



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:45 AM UTC

PDB ID : 7M7J / pdb_00007m7j
EMDB ID : EMD-23715
Title : 6-Deoxyerythronolide B synthase (DEBS) module 1 in complex with antibody fragment 1B2: "turnstile closed" state (TE-free)
Authors : Cogan, D.P.; Zhang, K.; Chiu, W.; Khosla, C.
Deposited on : 2021-03-28
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

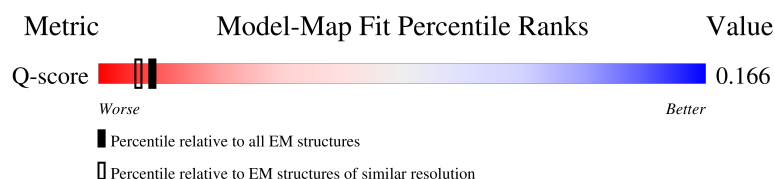
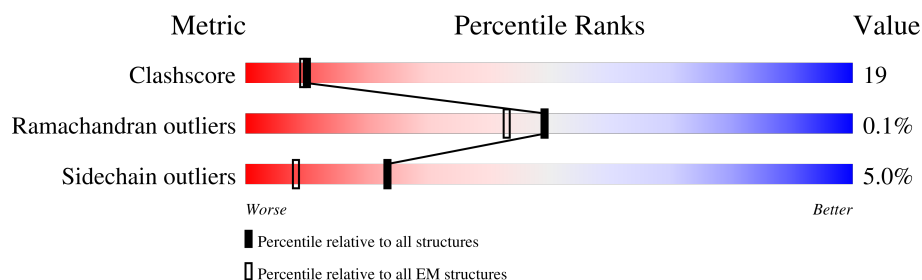
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

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	1593	18% 56% 30% 13%
1	B	1593	14% 35% 21% 43%
2	C	249	44% 36% 18%
2	E	249	48% 32% 18%

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Mol	Chain	Length	Quality of chain
3	D	236	
3	F	236	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23224 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 EryAI.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	912	Total	C	N	O	S	0	0
			6741	4190	1233	1291	27		
1	A	1390	Total	C	N	O	S	0	0
			10277	6381	1890	1971	35		

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP Q5UNP6
B	2	ALA	-	expression tag	UNP Q5UNP6
B	3	SER	-	expression tag	UNP Q5UNP6
B	4	THR	-	expression tag	UNP Q5UNP6
B	5	ASP	-	expression tag	UNP Q5UNP6
B	6	SER	-	expression tag	UNP Q5UNP6
B	7	GLU	-	expression tag	UNP Q5UNP6
B	8	LYS	-	expression tag	UNP Q5UNP6
B	9	VAL	-	expression tag	UNP Q5UNP6
B	10	ALA	-	expression tag	UNP Q5UNP6
B	11	GLU	-	expression tag	UNP Q5UNP6
B	12	TYR	-	expression tag	UNP Q5UNP6
B	13	LEU	-	expression tag	UNP Q5UNP6
B	14	ARG	-	expression tag	UNP Q5UNP6
B	15	ARG	-	expression tag	UNP Q5UNP6
B	16	ALA	-	expression tag	UNP Q5UNP6
B	17	THR	-	expression tag	UNP Q5UNP6
B	18	LEU	-	expression tag	UNP Q5UNP6
B	19	ASP	-	expression tag	UNP Q5UNP6
B	20	LEU	-	expression tag	UNP Q5UNP6
B	21	ARG	-	expression tag	UNP Q5UNP6
B	22	ALA	-	expression tag	UNP Q5UNP6
B	23	ALA	-	expression tag	UNP Q5UNP6
B	24	ARG	-	expression tag	UNP Q5UNP6
B	25	GLN	-	expression tag	UNP Q5UNP6
B	26	ARG	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	ILE	-	expression tag	UNP Q5UNP6
B	28	ARG	-	expression tag	UNP Q5UNP6
B	29	GLU	-	expression tag	UNP Q5UNP6
B	30	LEU	-	expression tag	UNP Q5UNP6
B	31	GLU	-	expression tag	UNP Q5UNP6
B	1574	PRO	-	expression tag	UNP Q5UNP6
B	1575	ASN	-	expression tag	UNP Q5UNP6
B	1576	SER	-	expression tag	UNP Q5UNP6
B	1577	SER	-	expression tag	UNP Q5UNP6
B	1578	SER	-	expression tag	UNP Q5UNP6
B	1579	VAL	-	expression tag	UNP Q5UNP6
B	1580	ASP	-	expression tag	UNP Q5UNP6
B	1581	LYS	-	expression tag	UNP Q5UNP6
B	1582	LEU	-	expression tag	UNP Q5UNP6
B	1583	ALA	-	expression tag	UNP Q5UNP6
B	1584	ALA	-	expression tag	UNP Q5UNP6
B	1585	ALA	-	expression tag	UNP Q5UNP6
B	1586	LEU	-	expression tag	UNP Q5UNP6
B	1587	GLU	-	expression tag	UNP Q5UNP6
B	1588	HIS	-	expression tag	UNP Q5UNP6
B	1589	HIS	-	expression tag	UNP Q5UNP6
B	1590	HIS	-	expression tag	UNP Q5UNP6
B	1591	HIS	-	expression tag	UNP Q5UNP6
B	1592	HIS	-	expression tag	UNP Q5UNP6
B	1593	HIS	-	expression tag	UNP Q5UNP6
A	1	MET	-	expression tag	UNP Q5UNP6
A	2	ALA	-	expression tag	UNP Q5UNP6
A	3	SER	-	expression tag	UNP Q5UNP6
A	4	THR	-	expression tag	UNP Q5UNP6
A	5	ASP	-	expression tag	UNP Q5UNP6
A	6	SER	-	expression tag	UNP Q5UNP6
A	7	GLU	-	expression tag	UNP Q5UNP6
A	8	LYS	-	expression tag	UNP Q5UNP6
A	9	VAL	-	expression tag	UNP Q5UNP6
A	10	ALA	-	expression tag	UNP Q5UNP6
A	11	GLU	-	expression tag	UNP Q5UNP6
A	12	TYR	-	expression tag	UNP Q5UNP6
A	13	LEU	-	expression tag	UNP Q5UNP6
A	14	ARG	-	expression tag	UNP Q5UNP6
A	15	ARG	-	expression tag	UNP Q5UNP6
A	16	ALA	-	expression tag	UNP Q5UNP6
A	17	THR	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	18	LEU	-	expression tag	UNP Q5UNP6
A	19	ASP	-	expression tag	UNP Q5UNP6
A	20	LEU	-	expression tag	UNP Q5UNP6
A	21	ARG	-	expression tag	UNP Q5UNP6
A	22	ALA	-	expression tag	UNP Q5UNP6
A	23	ALA	-	expression tag	UNP Q5UNP6
A	24	ARG	-	expression tag	UNP Q5UNP6
A	25	GLN	-	expression tag	UNP Q5UNP6
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6
A	28	ARG	-	expression tag	UNP Q5UNP6
A	29	GLU	-	expression tag	UNP Q5UNP6
A	30	LEU	-	expression tag	UNP Q5UNP6
A	31	GLU	-	expression tag	UNP Q5UNP6
A	1574	PRO	-	expression tag	UNP Q5UNP6
A	1575	ASN	-	expression tag	UNP Q5UNP6
A	1576	SER	-	expression tag	UNP Q5UNP6
A	1577	SER	-	expression tag	UNP Q5UNP6
A	1578	SER	-	expression tag	UNP Q5UNP6
A	1579	VAL	-	expression tag	UNP Q5UNP6
A	1580	ASP	-	expression tag	UNP Q5UNP6
A	1581	LYS	-	expression tag	UNP Q5UNP6
A	1582	LEU	-	expression tag	UNP Q5UNP6
A	1583	ALA	-	expression tag	UNP Q5UNP6
A	1584	ALA	-	expression tag	UNP Q5UNP6
A	1585	ALA	-	expression tag	UNP Q5UNP6
A	1586	LEU	-	expression tag	UNP Q5UNP6
A	1587	GLU	-	expression tag	UNP Q5UNP6
A	1588	HIS	-	expression tag	UNP Q5UNP6
A	1589	HIS	-	expression tag	UNP Q5UNP6
A	1590	HIS	-	expression tag	UNP Q5UNP6
A	1591	HIS	-	expression tag	UNP Q5UNP6
A	1592	HIS	-	expression tag	UNP Q5UNP6
A	1593	HIS	-	expression tag	UNP Q5UNP6

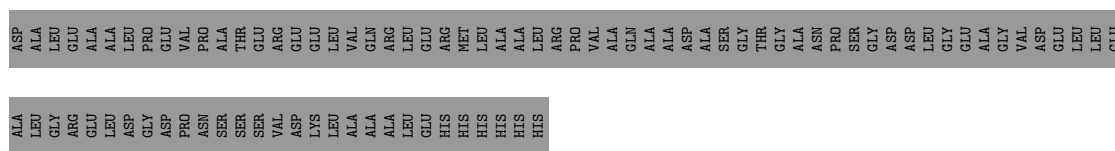
- Molecule 2 is a protein called 1B2 (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
2	E	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

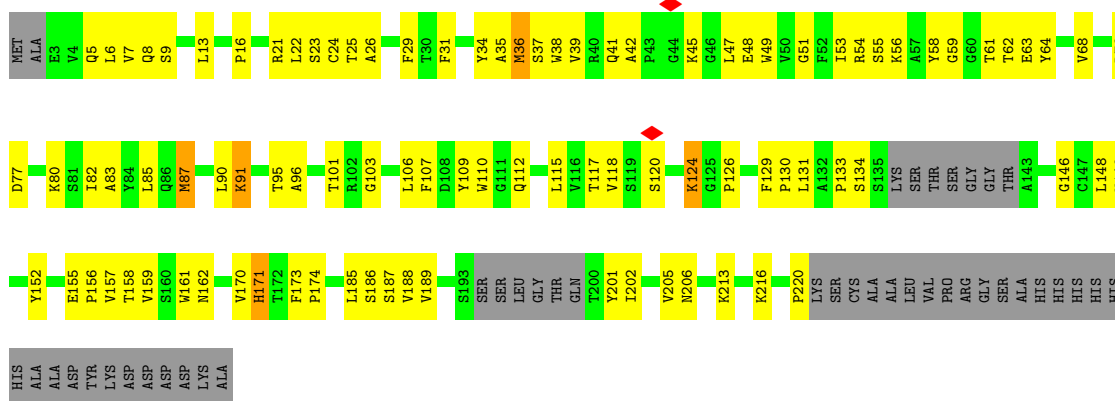
- Molecule 3 is a protein called 1B2 (light chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	206	Total	C	N	O	S	0	0
			1564	980	261	317	6		
3	F	206	Total	C	N	O	S	0	0
			1564	981	261	316	6		

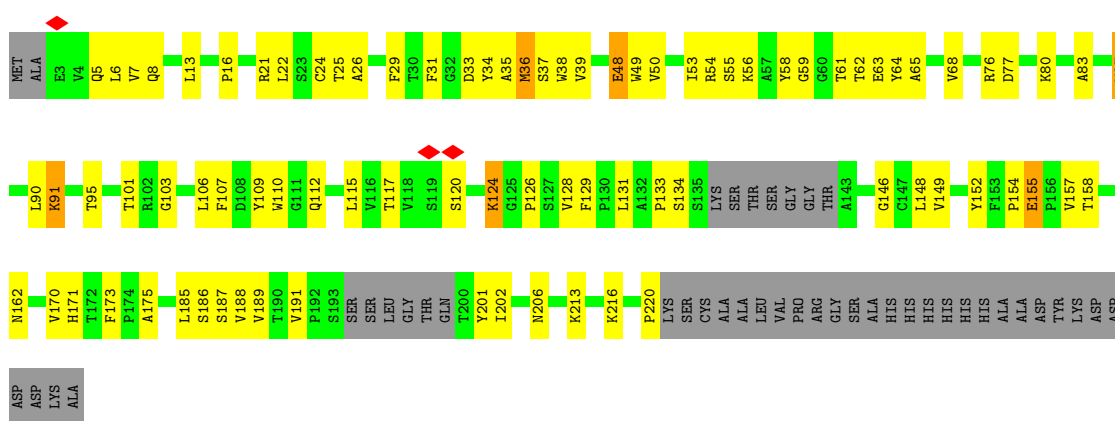




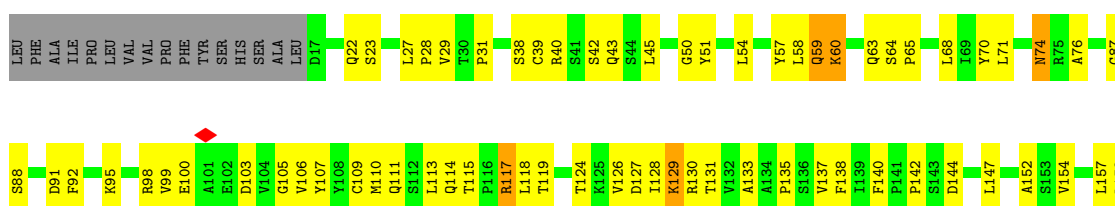
- Molecule 2: 1B2 (heavy chain)



- Molecule 2: 1B2 (heavy chain)

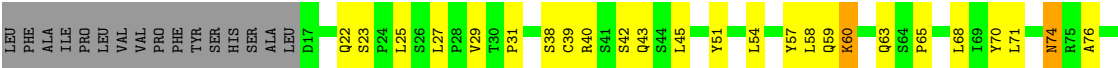


- Molecule 3: 1B2 (light chain)





• Molecule 3: 1B2 (light chain)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102772	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.481	Depositor
Minimum map value	-0.533	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/10473	0.55	5/14255 (0.0%)
1	B	0.34	0/6875	0.59	6/9353 (0.1%)
2	C	0.34	0/1575	0.60	0/2141
2	E	0.31	0/1575	0.55	0/2141
3	D	0.27	0/1597	0.60	1/2171 (0.0%)
3	F	0.37	0/1597	0.69	3/2170 (0.1%)
All	All	0.33	0/23692	0.58	15/32231 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	VAL	N-CA-C	-7.39	105.57	112.96
1	B	867	ASP	N-CA-C	-6.49	105.47	113.19
1	B	866	ALA	N-CA-C	-5.92	104.81	112.68
1	B	124	ARG	CB-CA-C	5.77	120.37	110.79
1	B	234	VAL	N-CA-C	-5.61	103.93	110.05
3	F	183	GLU	CA-CB-CG	5.60	125.30	114.10
3	D	183	GLU	CA-CB-CG	5.59	125.28	114.10
3	F	125	LYS	CA-CB-CG	5.41	124.92	114.10
1	A	250	LEU	CA-C-N	5.41	140.73	121.59
1	A	250	LEU	C-N-CA	5.41	140.73	121.59
3	F	113	LEU	N-CA-C	-5.27	107.02	113.50
1	B	158	GLN	CB-CA-C	-5.14	110.63	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	825	TYR	N-CA-C	-5.11	99.58	109.24
1	A	664	CYS	N-CA-C	-5.10	105.90	111.82
1	B	865	LEU	N-CA-C	-5.04	108.17	114.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	905	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10277	0	10118	381	0
1	B	6741	0	6618	279	0
2	C	1539	0	1511	77	0
2	E	1539	0	1511	74	0
3	D	1564	0	1517	72	0
3	F	1564	0	1522	71	0
All	All	23224	0	22797	889	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 19.

