



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 05:56 PM UTC

PDB ID : 3JAZ / pdb_00003jaz
EMDB ID : EMD-6371
Title : Atomic model of cytoplasmic polyhedrosis virus with ATP
Authors : Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on : 2015-07-06
Resolution : 3.10 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

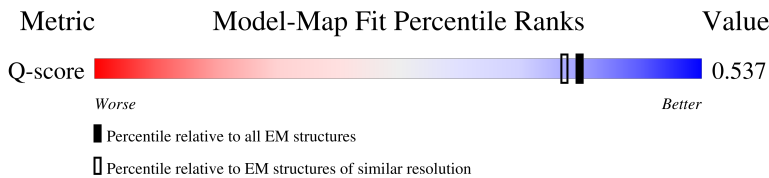
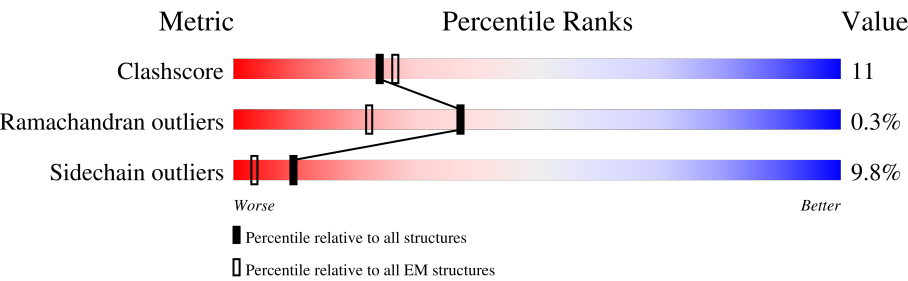
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1058	12% 66% 29% 5%
2	B	1333	61% 25% • 11%
2	C	1333	66% 25% • 6%
3	D	448	44% 19% • 35%

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Mol	Chain	Length	Quality of chain
3	E	448	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32244 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0
			8434	5345	1457	1587	45		

- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			9397	5937	1634	1789	37		
2	C	1250	Total	C	N	O	S	0	0
			9851	6219	1712	1882	38		

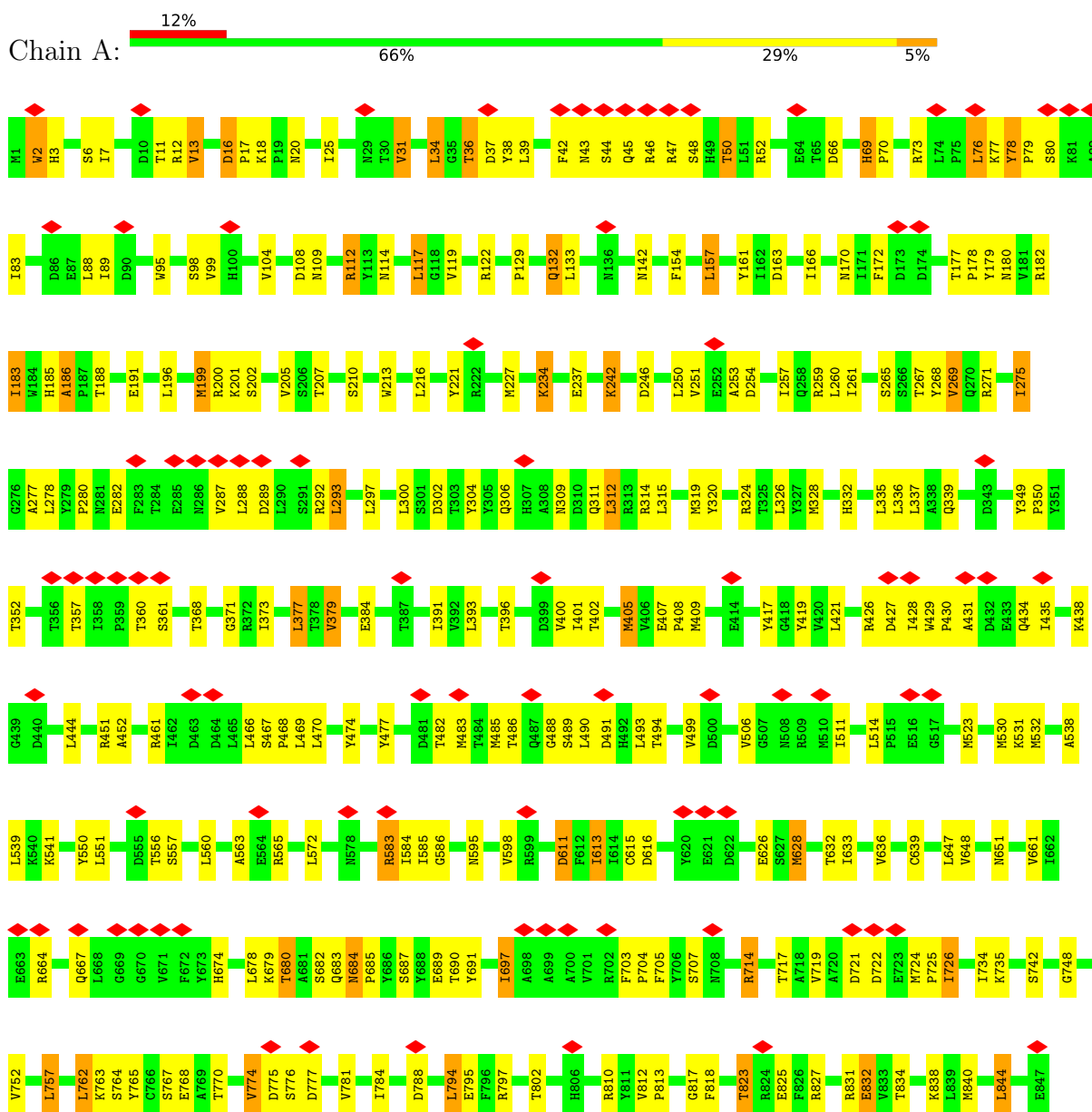
- Molecule 3 is a protein called Viral structural protein 5.

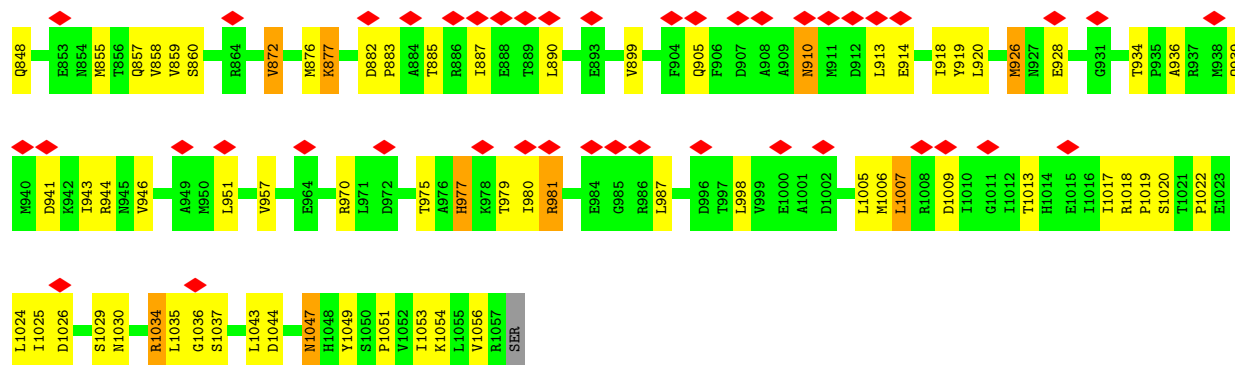
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

3 Residue-property plots

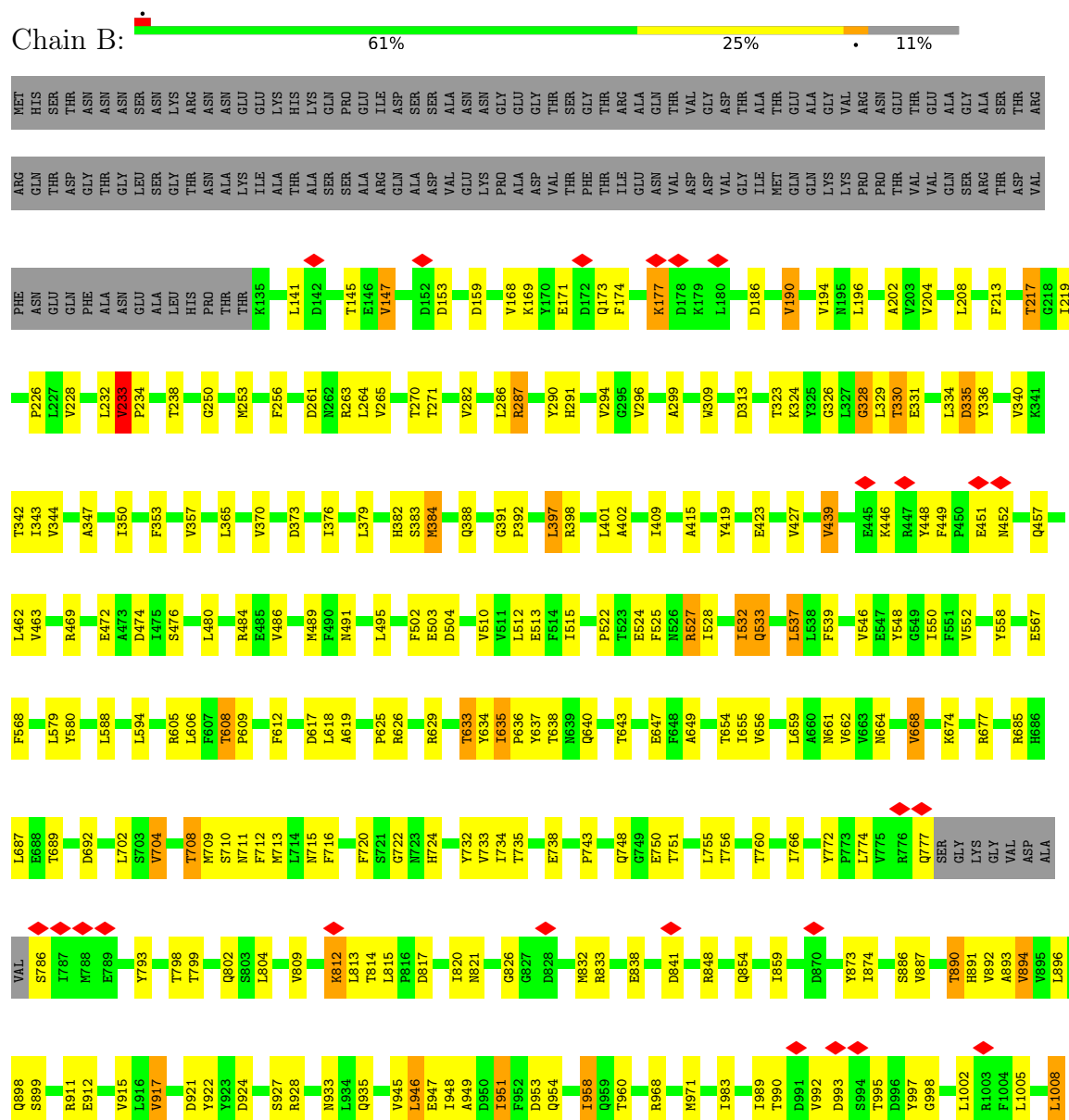
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

