15	0.46
4:BL:612:VAL:HB	4:BL:626:ILE:HG22	1.96	0.46
4:BT:731:ILE:HD13	4:BT:805:SER:HB2	1.98	0.46
1:C1:325:LYS:HB3	1:C3:51:GLU:HG2	1.98	0.46
1:C2:97:ILE:HD11	1:C2:272:LEU:HB3	1.98	0.46
1:C2:416:LEU:HD22	1:C2:437:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C3:115:ILE:HG22	1:C3:250:LEU:HB3	1.98	0.46
4:BT:423:GLU:HG3	4:BT:433:LYS:NZ	2.30	0.46
4:BT:684:LEU:HD21	4:BT:702:LEU:HD13	1.97	0.46
4:BT:762:PHE:CE2	4:BT:764:ASP:HB2	2.51	0.46
4:BO:52:ALA:HB1	4:BO:56:THR:OG1	2.15	0.46
4:BO:411:VAL:HG22	4:BO:974:PRO:HB3	1.97	0.46
4:BT:144:ASN:ND2	4:BT:320:GLY:O	2.45	0.46
1:C1:165:ARG:HG2	3:A1:132:LEU:HD21	1.98	0.46
1:C1:328:GLN:NE2	2:P1:109:SER:O	2.48	0.46
3:a2:37:MET:O	3:a2:374:LYS:NZ	2.48	0.46
4:BT:526:HIS:NE2	5:ZT:31:GLU:OE1	2.44	0.46
1:C1:158:GLN:HG2	1:C1:392:VAL:HG21	1.98	0.46
4:BT:23:GLY:HA3	4:BT:377:LEU:HB3	1.98	0.46
4:BO:137:LEU:HD23	4:BO:138:MET:HB3	1.98	0.46
3:A2:236:LYS:HB2	3:A2:301:LEU:HB2	1.97	0.46
3:a1:49:PRO:HA	3:a1:302:ASN:O	2.15	0.46
4:BT:509:LYS:HD2	4:BT:509:LYS:HA	1.78	0.46
4:BT:515:TRP:O	4:BT:519:MET:HE3	2.15	0.46
1:C1:40:ARG:NH2	2:P2:117:ARG:HG3	2.28	0.45
1:C2:161:GLN:HE21	1:C2:165:ARG:NH1	2.13	0.45
2:P2:96:ARG:HG3	2:P2:132:TRP:CE2	2.50	0.45
3:A1:221:ASN:OD1	3:A1:222:ASP:N	2.49	0.45
4:BL:355:MET:O	4:BL:359:LEU:HB2	2.16	0.45
4:BL:485:ALA:O	4:BL:489:THR:OG1	2.34	0.45
4:BL:601:LYS:HD3	4:BL:601:LYS:HA	1.71	0.45
4:BT:375:VAL:HG22	4:BT:484:VAL:HG21	1.99	0.45
4:BT:685:ILE:HG13	4:BT:824:SER:HB2	1.97	0.45
4:BT:687:GLN:OE1	4:BT:856:GLY:N	2.49	0.45
4:BO:352:PHE:HD1	4:BO:369:THR:HG21	1.81	0.45
4:BO:530:SER:O	4:BO:534:ILE:HG12	2.16	0.45
1:C1:284:SER:OG	1:C1:285:GLY:N	2.50	0.45
3:A3:141:GLN:NE2	3:a2:125:THR:OG1	2.49	0.45
4:BL:637:ARG:O	4:BL:643:LYS:NZ	2.49	0.45
4:BL:971:ARG:O	4:BL:974:PRO:HD2	2.17	0.45
4:BT:428:LYS:O	4:BT:432:ARG:HG3	2.15	0.45
4:BO:434:SER:O	4:BO:438:ILE:HG12	2.16	0.45
4:BO:943:ILE:HD12	4:BO:943:ILE:HA	1.82	0.45
2:P3:58:ASN:HD21	2:P3:99:LEU:HD22	1.82	0.45
3:A1:364:LEU:HD12	3:A1:364:LEU:H	1.80	0.45
3:A3:37:MET:HB3	3:A3:374:LYS:HD2	1.98	0.45
3:A3:282:ASN:HD21	3:A3:285:HIS:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:850:LYS:HA	4:BL:850:LYS:HD3	1.74	0.45
4:BO:1003:VAL:O	4:BO:1007:VAL:HG23	2.16	0.45
3:A1:284:ASP:HB2	3:A1:286:THR:HG23	1.99	0.45
4:BL:395:MET:HA	4:BL:395:MET:HE2	1.99	0.45
4:BT:566:ASP:OD1	4:BT:566:ASP:N	2.49	0.45
4:BO:954:ASP:OD2	4:BO:955:LYS:NZ	2.43	0.45
1:C2:205:ARG:O	1:C2:209:GLY:N	2.48	0.45
3:A2:210:ASP:HB3	3:A2:211:PRO:HD3	1.99	0.45
4:BL:497:LEU:HD23	4:BL:497:LEU:HA	1.78	0.45
4:BT:524:THR:HG23	4:BT:972:LEU:HD22	1.98	0.45
1:C3:111:LYS:O	1:C3:115:ILE:HG23	2.17	0.45
4:BL:732:ASP:HB3	4:BL:735:LYS:HB3	1.98	0.45
4:BL:108:GLN:NE2	4:BT:109:ASN:HB3	2.32	0.45
4:BT:169:THR:OG1	4:BT:170:SER:N	2.45	0.45
1:C1:256:ARG:HH12	2:P1:122:ARG:NH2	2.13	0.45
1:C2:111:LYS:O	1:C2:115:ILE:HG23	2.16	0.45
2:P2:19:CYS:O	2:P2:20:THR:OG1	2.35	0.45
3:A1:354:LYS:HD3	3:A1:355:ALA:N	2.32	0.45
4:BT:376:LEU:HD11	4:BT:402:ILE:HD11	1.98	0.45
1:C2:356:ILE:O	1:C2:360:ILE:HG12	2.17	0.45
1:C3:100:MET:HE3	1:C3:104:ARG:HD3	1.99	0.45
1:C3:272:LEU:HD12	1:C3:308:LEU:HD11	1.99	0.45
2:P1:136:VAL:HB	2:P1:147:ILE:HD11	1.99	0.45
3:A2:141:GLN:OE1	3:a1:128:ARG:NH1	2.41	0.45
4:BL:705:GLU:OE2	4:BL:708:LYS:NZ	2.40	0.45
4:BT:730:ASP:OD1	4:BT:730:ASP:N	2.39	0.45
3:A1:212:ILE:HG22	3:A1:280:PHE:HB2	1.99	0.45
3:a3:310:GLN:HA	3:a3:347:TRP:HD1	1.82	0.45
3:A2:82:LYS:HB2	3:A2:82:LYS:HE3	1.63	0.44
3:a3:315:ARG:NH2	3:a3:339:ALA:O	2.51	0.44
4:BL:462:SER:O	4:BL:466:ILE:HG13	2.16	0.44
4:BT:36:PRO:HD2	4:BT:38:ILE:HD11	1.99	0.44
1:C3:107:THR:O	1:C3:111:LYS:HG3	2.17	0.44
3:A3:265:VAL:HG11	3:a2:209:LEU:HD11	2.00	0.44
4:BL:570:GLY:O	4:BL:631:LEU:N	2.50	0.44
4:BT:825:MET:HE3	4:BT:825:MET:HB3	1.85	0.44
4:BO:182:TYR:HD2	4:BO:270:LEU:HD22	1.82	0.44
1:C1:194:ARG:NH1	1:C1:453:ALA:O	2.41	0.44
3:A2:366:LYS:NZ	4:BT:661:ALA:O	2.49	0.44
4:BL:30:LEU:HD12	4:BL:30:LEU:HA	1.85	0.44
1:C1:314:ILE:HD12	1:C3:65:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P1:49:TYR:O	2:P1:53:ILE:HG12	2.17	0.44
3:a2:339:ALA:HB1	3:a2:347:TRP:HB3	1.99	0.44
3:a1:247:ILE:HG23	3:a1:253:LYS:HD3	1.99	0.44
4:BO:703:LEU:HD11	4:BO:718:PRO:HG3	2.00	0.44
1:C1:100:MET:HA	1:C1:103:TRP:CD1	2.52	0.44
1:C2:104:ARG:NH1	1:C2:260:ARG:HD2	2.32	0.44
3:A3:212:ILE:HG22	3:A3:280:PHE:HB2	1.99	0.44
4:BT:174:ASP:OD2	4:BT:175:VAL:N	2.50	0.44
1:C3:319:MET:HB3	1:C3:320:VAL:H	1.67	0.44
2:P2:48:PHE:HE2	2:P2:63:LEU:HD13	1.82	0.44
3:A1:39:ALA:HB2	3:A1:374:LYS:HD3	2.00	0.44
4:BL:376:LEU:O	4:BL:379:THR:OG1	2.36	0.44
1:C2:332:VAL:O	1:C2:336:GLU:HG2	2.17	0.44
2:P1:37:VAL:HG12	2:P1:38:GLU:H	1.83	0.44
3:A3:148:ALA:O	3:A3:152:GLN:HG3	2.17	0.44
3:a2:147:LEU:HD12	3:a2:147:LEU:HA	1.88	0.44
3:a2:236:LYS:HD2	3:a2:236:LYS:HA	1.69	0.44
3:a1:58:GLY:HA3	3:a1:216:VAL:HG12	2.00	0.44
4:BO:58:GLN:HA	4:BO:62:THR:HG22	2.00	0.44
2:P1:70:LYS:HA	2:P1:73:THR:HG23	2.00	0.44
2:P2:156:SER:OG	2:P2:156:SER:O	2.27	0.44
3:A1:141:GLN:OE1	3:a3:128:ARG:NH1	2.42	0.44
3:a1:73:SER:OG	3:a1:197:ASN:N	2.51	0.44
3:a1:365:GLN:C	3:a1:368:ARG:HH22	2.26	0.44
4:BL:129:VAL:HG12	4:BT:113:LEU:HD11	2.00	0.44
4:BL:186:ILE:HD11	4:BL:246:PHE:HE2	1.83	0.44
4:BL:401:ALA:O	4:BL:405:LEU:HG	2.18	0.44
4:BL:727:PHE:CZ	4:BL:807:SER:HB2	2.53	0.44
4:BL:940:LYS:HE3	4:BL:940:LYS:HB3	1.85	0.44
4:BT:952:LEU:HD12	4:BT:952:LEU:HA	1.84	0.44
4:BO:172:VAL:HG11	4:BO:306:ILE:HD11	2.00	0.44
4:BL:361:ASN:O	4:BL:365:THR:HG23	2.18	0.44
1:C3:332:VAL:O	1:C3:336:GLU:HG2	2.18	0.43
3:A3:214:VAL:HG12	3:A3:216:VAL:HG23	1.99	0.43
4:BL:270:LEU:HD23	4:BL:270:LEU:HA	1.86	0.43
4:BL:685:ILE:HD11	4:BL:819:TYR:HD2	1.83	0.43
4:BL:712:MET:SD	4:BL:843:LEU:HD22	2.58	0.43
4:BO:699:ARG:HD3	4:BO:825:MET:HE2	2.00	0.43
1:C1:328:GLN:HE22	2:P1:109:SER:HB2	1.83	0.43
1:C3:157:ARG:HD2	1:C3:157:ARG:HA	1.60	0.43
2:P1:164:LEU:O	2:P1:168:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P2:36:CYS:HB3	2:P2:144:CYS:HB3	1.63	0.43
3:A2:70:PRO:HD3	3:A2:203:LEU:HG	2.00	0.43
4:BT:375:VAL:HG11	4:BT:405:LEU:HD22	2.00	0.43
4:BT:904:VAL:HG23	4:BT:907:LEU:HD12	2.00	0.43
4:BO:80:SER:HB2	4:BO:90:ILE:HG13	2.00	0.43
4:BO:456:MET:HE2	4:BO:932:LEU:HD13	2.00	0.43
1:C1:41:LYS:HE2	1:C2:337:GLN:HB2	1.99	0.43
1:C3:205:ARG:O	1:C3:209:GLY:N	2.41	0.43
1:C3:325:LYS:HB2	1:C3:325:LYS:HE2	1.87	0.43
4:BO:146:ASP:OD1	4:BO:146:ASP:N	2.51	0.43
4:BO:564:LEU:HD12	4:BO:564:LEU:HA	1.89	0.43
1:C1:236:LYS:HG3	2:P1:162:GLY:H	1.83	0.43
1:C1:324:VAL:O	1:C1:328:GLN:HG2	2.19	0.43
1:C2:41:LYS:HD2	1:C3:337:GLN:HG2	2.00	0.43
1:C2:56:ALA:O	1:C2:59:PRO:HD2	2.19	0.43
1:C2:157:ARG:HD2	1:C2:157:ARG:HA	1.61	0.43
1:C2:301:MET:SD	1:C2:301:MET:N	2.91	0.43
2:P2:90:ASN:HB2	2:P2:158:HIS:CE1	2.53	0.43
3:A3:302:ASN:N	3:A3:302:ASN:OD1	2.50	0.43
4:BL:940:LYS:NZ	4:BL:941:ASN:OD1	2.39	0.43
4:BL:1022:VAL:HG12	4:BL:1023:PRO:HD3	2.01	0.43
4:BO:971:ARG:NH2	4:BO:974:PRO:HG2	2.34	0.43
1:C1:35:SER:HB2	2:P2:117:ARG:NH2	2.33	0.43
2:P3:68:SER:HB3	2:P3:146:VAL:HG21	2.00	0.43
4:BL:960:LEU:HD11	4:BL:1027:VAL:HG22	1.99	0.43
4:BT:398:MET:O	4:BT:402:ILE:HG12	2.19	0.43
4:BO:38:ILE:HG22	4:BO:465:ALA:HB3	2.00	0.43
4:BO:291:ILE:HD13	4:BO:306:ILE:HD12	2.00	0.43
4:BO:492:LEU:HD23	4:BO:492:LEU:HA	1.86	0.43
2:P3:50:ASP:HA	2:P3:53:ILE:HG22	2.00	0.43
3:a1:140:LYS:HB2	3:a1:140:LYS:HE3	1.81	0.43
3:a3:89:ALA:N	3:a3:181:SER:OG	2.50	0.43
3:a3:187:SER:OG	3:a3:189:VAL:O	2.32	0.43
4:BL:989:LEU:HD22	4:BL:1000:GLN:HG2	2.01	0.43
4:BL:1033:PHE:O	4:BL:1035:ARG:N	2.52	0.43
5:ZL:9:VAL:O	5:ZL:13:ILE:HG12	2.18	0.43
4:BT:395:MET:N	4:BT:395:MET:SD	2.92	0.43
1:C2:270:LEU:HD13	1:C2:310:PHE:HB2	2.00	0.43
3:A1:214:VAL:HG12	3:A1:216:VAL:HG23	2.01	0.43
3:a3:52:ILE:HD11	3:a3:235:LEU:HD11	2.00	0.43
4:BL:583:THR:HG22	4:BL:584:GLN:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:904:VAL:O	4:BL:907:LEU:HB2	2.18	0.43
4:BT:414:GLU:CD	4:BT:973:ARG:HE	2.27	0.43
4:BT:493:CYS:HA	4:BT:497:LEU:HD23	2.00	0.43
4:BO:254:ASN:ND2	4:BO:258:SER:OG	2.36	0.43
4:BO:310:LEU:HD23	4:BO:310:LEU:HA	1.85	0.43
4:BO:966:ASP:O	4:BO:970:MET:HG2	2.18	0.43
3:A1:83:GLU:HG2	3:A1:186:LYS:HA	2.01	0.43
3:A1:345:ASP:OD1	3:A1:345:ASP:N	2.47	0.43
4:BL:760:ASN:O	4:BL:771:VAL:HG12	2.18	0.43
4:BO:19:ILE:HD13	4:BO:19:ILE:HA	1.88	0.43
4:BO:219:LEU:O	4:BO:231:ASN:HA	2.19	0.43
4:BO:355:MET:SD	4:BO:410:ILE:HG21	2.58	0.43
4:BO:986:VAL:HG21	4:BO:1007:VAL:HB	2.01	0.43
1:C3:104:ARG:HH21	1:C3:257:GLU:CD	2.27	0.43
1:C3:314:ILE:O	1:C3:316:GLN:HG3	2.19	0.43
2:P3:32:ARG:NH2	2:P3:35:PRO:O	2.52	0.43
3:A3:332:VAL:HG23	3:A3:369:PRO:HA	1.99	0.43
3:a3:353:LEU:HD23	3:a3:353:LEU:HA	1.86	0.43
4:BL:885:PHE:HB2	4:BL:902:MET:HE1	2.01	0.43
4:BL:890:ALA:HB2	4:BO:14:VAL:HG11	1.99	0.43
5:ZT:6:LYS:HA	5:ZT:9:VAL:HG12	2.00	0.43
4:BO:407:ASP:HB2	4:BO:978:THR:HG22	2.00	0.43
2:P2:71:LEU:HD23	2:P2:71:LEU:HA	1.79	0.43
3:a1:222:ASP:OD1	3:a1:222:ASP:N	2.51	0.43
4:BT:403:GLY:HA3	4:BT:982:PHE:CE2	2.53	0.43
5:ZT:6:LYS:HG3	5:ZT:7:SER:N	2.34	0.43
4:BO:134:SER:OG	4:BO:675:GLY:O	2.37	0.43
4:BO:572:PHE:HB2	4:BO:666:PHE:O	2.18	0.43
4:BO:999:ALA:O	4:BO:1003:VAL:HG12	2.19	0.43
1:C3:123:ASP:HA	1:C3:126:THR:HG22	2.01	0.42
1:C3:164:GLN:O	1:C3:168:VAL:HG12	2.18	0.42
2:P2:125:LEU:HD11	2:P2:134:ASP:HB2	2.01	0.42
3:A2:49:PRO:HB3	3:A2:303:PRO:HA	1.99	0.42
3:A2:229:GLU:HG2	3:A2:235:LEU:HD23	2.01	0.42
4:BL:64:VAL:HG11	4:BL:117:LEU:HB3	2.01	0.42
4:BL:104:GLN:HA	4:BL:107:VAL:HG22	2.00	0.42
4:BL:367:ILE:HB	4:BL:368:PRO:HD3	2.01	0.42
4:BT:741:VAL:HG21	4:BT:799:VAL:HG11	2.00	0.42
3:A1:254:PHE:CE2	3:A1:256:GLN:HB2	2.54	0.42
3:A2:45:VAL:HG21	3:A2:353:LEU:HD12	2.01	0.42
4:BL:350:LEU:HD11	4:BL:984:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:355:MET:HE3	4:BL:368:PRO:HG2	2.01	0.42
4:BT:351:VAL:HA	4:BT:354:VAL:HG12	2.01	0.42
4:BT:500:ILE:HD12	4:BT:500:ILE:HA	1.91	0.42
4:BO:994:GLY:O	4:BO:997:SER:OG	2.34	0.42
1:C2:314:ILE:O	1:C2:316:GLN:HG3	2.19	0.42
3:a1:175:LYS:HE3	3:a1:175:LYS:HB2	1.90	0.42
4:BL:186:ILE:HD11	4:BL:246:PHE:CE2	2.54	0.42
4:BT:131:LYS:HB3	4:BT:131:LYS:HE2	1.65	0.42
3:A1:144:ASP:OD2	3:a3:128:ARG:NH2	2.37	0.42
3:a3:87:ILE:HD13	3:a3:87:ILE:HA	1.87	0.42
3:a3:175:LYS:HB2	3:a3:175:LYS:HE3	1.84	0.42
4:BL:143:ILE:HG22	4:BL:286:ALA:HB2	2.02	0.42
4:BL:937:LEU:HA	4:BL:937:LEU:HD23	1.71	0.42
4:BL:1020:PHE:CE2	5:ZL:29:LEU:HD22	2.53	0.42
4:BT:391:ASN:O	4:BT:395:MET:HG2	2.19	0.42
4:BO:143:ILE:HG22	4:BO:286:ALA:HB2	2.01	0.42
4:BO:680:PHE:HZ	4:BO:844:MET:HE3	1.85	0.42
1:C2:111:LYS:HB2	1:C2:254:LEU:HD13	2.00	0.42