All (889) 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:F:125:LYS:H	3:F:125:LYS:HD3	1.23	1.02
1:B:151:VAL:HA	1:B:228:MET:HB2	1.62	0.82
1:B:121:PRO:HB2	1:B:234:VAL:HG11	1.61	0.81
1:A:966:ARG:HG2	1:A:976:VAL:HG11	1.62	0.80
1:A:235:MET:HG2	1:A:240:MET:HG3	1.68	0.76
1:A:718:ASN:H	1:A:723:VAL:HG12	1.51	0.75
2:E:155:GLU:HG3	2:E:175:ALA:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:125:LYS:H	3:F:125:LYS:CD	2.00	0.74
1:A:653:ILE:HG12	1:A:820:LEU:HD21	1.70	0.73
1:A:120:ASP:HB2	1:A:179:THR:HA	1.71	0.72
2:E:39:VAL:HG22	2:E:49:TRP:HD1	1.55	0.71
2:C:24:CYS:HB3	2:C:83:ALA:HB3	1.71	0.71
2:E:24:CYS:HB3	2:E:83:ALA:HB3	1.73	0.71
1:A:120:ASP:HB3	1:A:123:GLN:HG3	1.72	0.71
1:B:724:VAL:HG22	1:B:745:ARG:HH12	1.56	0.70
1:A:1252:VAL:HG23	1:A:1253:LEU:HD12	1.72	0.70
1:A:318:ARG:O	1:A:322:GLN:NE2	2.23	0.70
1:B:294:LEU:HD11	1:B:452:ALA:HB1	1.72	0.70
2:C:188:VAL:HG11	3:D:157:LEU:HD11	1.74	0.70
3:F:125:LYS:HD3	3:F:125:LYS:N	2.04	0.70
1:A:692:LYS:HD3	1:A:759:HIS:HB3	1.74	0.69
1:B:331:PRO:HB3	1:B:359:TYR:HA	1.75	0.69
1:A:330:GLY:N	3:F:98:ARG:HH12	1.90	0.69
1:B:243:ASP:HB2	1:A:176:MET:HE1	1.73	0.69
1:B:205:CYS:HB2	1:B:444:GLY:HA2	1.75	0.69
1:A:301:SER:HA	1:A:448:THR:HA	1.75	0.69
1:A:628:GLN:HA	1:A:631:MET:HG2	1.75	0.69
3:D:42:SER:OG	3:D:43:GLN:OE1	2.12	0.68
1:B:163:ARG:NH2	1:A:161:GLY:O	2.27	0.68
3:F:42:SER:OG	3:F:43:GLN:OE1	2.12	0.68
1:A:226:LEU:HD12	1:A:227:ALA:H	1.58	0.68
3:D:29:VAL:HB	3:D:99:VAL:HG21	1.76	0.68
1:B:240:MET:HE1	1:B:268:MET:HE3	1.76	0.68
1:B:638:LEU:HA	1:B:641:MET:HG2	1.73	0.68
1:A:126:MET:HE2	1:A:232:VAL:HB	1.74	0.68
1:B:126:MET:HE2	1:B:232:VAL:HB	1.75	0.67
1:B:333:ASP:OD2	3:D:98:ARG:NH1	2.28	0.67
1:A:1332:ARG:HG2	1:A:1337:ILE:HG13	1.77	0.67
2:E:173:PHE:CD2	2:E:186:SER:HB2	2.29	0.67
1:A:558:ALA:HA	1:A:827:THR:HB	1.77	0.67
3:D:40:ARG:NH2	3:D:91:ASP:OD1	2.28	0.67
1:A:561:VAL:HG11	1:A:837:LEU:HD13	1.76	0.67
3:F:29:VAL:HB	3:F:99:VAL:HG21	1.76	0.67
3:F:40:ARG:NH2	3:F:91:ASP:OD1	2.28	0.66
2:C:173:PHE:CD2	2:C:186:SER:HB2	2.29	0.66
2:E:126:PRO:HB3	2:E:152:TYR:HB3	1.78	0.66
1:B:60:GLU:HG3	1:B:62:ARG:HG3	1.78	0.66
3:D:113:LEU:HD23	3:D:114:GLN:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HD11	1:A:268:MET:HG3	1.78	0.65
1:B:558:ALA:HA	1:B:827:THR:HB	1.77	0.65
1:B:208:SER:HB2	1:B:385:VAL:HB	1.77	0.65
1:B:491:ARG:HD3	1:B:902:PRO:HG3	1.79	0.65
1:A:1076:LEU:HD13	1:A:1281:GLY:HA3	1.78	0.65
1:A:29:GLU:HA	1:A:33:GLU:HB2	1.77	0.65
1:B:903:PHE:HB3	1:B:905:ARG:HH11	1.61	0.65
1:A:1205:ARG:HH12	1:A:1253:LEU:HD23	1.61	0.65
2:C:126:PRO:HB3	2:C:152:TYR:HB3	1.79	0.65
1:B:903:PHE:HB3	1:B:905:ARG:NH1	2.12	0.65
1:A:656:SER:HB3	1:A:659:GLU:HG3	1.79	0.65
1:A:390:LYS:HE3	1:A:401:PRO:HG2	1.79	0.64
3:D:130:ARG:HH12	3:D:133:ALA:HB2	1.62	0.64
3:F:130:ARG:HH12	3:F:133:ALA:HB2	1.62	0.64
1:A:1276:PHE:HD1	1:A:1315:GLY:HA2	1.62	0.64
1:B:344:THR:HG23	1:B:347:GLY:H	1.62	0.64
1:B:905:ARG:CZ	1:B:905:ARG:HA	2.26	0.64
1:B:595:GLU:HB2	1:B:671:LEU:HD21	1.80	0.64
1:B:681:ARG:HH11	1:B:685:ILE:HD11	1.61	0.64
1:A:1019:LEU:HD13	1:A:1244:ILE:HG22	1.78	0.64
1:A:111:MET:HE1	1:A:116:ALA:HB2	1.80	0.64
1:A:577:LEU:HB3	1:A:588:ARG:HH12	1.62	0.64
1:A:681:ARG:HH11	1:A:685:ILE:HD11	1.63	0.64
1:A:602:VAL:HG22	1:A:606:LEU:HG	1.80	0.63
1:A:1203:THR:OG1	1:A:1249:ARG:NH1	2.30	0.63
1:A:219:LEU:O	1:A:279:ARG:NH1	2.31	0.63
1:A:36:ALA:N	1:A:278:GLU:O	2.32	0.63
1:A:338:GLU:HB3	1:A:440:VAL:HA	1.81	0.63
1:A:980:VAL:O	1:A:993:ARG:NH1	2.30	0.63
1:A:1363:ASP:HB3	1:A:1365:ARG:HH12	1.64	0.63
1:A:127:LEU:HD23	1:A:188:ILE:HD13	1.81	0.63
1:A:148:PRO:HB2	1:A:224:SER:HA	1.81	0.63
2:E:50:VAL:O	2:E:65:ALA:N	2.31	0.63
2:E:101:THR:HG22	2:E:110:TRP:CD1	2.34	0.63
1:B:561:VAL:HG11	1:B:837:LEU:HD13	1.81	0.62
1:B:716:ALA:HB3	1:B:724:VAL:HB	1.81	0.62
1:A:312:ASN:OD1	1:A:314:ARG:NH1	2.32	0.62
3:D:168:VAL:HA	3:D:217:GLU:O	1.99	0.62
2:E:54:ARG:HD2	2:E:61:THR:H	1.64	0.62
1:B:718:ASN:H	1:B:723:VAL:HG12	1.63	0.62
2:C:54:ARG:HD2	2:C:61:THR:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:SER:HB2	1:A:1045:THR:HA	1.80	0.62
1:B:76:LEU:H	1:B:79:LEU:HD13	1.64	0.62
1:A:379:THR:HB	1:A:382:ALA:HB3	1.82	0.62
1:A:505:ARG:HH21	1:A:894:ARG:HH22	1.47	0.62
2:C:101:THR:HG22	2:C:110:TRP:CD1	2.34	0.62
3:D:185:VAL:HG23	3:D:197:LEU:HD12	1.81	0.62
1:B:13:LEU:HD11	1:A:12:TYR:HB3	1.81	0.62
1:B:42:CYS:HB3	1:B:389:ILE:HD13	1.82	0.62
1:B:296:GLY:HA3	1:B:327:SER:HB3	1.81	0.62
1:A:334:ILE:HD13	1:A:359:TYR:HE1	1.64	0.62
2:C:37:SER:HB2	2:C:101:THR:OG1	2.00	0.62
3:F:185:VAL:HG23	3:F:197:LEU:HD12	1.81	0.62
1:A:71:ASP:O	1:A:907:ARG:NH2	2.33	0.61
1:B:43:ARG:HG3	1:B:129:LEU:HD21	1.82	0.61
1:B:683:ARG:HE	1:B:687:THR:HB	1.64	0.61
1:B:519:PRO:HB3	1:B:552:SER:HB3	1.82	0.61
1:A:35:VAL:HG12	1:A:277:LEU:HD12	1.82	0.61
1:A:334:ILE:O	1:A:363:ARG:NH2	2.33	0.61
1:B:513:THR:O	1:B:895:ARG:NH1	2.33	0.61
1:A:683:ARG:HE	1:A:687:THR:HB	1.65	0.61
1:A:1087:ASP:HB3	1:A:1114:ALA:HA	1.82	0.61
2:C:8:GLN:H	2:C:112:GLN:HE22	1.49	0.61
2:C:77:ASP:HB3	2:C:80:LYS:HE3	1.83	0.61
1:A:1176:PRO:HD2	1:A:1199:ALA:HB2	1.83	0.61
1:A:485:LEU:HD21	1:A:522:ALA:HB2	1.81	0.61
1:B:123:GLN:NE2	1:B:180:THR:O	2.34	0.61
1:A:1354:ARG:HB2	1:A:1356:GLU:HG2	1.82	0.61
2:C:149:VAL:N	2:C:185:LEU:O	2.30	0.61
1:B:335:ASP:HB2	1:B:429:TRP:CZ2	2.36	0.61
1:A:208:SER:HB2	1:A:385:VAL:HB	1.83	0.61
2:E:77:ASP:HB3	2:E:80:LYS:HE3	1.83	0.61
1:A:756:HIS:HE1	1:A:788:VAL:HB	1.65	0.60
3:D:110:MET:SD	3:D:117:ARG:HD2	2.41	0.60
2:E:37:SER:HB2	2:E:101:THR:OG1	2.00	0.60
1:A:215:ALA:HB1	1:A:227:ALA:HB1	1.84	0.60
1:A:156:ILE:HG13	1:A:381:ALA:HB2	1.83	0.60
3:F:168:VAL:HA	3:F:217:GLU:O	2.00	0.60
1:B:9:VAL:HG11	1:A:9:VAL:HG13	1.84	0.60
1:A:283:ALA:HB1	1:A:288:HIS:HB2	1.83	0.60
1:A:1222:SER:HB3	1:A:1268:THR:H	1.67	0.60
1:A:694:MET:SD	1:A:724:VAL:HG13	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:VAL:HG11	1:A:199:ILE:HD11	1.84	0.60
1:B:829:LEU:HG	1:B:855:ILE:HD12	1.84	0.59
3:D:128:ILE:HB	3:D:188:GLN:HE22	1.67	0.59
1:A:180:THR:HG22	1:A:182:SER:H	1.67	0.59
2:E:8:GLN:H	2:E:112:GLN:HE22	1.49	0.59
2:E:49:TRP:CZ3	3:F:116:PRO:HB3	2.38	0.59
1:A:257:LYS:HB2	1:A:263:ALA:HA	1.83	0.59
1:B:9:VAL:HG13	1:A:13:LEU:HD21	1.84	0.59
1:B:694:MET:HB2	1:B:749:LEU:HD12	1.85	0.59
1:B:213:HIS:HA	1:B:297:THR:HG21	1.84	0.59
1:B:863:GLY:HA3	1:B:867:ASP:HB3	1.83	0.59
1:A:715:ALA:HB3	1:A:724:VAL:HG12	1.85	0.59
2:E:49:TRP:HZ3	3:F:116:PRO:HB3	1.67	0.59
1:B:561:VAL:HG22	1:B:653:ILE:HD11	1.84	0.59
1:A:337:VAL:HG23	1:A:367:LEU:HD11	1.85	0.59
1:A:1363:ASP:HB3	1:A:1365:ARG:NH1	2.17	0.59
1:B:334:ILE:O	1:B:363:ARG:NH1	2.27	0.59
1:A:329:LEU:C	3:F:98:ARG:HH12	2.11	0.59
1:A:340:HIS:N	1:A:351:GLU:OE2	2.32	0.59
1:A:1276:PHE:CD1	1:A:1315:GLY:HA2	2.38	0.59
2:E:149:VAL:N	2:E:185:LEU:O	2.30	0.59
1:B:866:ALA:C	1:B:868:PHE:H	2.10	0.59
1:B:205:CYS:HB3	1:B:378:HIS:HE2	1.67	0.58
1:A:1000:VAL:HG12	1:A:1002:GLY:H	1.68	0.58
1:A:1072:ARG:HG2	1:A:1112:GLN:HE21	1.67	0.58
1:B:553:ARG:HB2	1:B:853:SER:HA	1.84	0.58
1:B:101:ALA:HA	1:B:125:LEU:HD21	1.86	0.58
3:F:128:ILE:HB	3:F:188:GLN:HE22	1.67	0.58
1:B:76:LEU:HD23	1:B:79:LEU:HD22	1.86	0.58
1:B:709:GLY:H	1:B:713:GLU:HB2	1.69	0.58
1:A:437:ARG:HG2	1:A:455:GLU:HG3	1.86	0.58
1:A:74:TRP:NE1	1:A:236:PRO:O	2.25	0.58
1:A:466:VAL:HG23	1:A:505:ARG:HH22	1.67	0.58
1:A:561:VAL:HG13	1:A:654:GLY:HA3	1.85	0.58
1:B:92:GLN:HE22	1:B:268:MET:HB3	1.69	0.58
1:B:134:LEU:HD21	1:B:228:MET:HE1	1.85	0.58
1:B:670:SER:H	1:B:673:ASP:HB2	1.68	0.57
2:E:129:PHE:O	2:E:148:LEU:N	2.36	0.57
1:B:216:CYS:HB3	1:B:220:ARG:HE	1.68	0.57
1:B:642:TRP:HE3	1:B:829:LEU:HD21	1.69	0.57
1:B:714:ILE:HG22	1:B:725:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:THR:N	1:A:1057:GLU:OE2	2.33	0.57
1:B:332:ALA:O	1:B:434:ARG:NH2	2.38	0.57
2:E:8:GLN:HE21	2:E:38:TRP:HZ3	1.51	0.57
1:A:226:LEU:HD11	1:A:276:LEU:HG	1.86	0.57
2:C:129:PHE:O	2:C:148:LEU:N	2.36	0.57
1:A:597:HIS:HB2	1:A:675:ALA:HB1	1.87	0.57
2:C:161:TRP:NE1	2:C:187:SER:OG	2.38	0.57
3:D:29:VAL:N	3:D:127:ASP:O	2.34	0.57
3:F:29:VAL:N	3:F:127:ASP:O	2.34	0.57
1:A:492:LEU:HD23	1:A:536:LEU:HD21	1.86	0.57
2:C:8:GLN:HE21	2:C:38:TRP:HZ3	1.51	0.57
1:B:379:THR:HB	1:B:382:ALA:HB3	1.85	0.56
1:A:1066:ALA:HB1	1:A:1290:PRO:HB3	1.85	0.56
1:B:577:LEU:HD22	1:B:607:ARG:HG2	1.86	0.56
1:A:930:TYR:OH	1:A:1127:ARG:NH1	2.38	0.56
2:C:41:GLN:NE2	2:C:45:LYS:O	2.33	0.56
3:D:29:VAL:O	3:D:128:ILE:HA	2.05	0.56
1:B:149:THR:HB	1:B:194:LEU:HD22	1.88	0.56
1:B:278:GLU:OE2	1:B:283:ALA:HB2	2.05	0.56
1:B:594:LEU:HD22	1:B:675:ALA:HA	1.88	0.56
1:B:503:ASP:OD2	1:B:505:ARG:HG2	2.04	0.56
1:A:930:TYR:O	1:A:1360:ILE:N	2.38	0.56
2:E:161:TRP:NE1	2:E:187:SER:OG	2.38	0.56
3:F:59:GLN:HB3	3:F:106:VAL:HB	1.88	0.56
1:B:163:ARG:N	1:A:163:ARG:HH22	2.04	0.56
1:A:338:GLU:HB2	1:A:391:MET:HE2	1.88	0.56
1:A:429:TRP:HH2	1:A:438:ALA:HB2	1.71	0.56
1:A:959:ASP:HB3	1:A:961:THR:HG22	1.88	0.56
1:A:1143:VAL:HG11	1:A:1160:LEU:HD13	1.87	0.56
3:F:43:GLN:OE1	3:F:43:GLN:N	2.36	0.56
1:B:13:LEU:HD22	1:A:13:LEU:HD22	1.88	0.56
1:A:302:ASP:O	1:A:312:ASN:ND2	2.39	0.56
1:A:474:PRO:HG3	1:A:869:GLY:HA2	1.88	0.56
1:A:33:GLU:O	1:A:220:ARG:NE	2.39	0.56
1:A:133:VAL:HG11	1:A:228:MET:HE1	1.87	0.56
1:A:493:ALA:HB2	1:A:536:LEU:HB3	1.87	0.56
1:A:594:LEU:HD22	1:A:675:ALA:HA	1.87	0.56
1:A:30:LEU:O	1:A:220:ARG:HB3	2.06	0.55
2:E:31:PHE:HE2	2:E:76:ARG:HB2	1.71	0.55
3:F:29:VAL:O	3:F:128:ILE:HA	2.05	0.55
1:A:244:PHE:HB3	1:A:250:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:THR:HG23	2:C:117:THR:HG23	1.88	0.55
3:D:27:LEU:O	3:D:126:VAL:HG13	2.06	0.55
1:A:1260:GLU:O	1:A:1263:ARG:NE	2.39	0.55
1:A:1383:ASP:HA	1:A:1389:ARG:HH22	1.71	0.55
1:B:69:PRO:HD3	1:B:97:PHE:CD2	2.42	0.55
3:D:43:GLN:OE1	3:D:43:GLN:N	2.36	0.55
1:B:41:ALA:HB3	1:B:274:MET:HB3	1.88	0.55
1:B:429:TRP:O	1:B:436:ARG:NH1	2.37	0.55
1:A:561:VAL:HG13	1:A:655:HIS:H	1.71	0.55
3:F:27:LEU:O	3:F:126:VAL:HG13	2.06	0.55
3:F:135:PRO:HB2	3:F:158:LEU:HD11	1.88	0.55