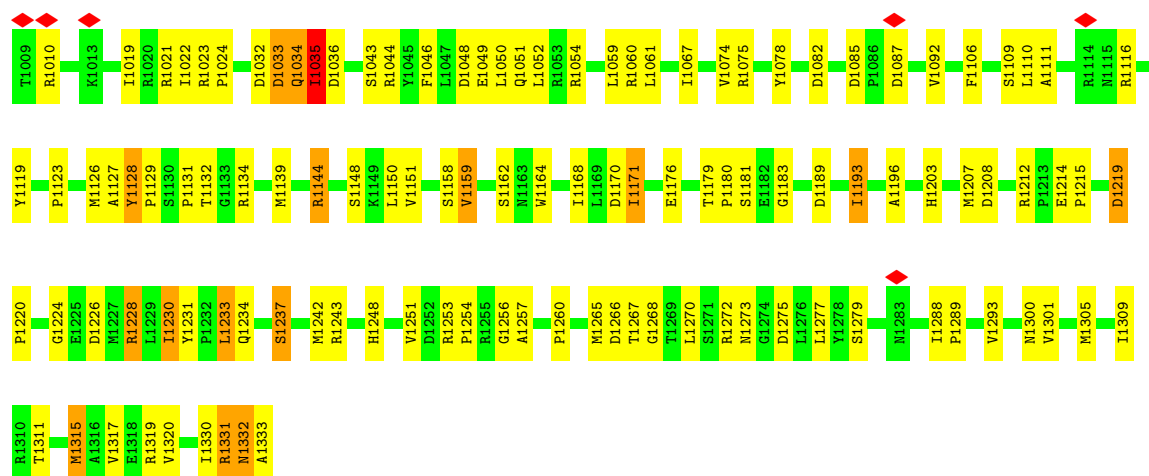
• Molecule 1: Structural protein VP3





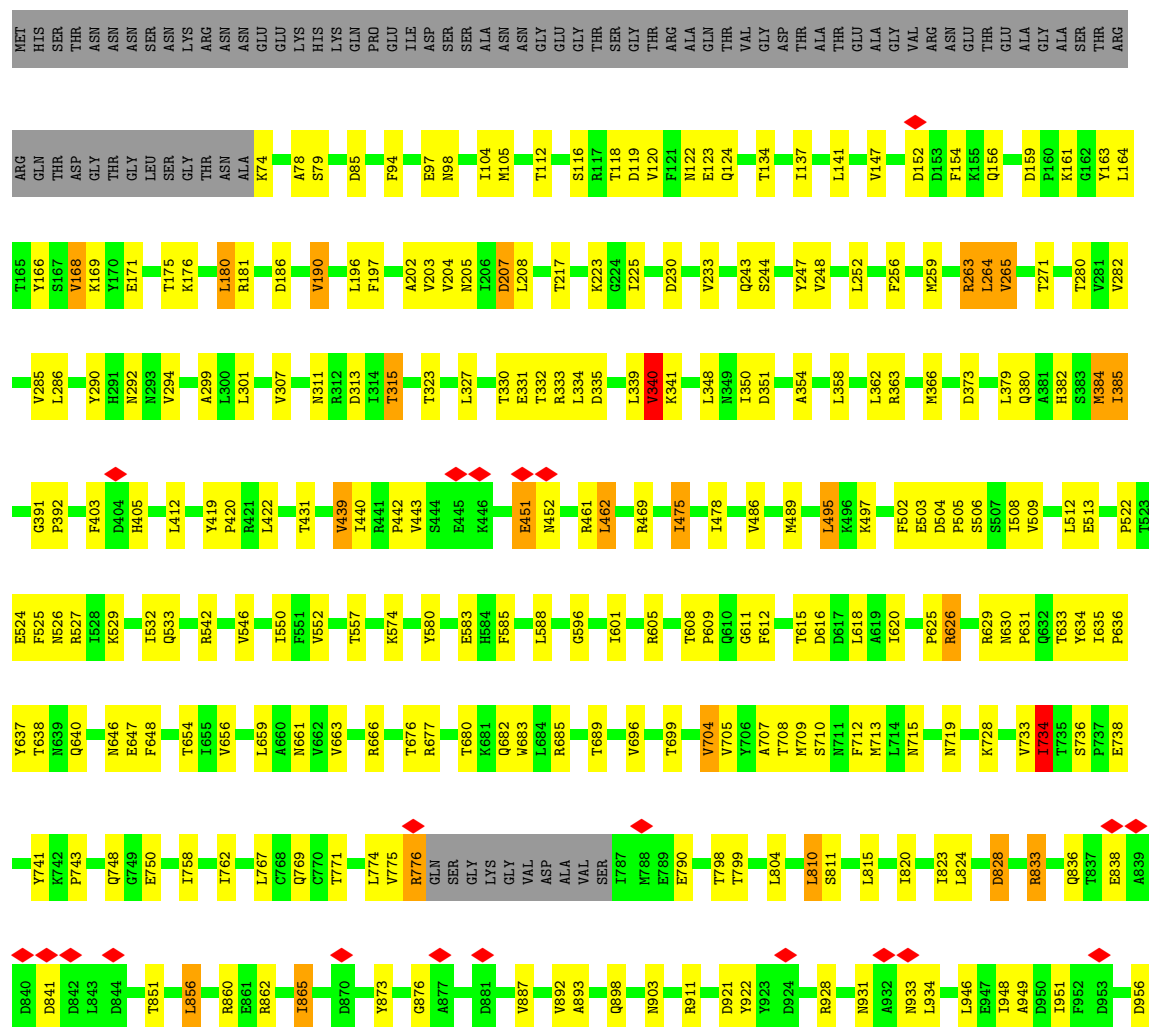
• Molecule 2: Capsid protein VP1

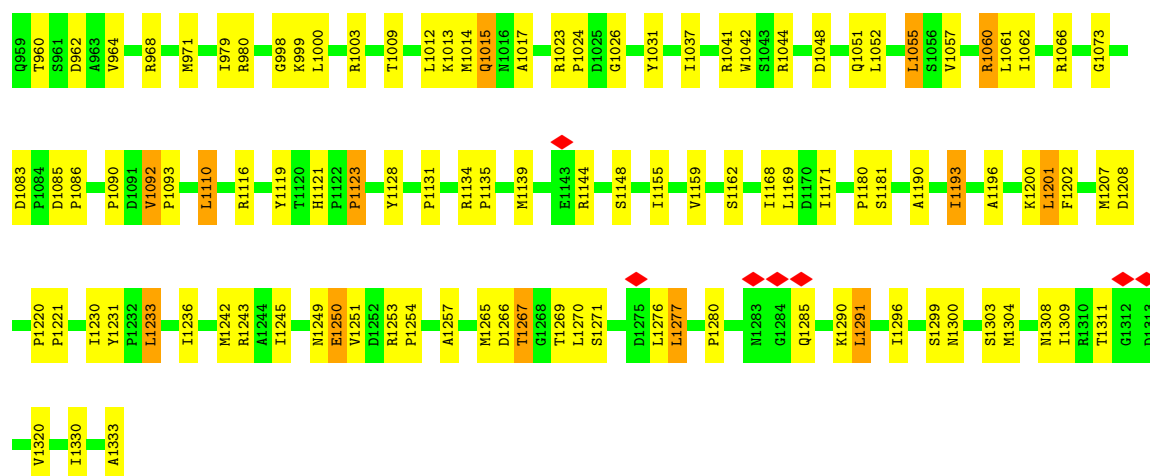




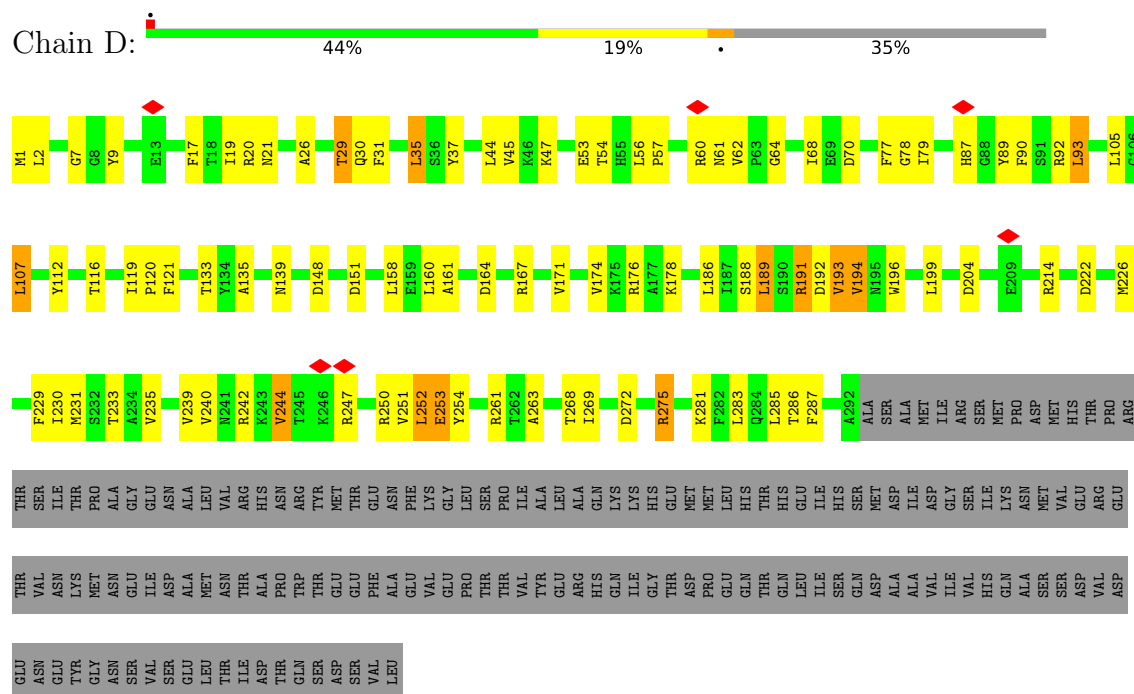
• Molecule 2: Capsid protein VP1

Chain C: 66% 25% 6%

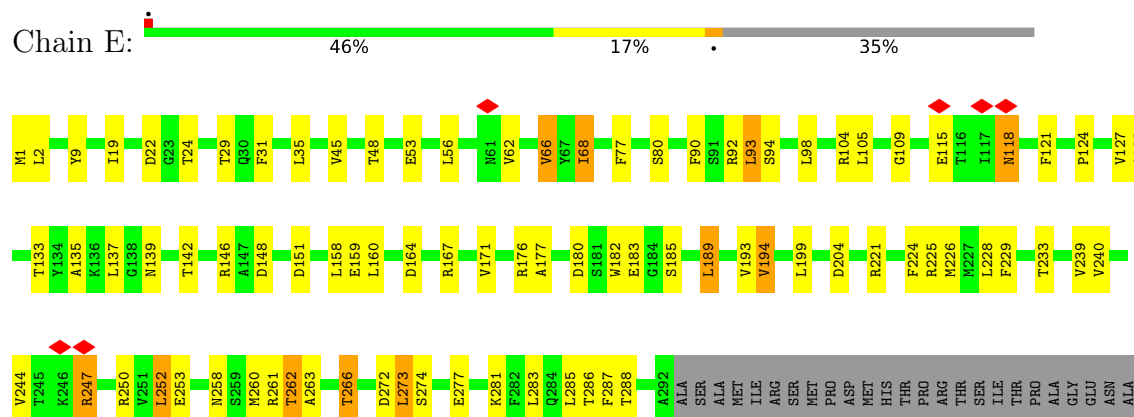




• Molecule 3: Viral structural protein 5



• Molecule 3: Viral structural protein 5



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	19447	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	60535	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	26.030	Depositor
Minimum map value	-16.162	Depositor
Average map value	0.072	Depositor
Map value standard deviation	1.603	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	772.8, 772.8, 772.8	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.104, 1.104, 1.104	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	0.37	0/8619	0.83	14/11737 (0.1%)
2	B	0.45	0/9590	0.90	25/13056 (0.2%)
2	C	0.45	0/10052	0.86	10/13687 (0.1%)
3	D	0.42	0/2327	0.86	5/3163 (0.2%)
3	E	0.41	0/2327	0.84	1/3163 (0.0%)
All	All	0.43	0/32915	0.86	55/44806 (0.1%)