2:P2:49:TYR:CE2	2:P2:123:VAL:HG21	2.55	0.42
3:A1:148:ALA:O	3:A1:152:GLN:HG3	2.19	0.42
3:a1:248:THR:HG22	3:a1:249:SER:H	1.85	0.42
4:BL:169:THR:O	4:BL:172:VAL:HG22	2.19	0.42
4:BT:360:GLN:HG2	4:BT:513:PHE:CD2	2.54	0.42
4:BT:939:ALA:O	4:BT:943:ILE:HG12	2.20	0.42
4:BO:530:SER:HA	5:ZO:34:ASN:HD21	1.83	0.42
1:C1:249:ARG:NH1	2:P1:135:GLU:OE1	2.53	0.42
1:C2:237:GLU:HG2	1:C2:426:LEU:HD21	2.02	0.42
1:C3:183:TYR:O	1:C3:186:VAL:HG12	2.19	0.42
3:a2:42:VAL:HG23	3:a2:359:VAL:O	2.20	0.42
3:a1:343:ILE:HD13	3:a1:343:ILE:HA	1.90	0.42
3:a3:53:THR:HG22	3:a3:298:GLU:HG2	2.01	0.42
4:BL:53:ASP:OD1	4:BL:53:ASP:N	2.40	0.42
4:BL:846:GLN:O	4:BL:849:SER:OG	2.29	0.42
4:BT:589:LYS:HB2	4:BT:589:LYS:HE3	1.78	0.42
4:BO:655:PHE:HB3	4:BO:663:VAL:CG1	2.49	0.42
2:P1:127:GLN:HB2	2:P1:132:TRP:CH2	2.55	0.42
2:P2:148:ASP:OD1	2:P2:149:ASP:N	2.51	0.42
3:A1:270:THR:O	3:A1:270:THR:OG1	2.38	0.42
3:A2:368:ARG:HG2	3:A2:369:PRO:HD2	2.00	0.42
4:BL:27:ILE:HD11	4:BL:380:PHE:CD2	2.55	0.42
4:BO:904:VAL:HG11	4:BO:942:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:256:ARG:NH1	1:C2:260:ARG:HG3	2.33	0.42
2:P3:128:GLY:O	2:P3:130:GLN:HG3	2.19	0.42
4:BL:355:MET:HE2	4:BL:355:MET:HB2	1.81	0.42
4:BT:10:ILE:HA	4:BT:13:TRP:HB2	2.02	0.42
4:BT:612:VAL:HB	4:BT:626:ILE:HG22	2.02	0.42
4:BO:118:LEU:HG	4:BO:119:PRO:HD2	2.02	0.42
4:BO:348:ILE:HG13	4:BO:349:ILE:N	2.34	0.42
4:BO:922:THR:OG1	4:BO:923:ASN:N	2.53	0.42
1:C1:70:TYR:HD1	1:C1:87:THR:HG22	1.84	0.42
1:C1:363:ILE:HD13	1:C1:363:ILE:HA	1.93	0.42
1:C2:103:TRP:CD1	1:C2:103:TRP:H	2.37	0.42
1:C2:256:ARG:HA	1:C2:256:ARG:HD2	1.78	0.42
2:P1:70:LYS:HE2	2:P1:165:ARG:NH1	2.30	0.42
2:P2:32:ARG:NH1	2:P2:68:SER:HA	2.35	0.42
3:A3:227:LYS:HE2	3:A3:227:LYS:HB2	1.92	0.42
3:a2:42:VAL:HG11	3:a2:375:ALA:HB1	2.02	0.42
4:BL:29:LYS:HA	4:BL:29:LYS:HD3	1.94	0.42
4:BL:649:MET:SD	4:BL:653:ARG:NH2	2.93	0.42
4:BL:901:VAL:HG11	4:BL:943:ILE:HG13	2.02	0.42
4:BO:350:LEU:O	4:BO:354:VAL:HG12	2.20	0.42
4:BO:606:VAL:HA	4:BO:631:LEU:HA	2.02	0.42
1:C2:347:GLN:HE21	1:C2:347:GLN:C	2.28	0.42
2:P2:37:VAL:HG12	2:P2:38:GLU:H	1.85	0.42
2:P2:122:ARG:H	2:P2:122:ARG:HG2	1.72	0.42
3:A1:65:ILE:HG13	3:A1:207:GLN:HG3	2.02	0.42
3:a2:42:VAL:HG23	3:a2:359:VAL:C	2.44	0.42
3:a1:186:LYS:NZ	3:a1:187:SER:O	2.53	0.42
4:BL:875:SER:O	4:BL:879:ILE:HG23	2.20	0.42
4:BL:1020:PHE:CD2	5:ZL:29:LEU:HD22	2.55	0.42
4:BT:438:ILE:HG13	4:BT:442:LEU:HD23	2.02	0.42
4:BO:354:VAL:HG13	4:BO:355:MET:HE3	2.02	0.42
4:BO:365:THR:O	4:BO:368:PRO:HD2	2.20	0.42
4:BO:367:ILE:HB	4:BO:368:PRO:HD3	2.01	0.42
4:BO:380:PHE:HE2	4:BO:390:ILE:HG12	1.84	0.42
1:C1:183:TYR:O	1:C1:186:VAL:HG12	2.20	0.41
1:C2:104:ARG:HD2	1:C2:261:GLN:HA	2.00	0.41
1:C2:423:LYS:HB3	1:C2:429:LEU:HD13	2.02	0.41
1:C3:367:LYS:O	1:C3:370:VAL:HG12	2.19	0.41
3:A3:261:GLU:O	3:A3:261:GLU:HG3	2.19	0.41
5:ZL:28:GLY:O	5:ZL:31:GLU:HG2	2.19	0.41
4:BT:376:LEU:HD23	4:BT:376:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:245:LEU:HD12	1:C1:245:LEU:HA	1.80	0.41
2:P3:165:ARG:HE	2:P3:165:ARG:HB3	1.68	0.41
3:A1:45:VAL:HG11	3:A1:353:LEU:HD22	2.01	0.41
3:a1:36:GLN:HB3	3:a1:37:MET:H	1.57	0.41
3:a1:42:VAL:HG22	3:a1:360:VAL:HG22	2.02	0.41
4:BT:534:ILE:HG13	4:BT:535:LEU:N	2.33	0.41
4:BT:583:THR:OG1	4:BT:584:GLN:N	2.50	0.41
4:BO:346:GLU:O	4:BO:350:LEU:HD12	2.19	0.41
4:BL:564:LEU:HD12	4:BL:564:LEU:HA	1.92	0.41
4:BL:685:ILE:HG22	4:BL:687:GLN:HG2	2.02	0.41
4:BL:790:TYR:HB3	4:BL:798:MET:HB3	2.02	0.41
4:BO:445:ILE:CG2	4:BO:940:LYS:HG3	2.50	0.41
4:BO:453:PHE:N	4:BO:453:PHE:CD1	2.88	0.41
4:BO:664:PHE:CD2	4:BO:717:ARG:HD2	2.55	0.41
4:BO:727:PHE:CZ	4:BO:783:PRO:HB3	2.55	0.41
4:BO:859:TRP:CD1	4:BO:867:ARG:HE	2.38	0.41
1:C1:325:LYS:HB2	1:C1:325:LYS:HE2	1.87	0.41
1:C2:107:THR:O	1:C2:111:LYS:HG3	2.20	0.41
2:P3:68:SER:HB3	2:P3:146:VAL:HG11	2.02	0.41
2:P3:137:LEU:HB3	2:P3:148:ASP:HB3	2.02	0.41
3:A1:63:TYR:CD2	3:A1:211:PRO:HG2	2.55	0.41
3:A1:246:LEU:HA	3:A1:246:LEU:HD23	1.78	0.41
3:a2:241:LYS:HB3	3:a2:260:LEU:O	2.21	0.41
4:BL:16:ALA:HB2	4:BL:488:LEU:HD22	2.01	0.41
4:BT:673:GLU:H	4:BT:673:GLU:HG2	1.70	0.41
4:BO:30:LEU:HD12	4:BO:30:LEU:HA	1.84	0.41
4:BO:970:MET:HG3	4:BO:971:ARG:HG2	2.01	0.41
1:C2:268:PRO:HB3	1:C2:312:LEU:HD13	2.01	0.41
1:C3:104:ARG:HH22	1:C3:260:ARG:NE	2.18	0.41
1:C3:224:LYS:HD2	1:C3:224:LYS:HA	1.84	0.41
1:C3:328:GLN:HE21	1:C3:328:GLN:HB3	1.69	0.41
3:a1:312:GLY:HA2	3:a1:364:LEU:HD11	2.03	0.41
4:BL:259:ARG:HE	4:BL:261:LEU:HD21	1.85	0.41
4:BL:758:TYR:CE1	4:BL:770:LYS:HB3	2.55	0.41
4:BT:187:TRP:HB3	4:BT:776:GLU:HB2	2.02	0.41
4:BT:462:SER:O	4:BT:466:ILE:HG13	2.20	0.41
4:BO:321:LEU:HD12	4:BO:321:LEU:HA	1.85	0.41
1:C1:232:ASN:HB3	2:P1:161:ALA:HB3	2.02	0.41
2:P1:160:THR:HG22	2:P1:161:ALA:N	2.36	0.41
3:A1:72:VAL:HG21	3:A1:174:THR:HG22	2.02	0.41
3:A1:326:VAL:HG12	3:A1:358:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a3:271:THR:HG21	4:BO:258:SER:HB2	2.03	0.41
4:BL:388:PHE:HE2	4:BL:472:ILE:HG21	1.85	0.41
4:BL:472:ILE:O	4:BL:476:SER:OG	2.31	0.41
4:BL:885:PHE:HD1	4:BL:902:MET:HE1	1.85	0.41
4:BL:903:LEU:HD23	4:BL:903:LEU:HA	1.88	0.41
4:BO:859:TRP:HD1	4:BO:867:ARG:HE	1.68	0.41
2:P1:67:LEU:HD13	2:P1:147:ILE:HG23	2.03	0.41
2:P2:85:ARG:H	2:P2:85:ARG:HG3	1.64	0.41
2:P3:32:ARG:NE	2:P3:36:CYS:SG	2.87	0.41
3:A3:82:LYS:HB2	3:A3:82:LYS:HE3	1.71	0.41
3:A3:84:GLY:HA3	3:a3:262:PHE:HD1	1.86	0.41
4:BT:31:PRO:HG2	4:BT:389:SER:HB3	2.02	0.41
4:BT:184:MET:HE3	4:BT:246:PHE:CD2	2.55	0.41
4:BT:390:ILE:HG23	4:BT:395:MET:SD	2.60	0.41
4:BT:735:LYS:HE2	4:BT:735:LYS:HB3	1.85	0.41
5:ZT:18:VAL:HA	5:ZT:21:ILE:HD12	2.03	0.41
4:BO:955:LYS:HA	4:BO:955:LYS:HD3	1.78	0.41
1:C1:417:ILE:HD13	1:C1:417:ILE:HA	1.96	0.41
1:C1:420:LEU:HD23	1:C1:420:LEU:HA	1.84	0.41
4:BL:540:ARG:HA	4:BL:540:ARG:HD3	1.74	0.41
4:BL:566:ASP:OD1	4:BL:566:ASP:N	2.53	0.41
4:BT:58:GLN:HA	4:BT:62:THR:HG22	2.02	0.41
4:BT:406:VAL:O	4:BT:410:ILE:HG12	2.20	0.41
4:BO:901:VAL:O	4:BO:904:VAL:HG12	2.21	0.41
1:C2:147:TYR:CE1	1:C2:403:ASN:HB2	2.56	0.41
1:C2:240:LYS:HB3	1:C2:240:LYS:HE3	1.88	0.41
1:C2:322:SER:O	1:C2:326:GLN:HG3	2.20	0.41
1:C3:103:TRP:CD1	1:C3:103:TRP:H	2.38	0.41
2:P3:102:SER:OG	2:P3:126:LYS:HB3	2.21	0.41
3:A2:132:LEU:HD12	3:A2:132:LEU:HA	1.85	0.41
3:A2:246:LEU:HD23	3:A2:246:LEU:HA	1.85	0.41
3:A3:119:ALA:HA	3:A3:153:ALA:HB1	2.02	0.41
3:A3:212:ILE:HD12	3:A3:212:ILE:HA	1.95	0.41
3:A3:311:GLN:HG2	3:A3:361:ILE:HD11	2.03	0.41
3:a2:175:LYS:HE3	3:a2:175:LYS:HB2	1.90	0.41
3:a2:311:GLN:HB3	3:a2:361:ILE:HG22	2.03	0.41
4:BL:26:ALA:O	4:BL:30:LEU:HB2	2.21	0.41
4:BL:188:MET:SD	4:BL:773:VAL:HG13	2.61	0.41
4:BL:530:SER:O	4:BL:534:ILE:HG22	2.21	0.41
4:BL:535:LEU:HD21	4:BL:1027:VAL:HG21	2.03	0.41
4:BL:555:LEU:HD23	4:BL:913:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BT:202:ASP:OD2	4:BT:792:ARG:NH2	2.54	0.41
4:BT:423:GLU:HG3	4:BT:433:LYS:HZ2	1.85	0.41
5:ZT:22:ILE:HD12	5:ZT:25:LEU:HD23	2.03	0.41
4:BO:36:PRO:HG2	4:BO:38:ILE:HG23	2.02	0.41
5:ZO:13:ILE:O	5:ZO:17:VAL:HG22	2.21	0.41
1:C1:111:LYS:HE3	1:C1:253:ASP:HB3	2.02	0.41
1:C1:112:ALA:O	1:C1:115:ILE:HG12	2.21	0.41
1:C1:423:LYS:HB3	1:C1:429:LEU:HD13	2.03	0.41
1:C2:40:ARG:HH22	2:P3:117:ARG:HG3	1.86	0.41
1:C2:197:LEU:HD22	1:C2:449:PRO:HG3	2.03	0.41
1:C3:51:GLU:OE2	1:C3:54:ASN:ND2	2.54	0.41
1:C3:226:ASP:OD1	1:C3:226:ASP:N	2.53	0.41
3:A3:212:ILE:HG21	3:A3:287:LEU:HD11	2.02	0.41
3:a1:345:ASP:OD2	3:a1:345:ASP:C	2.64	0.41
4:BT:472:ILE:HD13	4:BT:472:ILE:HA	1.90	0.41
2:P3:37:VAL:HG12	2:P3:38:GLU:H	1.85	0.40
4:BT:418:ARG:HG3	4:BT:419:VAL:N	2.35	0.40
5:ZT:19:MET:O	5:ZT:22:ILE:HG22	2.22	0.40
4:BO:438:ILE:O	4:BO:442:LEU:HG	2.20	0.40
4:BO:727:PHE:CE1	4:BO:807:SER:HB2	2.55	0.40
4:BO:786:ILE:HD12	4:BO:786:ILE:HA	1.92	0.40
1:C1:76:TYR:N	1:C2:302:GLY:O	2.53	0.40
1:C2:26:MET:HE1	1:C2:434:LEU:C	2.47	0.40
1:C2:70:TYR:HD1	1:C2:87:THR:HG22	1.86	0.40
4:BT:45:ILE:HD13	4:BT:111:LEU:HD22	2.02	0.40
4:BT:303:ALA:O	4:BT:307:ARG:HG2	2.21	0.40
1:C1:391:ILE:O	1:C1:394:VAL:HG22	2.21	0.40
1:C3:100:MET:HE2	1:C3:100:MET:HB3	1.85	0.40
2:P1:139:ILE:HG13	2:P1:146:VAL:HG23	2.02	0.40
3:A2:270:THR:O	3:A2:270:THR:OG1	2.37	0.40
3:A2:310:GLN:HG2	3:A2:347:TRP:CD1	2.56	0.40
3:a1:260:LEU:HD11	3:a1:276:LEU:HB3	2.02	0.40
3:a3:354:LYS:HE2	3:a3:354:LYS:HB2	1.90	0.40
4:BL:781:MET:HB3	4:BO:228:GLN:HE21	1.86	0.40
5:ZT:22:ILE:O	5:ZT:26:ILE:HG12	2.21	0.40
5:ZT:25:LEU:O	5:ZT:29:LEU:HD23	2.22	0.40
4:BO:137:LEU:N	4:BO:291:ILE:O	2.51	0.40
4:BO:760:ASN:O	4:BO:771:VAL:HG12	2.22	0.40
4:BO:1022:VAL:N	4:BO:1023:PRO:HD2	2.37	0.40
1:C3:147:TYR:CE1	1:C3:403:ASN:HB2	2.56	0.40
1:C3:268:PRO:HB3	1:C3:312:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P2:149:ASP:O	2:P2:164:LEU:HB3	2.22	0.40
3:A1:125:THR:OG1	3:a1:141:GLN:NE2	2.49	0.40
3:a3:46:LYS:HE2	3:a3:46:LYS:HB2	1.95	0.40
4:BL:976:LEU:HD12	5:ZL:22:ILE:HD12	2.03	0.40
4:BT:14:VAL:HG21	4:BO:890:ALA:HB2	2.04	0.40
4:BT:30:LEU:HD12	4:BT:30:LEU:HA	1.80	0.40
4:BO:907:LEU:HD12	4:BO:1017:LEU:HB3	2.03	0.40
1:C2:245:LEU:HD23	1:C2:245:LEU:HA	1.87	0.40
4:BL:275:TYR:CG	4:BO:223:PRO:HG3	2.56	0.40
4:BL:472:ILE:HD13	4:BL:472:ILE:HA	1.91	0.40
4:BL:873:ALA:N	4:BL:874:PRO:HD2	2.36	0.40
4:BT:431:THR:O	4:BT:435:MET:HG2	2.22	0.40
4:BO:182:TYR:CD2	4:BO:270:LEU:HD22	2.57	0.40
4:BO:580:ALA:HB1	4:BO:724:THR:HG22	2.02	0.40
4:BO:879:ILE:HD13	4:BO:879:ILE:HA	1.96	0.40
4:BO:973:ARG:O	4:BO:977:MET:HG2	2.21	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	C1	430/493 (87%)	420 (98%)	10 (2%)	0	100	100
1	C2	430/493 (87%)	421 (98%)	9 (2%)	0	100	100
1	C3	430/493 (87%)	420 (98%)	9 (2%)	1 (0%)	44	72
2	P1	150/171 (88%)	122 (81%)	27 (18%)	1 (1%)	19	47
2	P2	150/171 (88%)	125 (83%)	24 (16%)	1 (1%)	19	47
2	P3	150/171 (88%)	127 (85%)	22 (15%)	1 (1%)	19	47
3	A1	342/397 (86%)	335 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A2	342/397 (86%)	333 (97%)	9 (3%)	0	100	100
3	A3	342/397 (86%)	332 (97%)	10 (3%)	0	100	100
3	a1	342/397 (86%)	333 (97%)	8 (2%)	1 (0%)	37	66
3	a2	342/397 (86%)	332 (97%)	10 (3%)	0	100	100
3	a3	342/397 (86%)	333 (97%)	8 (2%)	1 (0%)	37	66
4	BL	1034/1049 (99%)	1008 (98%)	25 (2%)	1 (0%)	48	78
4	BO	1032/1049 (98%)	995 (96%)	35 (3%)	2 (0%)	44	72
4	BT	1032/1049 (98%)	1006 (98%)	25 (2%)	1 (0%)	48	78
5	ZL	37/49 (76%)	36 (97%)	1 (3%)	0	100	100
5	ZO	37/49 (76%)	37 (100%)	0	0	100	100
5	ZT	37/49 (76%)	37 (100%)	0	0	100	100
All	All	7001/7668 (91%)	6752 (96%)	239 (3%)	10 (0%)	50	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C3	286	SER
4	BT	777	ALA
4	BO	777	ALA
4	BL	1034	SER
4	BO	222	THR
3	a3	262	PHE
2	P1	150	VAL
2	P2	150	VAL
2	P3	150	VAL
3	a1	262	PHE