1:B:300:ASN:O	1:B:449:ASN:N	2.38	0.55
1:A:69:PRO:HG2	1:A:72:ARG:HH21	1.72	0.55
1:A:709:GLY:H	1:A:713:GLU:HB2	1.71	0.55
1:B:150:GLY:O	1:B:228:MET:N	2.39	0.55
1:B:905:ARG:HA	1:B:905:ARG:NE	2.22	0.55
1:B:597:HIS:HB2	1:B:675:ALA:HB1	1.88	0.55
1:B:700:PRO:HA	1:B:720:PRO:HA	1.89	0.55
2:C:31:PHE:HE2	2:C:76:ARG:HB2	1.71	0.55
3:D:135:PRO:HB2	3:D:158:LEU:HD11	1.88	0.55
1:B:114:ARG:NH2	1:B:172:GLU:H	2.04	0.54
1:A:638:LEU:HD22	1:A:641:MET:HE2	1.89	0.54
2:E:162:ASN:N	2:E:202:ILE:O	2.32	0.54
1:A:279:ARG:NE	1:A:282:ASP:OD2	2.40	0.54
1:A:992:GLU:HA	1:A:995:ARG:HE	1.73	0.54
2:C:162:ASN:N	2:C:202:ILE:O	2.32	0.54
3:D:54:LEU:HD13	3:D:92:PHE:HD2	1.72	0.54
1:A:368:HIS:HB3	1:A:423:LEU:HD21	1.90	0.54
1:A:570:ALA:HA	1:A:630:VAL:HG11	1.89	0.54
3:D:54:LEU:HD13	3:D:92:PHE:CD2	2.42	0.54
1:B:676:ARG:HD3	1:B:772:GLY:H	1.72	0.54
1:B:767:LEU:HD23	1:B:803:TRP:HB2	1.90	0.54
1:A:357:GLU:N	1:A:357:GLU:OE1	2.40	0.54
2:E:95:THR:HG23	2:E:117:THR:HG23	1.88	0.54
3:F:54:LEU:HD13	3:F:92:PHE:CD2	2.42	0.54
1:B:175:LEU:HB2	1:A:243:ASP:OD2	2.07	0.54
1:A:700:PRO:HA	1:A:720:PRO:HA	1.90	0.54
2:C:6:LEU:H	2:C:109:TYR:HE2	1.56	0.54
1:B:724:VAL:HG22	1:B:745:ARG:NH1	2.23	0.54
1:A:1034:MET:HE1	1:A:1043:LEU:HB2	1.90	0.54
2:E:16:PRO:HB3	2:E:91:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:SD	1:B:3:SER:N	2.81	0.54
1:A:1147:GLY:N	1:A:1171:VAL:O	2.40	0.54
1:B:40:MET:SD	1:B:389:ILE:HG12	2.49	0.54
1:A:1142:THR:HA	1:A:1167:HIS:HB2	1.88	0.54
1:A:121:PRO:HA	1:A:124:ARG:HG2	1.91	0.53
1:A:235:MET:HG2	1:A:240:MET:CG	2.37	0.53
1:A:660:ILE:HG21	1:A:681:ARG:HE	1.74	0.53
1:A:767:LEU:HD23	1:A:803:TRP:HB2	1.90	0.53
1:A:1239:LEU:HD23	1:A:1243:ARG:HD3	1.90	0.53
1:B:694:MET:HE1	1:B:715:ALA:HB3	1.90	0.53
1:A:43:ARG:O	1:A:272:ALA:N	2.40	0.53
2:C:16:PRO:HB3	2:C:91:LYS:HA	1.90	0.53
3:D:124:THR:HG22	3:D:126:VAL:HG23	1.89	0.53
3:F:54:LEU:HD13	3:F:92:PHE:HD2	1.72	0.53
1:A:618:ALA:HB3	1:A:623:ARG:HD3	1.89	0.53
3:D:31:PRO:HD3	3:D:128:ILE:HD12	1.91	0.53
3:F:58:LEU:HB3	3:F:68:LEU:HD11	1.91	0.53
3:F:137:VAL:HG12	3:F:229:LYS:HD2	1.90	0.53
1:B:291:LEU:HA	1:B:396:ARG:HH22	1.73	0.53
1:A:776:HIS:ND1	2:C:201:TYR:HE1	2.07	0.53
3:F:59:GLN:HB2	3:F:108:TYR:HE2	1.73	0.53
1:B:44:LEU:HD13	1:B:376:LEU:HD11	1.91	0.53
2:C:56:LYS:NZ	2:C:76:ARG:HE	2.07	0.53
2:E:56:LYS:NZ	2:E:76:ARG:HE	2.07	0.53
3:F:31:PRO:HD3	3:F:128:ILE:HD12	1.91	0.53
1:B:1:MET:SD	1:B:2:ALA:N	2.82	0.53
1:B:219:LEU:HD22	1:B:278:GLU:HA	1.91	0.53
1:A:565:GLN:HA	1:A:751:VAL:HG21	1.91	0.53
3:D:183:GLU:OE1	3:D:183:GLU:O	2.26	0.53
1:B:97:PHE:HA	1:B:270:GLU:HG2	1.91	0.53
1:A:372:VAL:HG22	1:A:376:LEU:HD13	1.89	0.53
1:A:429:TRP:O	1:A:436:ARG:NH1	2.40	0.53
1:A:43:ARG:NH1	1:A:49:SER:OG	2.42	0.52
1:A:610:ALA:HB3	1:A:862:ASP:HB2	1.91	0.52
3:D:137:VAL:HG12	3:D:229:LYS:HD2	1.90	0.52
1:B:36:ALA:HB1	1:B:290:VAL:HG13	1.91	0.52
1:B:567:TRP:HE3	1:B:857:SER:HB3	1.73	0.52
1:A:714:ILE:HG22	1:A:725:VAL:HG12	1.90	0.52
1:A:945:LEU:N	1:A:972:ALA:O	2.41	0.52
1:B:91:HIS:N	1:B:245:SER:OG	2.43	0.52
1:A:829:LEU:HG	1:A:855:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1168:LEU:HD13	1:A:1195:THR:HG22	1.92	0.52
3:F:183:GLU:OE1	3:F:183:GLU:O	2.26	0.52
1:B:120:ASP:HB3	1:B:123:GLN:HG3	1.91	0.52
1:A:26:ARG:HA	1:A:29:GLU:HG2	1.91	0.52
1:B:14:ARG:HB3	2:E:34:TYR:HE1	1.75	0.52
1:B:34:PRO:HG2	1:B:280:LEU:HD22	1.92	0.52
1:A:37:VAL:N	1:A:292:ALA:O	2.34	0.52
1:B:11:GLU:HG3	2:E:106:LEU:HD12	1.91	0.52
1:B:641:MET:HG3	1:B:642:TRP:CD1	2.44	0.52
1:A:14:ARG:HD2	2:C:34:TYR:CE1	2.44	0.52
1:B:331:PRO:O	1:B:363:ARG:NH1	2.43	0.52
1:A:1205:ARG:O	1:A:1209:ARG:HD3	2.10	0.52
2:C:55:SER:O	2:C:59:GLY:N	2.41	0.52
2:E:107:PHE:HB3	2:E:110:TRP:HE1	1.75	0.52
2:E:188:VAL:HG11	3:F:157:LEU:HD11	1.90	0.52
1:B:2:ALA:O	1:B:5:ASP:N	2.43	0.52
1:B:693:GLY:HA3	1:B:732:LEU:HD11	1.90	0.52
1:A:10:ALA:HA	1:A:13:LEU:HD23	1.92	0.52
1:A:162:PRO:HB3	1:A:913:LYS:HZ1	1.75	0.52
2:E:133:PRO:HG2	2:E:220:PRO:HB3	1.92	0.52
3:F:25:LEU:HA	3:F:124:THR:HG23	1.91	0.52
1:A:1030:LEU:HG	1:A:1034:MET:HE2	1.93	0.51
3:D:144:ASP:HA	3:D:147:LEU:HD12	1.91	0.51
1:B:717:VAL:O	1:B:814:ALA:N	2.43	0.51
1:A:676:ARG:HD3	1:A:772:GLY:H	1.75	0.51
2:C:133:PRO:HG2	2:C:220:PRO:HB3	1.92	0.51
1:B:133:VAL:HG22	1:B:276:LEU:HG	1.91	0.51
1:A:724:VAL:HG22	1:A:745:ARG:HH12	1.74	0.51
1:A:1188:LEU:HB3	1:A:1195:THR:HG21	1.92	0.51
3:D:54:LEU:HA	3:D:111:GLN:HA	1.93	0.51
3:F:163:PRO:HD2	3:F:221:GLN:HE21	1.74	0.51
1:B:49:SER:OG	1:B:100:GLU:OE2	2.27	0.51
1:A:154:GLY:N	1:A:230:GLY:O	2.41	0.51
2:C:107:PHE:HB3	2:C:110:TRP:HE1	1.75	0.51
2:E:6:LEU:H	2:E:109:TYR:HE2	1.56	0.51
3:F:116:PRO:HB2	3:F:118:LEU:HG	1.93	0.51
1:B:12:TYR:CZ	2:E:106:LEU:HD21	2.46	0.51
1:A:141:PRO:HG2	1:A:516:ALA:HB2	1.92	0.51
1:A:717:VAL:O	1:A:814:ALA:N	2.44	0.51
1:A:810:THR:HG23	1:A:812:ARG:HG2	1.92	0.51
2:C:110:TRP:CZ3	3:D:65:PRO:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:VAL:HG13	1:A:13:LEU:CD2	2.40	0.51
1:B:602:VAL:HG22	1:B:606:LEU:HG	1.93	0.51
1:A:1087:ASP:O	1:A:1115:LEU:N	2.35	0.51
1:B:635:MET:CE	1:B:661:ALA:HB1	2.41	0.51
1:B:776:HIS:ND1	2:E:201:TYR:HE1	2.09	0.51
1:A:945:LEU:HD21	1:A:1105:SER:HB3	1.91	0.51
1:A:1315:GLY:H	1:A:1339:MET:HE1	1.76	0.51
3:F:144:ASP:HA	3:F:147:LEU:HD12	1.91	0.51
1:A:64:ALA:HB3	1:A:376:LEU:HA	1.92	0.51
1:A:1334:HIS:O	1:A:1334:HIS:ND1	2.44	0.51
1:A:680:LEU:O	1:A:684:VAL:HG23	2.10	0.51
1:A:1068:TRP:HZ2	1:A:1087:ASP:HB2	1.75	0.51
1:A:1317:TRP:HB3	1:A:1320:SER:HB3	1.93	0.51
1:B:577:LEU:HB2	1:B:607:ARG:HD3	1.93	0.51
1:A:241:LEU:HA	1:A:268:MET:HE1	1.91	0.51
1:A:324:LEU:HD11	1:A:330:GLY:CA	2.41	0.51
2:E:39:VAL:HG23	2:E:101:THR:HG21	1.93	0.51
1:B:155:LEU:HB2	1:B:181:THR:HG23	1.93	0.50
3:F:135:PRO:HG3	3:F:220:HIS:HB3	1.93	0.50
1:B:330:GLY:N	3:D:98:ARG:HH12	2.09	0.50
1:B:755:SER:OG	1:B:806:ASN:O	2.29	0.50
1:A:65:VAL:HG12	1:A:96:GLY:N	2.26	0.50
1:B:68:LEU:HD23	1:B:97:PHE:HE2	1.74	0.50
1:B:316:GLN:O	1:B:320:ILE:HG12	2.10	0.50
1:B:351:GLU:HG3	1:B:443:PHE:HE2	1.76	0.50
1:B:777:PRO:HG3	2:E:191:VAL:HG21	1.91	0.50
1:A:598:LEU:HD21	1:A:679:ALA:HB2	1.92	0.50
1:A:1088:VAL:HG12	1:A:1115:LEU:HD12	1.93	0.50
1:B:4:THR:OG1	1:A:5:ASP:HB2	2.11	0.50
1:B:680:LEU:O	1:B:684:VAL:HG23	2.11	0.50
1:A:657:GLN:HG2	1:A:755:SER:HB2	1.92	0.50
1:A:1336:VAL:HG12	1:A:1364:VAL:HA	1.94	0.50
3:F:51:TYR:HB3	3:F:71:LEU:HD12	1.93	0.50
1:B:92:GLN:HA	1:B:252:PRO:HA	1.94	0.50
1:B:212:VAL:HG12	1:B:229:ALA:HB1	1.94	0.50
1:B:628:GLN:HA	1:B:631:MET:HG3	1.94	0.50
1:B:810:THR:HG23	1:B:812:ARG:HG2	1.94	0.50
3:D:135:PRO:HG3	3:D:220:HIS:HB3	1.94	0.50
1:A:41:ALA:O	1:A:274:MET:N	2.44	0.50
3:D:87:GLY:HA3	3:D:92:PHE:HD1	1.77	0.50
1:B:388:VAL:HG23	1:B:454:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:PRO:O	1:B:520:HIS:ND1	2.45	0.49
1:B:548:ALA:HB3	1:B:874:ARG:HH21	1.76	0.49
1:B:598:LEU:HD21	1:B:679:ALA:HB2	1.93	0.49
1:B:862:ASP:HB2	1:B:868:PHE:HA	1.93	0.49
1:B:55:TRP:CZ3	1:B:401:PRO:HG3	2.47	0.49
1:A:92:GLN:HB3	1:A:241:LEU:HD23	1.95	0.49
1:A:1203:THR:O	1:A:1257:ASN:ND2	2.45	0.49
1:A:1231:LEU:HD13	1:A:1288:TYR:HB2	1.93	0.49
2:C:13:LEU:HD13	2:C:117:THR:HB	1.95	0.49
3:D:130:ARG:HH21	3:D:194:THR:HG22	1.77	0.49
3:D:58:LEU:HD13	3:D:107:TYR:CE1	2.47	0.49
3:D:63:GLN:N	3:D:63:GLN:OE1	2.46	0.49
1:B:141:PRO:HD2	1:B:516:ALA:HB2	1.94	0.49
3:D:51:TYR:HB3	3:D:71:LEU:HD12	1.93	0.49
2:E:36:MET:H	2:E:76:ARG:HH12	1.59	0.49
3:F:87:GLY:HA3	3:F:92:PHE:HD1	1.77	0.49
1:A:1068:TRP:CZ2	1:A:1087:ASP:HB2	2.47	0.49
2:E:107:PHE:HB3	2:E:110:TRP:NE1	2.28	0.49
1:B:176:MET:HG3	1:A:244:PHE:CE1	2.47	0.49
1:B:243:ASP:CB	1:A:176:MET:HE1	2.43	0.49
1:B:700:PRO:HB2	1:B:703:GLU:HB2	1.95	0.49
1:A:135:GLU:OE1	1:A:901:TYR:N	2.45	0.49
1:A:340:HIS:HD2	1:A:442:SER:HA	1.77	0.49
2:C:36:MET:H	2:C:76:ARG:HH12	1.59	0.49
2:C:171:HIS:CE1	3:D:186:THR:HG21	2.48	0.49
3:F:130:ARG:HH21	3:F:194:THR:HG22	1.77	0.49
1:B:291:LEU:O	1:B:396:ARG:NH2	2.45	0.49
1:B:338:GLU:OE2	1:B:372:VAL:N	2.44	0.49
1:B:577:LEU:HD11	1:B:606:LEU:HB3	1.95	0.49
2:C:56:LYS:HZ3	2:C:76:ARG:HE	1.61	0.49
2:C:107:PHE:HB3	2:C:110:TRP:NE1	2.28	0.49
1:B:176:MET:HE2	1:B:176:MET:HA	1.94	0.49
1:B:866:ALA:C	1:B:868:PHE:N	2.70	0.49
1:B:39:ALA:HB3	1:B:276:LEU:HD12	1.93	0.49
1:A:15:ARG:HH21	3:D:76:ALA:HB1	1.78	0.49
1:A:928:LEU:HB3	1:A:1361:VAL:HG13	1.94	0.49
1:A:1272:LEU:HD13	1:A:1299:ALA:HB2	1.94	0.49
2:E:34:TYR:O	2:E:76:ARG:NH2	2.44	0.49
3:F:59:GLN:HB2	3:F:108:TYR:CE2	2.47	0.49
3:F:63:GLN:N	3:F:63:GLN:OE1	2.46	0.49
1:A:694:MET:HG3	1:A:836:ILE:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:TRP:CG	1:A:1345:CYS:HB2	2.48	0.49
3:F:152:ALA:HB3	3:F:203:LEU:HB3	1.95	0.49
1:B:410:SER:HB3	1:B:413:ILE:HD12	1.93	0.48
1:B:892:GLY:O	1:B:894:ARG:NH1	2.46	0.48
3:D:163:PRO:O	3:D:220:HIS:NE2	2.46	0.48
1:B:776:HIS:CG	2:E:201:TYR:HE1	2.31	0.48
1:A:700:PRO:HB2	1:A:703:GLU:HB2	1.95	0.48
1:A:1236:VAL:HA	1:A:1239:LEU:HB2	1.94	0.48
1:B:210:VAL:HG11	1:A:199:ILE:HD12	1.94	0.48
1:A:67:GLY:HA2	1:A:94:GLY:HA2	1.94	0.48
1:B:572:MET:HA	1:B:576:LEU:HD23	1.95	0.48
1:A:324:LEU:HD21	1:A:331:PRO:HD3	1.95	0.48
1:A:1171:VAL:HG21	1:A:1211:LEU:HD21	1.95	0.48
2:E:56:LYS:HZ3	2:E:76:ARG:HE	1.61	0.48
3:F:38:SER:OG	3:F:39:CYS:N	2.47	0.48
1:B:52:GLU:O	1:B:56:GLU:HG3	2.13	0.48
1:B:485:LEU:HD21	1:B:522:ALA:HB2	1.95	0.48
1:A:367:LEU:HB3	1:A:420:ILE:HG12	1.94	0.48
1:A:466:VAL:HG23	1:A:505:ARG:NH2	2.29	0.48
1:A:641:MET:HE3	1:A:642:TRP:NE1	2.28	0.48
1:A:1043:LEU:HD23	1:A:1082:TRP:HZ3	1.77	0.48
2:C:36:MET:HE2	2:C:36:MET:HA	1.96	0.48
3:D:130:ARG:HH22	3:D:133:ALA:HB2	1.79	0.48
3:F:130:ARG:HH22	3:F:133:ALA:HB2	1.78	0.48
1:B:862:ASP:HB3	1:B:868:PHE:HD1	1.78	0.48
1:A:716:ALA:HB3	1:A:724:VAL:HB	1.96	0.48
1:A:1019:LEU:HG	1:A:1252:VAL:HG21	1.94	0.48
3:D:28:PRO:HB2	3:D:129:LYS:HG3	1.95	0.48
3:D:38:SER:OG	3:D:39:CYS:N	2.47	0.48
1:A:340:HIS:CD2	1:A:443:PHE:H	2.32	0.48
2:C:87:MET:HG3	2:C:90:LEU:HD21	1.96	0.48
2:E:13:LEU:HD13	2:E:117:THR:HB	1.95	0.48