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

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

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	ASP	CA-C-N	8.72	128.87	119.28
2	B	504	ASP	C-N-CA	8.72	128.87	119.28
1	A	186	ALA	C-N-CD	-8.47	101.96	120.60
1	A	186	ALA	CA-C-N	8.33	146.99	127.00
1	A	186	ALA	C-N-CA	8.33	146.99	127.00
2	B	233	VAL	CA-C-N	7.83	127.85	119.78
2	B	233	VAL	C-N-CA	7.83	127.85	119.78
1	A	872	VAL	N-CA-C	6.97	114.80	107.76
2	B	1033	ASP	N-CA-C	-6.91	100.21	110.23
1	A	16	ASP	CA-C-N	6.88	126.80	119.85
1	A	16	ASP	C-N-CA	6.88	126.80	119.85
2	B	1132	THR	N-CA-C	6.79	118.75	111.36
2	B	608	THR	CA-C-N	6.71	126.70	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	608	THR	C-N-CA	6.71	126.70	119.78
3	D	192	ASP	N-CA-C	-6.59	104.18	111.82
2	B	1168	ILE	CB-CA-C	-6.51	103.49	111.88
2	B	159	ASP	CA-C-N	6.50	126.45	119.76
2	B	159	ASP	C-N-CA	6.50	126.45	119.76
2	B	1128	TYR	CA-C-N	6.38	126.30	119.28
2	B	1128	TYR	C-N-CA	6.38	126.30	119.28
1	A	78	TYR	CA-C-N	6.09	141.63	127.00
1	A	78	TYR	C-N-CA	6.09	141.63	127.00
2	B	398	ARG	CA-C-N	6.07	126.04	120.03
2	B	398	ARG	C-N-CA	6.07	126.04	120.03
2	C	223	LYS	N-CA-C	-5.99	102.06	110.50
2	C	1092	VAL	CA-C-N	5.99	125.96	120.03
2	C	1092	VAL	C-N-CA	5.99	125.96	120.03
2	B	635	ILE	CA-C-N	5.93	125.80	119.28
2	B	635	ILE	C-N-CA	5.93	125.80	119.28
3	D	272	ASP	N-CA-C	-5.90	103.16	110.41
2	B	1332	ASN	N-CA-C	5.89	118.77	110.23
3	D	7	GLY	N-CA-C	-5.84	103.03	112.31
1	A	78	TYR	C-N-CD	-5.78	107.88	120.60
1	A	265	SER	N-CA-C	5.66	116.74	108.14
2	C	734	ILE	N-CA-C	-5.61	101.58	109.21
1	A	69	HIS	CA-C-N	5.58	125.42	119.28
1	A	69	HIS	C-N-CA	5.58	125.42	119.28
2	B	958	ILE	CB-CA-C	-5.53	104.14	110.73
2	C	159	ASP	CA-C-N	5.52	125.46	119.78
2	C	159	ASP	C-N-CA	5.52	125.46	119.78
3	D	37	TYR	N-CA-C	5.50	117.76	109.23
2	C	719	ASN	N-CA-C	5.48	118.18	111.82
1	A	31	VAL	CA-C-N	5.45	125.39	119.78
1	A	31	VAL	C-N-CA	5.45	125.39	119.78
2	B	1219	ASP	CA-C-N	5.42	123.62	119.66
2	B	1219	ASP	C-N-CA	5.42	123.62	119.66
3	E	128	ALA	N-CA-C	-5.42	105.45	111.36
3	D	251	VAL	CB-CA-C	-5.33	104.33	110.41
2	C	1266	ASP	N-CA-C	5.33	118.00	111.82
2	B	793	TYR	CA-C-N	5.31	125.25	119.78
2	B	793	TYR	C-N-CA	5.31	125.25	119.78
2	B	716	PHE	N-CA-C	5.29	118.99	112.54
2	C	1083	ASP	CA-C-N	5.28	124.91	119.05
2	C	1083	ASP	C-N-CA	5.28	124.91	119.05
2	B	1171	ILE	N-CA-C	5.21	116.30	109.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	328	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8434	0	8399	198	0
2	B	9397	0	9315	221	0
2	C	9851	0	9762	204	0
3	D	2281	0	2282	54	0
3	E	2281	0	2282	48	0
All	All	32244	0	32040	696	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (696) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:812:LYS:NZ	2:B:812:LYS:HB3	1.55	1.12
2:B:812:LYS:NZ	2:B:812:LYS:CB	2.12	1.11
2:B:812:LYS:HB3	2:B:812:LYS:HZ3	0.95	1.10
2:B:812:LYS:CB	2:B:812:LYS:HZ2	1.86	0.88
2:B:328:GLY:H	2:B:347:ALA:HB3	1.41	0.85
1:A:797:ARG:NH2	1:A:876:MET:O	2.09	0.85
2:B:812:LYS:HZ2	2:B:812:LYS:HB2	1.44	0.82
2:C:363:ARG:NH1	3:E:183:GLU:OE1	2.14	0.81
2:C:1116:ARG:HH11	2:C:1116:ARG:HG2	1.47	0.79
1:A:277:ALA:HB3	1:A:319:MET:HE1	1.64	0.79
1:A:685:PRO:O	1:A:714:ARG:NH2	2.19	0.76
2:B:392:PRO:HD2	2:B:1315:MET:HE2	1.65	0.76
2:B:376:ILE:HD11	2:B:1317:VAL:HG11	1.69	0.75
1:A:680:THR:HG22	1:A:683:GLN:HG3	1.69	0.75
3:E:77:PHE:HB2	3:E:194:VAL:HG23	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:ARG:NE	2:B:524:GLU:OE2	2.19	0.74
2:C:161:LYS:O	2:C:263:ARG:NH2	2.20	0.74
2:C:734:ILE:HG22	2:C:1017:ALA:HB1	1.69	0.74
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.20	0.74
2:C:815:LEU:HD11	2:C:1051:GLN:HE22	1.53	0.74
2:B:1208:ASP:OD1	2:B:1243:ARG:NH2	2.20	0.73
2:C:1208:ASP:OD1	2:C:1243:ARG:NH2	2.21	0.73
1:A:752:VAL:HG12	1:A:781:VAL:HG23	1.70	0.73
1:A:200:ARG:HG2	1:A:324:ARG:HE	1.52	0.73
2:C:384:MET:HA	2:C:708:THR:HG21	1.71	0.73
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.21	0.72
2:C:887:VAL:HG22	2:C:893:ALA:HA	1.70	0.72
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.71	0.72
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.23	0.72
2:B:1131:PRO:O	2:B:1162:SER:OG	2.07	0.72
1:A:563:ALA:O	1:A:565:ARG:NH1	2.23	0.72
3:E:283:LEU:HA	3:E:286:THR:HG22	1.72	0.72
2:C:1057:VAL:HG22	2:C:1291:LEU:HD21	1.72	0.71
2:C:841:ASP:OD2	2:C:911:ARG:NH2	2.24	0.71
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.72	0.71
2:C:156:GLN:NE2	2:C:1308:ASN:OD1	2.26	0.69
1:A:328:MET:HE2	1:A:332:HIS:HB3	1.74	0.68
2:B:469:ARG:NH1	2:B:472:GLU:OE1	2.27	0.68
2:B:921:ASP:OD1	2:B:928:ARG:NH2	2.26	0.68
1:A:408:PRO:HB2	1:A:468:PRO:HG3	1.75	0.68
1:A:680:THR:HG23	1:A:682:SER:H	1.59	0.67
2:B:1144:ARG:NH2	2:B:1196:ALA:O	2.27	0.67
1:A:66:ASP:OD1	1:A:122:ARG:NH2	2.27	0.67
1:A:489:SER:OG	1:A:491:ASP:OD1	2.10	0.67
1:A:326:LEU:HB3	1:A:352:THR:HG22	1.74	0.67
2:B:1021:ARG:NE	2:B:1036:ASP:OD1	2.28	0.67
2:B:817:ASP:HA	2:B:983:ILE:HG12	1.77	0.66
3:E:164:ASP:OD2	3:E:167:ARG:NH2	2.28	0.66
2:B:365:LEU:HD22	2:B:1305:MET:HE1	1.76	0.66
2:B:841:ASP:OD1	2:B:911:ARG:NH2	2.27	0.66
2:C:366:MET:HG2	3:E:266:THR:HG21	1.77	0.66
1:A:674:HIS:HB2	1:A:697:ILE:HD12	1.78	0.66
2:B:1254:PRO:HG2	2:B:1257:ALA:HB2	1.77	0.66
1:A:242:LYS:NZ	1:A:246:ASP:OD2	2.26	0.65
3:D:193:VAL:HG11	3:D:230:ILE:HG13	1.79	0.65
1:A:13:VAL:HG23	1:A:213:TRP:CD1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1331:ARG:HB3	2:B:1331:ARG:HH11	1.62	0.64
1:A:427:ASP:HA	1:A:703:PHE:HA	1.80	0.64
3:E:272:ASP:OD2	3:E:274:SER:OG	2.14	0.64
3:D:164:ASP:OD1	3:D:167:ARG:NH2	2.30	0.64
2:B:1085:ASP:OD2	2:B:1243:ARG:NH2	2.31	0.64
2:C:1254:PRO:HG2	2:C:1257:ALA:HB2	1.80	0.64
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.80	0.63
2:C:169:LYS:O	2:C:202:ALA:N	2.31	0.63
2:C:462:LEU:HD13	2:C:680:THR:HG22	1.81	0.63
1:A:282:GLU:OE1	1:A:810:ARG:NH2	2.31	0.63
3:E:180:ASP:OD1	3:E:247:ARG:NH1	2.32	0.63
1:A:36:THR:OG1	1:A:37:ASP:N	2.27	0.62
2:B:1023:ARG:HG2	2:B:1024:PRO:HD2	1.79	0.62
2:C:313:ASP:OD2	2:C:1253:ARG:NH2	2.31	0.62
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.16	0.62
1:A:2:TRP:CD1	1:A:3:HIS:H	2.18	0.62
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.32	0.62
2:B:750:GLU:OE1	2:C:452:ASN:ND2	2.33	0.62
2:B:1228:ARG:HG2	2:B:1231:TYR:CZ	2.35	0.62
2:B:921:ASP:O	2:B:928:ARG:NH1	2.32	0.61
2:B:1048:ASP:HB3	2:B:1051:GLN:HG3	1.80	0.61
2:C:626:ARG:NH2	2:C:712:PHE:O	2.26	0.61
3:D:112:TYR:CE2	3:D:119:ILE:HG21	2.36	0.61
1:A:419:TYR:HE1	1:A:421:LEU:HD23	1.65	0.61
2:C:615:THR:H	2:C:1333:ALA:HA	1.64	0.61
2:C:163:TYR:N	2:C:351:ASP:OD2	2.32	0.61
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.83	0.61
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.81	0.61
2:C:78:ALA:HB2	2:C:1181:SER:HB2	1.81	0.61
2:C:443:VAL:HB	2:C:771:THR:HG23	1.81	0.61
2:C:469:ARG:NH2	2:C:513:GLU:OE2	2.26	0.61
1:A:161:TYR:CE2	2:B:1333:ALA:HB1	2.36	0.61
1:A:477:TYR:HA	1:A:482:THR:HG22	1.82	0.61
2:C:704:VAL:O	2:C:708:THR:HG23	2.00	0.61
2:C:709:MET:O	2:C:715:ASN:ND2	2.34	0.61
2:B:1144:ARG:NH1	2:B:1170:ASP:OD1	2.34	0.60
2:C:271:THR:OG1	2:C:292:ASN:OD1	2.18	0.60
2:B:992:VAL:HG12	2:B:992:VAL:O	2.01	0.60
2:B:709:MET:O	2:B:715:ASN:ND2	2.33	0.60
2:C:921:ASP:OD1	2:C:928:ARG:NH2	2.34	0.60
2:B:626:ARG:NH2	2:B:712:PHE:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:ARG:NH1	3:D:263:ALA:O	2.35	0.60
3:E:148:ASP:OD1	3:E:151:ASP:N	2.32	0.60
1:A:288:LEU:HD22	1:A:368:THR:HG22	1.84	0.59
2:B:489:MET:HE1	2:B:580:TYR:HE2	1.67	0.59
2:B:384:MET:HA	2:B:708:THR:HG21	1.84	0.59
1:A:129:PRO:HB2	2:B:1332:ASN:HD22	1.67	0.59
1:A:227:MET:HG2	1:A:269:VAL:HG21	1.84	0.59
1:A:957:VAL:HG22	1:A:1056:VAL:HG23	1.85	0.59
1:A:47:ARG:NH1	1:A:80:SER:OG	2.35	0.59
1:A:1026:ASP:OD1	1:A:1030:ASN:ND2	2.35	0.59
2:B:640:GLN:OE1	2:B:647:GLU:N	2.33	0.58
1:A:114:ASN:ND2	1:A:117:LEU:HB2	2.17	0.58
1:A:848:GLN:OE1	1:A:1054:LYS:NZ	2.35	0.58
2:B:335:ASP:OD1	2:B:340:VAL:N	2.33	0.58
2:B:891:HIS:CG	3:D:240:VAL:HG21	2.38	0.58
1:A:234:LYS:NZ	1:A:237:GLU:OE2	2.37	0.58
2:C:949:ALA:HA	2:C:958:ILE:HD13	1.86	0.58
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.86	0.57
2:B:226:PRO:HB2	2:B:250:GLY:HA3	1.85	0.57
2:C:307:VAL:HG21	2:C:1245:ILE:HG22	1.86	0.57
1:A:129:PRO:HG2	2:B:1332:ASN:HB2	1.85	0.57
2:B:537:LEU:HD13	2:B:548:TYR:HE1	1.69	0.57
1:A:292:ARG:NH1	1:A:777:ASP:OD1	2.35	0.57
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.86	0.57
2:B:528:ILE:HG13	2:B:532:ILE:HD12	1.85	0.57
2:C:207:ASP:OD1	2:C:207:ASP:N	2.37	0.57
2:C:533:GLN:HG3	2:C:588:LEU:HD12	1.85	0.57
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.87	0.57
2:C:741:TYR:OH	2:C:1026:GLY:O	2.21	0.57
2:B:704:VAL:O	2:B:708:THR:HG23	2.05	0.57
2:C:171:GLU:OE2	2:C:1181:SER:OG	2.23	0.57
2:C:550:ILE:HD13	2:C:596:GLY:HA3	1.87	0.57
2:B:484:ARG:HE	2:B:524:GLU:CD	2.13	0.56
2:C:204:VAL:HG21	2:C:1242:MET:HE3	1.85	0.56
2:C:244:SER:HA	2:C:1201:LEU:HD22	1.85	0.56
1:A:651:ASN:HA	1:A:689:GLU:HG3	1.88	0.56
2:C:104:ILE:HG12	2:C:1311:THR:HG23	1.88	0.56
2:B:491:ASN:HD22	2:B:756:THR:HG21	1.69	0.56
2:B:1032:ASP:HB3	2:B:1035:ILE:HG23	1.87	0.56
3:E:90:PHE:HA	3:E:93:LEU:HB2	1.87	0.56
1:A:687:SER:OG	1:A:689:GLU:OE1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASP:OD1	1:A:182:ARG:NE	2.32	0.56
1:A:257:ILE:HG21	1:A:326:LEU:HD11	1.87	0.56
2:B:606:LEU:HD13	2:B:655:ILE:HG23	1.88	0.56
1:A:565:ARG:NH2	1:A:616:ASP:OD2	2.37	0.56
2:C:838:GLU:OE1	2:C:933:ASN:ND2	2.39	0.56
2:C:931:ASN:HB3	2:C:934:LEU:HD23	1.87	0.56
3:E:45:VAL:HA	3:E:171:VAL:HG12	1.87	0.56
2:B:147:VAL:HG22	2:B:379:LEU:HD11	1.88	0.55
1:A:36:THR:OG1	1:A:37:ASP:OD1	2.24	0.55
1:A:541:LYS:HD3	1:A:550:TYR:HE1	1.70	0.55
2:B:633:THR:HG21	2:B:710:SER:HB3	1.87	0.55
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.89	0.55
1:A:714:ARG:NH1	1:A:1044:ASP:OD1	2.40	0.55
2:B:474:ASP:OD2	2:B:476:SER:OG	2.24	0.55
2:B:1171:ILE:HD11	2:B:1193:ILE:HG23	1.88	0.55
2:C:469:ARG:NE	2:C:513:GLU:OE1	2.39	0.55
1:A:636:VAL:HG11	1:A:661:VAL:HG13	1.88	0.55
2:B:873:TYR:HB3	2:B:898:GLN:HB2	1.88	0.55
2:B:1127:ALA:O	3:E:146:ARG:NH2	2.39	0.55
2:C:1048:ASP:HB3	2:C:1051:GLN:HG3	1.88	0.55
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.89	0.55
2:C:180:LEU:HD12	2:C:181:ARG:H	1.72	0.54
2:B:342:THR:OG1	2:B:343:ILE:N	2.36	0.54
2:B:1109:SER:HB2	3:E:262:THR:HG21	1.88	0.54
2:C:203:VAL:HG12	2:C:1243:ARG:HG3	1.89	0.54
2:C:230:ASP:HA	2:C:233:VAL:HG11	1.89	0.54
2:C:1128:TYR:CZ	2:C:1135:PRO:HD3	2.42	0.54
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.40	0.54
2:C:461:ARG:HB3	2:C:676:THR:HG21	1.88	0.54
1:A:78:TYR:CE2	1:A:83:ILE:HA	2.42	0.54
2:B:1273:ASN:ND2	2:B:1275:ASP:OD1	2.35	0.54
1:A:664:ARG:HD2	1:A:667:GLN:HE21	1.72	0.54
1:A:928:GLU:HG2	1:A:934:THR:HG22	1.89	0.54
2:B:1226:ASP:OD1	2:C:122:ASN:ND2	2.35	0.54
2:C:451:GLU:OE2	2:C:452:ASN:ND2	2.41	0.54
3:D:186:LEU:HD22	3:D:233:THR:HG21	1.89	0.54
3:E:19:ILE:HD11	3:E:31:PHE:HB2	1.89	0.54
3:E:239:VAL:HG12	3:E:250:ARG:HD2	1.90	0.54
2:C:1119:TYR:HH	2:C:1121:HIS:HD1	1.55	0.54
1:A:882:ASP:OD2	1:A:885:THR:OG1	2.24	0.54
2:B:748:GLN:HA	2:C:682:GLN:HE22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:504:ASP:OD2	2:C:506:SER:OG	2.26	0.53
3:D:60:ARG:NH2	3:D:87:HIS:O	2.41	0.53
2:C:505:PRO:HG2	2:C:677:ARG:HB2	1.89	0.53
2:B:892:VAL:HG12	2:B:894:VAL:HB	1.91	0.53
2:C:640:GLN:HB2	2:C:646:ASN:HD22	1.71	0.53
1:A:572:LEU:HB3	1:A:584:ILE:HD13	1.89	0.53
2:C:611:GLY:HA3	2:C:635:ILE:O	2.08	0.53
1:A:44:SER:O	1:A:45:GLN:HB2	2.09	0.53
1:A:170:ASN:OD1	1:A:172:PHE:N	2.42	0.53
1:A:532:MET:HE3	1:A:560:LEU:HD12	1.89	0.53
