



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:43 PM UTC

PDB ID : 3JB0 / pdb_00003jb0
EMDB ID : EMD-6374
Title : Atomic model of cytoplasmic polyhedrosis virus with GTP
Authors : Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on : 2015-07-06
Resolution : 2.90 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:

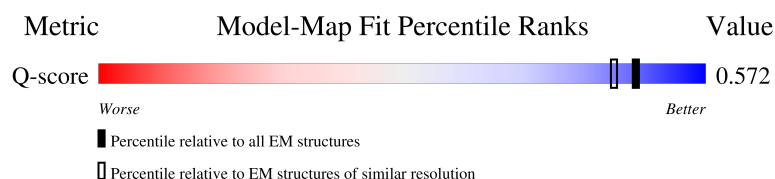
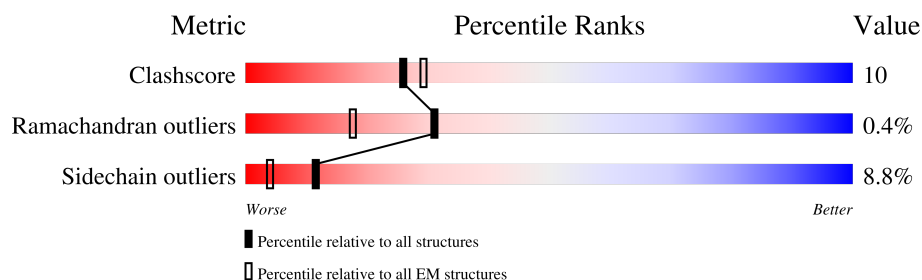
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	
2	B	1333	
2	C	1333	
3	D	448	

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Mol	Chain	Length	Quality of chain
3	E	448	48% 16% 35%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32276 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		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

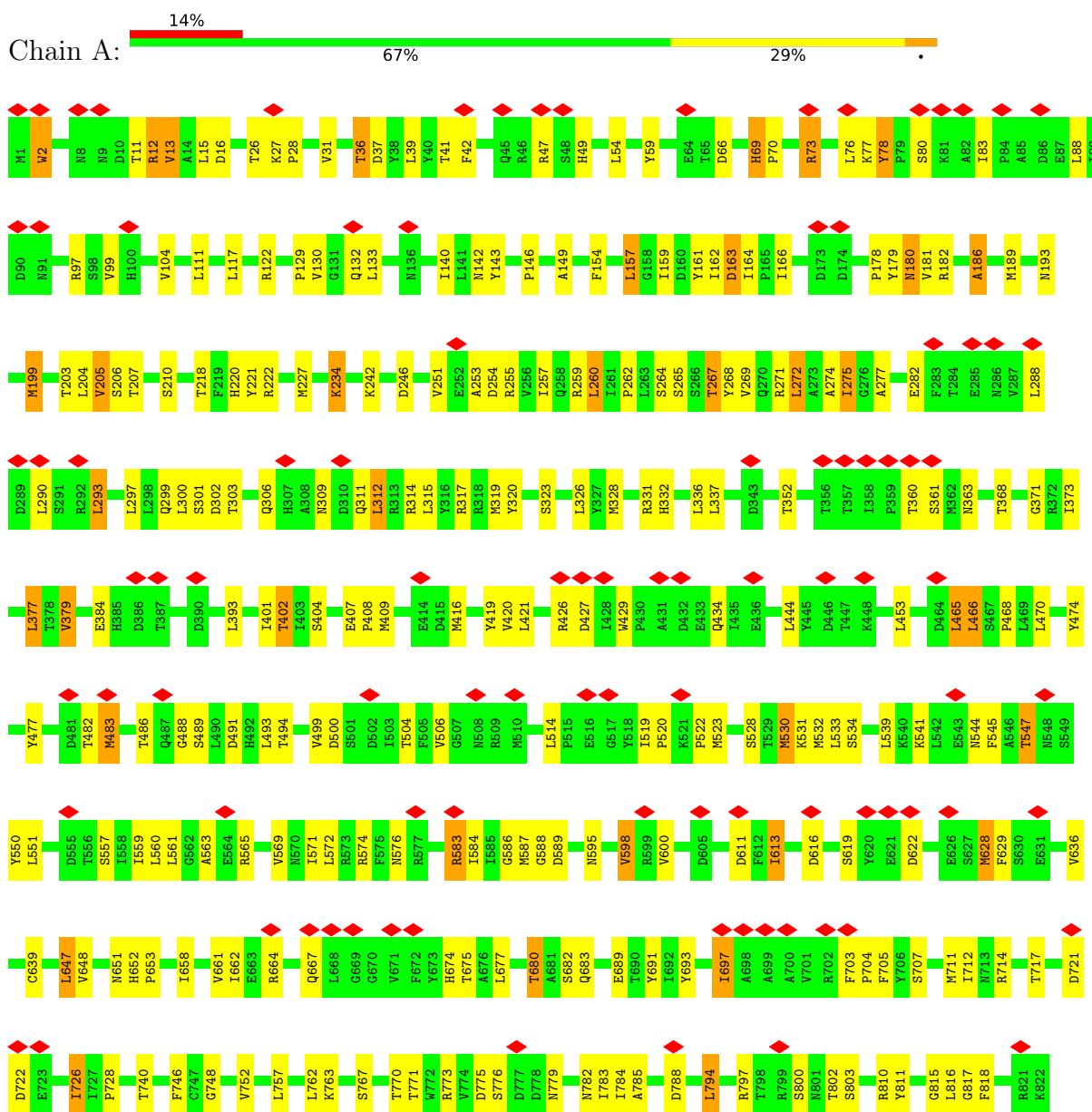


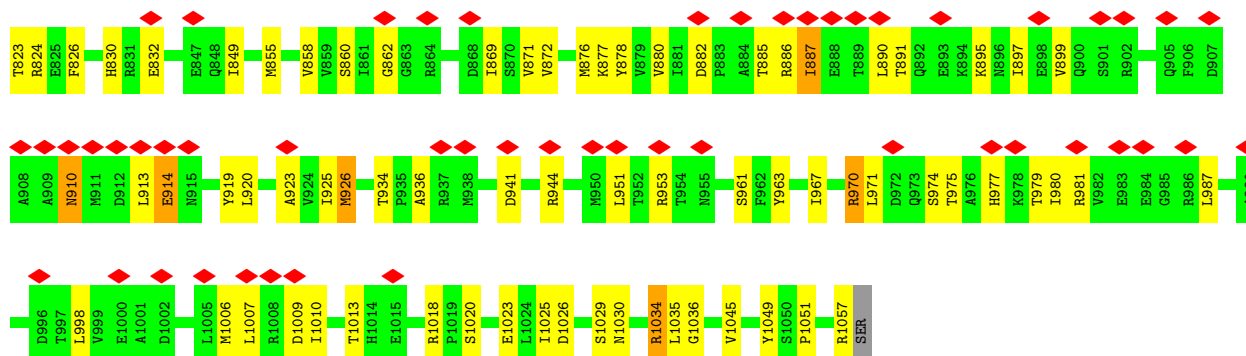
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

