Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 05:20 pm BST

PDB ID	:	1UPN
EMDB ID	:	EMD-1057
Title	:	COMPLEX OF ECHOVIRUS TYPE 12 WITH DOMAINS 3 AND 4 OF ITS RECEPTOR DECAY ACCELERATING FACTOR (CD55) BY CRYO ELECTRON MICROSCOPY AT 16 A
Authors	:	Bhella, D.; Goodfellow, I.G.; Roversi, P.; Pettigrew, D.; Chaudry, Y.; Evans, D.J.; Lea, S.M.
Deposited on	:	2003-10-08
Resolution	:	16.00 Å(reported)
Based on initial model	:	1UPN

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 (i) 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 (i)) were used in the production of this report:

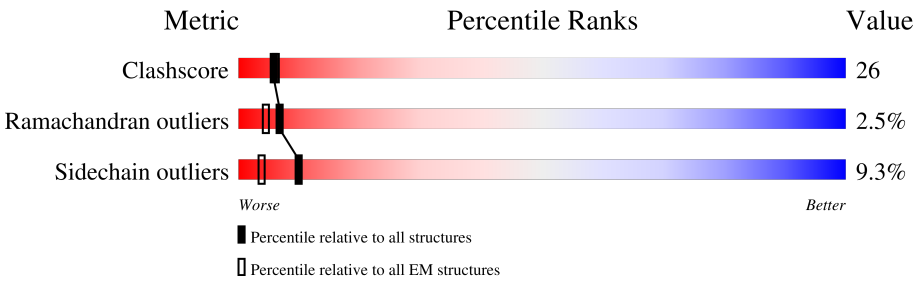
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 16.00 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	292	29%; 60%; 32%; 8%; •
2	B	262	17%; 64%; 25%; 5%; •; •
3	C	238	16%; 65%; 28%; 5%; •
4	D	69	38%; 36%; 13%; 13%
5	E	129	97%; 76%; 18%; •; •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7463 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 ECHOVIRUS 11 COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	289	2283	1439	398	435	11	0	0

- Molecule 2 is a protein called ECHOVIRUS 11 COAT PROTEIN VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	252	1963	1240	331	376	16	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	226	PHE	SER	conflict	UNP Q8JKE8

- Molecule 3 is a protein called ECHOVIRUS 11 COAT PROTEIN VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	238	1818	1161	299	345	13	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	63	GLU	GLN	conflict	UNP Q8JKE8

- Molecule 4 is a protein called ECHOVIRUS 11 COAT PROTEIN VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	60	466	289	81	95	1	0	0

- Molecule 5 is a protein called COMPLEMENT DECAY-ACCELERATING FACTOR.

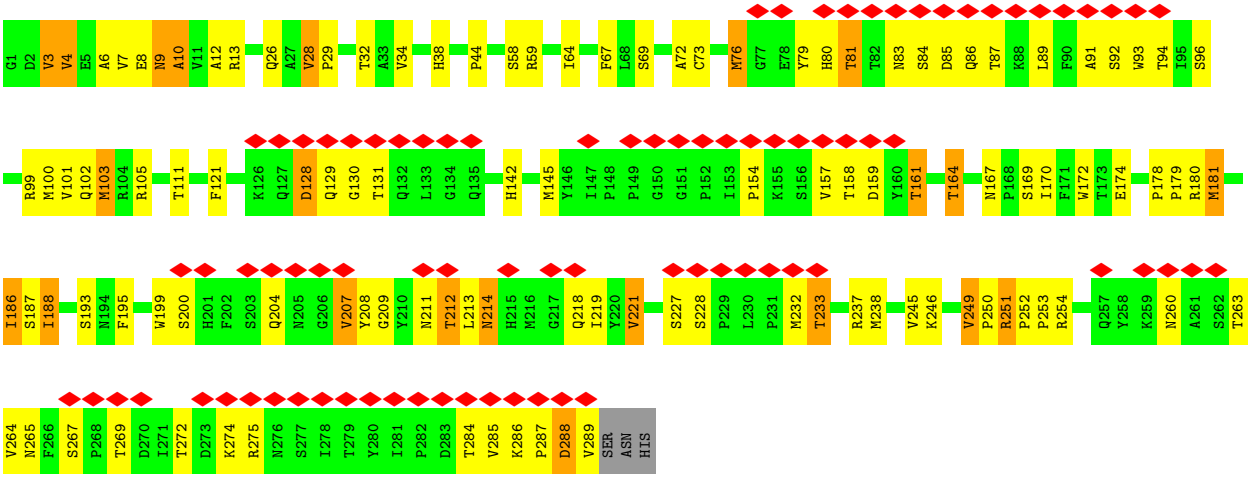
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	125	933	583	159	182	9	0	0

3 Residue-property plots (i)

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.

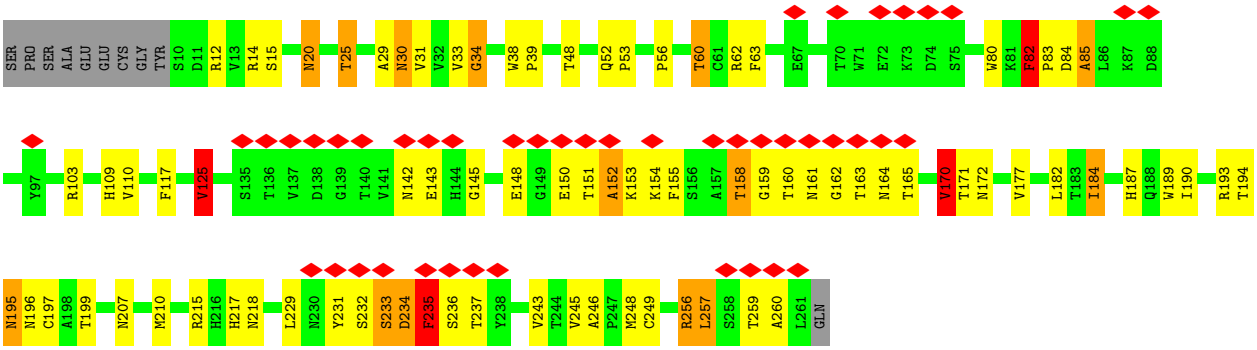
- Molecule 1: ECHOVIRUS 11 COAT PROTEIN VP1