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	C1	361/412 (88%)	361 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C2	361/412 (88%)	360 (100%)	1 (0%)	91	95
1	C3	361/412 (88%)	361 (100%)	0	100	100
2	P1	131/148 (88%)	131 (100%)	0	100	100
2	P2	131/148 (88%)	129 (98%)	2 (2%)	60	76
2	P3	131/148 (88%)	130 (99%)	1 (1%)	79	87
3	A1	278/318 (87%)	278 (100%)	0	100	100
3	A2	278/318 (87%)	277 (100%)	1 (0%)	89	93
3	A3	278/318 (87%)	277 (100%)	1 (0%)	89	93
3	a1	278/318 (87%)	278 (100%)	0	100	100
3	a2	278/318 (87%)	277 (100%)	1 (0%)	89	93
3	a3	278/318 (87%)	278 (100%)	0	100	100
4	BL	834/855 (98%)	831 (100%)	3 (0%)	89	93
4	BO	834/855 (98%)	832 (100%)	2 (0%)	92	96
4	BT	834/855 (98%)	833 (100%)	1 (0%)	92	97
5	ZL	33/41 (80%)	33 (100%)	0	100	100
5	ZO	33/41 (80%)	33 (100%)	0	100	100
5	ZT	33/41 (80%)	32 (97%)	1 (3%)	36	61
All	All	5745/6276 (92%)	5731 (100%)	14 (0%)	91	96