2:E:206:ASN:HB2	2:E:213:LYS:NZ	2.29	0.48
1:B:131:TRP:CZ2	1:B:518:LEU:HD21	2.49	0.48
1:A:103:ALA:HB1	1:A:905:ARG:HB3	1.95	0.48
1:A:704:VAL:HG11	1:A:723:VAL:HG11	1.96	0.48
1:A:1274:SER:HB2	1:A:1292:ASN:HB3	1.96	0.48
3:F:70:TYR:CD2	3:F:71:LEU:HD23	2.48	0.48
1:B:202:ASP:OD2	1:A:181:THR:OG1	2.27	0.48
1:A:1212:LEU:HD13	1:A:1261:LEU:HG	1.95	0.48
3:D:70:TYR:CD2	3:D:71:LEU:HD23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:111:GLN:O	3:D:117:ARG:NH1	2.47	0.48
2:E:48:GLU:HA	3:F:119:THR:HA	1.96	0.48
3:F:166:ALA:HB2	3:F:220:HIS:HB2	1.95	0.48
2:C:54:ARG:HD3	2:C:58:TYR:HE2	1.79	0.48
1:B:149:THR:C	1:B:196:GLY:HA3	2.39	0.47
1:B:251:ALA:H	1:B:267:GLY:H	1.62	0.47
1:B:385:VAL:O	1:B:389:ILE:HG13	2.14	0.47
1:B:704:VAL:HG11	1:B:723:VAL:HG11	1.96	0.47
1:A:9:VAL:HA	1:A:12:TYR:HD2	1.79	0.47
1:A:561:VAL:HA	1:A:654:GLY:HA3	1.96	0.47
2:C:206:ASN:HB2	2:C:213:LYS:NZ	2.29	0.47
1:B:202:ASP:O	1:A:200:SER:HB3	2.15	0.47
1:B:338:GLU:HB2	1:B:391:MET:SD	2.54	0.47
1:A:1025:ALA:HB2	1:A:1241:GLY:HA3	1.95	0.47
2:C:174:PRO:HD2	3:D:184:SER:OG	2.14	0.47
3:D:152:ALA:HB3	3:D:203:LEU:HB3	1.95	0.47
2:E:87:MET:HB3	2:E:90:LEU:HD21	1.96	0.47
1:B:618:ALA:HB3	1:B:623:ARG:HD3	1.96	0.47
1:B:705:ARG:HH21	1:B:814:ALA:HB3	1.79	0.47
1:A:12:TYR:CZ	2:C:106:LEU:HD21	2.50	0.47
1:A:162:PRO:HB3	1:A:913:LYS:NZ	2.28	0.47
1:A:717:VAL:HG12	1:A:812:ARG:HA	1.95	0.47
2:C:34:TYR:O	2:C:76:ARG:NH2	2.44	0.47
2:E:36:MET:HE2	2:E:36:MET:HA	1.96	0.47
2:E:87:MET:HG3	2:E:90:LEU:HD21	1.96	0.47
1:B:189:ALA:HA	1:B:194:LEU:HB2	1.95	0.47
1:B:635:MET:HE1	1:B:661:ALA:HB1	1.95	0.47
3:F:54:LEU:HD11	3:F:109:CYS:SG	2.55	0.47
1:B:817:VAL:HG21	1:B:840:ALA:HB1	1.96	0.47
1:A:30:LEU:O	1:A:30:LEU:HD23	2.15	0.47
1:A:660:ILE:HA	1:A:663:ALA:HB3	1.96	0.47
2:C:41:GLN:O	2:C:96:ALA:HB1	2.15	0.47
3:D:129:LYS:HB2	3:D:129:LYS:HE2	1.52	0.47
1:B:26:ARG:HA	1:B:29:GLU:HG2	1.96	0.47
1:B:862:ASP:HB3	1:B:868:PHE:CD1	2.50	0.47
1:A:226:LEU:HD12	1:A:227:ALA:N	2.28	0.47
1:A:476:VAL:HG13	1:A:876:PHE:CE2	2.50	0.47
1:A:705:ARG:HH21	1:A:814:ALA:HB3	1.80	0.47
2:C:87:MET:HB3	2:C:90:LEU:HD21	1.96	0.47
1:A:40:MET:SD	1:A:389:ILE:HA	2.54	0.47
1:B:126:MET:HG3	1:B:153:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:ARG:HD2	1:A:1250:ALA:N	2.31	0.47
1:A:631:MET:O	1:A:635:MET:HB2	2.15	0.46
1:A:1000:VAL:HB	1:A:1039:LEU:HD21	1.95	0.46
1:A:1147:GLY:HA2	1:A:1172:SER:HB3	1.97	0.46
1:B:308:LEU:HD21	1:A:183:VAL:HB	1.96	0.46
1:A:151:VAL:HA	1:A:228:MET:HB3	1.97	0.46
2:E:54:ARG:HD3	2:E:58:TYR:CE2	2.50	0.46
3:F:110:MET:SD	3:F:117:ARG:HB3	2.55	0.46
1:B:14:ARG:HB3	2:E:34:TYR:CE1	2.51	0.46
1:B:709:GLY:N	1:B:713:GLU:HB2	2.30	0.46
1:B:828:PHE:HB3	1:B:837:LEU:HD11	1.97	0.46
1:A:994:LEU:HA	1:A:997:VAL:HG12	1.97	0.46
1:A:1133:THR:HG22	1:A:1135:ASP:H	1.80	0.46
2:C:54:ARG:HD3	2:C:58:TYR:CE2	2.50	0.46
2:C:80:LYS:NZ	2:C:82:ILE:O	2.38	0.46
3:D:54:LEU:HD11	3:D:109:CYS:SG	2.55	0.46
2:E:31:PHE:CE2	2:E:76:ARG:HB2	2.50	0.46
2:E:54:ARG:HD3	2:E:58:TYR:HE2	1.79	0.46
1:B:108:PHE:HZ	1:B:131:TRP:CE2	2.34	0.46
1:B:188:ILE:HD12	1:B:188:ILE:H	1.79	0.46
1:A:189:ALA:O	1:A:194:LEU:N	2.47	0.46
1:A:526:PRO:HG3	1:A:532:ALA:HB2	1.97	0.46
1:A:656:SER:HB3	1:A:659:GLU:CG	2.45	0.46
1:A:929:ARG:HH22	1:A:1354:ARG:NH1	2.13	0.46
1:A:987:ARG:NH1	1:A:1239:LEU:O	2.48	0.46
2:C:36:MET:H	2:C:76:ARG:NH1	2.13	0.46
1:A:164:LEU:HG	1:A:176:MET:HE3	1.98	0.46
1:A:296:GLY:O	1:A:453:ILE:HG22	2.15	0.46
1:A:503:ASP:O	1:A:507:ILE:HD12	2.16	0.46
1:A:511:LEU:HD12	1:A:515:ARG:HD3	1.98	0.46
1:A:1259:HIS:O	1:A:1263:ARG:HD3	2.16	0.46
2:C:7:VAL:HG23	2:C:25:THR:HB	1.98	0.46
2:C:35:ALA:HA	2:C:76:ARG:HH12	1.80	0.46
2:C:49:TRP:CZ2	2:C:51:GLY:HA2	2.51	0.46
3:F:80:PRO:HB2	3:F:82:ARG:HG3	1.98	0.46
1:B:29:GLU:HA	1:B:33:GLU:HB2	1.98	0.46
1:A:1159:TRP:CZ2	1:A:1349:GLN:HB2	2.50	0.46
2:C:101:THR:HG22	2:C:110:TRP:HD1	1.80	0.46
3:D:100:GLU:H	3:D:103:ASP:HB2	1.81	0.46
2:E:36:MET:H	2:E:76:ARG:NH1	2.13	0.46
1:B:239:GLY:HA2	1:A:165:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:868:PHE:CE2	1:B:887:VAL:HG13	2.50	0.46
2:C:115:LEU:HD12	2:C:115:LEU:O	2.15	0.46
1:B:92:GLN:NE2	1:B:268:MET:HB3	2.31	0.46
1:B:596:PRO:HD3	1:B:671:LEU:HG	1.97	0.46
1:B:717:VAL:HG12	1:B:812:ARG:HA	1.96	0.46
3:F:60:LYS:HD3	3:F:60:LYS:HA	1.59	0.46
1:B:681:ARG:NH1	1:B:685:ILE:HD11	2.31	0.46
1:A:38:VAL:HB	1:A:276:LEU:HD23	1.97	0.46
1:A:1262:THR:HA	1:A:1265:LEU:HD13	1.97	0.46
1:A:98:LEU:HD13	1:A:100:GLU:HB2	1.97	0.46
3:D:71:LEU:HB2	3:D:74:ASN:HB2	1.98	0.46
1:B:512:ALA:HB1	1:B:884:TRP:HB3	1.98	0.45
1:B:596:PRO:HG3	1:B:672:ASP:OD1	2.16	0.45
1:B:656:SER:HB2	1:B:755:SER:HB3	1.97	0.45
1:A:244:PHE:O	1:A:250:LEU:HD23	2.16	0.45
1:A:1339:MET:HG3	1:A:1363:ASP:OD2	2.16	0.45
1:B:904:GLN:O	1:B:905:ARG:NH2	2.48	0.45
1:A:97:PHE:HA	1:A:270:GLU:HG2	1.98	0.45
1:A:208:SER:HB3	1:A:231:GLY:HA3	1.98	0.45
1:A:596:PRO:HG3	1:A:672:ASP:OD1	2.15	0.45
2:E:7:VAL:HG23	2:E:25:THR:HB	1.98	0.45
2:E:128:VAL:HG12	2:E:216:LYS:HZ2	1.80	0.45
3:F:60:LYS:HG3	3:F:63:GLN:CD	2.41	0.45
1:B:12:TYR:HB3	1:A:13:LEU:HD11	1.98	0.45
1:B:120:ASP:HB2	1:B:178:GLY:O	2.16	0.45
1:A:1310:THR:HG22	1:A:1312:VAL:HG13	1.98	0.45
2:E:55:SER:O	2:E:59:GLY:N	2.41	0.45
1:B:81:HIS:HB2	1:B:89:THR:HG21	1.97	0.45
2:E:35:ALA:HA	2:E:76:ARG:HH12	1.80	0.45
2:E:115:LEU:HD12	2:E:115:LEU:O	2.15	0.45
1:B:275:LEU:HD23	1:B:385:VAL:HG23	1.99	0.45
1:B:329:LEU:HD12	1:B:453:ILE:HG21	1.99	0.45
1:A:335:ASP:HB2	1:A:429:TRP:CZ2	2.51	0.45
1:A:1282:ALA:HB1	1:A:1285:LEU:HD12	1.98	0.45
3:D:60:LYS:HG3	3:D:63:GLN:CD	2.41	0.45
1:B:97:PHE:HD1	1:B:270:GLU:HG2	1.82	0.45
1:A:680:LEU:HD12	1:A:770:GLU:HB2	1.97	0.45
1:A:1205:ARG:NE	1:A:1257:ASN:OD1	2.49	0.45
1:A:1291:GLY:O	1:A:1295:LEU:HG	2.16	0.45
2:C:206:ASN:HB2	2:C:213:LYS:HZ2	1.79	0.45
3:D:106:VAL:HA	3:D:124:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLU:HA	1:A:14:ARG:HE	1.82	0.45
1:A:77:ASP:OD1	1:A:78:SER:N	2.50	0.45
1:A:257:LYS:HE3	1:A:257:LYS:HB3	1.72	0.45
1:A:334:ILE:HD13	1:A:359:TYR:CE1	2.48	0.45
1:A:378:HIS:CD2	1:A:380:GLN:H	2.34	0.45
1:A:785:PHE:HD1	1:A:785:PHE:HA	1.65	0.45
2:C:31:PHE:CE2	2:C:76:ARG:HB2	2.50	0.45
1:B:42:CYS:HB2	1:B:44:LEU:HG	1.99	0.45
1:B:55:TRP:HZ3	1:B:401:PRO:HG3	1.82	0.45
1:B:93:ARG:N	1:B:252:PRO:O	2.42	0.45
1:B:121:PRO:HA	1:B:124:ARG:HD2	1.99	0.45
1:B:475:TRP:CD1	1:B:508:ALA:HB2	2.51	0.45
1:A:127:LEU:HD21	1:A:187:ARG:HB3	1.99	0.45
1:A:711:ARG:HH21	1:A:759:HIS:HB2	1.81	0.45
1:A:929:ARG:HG3	1:A:1359:PRO:HB3	1.99	0.45
3:D:58:LEU:HD13	3:D:107:TYR:CD1	2.52	0.45
1:B:15:ARG:HH21	3:F:76:ALA:HB1	1.81	0.45
1:A:139:ILE:HD11	1:A:288:HIS:CG	2.51	0.45
1:A:50:THR:OG1	1:A:136:ARG:NH1	2.37	0.45
1:A:240:MET:HE2	1:A:244:PHE:CE2	2.52	0.45
1:A:553:ARG:NE	1:A:852:LEU:O	2.49	0.45
1:A:583:PHE:CE2	1:A:587:LEU:HD11	2.52	0.45
1:A:595:GLU:HB2	1:A:671:LEU:HD21	1.97	0.45
1:A:874:ARG:HA	1:A:874:ARG:NE	2.32	0.45
2:C:39:VAL:HG23	2:C:101:THR:HG21	1.99	0.45
1:A:1031:VAL:HG21	1:A:1074:ILE:HD13	1.98	0.44
3:D:169:GLN:O	3:D:216:CYS:HA	2.18	0.44
1:B:30:LEU:HD21	1:A:30:LEU:HD22	1.98	0.44
1:B:104:PHE:HD2	1:B:116:ALA:HB1	1.82	0.44
1:B:256:CYS:SG	1:B:378:HIS:N	2.90	0.44
1:B:342:THR:HG23	1:B:344:THR:HG22	1.99	0.44
1:B:668:ALA:H	1:B:780:GLY:HA2	1.82	0.44
1:A:331:PRO:O	1:A:363:ARG:NH1	2.51	0.44
1:A:1043:LEU:HD23	1:A:1082:TRP:CZ3	2.52	0.44
2:E:101:THR:HG22	2:E:110:TRP:HD1	1.80	0.44
1:B:45:PRO:HB3	1:B:96:GLY:C	2.42	0.44
1:B:680:LEU:HD12	1:B:770:GLU:HB2	1.99	0.44
1:A:637:SER:O	1:A:641:MET:HG2	2.17	0.44
1:A:817:VAL:HG21	1:A:840:ALA:HB1	1.99	0.44
1:A:1076:LEU:HA	1:A:1376:GLN:NE2	2.32	0.44
1:A:1125:TRP:N	1:A:1381:LEU:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:71:LEU:HB2	3:F:74:ASN:HB2	1.98	0.44
3:F:112:SER:HA	3:F:117:ARG:CZ	2.47	0.44
3:F:169:GLN:O	3:F:216:CYS:HA	2.18	0.44
1:B:335:ASP:HB2	1:B:429:TRP:HZ2	1.80	0.44
1:A:828:PHE:HB3	1:A:837:LEU:HD11	1.98	0.44
1:B:648:GLU:OE2	1:A:314:ARG:NH2	2.51	0.44
1:A:560:PHE:CE1	1:A:829:LEU:HD13	2.52	0.44
1:A:1125:TRP:HD1	1:A:1385:ILE:HD11	1.82	0.44
1:A:1383:ASP:HA	1:A:1389:ARG:HH12	1.83	0.44
2:C:161:TRP:HD1	2:C:170:VAL:HG13	1.82	0.44
1:B:30:LEU:CD2	1:A:30:LEU:HD22	2.48	0.44
1:B:79:LEU:O	1:B:90:ALA:N	2.30	0.44
1:B:189:ALA:O	1:B:194:LEU:N	2.51	0.44
1:B:493:ALA:HB2	1:B:536:LEU:HB3	1.99	0.44
2:C:41:GLN:NE2	2:C:42:ALA:O	2.51	0.44
2:E:155:GLU:HG3	2:E:175:ALA:CB	2.43	0.44
2:E:161:TRP:HD1	2:E:170:VAL:HG13	1.82	0.44
1:B:43:ARG:CG	1:B:129:LEU:HD21	2.48	0.44
1:B:215:ALA:HB1	1:B:227:ALA:HB1	1.99	0.44
1:A:502:GLN:HB3	1:A:507:ILE:HD11	2.00	0.44
1:A:665:VAL:O	1:A:781:PHE:HB3	2.17	0.44
1:A:954:TYR:HD2	1:A:956:GLY:H	1.66	0.44
1:A:1259:HIS:CE1	1:A:1302:ARG:HG2	2.52	0.44
2:E:124:LYS:HE2	2:E:124:LYS:HB2	1.66	0.44
1:B:92:GLN:NE2	1:B:241:LEU:HD22	2.32	0.44
1:B:363:ARG:HA	1:B:363:ARG:HD2	1.80	0.44
1:A:1103:VAL:HG13	1:A:1113:LEU:HG	1.98	0.44
1:A:1212:LEU:HD11	1:A:1265:LEU:HD21	2.00	0.44
1:A:1227:ALA:HB2	1:A:1273:PHE:HD2	1.82	0.44
1:B:513:THR:OG1	1:B:895:ARG:NH2	2.51	0.44
1:B:602:VAL:O	1:B:606:LEU:HG	2.18	0.44
1:A:103:ALA:HB1	1:A:905:ARG:HD3	2.00	0.44
1:A:216:CYS:O	1:A:220:ARG:HG2	2.18	0.44
1:A:693:GLY:HA3	1:A:732:LEU:HD11	2.00	0.44
1:A:953:LYS:HA	1:A:1007:LEU:HB3	2.00	0.44
1:A:1068:TRP:CG	1:A:1085:LEU:HD22	2.53	0.44
1:A:1144:LEU:HD22	1:A:1224:VAL:HG13	2.00	0.44
3:D:70:TYR:HD2	3:D:71:LEU:HD23	1.83	0.44
2:E:189:VAL:HG21	2:E:201:TYR:CD2	2.53	0.44
1:B:10:ALA:O	1:B:13:LEU:HB2	2.18	0.43
1:B:339:ALA:HB1	1:B:351:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:HZ	1:A:131:TRP:CE2	2.36	0.43
1:A:264:ASN:O	1:A:345:ARG:NH1	2.51	0.43
1:A:302:ASP:OD1	1:A:449:ASN:ND2	2.40	0.43
1:A:318:ARG:HB3	1:A:322:GLN:HE22	1.83	0.43
1:B:390:LYS:HE2	1:B:401:PRO:HB2	1.99	0.43
1:A:756:HIS:HB3	1:A:810:THR:HA	2.00	0.43
1:A:1262:THR:HG22	1:A:1265:LEU:HD22	2.00	0.43
3:F:130:ARG:NH2	3:F:194:THR:HG22	2.34	0.43
1:A:14:ARG:HA	3:F:51:TYR:OH	2.18	0.43
1:A:55:TRP:HB2	1:A:393:LEU:HD13	1.99	0.43
2:C:37:SER:OG	2:C:103:GLY:O	2.34	0.43