Chain A:



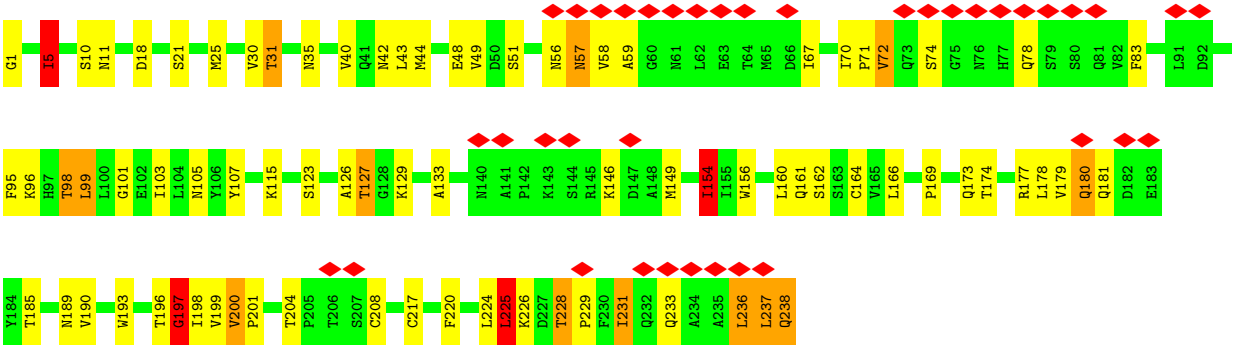
- Molecule 2: ECHOVIRUS 11 COAT PROTEIN VP2

Chain B:



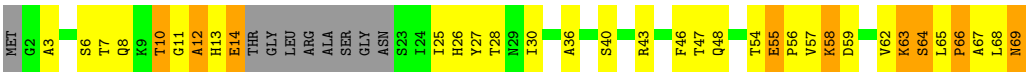
- Molecule 3: ECHOVIRUS 11 COAT PROTEIN VP3

Chain C:



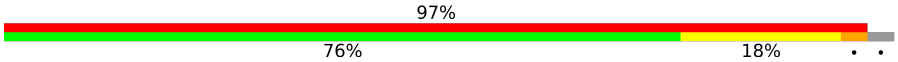
- Molecule 4: ECHOVIRUS 11 COAT PROTEIN VP4

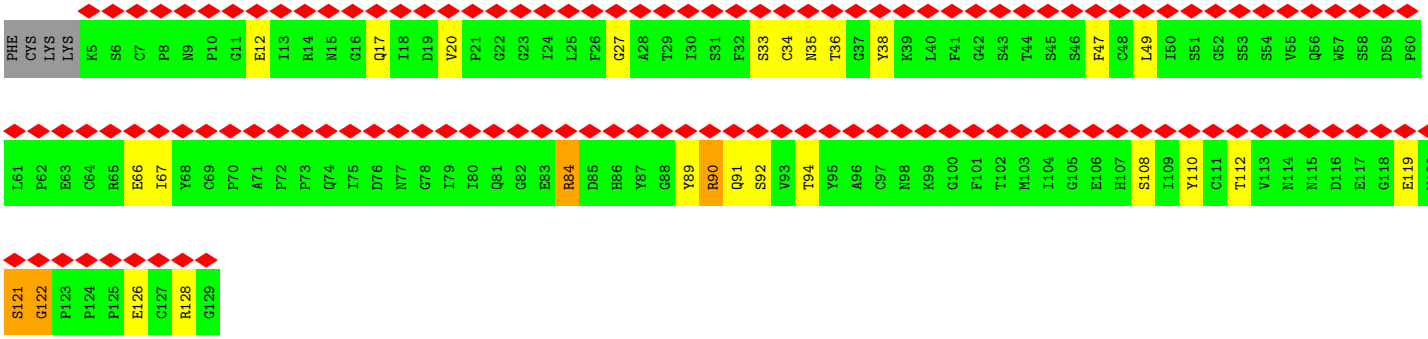
Chain D:



- Molecule 5: COMPLEMENT DECAY-ACCELERATING FACTOR

Chain E:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	903	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	JEOL 2000EXII	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	29200	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	255.000	Depositor
Minimum map value	0.000	Depositor
Average map value	66.186	Depositor
Map value standard deviation	31.678	Depositor
Recommended contour level	169	Depositor
Map size (Å)	598.5, 598.5, 598.5	wwPDB
Map dimensions	175, 175, 175	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	3.42, 3.42, 3.42	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.77	2/2348 (0.1%)	0.95	3/3206 (0.1%)
2	B	0.76	0/2015	1.05	8/2753 (0.3%)
3	C	0.77	1/1865 (0.1%)	0.99	6/2549 (0.2%)
4	D	0.87	0/474	1.04	3/639 (0.5%)
5	E	0.64	0/959	0.81	2/1299 (0.2%)
All	All	0.76	3/7661 (0.0%)	0.98	22/10446 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	MET	SD-CE	6.53	2.14	1.77
3	C	1	GLY	N-CA	6.17	1.55	1.46
1	A	3	VAL	CA-CB	5.00	1.65	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	195	ASN	N-CA-CB	-8.59	95.15	110.60
2	B	82	PHE	N-CA-C	8.56	134.11	111.00
3	C	237	LEU	CB-CG-CD1	-7.95	97.49	111.00
3	C	197	GLY	N-CA-C	7.88	132.81	113.10
1	A	237	ARG	NE-CZ-NH2	-7.41	116.59	120.30
2	B	14	ARG	NE-CZ-NH2	-6.87	116.87	120.30
3	C	237	LEU	CB-CG-CD2	6.77	122.51	111.00
3	C	5	ILE	CB-CA-C	-5.96	99.69	111.60
3	C	225	LEU	CA-CB-CG	5.94	128.96	115.30
2	B	29	ALA	N-CA-C	-5.84	95.23	111.00
2	B	125	VAL	CB-CA-C	-5.79	100.40	111.40
2	B	215	ARG	CG-CD-NE	5.62	123.61	111.80
4	D	12	ALA	N-CA-C	5.60	126.11	111.00
2	B	82	PHE	C-N-CA	-5.59	98.52	122.00
1	A	284	THR	N-CA-C	-5.57	95.96	111.00
3	C	154	ILE	CB-CA-C	-5.42	100.77	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	ASP	CB-CG-OD2	-5.35	113.49	118.30
4	D	58	LYS	N-CA-C	-5.25	96.81	111.00
5	E	84	ARG	NE-CZ-NH1	5.25	122.93	120.30
5	E	84	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	B	170	VAL	CB-CA-C	-5.09	101.73	111.40
4	D	64	SER	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2283	0	2212	148	0
2	B	1963	0	1872	131	0
3	C	1818	0	1775	114	0
4	D	466	0	447	47	0
5	E	933	0	852	87	0
All	All	7463	0	7158	387	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 26.