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C2	347	GLN
2	P2	136	VAL
2	P2	144	CYS
2	P3	46	GLN
3	A2	36	GLN
3	A3	36	GLN
3	a2	216	VAL
4	BL	492	LEU
4	BL	822	LEU
4	BL	914	LEU
4	BT	125	GLN
5	ZT	31	GLU
4	BO	552	MET
4	BO	741	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	C1	74	ASN
1	C1	206	GLN
1	C1	300	ASN
1	C1	321	ASN
1	C1	328	GLN
1	C1	330	ASN
1	C1	414	ASN
1	C1	419	GLN
1	C1	451	ASN
1	C2	63	GLN
1	C2	74	ASN
1	C2	83	ASN
1	C2	140	ASN
1	C2	161	GLN
1	C2	199	ASN
1	C2	321	ASN
1	C2	403	ASN
1	C2	410	ASN
1	C2	418	ASN
1	C3	36	ASN
1	C3	316	GLN
1	C3	323	GLN
1	C3	414	ASN
1	C3	451	ASN
2	P1	55	HIS
2	P1	84	HIS
2	P2	83	ASN
2	P2	127	GLN
2	P2	133	GLN
2	P2	158	HIS
3	A2	102	GLN
3	A2	196	GLN
3	A2	237	GLN
3	A2	376	GLN
3	A3	218	GLN
3	a2	102	GLN
3	a2	310	GLN
3	a2	341	GLN
3	a1	102	GLN
3	a1	152	GLN
3	a1	196	GLN