3:D:45:LEU:HD12	3:D:92:PHE:HE2	1.83	0.43
2:E:22:LEU:HD23	2:E:22:LEU:HA	1.91	0.43
3:F:88:SER:N	3:F:91:ASP:O	2.48	0.43
1:A:220:ARG:NH2	1:A:295:ARG:O	2.51	0.43
1:A:515:ARG:NH2	1:A:899:PRO:O	2.50	0.43
1:A:596:PRO:HD3	1:A:671:LEU:HG	2.01	0.43
1:A:950:LEU:HG	1:A:977:ARG:HB3	2.00	0.43
1:A:1034:MET:HE1	1:A:1043:LEU:HD22	2.00	0.43
1:A:1327:VAL:HA	1:A:1330:ARG:HD2	2.00	0.43
1:B:509:TYR:O	1:B:895:ARG:NH2	2.52	0.43
1:B:711:ARG:HH21	1:B:759:HIS:HB2	1.83	0.43
1:A:531:ALA:O	1:A:535:VAL:HG23	2.18	0.43
3:D:59:GLN:HB3	3:D:106:VAL:HB	2.00	0.43
1:B:12:TYR:HE1	3:F:70:TYR:HB2	1.83	0.43
1:B:30:LEU:HD11	1:A:31:GLU:HG3	2.00	0.43
1:A:51:PRO:HD2	1:A:136:ARG:CZ	2.48	0.43
1:A:300:ASN:O	1:A:449:ASN:N	2.51	0.43
1:A:333:ASP:OD2	3:F:98:ARG:NH1	2.52	0.43
2:E:21:ARG:HE	2:E:22:LEU:N	2.17	0.43
3:F:45:LEU:HD12	3:F:92:PHE:HE2	1.83	0.43
3:F:70:TYR:HD2	3:F:71:LEU:HD23	1.83	0.43
1:B:208:SER:O	1:B:212:VAL:HG13	2.19	0.43
1:B:209:LEU:O	1:B:212:VAL:HG22	2.18	0.43
1:A:155:LEU:HD11	1:A:184:ALA:HB3	2.00	0.43
1:A:1013:GLU:HB2	1:A:1061:ASN:HD21	1.84	0.43
2:C:9:SER:OG	2:C:23:SER:OG	2.35	0.43
2:C:21:ARG:HE	2:C:22:LEU:N	2.17	0.43
2:C:87:MET:N	2:C:87:MET:SD	2.91	0.43
2:C:189:VAL:HG21	2:C:201:TYR:CD2	2.53	0.43
1:B:662:ALA:HA	1:B:665:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:GLY:HA3	1:A:874:ARG:HG3	2.01	0.43
1:B:235:MET:N	1:B:270:GLU:OE1	2.52	0.43
1:B:774:ASP:HB3	1:B:776:HIS:CD2	2.54	0.43
1:A:479:ALA:O	1:A:520:HIS:N	2.47	0.43
1:A:868:PHE:CE2	1:A:872:LEU:HD11	2.53	0.43
1:B:266:PHE:HB3	1:B:344:THR:HB	2.01	0.43
1:B:621:THR:HB	1:B:751:VAL:HA	2.01	0.43
1:B:802:TYR:O	1:B:805:ARG:HG2	2.19	0.43
1:B:828:PHE:CD2	1:B:852:LEU:HB3	2.54	0.43
1:A:103:ALA:HA	1:A:906:GLU:O	2.19	0.43
1:A:115:GLU:HG3	1:A:174:TYR:CG	2.54	0.43
1:A:561:VAL:HG13	1:A:654:GLY:CA	2.48	0.43
1:A:914:PRO:HA	1:A:918:ARG:HH21	1.84	0.43
2:E:110:TRP:CZ3	3:F:65:PRO:HB2	2.54	0.43
1:B:3:SER:HB3	1:B:6:SER:OG	2.18	0.42
1:B:43:ARG:HD3	1:B:49:SER:HA	2.01	0.42
1:A:124:ARG:NH1	1:A:908:VAL:O	2.52	0.42
1:B:36:ALA:HA	1:B:293:VAL:HA	2.01	0.42
1:B:162:PRO:HA	1:A:163:ARG:HH22	1.83	0.42
1:B:216:CYS:SG	1:B:277:LEU:HD21	2.59	0.42
1:B:596:PRO:HG2	1:B:597:HIS:ND1	2.34	0.42
1:B:708:ILE:HA	1:B:713:GLU:HG3	2.01	0.42
1:B:908:VAL:HG23	1:B:908:VAL:O	2.19	0.42
1:A:42:CYS:HB3	1:A:389:ILE:HD13	2.00	0.42
1:A:704:VAL:HG21	1:A:723:VAL:HG21	2.01	0.42
1:A:709:GLY:N	1:A:713:GLU:HB2	2.34	0.42
2:C:110:TRP:HH2	3:D:57:TYR:CG	2.36	0.42
2:C:130:PRO:HD3	2:C:216:LYS:HZ1	1.84	0.42
1:B:122:GLN:HG3	1:B:234:VAL:HB	2.02	0.42
1:B:158:GLN:HB3	1:B:159:GLU:H	1.58	0.42
1:A:226:LEU:HD21	1:A:276:LEU:HD11	2.01	0.42
3:D:58:LEU:HB3	3:D:68:LEU:HD11	2.01	0.42
2:E:39:VAL:HG13	2:E:49:TRP:HA	1.99	0.42
1:B:402:ARG:HE	1:B:426:PRO:HG3	1.85	0.42
1:B:704:VAL:HG11	1:B:723:VAL:HG21	2.00	0.42
1:A:250:LEU:HG	1:A:268:MET:HE2	2.02	0.42
1:A:828:PHE:CD2	1:A:852:LEU:HB3	2.54	0.42
3:D:23:SER:HA	3:D:39:CYS:HA	2.02	0.42
3:D:127:ASP:OD2	3:D:162:TYR:HE1	2.02	0.42
2:E:131:LEU:HD21	3:F:140:PHE:CD2	2.54	0.42
3:F:23:SER:HA	3:F:39:CYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TYR:HA	1:A:177:THR:OG1	2.19	0.42
1:A:316:GLN:O	1:A:319:VAL:HG12	2.20	0.42
1:A:1169:LEU:HD23	1:A:1196:THR:HB	2.01	0.42
1:A:1315:GLY:H	1:A:1339:MET:CE	2.32	0.42
1:A:1315:GLY:N	1:A:1339:MET:HE1	2.34	0.42
3:D:88:SER:N	3:D:91:ASP:O	2.48	0.42
2:E:64:TYR:HB3	2:E:68:VAL:HG23	2.02	0.42
3:F:127:ASP:OD2	3:F:162:TYR:HE1	2.02	0.42
1:B:163:ARG:O	1:B:166:GLU:HG2	2.19	0.42
1:B:506:ASP:OD1	1:B:894:ARG:N	2.39	0.42
1:A:12:TYR:CE1	2:C:106:LEU:HD21	2.55	0.42
1:A:373:LYS:HD3	1:A:378:HIS:HA	2.01	0.42
1:A:1350:ASN:C	1:A:1350:ASN:HD22	2.28	0.42
2:C:110:TRP:CE3	3:D:65:PRO:HB2	2.54	0.42
2:E:87:MET:SD	2:E:87:MET:N	2.91	0.42
2:E:146:GLY:HA2	2:E:161:TRP:CZ2	2.55	0.42
1:B:97:PHE:CD1	1:B:270:GLU:HG2	2.55	0.42
1:A:330:GLY:N	1:A:333:ASP:OD2	2.53	0.42
3:F:138:PHE:O	3:F:157:LEU:N	2.52	0.42
1:B:240:MET:HB3	1:A:164:LEU:HD23	2.00	0.42
1:B:632:PHE:O	1:B:635:MET:HE2	2.20	0.42
1:A:510:SER:HB3	1:A:895:ARG:HA	2.00	0.42
1:A:704:VAL:HG11	1:A:723:VAL:HG21	2.02	0.42
1:A:718:ASN:ND2	1:A:840:ALA:HB2	2.35	0.42
2:C:64:TYR:HB3	2:C:68:VAL:HG23	2.02	0.42
1:B:774:ASP:HB3	1:B:776:HIS:HD2	1.84	0.42
1:A:69:PRO:HG3	1:A:97:PHE:HB3	2.02	0.42
1:A:565:GLN:HB3	1:A:751:VAL:HG11	2.02	0.42
1:A:42:CYS:HA	1:A:273:GLY:HA2	2.01	0.42
1:A:338:GLU:HG2	1:A:440:VAL:HG13	2.01	0.42
1:A:1322:MET:HE3	1:A:1322:MET:HB3	1.71	0.42
3:D:58:LEU:HD11	3:D:105:GLY:HA3	2.02	0.42
2:E:110:TRP:HH2	3:F:57:TYR:CG	2.38	0.42
3:F:70:TYR:O	3:F:74:ASN:N	2.52	0.42
1:B:58:LEU:HB3	1:B:401:PRO:HB3	2.02	0.41
1:A:1:MET:HE1	2:C:54:ARG:HH21	1.85	0.41
1:A:718:ASN:HD21	1:A:813:PHE:HB3	1.84	0.41
1:A:1159:TRP:CD1	1:A:1345:CYS:HB2	2.54	0.41
1:B:23:ALA:O	1:B:27:ILE:HG12	2.20	0.41
1:B:479:ALA:HA	1:B:901:TYR:HE2	1.85	0.41
1:B:872:LEU:HD21	1:B:882:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:THR:HG22	1:A:909:TRP:CD2	2.55	0.41
1:A:259:PHE:CE2	1:A:369:LEU:HD21	2.55	0.41
1:A:602:VAL:O	1:A:606:LEU:N	2.50	0.41
1:A:724:VAL:HG21	1:A:836:ILE:O	2.20	0.41
2:C:131:LEU:HD21	3:D:140:PHE:CD2	2.55	0.41
3:D:70:TYR:O	3:D:74:ASN:N	2.52	0.41
2:E:37:SER:OG	2:E:103:GLY:O	2.34	0.41
1:B:406:ALA:HB1	1:B:422:LEU:HD21	2.02	0.41
1:B:830:GLU:HG2	1:B:837:LEU:HD21	2.02	0.41
1:A:277:LEU:HD11	1:A:294:LEU:HD23	2.02	0.41
1:A:596:PRO:HG2	1:A:597:HIS:ND1	2.35	0.41
1:A:944:ARG:HD3	1:A:944:ARG:HA	1.92	0.41
2:C:171:HIS:HE1	3:D:186:THR:HG21	1.85	0.41
1:B:91:HIS:CG	1:B:245:SER:HB3	2.56	0.41
1:B:313:GLY:O	1:B:317:VAL:HG23	2.20	0.41
1:B:373:LYS:O	1:B:377:GLY:N	2.52	0.41
1:A:681:ARG:NH1	1:A:685:ILE:HD11	2.31	0.41
2:C:53:ILE:HG13	2:C:62:THR:HG22	2.03	0.41
3:D:171:LYS:HD3	3:D:172:VAL:HB	2.02	0.41
1:B:568:GLN:HG2	1:B:634:VAL:HB	2.01	0.41
1:B:660:ILE:HG12	1:B:803:TRP:NE1	2.35	0.41
1:A:119:VAL:O	1:A:124:ARG:NH2	2.38	0.41
1:A:255:ARG:HG2	1:A:405:HIS:NE2	2.36	0.41
1:A:1108:ALA:O	1:A:1380:ARG:NH1	2.53	0.41
3:D:142:PRO:HD3	3:D:154:VAL:HB	2.01	0.41
2:E:189:VAL:HG21	2:E:201:TYR:HD2	1.86	0.41
1:B:10:ALA:O	1:B:14:ARG:HG3	2.21	0.41
1:A:438:ALA:O	1:A:454:ILE:HG22	2.20	0.41
1:A:577:LEU:HD11	1:A:606:LEU:HB3	2.02	0.41
1:A:1277:ALA:HB2	1:A:1285:LEU:HD13	2.03	0.41
2:C:146:GLY:HA2	2:C:161:TRP:CZ2	2.55	0.41
2:C:159:VAL:HG22	2:C:205:VAL:HG13	2.02	0.41
2:C:189:VAL:HG21	2:C:201:TYR:HD2	1.86	0.41
3:D:60:LYS:HA	3:D:60:LYS:HD3	1.59	0.41
1:B:240:MET:HE2	1:B:244:PHE:CD2	2.56	0.41
1:B:294:LEU:HD12	1:B:453:ILE:O	2.20	0.41
1:B:359:TYR:OH	1:B:451:HIS:NE2	2.53	0.41
1:B:627:VAL:HG12	1:B:631:MET:HG2	2.02	0.41
1:B:635:MET:SD	1:B:661:ALA:HB1	2.60	0.41
1:B:874:ARG:H	1:B:874:ARG:HG2	1.60	0.41
1:A:15:ARG:HD2	1:A:15:ARG:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:HIS:CG	1:A:899:PRO:HD3	2.56	0.41
1:A:694:MET:SD	1:A:695:ALA:N	2.93	0.41
1:A:1123:ARG:HH22	1:A:1279:ALA:HA	1.86	0.41
2:C:56:LYS:HE2	2:C:56:LYS:HB2	1.94	0.41
1:B:378:HIS:CD2	1:B:380:GLN:H	2.39	0.41
1:B:904:GLN:O	1:B:904:GLN:HG2	2.21	0.41
1:A:3:SER:O	1:A:4:THR:OG1	2.38	0.41
1:A:180:THR:O	1:A:183:VAL:HG22	2.21	0.41
1:A:692:LYS:HE2	1:A:692:LYS:HB3	1.93	0.41
3:D:50:GLY:HA3	2:E:33:ASP:OD1	2.21	0.41
3:D:130:ARG:NH2	3:D:194:THR:HG22	2.34	0.41
1:B:7:GLU:OE2	2:E:58:TYR:CZ	2.74	0.41
1:B:72:ARG:NE	1:B:235:MET:O	2.54	0.41
1:B:121:PRO:HA	1:B:124:ARG:CD	2.50	0.41
1:B:182:SER:HB2	1:A:202:ASP:OD1	2.21	0.41
1:B:559:VAL:HG11	1:B:820:LEU:HD13	2.03	0.41
1:A:40:MET:HG2	1:A:275:LEU:CD1	2.50	0.41
1:A:149:THR:HB	1:A:194:LEU:HD11	2.03	0.41
1:A:744:ILE:HG13	1:A:745:ARG:H	1.86	0.41
1:A:828:PHE:H	1:A:853:SER:H	1.69	0.41
1:A:1068:TRP:O	1:A:1072:ARG:HG3	2.21	0.41
2:C:26:ALA:HB1	2:C:29:PHE:CE1	2.56	0.41
2:E:53:ILE:HG13	2:E:62:THR:HG22	2.03	0.41
1:B:33:GLU:O	1:B:220:ARG:NH1	2.54	0.41
1:B:140:PRO:HB2	1:B:143:SER:HB3	2.02	0.41
1:A:57:LEU:HG	1:A:62:ARG:CG	2.51	0.41
1:A:642:TRP:HE3	1:A:829:LEU:HD21	1.86	0.41
3:F:142:PRO:HD3	3:F:154:VAL:HB	2.01	0.41
3:F:171:LYS:HD3	3:F:172:VAL:HB	2.02	0.41
1:B:320:ILE:HG22	1:B:451:HIS:CG	2.56	0.40
1:A:1151:GLY:HA3	1:A:1320:SER:HA	2.02	0.40
2:C:124:LYS:HE2	2:C:124:LYS:HB2	1.91	0.40
1:B:164:LEU:HD13	1:B:164:LEU:HA	1.91	0.40
1:B:257:LYS:HG3	1:B:405:HIS:HB3	2.02	0.40
1:B:565:GLN:HA	1:B:751:VAL:HG21	2.03	0.40
1:B:631:MET:O	1:B:635:MET:HB3	2.20	0.40
1:B:715:ALA:HB2	1:B:757:SER:HB2	2.02	0.40
2:C:95:THR:OG1	2:C:118:VAL:O	2.40	0.40
2:E:26:ALA:HB1	2:E:29:PHE:CE1	2.56	0.40
1:B:495:HIS:CG	1:B:899:PRO:HD3	2.55	0.40
1:A:3:SER:OG	2:C:58:TYR:OH	2.16	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ALA:HB1	1:A:290:VAL:HG13	2.03	0.40
2:C:49:TRP:CE2	2:C:51:GLY:HA2	2.57	0.40
2:E:56:LYS:HE2	2:E:56:LYS:HB2	1.94	0.40
3:F:130:ARG:NH1	3:F:131:THR:O	2.55	0.40
1:B:10:ALA:HA	1:B:13:LEU:HD23	2.03	0.40
1:B:124:ARG:HG2	1:B:125:LEU:HD22	2.04	0.40
1:B:485:LEU:HD13	1:B:520:HIS:O	2.22	0.40
1:A:318:ARG:NH1	1:A:321:GLN:OE1	2.54	0.40
1:A:453:ILE:HD12	1:A:453:ILE:HA	1.94	0.40
1:A:906:GLU:HG2	1:A:907:ARG:H	1.87	0.40
3:D:64:SER:HA	3:D:65:PRO:HD3	1.93	0.40
3:D:129:LYS:HA	3:D:162:TYR:OH	2.22	0.40
3:D:130:ARG:NH1	3:D:131:THR:O	2.55	0.40
3:F:139:ILE:HG22	3:F:229:LYS:HD3	2.04	0.40
1:B:218:SER:HA	1:B:221:ARG:CZ	2.52	0.40
1:A:34:PRO:HB2	1:A:280:LEU:HB2	2.04	0.40
1:A:312:ASN:HB3	1:A:315:ALA:HB3	2.02	0.40
1:A:718:ASN:ND2	1:A:813:PHE:HB3	2.36	0.40
1:A:1339:MET:HG3	1:A:1363:ASP:CG	2.47	0.40
2:C:38:TRP:CE2	2:C:85:LEU:HB2	2.57	0.40
3:D:138:PHE:O	3:D:157:LEU:N	2.53	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	1388/1593 (87%)	1300 (94%)	88 (6%)	0	100	100
1	B	910/1593 (57%)	844 (93%)	65 (7%)	1 (0%)	48	83
2	C	199/249 (80%)	193 (97%)	5 (2%)	1 (0%)	24	62
2	E	199/249 (80%)	191 (96%)	7 (4%)	1 (0%)	24	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	200/236 (85%)	187 (94%)	13 (6%)	0	100	100
3	F	200/236 (85%)	181 (90%)	19 (10%)	0	100	100
All	All	3096/4156 (74%)	2896 (94%)	197 (6%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	156	PRO
2	E	154	PRO
1	B	864	SER