All (387) 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:160:THR:HA	5:E:35:ASN:CB	1.34	1.48
5:E:66:GLU:C	5:E:67:ILE:HG13	1.21	1.48
2:B:165:THR:CG2	5:E:17:GLN:HB3	1.41	1.47
2:B:165:THR:CB	5:E:17:GLN:OE1	1.72	1.37
1:A:76:MET:SD	1:A:76:MET:CE	2.14	1.35
2:B:165:THR:HG21	5:E:17:GLN:CB	1.62	1.28
2:B:160:THR:HA	5:E:35:ASN:CA	1.65	1.25
5:E:66:GLU:O	5:E:67:ILE:HG13	1.36	1.22
2:B:162:GLY:HA3	5:E:33:SER:OG	1.42	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:THR:OG1	5:E:38:TYR:HE2	1.22	1.17
2:B:161:ASN:N	5:E:35:ASN:HA	1.63	1.14
2:B:165:THR:OG1	5:E:17:GLN:CG	1.96	1.13
2:B:165:THR:HB	5:E:17:GLN:OE1	0.97	1.13
5:E:66:GLU:C	5:E:67:ILE:CG1	2.17	1.11
2:B:162:GLY:CA	5:E:33:SER:OG	1.99	1.10
2:B:160:THR:CA	5:E:35:ASN:CB	2.25	1.10
4:D:54:THR:O	4:D:55:GLU:HB2	1.51	1.10
1:A:260:ASN:OD1	1:A:263:THR:HG22	1.49	1.09
2:B:160:THR:HA	5:E:35:ASN:HB3	1.16	1.09
2:B:161:ASN:ND2	5:E:34:CYS:O	1.84	1.09
2:B:165:THR:OG1	5:E:17:GLN:HG3	1.49	1.08
2:B:159:GLY:O	5:E:35:ASN:HB3	1.53	1.07
2:B:161:ASN:ND2	5:E:35:ASN:C	2.12	1.03
3:C:196:THR:O	3:C:196:THR:HG23	1.58	1.03
3:C:233:GLN:NE2	3:C:238:GLN:HG2	1.73	1.03
1:A:101:VAL:HB	3:C:238:GLN:OE1	1.60	1.02
2:B:234:ASP:O	2:B:236:SER:N	1.92	1.01
2:B:165:THR:HB	5:E:17:GLN:CD	1.80	1.00
3:C:98:THR:HG22	3:C:101:GLY:H	1.20	1.00
2:B:165:THR:CG2	5:E:17:GLN:CB	2.29	1.00
2:B:165:THR:HG21	5:E:17:GLN:HB3	1.04	0.99
2:B:160:THR:CA	5:E:35:ASN:HB3	1.91	0.98
2:B:25:THR:HG21	2:B:197:CYS:SG	2.03	0.97
2:B:165:THR:CB	5:E:17:GLN:CD	2.34	0.96
2:B:165:THR:HG21	5:E:17:GLN:CA	1.96	0.96
2:B:161:ASN:H	5:E:35:ASN:HA	1.23	0.95
5:E:66:GLU:O	5:E:67:ILE:CG1	2.15	0.94
1:A:275:ARG:HE	3:C:57:ASN:HD21	1.08	0.94
2:B:160:THR:CA	5:E:35:ASN:HA	1.99	0.93
2:B:160:THR:CA	5:E:35:ASN:CA	2.47	0.92
2:B:160:THR:HA	5:E:35:ASN:HA	1.51	0.91
3:C:233:GLN:CD	3:C:238:GLN:HE21	1.74	0.91
2:B:161:ASN:HB2	5:E:34:CYS:O	1.70	0.90
2:B:165:THR:HG23	5:E:17:GLN:HB3	1.53	0.90
3:C:233:GLN:HE22	3:C:238:GLN:HG2	1.34	0.90
1:A:101:VAL:HB	3:C:238:GLN:CD	1.92	0.89
2:B:154:LYS:CE	5:E:12:GLU:OE2	2.21	0.89
2:B:154:LYS:HE3	5:E:12:GLU:OE2	1.73	0.89
2:B:165:THR:CG2	5:E:17:GLN:OE1	2.21	0.88
2:B:142:ASN:HD21	5:E:20:VAL:H	1.19	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:PHE:O	2:B:83:PRO:C	2.01	0.87
2:B:165:THR:CB	5:E:17:GLN:HB3	2.05	0.86
1:A:38:HIS:HD2	4:D:55:GLU:HG3	1.40	0.85
2:B:158:THR:OG1	5:E:38:TYR:CE2	2.05	0.85
3:C:129:LYS:HB2	3:C:196:THR:HG22	1.59	0.84
1:A:128:ASP:OD2	1:A:233:THR:HG22	1.77	0.84
1:A:252:PRO:HD3	2:B:184:ILE:HD11	1.57	0.84
3:C:233:GLN:HB3	3:C:238:GLN:NE2	1.93	0.84
2:B:30:ASN:HD21	4:D:59:ASP:HB2	1.42	0.83
3:C:57:ASN:H	3:C:57:ASN:HD22	1.27	0.82
3:C:154:ILE:HD11	3:C:166:LEU:HA	1.59	0.82
1:A:159:ASP:OD1	1:A:161:THR:HB	1.79	0.82
2:B:161:ASN:CB	5:E:34:CYS:O	2.27	0.82
1:A:101:VAL:HB	3:C:238:GLN:NE2	1.95	0.81
2:B:160:THR:C	5:E:35:ASN:HA	2.00	0.81
2:B:161:ASN:HD22	5:E:34:CYS:C	1.83	0.81
4:D:47:THR:HG22	4:D:48:GLN:H	1.44	0.81
1:A:59:ARG:NH1	4:D:48:GLN:HE22	1.79	0.80
2:B:161:ASN:HD21	5:E:35:ASN:C	1.81	0.80
2:B:159:GLY:C	5:E:35:ASN:HB3	2.02	0.79
1:A:81:THR:HG21	1:A:232:MET:HB2	1.64	0.79
1:A:6:ALA:O	1:A:7:VAL:HG23	1.82	0.79
2:B:193:ARG:HG3	2:B:194:THR:HG23	1.63	0.79
1:A:83:ASN:ND2	1:A:84:SER:H	1.80	0.78
3:C:95:PHE:O	3:C:98:THR:HB	1.82	0.78
1:A:38:HIS:CD2	4:D:55:GLU:HG3	2.19	0.78
3:C:228:THR:HG22	3:C:229:PRO:HD2	1.65	0.78
2:B:233:SER:O	2:B:235:PHE:CD2	2.36	0.77