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Mol	Chain	Res	Type
3	a3	136	GLN
3	a3	237	GLN
4	BL	3	ASN
4	BL	70	ASN
4	BL	108	GLN
4	BL	109	ASN
4	BL	112	GLN
4	BL	120	GLN
4	BL	124	GLN
4	BL	189	ASN
4	BL	284	GLN
4	BL	360	GLN
4	BL	439	GLN
4	BL	517	ASN
4	BL	584	GLN
4	BL	797	GLN
4	BT	106	GLN
4	BT	228	GLN
4	BT	284	GLN
4	BT	697	GLN
4	BT	737	GLN
4	BO	3	ASN
4	BO	70	ASN
4	BO	104	GLN
4	BO	517	ASN
4	BO	526	HIS
4	BO	657	GLN
4	BO	737	GLN
5	ZO	34	ASN

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 [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.

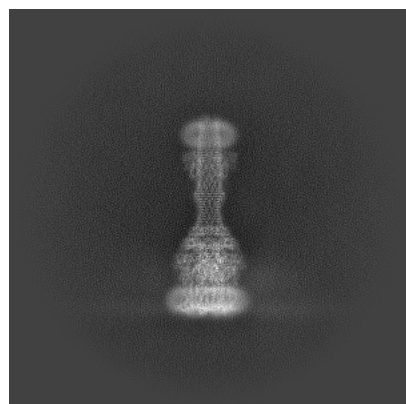
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64785. These allow visual inspection of the internal detail of the map and identification of artifacts.

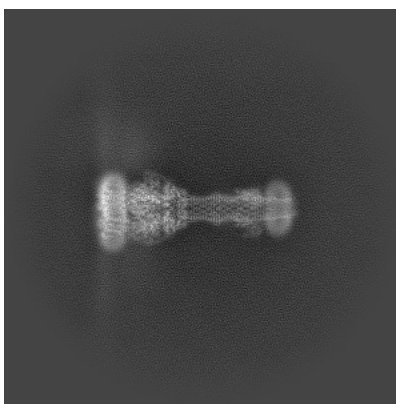
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

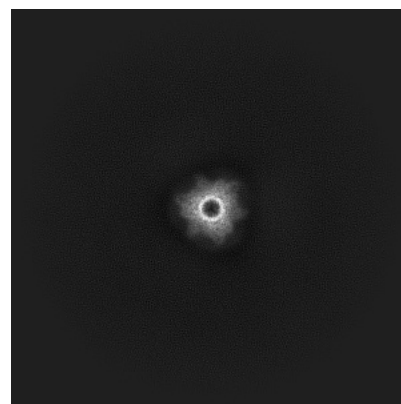
6.1.1 Primary map



X

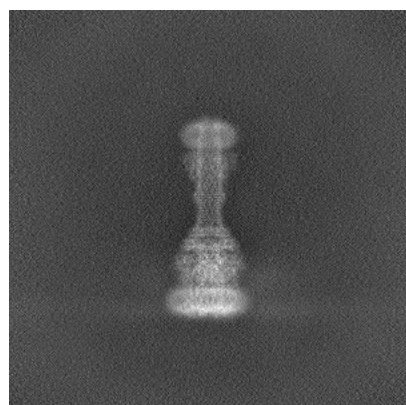


Y

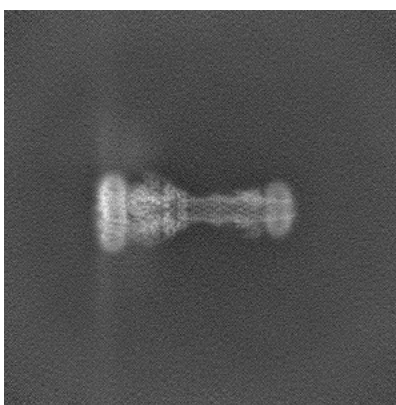


Z

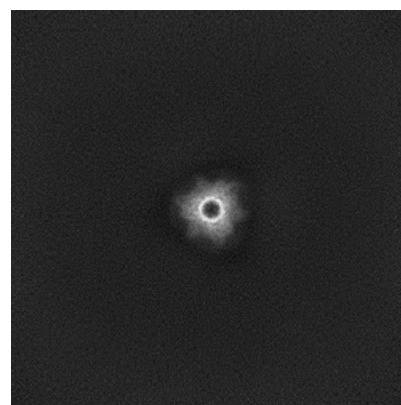
6.1.2 Raw map



X



Y

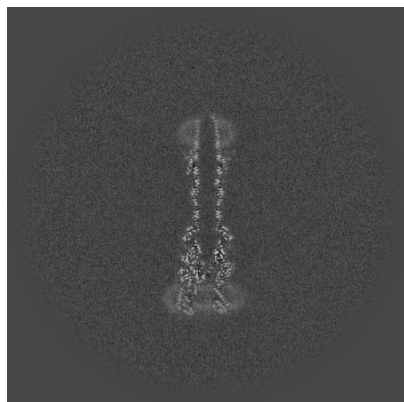


Z

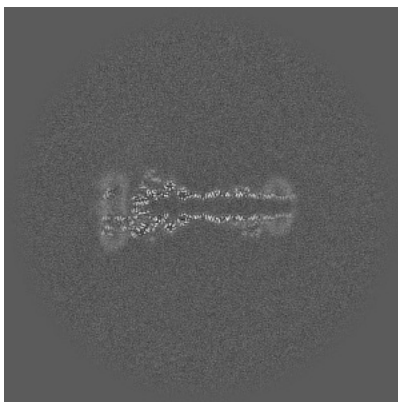
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

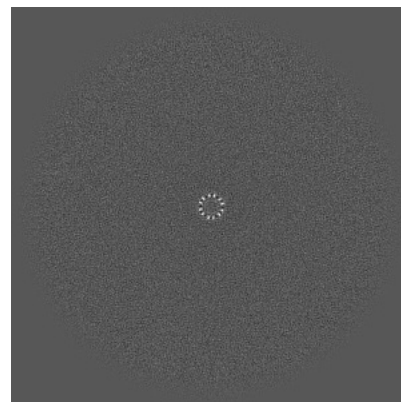
6.2.1 Primary map



X Index: 256

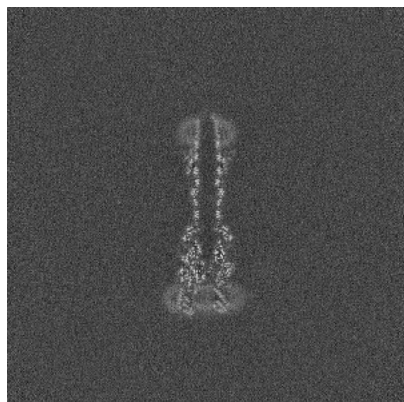


Y Index: 256

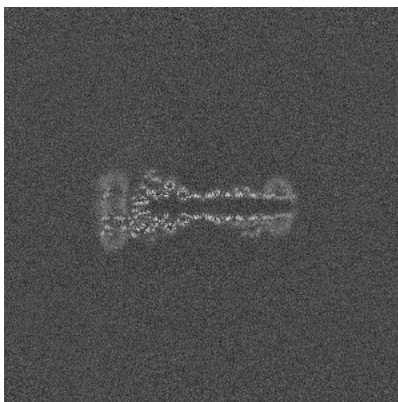


Z Index: 256

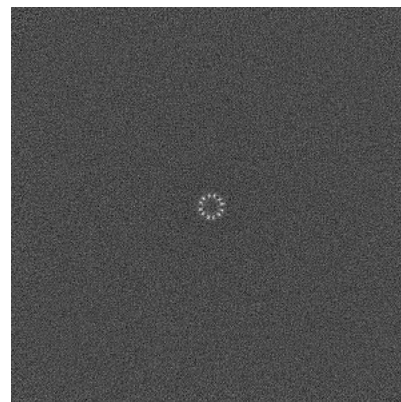
6.2.2 Raw map



X Index: 256



Y Index: 256

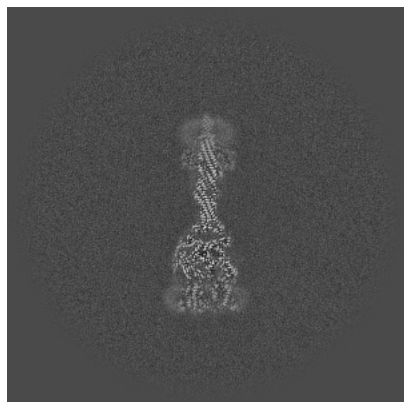


Z Index: 256

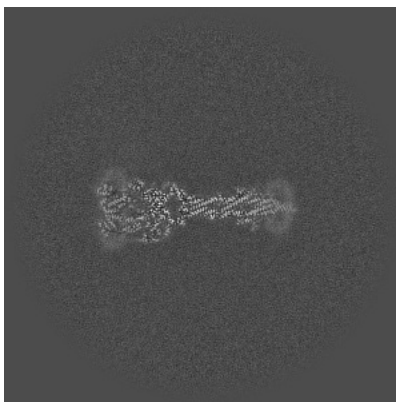
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