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	1022/1173 (87%)	990 (97%)	32 (3%)	35	56
1	B	675/1173 (58%)	644 (95%)	31 (5%)	24	46
2	C	170/203 (84%)	156 (92%)	14 (8%)	10	31
2	E	170/203 (84%)	157 (92%)	13 (8%)	12	33
3	D	181/208 (87%)	165 (91%)	16 (9%)	9	29
3	F	181/208 (87%)	166 (92%)	15 (8%)	10	31
All	All	2399/3168 (76%)	2278 (95%)	121 (5%)	23	44

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	86	ARG
1	B	124	ARG
1	B	155	LEU
1	B	158	GLN
1	B	214	LEU
1	B	537	ASP
1	B	551	THR

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Mol	Chain	Res	Type
1	B	553	ARG
1	B	555	GLN
1	B	557	ARG
1	B	569	TRP
1	B	572	MET
1	B	574	VAL
1	B	577	LEU
1	B	643	ARG
1	B	657	GLN
1	B	692	LYS
1	B	786	SER
1	B	788	VAL
1	B	789	THR
1	B	791	ARG
1	B	794	GLN
1	B	857	SER
1	B	858	LEU
1	B	864	SER
1	B	865	LEU
1	B	867	ASP
1	B	872	LEU
1	B	874	ARG
1	B	880	VAL
1	B	882	VAL
1	A	194	LEU
1	A	203	THR
1	A	205	CYS
1	A	208	SER
1	A	210	VAL
1	A	235	MET
1	A	559	VAL
1	A	572	MET
1	A	612	ARG
1	A	630	VAL
1	A	635	MET
1	A	638	LEU
1	A	643	ARG
1	A	653	ILE
1	A	659	GLU
1	A	660	ILE
1	A	664	CYS
1	A	665	VAL