4:D:54:THR:O	4:D:55:GLU:CB	2.31	0.77
3:C:42:ASN:HD22	3:C:44:MET:H	1.28	0.77
3:C:196:THR:O	3:C:196:THR:CG2	2.28	0.77
5:E:94:THR:HG22	5:E:108:SER:HB3	1.65	0.77
3:C:57:ASN:HA	3:C:67:ILE:HG13	1.67	0.76
1:A:4:VAL:CG1	4:D:36:ALA:HB1	2.15	0.76
2:B:117:PHE:CD2	3:C:204:THR:HG22	2.22	0.74
1:A:164:THR:HG21	1:A:169:SER:OG	1.87	0.73
3:C:57:ASN:HD22	3:C:57:ASN:N	1.87	0.73
4:D:58:LYS:O	4:D:59:ASP:HB2	1.86	0.73
1:A:128:ASP:OD2	1:A:233:THR:CG2	2.36	0.72
1:A:99:ARG:C	3:C:238:GLN:HB2	2.10	0.72
1:A:3:VAL:HG23	1:A:3:VAL:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:GLY:HA2	5:E:33:SER:CB	2.19	0.72
2:B:190:ILE:HA	2:B:195:ASN:ND2	2.05	0.71
2:B:162:GLY:HA2	5:E:33:SER:OG	1.90	0.71
1:A:32:THR:HB	4:D:63:LYS:HE3	1.70	0.71
3:C:107:TYR:O	3:C:226:LYS:HE3	1.92	0.70
3:C:173:GLN:HG2	3:C:174:THR:HG23	1.73	0.70
2:B:159:GLY:O	5:E:35:ASN:CB	2.36	0.70
1:A:209:GLY:O	1:A:212:THR:HG23	1.91	0.70
2:B:165:THR:CB	5:E:17:GLN:CG	2.68	0.70
1:A:101:VAL:CG1	3:C:238:GLN:NE2	2.55	0.70
2:B:142:ASN:HB3	2:B:145:GLY:H	1.55	0.70
2:B:165:THR:OG1	5:E:17:GLN:CB	2.39	0.70
3:C:233:GLN:HB3	3:C:238:GLN:HE21	1.57	0.70
1:A:81:THR:HG22	1:A:232:MET:O	1.92	0.69
1:A:32:THR:HA	4:D:63:LYS:HE2	1.71	0.69
4:D:7:THR:HA	4:D:26:HIS:HB3	1.73	0.69
1:A:269:THR:H	2:B:172:ASN:HD21	1.39	0.69
1:A:4:VAL:HG12	4:D:36:ALA:HB1	1.75	0.69
3:C:5:ILE:HD12	3:C:5:ILE:H	1.58	0.69
5:E:66:GLU:HG2	5:E:67:ILE:N	2.07	0.69
3:C:72:VAL:HG13	3:C:198:ILE:CD1	2.23	0.69
1:A:85:ASP:O	1:A:87:THR:N	2.25	0.68
2:B:151:THR:O	2:B:152:ALA:HB2	1.93	0.68
1:A:99:ARG:O	3:C:238:GLN:HB2	1.93	0.67
2:B:159:GLY:O	5:E:36:THR:N	2.27	0.67
1:A:6:ALA:HB1	4:D:40:SER:OG	1.94	0.67
4:D:3:ALA:HB2	4:D:30:ILE:HG12	1.76	0.67
2:B:161:ASN:ND2	5:E:35:ASN:O	2.27	0.67
3:C:180:GLN:O	3:C:180:GLN:HG3	1.94	0.66
3:C:98:THR:HG22	3:C:101:GLY:N	2.04	0.66
1:A:105:ARG:HD3	3:C:231:ILE:HG12	1.76	0.66
2:B:194:THR:HG21	3:C:162:SER:HB3	1.78	0.65
5:E:89:TYR:O	5:E:90:ARG:HB2	1.94	0.65
2:B:158:THR:CB	5:E:38:TYR:HE2	2.08	0.65
1:A:100:MET:CA	3:C:238:GLN:HG3	2.26	0.65
1:A:263:THR:HG23	1:A:265:ASN:H	1.60	0.65
2:B:165:THR:OG1	5:E:17:GLN:CD	2.32	0.65
3:C:236:LEU:C	3:C:238:GLN:N	2.48	0.65
2:B:165:THR:HG21	5:E:17:GLN:HA	1.79	0.65
2:B:160:THR:HB	5:E:17:GLN:HE21	1.62	0.65
1:A:286:LYS:HD2	1:A:289:VAL:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ASP:O	2:B:85:ALA:CB	2.46	0.64
4:D:55:GLU:H	4:D:56:PRO:CD	2.11	0.64
1:A:80:HIS:CD2	1:A:233:THR:HB	2.33	0.64
1:A:101:VAL:CB	3:C:238:GLN:NE2	2.60	0.64
3:C:72:VAL:HG13	3:C:198:ILE:HD12	1.80	0.64
1:A:101:VAL:CG1	3:C:238:GLN:HE22	2.10	0.63
1:A:12:ALA:HB2	4:D:46:PHE:HB3	1.80	0.63
5:E:66:GLU:O	5:E:67:ILE:N	2.32	0.63
2:B:184:ILE:N	2:B:184:ILE:HD12	2.14	0.63
2:B:162:GLY:CA	5:E:33:SER:CB	2.74	0.63
1:A:101:VAL:CB	3:C:238:GLN:OE1	2.43	0.63
3:C:200:VAL:HG22	3:C:201:PRO:HD2	1.79	0.63
1:A:81:THR:CG2	1:A:232:MET:H	2.12	0.63
2:B:161:ASN:O	5:E:17:GLN:HG3	1.99	0.63
1:A:72:ALA:CB	1:A:103:MET:HG2	2.29	0.62
4:D:66:PRO:O	4:D:67:ALA:HB3	1.98	0.62
2:B:117:PHE:HD2	3:C:204:THR:HG22	1.63	0.62
3:C:228:THR:HG22	3:C:229:PRO:CD	2.29	0.62
1:A:145:MET:SD	1:A:164:THR:HG23	2.39	0.62
3:C:129:LYS:HB2	3:C:196:THR:CG2	2.28	0.62
2:B:161:ASN:ND2	5:E:36:THR:N	2.47	0.62
1:A:101:VAL:HG12	3:C:238:GLN:NE2	2.15	0.61
4:D:47:THR:HG22	4:D:48:GLN:N	2.15	0.61
1:A:100:MET:HA	3:C:238:GLN:HG3	1.82	0.61
2:B:56:PRO:HB2	2:B:60:THR:HB	1.82	0.61
1:A:101:VAL:HB	3:C:238:GLN:HE22	1.65	0.61