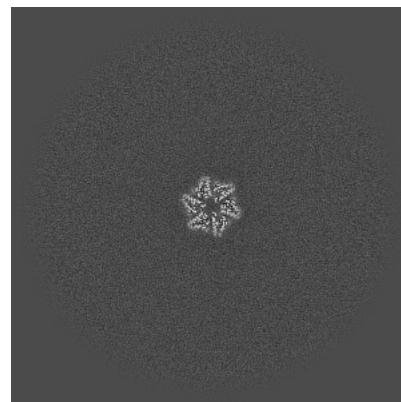
6.3.1 Primary map



X Index: 269

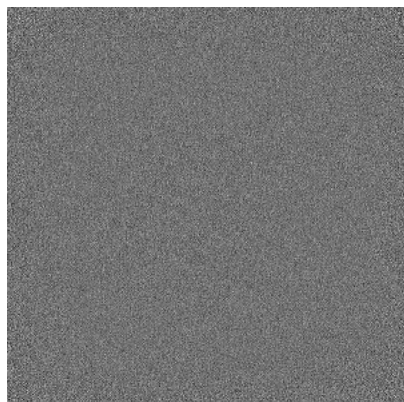


Y Index: 268

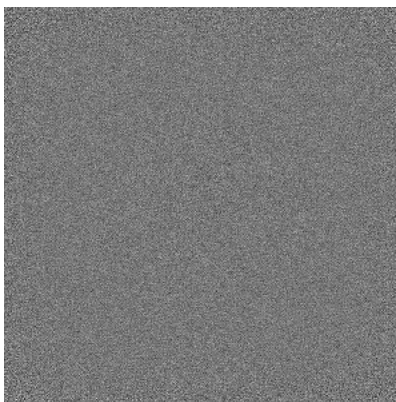


Z Index: 209

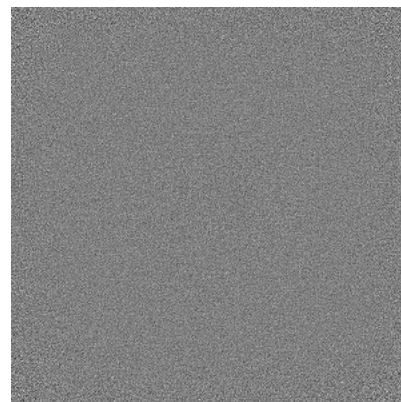
6.3.2 Raw map



X Index: 0



Y Index: 0

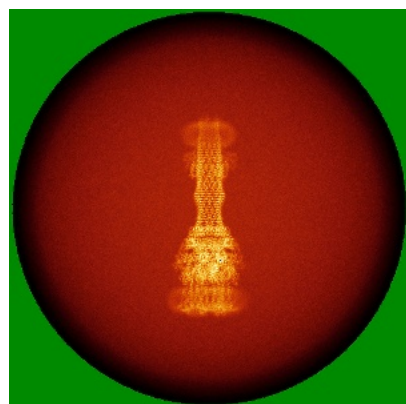


Z Index: 0

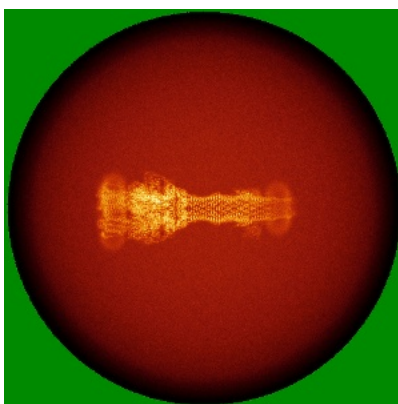
The images above show the largest variance slices of the map in three orthogonal directions.

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

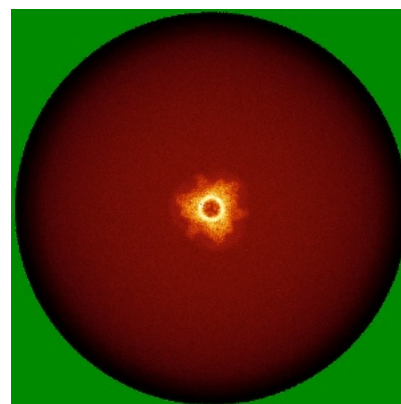
6.4.1 Primary map



X

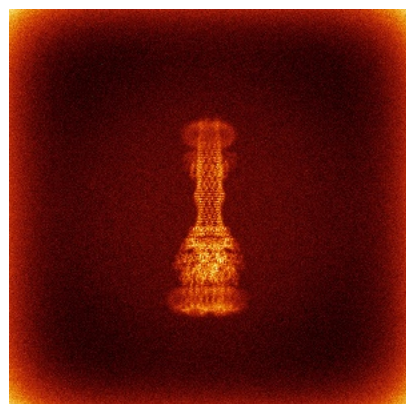


Y

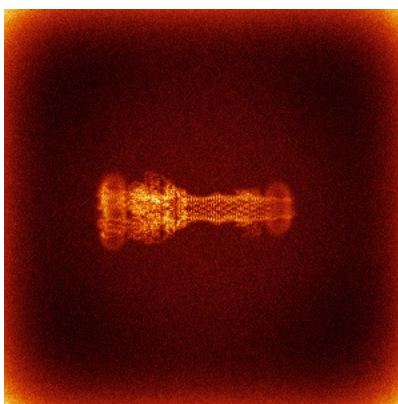


Z

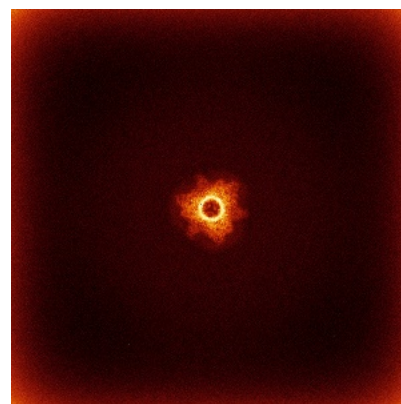
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

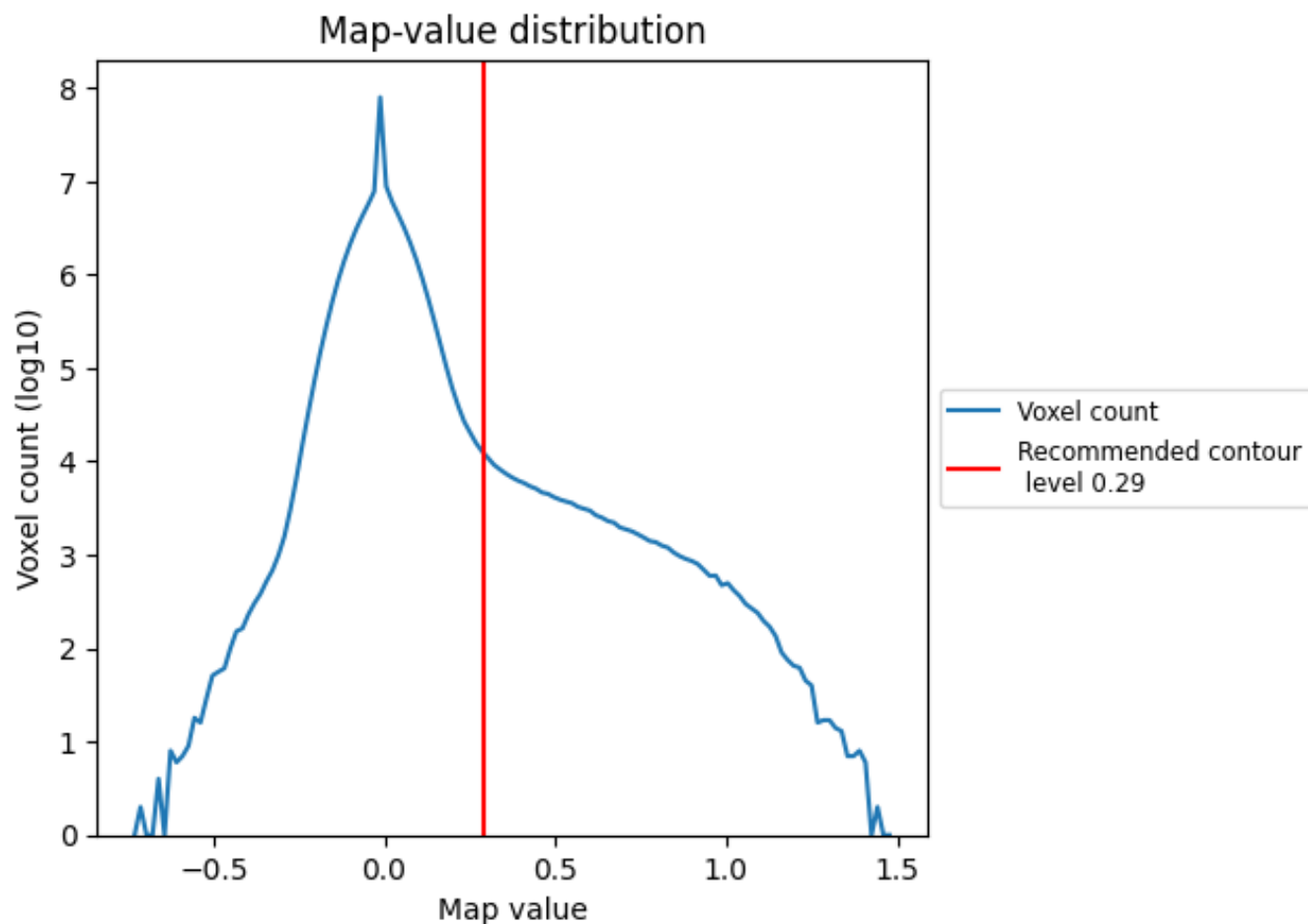
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