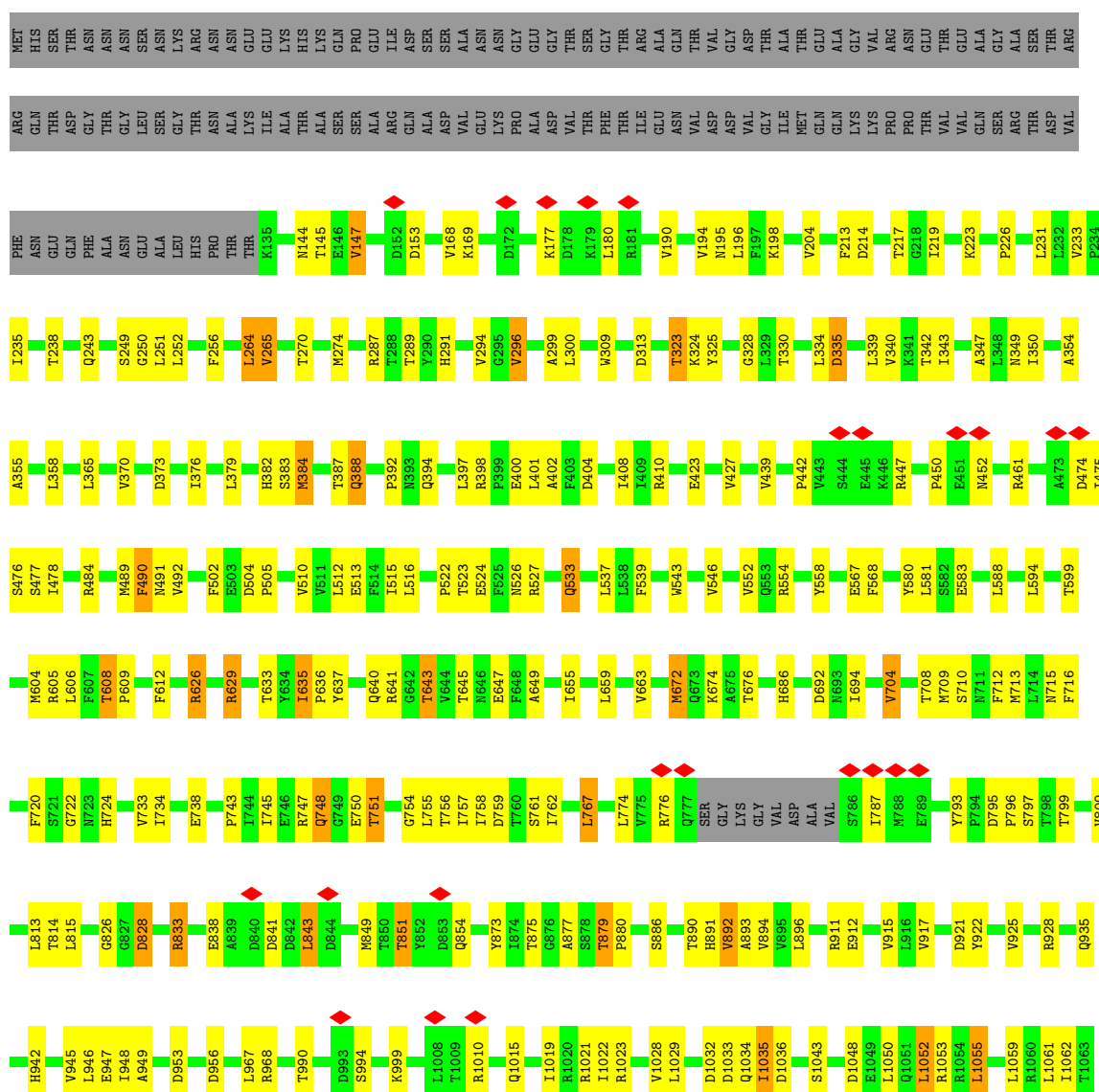
• Molecule 1: Structural protein VP3

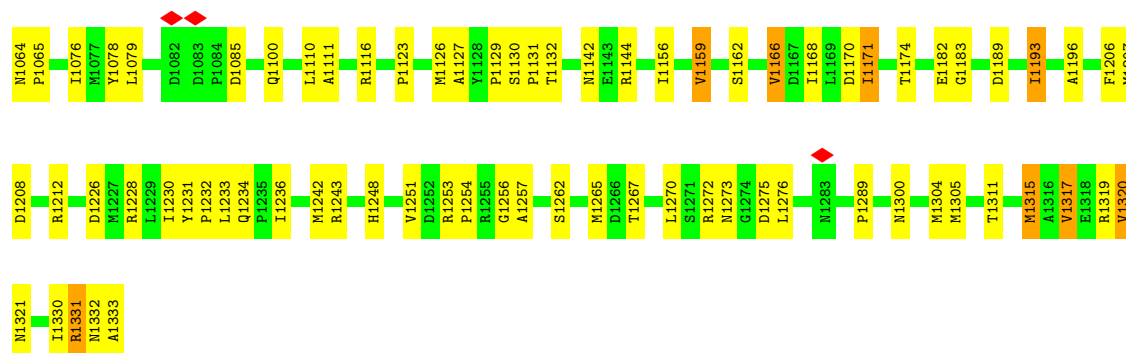




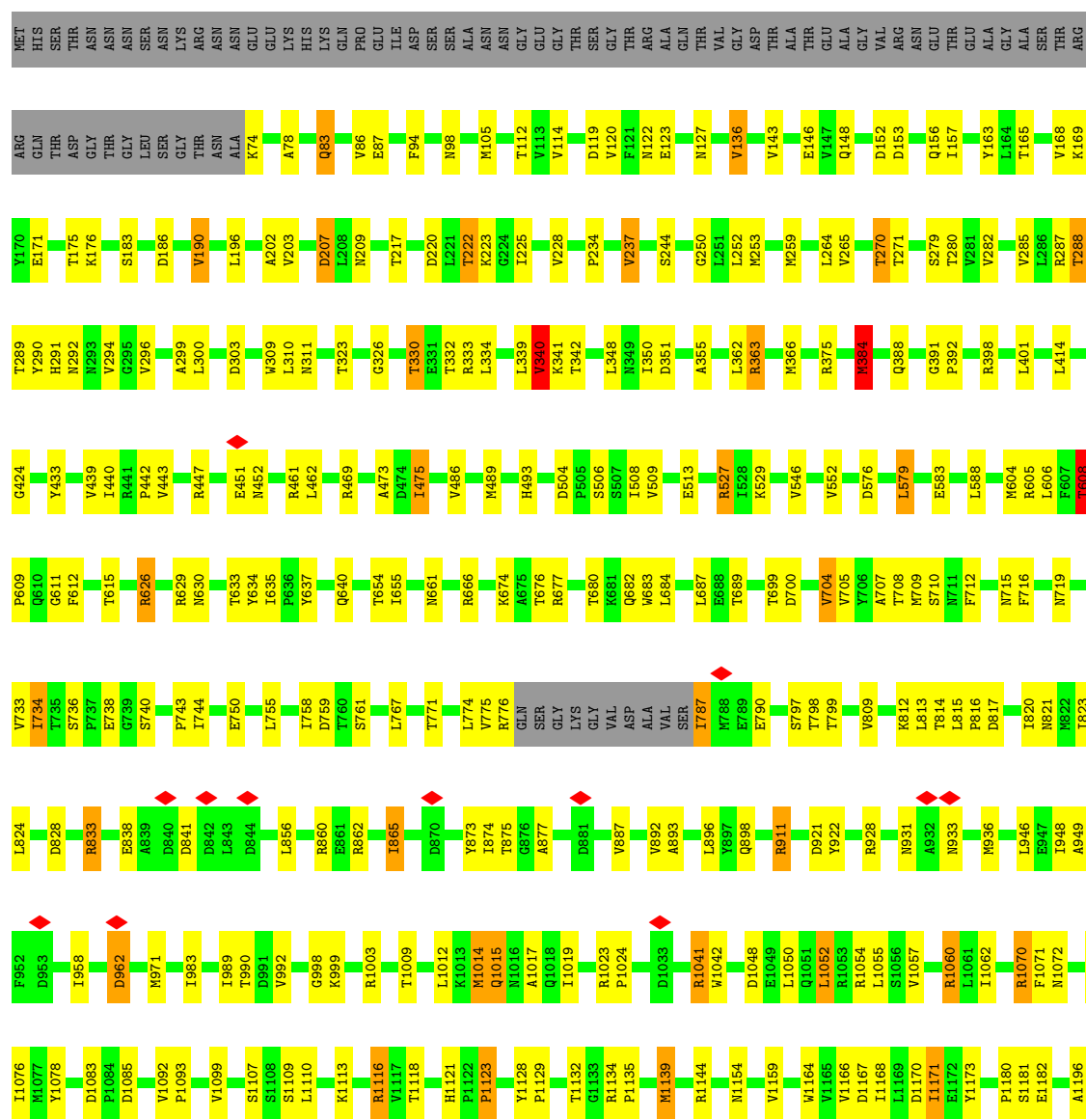
• Molecule 2: Capsid protein VP1

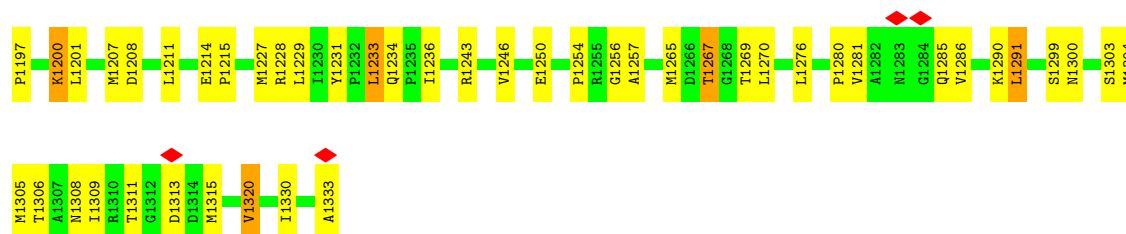
Chain B: 64% 22% 11%



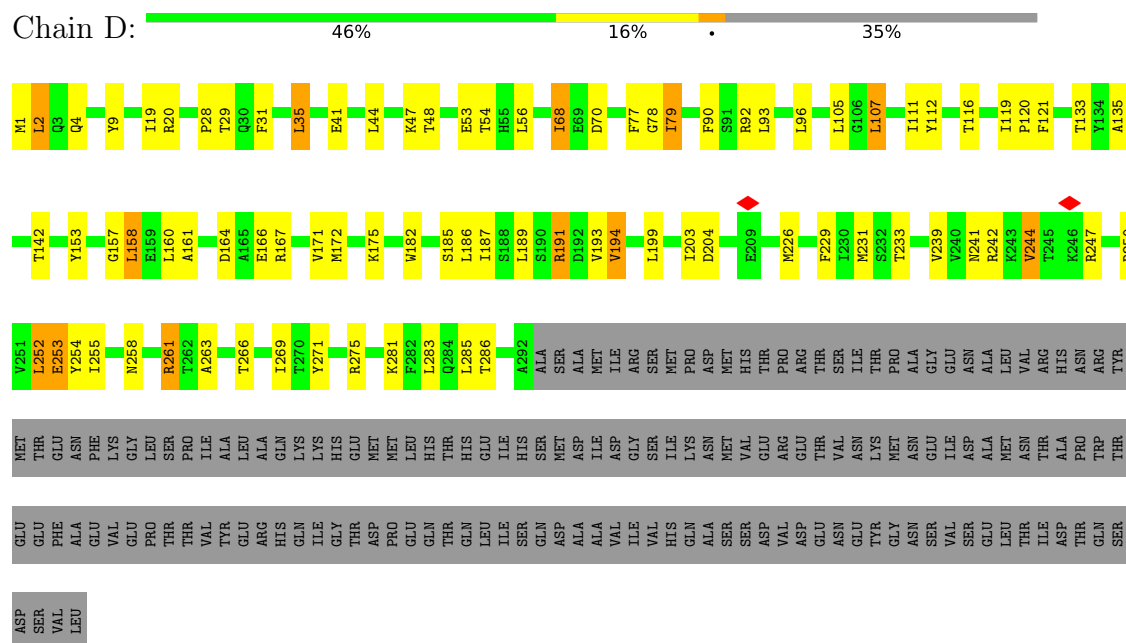


• Molecule 2: Capsid protein VP1

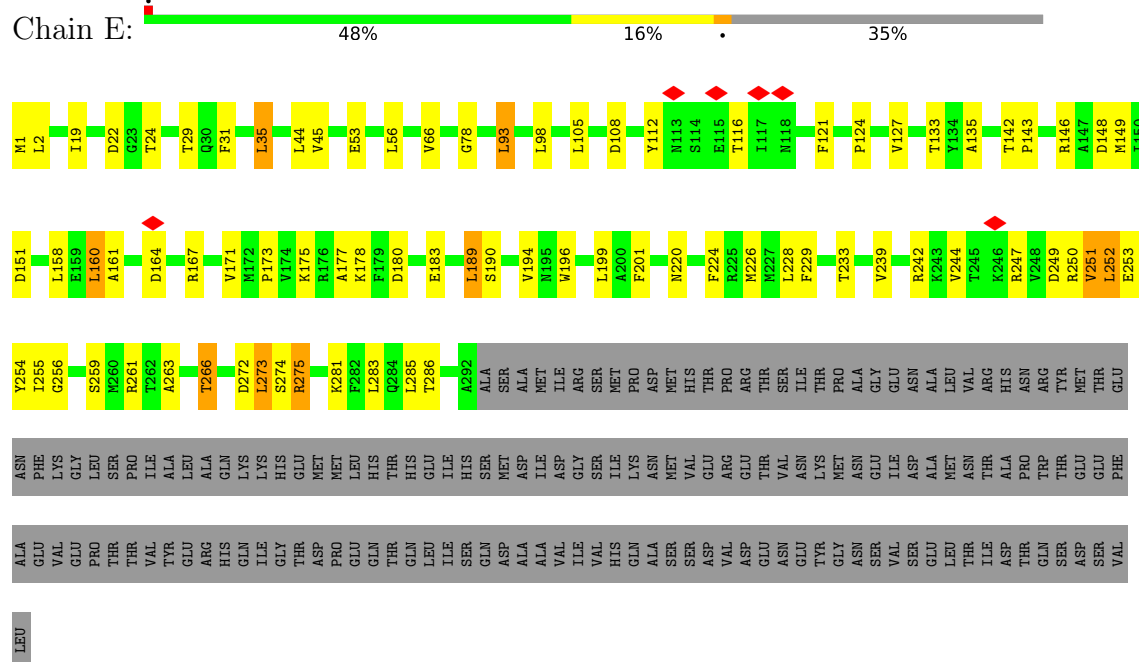




• Molecule 3: Viral structural protein 5



• Molecule 3: Viral structural protein 5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	71946	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	30.516	Depositor
Minimum map value	-18.951	Depositor
Average map value	0.020	Depositor
Map value standard deviation	1.606	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

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

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	0.36	0/8619	0.80	9/11737 (0.1%)
2	B	0.46	0/9590	0.87	12/13056 (0.1%)
2	C	0.46	0/10052	0.86	11/13687 (0.1%)
3	D	0.42	0/2327	0.83	1/3163 (0.0%)
3	E	0.41	0/2327	0.82	0/3163
All	All	0.43	0/32915	0.84	33/44806 (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	C	0	1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ALA	C-N-CD	-8.43	102.05	120.60
1	A	186	ALA	CA-C-N	8.33	147.00	127.00
1	A	186	ALA	C-N-CA	8.33	147.00	127.00
2	C	716	PHE	N-CA-C	7.27	120.25	111.82
2	B	716	PHE	N-CA-C	7.17	121.29	112.54
2	C	719	ASN	N-CA-C	6.96	119.90	111.82
1	A	78	TYR	CA-C-N	6.82	143.36	127.00
1	A	78	TYR	C-N-CA	6.82	143.36	127.00
1	A	78	TYR	C-N-CD	-6.39	106.53	120.60
2	B	1171	ILE	N-CA-C	6.37	117.26	109.30
2	B	608	THR	CA-C-N	5.95	125.90	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	608	THR	C-N-CA	5.95	125.90	119.78
2	B	1130	SER	CA-C-N	5.93	125.80	119.28
2	B	1130	SER	C-N-CA	5.93	125.80	119.28
2	C	529	LYS	N-CA-C	5.92	118.68	111.82
2	C	1083	ASP	CA-C-N	5.91	125.78	119.28
2	C	1083	ASP	C-N-CA	5.91	125.78	119.28
2	B	513	GLU	N-CA-C	-5.74	104.93	111.07
2	C	1085	ASP	CA-C-N	5.71	125.56	119.28
2	C	1085	ASP	C-N-CA	5.71	125.56	119.28
2	B	1132	THR	N-CA-C	5.50	117.28	111.28
1	A	872	VAL	N-CA-C	5.48	113.35	108.63
2	B	635	ILE	CA-C-N	5.47	125.30	119.28
2	B	635	ILE	C-N-CA	5.47	125.30	119.28
3	D	68	ILE	N-CA-C	5.38	116.15	110.72
2	B	490	PHE	N-CA-C	-5.37	104.92	112.12
2	B	243	GLN	N-CA-C	5.35	117.11	111.28
2	C	608	THR	CA-C-N	5.17	125.07	119.85
2	C	608	THR	C-N-CA	5.17	125.07	119.85
2	C	143	VAL	N-CA-C	5.11	117.48	111.09
1	A	69	HIS	CA-C-N	5.05	124.83	119.28
1	A	69	HIS	C-N-CA	5.05	124.83	119.28
2	C	734	ILE	N-CA-C	-5.00	102.28	108.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	384	MET	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	196	0
2	B	9397	0	9315	195	0
2	C	9851	0	9762	193	0
3	D	2281	0	2282	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2281	0	2282	47	0
4	A	32	0	12	2	0
All	All	32276	0	32052	653	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 10.