2:B:162:GLY:HA3	5:E:33:SER:HG	1.63	0.61
4:D:6:SER:O	4:D:26:HIS:HB2	2.00	0.61
1:A:286:LYS:C	1:A:288:ASP:H	2.04	0.61
1:A:164:THR:HG22	1:A:167:ASN:HB2	1.82	0.61
1:A:207:VAL:HG22	1:A:212:THR:HG22	1.82	0.61
2:B:151:THR:OG1	2:B:152:ALA:N	2.34	0.61
1:A:13:ARG:HH11	1:A:13:ARG:HG3	1.66	0.60
1:A:81:THR:CG2	1:A:232:MET:HB2	2.30	0.60
1:A:105:ARG:HD3	3:C:231:ILE:CG1	2.31	0.60
3:C:18:ASP:OD2	4:D:43:ARG:HD2	2.01	0.60
2:B:151:THR:O	2:B:152:ALA:CB	2.49	0.60
2:B:161:ASN:CG	5:E:34:CYS:O	2.40	0.59
1:A:81:THR:HG21	1:A:232:MET:CB	2.32	0.59
1:A:59:ARG:NH1	4:D:48:GLN:NE2	2.50	0.59
1:A:72:ALA:HB3	1:A:103:MET:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:SER:HB3	1:A:207:VAL:HG13	1.83	0.59
5:E:94:THR:HG22	5:E:108:SER:CB	2.32	0.59
4:D:55:GLU:H	4:D:56:PRO:HD3	1.67	0.59
2:B:161:ASN:O	5:E:17:GLN:CG	2.50	0.59
2:B:160:THR:N	5:E:35:ASN:HB3	2.18	0.58
3:C:233:GLN:CB	3:C:238:GLN:HE21	2.15	0.58
2:B:184:ILE:HD12	2:B:184:ILE:H	1.67	0.58
5:E:84:ARG:HH22	5:E:91:GLN:NE2	2.01	0.58
1:A:3:VAL:HG21	1:A:246:LYS:HG3	1.86	0.58
1:A:101:VAL:CB	3:C:238:GLN:CD	2.71	0.58
2:B:165:THR:CB	5:E:17:GLN:CB	2.74	0.58
3:C:42:ASN:ND2	3:C:44:MET:H	1.99	0.57
2:B:160:THR:CB	5:E:17:GLN:HE21	2.16	0.57
1:A:275:ARG:HE	3:C:57:ASN:ND2	1.92	0.57
1:A:9:ASN:O	1:A:10:ALA:HB3	2.04	0.57
1:A:275:ARG:NE	3:C:57:ASN:HD21	1.92	0.57
1:A:195:PHE:CE1	1:A:251:ARG:HD2	2.39	0.57
5:E:66:GLU:C	5:E:67:ILE:N	2.58	0.57
1:A:44:PRO:HB3	3:C:169:PRO:HB3	1.87	0.56
1:A:249:VAL:O	1:A:249:VAL:HG22	2.05	0.56
1:A:252:PRO:HG2	2:B:177:VAL:HG11	1.86	0.56
3:C:49:VAL:HA	4:D:54:THR:HG22	1.87	0.56
3:C:107:TYR:CE2	3:C:225:LEU:HD13	2.40	0.56
1:A:12:ALA:HB2	4:D:46:PHE:CB	2.35	0.56
2:B:20:ASN:HD21	2:B:62:ARG:HH21	1.51	0.56
1:A:85:ASP:O	1:A:85:ASP:OD1	2.22	0.56
1:A:99:ARG:HA	3:C:238:GLN:HB2	1.87	0.56
3:C:233:GLN:CG	3:C:238:GLN:HE21	2.18	0.56
5:E:84:ARG:HH22	5:E:91:GLN:HE21	1.53	0.56
4:D:66:PRO:O	4:D:67:ALA:CB	2.54	0.55
1:A:59:ARG:HH11	4:D:48:GLN:HE22	1.55	0.55
2:B:63:PHE:CD1	2:B:246:ALA:HB2	2.41	0.55
3:C:233:GLN:CD	3:C:238:GLN:NE2	2.54	0.55
1:A:59:ARG:HH11	4:D:48:GLN:NE2	2.05	0.55
2:B:12:ARG:HH11	2:B:12:ARG:HG3	1.70	0.55
3:C:57:ASN:H	3:C:57:ASN:ND2	2.00	0.55
2:B:154:LYS:CD	5:E:12:GLU:OE2	2.54	0.54
2:B:193:ARG:NH1	3:C:123:SER:O	2.40	0.54
1:A:180:ARG:C	1:A:181:MET:HG3	2.28	0.54
1:A:272:THR:HG22	3:C:67:ILE:HD11	1.88	0.54
1:A:245:VAL:HG12	1:A:246:LYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:THR:OG1	5:E:17:GLN:HB3	2.06	0.54
1:A:93:TRP:O	1:A:218:GLN:HB2	2.08	0.53
1:A:99:ARG:O	3:C:238:GLN:CG	2.56	0.53
2:B:12:ARG:HG3	2:B:12:ARG:NH1	2.24	0.53
1:A:7:VAL:HG22	4:D:27:TYR:OH	2.08	0.53
1:A:83:ASN:ND2	1:A:84:SER:N	2.53	0.53
3:C:107:TYR:O	3:C:179:VAL:HG11	2.09	0.53
3:C:236:LEU:C	3:C:238:GLN:H	2.11	0.53
1:A:28:VAL:HG13	1:A:28:VAL:O	2.09	0.52
1:A:32:THR:CB	4:D:63:LYS:HE3	2.37	0.52
5:E:112:THR:HG22	5:E:119:GLU:O	2.09	0.52
2:B:233:SER:O	2:B:235:PHE:HD2	1.90	0.52
1:A:170:ILE:HD11	1:A:181:MET:HG2	1.92	0.52
2:B:84:ASP:O	2:B:85:ALA:HB2	2.09	0.52
1:A:13:ARG:HG3	1:A:13:ARG:NH1	2.24	0.52
1:A:99:ARG:O	3:C:238:GLN:CB	2.57	0.52
1:A:101:VAL:CB	3:C:238:GLN:HE22	2.23	0.51
3:C:51:SER:HB3	3:C:99:LEU:HD22	1.93	0.51
1:A:28:VAL:N	1:A:29:PRO:HD3	2.24	0.51
1:A:73:CYS:SG	1:A:100:MET:CE	2.99	0.51
1:A:111:THR:OG1	1:A:249:VAL:HG22	2.11	0.51
1:A:99:ARG:CA	3:C:238:GLN:HB2	2.41	0.51
2:B:125:VAL:HG13	2:B:187:HIS:HB3	1.93	0.51
1:A:79:TYR:OH	1:A:142:HIS:CD2	2.63	0.51