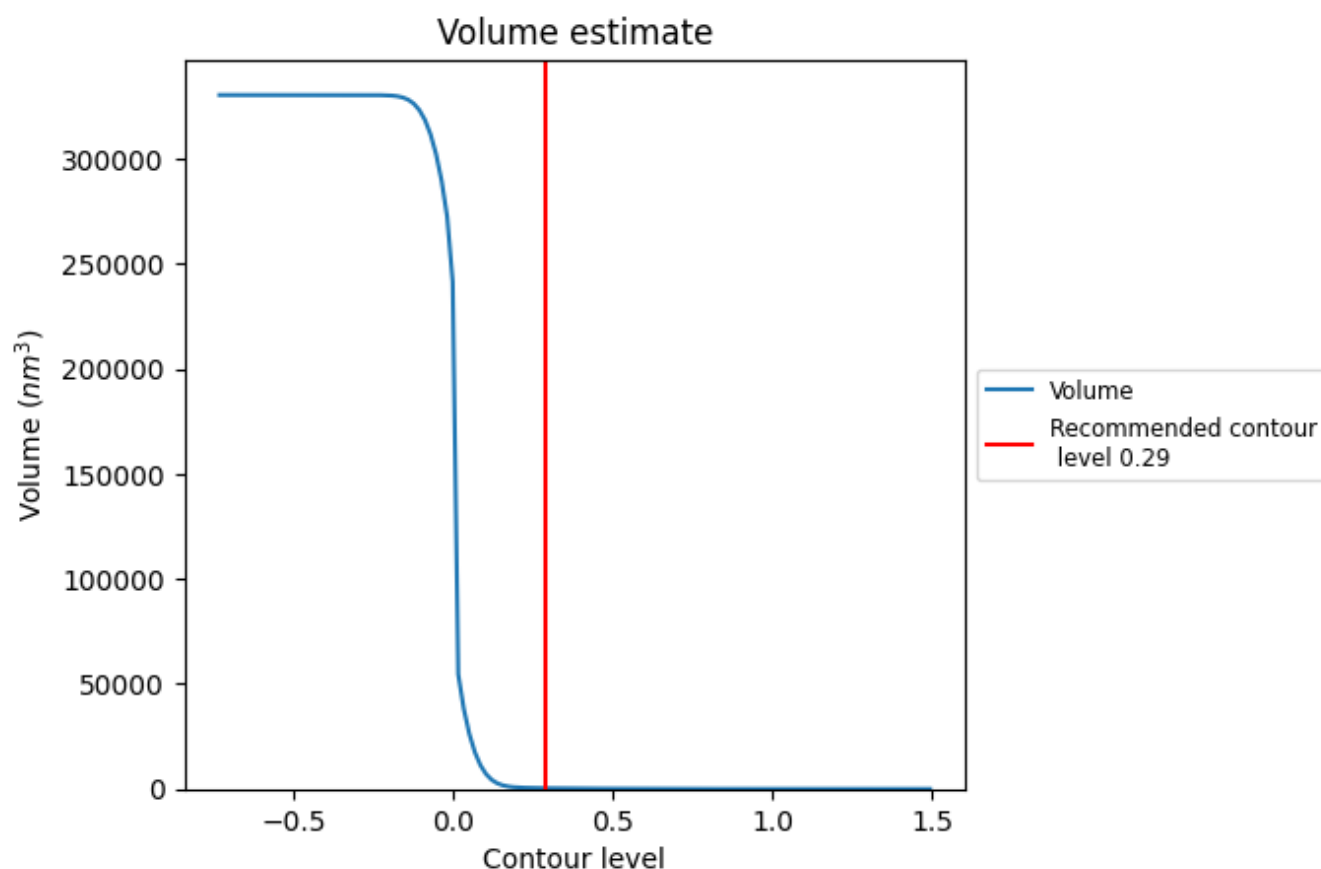
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

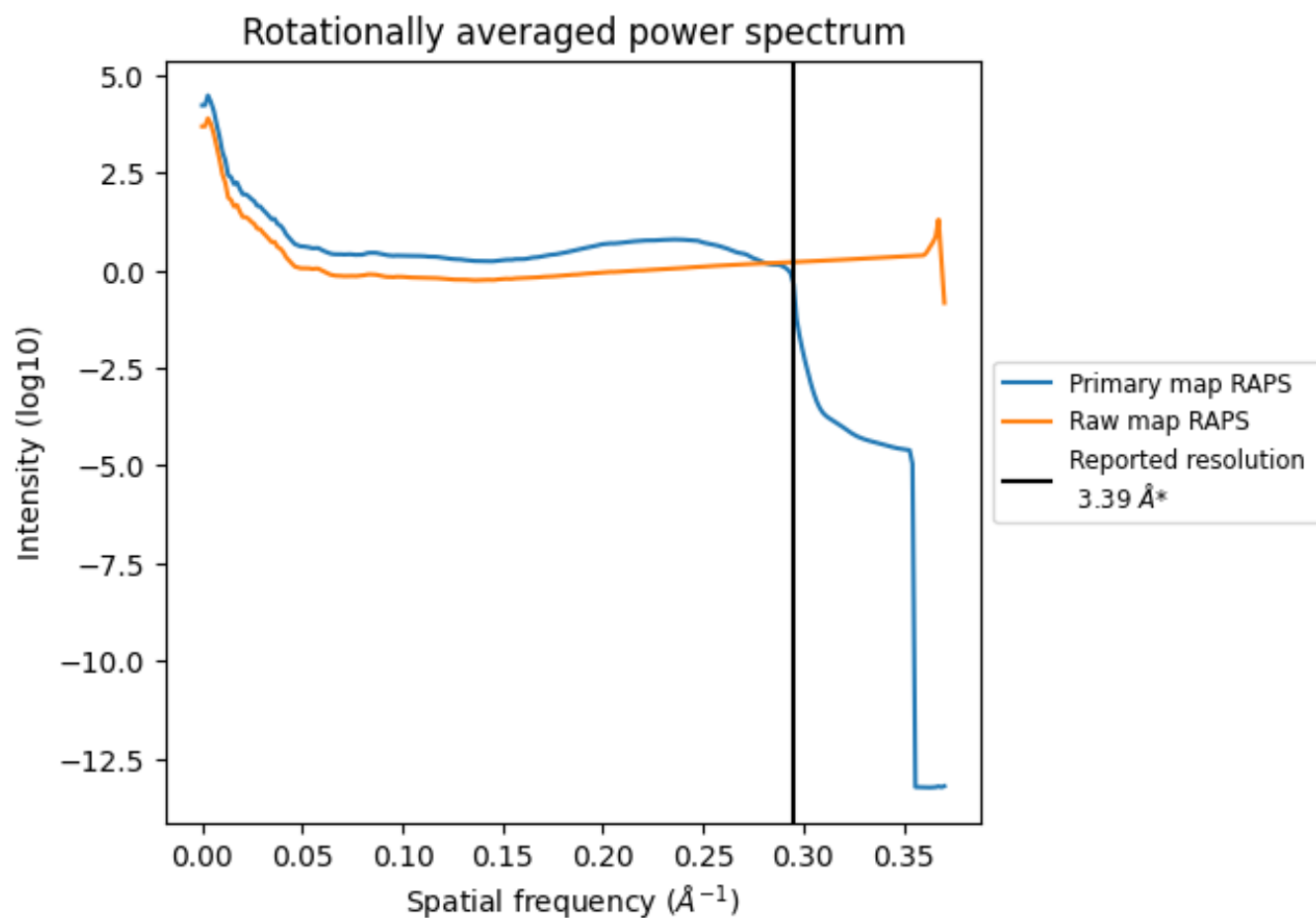
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 351 nm³; this corresponds to an approximate mass of 317 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 ⓘ