All (653) 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:392:PRO:HD2	2:B:1315:MET:HE2	1.57	0.85
1:A:111:LEU:HD13	1:A:142:ASN:HB3	1.60	0.84
2:B:709:MET:O	2:B:715:ASN:ND2	2.13	0.82
2:B:491:ASN:HD22	2:B:756:THR:HG21	1.44	0.82
1:A:277:ALA:HB3	1:A:319:MET:HE1	1.62	0.81
2:B:461:ARG:HH21	2:B:504:ASP:HB2	1.48	0.79
1:A:255:ARG:NH2	4:A:1101:GTP:O2A	2.15	0.79
2:C:363:ARG:NH1	3:E:183:GLU:OE1	2.16	0.78
1:A:583:ARG:HH11	1:A:583:ARG:H	1.30	0.78
2:C:1116:ARG:HH11	2:C:1116:ARG:HG2	1.49	0.77
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.18	0.76
2:B:626:ARG:NH2	2:B:712:PHE:O	2.19	0.76
2:C:332:THR:HG22	2:C:334:LEU:H	1.50	0.76
2:C:709:MET:O	2:C:715:ASN:ND2	2.19	0.75
2:B:328:GLY:H	2:B:347:ALA:HB3	1.52	0.74
1:A:2:TRP:H	1:A:2:TRP:CD1	2.05	0.74
3:D:77:PHE:HB2	3:D:194:VAL:HG23	1.70	0.72
1:A:427:ASP:HA	1:A:703:PHE:HA	1.72	0.71
2:B:629:ARG:NH1	2:B:1036:ASP:O	2.22	0.71
2:B:841:ASP:OD1	2:B:911:ARG:NH2	2.22	0.71
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.72	0.71
2:B:1144:ARG:NH2	2:B:1196:ALA:O	2.23	0.71
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.24	0.70
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.73	0.70
2:C:439:VAL:HG11	2:C:705:VAL:HG21	1.75	0.69
1:A:282:GLU:OE1	1:A:810:ARG:NH2	2.25	0.69
1:A:1026:ASP:OD1	1:A:1030:ASN:ND2	2.26	0.69
2:C:271:THR:OG1	2:C:292:ASN:OD1	2.11	0.69
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.74	0.69
2:C:841:ASP:OD2	2:C:911:ARG:NH2	2.25	0.69
2:C:1208:ASP:OD2	2:C:1243:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.26	0.68
2:B:484:ARG:NE	2:B:524:GLU:OE2	2.26	0.68
1:A:541:LYS:HG2	1:A:975:THR:HG21	1.75	0.68
1:A:680:THR:HG22	1:A:683:GLN:HG3	1.76	0.68
1:A:628:MET:SD	1:A:652:HIS:ND1	2.66	0.68
1:A:66:ASP:OD1	1:A:122:ARG:NH2	2.27	0.68
1:A:129:PRO:HB2	2:B:1332:ASN:HD22	1.57	0.67
2:B:921:ASP:OD1	2:B:928:ARG:NH2	2.24	0.67
2:B:1131:PRO:O	2:B:1162:SER:OG	2.11	0.67
2:B:814:THR:HA	2:B:1010:ARG:HH12	1.59	0.67
2:B:1126:MET:HE1	3:E:146:ARG:HB3	1.75	0.67
1:A:161:TYR:CE1	2:B:1333:ALA:HB1	2.29	0.67
2:C:443:VAL:HB	2:C:771:THR:HG23	1.76	0.67
2:C:812:LYS:NZ	2:C:990:THR:O	2.28	0.67
1:A:489:SER:OG	1:A:491:ASP:OD2	2.13	0.66
2:B:750:GLU:OE1	2:C:452:ASN:ND2	2.28	0.66
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.77	0.66
2:B:1021:ARG:NE	2:B:1036:ASP:OD1	2.28	0.66
2:C:704:VAL:O	2:C:708:THR:HG23	1.96	0.66
1:A:312:LEU:HD11	1:A:361:SER:HB3	1.78	0.65
2:B:1171:ILE:HD13	2:B:1193:ILE:HD12	1.78	0.65
2:B:145:THR:HB	2:B:1317:VAL:HG23	1.77	0.65
2:C:1254:PRO:HG2	2:C:1257:ALA:HB2	1.78	0.65
1:A:178:PRO:HB2	1:A:179:TYR:HD2	1.61	0.65
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.77	0.65
1:A:797:ARG:NH2	1:A:876:MET:O	2.30	0.65
2:B:704:VAL:O	2:B:708:THR:HG23	1.97	0.64
2:B:1023:ARG:HG3	2:B:1029:LEU:HD21	1.77	0.64
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.80	0.64
2:C:1116:ARG:HH11	2:C:1116:ARG:CG	2.11	0.64
1:A:73:ARG:HH11	1:A:73:ARG:HB2	1.61	0.64
2:B:376:ILE:HD11	2:B:1317:VAL:HG11	1.78	0.64
2:C:824:LEU:HB3	2:C:1015:GLN:HE21	1.63	0.63
3:E:233:THR:HG22	3:E:252:LEU:HD13	1.80	0.63
2:C:736:SER:OG	2:C:738:GLU:OE1	2.13	0.63
1:A:408:PRO:HB2	1:A:468:PRO:HG3	1.81	0.63
2:C:633:THR:HG21	2:C:710:SER:HB2	1.80	0.63
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.79	0.63
1:A:317:ARG:NH1	3:D:41:GLU:OE1	2.32	0.63
3:E:78:GLY:O	3:E:275:ARG:NH2	2.30	0.63
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:GLY:HA3	2:B:347:ALA:H	1.62	0.62
2:C:183:SER:OG	2:C:186:ASP:OD2	2.17	0.62
1:A:979:THR:HG23	1:A:980:ILE:HG12	1.80	0.62
2:C:626:ARG:NH2	2:C:712:PHE:O	2.31	0.62
2:B:153:ASP:OD1	2:B:153:ASP:N	2.33	0.62
2:B:1100:GLN:OE1	2:B:1142:ASN:ND2	2.31	0.62
1:A:129:PRO:HG2	2:B:1332:ASN:HB2	1.81	0.62
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.33	0.62
1:A:326:LEU:HB3	1:A:352:THR:HG22	1.82	0.62
1:A:531:LYS:HD3	1:A:683:GLN:HG2	1.81	0.61
2:C:388:GLN:HB3	2:C:1320:VAL:HG13	1.82	0.61
2:C:887:VAL:HG22	2:C:893:ALA:HA	1.81	0.61
1:A:2:TRP:H	1:A:2:TRP:HD1	1.48	0.61
1:A:674:HIS:HB2	1:A:697:ILE:HD12	1.83	0.61
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.34	0.61
1:A:404:SER:OG	1:A:824:ARG:NH1	2.34	0.61
1:A:47:ARG:NH1	1:A:80:SER:OG	2.34	0.60
2:B:313:ASP:OD1	2:B:1253:ARG:NH1	2.34	0.60
3:E:242:ARG:HG3	3:E:251:VAL:HG21	1.83	0.60
1:A:234:LYS:HG2	1:A:260:LEU:HD22	1.84	0.60
1:A:563:ALA:O	1:A:565:ARG:NH1	2.35	0.60
2:C:734:ILE:HG22	2:C:1017:ALA:HB1	1.84	0.60
1:A:658:ILE:HD12	1:A:712:ILE:HG12	1.84	0.60
2:B:335:ASP:OD2	2:B:340:VAL:N	2.32	0.60
1:A:419:TYR:HE1	1:A:421:LEU:HD23	1.66	0.59
1:A:541:LYS:HD3	1:A:550:TYR:HE2	1.65	0.59
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.36	0.59
3:E:177:ALA:HB3	3:E:252:LEU:HG	1.84	0.59
2:B:1289:PRO:HD2	3:D:20:ARG:HD2	1.84	0.59
1:A:328:MET:HE2	1:A:332:HIS:HB3	1.83	0.59
1:A:887:ILE:HG13	1:A:899:VAL:HG21	1.84	0.59
2:B:474:ASP:OD1	2:B:476:SER:OG	2.21	0.58
2:C:462:LEU:HD13	2:C:680:THR:HG22	1.84	0.58
2:C:156:GLN:NE2	2:C:1308:ASN:OD1	2.36	0.58
3:E:19:ILE:HD11	3:E:31:PHE:HB2	1.84	0.58
1:A:541:LYS:NZ	1:A:545:PHE:O	2.36	0.58
1:A:477:TYR:HA	1:A:482:THR:HG22	1.86	0.58
3:D:164:ASP:OD2	3:D:167:ARG:NH2	2.31	0.58
3:D:283:LEU:HA	3:D:286:THR:HG22	1.86	0.58
3:E:283:LEU:HA	3:E:286:THR:HG22	1.86	0.57
2:B:223:LYS:HB3	2:B:1174:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:LEU:HD13	2:B:659:LEU:HD12	1.86	0.57
2:C:171:GLU:OE2	2:C:1181:SER:OG	2.22	0.57
1:A:206:SER:HB3	1:A:227:MET:HE3	1.87	0.57
2:B:264:LEU:HD11	2:B:365:LEU:HD22	1.85	0.57
1:A:59:TYR:HB3	4:A:1101:GTP:C6	2.38	0.57
1:A:420:VAL:HA	1:A:974:SER:HB2	1.86	0.57
2:B:410:ARG:HD3	2:B:1043:SER:HA	1.86	0.57
1:A:474:TYR:HD1	1:A:499:VAL:HG22	1.68	0.57
2:B:851:THR:HG22	2:B:854:GLN:HG2	1.87	0.57
2:C:824:LEU:HD23	2:C:971:MET:HE1	1.86	0.57
1:A:42:PHE:HD1	1:A:49:HIS:HD2	1.52	0.57
2:B:1208:ASP:OD1	2:B:1243:ARG:NH2	2.27	0.57
2:C:163:TYR:N	2:C:351:ASP:OD1	2.38	0.57
2:B:712:PHE:HB2	2:B:715:ASN:ND2	2.20	0.56
3:D:78:GLY:O	3:D:275:ARG:NH2	2.38	0.56
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.87	0.56
1:A:288:LEU:HD22	1:A:368:THR:HG22	1.86	0.56
1:A:514:LEU:H	1:A:514:LEU:HD12	1.70	0.56
2:C:865:ILE:HD11	2:C:1041:ARG:O	2.05	0.56
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.23	0.56
1:A:203:THR:HG22	1:A:204:LEU:HG	1.88	0.56
2:C:921:ASP:OD1	2:C:928:ARG:NH2	2.33	0.56
1:A:13:VAL:HG21	1:A:146:PRO:HB3	1.87	0.56
2:B:492:VAL:HB	2:B:747:ARG:HG2	1.88	0.56
2:B:1129:PRO:HD3	3:E:273:LEU:HD23	1.88	0.56
2:C:949:ALA:HA	2:C:958:ILE:HD13	1.88	0.56
3:E:272:ASP:OD2	3:E:274:SER:OG	2.16	0.56
1:A:717:THR:HB	1:A:1020:SER:HB2	1.88	0.55
2:C:259:MET:O	2:C:1054:ARG:NH1	2.36	0.55
1:A:154:PHE:HE1	1:A:162:ILE:HG13	1.72	0.55
2:B:328:GLY:N	2:B:347:ALA:HB3	2.22	0.55
2:B:612:PHE:HZ	2:B:1330:ILE:HG22	1.71	0.55
2:B:826:GLY:HA3	2:B:949:ALA:HB2	1.89	0.55
2:C:114:VAL:HG22	2:C:136:VAL:HG12	1.88	0.55
3:D:186:LEU:HD22	3:D:233:THR:HG21	1.87	0.55
3:E:148:ASP:OD2	3:E:151:ASP:N	2.34	0.55
1:A:275:ILE:HD12	1:A:301:SER:HA	1.88	0.55
3:D:239:VAL:HG12	3:D:250:ARG:HD2	1.88	0.55
1:A:466:LEU:HD23	1:A:530:MET:HG2	1.89	0.55
1:A:178:PRO:HB2	1:A:179:TYR:CD2	2.42	0.55
2:C:750:GLU:OE1	2:C:1003:ARG:NH1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:THR:HG1	1:A:220:HIS:HE2	1.54	0.54
3:D:9:TYR:H	3:D:204:ASP:CG	2.16	0.54
1:A:1020:SER:OG	1:A:1023:GLU:OE2	2.18	0.54
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.39	0.54
2:C:999:LYS:HG2	2:C:1009:THR:HG22	1.88	0.54
3:E:108:ASP:OD2	3:E:112:TYR:OH	2.22	0.54
1:A:539:LEU:HG	1:A:647:LEU:HD12	1.90	0.54
2:B:270:THR:HG22	2:B:291:HIS:HA	1.88	0.54
2:C:253:MET:HE2	2:C:989:ILE:HG21	1.89	0.54
2:C:461:ARG:HB3	2:C:676:THR:HG21	1.89	0.54
2:B:252:LEU:HD23	2:B:967:LEU:HD21	1.90	0.54
2:B:1230:ILE:HG12	2:C:119:ASP:HA	1.90	0.54
2:B:1076:ILE:HB	2:B:1166:VAL:HG22	1.90	0.53
2:B:370:VAL:HG12	2:B:400:GLU:HG3	1.90	0.53
1:A:12:ARG:NH2	1:A:16:ASP:OD2	2.41	0.53
1:A:189:MET:O	1:A:193:ASN:ND2	2.40	0.53
2:C:504:ASP:OD2	2:C:506:SER:OG	2.26	0.53
2:B:450:PRO:HG3	2:B:686:HIS:HB2	1.91	0.53
2:C:340:VAL:HG22	2:C:1309:ILE:HD12	1.90	0.53
2:C:439:VAL:HG23	2:C:440:ILE:HG22	1.90	0.53
2:C:736:SER:HB3	2:C:740:SER:HB3	1.90	0.53
3:E:164:ASP:OD1	3:E:167:ARG:NH2	2.34	0.53
2:C:78:ALA:HB2	2:C:1181:SER:HB2	1.90	0.53
2:C:666:ARG:O	2:C:677:ARG:NH1	2.39	0.53
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.90	0.53
2:C:169:LYS:NZ	2:C:1182:GLU:OE2	2.32	0.53
1:A:274:ALA:HA	1:A:319:MET:HE2	1.91	0.52
1:A:299:GLN:O	1:A:303:THR:HG23	2.08	0.52
2:B:384:MET:HA	2:B:708:THR:HG21	1.91	0.52
2:C:1116:ARG:HG2	2:C:1116:ARG:NH1	2.22	0.52
2:B:1032:ASP:HB3	2:B:1035:ILE:CG2	2.40	0.52
2:C:699:THR:OG1	2:C:700:ASP:OD2	2.24	0.52
2:C:865:ILE:HD11	2:C:1041:ARG:C	2.35	0.52
3:E:124:PRO:HA	3:E:127:VAL:HG22	1.92	0.52
3:E:261:ARG:NH1	3:E:263:ALA:O	2.42	0.52
2:B:256:PHE:CE2	2:B:990:THR:HG21	2.44	0.52
2:C:442:PRO:HB3	2:C:473:ALA:HB1	1.91	0.52
2:C:489:MET:SD	2:C:527:ARG:HD2	2.50	0.52
2:B:1111:ALA:HB3	2:B:1116:ARG:HD2	1.92	0.52
1:A:39:LEU:HD23	1:A:54:LEU:HD11	1.92	0.52
1:A:143:TYR:CG	1:A:149:ALA:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASP:OD2	1:A:182:ARG:NE	2.39	0.52
2:C:611:GLY:HA3	2:C:635:ILE:O	2.10	0.52
2:B:190:VAL:HG22	2:B:194:VAL:HG23	1.92	0.52
1:A:262:PRO:HG2	1:A:323:SER:HB2	1.91	0.52
1:A:532:MET:HE3	1:A:560:LEU:HD12	1.91	0.52
1:A:951:LEU:O	1:A:1057:ARG:NH1	2.43	0.52
2:B:388:GLN:HB3	2:B:1320:VAL:HG13	1.92	0.52
2:B:1248:HIS:ND1	2:B:1251:VAL:HG22	2.25	0.52
2:C:228:VAL:HG23	2:C:250:GLY:HA2	1.92	0.51
2:B:324:LYS:O	2:B:1267:THR:HG22	2.10	0.51
2:B:748:GLN:HA	2:C:682:GLN:HE22	1.74	0.51
2:C:443:VAL:HG11	2:C:447:ARG:HH22	1.75	0.51
2:C:833:ARG:HG3	2:C:922:TYR:CZ	2.45	0.51
1:A:636:VAL:HG11	1:A:661:VAL:HG13	1.92	0.51
2:B:893:ALA:HB1	2:B:915:VAL:HA	1.92	0.51
2:C:962:ASP:OD1	2:C:962:ASP:N	2.43	0.51
1:A:157:LEU:HB3	1:A:159:ILE:HG23	1.93	0.51
1:A:849:ILE:HD12	1:A:871:VAL:HG12	1.90	0.51
2:B:190:VAL:HG23	2:B:300:LEU:HB3	1.92	0.51
2:B:833:ARG:HG3	2:B:922:TYR:CZ	2.45	0.51
2:C:1211:LEU:HD21	2:C:1246:VAL:HG21	1.93	0.51