3:C:44:MET:HE2	3:C:220:PHE:HD1	1.75	0.50
4:D:62:VAL:HB	4:D:65:LEU:HD13	1.91	0.50
5:E:126:GLU:OE1	5:E:128:ARG:NH2	2.44	0.50
1:A:79:TYR:OH	1:A:142:HIS:HD2	1.93	0.50
4:D:11:GLY:O	4:D:13:HIS:N	2.41	0.50
1:A:99:ARG:O	3:C:238:GLN:HG3	2.12	0.50
1:A:99:ARG:HD3	3:C:237:LEU:HA	1.92	0.50
3:C:154:ILE:HD11	3:C:166:LEU:CA	2.35	0.50
1:A:3:VAL:O	1:A:3:VAL:CG2	2.59	0.49
1:A:172:TRP:CD1	1:A:179:PRO:HG3	2.46	0.49
2:B:31:VAL:HB	4:D:58:LYS:HG2	1.94	0.49
3:C:133:ALA:O	3:C:190:VAL:HA	2.13	0.49
1:A:101:VAL:HG21	3:C:231:ILE:HD12	1.94	0.49
1:A:129:GLN:NE2	1:A:130:GLY:H	2.10	0.49
1:A:249:VAL:O	1:A:249:VAL:CG2	2.61	0.49
1:A:250:PRO:HD3	3:C:40:VAL:CG2	2.42	0.49
1:A:85:ASP:OD1	1:A:87:THR:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:VAL:HG13	3:C:198:ILE:HD11	1.94	0.49
1:A:101:VAL:CG2	3:C:231:ILE:HG13	2.42	0.48
2:B:33:VAL:O	2:B:34:GLY:C	2.51	0.48
1:A:64:ILE:HD12	3:C:40:VAL:O	2.12	0.48
2:B:80:TRP:CE2	2:B:152:ALA:HB2	2.47	0.48
3:C:180:GLN:O	3:C:180:GLN:CG	2.57	0.48
1:A:154:PRO:HG3	1:A:161:THR:CG2	2.43	0.48
2:B:234:ASP:C	2:B:236:SER:N	2.66	0.48
1:A:157:VAL:HG23	1:A:158:THR:HG23	1.94	0.48
2:B:148:GLU:OE2	2:B:153:LYS:HE3	2.12	0.48
4:D:55:GLU:N	4:D:56:PRO:CD	2.77	0.48
3:C:57:ASN:N	3:C:57:ASN:ND2	2.59	0.48
3:C:173:GLN:HG2	3:C:174:THR:N	2.27	0.48
1:A:121:PHE:CZ	1:A:238:MET:HE2	2.49	0.47
1:A:286:LYS:O	1:A:288:ASP:N	2.44	0.47
2:B:52:GLN:HE21	2:B:53:PRO:HD2	1.78	0.47
3:C:233:GLN:CD	3:C:238:GLN:HG2	2.33	0.47
2:B:20:ASN:HD21	2:B:62:ARG:HE	1.62	0.47
1:A:81:THR:HG23	1:A:232:MET:H	1.78	0.47
1:A:285:VAL:HG12	1:A:285:VAL:O	2.14	0.47
1:A:252:PRO:HD3	2:B:184:ILE:CD1	2.37	0.47
1:A:263:THR:HG21	1:A:265:ASN:HB2	1.96	0.47
1:A:274:LYS:HD2	3:C:59:ALA:HB2	1.97	0.47
2:B:189:TRP:O	2:B:195:ASN:ND2	2.47	0.47
3:C:115:LYS:HG3	3:C:217:CYS:SG	2.55	0.47
2:B:103:ARG:HB2	2:B:210:MET:HG2	1.96	0.47
3:C:5:ILE:HD12	3:C:5:ILE:N	2.25	0.47
2:B:62:ARG:HH11	2:B:62:ARG:HG3	1.80	0.47
1:A:128:ASP:CG	1:A:233:THR:HG22	2.34	0.46
2:B:109:HIS:HD2	2:B:199:THR:OG1	1.97	0.46
1:A:172:TRP:CG	1:A:179:PRO:HG3	2.50	0.46
1:A:9:ASN:O	1:A:10:ALA:CB	2.63	0.46
3:C:156:TRP:CD1	3:C:164:CYS:HB2	2.50	0.46
1:A:260:ASN:CG	1:A:263:THR:HG22	2.29	0.46
1:A:263:THR:CG2	1:A:265:ASN:HB2	2.46	0.46
3:C:177:ARG:HG2	3:C:185:THR:HB	1.98	0.46
2:B:142:ASN:HB2	2:B:164:ASN:HB3	1.98	0.46
2:B:20:ASN:HD21	2:B:62:ARG:NH2	2.14	0.46
3:C:146:LYS:HB2	3:C:146:LYS:HE2	1.68	0.45
5:E:92:SER:HB3	5:E:110:TYR:CD2	2.50	0.45
1:A:252:PRO:HA	1:A:253:PRO:HD3	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LYS:HD2	1:A:289:VAL:CB	2.45	0.45
1:A:249:VAL:HA	1:A:250:PRO:HD2	1.81	0.45
3:C:201:PRO:HG2	3:C:204:THR:HG21	1.98	0.45
1:A:105:ARG:HG3	1:A:254:ARG:HB3	1.99	0.45
2:B:161:ASN:ND2	5:E:35:ASN:CA	2.79	0.45
2:B:190:ILE:HA	2:B:195:ASN:HD21	1.81	0.45
2:B:232:SER:C	2:B:234:ASP:H	2.19	0.45
3:C:196:THR:O	3:C:197:GLY:O	2.34	0.45
1:A:154:PRO:CA	1:A:161:THR:HG21	2.46	0.45
3:C:160:LEU:HD21	4:D:69:ASN:H	1.82	0.45
4:D:68:LEU:O	4:D:69:ASN:HB2	2.16	0.45
1:A:81:THR:HG22	1:A:232:MET:C	2.37	0.45
1:A:267:SER:O	1:A:269:THR:HG23	2.17	0.45
1:A:154:PRO:HG3	1:A:161:THR:HG21	1.99	0.44
2:B:154:LYS:HD2	5:E:12:GLU:OE2	2.17	0.44
4:D:3:ALA:HB2	4:D:30:ILE:CG1	2.47	0.44
1:A:188:ILE:HG21	1:A:188:ILE:HD13	1.62	0.44
1:A:211:ASN:HD22	1:A:211:ASN:HA	1.53	0.44
1:A:92:SER:HA	1:A:219:ILE:O	2.17	0.44
3:C:44:MET:O	3:C:48:GLU:HG3	2.18	0.44
3:C:10:SER:O	3:C:11:ASN:HB2	2.18	0.44