2:B:674:LYS:HA	2:B:677:ARG:HD3	1.90	0.53
2:C:252:LEU:HD22	2:C:823:ILE:HD13	1.90	0.53
2:B:891:HIS:HA	3:D:242:ARG:HD3	1.90	0.53
3:D:244:VAL:HG13	3:D:247:ARG:HB2	1.90	0.53
2:C:348:LEU:HD11	2:C:1304:MET:HE1	1.88	0.53
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.91	0.53
3:E:176:ARG:HG3	3:E:253:GLU:HB3	1.90	0.53
1:A:943:ILE:HA	1:A:946:VAL:HG12	1.90	0.53
1:A:393:LEU:HB3	1:A:748:GLY:HA3	1.90	0.52
1:A:541:LYS:HG2	1:A:975:THR:HG21	1.90	0.52
2:B:217:THR:HB	2:B:219:ILE:HG13	1.91	0.52
2:B:486:VAL:HG21	2:B:709:MET:HB3	1.91	0.52
2:C:865:ILE:HG12	2:C:1041:ARG:HG2	1.91	0.52
1:A:161:TYR:CD2	2:B:1333:ALA:HB1	2.45	0.52
2:B:261:ASP:OD1	2:B:263:ARG:NE	2.41	0.52
2:B:813:LEU:HD11	2:B:1008:LEU:HD13	1.91	0.52
3:E:66:VAL:HG11	3:E:92:ARG:HG3	1.91	0.52
1:A:486:THR:HB	1:A:489:SER:HB3	1.92	0.52
2:C:439:VAL:HG11	2:C:705:VAL:HG21	1.92	0.52
3:D:229:PHE:CE1	3:D:252:LEU:HD11	2.44	0.52
2:C:707:ALA:HB2	2:C:1330:ILE:HG23	1.92	0.52
1:A:429:TRP:CE2	1:A:434:GLN:HG2	2.45	0.52
2:B:328:GLY:HA3	2:B:347:ALA:H	1.74	0.52
2:C:495:LEU:HD13	2:C:532:ILE:HG13	1.92	0.52
2:C:156:GLN:HE22	2:C:1309:ILE:H	1.58	0.52
1:A:775:ASP:OD1	1:A:776:SER:N	2.42	0.51
2:C:489:MET:HE1	2:C:580:TYR:HE2	1.75	0.51
3:D:68:ILE:HD11	3:D:90:PHE:HA	1.91	0.51
1:A:379:VAL:HG21	1:A:794:LEU:HD13	1.90	0.51
2:C:828:ASP:OD2	2:C:862:ARG:NH2	2.44	0.51
2:C:633:THR:HG21	2:C:710:SER:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1289:PRO:HD2	3:D:20:ARG:HD2	1.92	0.51
2:C:1116:ARG:HG2	2:C:1116:ARG:NH1	2.23	0.51
3:D:112:TYR:CZ	3:D:119:ILE:HD13	2.45	0.51
2:B:299:ALA:HB2	2:B:1265:MET:HB3	1.92	0.51
2:B:1134:ARG:NH1	2:B:1158:SER:OG	2.40	0.51
2:C:676:THR:O	2:C:680:THR:HG23	2.11	0.51
3:D:233:THR:HB	3:D:268:THR:HG21	1.93	0.51
2:B:1183:GLY:HA2	2:B:1207:MET:HE1	1.93	0.51
1:A:831:ARG:NH1	1:A:832:GLU:OE2	2.44	0.51
2:B:629:ARG:NH1	2:B:1036:ASP:O	2.44	0.50
1:A:840:MET:HE2	1:A:1019:PRO:HB2	1.93	0.50
2:B:550:ILE:HG22	2:B:594:LEU:HD21	1.93	0.50
2:B:1248:HIS:ND1	2:B:1251:VAL:HG22	2.26	0.50
2:B:1288:ILE:HG12	3:D:20:ARG:NH2	2.26	0.50
1:A:704:PRO:HG2	1:A:705:PHE:CD2	2.46	0.50
1:A:860:SER:HA	1:A:920:LEU:HB2	1.94	0.50
2:C:204:VAL:HB	2:C:1242:MET:HB2	1.94	0.50
2:C:713:MET:HE1	2:C:804:LEU:HG	1.92	0.50
1:A:887:ILE:HG13	1:A:899:VAL:HG21	1.93	0.50
2:B:357:VAL:HG13	2:B:1054:ARG:HG2	1.92	0.50
2:B:513:GLU:OE2	2:B:760:THR:OG1	2.23	0.50
1:A:539:LEU:HG	1:A:647:LEU:HD12	1.93	0.50
2:B:766:ILE:O	2:B:772:TYR:OH	2.25	0.50
2:B:874:ILE:HD11	2:B:917:VAL:HG13	1.93	0.50
2:C:382:HIS:HE2	2:C:713:MET:H	1.60	0.50
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.94	0.50
2:B:1126:MET:HE1	3:E:146:ARG:HB3	1.93	0.50
3:D:53:GLU:CD	3:D:53:GLU:H	2.20	0.50
2:B:1243:ARG:HD3	2:B:1256:GLY:O	2.12	0.50
3:D:19:ILE:HD12	3:D:19:ILE:O	2.12	0.50
1:A:18:LYS:HA	1:A:112:ARG:HA	1.94	0.50
2:C:748:GLN:HG3	2:C:1000:LEU:HD22	1.92	0.50
2:C:828:ASP:OD1	2:C:828:ASP:N	2.45	0.50
1:A:42:PHE:CE1	1:A:47:ARG:HA	2.47	0.49
1:A:371:GLY:N	1:A:818:PHE:O	2.42	0.49
2:B:734:ILE:HD13	2:B:1019:ILE:HG12	1.93	0.49
3:D:176:ARG:HD3	3:D:253:GLU:HB3	1.94	0.49
3:E:1:MET:HB2	3:E:121:PHE:CE2	2.48	0.49
3:E:221:ARG:O	3:E:225:ARG:HG3	2.11	0.49
1:A:409:MET:HE1	1:A:1036:GLY:HA2	1.93	0.49
2:B:1087:ASP:OD2	2:B:1237:SER:OG	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:177:ALA:HB3	3:E:252:LEU:HG	1.93	0.49
2:B:990:THR:O	2:B:992:VAL:HG23	2.12	0.49
2:C:522:PRO:HB3	2:C:609:PRO:HB3	1.93	0.49
2:C:824:LEU:HD23	2:C:971:MET:HE1	1.94	0.49
2:C:1276:LEU:HB3	2:C:1290:LYS:HD2	1.94	0.49
1:A:391:ILE:HD11	1:A:757:LEU:HD22	1.95	0.49
1:A:939:GLN:HB2	1:A:998:LEU:HD21	1.95	0.49
2:B:1033:ASP:O	2:B:1034:GLN:HB2	2.12	0.49
1:A:275:ILE:HA	1:A:278:LEU:HD12	1.95	0.49
1:A:557:SER:N	1:A:611:ASP:OD1	2.29	0.49
2:B:704:VAL:HG12	2:B:1330:ILE:HD11	1.93	0.49
2:C:633:THR:HG21	2:C:710:SER:HB2	1.94	0.49
2:C:865:ILE:HD12	2:C:1042:TRP:HE3	1.77	0.49
2:C:1042:TRP:HD1	2:C:1044:ARG:HG2	1.77	0.49
3:D:79:ILE:HA	3:D:269:ILE:HG22	1.94	0.49
3:D:148:ASP:OD2	3:D:151:ASP:N	2.41	0.49
3:E:159:GLU:O	3:E:225:ARG:HG2	2.13	0.49
1:A:1006:MET:HA	1:A:1009:ASP:OD2	2.13	0.49
2:C:225:ILE:HB	2:C:247:TYR:HD1	1.78	0.49
2:C:354:ALA:O	2:C:358:LEU:HG	2.12	0.49
3:E:233:THR:HG22	3:E:252:LEU:HD13	1.94	0.49
2:B:1230:ILE:HG12	2:C:119:ASP:HA	1.95	0.49
2:C:164:LEU:HD23	2:C:208:LEU:HA	1.95	0.49
2:B:1150:LEU:HD23	2:C:141:LEU:HD22	1.95	0.49
2:C:503:GLU:O	2:C:666:ARG:NH2	2.39	0.48
1:A:163:ASP:HB3	1:A:180:ASN:ND2	2.28	0.48
1:A:910:ASN:OD1	1:A:910:ASN:N	2.39	0.48
2:B:558:TYR:HB3	2:B:568:PHE:CD2	2.47	0.48
2:B:1214:GLU:HG2	2:B:1215:PRO:HD2	1.95	0.48
3:D:57:PRO:HD3	3:D:139:ASN:ND2	2.28	0.48
2:C:85:ASP:HB2	2:C:161:LYS:HE2	1.96	0.48
2:C:248:VAL:HG11	2:C:971:MET:HG2	1.95	0.48
2:C:525:PHE:CE1	2:C:532:ILE:HD13	2.48	0.48
3:E:53:GLU:CD	3:E:53:GLU:H	2.21	0.48
1:A:16:ASP:HA	1:A:17:PRO:HD3	1.69	0.48
2:C:862:ARG:O	2:C:865:ILE:HG22	2.13	0.48
2:B:1111:ALA:HB3	2:B:1116:ARG:HD2	1.95	0.48
2:B:1189:ASP:HA	2:C:118:THR:HG22	1.96	0.48
2:C:168:VAL:HG11	2:C:196:LEU:HG	1.94	0.48
2:B:419:TYR:HB3	2:B:1005:LEU:HD22	1.95	0.48
2:C:366:MET:HE2	2:C:366:MET:HB3	1.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:THR:HB	1:A:1020:SER:HB2	1.96	0.48
2:B:330:THR:OG1	2:B:331:GLU:N	2.47	0.48
2:C:94:PHE:HB3	2:C:105:MET:HG2	1.95	0.48
2:C:286:LEU:HD11	2:C:290:TYR:HB3	1.96	0.48
2:C:616:ASP:O	2:C:620:ILE:HG13	2.13	0.48
1:A:2:TRP:HD1	1:A:3:HIS:H	1.57	0.48
2:B:1266:ASP:OD1	2:B:1279:SER:OG	2.27	0.48
2:C:526:ASN:OD1	2:C:529:LYS:NZ	2.42	0.48
2:C:1090:PRO:HD3	2:C:1231:TYR:CD2	2.49	0.48
2:B:213:PHE:HB3	2:B:219:ILE:HD12	1.96	0.48
2:B:634:TYR:CE1	2:B:722:GLY:HA3	2.49	0.48
2:B:995:THR:O	2:B:998:GLY:N	2.45	0.48
2:C:422:LEU:HD13	2:C:810:LEU:HD11	1.96	0.48
3:D:26:ALA:HB1	3:D:30:GLN:HG3	1.96	0.48
1:A:377:LEU:HB3	1:A:763:LYS:HB3	1.96	0.48
2:C:704:VAL:HB	2:C:1330:ILE:HD11	1.96	0.48
1:A:43:ASN:HD21	1:A:46:ARG:HD2	1.77	0.47
1:A:724:MET:HG3	1:A:725:PRO:HD2	1.95	0.47
1:A:726:ILE:HG13	1:A:1029:SER:HB2	1.96	0.47
2:B:1159:VAL:HA	2:B:1164:TRP:HB2	1.97	0.47
2:C:626:ARG:HG2	2:C:631:PRO:HB3	1.96	0.47
2:C:1060:ARG:HD3	2:C:1291:LEU:O	2.14	0.47
1:A:328:MET:HE1	1:A:336:LEU:HD11	1.95	0.47
1:A:426:ARG:HG3	1:A:707:SER:HB3	1.96	0.47
1:A:979:THR:HG23	1:A:980:ILE:HG12	1.97	0.47
2:B:256:PHE:CE2	2:B:990:THR:HG21	2.48	0.47
1:A:43:ASN:ND2	1:A:46:ARG:HD2	2.29	0.47
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.96	0.47
1:A:39:LEU:HD11	1:A:52:ARG:HH11	1.79	0.47
2:C:380:GLN:HB3	2:C:618:LEU:HD22	1.97	0.47
2:C:750:GLU:OE1	2:C:1003:ARG:NH1	2.46	0.47
2:C:998:GLY:HA3	2:C:1012:LEU:HD21	1.97	0.47
2:C:1073:GLY:HA2	2:C:1168:ILE:O	2.13	0.47
3:E:229:PHE:O	3:E:233:THR:HG23	2.15	0.47
1:A:6:SER:HB2	1:A:251:VAL:O	2.15	0.47
1:A:275:ILE:HD11	1:A:300:LEU:HD22	1.97	0.47
1:A:531:LYS:HD3	1:A:683:GLN:HG2	1.97	0.47
2:B:313:ASP:OD2	2:B:1253:ARG:NH1	2.48	0.47
2:B:886:SER:O	2:B:890:THR:HG23	2.14	0.47
2:B:992:VAL:O	2:B:993:ASP:HB2	2.15	0.47
2:C:119:ASP:OD1	2:C:119:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:PHE:HB2	2:C:301:LEU:HD21	1.96	0.47
3:D:78:GLY:O	3:D:275:ARG:NH2	2.47	0.47
1:A:488:GLY:HA2	1:A:551:LEU:HD13	1.97	0.47
2:B:1268:GLY:HA3	2:B:1277:LEU:O	2.14	0.47
2:C:629:ARG:HA	2:C:1037:ILE:HG22	1.96	0.47
2:B:270:THR:HG22	2:B:291:HIS:HA	1.97	0.47
2:B:512:LEU:HD13	2:B:659:LEU:HD12	1.97	0.47
2:B:522:PRO:HB3	2:B:609:PRO:HB3	1.96	0.47
2:B:612:PHE:CD1	2:B:638:THR:HG22	2.49	0.47
2:C:833:ARG:HG3	2:C:922:TYR:CZ	2.49	0.47
2:B:838:GLU:C	2:B:935:GLN:HG2	2.40	0.47
3:D:93:LEU:HD12	3:D:93:LEU:HA	1.74	0.47
2:B:153:ASP:OD1	2:B:153:ASP:N	2.43	0.46
2:B:720:PHE:CE2	2:B:722:GLY:HA2	2.50	0.46
3:D:17:PHE:HB3	3:D:196:TRP:CE2	2.50	0.46
1:A:302:ASP:O	1:A:306:GLN:HB2	2.16	0.46
1:A:812:VAL:HA	1:A:813:PRO:HA	1.70	0.46
2:B:141:LEU:HD22	2:B:391:GLY:HA3	1.97	0.46
2:B:287:ARG:NH2	2:B:326:GLY:HA3	2.30	0.46
2:C:856:LEU:HD23	2:C:860:ARG:HD3	1.98	0.46
3:D:45:VAL:HG13	3:D:171:VAL:HG12	1.98	0.46
2:B:1139:MET:HB2	2:B:1139:MET:HE3	1.62	0.46
2:B:1180:PRO:HA	2:B:1207:MET:SD	2.55	0.46
2:C:1180:PRO:HD3	2:C:1208:ASP:O	2.15	0.46
3:D:281:LYS:O	3:D:285:LEU:HG	2.15	0.46
2:B:347:ALA:HA	2:B:1301:VAL:HA	1.97	0.46
2:B:832:MET:SD	2:B:946:LEU:HG	2.55	0.46
2:C:495:LEU:HD23	2:C:497:LYS:HA	1.98	0.46
2:C:524:GLU:OE1	2:C:758:ILE:HG12	2.15	0.46
1:A:78:TYR:HB3	1:A:79:PRO:HA	1.98	0.46
2:C:332:THR:HG22	2:C:334:LEU:H	1.81	0.46
2:C:1131:PRO:O	2:C:1162:SER:OG	2.28	0.46
2:C:362:LEU:HD22	2:C:1303:SER:HB3	1.98	0.46
1:A:461:ARG:HH21	1:A:684:ASN:CG	2.23	0.46
2:B:446:LYS:HB3	2:B:448:TYR:HD2	1.80	0.46
2:B:713:MET:HE1	2:B:804:LEU:HG	1.98	0.46
2:B:833:ARG:HG3	2:B:922:TYR:CZ	2.50	0.46
3:D:35:LEU:HD12	3:D:35:LEU:HA	1.78	0.46
2:B:873:TYR:HA	2:B:896:LEU:O	2.16	0.46
2:B:949:ALA:HB1	2:B:960:THR:HG22	1.98	0.46
2:B:1106:PHE:CE2	2:B:1119:TYR:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9:TYR:H	3:E:204:ASP:CG	2.24	0.46
2:B:854:GLN:NE2	2:C:647:GLU:OE1	2.48	0.46
2:C:1031:TYR:CE2	2:C:1041:ARG:HG3	2.51	0.46
1:A:438:LYS:NZ	1:A:626:GLU:OE2	2.47	0.45
2:B:196:LEU:HD22	2:B:296:VAL:HG11	1.98	0.45
2:B:525:PHE:CE1	2:B:532:ILE:HD13	2.51	0.45
2:B:1044:ARG:HH22	2:B:1049:GLU:CD	2.24	0.45
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.97	0.45
1:A:129:PRO:CG	2:B:1332:ASN:HB2	2.46	0.45
2:B:253:MET:HE2	2:B:989:ILE:HG21	1.98	0.45
2:B:489:MET:SD	2:B:527:ARG:HD2	2.56	0.45
2:B:515:ILE:HD12	2:B:659:LEU:HD11	1.97	0.45
2:C:615:THR:HB	2:C:1333:ALA:HB1	1.97	0.45
3:D:9:TYR:H	3:D:204:ASP:CG	2.23	0.45
3:D:29:THR:HG22	3:D:222:ASP:HB2	1.98	0.45
3:E:137:LEU:HD23	3:E:281:LYS:HG3	1.98	0.45
2:B:384:MET:HA	2:B:708:THR:CG2	2.45	0.45
2:B:510:VAL:O	2:B:513:GLU:HB3	2.16	0.45
2:B:1075:ARG:HB2	2:B:1233:LEU:HD11	1.98	0.45
2:C:979:ILE:HD13	2:C:1013:LYS:HB2	1.98	0.45
3:E:62:VAL:HB	3:E:92:ARG:HD3	1.99	0.45
1:A:201:LYS:O	2:B:629:ARG:HG2	2.16	0.45
1:A:613:ILE:HG21	1:A:639:CYS:HB3	1.98	0.45
2:B:309:TRP:CZ2	2:B:1257:ALA:HB1	2.50	0.45
3:E:146:ARG:NH1	3:E:277:GLU:OE2	2.49	0.45
1:A:735:LYS:O	1:A:765:TYR:OH	2.24	0.45
1:A:1020:SER:OG	1:A:1022:PRO:HD2	2.15	0.45
2:B:609:PRO:HD3	2:B:724:HIS:CD2	2.52	0.45
1:A:428:ILE:HG23	1:A:430:PRO:HD3	1.98	0.45
1:A:452:ALA:HB2	1:A:725:PRO:HB3	1.99	0.45
1:A:926:MET:HE2	1:A:926:MET:HB2	1.76	0.45
2:B:1176:GLU:HB2	2:B:1203:HIS:NE2	2.32	0.45
2:C:311:ASN:O	2:C:315:THR:HB	2.16	0.45
1:A:474:TYR:HD1	1:A:499:VAL:HG22	1.81	0.45
1:A:722:ASP:OD1	1:A:722:ASP:N	2.44	0.45
2:B:287:ARG:HB2	2:B:329:LEU:O	2.16	0.45
2:B:489:MET:HE1	2:B:580:TYR:CE2	2.48	0.45
2:C:405:HIS:ND1	2:C:625:PRO:HA	2.31	0.45
2:B:423:GLU:O	2:B:427:VAL:HG23	2.16	0.45
2:B:777:GLN:O	2:B:786:SER:N	2.49	0.45
2:C:1110:LEU:HD23	2:C:1110:LEU:HA	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:TYR:O	1:A:271:ARG:HG2	2.17	0.45
2:B:370:VAL:HG21	2:B:402:ALA:HB2	1.98	0.45
2:B:449:PHE:CE1	2:B:463:VAL:HG22	2.51	0.45
2:C:585:PHE:CE1	2:C:728:LYS:HE2	2.52	0.45
2:C:775:VAL:HA	2:C:776:ARG:HA	1.72	0.45
1:A:42:PHE:HE1	1:A:47:ARG:HA	1.82	0.45
1:A:280:PRO:HB3	1:A:304:TYR:CE2	2.52	0.45
1:A:1007:LEU:HD12	1:A:1007:LEU:HA	1.86	0.45
2:B:502:PHE:CE1	2:B:539:PHE:HB2	2.52	0.45
2:B:619:ALA:HB2	2:B:711:ASN:HA	1.98	0.45
2:B:813:LEU:HG	2:B:1010:ARG:HH11	1.82	0.45
2:C:264:LEU:HD21	2:C:362:LEU:HA	1.99	0.45
1:A:25:ILE:HD12	1:A:25:ILE:HA	1.82	0.44
1:A:179:TYR:HB3	1:A:221:TYR:CD1	2.52	0.44
1:A:857:GLN:HB3	1:A:877:LYS:HG3	1.98	0.44
1:A:1007:LEU:HD21	1:A:1053:ILE:HG21	1.99	0.44
2:C:999:LYS:HG2	2:C:1009:THR:HA	1.99	0.44
1:A:315:LEU:O	1:A:319:MET:HG3	2.17	0.44
2:C:332:THR:HG23	2:C:1270:LEU:HD12	2.00	0.44
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.49	0.44
2:C:583:GLU:H	2:C:583:GLU:CD	2.24	0.44
2:C:605:ARG:O	2:C:608:THR:HG23	2.18	0.44