1:A:129:PRO:CG	2:B:1332:ASN:HB2	2.41	0.51
2:C:424:GLY:HA2	2:C:755:LEU:HD11	1.92	0.51
1:A:246:ASP:OD1	1:A:331:ARG:NH2	2.43	0.51
1:A:572:LEU:HB3	1:A:584:ILE:HD13	1.91	0.51
2:B:1189:ASP:OD2	2:B:1189:ASP:N	2.42	0.51
2:C:156:GLN:HE22	2:C:1309:ILE:H	1.57	0.51
3:D:161:ALA:HB3	3:D:172:MET:HE1	1.93	0.51
2:C:299:ALA:HB2	2:C:1265:MET:HB3	1.92	0.51
2:C:828:ASP:OD1	2:C:862:ARG:NH2	2.44	0.51
1:A:420:VAL:HG23	1:A:711:MET:HE1	1.93	0.51
1:A:613:ILE:HG21	1:A:639:CYS:HB3	1.93	0.51
2:B:226:PRO:HG2	2:B:251:LEU:HD23	1.92	0.51
2:C:588:LEU:HB3	2:C:604:MET:HE2	1.92	0.51
3:E:45:VAL:HA	3:E:171:VAL:HG12	1.92	0.50
2:C:1144:ARG:NH1	2:C:1170:ASP:OD1	2.43	0.50
1:A:775:ASP:OD1	1:A:776:SER:N	2.44	0.50
2:B:442:PRO:HB3	2:B:475:ILE:HG21	1.93	0.50
1:A:393:LEU:HB3	1:A:748:GLY:HA3	1.94	0.50
2:C:615:THR:H	2:C:1333:ALA:HA	1.76	0.50
2:B:1144:ARG:NH1	2:B:1170:ASP:OD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:606:LEU:HD22	2:C:655:ILE:HG12	1.92	0.50
2:C:1276:LEU:HB3	2:C:1290:LYS:HD2	1.94	0.50
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.94	0.50
1:A:491:ASP:O	1:A:494:THR:HG22	2.11	0.50
1:A:923:ALA:N	1:A:961:SER:OG	2.31	0.50
1:A:379:VAL:HG21	1:A:794:LEU:HD13	1.92	0.50
2:B:1289:PRO:HG2	3:D:191:ARG:NH2	2.26	0.50
2:C:469:ARG:NE	2:C:513:GLU:OE1	2.43	0.50
1:A:882:ASP:OD2	1:A:885:THR:OG1	2.29	0.50
2:B:838:GLU:C	2:B:935:GLN:HG2	2.36	0.50
2:B:956:ASP:OD2	3:D:266:THR:OG1	2.23	0.50
2:B:1144:ARG:HD2	2:B:1168:ILE:HG21	1.93	0.50
3:E:252:LEU:HD12	3:E:255:ILE:HD11	1.93	0.50
2:B:828:ASP:OD2	2:B:1015:GLN:NE2	2.45	0.49
2:C:207:ASP:OD1	2:C:207:ASP:N	2.45	0.49
2:C:362:LEU:HD22	2:C:1303:SER:HB3	1.94	0.49
2:C:366:MET:HG2	3:E:266:THR:HG21	1.94	0.49
1:A:328:MET:HE1	1:A:336:LEU:HD11	1.94	0.49
2:B:484:ARG:O	2:B:527:ARG:NH2	2.46	0.49
1:A:588:GLY:H	1:A:598:VAL:HG23	1.76	0.49
2:C:119:ASP:OD1	2:C:119:ASP:N	2.45	0.49
2:C:817:ASP:OD1	2:C:821:ASN:ND2	2.45	0.49
1:A:771:THR:HG22	1:A:783:ILE:HG23	1.93	0.49
2:B:342:THR:OG1	2:B:343:ILE:N	2.45	0.49
2:B:759:ASP:OD2	2:B:761:SER:OG	2.31	0.49
2:B:813:LEU:HG	2:B:1010:ARG:NH1	2.27	0.49
1:A:533:LEU:HD21	1:A:571:ILE:HG21	1.95	0.49
2:B:365:LEU:HD23	2:B:1305:MET:HE1	1.93	0.49
2:C:326:GLY:H	2:C:1267:THR:HG21	1.77	0.49
2:C:759:ASP:OD1	2:C:761:SER:OG	2.28	0.49
2:C:1075:ARG:NH2	2:C:1167:ASP:OD2	2.32	0.49
1:A:680:THR:HG23	1:A:682:SER:H	1.77	0.49
2:B:704:VAL:HB	2:B:1330:ILE:HD11	1.93	0.49
2:B:734:ILE:HD13	2:B:1019:ILE:HG12	1.94	0.49
1:A:595:ASN:HD22	1:A:595:ASN:H	1.61	0.49
1:A:882:ASP:OD1	1:A:882:ASP:N	2.45	0.49
2:C:287:ARG:HH11	2:C:330:THR:HB	1.76	0.49
2:C:1305:MET:HE2	2:C:1309:ILE:HD11	1.94	0.49
1:A:12:ARG:HH21	1:A:15:LEU:HB3	1.78	0.48
1:A:409:MET:HE1	1:A:1036:GLY:HA2	1.95	0.48
1:A:420:VAL:HA	1:A:974:SER:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:LEU:HD13	2:B:655:ILE:HG23	1.94	0.48
1:A:179:TYR:HB3	1:A:221:TYR:CD1	2.47	0.48
1:A:628:MET:HG3	1:A:629:PHE:N	2.28	0.48
1:A:651:ASN:HA	1:A:689:GLU:HG3	1.95	0.48
1:A:1006:MET:HA	1:A:1009:ASP:OD2	2.13	0.48
2:C:705:VAL:HG12	2:C:709:MET:HE2	1.94	0.48
1:A:658:ILE:O	1:A:662:ILE:HG12	2.13	0.48
2:B:1171:ILE:CD1	2:B:1193:ILE:HG23	2.44	0.48
3:D:4:GLN:NE2	3:D:204:ASP:OD1	2.46	0.48
1:A:586:GLY:HA3	1:A:595:ASN:OD1	2.13	0.48
1:A:704:PRO:HG2	1:A:705:PHE:CD2	2.48	0.48
1:A:251:VAL:HG12	1:A:253:ALA:H	1.79	0.48
1:A:664:ARG:HD2	1:A:667:GLN:HE21	1.78	0.48
1:A:830:HIS:HB2	1:A:1034:ARG:CZ	2.44	0.48
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.94	0.48
2:B:355:ALA:HB3	2:B:1276:LEU:HD11	1.94	0.48
2:B:1127:ALA:O	3:E:146:ARG:NH2	2.35	0.48
2:C:838:GLU:OE1	2:C:933:ASN:ND2	2.46	0.48
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.95	0.48
1:A:302:ASP:O	1:A:306:GLN:HB2	2.13	0.48
2:C:392:PRO:HG2	2:C:1315:MET:HE3	1.95	0.48
2:C:1057:VAL:HG22	2:C:1291:LEU:HD21	1.94	0.48
2:C:1311:THR:HB	2:C:1313:ASP:OD2	2.13	0.48
1:A:429:TRP:CE2	1:A:434:GLN:HG2	2.48	0.48
2:C:398:ARG:HG2	2:C:398:ARG:HH11	1.79	0.48
1:A:560:LEU:HD22	1:A:560:LEU:H	1.78	0.48
2:B:720:PHE:CE1	2:B:722:GLY:HA2	2.49	0.48
3:E:253:GLU:HA	3:E:254:TYR:HA	1.55	0.48
1:A:377:LEU:HB3	1:A:763:LYS:HB3	1.94	0.48
2:B:891:HIS:HA	3:D:242:ARG:HD3	1.96	0.48
2:B:1243:ARG:HD3	2:B:1256:GLY:O	2.14	0.48
2:C:252:LEU:HD22	2:C:823:ILE:HD13	1.95	0.48
3:D:1:MET:HB2	3:D:121:PHE:CE1	2.49	0.48
3:D:44:LEU:HD12	3:D:172:MET:HE2	1.94	0.48
1:A:544:ASN:HB3	1:A:547:THR:OG1	2.14	0.47
1:A:180:ASN:HD22	1:A:180:ASN:C	2.19	0.47
2:B:640:GLN:OE1	2:B:647:GLU:N	2.37	0.47
1:A:858:VAL:HG23	1:A:876:MET:HE2	1.96	0.47
2:C:165:THR:HG23	2:C:209:ASN:HB2	1.95	0.47
3:D:105:LEU:HD23	3:D:203:ILE:HD11	1.96	0.47
3:E:44:LEU:HD11	3:E:256:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:CE1	1:A:162:ILE:HG13	2.49	0.47
2:B:633:THR:HG21	2:B:710:SER:CB	2.45	0.47
2:C:342:THR:O	2:C:1306:THR:HG23	2.14	0.47
2:C:605:ARG:O	2:C:608:THR:HG23	2.13	0.47
1:A:199:MET:HG3	1:A:205:VAL:HG21	1.96	0.47
1:A:528:SER:O	1:A:532:MET:HG2	2.15	0.47
2:B:1273:ASN:ND2	2:B:1275:ASP:OD1	2.44	0.47
1:A:164:ILE:HB	1:A:181:VAL:HG12	1.96	0.47
2:B:523:THR:O	2:B:527:ARG:HG3	2.15	0.47
2:B:843:LEU:HG	2:B:942:HIS:HB2	1.96	0.47
3:E:239:VAL:HG12	3:E:250:ARG:HD2	1.97	0.47
1:A:42:PHE:HD1	1:A:49:HIS:CD2	2.32	0.47
1:A:419:TYR:CE1	1:A:421:LEU:HD23	2.50	0.47
1:A:926:MET:HE2	1:A:926:MET:HB2	1.79	0.47
2:B:522:PRO:HB3	2:B:609:PRO:HB3	1.95	0.47
2:B:925:VAL:HA	2:B:928:ARG:HD2	1.97	0.47
2:C:1159:VAL:HA	2:C:1164:TRP:HB2	1.97	0.47
1:A:488:GLY:HA2	1:A:551:LEU:HD13	1.96	0.47
1:A:977:HIS:HB2	1:A:981:ARG:HB3	1.97	0.47
2:C:640:GLN:N	2:C:700:ASP:OD1	2.46	0.47
2:C:1243:ARG:HD3	2:C:1256:GLY:O	2.14	0.47
1:A:967:ILE:HG13	1:A:1045:VAL:HG12	1.96	0.47
2:B:558:TYR:HB3	2:B:568:PHE:CD1	2.49	0.47
2:C:384:MET:HA	2:C:708:THR:CG2	2.44	0.47
2:B:1331:ARG:HB3	2:B:1331:ARG:HH11	1.80	0.47
1:A:416:MET:HE3	1:A:530:MET:HE2	1.96	0.46
1:A:653:PRO:HB3	1:A:658:ILE:HD11	1.97	0.46
2:B:879:THR:HG22	2:B:880:PRO:HD2	1.96	0.46
1:A:129:PRO:HA	1:A:132:GLN:HG2	1.97	0.46
1:A:242:LYS:NZ	1:A:246:ASP:OD2	2.32	0.46
1:A:265:SER:HB2	1:A:269:VAL:HB	1.97	0.46
2:B:147:VAL:HG22	2:B:379:LEU:HD11	1.96	0.46
2:C:1267:THR:HB	2:C:1299:SER:HB3	1.96	0.46
3:E:281:LYS:O	3:E:285:LEU:HG	2.15	0.46
1:A:726:ILE:HG13	1:A:1029:SER:HB2	1.97	0.46
1:A:970:ARG:NH1	1:A:1049:TYR:OH	2.49	0.46
2:C:384:MET:SD	2:C:433:TYR:OH	2.70	0.46
2:C:1211:LEU:HD23	2:C:1211:LEU:HA	1.60	0.46
1:A:560:LEU:HD23	1:A:569:VAL:HG22	1.96	0.46
2:B:484:ARG:HE	2:B:524:GLU:CD	2.23	0.46
2:C:220:ASP:OD1	2:C:222:THR:OG1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:375:ARG:O	2:C:375:ARG:HD3	2.16	0.46
2:C:1139:MET:HB3	2:C:1166:VAL:HG12	1.96	0.46
2:C:1228:ARG:HG2	2:C:1231:TYR:CZ	2.50	0.46
2:C:1139:MET:HE3	2:C:1139:MET:HB2	1.66	0.46
3:E:19:ILE:HD13	3:E:189:LEU:HD11	1.98	0.46
2:B:502:PHE:CE1	2:B:539:PHE:HB2	2.51	0.46
2:B:533:GLN:HB2	2:B:588:LEU:HD12	1.96	0.46
2:C:824:LEU:HB3	2:C:1015:GLN:NE2	2.27	0.46
2:C:384:MET:HA	2:C:708:THR:HG21	1.98	0.46
2:C:493:HIS:HB3	2:C:758:ILE:HD13	1.98	0.46
2:C:816:PRO:HB2	2:C:983:ILE:HG23	1.96	0.46
3:E:229:PHE:O	3:E:233:THR:HG23	2.15	0.46
1:A:914:GLU:N	1:A:919:TYR:OH	2.49	0.46
2:C:609:PRO:HB2	2:C:634:TYR:CE2	2.50	0.46
2:C:609:PRO:HB2	2:C:634:TYR:HE2	1.81	0.46
1:A:895:LYS:HA	1:A:895:LYS:HD3	1.76	0.46
3:E:253:GLU:HB2	3:E:254:TYR:CD1	2.51	0.46
1:A:309:ASN:OD1	1:A:311:GLN:HG3	2.15	0.46
2:C:169:LYS:O	2:C:202:ALA:N	2.42	0.46
2:C:856:LEU:HD23	2:C:860:ARG:HD3	1.98	0.46
2:C:1076:ILE:HG22	2:C:1159:VAL:HG11	1.97	0.46
3:E:178:LYS:HA	3:E:250:ARG:O	2.16	0.46
1:A:426:ARG:HG3	1:A:707:SER:HB3	1.98	0.45
2:B:423:GLU:O	2:B:427:VAL:HG23	2.16	0.45
2:B:776:ARG:HD3	2:B:787:ILE:HB	1.97	0.45
2:B:833:ARG:HG3	2:B:922:TYR:CE2	2.51	0.45
1:A:257:ILE:HG22	1:A:259:ARG:H	1.81	0.45
1:A:404:SER:O	1:A:826:PHE:HA	2.16	0.45
2:B:1228:ARG:HB3	2:B:1231:TYR:OH	2.16	0.45
2:C:348:LEU:HD11	2:C:1304:MET:HE1	1.98	0.45
2:C:828:ASP:OD2	2:C:828:ASP:N	2.49	0.45
2:C:1180:PRO:HA	2:C:1207:MET:SD	2.56	0.45
2:C:1233:LEU:HD13	2:C:1233:LEU:HA	1.76	0.45
3:E:253:GLU:HB2	3:E:254:TYR:CE1	2.51	0.45
1:A:161:TYR:CD1	2:B:1333:ALA:HB1	2.52	0.45
1:A:963:TYR:CD2	1:A:987:LEU:HD21	2.52	0.45
2:C:303:ASP:N	2:C:311:ASN:OD1	2.45	0.45
2:C:583:GLU:H	2:C:583:GLU:CD	2.24	0.45
2:C:931:ASN:HD21	2:C:936:MET:HB3	1.81	0.45
2:B:886:SER:O	2:B:890:THR:HG23	2.16	0.45
2:C:152:ASP:OD1	2:C:152:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:ILE:HD11	3:D:90:PHE:HA	1.99	0.45
3:D:281:LYS:O	3:D:285:LEU:HG	2.17	0.45
2:B:1305:MET:HB3	2:B:1305:MET:HE2	1.67	0.45
2:C:339:LEU:C	2:C:341:LYS:H	2.25	0.45
2:C:362:LEU:HD11	2:C:1305:MET:SD	2.57	0.45
1:A:910:ASN:OD1	1:A:910:ASN:N	2.39	0.45
2:B:370:VAL:HG21	2:B:402:ALA:HB2	1.99	0.45
2:B:392:PRO:HG2	2:B:394:GLN:HG3	1.98	0.45
2:B:588:LEU:HB3	2:B:604:MET:HE2	1.99	0.45
2:B:757:ILE:C	2:B:758:ILE:HD13	2.42	0.45
2:B:774:LEU:HD23	2:B:774:LEU:HA	1.79	0.45
3:E:93:LEU:HD23	3:E:93:LEU:HA	1.74	0.45
2:B:649:ALA:HB1	2:B:692:ASP:OD1	2.17	0.45
2:C:1280:PRO:HB3	2:C:1285:GLN:O	2.17	0.45
1:A:2:TRP:CD1	1:A:2:TRP:N	2.78	0.45
2:B:515:ILE:HG21	2:B:655:ILE:HG21	1.99	0.45
2:C:94:PHE:HB3	2:C:105:MET:HG2	1.98	0.45
2:C:270:THR:HG22	2:C:291:HIS:HA	1.99	0.45
2:C:1144:ARG:HD2	2:C:1168:ILE:CG2	2.47	0.45
1:A:271:ARG:HE	1:A:271:ARG:HB3	1.63	0.45
1:A:419:TYR:O	1:A:974:SER:HB2	2.16	0.45
2:B:196:LEU:HD22	2:B:296:VAL:HG11	1.98	0.45
2:B:581:LEU:HD11	2:B:745:ILE:HG22	1.97	0.45
2:B:659:LEU:O	2:B:663:VAL:HG23	2.17	0.45
2:B:953:ASP:HB3	3:D:241:ASN:HB2	1.98	0.45
2:B:1033:ASP:OD1	2:B:1033:ASP:N	2.50	0.45
1:A:66:ASP:CG	1:A:122:ARG:HH21	2.24	0.44
2:B:489:MET:SD	2:B:527:ARG:HD2	2.57	0.44
1:A:267:THR:OG1	1:A:320:TYR:OH	2.14	0.44
1:A:282:GLU:HB2	1:A:363:ASN:HB3	1.99	0.44
1:A:944:ARG:HG3	1:A:1010:ILE:HD11	1.99	0.44
1:A:752:VAL:HG13	1:A:779:ASN:O	2.17	0.44
2:B:635:ILE:HA	2:B:636:PRO:HD3	1.80	0.44
2:B:1022:ILE:HG22	2:B:1028:VAL:HG22	1.99	0.44
2:C:169:LYS:HB2	2:C:203:VAL:HG22	2.00	0.44
3:D:153:TYR:CD2	3:D:258:ASN:HB2	2.53	0.44
3:D:157:GLY:HA2	3:D:255:ILE:HG22	2.00	0.44
1:A:967:ILE:HG12	1:A:971:LEU:HD23	2.00	0.44