4:D:67:ALA:O	4:D:68:LEU:HD23	2.18	0.44
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.62	0.44
4:D:10:THR:O	4:D:10:THR:CG2	2.61	0.44
4:D:63:LYS:CD	4:D:67:ALA:HB2	2.48	0.44
4:D:47:THR:CG2	4:D:48:GLN:H	2.24	0.43
1:A:193:SER:HB2	2:B:207:ASN:ND2	2.33	0.43
2:B:161:ASN:H	5:E:35:ASN:CA	2.11	0.43
2:B:256:ARG:HD2	2:B:257:LEU:O	2.18	0.43
4:D:10:THR:O	4:D:10:THR:HG22	2.18	0.43
1:A:121:PHE:CZ	1:A:238:MET:CE	3.01	0.43
2:B:193:ARG:HG3	2:B:194:THR:CG2	2.42	0.43
2:B:248:MET:O	2:B:249:CYS:HB2	2.18	0.43
3:C:74:SER:HA	3:C:198:ILE:O	2.19	0.43
1:A:81:THR:CG2	1:A:232:MET:O	2.62	0.43
3:C:173:GLN:CG	3:C:174:THR:HG23	2.47	0.43
5:E:66:GLU:CG	5:E:67:ILE:N	2.79	0.43
1:A:187:SER:O	3:C:31:THR:HG21	2.19	0.42
1:A:245:VAL:CG1	1:A:246:LYS:N	2.82	0.42
1:A:263:THR:HG23	1:A:265:ASN:N	2.29	0.42
1:A:81:THR:CG2	1:A:232:MET:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:HIS:HE1	1:A:174:GLU:OE1	2.02	0.42
1:A:178:PRO:HA	1:A:179:PRO:HD3	1.83	0.42
2:B:161:ASN:HD21	5:E:36:THR:N	2.10	0.42
1:A:101:VAL:N	3:C:238:GLN:CD	2.72	0.42
2:B:83:PRO:HD2	2:B:217:HIS:HA	2.01	0.42
2:B:184:ILE:H	2:B:184:ILE:CD1	2.28	0.42
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.85	0.42
2:B:165:THR:HG21	5:E:17:GLN:OE1	2.11	0.42
3:C:201:PRO:HG2	3:C:204:THR:CG2	2.50	0.42
1:A:93:TRP:O	1:A:218:GLN:CB	2.67	0.42
2:B:38:TRP:CD1	2:B:39:PRO:HD2	2.55	0.42
3:C:127:THR:HG22	3:C:199:VAL:HB	2.02	0.42
3:C:161:GLN:NE2	4:D:66:PRO:HB3	2.35	0.42
3:C:193:TRP:CD1	3:C:193:TRP:N	2.87	0.42
3:C:72:VAL:CG1	3:C:198:ILE:HD11	2.49	0.42
1:A:186:ILE:HD11	3:C:25:MET:CE	2.50	0.42
1:A:101:VAL:HG21	3:C:231:ILE:CD1	2.50	0.42
2:B:154:LYS:NZ	5:E:12:GLU:OE2	2.53	0.42
3:C:129:LYS:CB	3:C:196:THR:HG22	2.40	0.42
1:A:12:ALA:O	1:A:58:SER:HA	2.19	0.41
2:B:231:TYR:CE1	2:B:237:THR:HG22	2.55	0.41
2:B:259:THR:HG22	2:B:260:ALA:N	2.35	0.41
3:C:115:LYS:HB2	3:C:115:LYS:HE3	1.75	0.41
2:B:155:PHE:HB3	2:B:170:VAL:HG13	2.02	0.41
1:A:199:TRP:CZ3	1:A:208:TYR:HB2	2.54	0.41
4:D:14:GLU:HA	4:D:14:GLU:OE2	2.20	0.41
1:A:204:GLN:NE2	2:B:143:GLU:HG2	2.34	0.41
3:C:18:ASP:OD1	4:D:40:SER:HB2	2.20	0.41
2:B:233:SER:O	2:B:235:PHE:N	2.53	0.41
2:B:159:GLY:O	5:E:35:ASN:C	2.59	0.41
3:C:70:ILE:HA	3:C:71:PRO:HD3	1.81	0.41
3:C:105:ASN:HB3	3:C:228:THR:HG23	2.03	0.41
3:C:126:ALA:HA	3:C:200:VAL:HG23	2.03	0.41
5:E:27:GLY:HA2	5:E:47:PHE:CZ	2.55	0.41
1:A:89:LEU:HB3	1:A:157:VAL:HG11	2.03	0.41
1:A:91:ALA:HB3	1:A:221:VAL:HG13	2.01	0.41
2:B:196:ASN:OD1	2:B:196:ASN:C	2.59	0.41
3:C:228:THR:HA	3:C:229:PRO:HD3	1.83	0.41
5:E:121:SER:O	5:E:122:GLY:O	2.39	0.41
2:B:110:VAL:HG22	2:B:243:VAL:HG22	2.03	0.41
2:B:256:ARG:HD3	2:B:257:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:GLN:HG3	4:D:26:HIS:HA	2.04	0.40
1:A:129:GLN:NE2	1:A:130:GLY:N	2.68	0.40
1:A:67:PHE:CG	3:C:43:LEU:HD11	2.55	0.40
1:A:101:VAL:O	1:A:102:GLN:C	2.59	0.40
2:B:182:LEU:HD23	2:B:182:LEU:HA	1.82	0.40
3:C:83:PHE:CD1	3:C:83:PHE:C	2.95	0.40
1:A:99:ARG:C	3:C:238:GLN:HG3	2.42	0.40
2:B:83:PRO:HD3	2:B:218:ASN:H	1.86	0.40
4:D:57:VAL:O	4:D:57:VAL:HG23	2.22	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	287/292 (98%)	258 (90%)	20 (7%)	9 (3%)	3 22
2	B	250/262 (95%)	220 (88%)	23 (9%)	7 (3%)	4 24
3	C	236/238 (99%)	224 (95%)	10 (4%)	2 (1%)	16 55
4	D	56/69 (81%)	43 (77%)	9 (16%)	4 (7%)	1 11
5	E	121/129 (94%)	117 (97%)	2 (2%)	2 (2%)	7 37
All	All	950/990 (96%)	862 (91%)	64 (7%)	24 (2%)	7 26