2:C:1249:ASN:HB3	2:C:1250:GLU:H	1.65	0.44
2:C:186:ASP:O	2:C:190:VAL:HB	2.17	0.44
2:C:962:ASP:OD1	2:C:962:ASP:N	2.48	0.44
1:A:7:ILE:HD11	1:A:250:LEU:HD21	1.98	0.44
1:A:417:TYR:CD2	1:A:490:LEU:HD22	2.52	0.44
2:B:347:ALA:HB2	2:B:1301:VAL:HG22	1.98	0.44
2:C:1085:ASP:HA	2:C:1086:PRO:HD3	1.88	0.44
1:A:50:THR:HA	1:A:170:ASN:ND2	2.33	0.44
1:A:267:THR:OG1	1:A:320:TYR:OH	2.26	0.44
1:A:491:ASP:HA	1:A:494:THR:HG22	1.99	0.44
2:B:933:ASN:HB3	2:B:935:GLN:HB2	1.98	0.44
2:C:1051:GLN:O	2:C:1055:LEU:HB2	2.16	0.44
3:D:231:MET:HB2	3:D:231:MET:HE3	1.57	0.44
1:A:43:ASN:HB3	1:A:48:SER:OG	2.16	0.44
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.52	0.44
1:A:154:PHE:CD2	1:A:185:HIS:HA	2.52	0.44
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.49	0.44
1:A:485:MET:HB2	1:A:491:ASP:OD1	2.18	0.44
1:A:1049:TYR:C	1:A:1051:PRO:HD3	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:649:ALA:HB1	2:B:692:ASP:OD1	2.17	0.44
2:C:1201:LEU:HD12	2:C:1201:LEU:HA	1.80	0.44
3:E:68:ILE:HA	3:E:68:ILE:HD12	1.89	0.44
1:A:196:LEU:HD13	1:A:349:TYR:CE1	2.52	0.44
1:A:767:SER:HB2	1:A:788:ASP:CG	2.43	0.44
2:B:186:ASP:O	2:B:190:VAL:HB	2.17	0.44
1:A:400:VAL:HG22	1:A:774:VAL:HG21	1.99	0.44
1:A:680:THR:HG23	1:A:682:SER:N	2.30	0.44
2:B:169:LYS:O	2:B:202:ALA:N	2.47	0.44
2:B:685:ARG:O	2:B:689:THR:HG23	2.18	0.44
2:B:953:ASP:OD1	2:B:960:THR:OG1	2.34	0.44
2:C:478:ILE:HG13	2:C:762:ILE:HD11	1.98	0.44
2:C:1236:ILE:HD13	2:C:1236:ILE:HA	1.85	0.44
3:E:104:ARG:NH2	3:E:115:GLU:OE2	2.50	0.44
1:A:11:THR:OG1	1:A:254:ASP:OD2	2.36	0.44
1:A:913:LEU:HD22	1:A:919:TYR:CZ	2.53	0.44
2:B:261:ASP:CG	2:B:263:ARG:HE	2.26	0.44
3:E:258:ASN:ND2	3:E:260:MET:SD	2.90	0.44
1:A:154:PHE:HZ	1:A:183:ILE:HB	1.82	0.43
1:A:467:SER:N	1:A:468:PRO:HD2	2.33	0.43
1:A:823:THR:OG1	1:A:825:GLU:OE1	2.36	0.43
3:E:283:LEU:O	3:E:287:PHE:HB2	2.17	0.43
1:A:615:CYS:HB2	1:A:639:CYS:SG	2.58	0.43
2:B:171:GLU:OE2	2:B:174:PHE:N	2.51	0.43
2:C:502:PHE:O	2:C:542:ARG:HG2	2.18	0.43
1:A:844:LEU:HD11	1:A:1017:ILE:HD12	2.00	0.43
2:B:826:GLY:HA3	2:B:949:ALA:HB2	2.00	0.43
2:B:893:ALA:HB1	2:B:915:VAL:HA	2.00	0.43
2:C:152:ASP:OD1	2:C:152:ASP:N	2.50	0.43
2:C:439:VAL:HG23	2:C:440:ILE:HG22	2.01	0.43
2:C:865:ILE:CG1	2:C:1041:ARG:HG2	2.49	0.43
2:C:1015:GLN:H	2:C:1015:GLN:HG2	1.44	0.43
2:C:1121:HIS:CD2	2:C:1123:PRO:HG2	2.53	0.43
1:A:1043:LEU:O	1:A:1047:ASN:HB3	2.19	0.43
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.70	0.43
3:D:60:ARG:O	3:D:62:VAL:HG23	2.18	0.43
1:A:470:LEU:HD21	1:A:530:MET:HE2	2.01	0.43
1:A:532:MET:HG3	1:A:565:ARG:HD2	2.01	0.43
2:C:299:ALA:HB2	2:C:1265:MET:HB3	1.99	0.43
3:D:178:LYS:HA	3:D:250:ARG:O	2.19	0.43
3:D:253:GLU:HA	3:D:254:TYR:HA	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:283:LEU:HA	3:D:286:THR:HG22	2.00	0.43
1:A:485:MET:HG2	1:A:511:ILE:HD11	1.99	0.43
1:A:944:ARG:HA	1:A:1006:MET:HE1	2.00	0.43
2:B:171:GLU:CD	2:B:173:GLN:HB3	2.44	0.43
2:B:617:ASP:OD1	2:B:618:LEU:N	2.51	0.43
2:B:1059:LEU:HD23	2:B:1059:LEU:HA	1.81	0.43
2:C:865:ILE:HD12	2:C:1042:TRP:CE3	2.52	0.43
1:A:95:TRP:O	1:A:98:SER:HB3	2.18	0.43
1:A:734:ILE:HD13	1:A:762:LEU:HD13	2.00	0.43
1:A:882:ASP:OD1	1:A:882:ASP:N	2.52	0.43
2:B:409:ILE:HD13	2:B:625:PRO:HB2	2.01	0.43
2:C:265:VAL:HB	2:C:1304:MET:HB3	2.00	0.43
2:C:340:VAL:HG23	2:C:341:LYS:HG2	2.00	0.43
2:C:685:ARG:O	2:C:689:THR:HG23	2.18	0.43
2:C:811:SER:O	2:C:815:LEU:HB2	2.19	0.43
1:A:199:MET:HG3	1:A:205:VAL:HG21	2.00	0.43
1:A:312:LEU:HD11	1:A:361:SER:HB3	2.00	0.43
1:A:767:SER:N	1:A:788:ASP:OD1	2.52	0.43
2:C:736:SER:HB2	2:C:738:GLU:OE1	2.19	0.43
2:C:1116:ARG:HH22	2:C:1131:PRO:HD2	1.84	0.43
3:E:176:ARG:NH1	3:E:253:GLU:OE2	2.45	0.43
1:A:34:LEU:HG	1:A:38:TYR:CZ	2.54	0.43
1:A:289:ASP:H	1:A:368:THR:HG23	1.84	0.43
1:A:377:LEU:HD22	1:A:768:GLU:HA	2.01	0.43
2:B:1148:SER:HB3	2:B:1151:VAL:HG23	2.01	0.43
2:C:442:PRO:HD2	2:C:475:ILE:HG23	2.00	0.43
2:C:489:MET:HE1	2:C:580:TYR:CE2	2.54	0.43
3:D:68:ILE:HG12	3:D:93:LEU:HD13	2.00	0.43
1:A:261:ILE:HD11	1:A:326:LEU:HD13	2.01	0.42
1:A:586:GLY:HA3	1:A:595:ASN:OD1	2.19	0.42
2:B:286:LEU:HD11	2:B:290:TYR:CD1	2.54	0.42
2:B:892:VAL:HG13	2:B:951:ILE:HG22	2.01	0.42
2:B:145:THR:HB	2:B:1317:VAL:HG23	2.00	0.42
2:C:154:PHE:HB3	2:C:264:LEU:HB2	2.02	0.42
2:C:1085:ASP:HA	2:C:1243:ARG:HH22	1.85	0.42
3:E:261:ARG:NH1	3:E:263:ALA:O	2.52	0.42
1:A:679:LYS:HE2	1:A:690:THR:HG22	2.01	0.42
2:B:439:VAL:HG11	2:B:702:LEU:HD13	2.01	0.42
2:B:484:ARG:O	2:B:527:ARG:NH2	2.53	0.42
2:C:391:GLY:HA3	2:C:392:PRO:HD3	1.84	0.42
2:C:334:LEU:HA	2:C:334:LEU:HD23	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1180:PRO:HA	2:C:1207:MET:SD	2.59	0.42
3:D:77:PHE:HB2	3:D:194:VAL:HG23	2.02	0.42
3:D:283:LEU:O	3:D:287:PHE:HB2	2.20	0.42
1:A:556:THR:HB	1:A:611:ASP:OD2	2.20	0.42
2:B:171:GLU:HG2	2:B:1181:SER:OG	2.19	0.42
2:B:515:ILE:HG21	2:B:655:ILE:HG21	2.02	0.42
2:B:1242:MET:HG2	2:B:1260:PRO:HD3	2.01	0.42
2:C:1066:ARG:HD2	2:C:1296:ILE:HG13	2.02	0.42
2:C:1267:THR:HB	2:C:1299:SER:HB3	2.01	0.42
3:D:189:LEU:HD12	3:D:189:LEU:HA	1.77	0.42
1:A:2:TRP:CD1	1:A:2:TRP:H	2.36	0.42
1:A:628:MET:O	1:A:632:THR:HG22	2.20	0.42
2:B:814:THR:HA	2:B:1010:ARG:HH12	1.84	0.42
2:B:859:ILE:H	2:B:859:ILE:HG13	1.68	0.42
1:A:18:LYS:NZ	1:A:109:ASN:O	2.52	0.42
1:A:565:ARG:HD3	1:A:565:ARG:HA	1.73	0.42
2:B:331:GLU:O	2:B:344:VAL:HA	2.20	0.42
2:B:732:TYR:CE1	2:B:1021:ARG:HG3	2.55	0.42
2:B:954:GLN:NE2	3:D:240:VAL:HG12	2.34	0.42
2:B:1043:SER:HB2	2:B:1046:PHE:CE2	2.55	0.42
2:B:1128:TYR:HB3	2:B:1134:ARG:HG2	2.01	0.42
2:C:1190:ALA:O	2:C:1193:ILE:HG22	2.20	0.42
1:A:251:VAL:HG12	1:A:253:ALA:H	1.84	0.42
1:A:373:ILE:HG12	1:A:817:GLY:N	2.35	0.42
1:A:595:ASN:HD22	1:A:595:ASN:H	1.66	0.42
1:A:936:ALA:HB1	1:A:998:LEU:HD23	2.02	0.42
2:B:664:ASN:O	2:B:668:VAL:HG13	2.20	0.42
2:B:887:VAL:O	2:B:891:HIS:N	2.51	0.42
2:B:924:ASP:O	2:B:927:SER:OG	2.33	0.42
3:D:188:SER:O	3:D:191:ARG:HG3	2.19	0.42
1:A:259:ARG:NH1	1:A:277:ALA:HB2	2.35	0.42
2:B:382:HIS:HD1	2:B:799:THR:HG23	1.84	0.42
2:B:491:ASN:ND2	2:B:750:GLU:O	2.53	0.42
2:C:385:ILE:HD13	2:C:385:ILE:HA	1.75	0.42
2:B:373:ASP:HA	2:B:1315:MET:HE1	2.01	0.41
1:A:409:MET:HE3	1:A:1037:SER:H	1.85	0.41
2:B:336:TYR:HA	3:D:64:GLY:HA3	2.01	0.41
2:B:533:GLN:HB2	2:B:588:LEU:HD12	2.01	0.41
2:B:1129:PRO:HD3	3:E:273:LEU:HD23	2.01	0.41
2:C:259:MET:HB3	2:C:259:MET:HE2	1.78	0.41
2:C:379:LEU:HD23	2:C:379:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:118:ASN:ND2	3:E:118:ASN:H	2.17	0.41
1:A:20:ASN:OD1	1:A:20:ASN:N	2.53	0.41
1:A:319:MET:HE2	1:A:319:MET:HB3	1.81	0.41
1:A:834:THR:O	1:A:838:LYS:HG2	2.20	0.41
2:B:1305:MET:H	2:B:1305:MET:HG2	1.65	0.41
2:C:405:HIS:CE1	2:C:625:PRO:HA	2.55	0.41
2:C:609:PRO:HB2	2:C:634:TYR:CE2	2.55	0.41
2:C:612:PHE:HZ	2:C:1330:ILE:HG22	1.84	0.41
2:C:828:ASP:OD1	2:C:960:THR:OG1	2.32	0.41
2:C:1139:MET:HE3	2:C:1139:MET:HB2	1.88	0.41
3:D:1:MET:HB2	3:D:121:PHE:CZ	2.55	0.41
3:D:87:HIS:CE1	3:D:89:TYR:H	2.38	0.41
3:D:160:LEU:HB3	3:D:161:ALA:H	1.77	0.41
1:A:384:GLU:HA	1:A:802:THR:HG22	2.01	0.41
1:A:538:ALA:HB1	1:A:678:LEU:HD11	2.02	0.41
1:A:595:ASN:HD22	1:A:595:ASN:N	2.18	0.41
2:B:147:VAL:HG13	2:B:379:LEU:HD21	2.01	0.41
2:B:233:VAL:HA	2:B:234:PRO:HD2	1.80	0.41
2:B:814:THR:HA	2:B:1010:ARG:NH1	2.36	0.41
2:B:1224:GLY:HA2	2:C:124:GLN:HG2	2.02	0.41
2:B:1305:MET:HE2	2:B:1305:MET:HB3	1.86	0.41
2:C:256:PHE:CE2	2:C:815:LEU:HD22	2.55	0.41
2:C:451:GLU:O	2:C:452:ASN:HB2	2.20	0.41
2:C:823:ILE:O	2:C:968:ARG:HD3	2.20	0.41
3:E:182:TRP:CE3	3:E:182:TRP:N	2.88	0.41
3:E:224:PHE:O	3:E:228:LEU:HG	2.20	0.41
1:A:178:PRO:HB2	1:A:179:TYR:CD1	2.55	0.41
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.90	0.41
2:B:208:LEU:HD22	2:B:213:PHE:CE2	2.55	0.41
2:B:376:ILE:HD13	2:B:379:LEU:HD12	2.01	0.41
2:B:537:LEU:HD22	2:B:537:LEU:HA	1.93	0.41
2:C:264:LEU:HD22	2:C:264:LEU:HA	1.87	0.41
2:C:659:LEU:O	2:C:663:VAL:HG23	2.20	0.41
1:A:50:THR:O	1:A:50:THR:OG1	2.39	0.41
1:A:132:GLN:H	1:A:132:GLN:HG2	1.70	0.41
1:A:309:ASN:OD1	1:A:311:GLN:HG3	2.20	0.41
1:A:882:ASP:HA	1:A:883:PRO:HD3	1.95	0.41
2:B:397:LEU:HA	2:B:1309:ILE:HD13	2.02	0.41
2:B:640:GLN:HE22	2:B:647:GLU:HB3	1.86	0.41
2:C:382:HIS:ND1	2:C:799:THR:HG23	2.35	0.41
2:C:1233:LEU:HD13	2:C:1233:LEU:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:281:LYS:O	3:E:285:LEU:HG	2.21	0.41
1:A:684:ASN:HA	1:A:685:PRO:HD3	1.91	0.41
2:B:232:LEU:HD11	2:B:971:MET:HE2	2.03	0.41
2:B:324:LYS:O	2:B:1267:THR:HG22	2.21	0.41
2:C:412:LEU:HD23	2:C:412:LEU:HA	1.80	0.41
2:C:419:TYR:HA	2:C:420:PRO:HD2	1.92	0.41
2:C:635:ILE:HA	2:C:636:PRO:HD3	1.89	0.41
2:C:836:GLN:N	2:C:836:GLN:OE1	2.54	0.41
3:E:93:LEU:HA	3:E:93:LEU:HD23	1.69	0.41
3:E:182:TRP:NE1	3:E:185:SER:HA	2.35	0.41
1:A:73:ARG:O	1:A:76:LEU:HB3	2.21	0.41
1:A:557:SER:HB3	1:A:583:ARG:HB2	2.01	0.41
2:B:1050:LEU:HA	2:B:1050:LEU:HD23	1.83	0.41
2:B:1219:ASP:HA	2:B:1220:PRO:HD3	1.86	0.41
2:C:339:LEU:C	2:C:341:LYS:H	2.29	0.41
2:C:648:PHE:HB2	2:C:699:THR:HG21	2.03	0.41
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.83	0.41
1:A:177:THR:HA	1:A:178:PRO:HD3	1.93	0.41
1:A:271:ARG:HE	1:A:271:ARG:HB3	1.66	0.41
1:A:583:ARG:HH11	1:A:583:ARG:H	1.68	0.41
1:A:647:LEU:HD22	1:A:691:TYR:HB3	2.03	0.41
2:B:353:PHE:CD2	2:B:1061:LEU:HD23	2.56	0.41
2:B:415:ALA:O	2:B:419:TYR:N	2.45	0.41
2:B:612:PHE:HZ	2:B:1330:ILE:HG22	1.86	0.41
2:B:635:ILE:HA	2:B:636:PRO:HD3	1.83	0.41
2:B:1074:VAL:HG22	2:B:1171:ILE:HD12	2.03	0.41
2:C:612:PHE:CZ	2:C:1330:ILE:HG22	2.56	0.41
2:C:1220:PRO:HA	2:C:1221:PRO:HD3	1.95	0.41
2:C:1280:PRO:HB3	2:C:1285:GLN:O	2.21	0.41
1:A:405:MET:HE2	1:A:827:ARG:HD2	2.03	0.41
1:A:616:ASP:OD1	1:A:691:TYR:OH	2.31	0.41
1:A:633:ILE:HD13	1:A:633:ILE:HA	1.87	0.41
2:B:802:GLN:HB2	2:B:997:TYR:CE2	2.56	0.41
2:B:1002:LEU:HD23	2:B:1002:LEU:HA	1.87	0.41
2:C:403:PHE:CE2	2:C:625:PRO:HD3	2.56	0.41
2:C:876:GLY:O	2:C:903:ASN:ND2	2.51	0.41
3:D:19:ILE:H	3:D:19:ILE:HG13	1.66	0.41
2:B:401:LEU:HD23	2:B:401:LEU:HA	1.87	0.40
2:B:817:ASP:OD1	2:B:821:ASN:ND2	2.55	0.40
3:E:273:LEU:O	3:E:277:GLU:HG3	2.21	0.40
1:A:951:LEU:HD12	1:A:951:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:475:ILE:H	2:C:475:ILE:HG13	1.55	0.40
2:C:833:ARG:HG3	2:C:922:TYR:CE1	2.56	0.40
2:C:1134:ARG:HB3	2:C:1135:PRO:HD2	2.03	0.40
3:E:109:GLY:HA2	3:E:199:LEU:HD12	2.02	0.40
1:A:431:ALA:O	1:A:435:ILE:HG12	2.22	0.40
2:B:177:LYS:HD3	2:B:177:LYS:O	2.22	0.40
2:C:166:TYR:HA	2:C:205:ASN:O	2.22	0.40
2:C:331:GLU:HA	2:C:335:ASP:OD2	2.22	0.40
2:C:956:ASP:O	2:C:1044:ARG:NH1	2.55	0.40
2:C:1271:SER:HB3	2:C:1277:LEU:HD21	2.03	0.40
3:E:124:PRO:HA	3:E:127:VAL:HG22	2.03	0.40
3:E:189:LEU:HD12	3:E:189:LEU:HA	1.85	0.40
1:A:66:ASP:CG	1:A:122:ARG:HH21	2.24	0.40
1:A:293:LEU:HD22	1:A:297:LEU:HG	2.02	0.40
1:A:858:VAL:HG22	1:A:918:ILE:HB	2.03	0.40
2:B:605:ARG:O	2:B:608:THR:HG23	2.21	0.40
2:B:1228:ARG:HG2	2:B:1231:TYR:CE1	2.55	0.40
2:C:509:VAL:HG22	2:C:683:TRP:CH2	2.55	0.40
2:C:820:ILE:HD13	2:C:820:ILE:HA	1.97	0.40
1:A:13:VAL:HG23	1:A:213:TRP:HD1	1.85	0.40
1:A:764:SER:HA	1:A:795:GLU:HG3	2.04	0.40
1:A:859:VAL:HB	1:A:919:TYR:CD1	2.56	0.40
1:A:977:HIS:HB2	1:A:981:ARG:HB3	2.03	0.40
2:B:832:MET:SD	2:B:848:ARG:HB3	2.61	0.40
3:D:44:LEU:HG	3:D:174:VAL:HG22	2.04	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	1055/1058 (100%)	1011 (96%)	41 (4%)	3 (0%)	36 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1187/1333 (89%)	1133 (96%)	49 (4%)	5 (0%)	30	61
2	C	1246/1333 (94%)	1180 (95%)	63 (5%)	3 (0%)	43	73
3	D	290/448 (65%)	283 (98%)	5 (2%)	2 (1%)	18	49
3	E	290/448 (65%)	282 (97%)	7 (2%)	1 (0%)	36	67
All	All	4068/4620 (88%)	3889 (96%)	165 (4%)	14 (0%)	37	67