1:A:797:ARG:HD2	1:A:869:ILE:HD11	1.99	0.44
2:B:354:ALA:O	2:B:358:LEU:HG	2.17	0.44
2:B:751:THR:HB	2:B:754:GLY:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:640:GLN:H	2:C:700:ASP:CG	2.25	0.44
1:A:222:ARG:HA	1:A:222:ARG:HD3	1.71	0.44
1:A:746:PHE:HB2	1:A:785:ALA:HB3	2.00	0.44
1:A:878:TYR:HD2	1:A:897:ILE:HD12	1.83	0.44
1:A:886:ARG:HD3	1:A:886:ARG:H	1.83	0.44
2:B:1144:ARG:HD2	2:B:1168:ILE:CG2	2.47	0.44
2:C:612:PHE:CZ	2:C:1330:ILE:HG22	2.53	0.44
2:C:865:ILE:HD12	2:C:1042:TRP:HE3	1.82	0.44
1:A:384:GLU:HA	1:A:802:THR:HG22	2.00	0.44
2:B:1053:ARG:HD3	2:B:1053:ARG:HA	1.75	0.44
2:C:1168:ILE:HG21	2:C:1171:ILE:HD12	1.99	0.44
1:A:26:THR:OG1	1:A:28:PRO:HG3	2.18	0.44
1:A:474:TYR:CE2	1:A:522:PRO:HG3	2.52	0.44
1:A:944:ARG:HA	1:A:1006:MET:HE1	1.98	0.44
2:C:127:ASN:O	2:C:127:ASN:ND2	2.51	0.44
1:A:1049:TYR:C	1:A:1051:PRO:HD3	2.43	0.44
2:B:849:MET:HE2	2:B:849:MET:HB3	1.68	0.44
1:A:675:THR:HA	1:A:693:TYR:O	2.18	0.43
1:A:913:LEU:O	1:A:953:ARG:NE	2.52	0.43
2:B:335:ASP:OD2	2:B:339:LEU:N	2.51	0.43
2:B:694:ILE:HD13	2:B:767:LEU:HD23	1.99	0.43
2:C:384:MET:HE3	2:C:705:VAL:HG22	2.00	0.43
2:C:475:ILE:H	2:C:475:ILE:HG13	1.51	0.43
2:B:478:ILE:HG13	2:B:762:ILE:HD11	2.00	0.43
2:C:469:ARG:O	2:C:761:SER:HB2	2.18	0.43
1:A:811:TYR:O	1:A:815:GLY:N	2.42	0.43
2:B:1226:ASP:OD2	2:C:122:ASN:ND2	2.41	0.43
2:C:366:MET:HE2	2:C:366:MET:HB3	1.73	0.43
3:D:158:LEU:HD13	3:D:158:LEU:HA	1.81	0.43
3:D:253:GLU:HA	3:D:254:TYR:HA	1.55	0.43
1:A:936:ALA:HB1	1:A:998:LEU:HD23	2.01	0.43
2:C:1060:ARG:HD3	2:C:1291:LEU:O	2.18	0.43
1:A:409:MET:HE2	1:A:465:LEU:HG	1.99	0.43
2:C:998:GLY:HA3	2:C:1012:LEU:HD21	2.01	0.43
3:E:173:PRO:O	3:E:175:LYS:HG3	2.18	0.43
1:A:42:PHE:CE1	1:A:47:ARG:HA	2.53	0.43
1:A:157:LEU:HD23	1:A:159:ILE:HD13	2.01	0.43
1:A:319:MET:HE2	1:A:319:MET:HB3	1.63	0.43
2:B:795:ASP:HA	2:B:796:PRO:HD2	1.84	0.43
2:C:146:GLU:O	2:C:148:GLN:NE2	2.52	0.43
2:C:391:GLY:HA3	2:C:392:PRO:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1118:THR:HA	2:C:1129:PRO:HA	1.99	0.43
3:D:112:TYR:CZ	3:D:119:ILE:HD13	2.53	0.43
1:A:373:ILE:HG12	1:A:817:GLY:N	2.33	0.43
2:B:1033:ASP:O	2:B:1034:GLN:HB2	2.18	0.43
3:D:1:MET:HE2	3:D:1:MET:HB3	1.95	0.43
3:D:182:TRP:NE1	3:D:185:SER:HA	2.34	0.43
2:B:1304:MET:HE2	2:B:1304:MET:HB3	1.87	0.43
2:C:612:PHE:HZ	2:C:1330:ILE:HG22	1.84	0.43
2:C:1012:LEU:HD23	2:C:1012:LEU:HA	1.83	0.43
2:C:1197:PRO:HG2	2:C:1200:LYS:HB2	2.00	0.43
3:E:180:ASP:OD2	3:E:247:ARG:NH1	2.51	0.43
3:E:201:PHE:HE1	3:E:220:ASN:HB3	1.82	0.43
1:A:69:HIS:CG	1:A:70:PRO:HD2	2.54	0.43
1:A:557:SER:HB3	1:A:583:ARG:HB2	2.00	0.43
2:B:554:ARG:HD3	2:B:594:LEU:HD13	2.00	0.43
1:A:561:LEU:HD22	1:A:587:MET:HB2	2.00	0.43
2:B:256:PHE:HE2	2:B:990:THR:HG21	1.84	0.43
2:B:299:ALA:HB2	2:B:1265:MET:HB3	2.01	0.43
2:B:490:PHE:O	2:B:745:ILE:HA	2.19	0.43
2:B:526:ASN:HB2	2:B:724:HIS:CE1	2.54	0.43
2:C:271:THR:HB	2:C:290:TYR:CE2	2.53	0.43
2:C:707:ALA:HB2	2:C:1330:ILE:HG23	2.01	0.43
2:C:1267:THR:HB	2:C:1299:SER:CB	2.49	0.43
3:E:53:GLU:OE1	3:E:281:LYS:NZ	2.52	0.43
3:E:142:THR:HA	3:E:143:PRO:HD3	1.85	0.43
1:A:486:THR:HB	1:A:489:SER:HB3	2.00	0.42
2:C:1128:TYR:CZ	2:C:1135:PRO:HD3	2.54	0.42
2:C:1214:GLU:HG2	2:C:1215:PRO:HD2	2.01	0.42
1:A:616:ASP:OD1	1:A:691:TYR:OH	2.31	0.42
2:B:309:TRP:CH2	2:B:1257:ALA:HB1	2.54	0.42
1:A:154:PHE:HD1	1:A:159:ILE:HG13	1.85	0.42
2:B:1254:PRO:HG2	2:B:1257:ALA:HB2	2.01	0.42
2:C:153:ASP:OD2	2:C:401:LEU:N	2.42	0.42
2:C:733:VAL:HG12	2:C:743:PRO:CA	2.46	0.42
1:A:860:SER:HA	1:A:920:LEU:HB2	2.00	0.42
2:B:213:PHE:HB3	2:B:219:ILE:HD12	2.01	0.42
2:B:404:ASP:O	2:B:408:ILE:HG12	2.19	0.42
2:B:672:MET:HE3	2:B:676:THR:OG1	2.19	0.42
2:B:1050:LEU:HD23	2:B:1050:LEU:HA	1.66	0.42
3:E:19:ILE:HG23	3:E:196:TRP:HZ2	1.84	0.42
1:A:36:THR:OG1	1:A:37:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:LYS:NZ	2:B:1182:GLU:OE2	2.42	0.42
2:B:265:VAL:HB	2:B:1304:MET:HB3	2.00	0.42
2:B:1183:GLY:HA2	2:B:1207:MET:HE1	2.01	0.42
2:C:309:TRP:CZ2	2:C:1257:ALA:HB1	2.55	0.42
2:C:633:THR:HG21	2:C:710:SER:CB	2.49	0.42
3:D:261:ARG:NH1	3:D:263:ALA:O	2.52	0.42
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.67	0.42
1:A:402:THR:HG23	1:A:824:ARG:HB3	2.01	0.42
2:B:235:ILE:HG21	2:C:774:LEU:HA	2.01	0.42
2:C:310:LEU:HD12	2:C:310:LEU:HA	1.82	0.42
2:C:1109:SER:OG	2:C:1118:THR:HB	2.19	0.42
2:C:1236:ILE:HD13	2:C:1236:ILE:HA	1.87	0.42
1:A:11:THR:OG1	1:A:254:ASP:OD2	2.37	0.42
1:A:293:LEU:HD22	1:A:297:LEU:HG	2.01	0.42
2:B:1048:ASP:O	2:B:1052:LEU:HD22	2.20	0.42
2:B:1055:LEU:O	2:B:1059:LEU:HG	2.19	0.42
2:C:190:VAL:HG23	2:C:300:LEU:HB3	2.00	0.42
2:C:776:ARG:HB3	2:C:787:ILE:HG13	2.02	0.42
2:C:874:ILE:HG12	2:C:896:LEU:O	2.19	0.42
1:A:773:ARG:O	1:A:818:PHE:HA	2.19	0.42
2:B:384:MET:O	2:B:387:THR:HG23	2.20	0.42
2:B:1064:ASN:HA	2:B:1065:PRO:HD3	1.94	0.42
2:B:1206:PHE:CE1	2:B:1232:PRO:HD3	2.55	0.42
2:B:1236:ILE:HD13	2:B:1236:ILE:HA	1.90	0.42
2:C:1071:PHE:HB2	2:C:1173:TYR:CZ	2.54	0.42
2:C:1121:HIS:CD2	2:C:1123:PRO:HG2	2.55	0.42
3:D:28:PRO:HB3	3:D:226:MET:HG3	2.01	0.42
2:B:231:LEU:HB3	2:B:249:SER:HB3	2.01	0.42
2:C:83:GLN:HG3	2:C:165:THR:HB	2.01	0.42
2:C:674:LYS:HA	2:C:674:LYS:HD2	1.82	0.42
2:C:1134:ARG:NH1	2:C:1154:ASN:OD1	2.50	0.42
3:D:244:VAL:HG13	3:D:247:ARG:HB2	2.02	0.42
3:E:178:LYS:HB2	3:E:249:ASP:OD2	2.20	0.42
1:A:290:LEU:O	1:A:293:LEU:HB2	2.20	0.42
2:C:332:THR:HG23	2:C:1270:LEU:HD12	2.02	0.41
2:C:355:ALA:HB3	2:C:1276:LEU:HD11	2.02	0.41
2:C:674:LYS:HE3	2:C:677:ARG:HH21	1.84	0.41
2:B:325:TYR:OH	2:B:349:ASN:OD1	2.22	0.41
2:B:537:LEU:HD23	2:B:537:LEU:HA	1.80	0.41
2:B:643:THR:HG22	2:B:645:THR:H	1.84	0.41
2:B:748:GLN:H	2:B:748:GLN:HG2	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:793:TYR:CD2	2:B:1321:ASN:HB3	2.55	0.41
2:B:994:SER:O	2:B:999:LYS:HE3	2.20	0.41
2:C:234:PRO:HB2	2:C:237:VAL:HG23	2.02	0.41
2:C:288:THR:OG1	2:C:289:THR:N	2.53	0.41
2:C:1208:ASP:CG	2:C:1243:ARG:HH21	2.27	0.41
3:D:96:LEU:HD21	3:D:111:ILE:HG23	2.02	0.41
2:B:323:THR:HG21	2:B:1262:SER:HB2	2.03	0.41
2:B:588:LEU:O	2:B:604:MET:HG3	2.20	0.41
2:B:605:ARG:O	2:B:608:THR:HG23	2.20	0.41
2:C:186:ASP:CG	2:C:279:SER:H	2.29	0.41
2:C:875:THR:HG23	2:C:877:ALA:H	1.85	0.41
2:C:1048:ASP:O	2:C:1052:LEU:HD22	2.21	0.41
1:A:70:PRO:HA	1:A:73:ARG:NH1	2.36	0.41
1:A:677:LEU:HD23	1:A:677:LEU:HA	1.95	0.41
1:A:794:LEU:O	1:A:797:ARG:HG3	2.20	0.41
2:B:474:ASP:O	2:B:477:SER:OG	2.31	0.41
3:D:2:LEU:HD12	3:D:107:LEU:HD21	2.01	0.41
3:D:79:ILE:HA	3:D:269:ILE:HG22	2.03	0.41
1:A:268:TYR:HD2	1:A:271:ARG:HD2	1.86	0.41
3:D:35:LEU:HD12	3:D:35:LEU:HA	1.79	0.41
3:D:229:PHE:CE2	3:D:252:LEU:HD11	2.55	0.41
3:E:224:PHE:O	3:E:228:LEU:HG	2.20	0.41
1:A:572:LEU:O	1:A:576:ASN:ND2	2.33	0.41
2:B:873:TYR:HA	2:B:896:LEU:O	2.20	0.41
2:B:1156:ILE:O	2:B:1159:VAL:HB	2.20	0.41
2:C:168:VAL:HG11	2:C:196:LEU:HG	2.02	0.41
2:C:509:VAL:HG22	2:C:683:TRP:CZ3	2.55	0.41
2:C:1076:ILE:HB	2:C:1166:VAL:CG2	2.50	0.41
3:E:35:LEU:HD12	3:E:35:LEU:HA	1.82	0.41
1:A:519:ILE:HA	1:A:520:PRO:HD2	1.97	0.41
1:A:726:ILE:H	1:A:726:ILE:HG12	1.64	0.41
1:A:862:GLY:HA2	1:A:882:ASP:HB3	2.03	0.41
2:B:287:ARG:HD2	2:B:328:GLY:HA2	2.02	0.41
2:C:1201:LEU:HD12	2:C:1201:LEU:HA	1.90	0.41
3:D:53:GLU:CD	3:D:53:GLU:H	2.28	0.41
2:B:505:PRO:HB3	2:B:663:VAL:HG13	2.02	0.41
2:B:583:GLU:CD	2:B:583:GLU:H	2.29	0.41
2:B:762:ILE:HD12	2:B:762:ILE:HA	1.89	0.41
2:B:814:THR:HA	2:B:1010:ARG:NH1	2.33	0.41
2:B:875:THR:HG23	2:B:877:ALA:H	1.85	0.41
2:C:820:ILE:HD13	2:C:820:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1099:VAL:O	2:C:1139:MET:HA	2.21	0.41
1:A:268:TYR:HA	1:A:271:ARG:HG2	2.01	0.41
1:A:371:GLY:N	1:A:818:PHE:O	2.51	0.41
2:B:195:ASN:O	2:B:198:LYS:HE3	2.21	0.41
2:B:447:ARG:O	2:B:686:HIS:NE2	2.52	0.41
2:B:505:PRO:HA	2:B:543:TRP:CH2	2.56	0.41
2:B:581:LEU:HD23	2:B:581:LEU:HA	1.85	0.41
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.83	0.41
3:E:259:SER:OG	3:E:261:ARG:HB2	2.20	0.41
1:A:583:ARG:HH11	1:A:583:ARG:N	2.08	0.41
1:A:763:LYS:HE2	1:A:803:SER:HB3	2.03	0.41
1:A:767:SER:N	1:A:788:ASP:OD1	2.54	0.41
2:B:383:SER:HB3	2:B:387:THR:HG21	2.03	0.41
2:B:401:LEU:HD23	2:B:401:LEU:HA	1.90	0.41
2:B:516:LEU:HD23	2:B:516:LEU:HA	1.92	0.41
3:D:187:ILE:HD13	3:D:187:ILE:HA	1.91	0.41
1:A:27:LYS:NZ	1:A:37:ASP:OD1	2.37	0.40
1:A:500:ASP:OD1	1:A:574:ARG:NH2	2.53	0.40
2:B:382:HIS:HE2	2:B:713:MET:H	1.69	0.40
3:D:166:GLU:OE1	3:D:175:LYS:NZ	2.42	0.40
2:B:489:MET:HE1	2:B:580:TYR:CE2	2.56	0.40
2:B:892:VAL:HG12	2:B:894:VAL:HB	2.04	0.40
3:D:231:MET:HG3	3:D:271:TYR:OH	2.21	0.40
2:B:214:ASP:OD2	2:B:217:THR:OG1	2.40	0.40
2:B:1127:ALA:H	3:E:149:MET:HE1	1.87	0.40
2:B:1289:PRO:CD	3:D:20:ARG:HD2	2.49	0.40
2:C:375:ARG:HH11	2:C:375:ARG:HD2	1.74	0.40
2:C:504:ASP:OD1	2:C:504:ASP:N	2.52	0.40
2:C:576:ASP:O	2:C:579:LEU:HB2	2.21	0.40
3:E:160:LEU:HB3	3:E:161:ALA:H	1.77	0.40
3:E:189:LEU:HD13	3:E:189:LEU:HA	1.92	0.40
1:A:272:LEU:HD21	1:A:297:LEU:HB3	2.02	0.40
1:A:563:ALA:HA	1:A:589:ASP:O	2.22	0.40
1:A:722:ASP:OD1	1:A:722:ASP:N	2.49	0.40
1:A:887:ILE:HG22	1:A:891:THR:HB	2.04	0.40
2:B:226:PRO:HB2	2:B:250:GLY:HA3	2.04	0.40
2:B:373:ASP:HA	2:B:1315:MET:HE1	2.03	0.40
2:B:394:GLN:HB3	2:B:398:ARG:HG3	2.03	0.40
2:C:225:ILE:HD13	2:C:1070:ARG:HB2	2.03	0.40
2:C:414:LEU:HD23	2:C:814:THR:HB	2.03	0.40
2:C:813:LEU:HA	2:C:992:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1050:LEU:HD12	2:C:1050:LEU:HA	1.78	0.40
2:C:1078:TYR:CE2	2:C:1227:MET:HE3	2.56	0.40
3:D:239:VAL:CG1	3:D:250:ARG:HD2	2.52	0.40
3:E:239:VAL:CG1	3:E:250:ARG:HD2	2.51	0.40
1:A:83:ILE:H	1:A:83:ILE:HG13	1.64	0.40
2:C:712:PHE:HB2	2:C:715:ASN:ND2	2.36	0.40
3:E:1:MET:HB2	3:E:121:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1055/1058 (100%)	1012 (96%)	40 (4%)	3 (0%)	36	65
2	B	1187/1333 (89%)	1145 (96%)	39 (3%)	3 (0%)	36	65
2	C	1246/1333 (94%)	1197 (96%)	41 (3%)	8 (1%)	21	51
3	D	290/448 (65%)	281 (97%)	8 (3%)	1 (0%)	36	65
3	E	290/448 (65%)	284 (98%)	6 (2%)	0	100	100
All	All	4068/4620 (88%)	3919 (96%)	134 (3%)	15 (0%)	31	59