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Mol	Chain	Res	Type
1	A	669	LEU
1	A	784	PHE
1	A	785	PHE
1	A	788	VAL
1	A	789	THR
1	A	793	THR
1	A	794	GLN
1	A	976	VAL
1	A	977	ARG
1	A	1058	ARG
1	A	1244	ILE
1	A	1316	THR
1	A	1320	SER
1	A	1322	MET
2	C	5	GLN
2	C	36	MET
2	C	47	LEU
2	C	48	GLU
2	C	63	GLU
2	C	87	MET
2	C	91	LYS
2	C	120	SER
2	C	124	LYS
2	C	134	SER
2	C	155	GLU
2	C	157	VAL
2	C	158	THR
2	C	171	HIS
3	D	22	GLN
3	D	59	GLN
3	D	60	LYS
3	D	74	ASN
3	D	95	LYS
3	D	115	THR
3	D	117	ARG
3	D	118	LEU
3	D	119	THR
3	D	129	LYS
3	D	167	LYS
3	D	183	GLU
3	D	185	VAL
3	D	197	LEU

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Mol	Chain	Res	Type
3	D	221	GLN
3	D	225	SER
2	E	5	GLN
2	E	36	MET
2	E	48	GLU
2	E	63	GLU
2	E	87	MET
2	E	91	LYS
2	E	120	SER
2	E	124	LYS
2	E	134	SER
2	E	155	GLU
2	E	157	VAL
2	E	158	THR
2	E	171	HIS
3	F	22	GLN
3	F	60	LYS
3	F	74	ASN
3	F	95	LYS
3	F	110	MET
3	F	112	SER
3	F	115	THR
3	F	117	ARG
3	F	125	LYS
3	F	167	LYS
3	F	183	GLU
3	F	185	VAL
3	F	197	LEU
3	F	221	GLN
3	F	225	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	92	GLN
1	B	300	ASN
1	B	322	GLN
1	B	375	ASN
1	B	380	GLN
1	B	405	HIS
1	B	776	HIS
1	A	122	GLN

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Mol	Chain	Res	Type
1	A	158	GLN
1	A	322	GLN
1	A	340	HIS
1	A	718	ASN
1	A	794	GLN
1	A	1112	GLN
1	A	1349	GLN
2	C	41	GLN
3	D	22	GLN
3	D	52	ASN
3	F	22	GLN
3	F	47	HIS
3	F	52	ASN
3	F	221	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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.

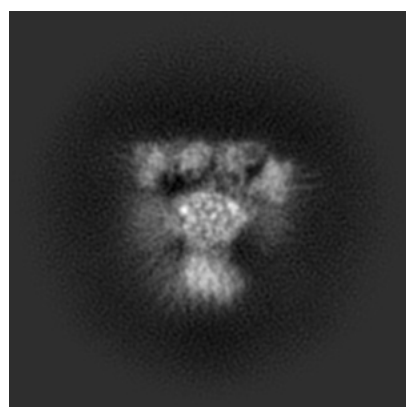
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23715. These allow visual inspection of the internal detail of the map and identification of artifacts.

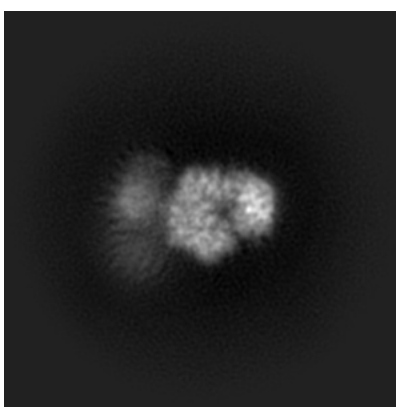
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

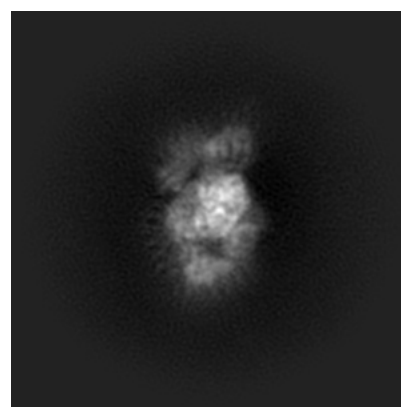
6.1.1 Primary map



X



Y

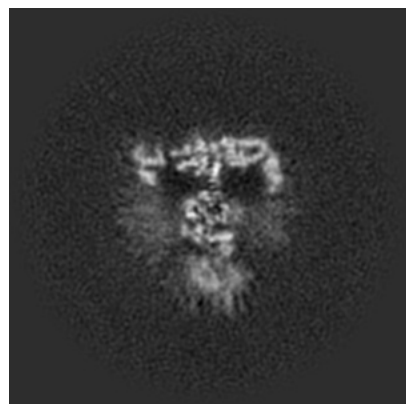


Z

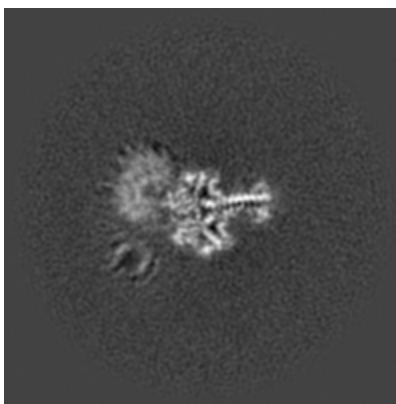
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

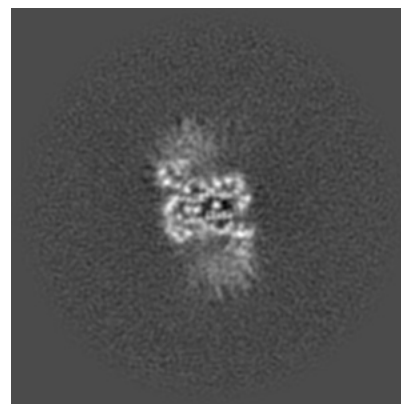
6.2.1 Primary map



X Index: 168



Y Index: 168

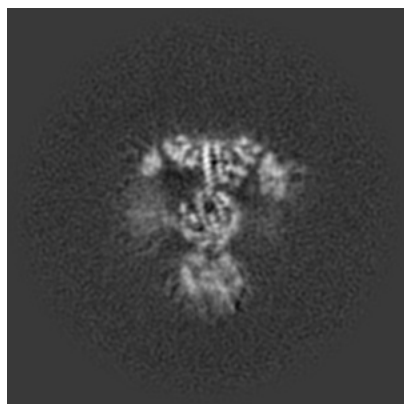


Z Index: 168

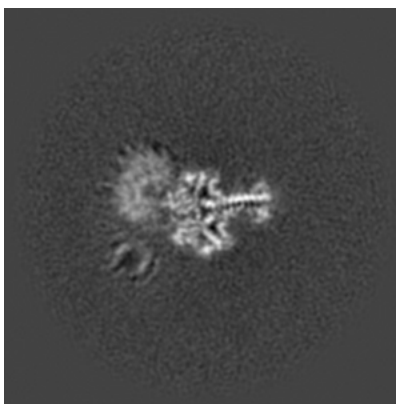
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

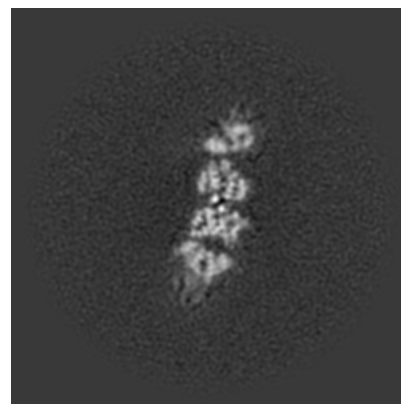
6.3.1 Primary map



X Index: 177



Y Index: 168

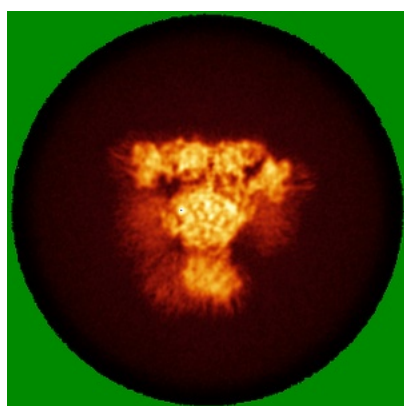


Z Index: 206

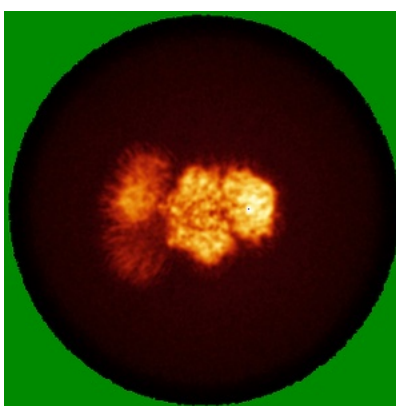
The images above show the largest variance slices of the map in three orthogonal directions.

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

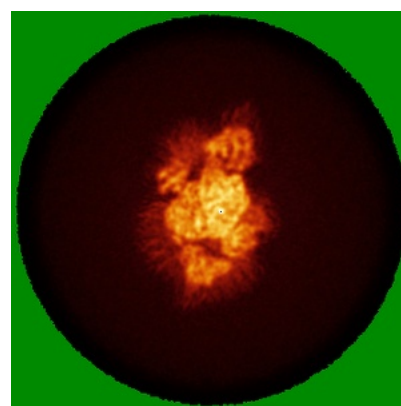
6.4.1 Primary map



X



Y

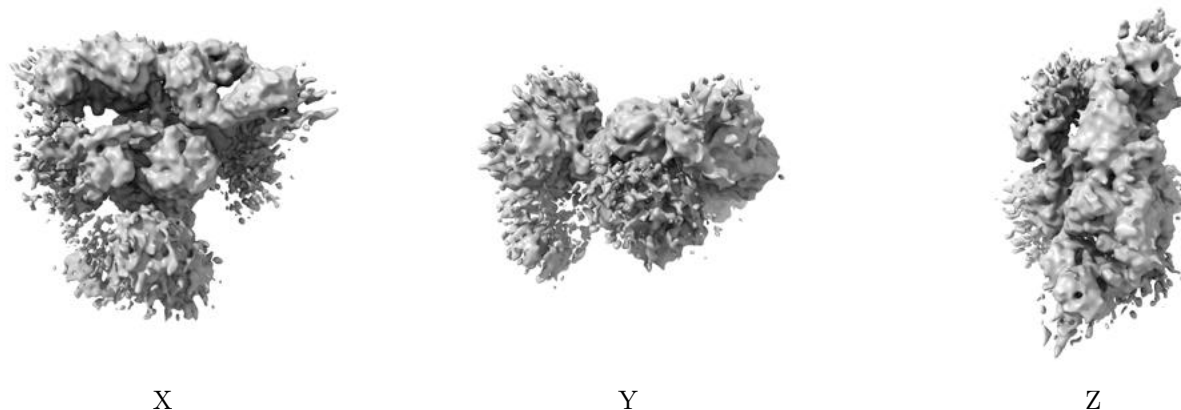


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

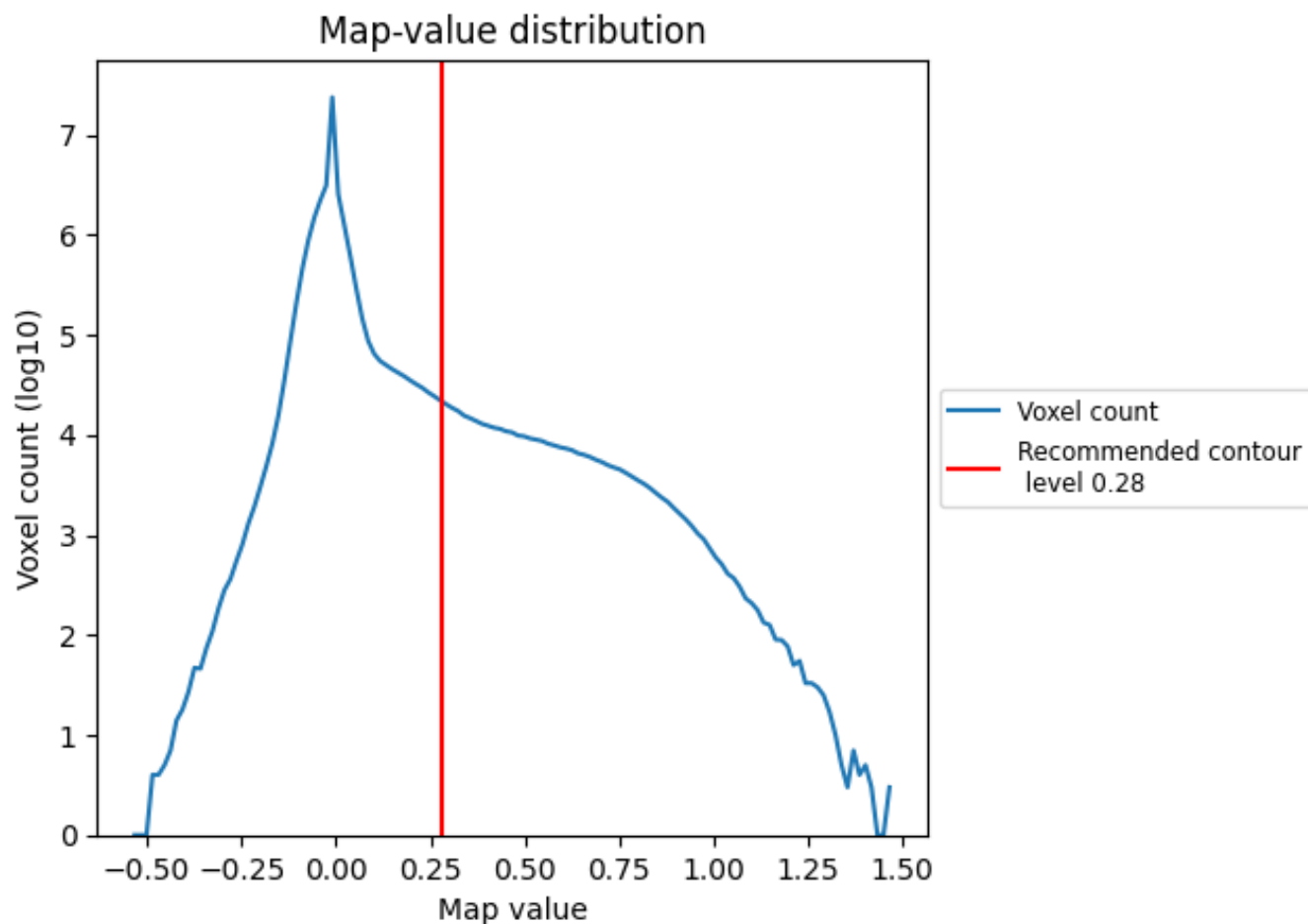
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