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	B	1035	ILE
2	B	1123	PRO
2	C	1267	THR
3	D	61	ASN
3	E	80	SER
2	C	1123	PRO
1	A	483	MET
2	B	503	GLU
2	B	738	GLU
1	A	350	PRO
2	C	340	VAL
2	B	1034	GLN
3	D	244	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	942/943 (100%)	839 (89%)	103 (11%)	6	24
2	B	1038/1153 (90%)	945 (91%)	93 (9%)	9	33
2	C	1089/1153 (94%)	988 (91%)	101 (9%)	8	31
3	D	240/379 (63%)	217 (90%)	23 (10%)	8	30
3	E	240/379 (63%)	212 (88%)	28 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3549/4007 (89%)	3201 (90%)	348 (10%)	10	29

All (348) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	12	ARG
1	A	13	VAL
1	A	31	VAL
1	A	34	LEU
1	A	36	THR
1	A	50	THR
1	A	76	LEU
1	A	77	LYS
1	A	88	LEU
1	A	89	ILE
1	A	99	VAL
1	A	104	VAL
1	A	108	ASP
1	A	112	ARG
1	A	117	LEU
1	A	119	VAL
1	A	132	GLN
1	A	133	LEU
1	A	142	ASN
1	A	157	LEU
1	A	166	ILE
1	A	183	ILE
1	A	188	THR
1	A	191	GLU
1	A	199	MET
1	A	202	SER
1	A	207	THR
1	A	210	SER
1	A	216	LEU
1	A	234	LYS
1	A	242	LYS
1	A	260	LEU
1	A	269	VAL
1	A	275	ILE
1	A	287	VAL
1	A	293	LEU

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Mol	Chain	Res	Type
1	A	312	LEU
1	A	314	ARG
1	A	337	LEU
1	A	339	GLN
1	A	357	THR
1	A	360	THR
1	A	377	LEU
1	A	379	VAL
1	A	396	THR
1	A	401	ILE
1	A	402	THR
1	A	405	MET
1	A	444	LEU
1	A	451	ARG
1	A	466	LEU
1	A	469	LEU
1	A	493	LEU
1	A	506	VAL
1	A	514	LEU
1	A	523	MET
1	A	583	ARG
1	A	585	ILE
1	A	598	VAL
1	A	611	ASP
1	A	613	ILE
1	A	628	MET
1	A	648	VAL
1	A	680	THR
1	A	684	ASN
1	A	697	ILE
1	A	714	ARG
1	A	719	VAL
1	A	721	ASP
1	A	726	ILE
1	A	742	SER
1	A	757	LEU
1	A	762	LEU
1	A	770	THR
1	A	774	VAL
1	A	784	ILE
1	A	794	LEU
1	A	823	THR

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Mol	Chain	Res	Type
1	A	832	GLU
1	A	844	LEU
1	A	855	MET
1	A	872	VAL
1	A	877	LYS
1	A	890	LEU
1	A	905	GLN
1	A	910	ASN
1	A	914	GLU
1	A	926	MET
1	A	941	ASP
1	A	970	ARG
1	A	977	HIS
1	A	981	ARG
1	A	987	LEU
1	A	1005	LEU
1	A	1007	LEU
1	A	1013	THR
1	A	1018	ARG
1	A	1024	LEU
1	A	1025	ILE
1	A	1034	ARG
1	A	1035	LEU
1	A	1047	ASN
2	B	147	VAL
2	B	168	VAL
2	B	177	LYS
2	B	190	VAL
2	B	194	VAL
2	B	217	THR
2	B	233	VAL
2	B	238	THR
2	B	264	LEU
2	B	265	VAL
2	B	271	THR
2	B	282	VAL
2	B	287	ARG
2	B	294	VAL
2	B	323	THR
2	B	330	THR
2	B	334	LEU
2	B	335	ASP

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Mol	Chain	Res	Type
2	B	383	SER
2	B	384	MET
2	B	388	GLN
2	B	397	LEU
2	B	439	VAL
2	B	451	GLU
2	B	452	ASN
2	B	457	GLN
2	B	462	LEU
2	B	480	LEU
2	B	495	LEU
2	B	527	ARG
2	B	532	ILE
2	B	533	GLN
2	B	537	LEU
2	B	546	VAL
2	B	552	VAL
2	B	567	GLU
2	B	579	LEU
2	B	633	THR
2	B	637	TYR
2	B	643	THR
2	B	654	THR
2	B	656	VAL
2	B	661	ASN
2	B	662	VAL
2	B	668	VAL
2	B	687	LEU
2	B	704	VAL
2	B	708	THR
2	B	735	THR
2	B	751	THR
2	B	755	LEU
2	B	774	LEU
2	B	798	THR
2	B	809	VAL
2	B	812	LYS
2	B	815	LEU
2	B	820	ILE
2	B	890	THR
2	B	894	VAL
2	B	899	SER

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Mol	Chain	Res	Type
2	B	912	GLU
2	B	917	VAL
2	B	945	VAL
2	B	946	LEU
2	B	948	ILE
2	B	951	ILE
2	B	958	ILE
2	B	1008	LEU
2	B	1022	ILE
2	B	1035	ILE
2	B	1052	LEU
2	B	1060	ARG
2	B	1067	ILE
2	B	1082	ASP
2	B	1092	VAL
2	B	1110	LEU
2	B	1144	ARG
2	B	1159	VAL
2	B	1179	THR
2	B	1193	ILE
2	B	1212	ARG
2	B	1228	ARG
2	B	1230	ILE
2	B	1233	LEU
2	B	1234	GLN
2	B	1237	SER
2	B	1270	LEU
2	B	1293	VAL
2	B	1311	THR
2	B	1315	MET
2	B	1319	ARG
2	B	1320	VAL
2	B	1331	ARG
2	C	74	LYS
2	C	79	SER
2	C	97	GLU
2	C	98	ASN
2	C	112	THR
2	C	116	SER
2	C	120	VAL
2	C	134	THR
2	C	137	ILE

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Mol	Chain	Res	Type
2	C	147	VAL
2	C	168	VAL
2	C	175	THR
2	C	176	LYS
2	C	180	LEU
2	C	190	VAL
2	C	207	ASP
2	C	217	THR
2	C	243	GLN
2	C	263	ARG
2	C	264	LEU
2	C	265	VAL
2	C	280	THR
2	C	282	VAL
2	C	285	VAL
2	C	294	VAL
2	C	315	THR
2	C	323	THR
2	C	327	LEU
2	C	330	THR
2	C	340	VAL
2	C	373	ASP
2	C	384	MET
2	C	385	ILE
2	C	431	THR
2	C	439	VAL
2	C	451	GLU
2	C	462	LEU
2	C	475	ILE
2	C	486	VAL
2	C	495	LEU
2	C	508	ILE
2	C	512	LEU
2	C	527	ARG
2	C	546	VAL
2	C	552	VAL
2	C	557	THR
2	C	574	LYS
2	C	601	ILE
2	C	626	ARG
2	C	630	ASN
2	C	637	TYR

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Mol	Chain	Res	Type
2	C	638	THR
2	C	654	THR
2	C	656	VAL
2	C	661	ASN
2	C	696	VAL
2	C	704	VAL
2	C	734	ILE
2	C	767	LEU
2	C	769	GLN
2	C	774	LEU
2	C	776	ARG
2	C	790	GLU
2	C	798	THR
2	C	810	LEU
2	C	828	ASP
2	C	833	ARG
2	C	851	THR
2	C	856	LEU
2	C	865	ILE
2	C	892	VAL
2	C	946	LEU
2	C	948	ILE
2	C	951	ILE
2	C	964	VAL
2	C	980	ARG
2	C	1014	MET
2	C	1015	GLN
2	C	1052	LEU
2	C	1055	LEU
2	C	1060	ARG
2	C	1061	LEU
2	C	1062	ILE
2	C	1110	LEU
2	C	1148	SER
2	C	1155	ILE
2	C	1159	VAL
2	C	1169	LEU
2	C	1171	ILE
2	C	1193	ILE
2	C	1200	LYS
2	C	1201	LEU
2	C	1202	PHE