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	B	1035	ILE
2	C	288	THR
2	C	1267	THR
1	A	483	MET
2	B	738	GLU
2	C	87	GLU

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Mol	Chain	Res	Type
2	C	1041	ARG
2	C	1123	PRO
2	C	340	VAL
2	B	1123	PRO
2	C	1014	MET
3	D	244	VAL
2	C	1281	VAL
1	A	728	PRO

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%)	841 (89%)	101 (11%)	6	22
2	B	1038/1153 (90%)	963 (93%)	75 (7%)	13	39
2	C	1089/1153 (94%)	997 (92%)	92 (8%)	10	31
3	D	240/379 (63%)	217 (90%)	23 (10%)	8	26
3	E	240/379 (63%)	219 (91%)	21 (9%)	9	29
All	All	3549/4007 (89%)	3237 (91%)	312 (9%)	11	29

All (312) 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	36	THR
1	A	41	THR
1	A	73	ARG
1	A	76	LEU
1	A	77	LYS
1	A	78	TYR
1	A	88	LEU

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Mol	Chain	Res	Type
1	A	97	ARG
1	A	99	VAL
1	A	104	VAL
1	A	117	LEU
1	A	130	VAL
1	A	133	LEU
1	A	140	ILE
1	A	157	LEU
1	A	163	ASP
1	A	166	ILE
1	A	180	ASN
1	A	199	MET
1	A	205	VAL
1	A	207	THR
1	A	210	SER
1	A	234	LYS
1	A	260	LEU
1	A	264	SER
1	A	267	THR
1	A	272	LEU
1	A	275	ILE
1	A	293	LEU
1	A	300	LEU
1	A	312	LEU
1	A	314	ARG
1	A	315	LEU
1	A	337	LEU
1	A	360	THR
1	A	377	LEU
1	A	379	VAL
1	A	401	ILE
1	A	402	THR
1	A	444	LEU
1	A	453	LEU
1	A	465	LEU
1	A	466	LEU
1	A	470	LEU
1	A	483	MET
1	A	493	LEU
1	A	504	THR
1	A	506	VAL
1	A	523	MET

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Mol	Chain	Res	Type
1	A	530	MET
1	A	534	SER
1	A	547	THR
1	A	559	ILE
1	A	583	ARG
1	A	598	VAL
1	A	600	VAL
1	A	611	ASP
1	A	613	ILE
1	A	619	SER
1	A	622	ASP
1	A	628	MET
1	A	647	LEU
1	A	648	VAL
1	A	680	THR
1	A	697	ILE
1	A	714	ARG
1	A	721	ASP
1	A	726	ILE
1	A	740	THR
1	A	757	LEU
1	A	762	LEU
1	A	770	THR
1	A	782	ASN
1	A	784	ILE
1	A	794	LEU
1	A	800	SER
1	A	816	LEU
1	A	823	THR
1	A	832	GLU
1	A	855	MET
1	A	877	LYS
1	A	880	VAL
1	A	887	ILE
1	A	890	LEU
1	A	910	ASN
1	A	914	GLU
1	A	925	ILE
1	A	926	MET
1	A	934	THR
1	A	941	ASP
1	A	970	ARG

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Mol	Chain	Res	Type
1	A	1007	LEU
1	A	1013	THR
1	A	1018	ARG
1	A	1025	ILE
1	A	1034	ARG
1	A	1035	LEU
2	B	144	ASN
2	B	147	VAL
2	B	168	VAL
2	B	177	LYS
2	B	180	LEU
2	B	233	VAL
2	B	238	THR
2	B	264	LEU
2	B	265	VAL
2	B	274	MET
2	B	289	THR
2	B	294	VAL
2	B	296	VAL
2	B	323	THR
2	B	330	THR
2	B	334	LEU
2	B	335	ASP
2	B	384	MET
2	B	388	GLN
2	B	397	LEU
2	B	439	VAL
2	B	452	ASN
2	B	510	VAL
2	B	533	GLN
2	B	546	VAL
2	B	552	VAL
2	B	567	GLU
2	B	599	THR
2	B	626	ARG
2	B	629	ARG
2	B	637	TYR
2	B	641	ARG
2	B	643	THR
2	B	672	MET
2	B	674	LYS
2	B	704	VAL

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Mol	Chain	Res	Type
2	B	748	GLN
2	B	751	THR
2	B	755	LEU
2	B	767	LEU
2	B	797	SER
2	B	799	THR
2	B	809	VAL
2	B	815	LEU
2	B	828	ASP
2	B	833	ARG
2	B	843	LEU
2	B	851	THR
2	B	879	THR
2	B	892	VAL
2	B	912	GLU
2	B	917	VAL
2	B	945	VAL
2	B	946	LEU
2	B	948	ILE
2	B	1052	LEU
2	B	1055	LEU
2	B	1061	LEU
2	B	1062	ILE
2	B	1079	LEU
2	B	1085	ASP
2	B	1110	LEU
2	B	1159	VAL
2	B	1166	VAL
2	B	1193	ILE
2	B	1212	ARG
2	B	1233	LEU
2	B	1234	GLN
2	B	1270	LEU
2	B	1311	THR
2	B	1315	MET
2	B	1317	VAL
2	B	1319	ARG
2	B	1320	VAL
2	B	1331	ARG
2	C	74	LYS
2	C	83	GLN
2	C	86	VAL

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Mol	Chain	Res	Type
2	C	98	ASN
2	C	112	THR
2	C	120	VAL
2	C	136	VAL
2	C	157	ILE
2	C	175	THR
2	C	176	LYS
2	C	190	VAL
2	C	207	ASP
2	C	217	THR
2	C	222	THR
2	C	223	LYS
2	C	237	VAL
2	C	244	SER
2	C	264	LEU
2	C	265	VAL
2	C	270	THR
2	C	280	THR
2	C	282	VAL
2	C	285	VAL
2	C	294	VAL
2	C	296	VAL
2	C	323	THR
2	C	330	THR
2	C	340	VAL
2	C	363	ARG
2	C	384	MET
2	C	451	GLU
2	C	475	ILE
2	C	486	VAL
2	C	508	ILE
2	C	527	ARG
2	C	546	VAL
2	C	552	VAL
2	C	579	LEU
2	C	608	THR
2	C	626	ARG
2	C	629	ARG
2	C	630	ASN
2	C	637	TYR
2	C	654	THR
2	C	661	ASN

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Mol	Chain	Res	Type
2	C	684	LEU
2	C	687	LEU
2	C	689	THR
2	C	704	VAL
2	C	744	ILE
2	C	767	LEU
2	C	775	VAL
2	C	787	ILE
2	C	790	GLU
2	C	797	SER
2	C	798	THR
2	C	799	THR
2	C	809	VAL
2	C	815	LEU
2	C	833	ARG
2	C	865	ILE
2	C	892	VAL
2	C	911	ARG
2	C	946	LEU
2	C	948	ILE
2	C	951	ILE
2	C	962	ASP
2	C	1014	MET
2	C	1015	GLN
2	C	1019	ILE
2	C	1052	LEU
2	C	1055	LEU
2	C	1060	ARG
2	C	1062	ILE
2	C	1070	ARG
2	C	1072	ASN
2	C	1107	SER
2	C	1110	LEU
2	C	1113	LYS
2	C	1116	ARG
2	C	1132	THR
2	C	1139	MET
2	C	1171	ILE
2	C	1200	LYS
2	C	1229	LEU
2	C	1233	LEU
2	C	1234	GLN

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Mol	Chain	Res	Type
2	C	1250	GLU
2	C	1269	THR
2	C	1286	VAL
2	C	1291	LEU
2	C	1320	VAL
3	D	2	LEU
3	D	29	THR
3	D	35	LEU
3	D	47	LYS
3	D	48	THR
3	D	54	THR
3	D	79	ILE
3	D	92	ARG
3	D	93	LEU
3	D	107	LEU
3	D	116	THR
3	D	133	THR
3	D	142	THR
3	D	158	LEU
3	D	160	LEU
3	D	171	VAL
3	D	189	LEU
3	D	191	ARG
3	D	193	VAL
3	D	194	VAL
3	D	252	LEU
3	D	253	GLU
3	D	261	ARG
3	E	2	LEU
3	E	24	THR
3	E	29	THR
3	E	35	LEU
3	E	66	VAL
3	E	93	LEU
3	E	98	LEU
3	E	116	THR
3	E	133	THR
3	E	158	LEU
3	E	160	LEU
3	E	189	LEU
3	E	190	SER
3	E	194	VAL

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Mol	Chain	Res	Type
3	E	226	MET
3	E	244	VAL
3	E	251	VAL
3	E	252	LEU
3	E	266	THR
3	E	273	LEU
3	E	275	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	49	HIS
1	A	114	ASN
1	A	125	ASN
1	A	145	ASN
1	A	180	ASN
1	A	194	HIS
1	A	457	ASN
1	A	508	ASN
1	A	527	ASN
1	A	544	ASN
1	A	595	ASN
1	A	623	GLN
1	A	779	ASN
1	A	916	ASN
1	A	955	ASN
1	A	1014	HIS
1	A	1047	ASN
2	B	491	ASN
2	B	661	ASN
2	B	682	GLN
2	B	724	HIS
2	B	1034	GLN
2	B	1138	HIS
2	B	1283	ASN
2	B	1295	HIS
2	B	1332	ASN
2	C	156	GLN
2	C	276	ASN
2	C	283	ASN
2	C	346	HIS

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Mol	Chain	Res	Type
2	C	430	ASN
2	C	526	ASN
2	C	610	GLN
2	C	664	ASN
2	C	682	GLN
2	C	711	ASN
2	C	731	GLN
2	C	981	HIS
2	C	1138	HIS
2	C	1273	ASN
2	C	1285	GLN
3	D	14	GLN
3	D	55	HIS
3	D	83	ASN
3	D	85	ASN
3	E	83	ASN
3	E	113	ASN
3	E	220	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GTP	A	1101	-	33,34,34	1.03	4 (12%)	50,54,54	1.67	10 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	1101	-	-	6/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	GTP	PA-O3A	2.32	1.62	1.59
4	A	1101	GTP	PB-O3A	2.26	1.61	1.59
4	A	1101	GTP	C2-N3	2.25	1.38	1.33
4	A	1101	GTP	C5-N7	-2.00	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	GTP	C5-C4-N3	-5.26	120.02	128.39
4	A	1101	GTP	C2-N3-C4	4.58	120.19	112.30
4	A	1101	GTP	N9-C4-N3	3.42	132.79	125.95
4	A	1101	GTP	C8-N7-C5	3.10	109.78	104.26
4	A	1101	GTP	N9-C8-N7	-3.05	107.74	113.40
4	A	1101	GTP	C2-N1-C6	-2.99	119.69	125.11
4	A	1101	GTP	C5-C6-N1	2.41	119.38	113.25
4	A	1101	GTP	O6-C6-C5	-2.34	120.36	126.53
4	A	1101	GTP	O2B-PB-O3A	2.27	113.41	107.27
4	A	1101	GTP	C4-C5-N7	-2.08	107.37	110.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	GTP	C5'-O5'-PA-O3A
4	A	1101	GTP	C5'-O5'-PA-O2A