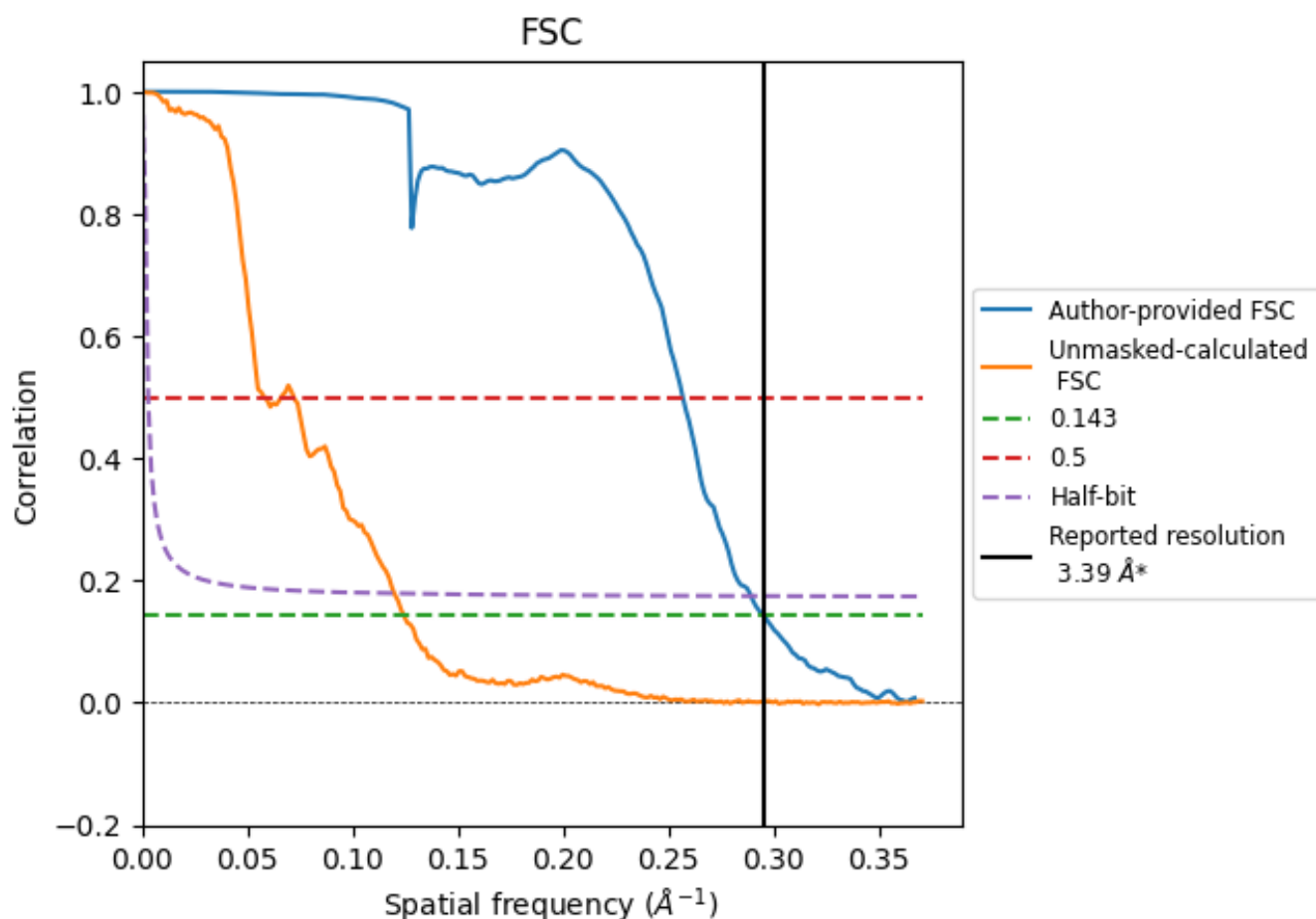


*Reported resolution corresponds to spatial frequency of 0.295 Å⁻¹

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 0.295 Å⁻¹

8.2 Resolution estimates [i](#)

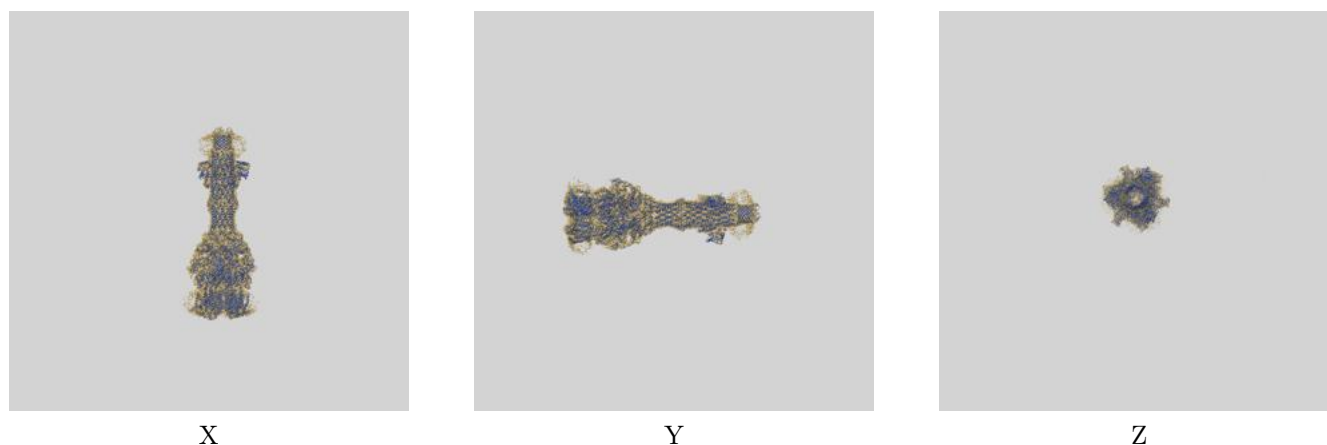
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	3.39	3.90	3.46
Unmasked-calculated*	8.05	17.27	8.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.05 differs from the reported value 3.39 by more than 10 %

9 Map-model fit [i](#)

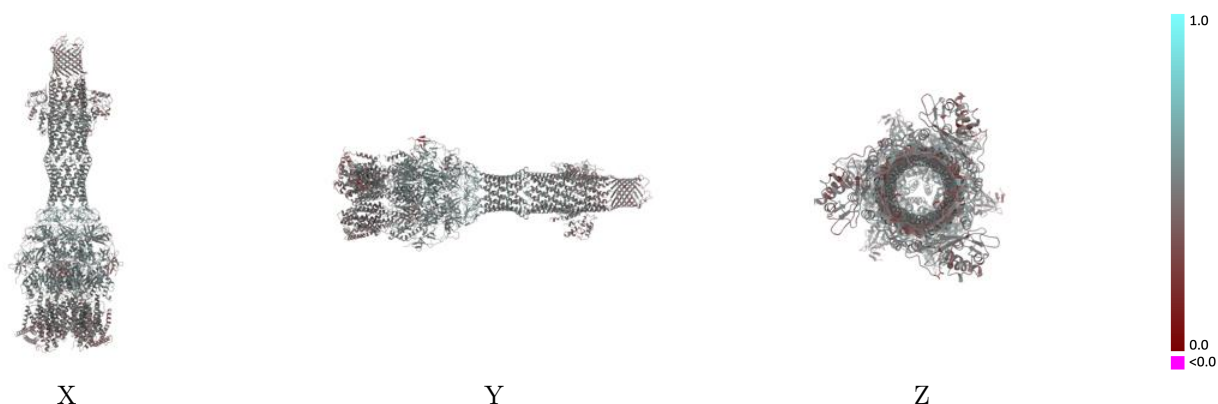
This section contains information regarding the fit between EMDB map EMD-64785 and PDB model 9V53. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



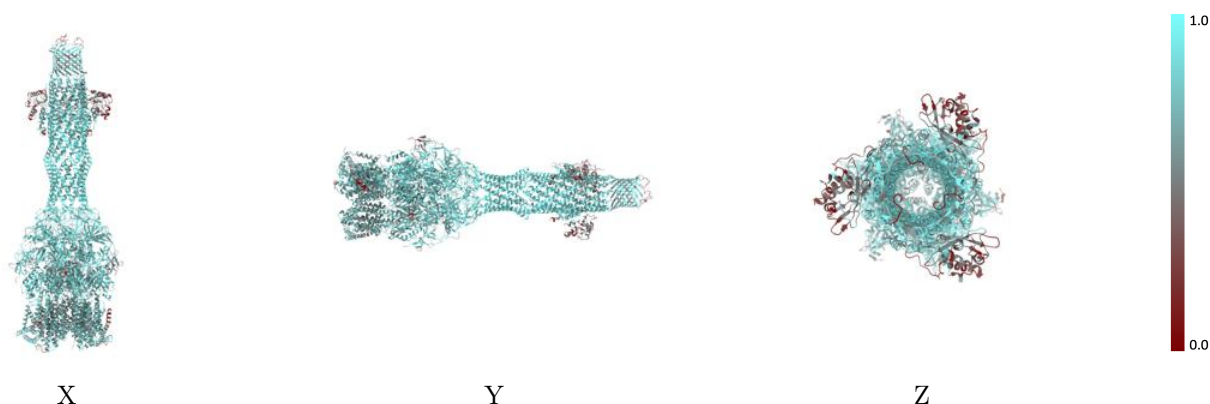
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



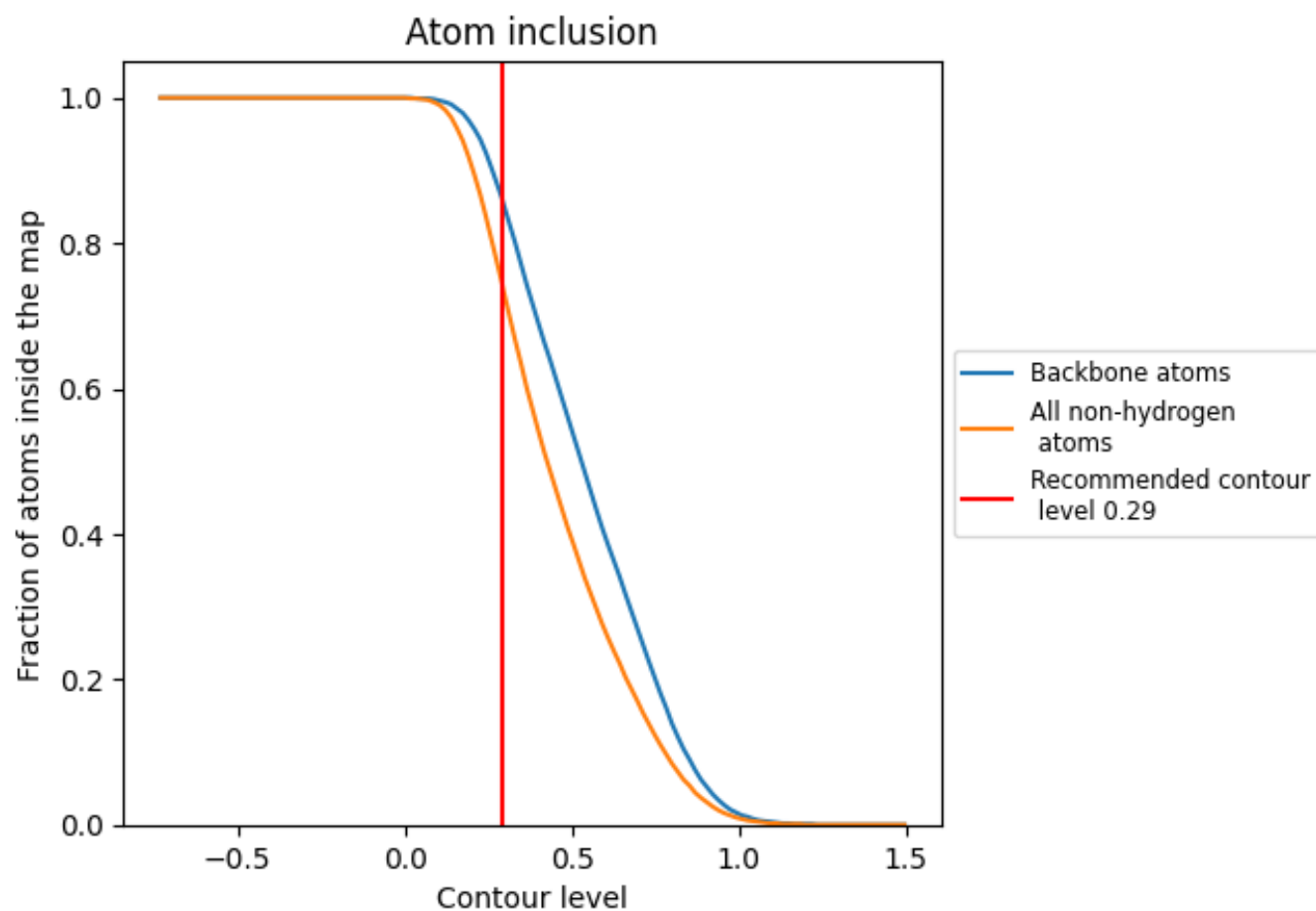
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.29).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.4820
A1	 0.8110	 0.5040
A2	 0.8140	 0.5110
A3	 0.8180	 0.5070
BL	 0.7600	 0.4900
BO	 0.7750	 0.4910
BT	 0.7560	 0.4870
C1	 0.7790	 0.4750
C2	 0.7740	 0.4630
C3	 0.7790	 0.4640
P1	 0.4240	 0.4430
P2	 0.3930	 0.4210
P3	 0.4080	 0.4140
ZL	 0.3990	 0.3690
ZO	 0.5600	 0.3850
ZT	 0.5260	 0.3920
a1	 0.7600	 0.4890
a2	 0.7730	 0.4930
a3	 0.7760	 0.4850