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Mol	Chain	Res	Type
2	C	1230	ILE
2	C	1233	LEU
2	C	1250	GLU
2	C	1251	VAL
2	C	1269	THR
2	C	1277	LEU
2	C	1291	LEU
2	C	1320	VAL
3	D	2	LEU
3	D	21	ASN
3	D	29	THR
3	D	35	LEU
3	D	47	LYS
3	D	54	THR
3	D	92	ARG
3	D	93	LEU
3	D	107	LEU
3	D	116	THR
3	D	133	THR
3	D	158	LEU
3	D	189	LEU
3	D	191	ARG
3	D	193	VAL
3	D	194	VAL
3	D	214	ARG
3	D	226	MET
3	D	235	VAL
3	D	239	VAL
3	D	252	LEU
3	D	253	GLU
3	D	275	ARG
3	E	2	LEU
3	E	24	THR
3	E	29	THR
3	E	35	LEU
3	E	48	THR
3	E	66	VAL
3	E	68	ILE
3	E	93	LEU
3	E	94	SER
3	E	98	LEU
3	E	118	ASN

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Mol	Chain	Res	Type
3	E	133	THR
3	E	139	ASN
3	E	142	THR
3	E	158	LEU
3	E	160	LEU
3	E	189	LEU
3	E	193	VAL
3	E	194	VAL
3	E	226	MET
3	E	240	VAL
3	E	244	VAL
3	E	247	ARG
3	E	252	LEU
3	E	262	THR
3	E	266	THR
3	E	273	LEU
3	E	288	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	58	GLN
1	A	114	ASN
1	A	125	ASN
1	A	457	ASN
1	A	527	ASN
1	A	595	ASN
1	A	779	ASN
1	A	955	ASN
1	A	1030	ASN
2	B	195	ASN
2	B	491	ASN
2	B	526	ASN
2	B	682	GLN
2	B	698	HIS
2	B	731	GLN
2	B	769	GLN
2	B	937	ASN
2	B	954	GLN
2	B	1064	ASN
2	B	1283	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1285	GLN
2	B	1321	ASN
2	C	283	ASN
2	C	430	ASN
2	C	646	ASN
2	C	664	ASN
2	C	682	GLN
2	C	769	GLN
2	C	858	HIS
2	C	864	HIS
2	C	981	HIS
2	C	1051	GLN
2	C	1138	HIS
2	C	1273	ASN
3	D	25	ASN
3	D	82	GLN
3	D	276	HIS
3	D	284	GLN
3	E	220	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

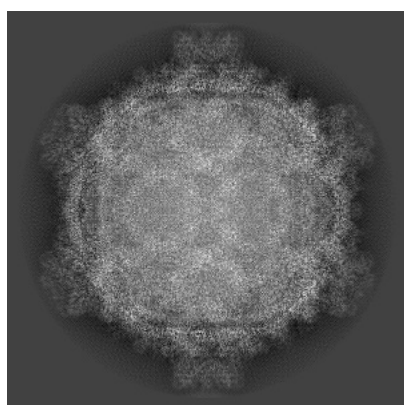
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6371. These allow visual inspection of the internal detail of the map and identification of artifacts.

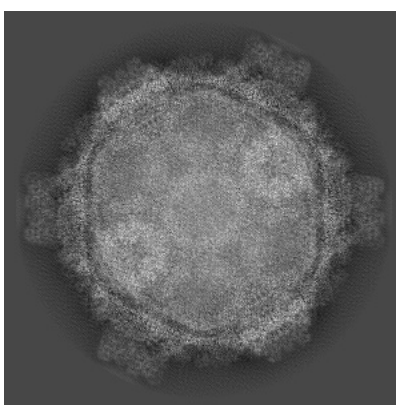
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

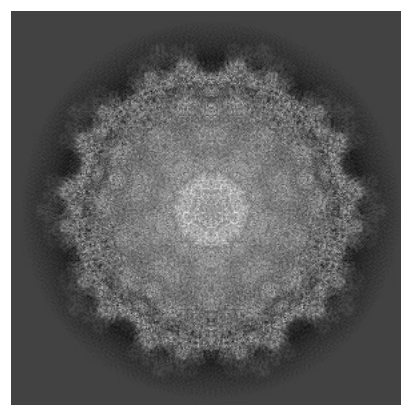
6.1.1 Primary map



X



Y

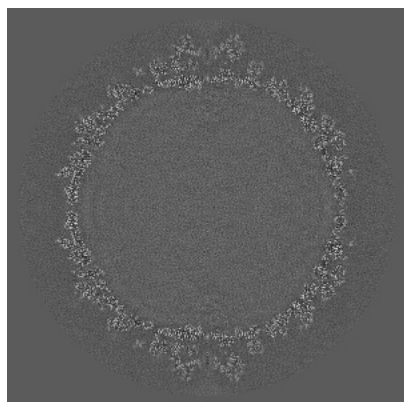


Z

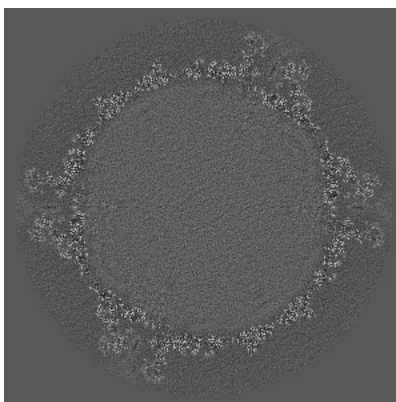
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

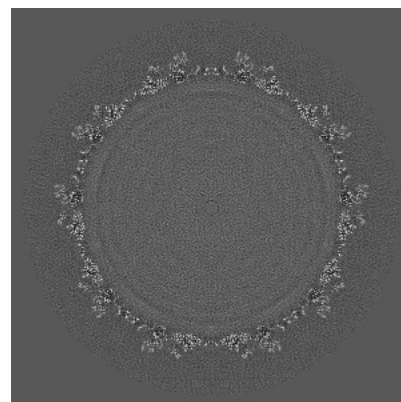
6.2.1 Primary map



X Index: 350



Y Index: 350

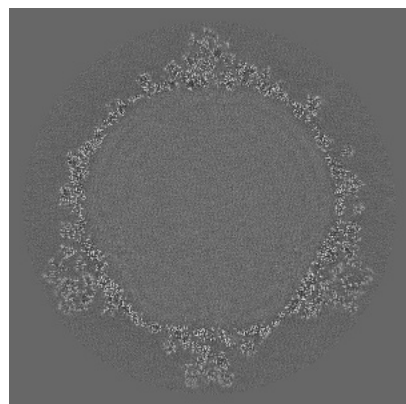


Z Index: 350

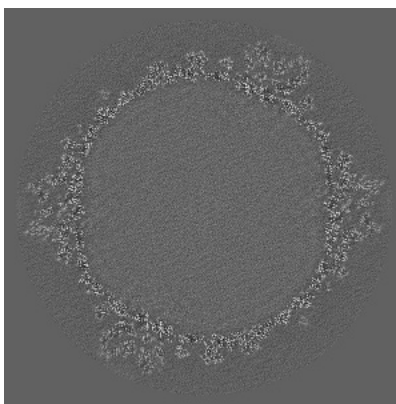
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

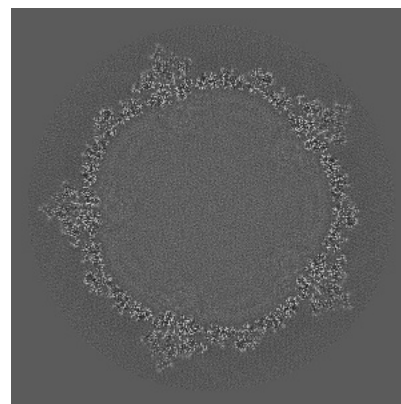
6.3.1 Primary map



X Index: 302



Y Index: 328

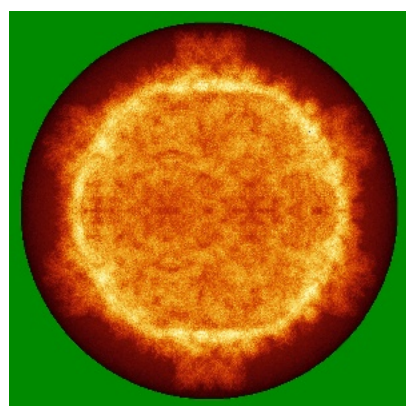


Z Index: 273

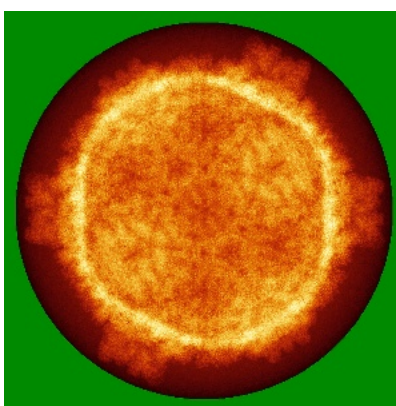
The images above show the largest variance slices of the map in three orthogonal directions.

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

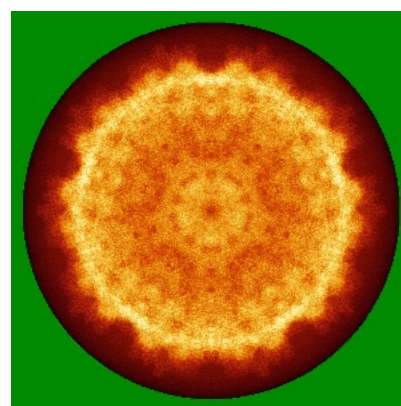
6.4.1 Primary map



X



Y

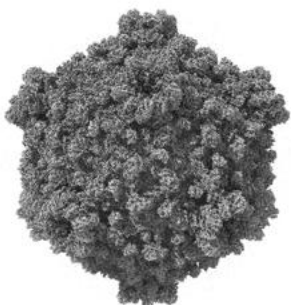


Z

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

6.5 Orthogonal surface views [i](#)

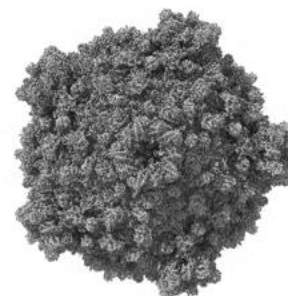
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

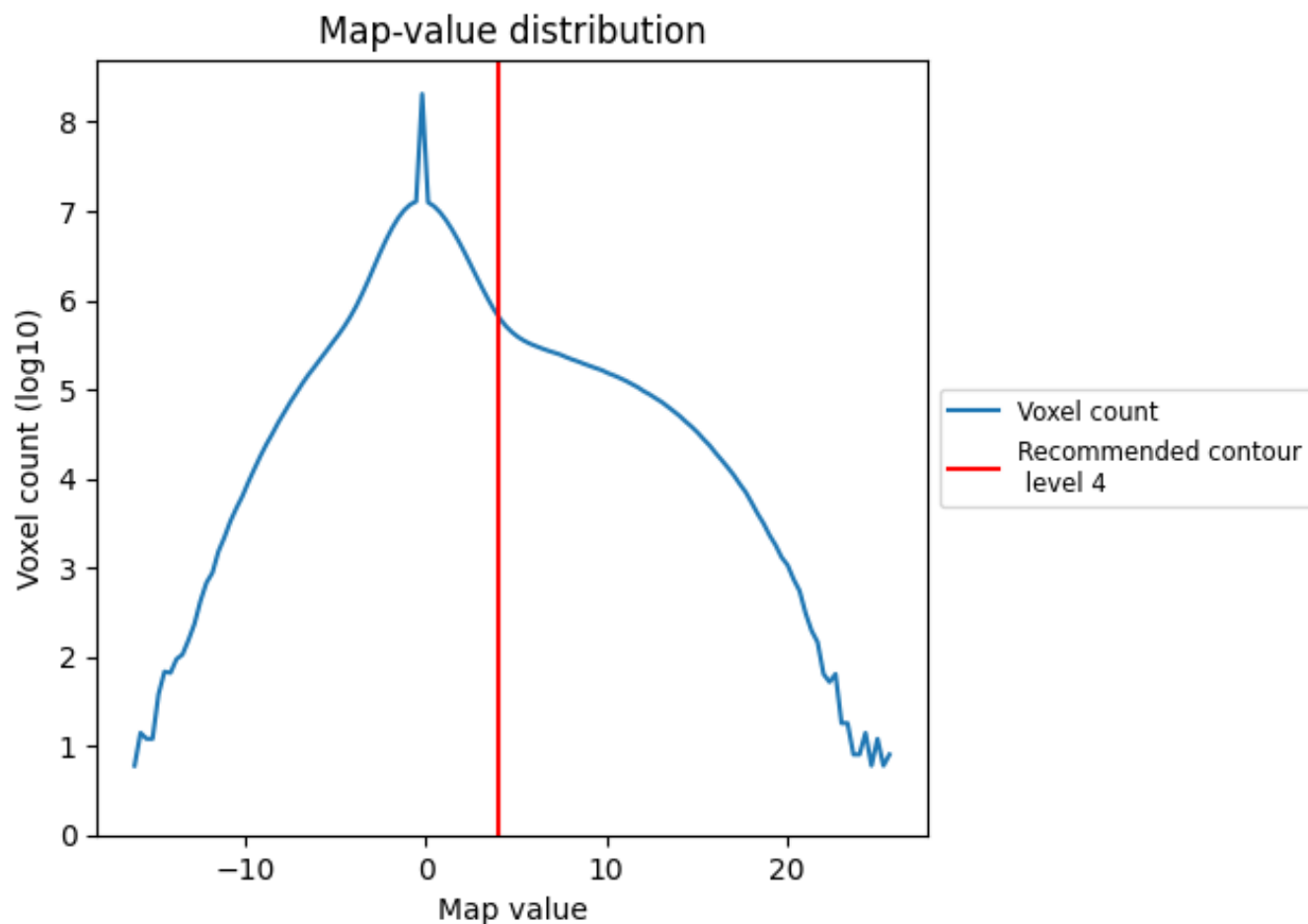
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