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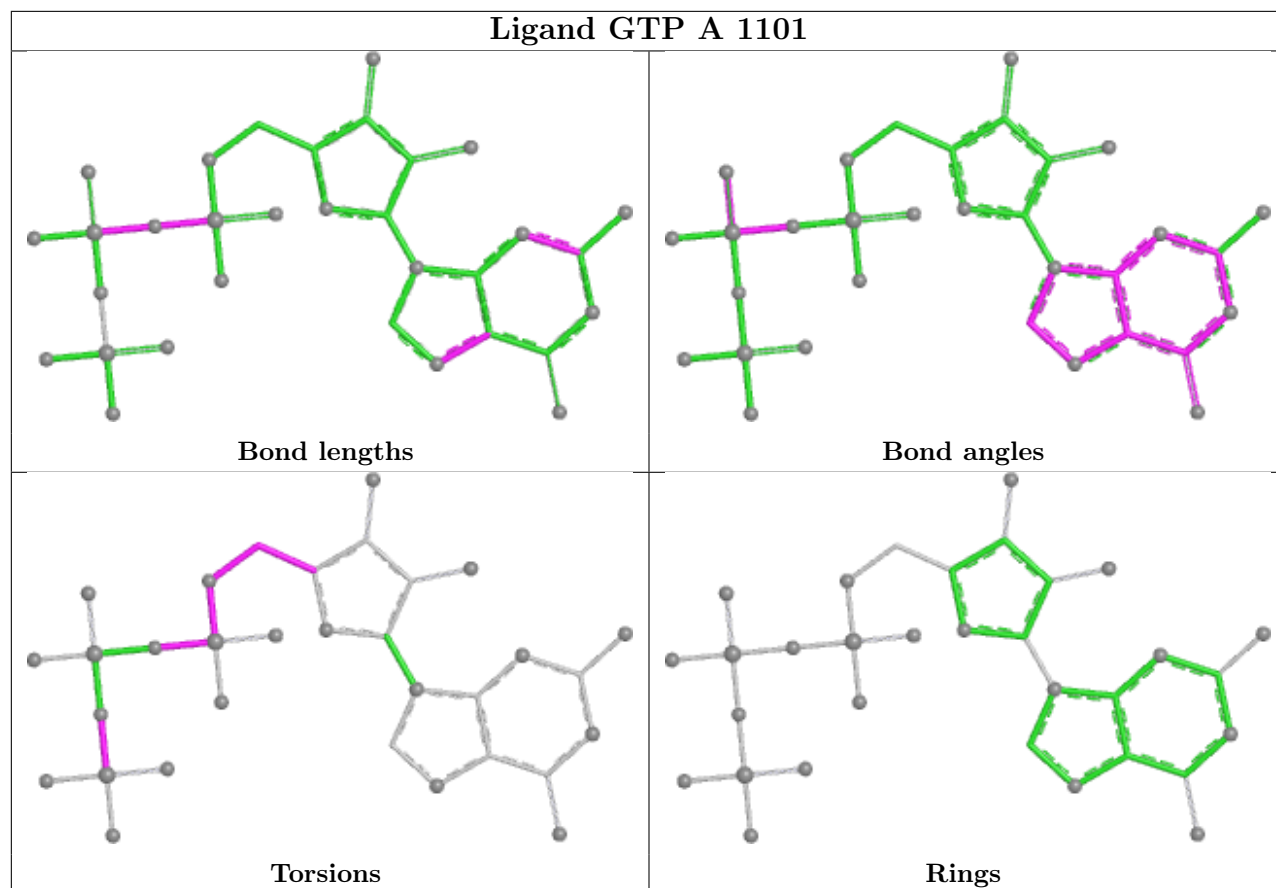
Mol	Chain	Res	Type	Atoms
4	A	1101	GTP	C4'-C5'-O5'-PA
4	A	1101	GTP	O4'-C4'-C5'-O5'
4	A	1101	GTP	PB-O3A-PA-O1A
4	A	1101	GTP	PB-O3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

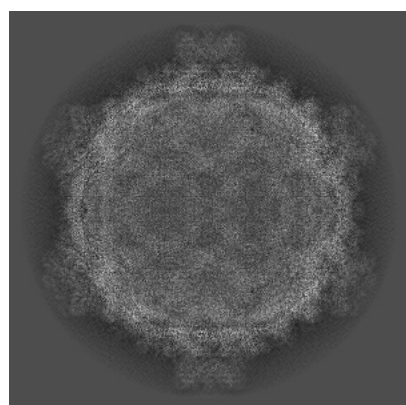
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6374. These allow visual inspection of the internal detail of the map and identification of artifacts.

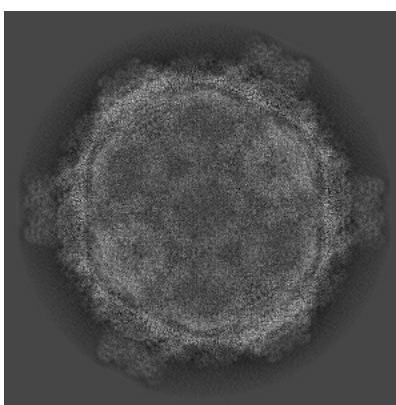
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

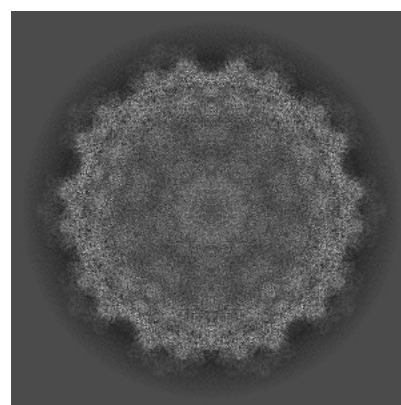
6.1.1 Primary map



X



Y

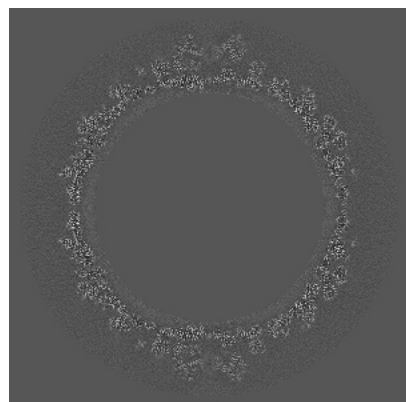


Z

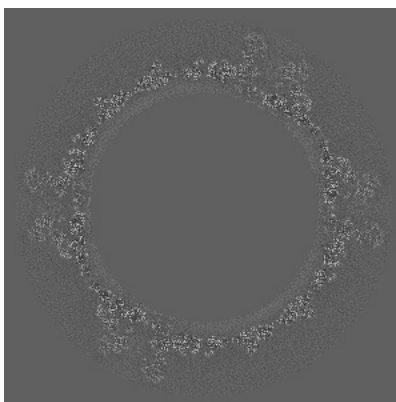
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

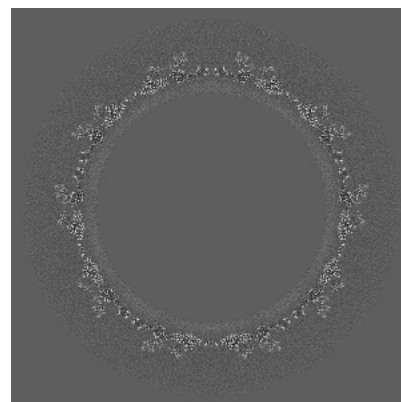
6.2.1 Primary map



X Index: 350



Y Index: 350

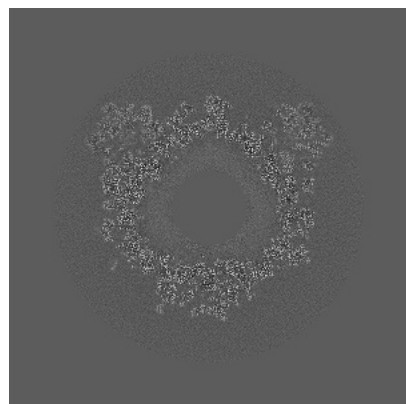


Z Index: 350

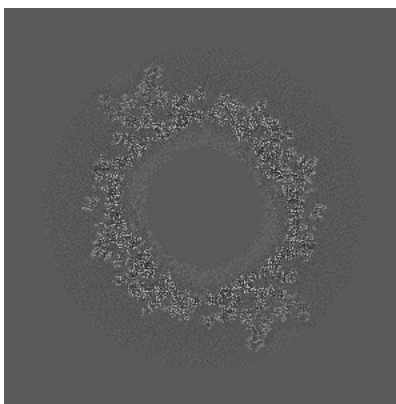
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

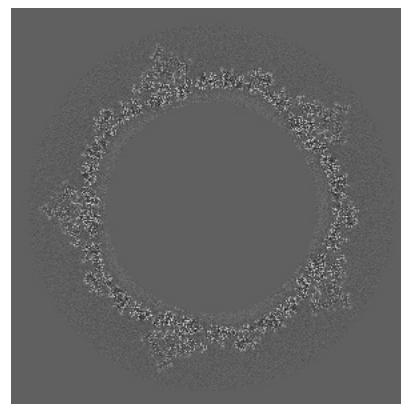
6.3.1 Primary map



X Index: 161



Y Index: 178

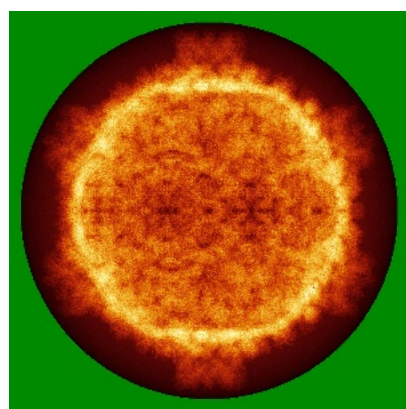


Z Index: 273

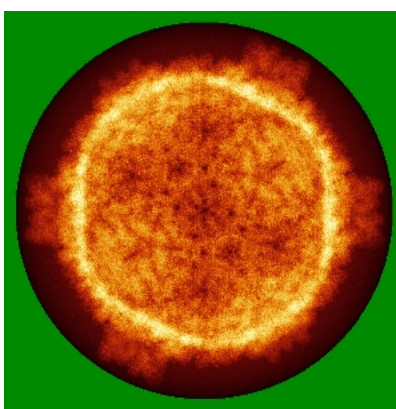
The images above show the largest variance slices of the map in three orthogonal directions.

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

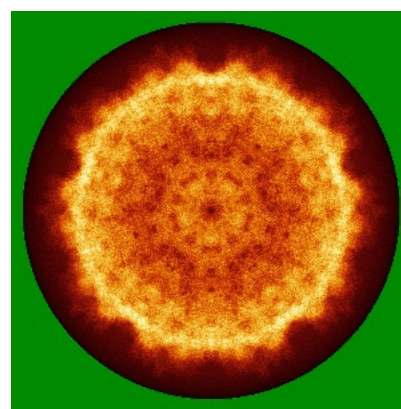
6.4.1 Primary map



X



Y

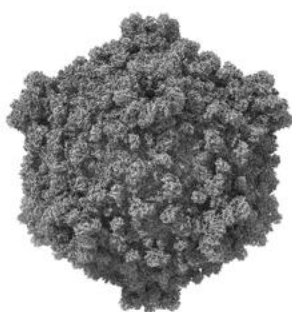


Z

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.

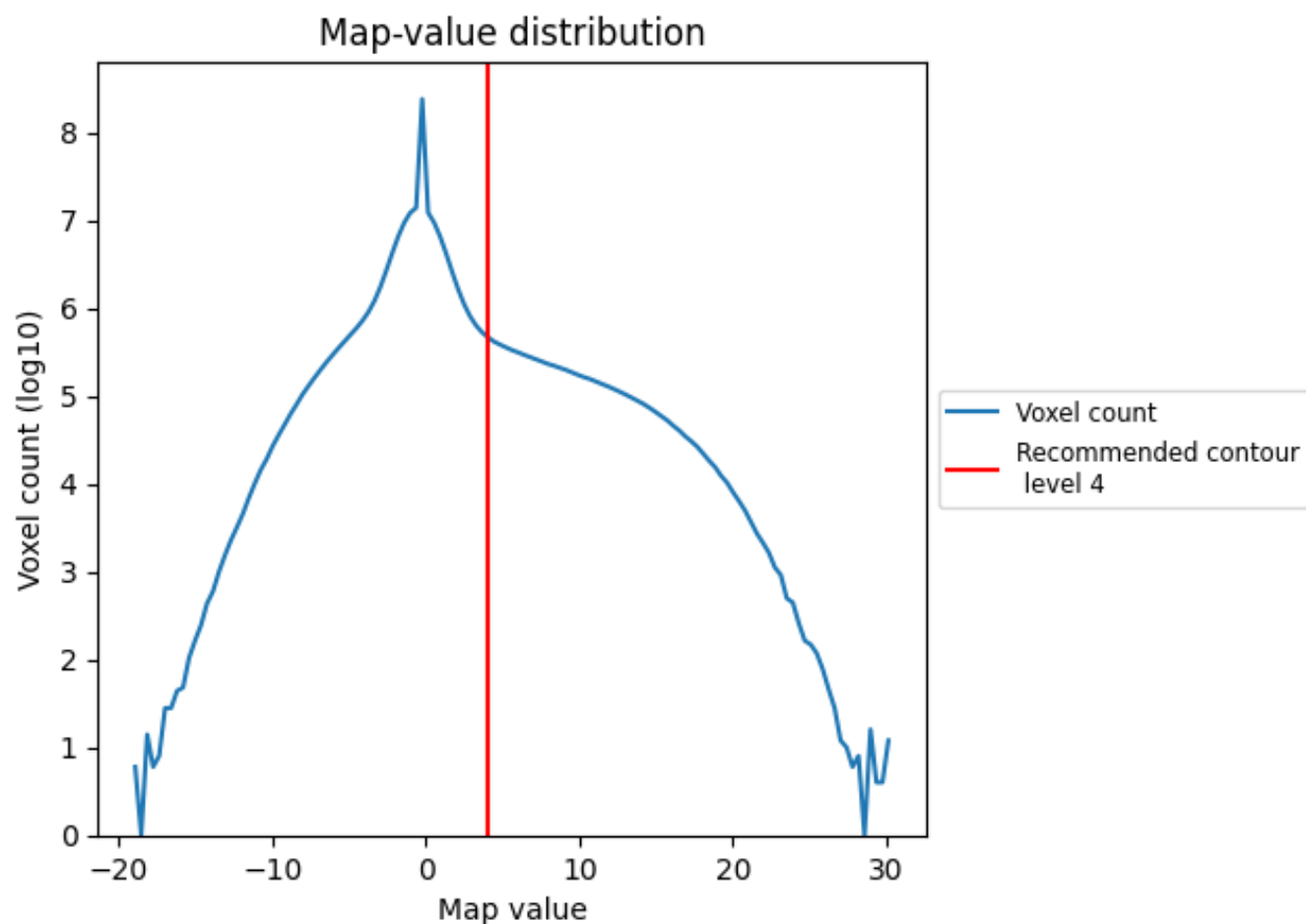
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

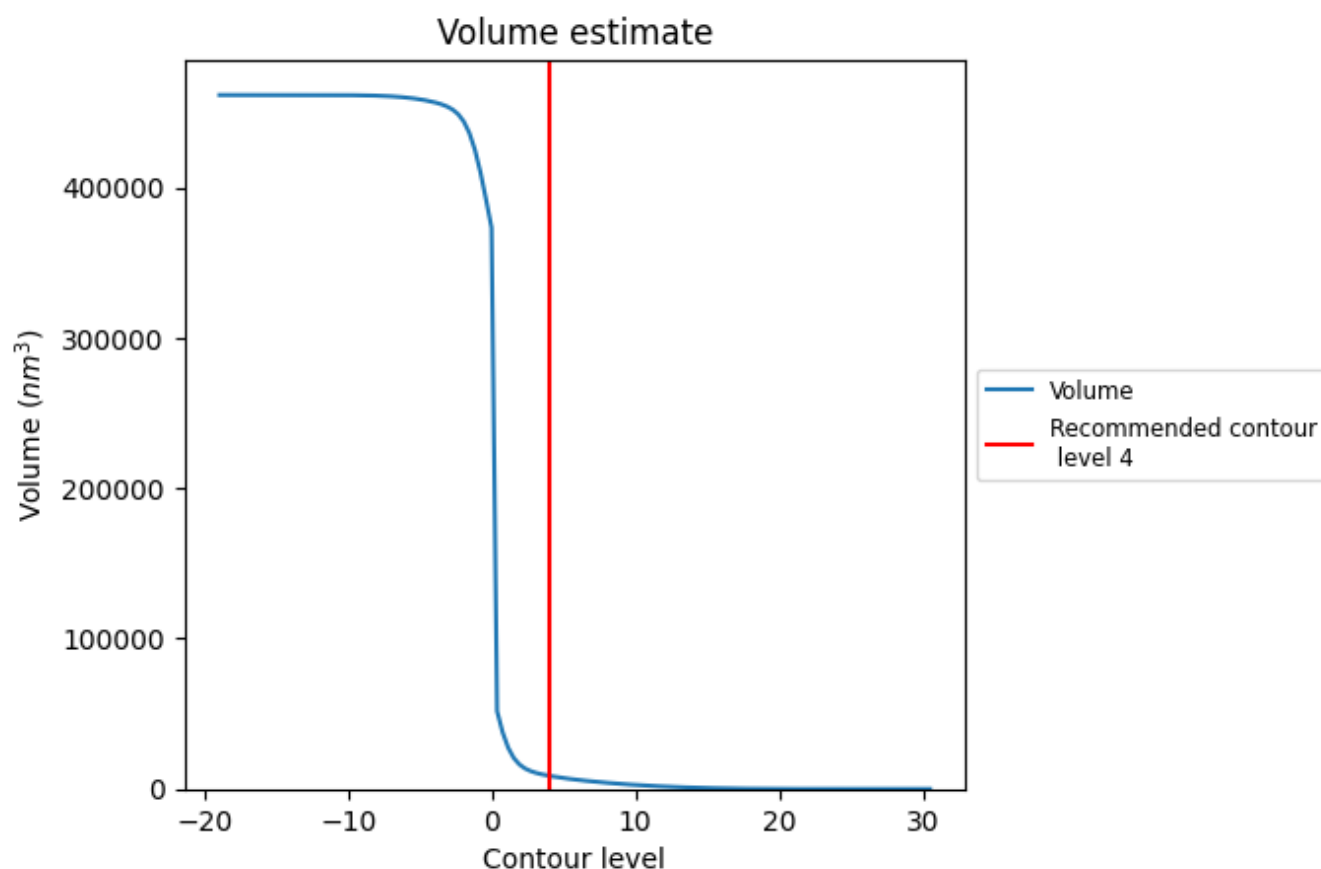
This section contains the results of statistical analysis of the map.