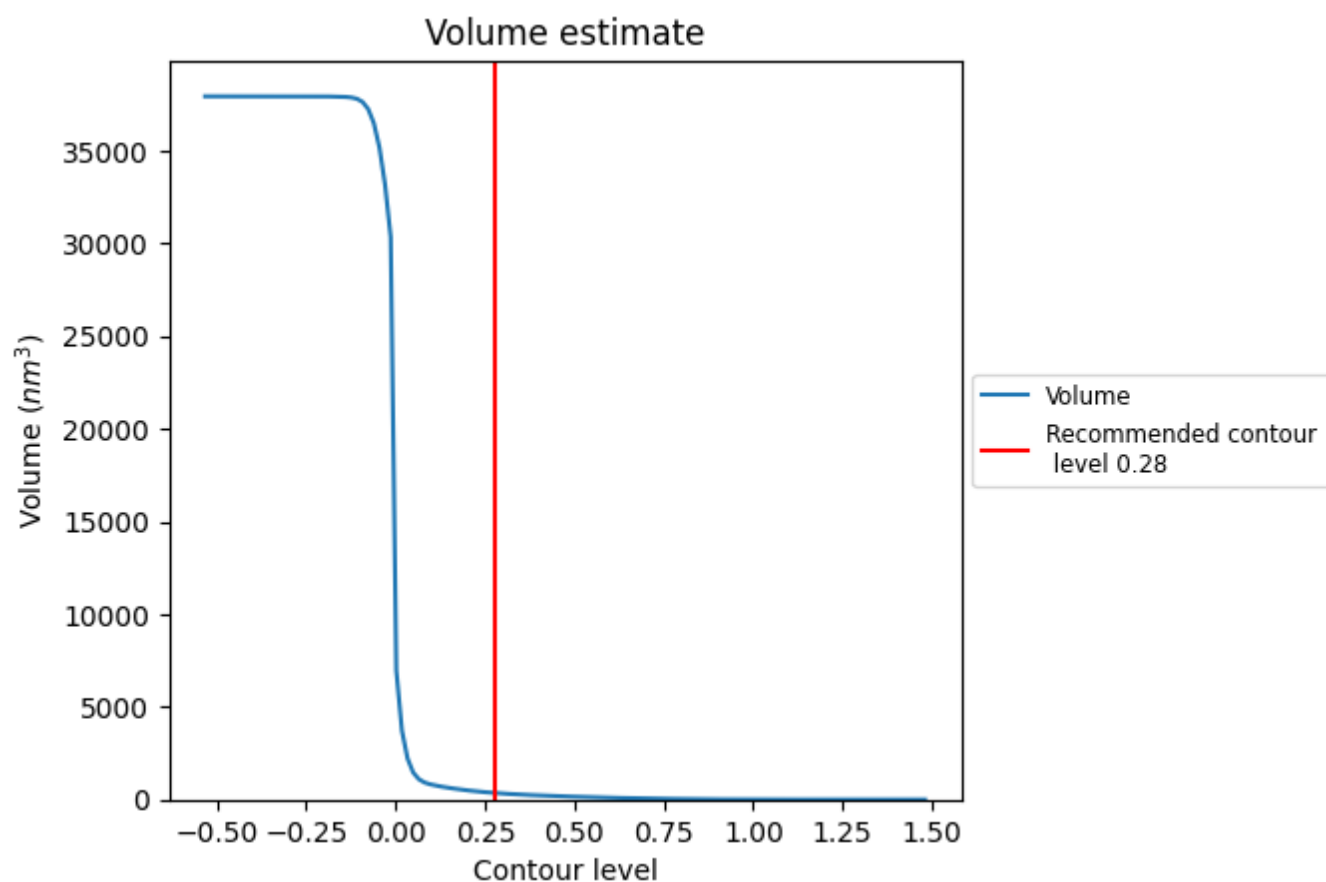
This section contains the results of statistical analysis of the map.

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.

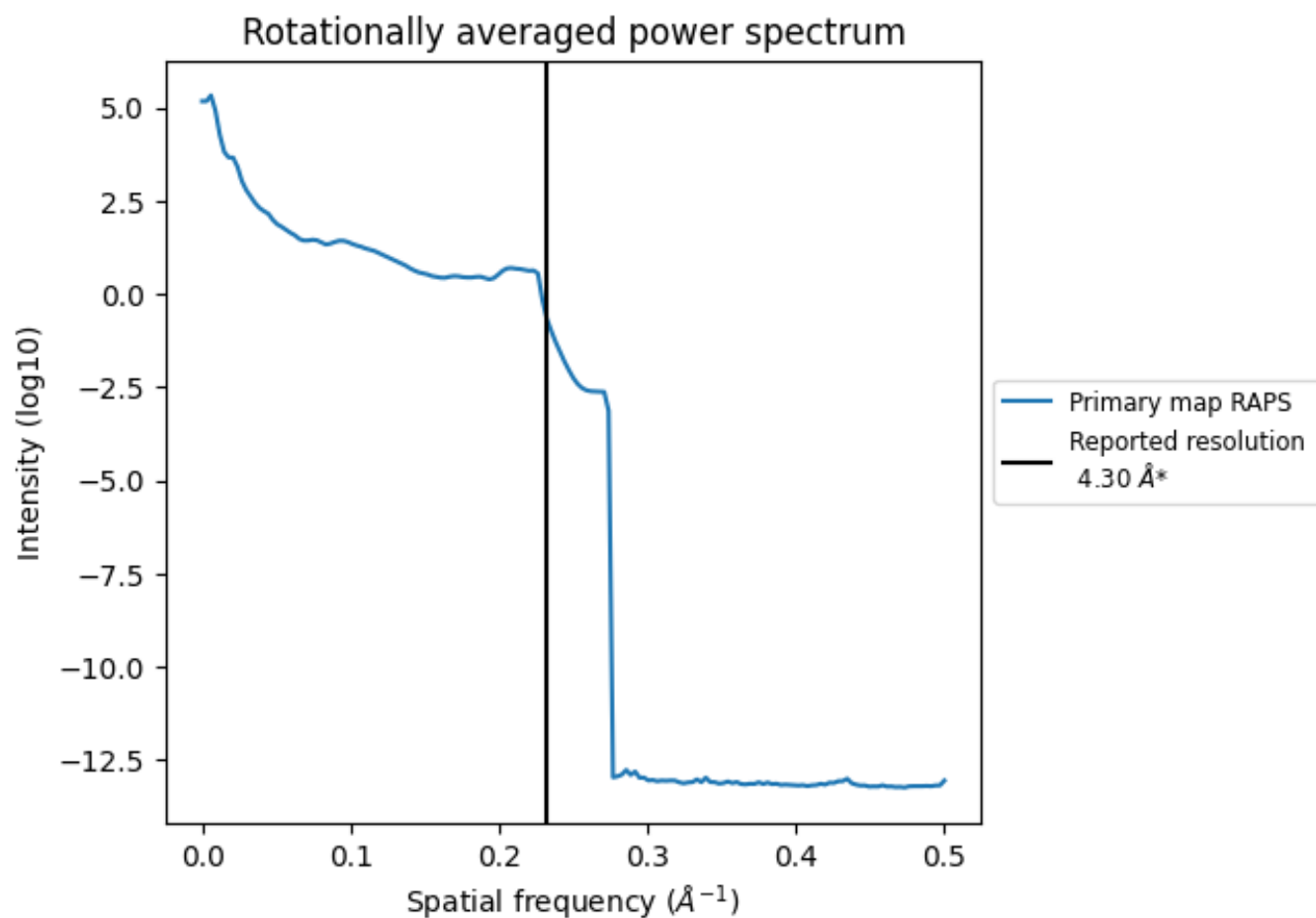
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm³; this corresponds to an approximate mass of 318 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 0.233 Å⁻¹

8 Fourier-Shell correlation

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

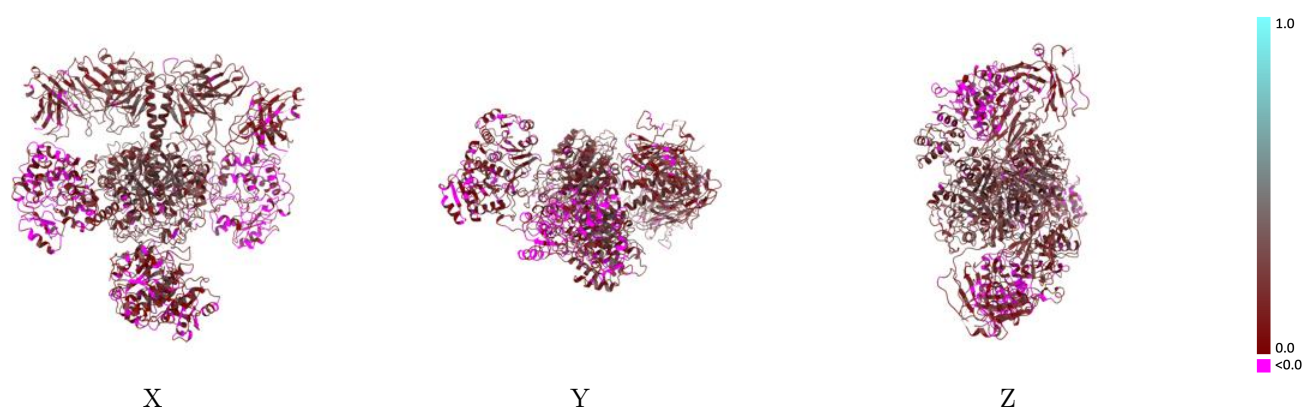
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23715 and PDB model 7M7J. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

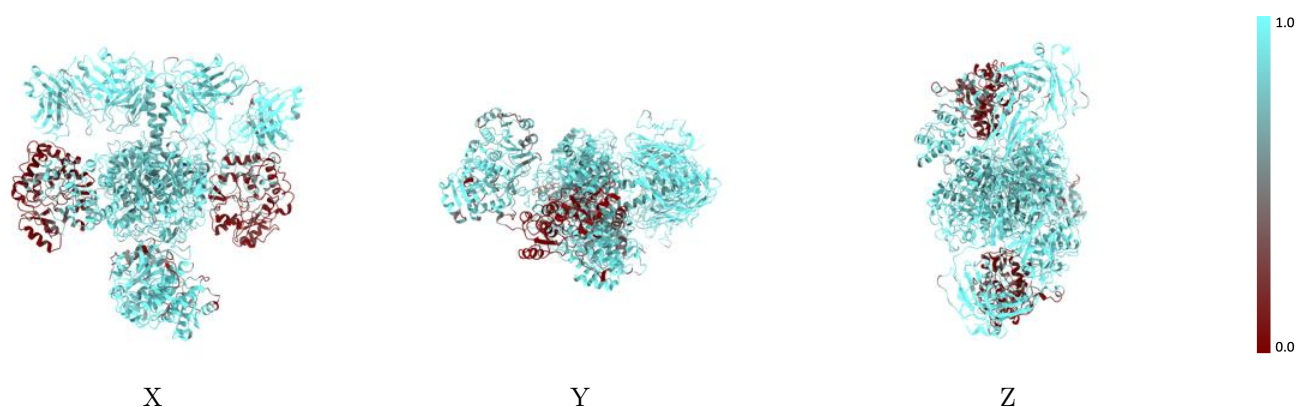
This section was not generated.

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



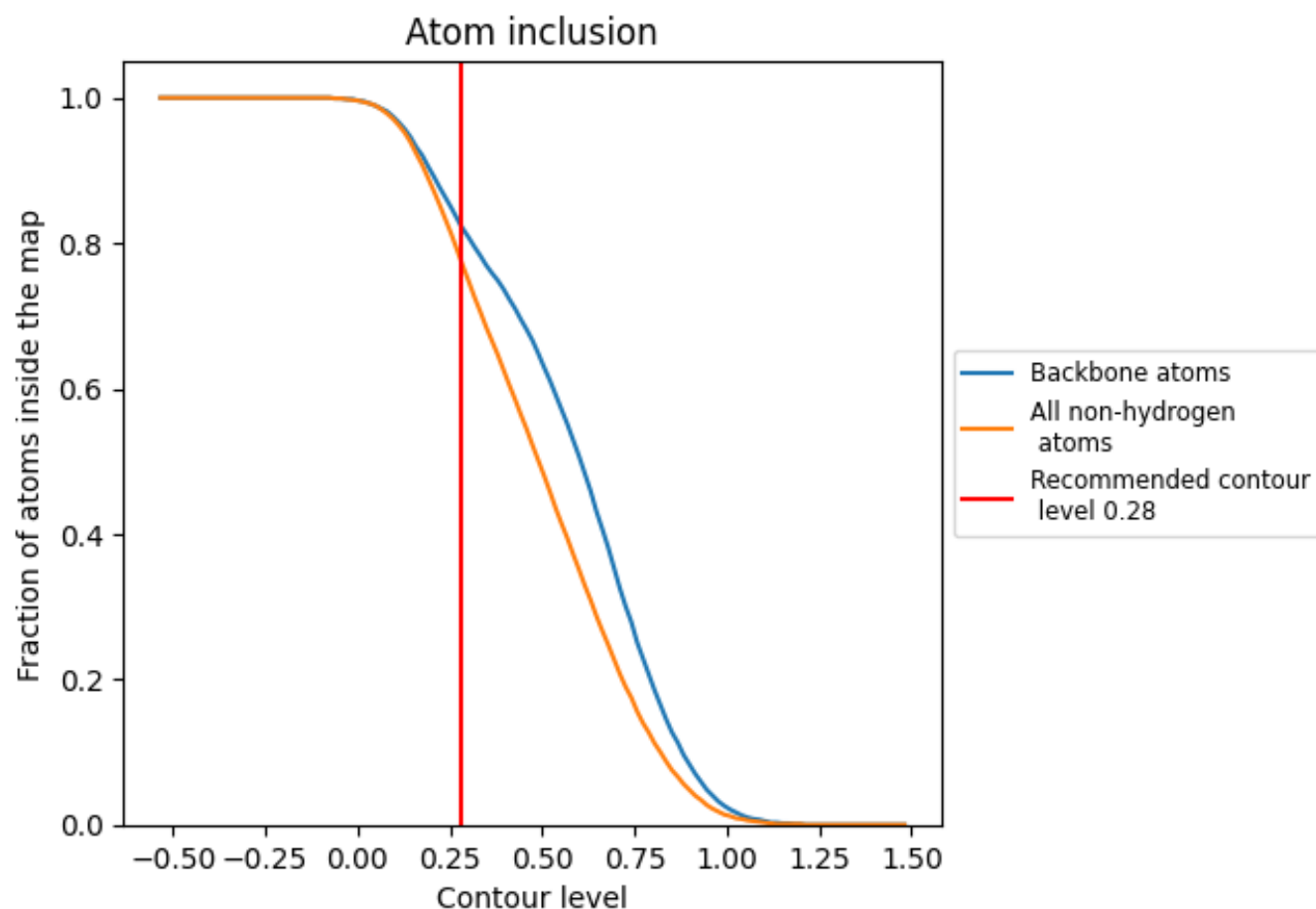
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.28).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.1660
A	0.7350	0.1410
B	0.6880	0.1610
C	0.9340	0.2010
D	0.9370	0.2120
E	0.9440	0.2050
F	0.9370	0.2280

1.0

0.0

<0.0