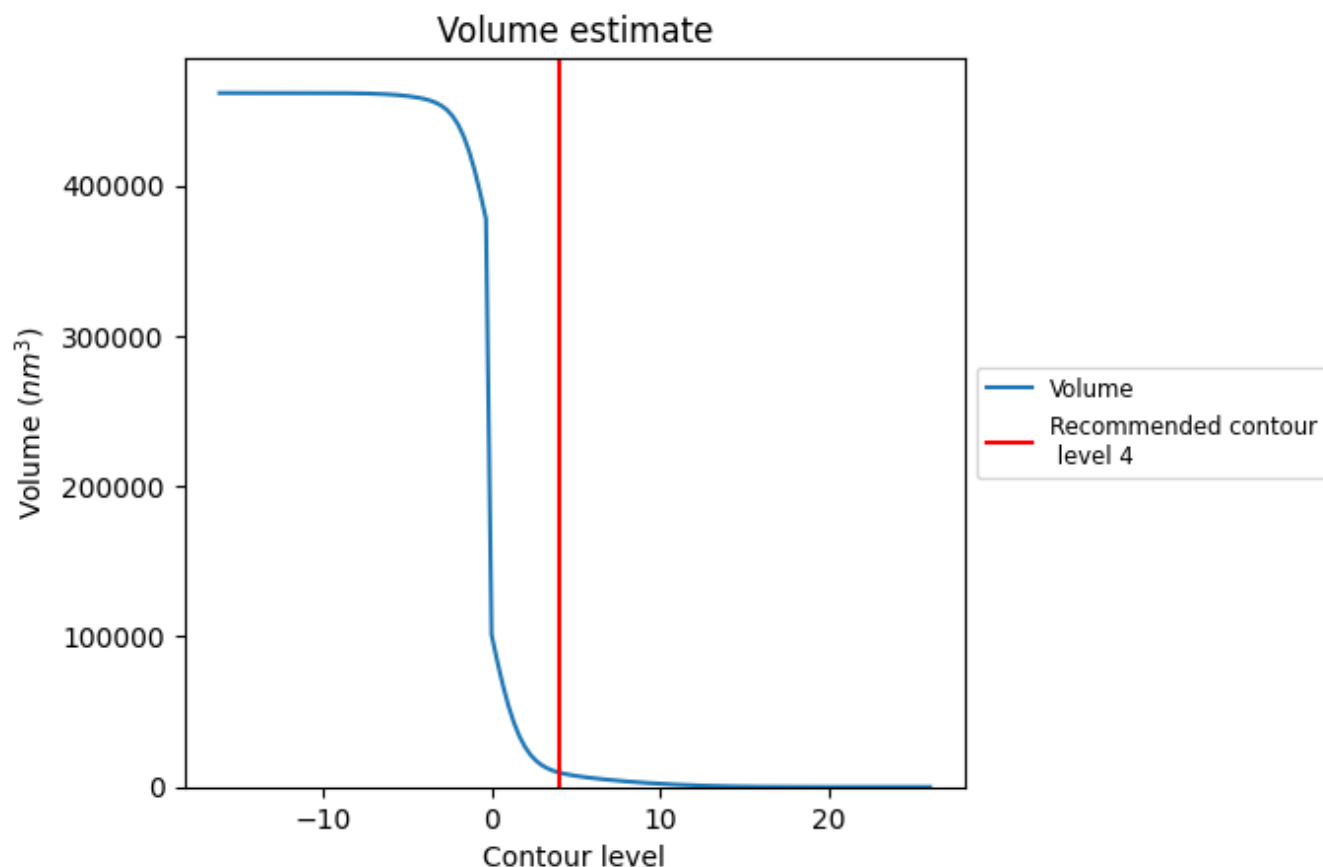
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

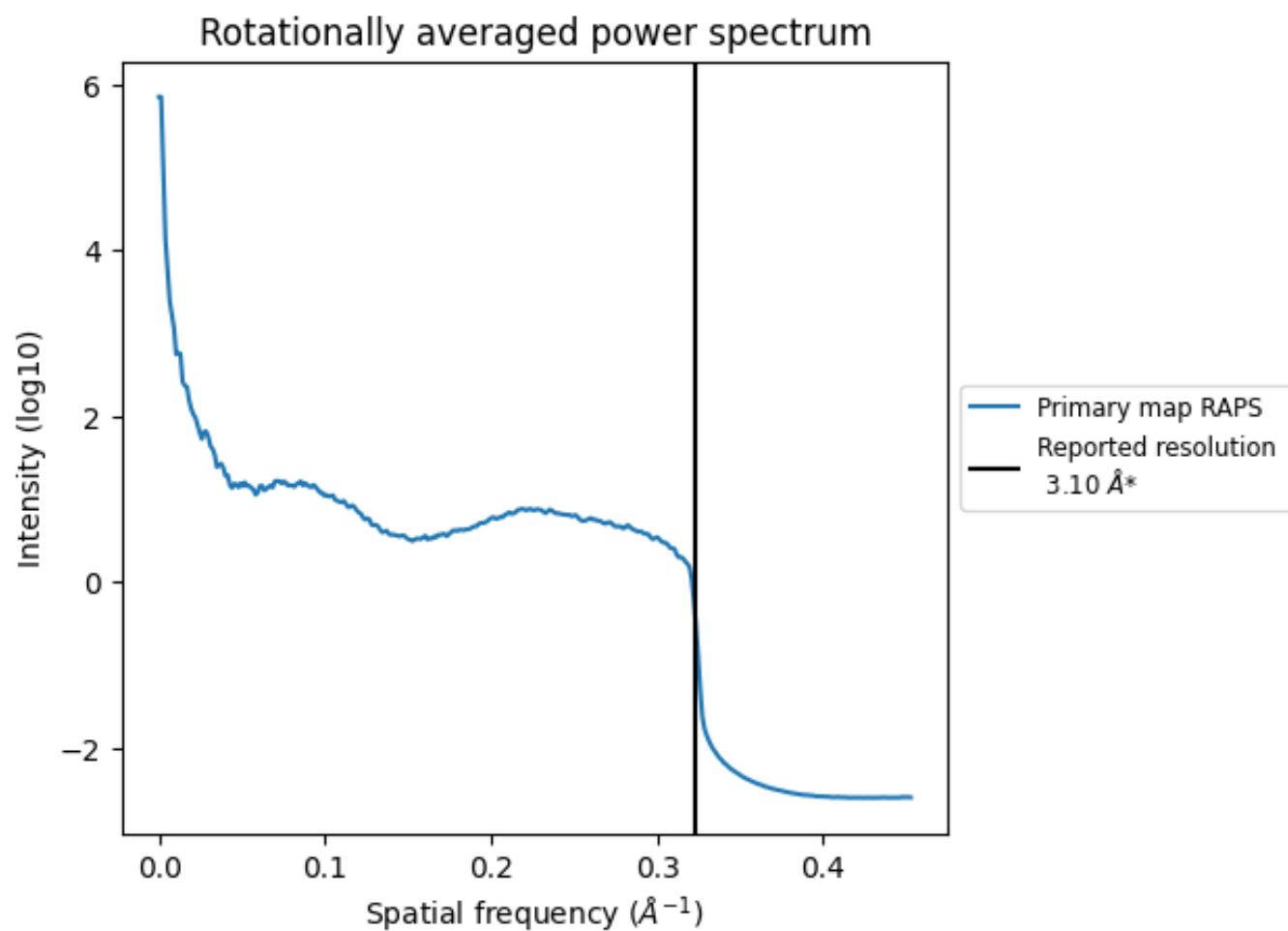
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9600 nm^3 ; this corresponds to an approximate mass of 8672 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 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

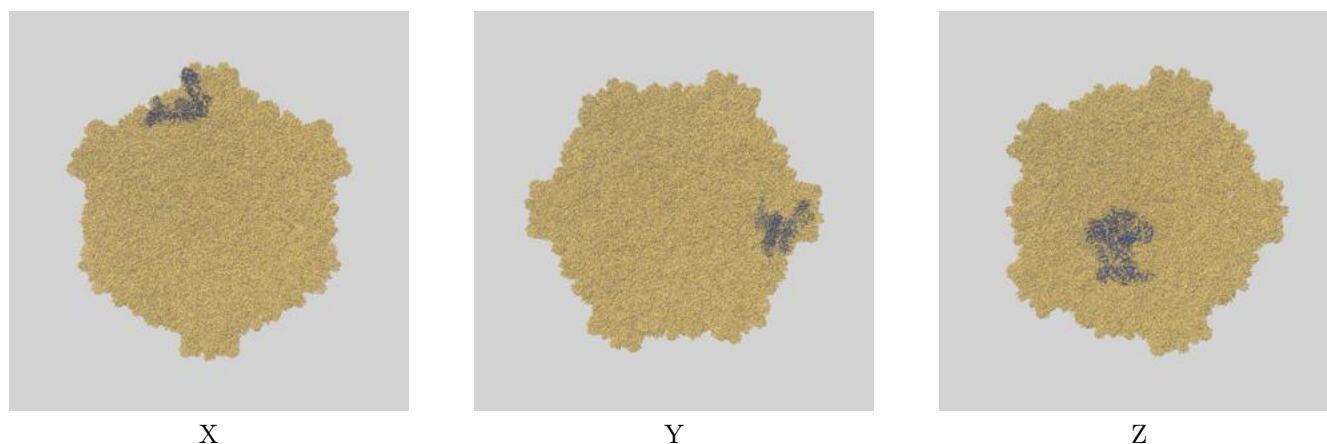
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

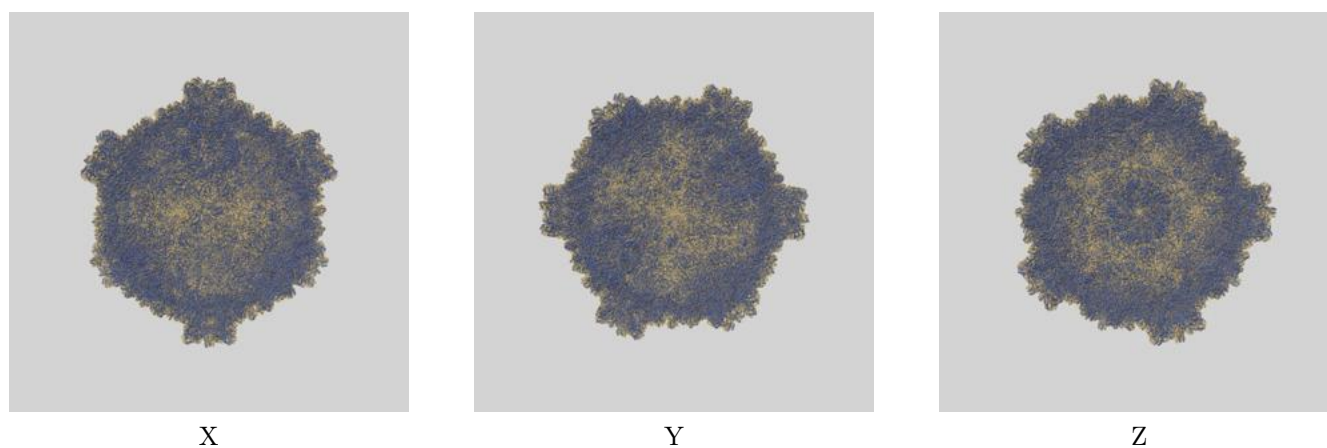
This section contains information regarding the fit between EMDB map EMD-6371 and PDB model 3JAZ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



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



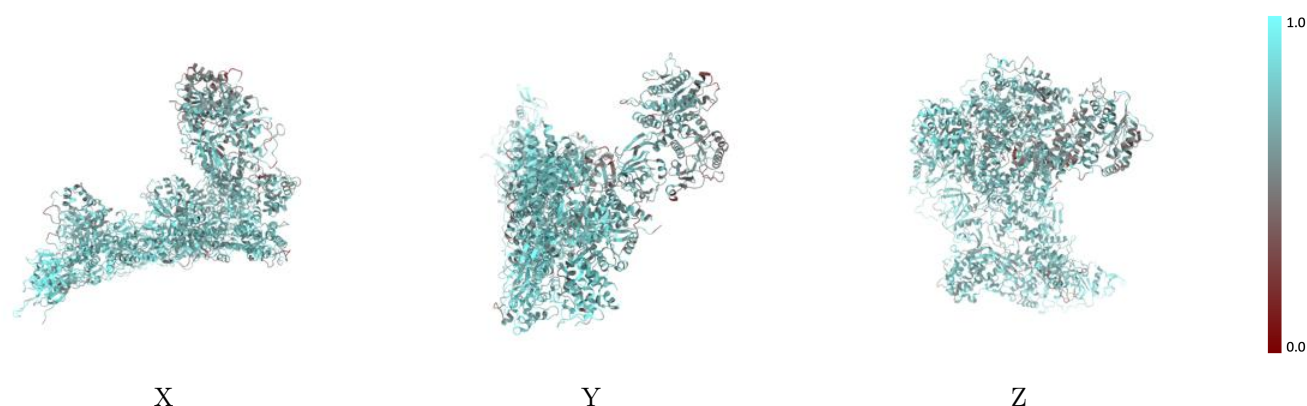
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



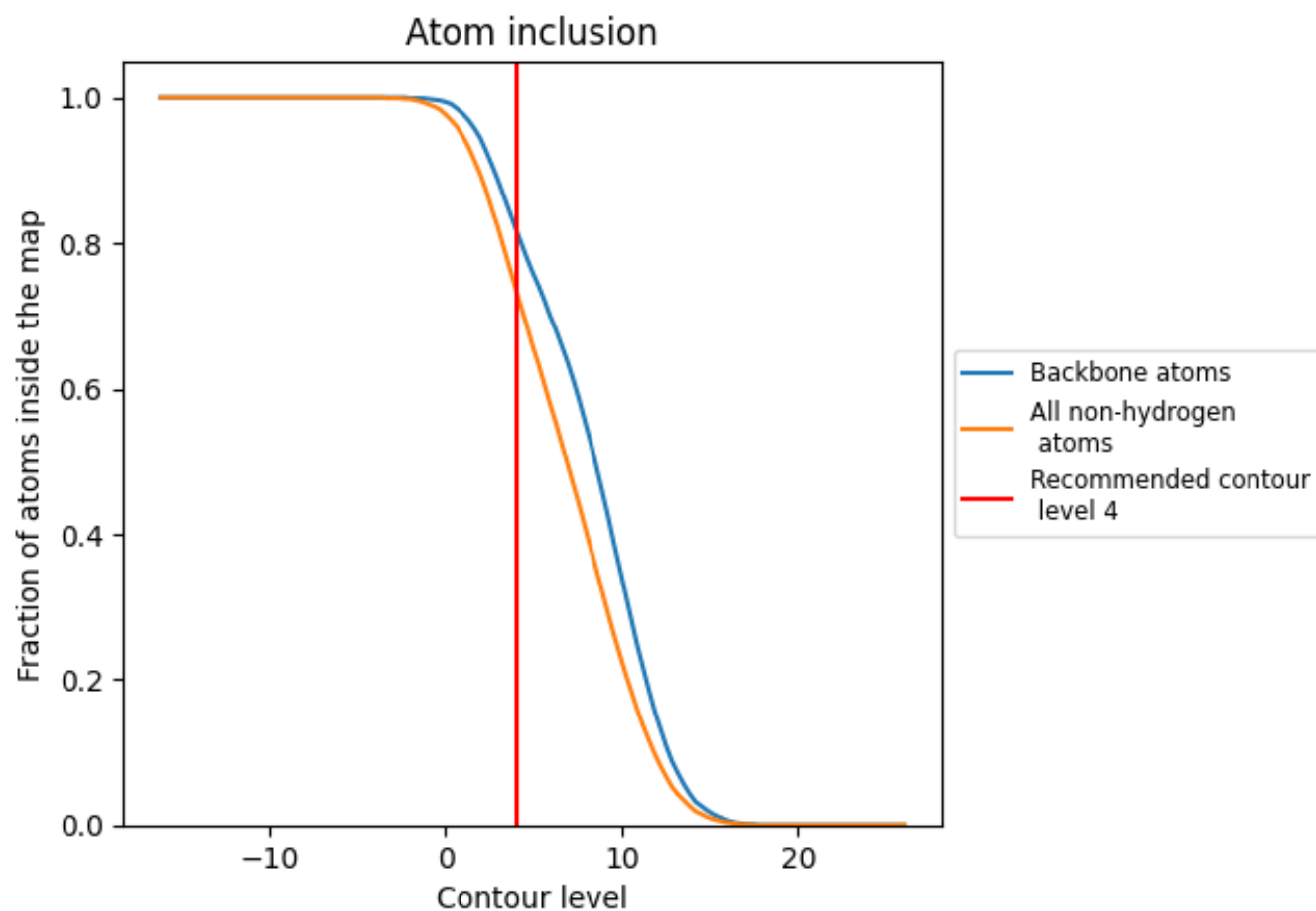
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.5370
A	0.6460	0.5100
B	0.7680	0.5470
C	0.7700	0.5480
D	0.7760	0.5510
E	0.7530	0.5390