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.

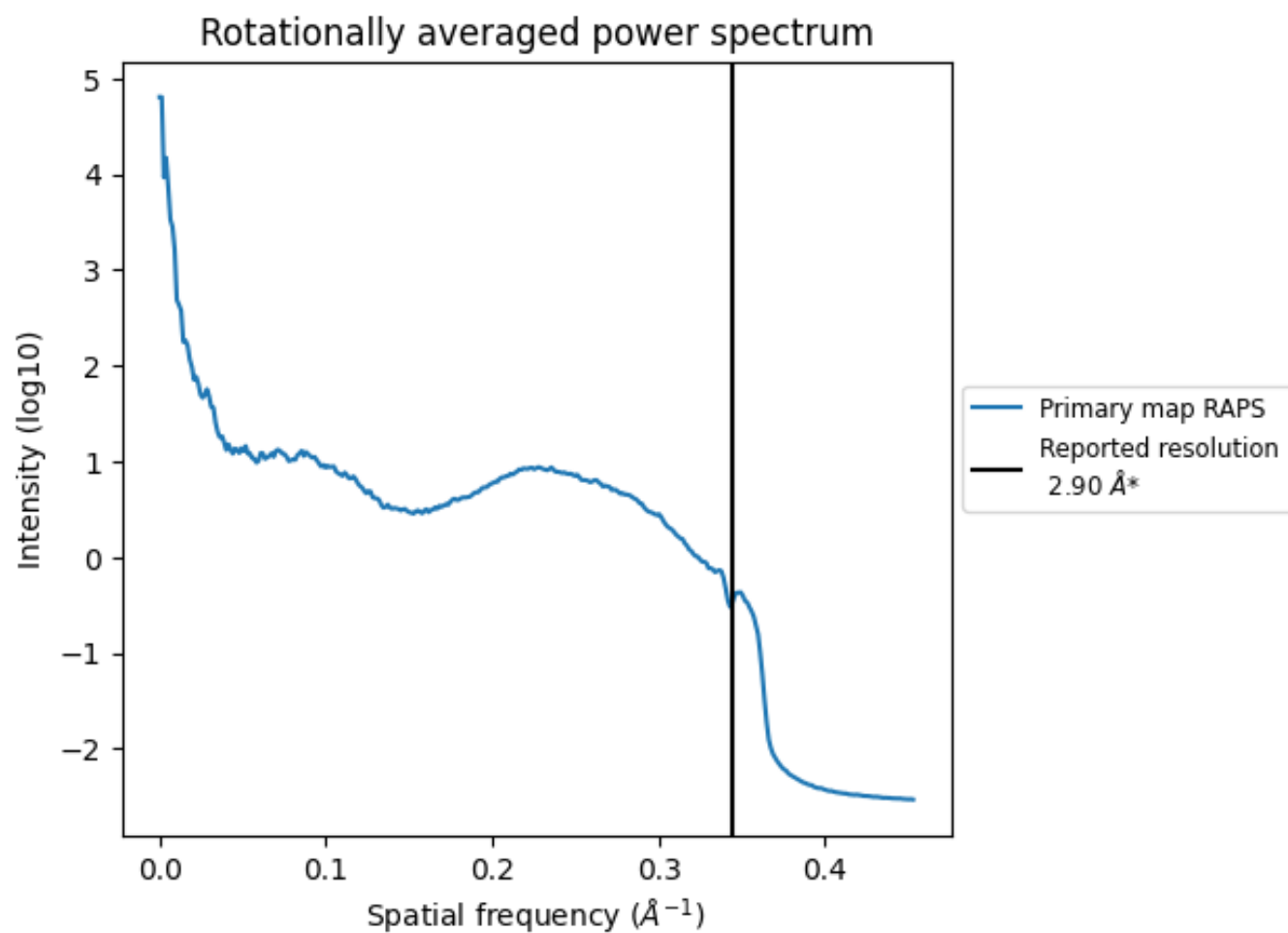
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8751 nm^3 ; this corresponds to an approximate mass of 7905 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 0.345 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

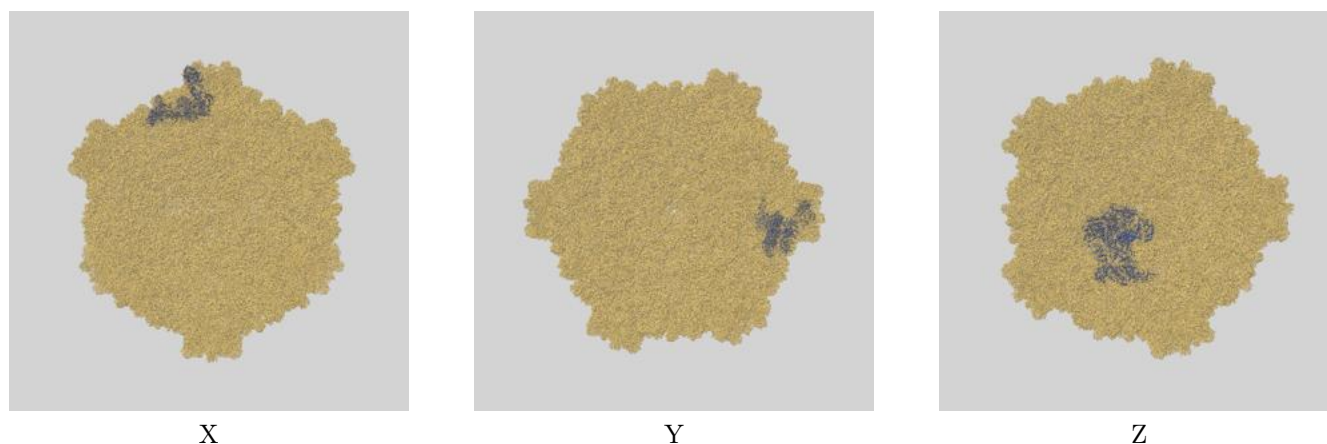
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

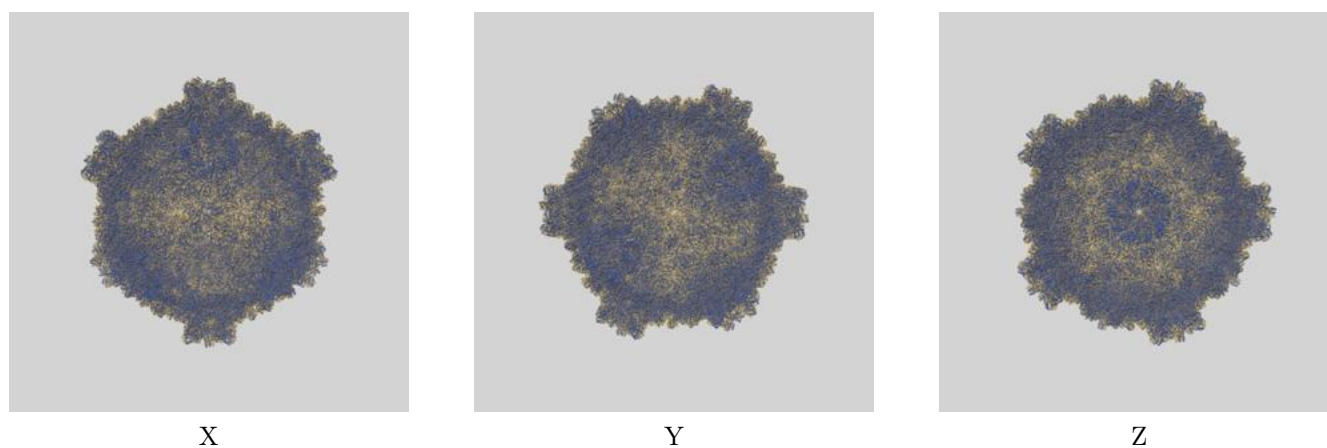
This section contains information regarding the fit between EMDB map EMD-6374 and PDB model 3JB0. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



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



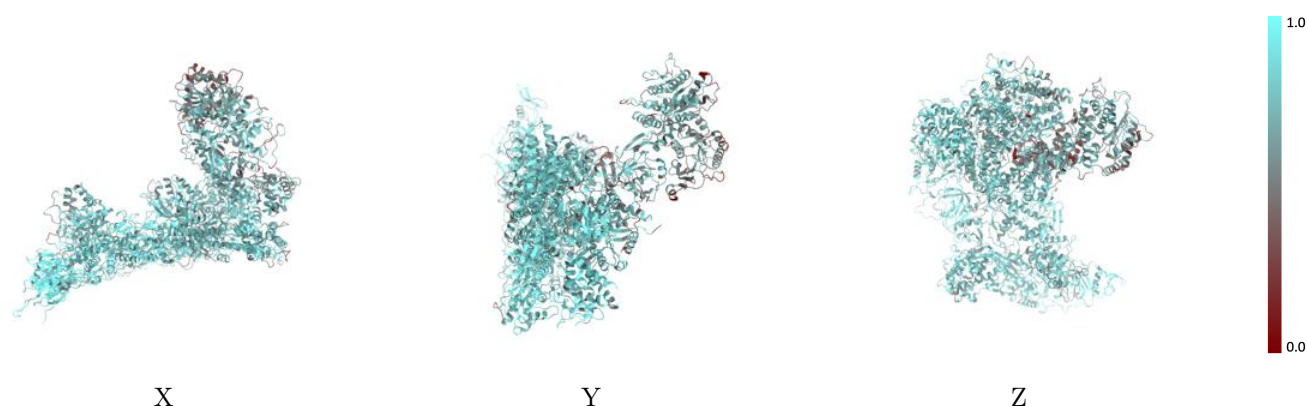
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



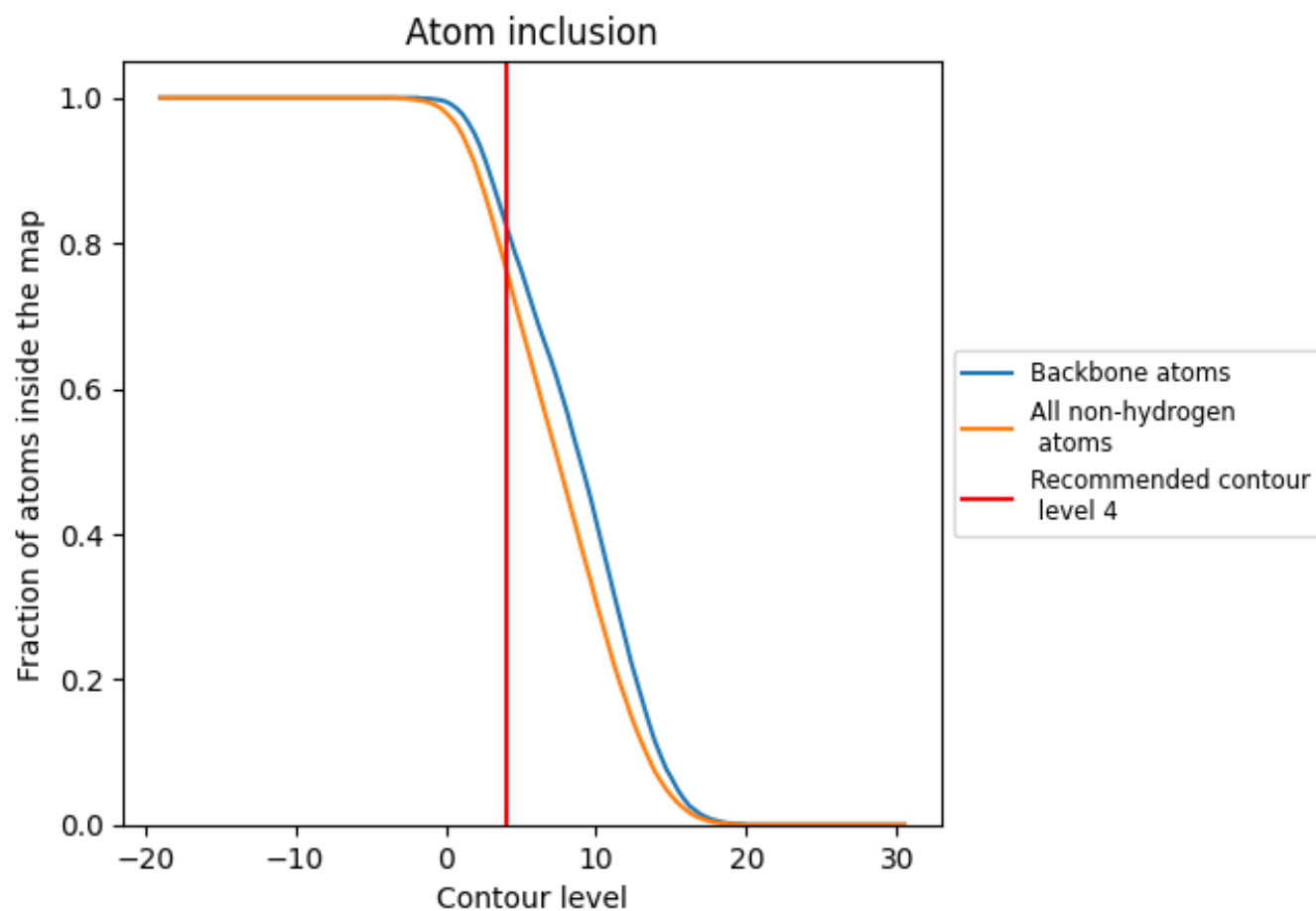
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 83% of all backbone atoms, 77% 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	0.7670	0.5720
A	0.6500	0.5510
B	0.8060	0.5790
C	0.8140	0.5800
D	0.8220	0.5870
E	0.7910	0.5730