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	ASN
1	A	214	ASN
1	A	228	SER
2	B	152	ALA

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Mol	Chain	Res	Type
2	B	234	ASP
2	B	235	PHE
3	C	197	GLY
4	D	12	ALA
4	D	55	GLU
4	D	64	SER
5	E	121	SER
1	A	227	SER
2	B	34	GLY
2	B	85	ALA
3	C	236	LEU
4	D	63	LYS
5	E	122	GLY
1	A	10	ALA
2	B	150	GLU
1	A	86	GLN
2	B	82	PHE
1	A	4	VAL
1	A	287	PRO

5.3.2 Protein sidechains (i)

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	259/262 (99%)	236 (91%)	23 (9%)	8 25
2	B	217/225 (96%)	199 (92%)	18 (8%)	9 27
3	C	204/204 (100%)	176 (86%)	28 (14%)	3 13
4	D	51/57 (90%)	45 (88%)	6 (12%)	4 16
5	E	101/110 (92%)	99 (98%)	2 (2%)	50 68
All	All	832/858 (97%)	755 (91%)	77 (9%)	10 23

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	28	VAL
1	A	34	VAL
1	A	69	SER
1	A	81	THR
1	A	94	THR
1	A	96	SER
1	A	103	MET
1	A	131	THR
1	A	161	THR
1	A	164	THR
1	A	181	MET
1	A	186	ILE
1	A	188	ILE
1	A	207	VAL
1	A	212	THR
1	A	214	ASN
1	A	221	VAL
1	A	233	THR
1	A	249	VAL
1	A	251	ARG
1	A	264	VAL
1	A	288	ASP
2	B	15	SER
2	B	20	ASN
2	B	25	THR
2	B	30	ASN
2	B	48	THR
2	B	60	THR
2	B	125	VAL
2	B	158	THR
2	B	163	THR
2	B	170	VAL
2	B	171	THR
2	B	184	ILE
2	B	229	LEU
2	B	233	SER
2	B	235	PHE
2	B	245	VAL
2	B	256	ARG
2	B	257	LEU
3	C	5	ILE
3	C	21	SER

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Mol	Chain	Res	Type
3	C	30	VAL
3	C	31	THR
3	C	35	ASN
3	C	56	ASN
3	C	57	ASN
3	C	58	VAL
3	C	72	VAL
3	C	78	GLN
3	C	96	LYS
3	C	98	THR
3	C	99	LEU
3	C	103	ILE
3	C	127	THR
3	C	149	MET
3	C	154	ILE
3	C	178	LEU
3	C	180	GLN
3	C	181	GLN
3	C	189	ASN
3	C	200	VAL
3	C	208	CYS
3	C	224	LEU
3	C	225	LEU
3	C	228	THR
3	C	231	ILE
3	C	238	GLN
4	D	10	THR
4	D	14	GLU
4	D	25	ILE
4	D	28	THR
4	D	66	PRO
4	D	69	ASN
5	E	49	LEU
5	E	90	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	83	ASN
1	A	129	GLN
1	A	142	HIS

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Mol	Chain	Res	Type
1	A	201	HIS
1	A	204	GLN
1	A	211	ASN
1	A	214	ASN
2	B	20	ASN
2	B	30	ASN
2	B	52	GLN
2	B	109	HIS
2	B	119	GLN
2	B	142	ASN
2	B	172	ASN
2	B	195	ASN
3	C	12	GLN
3	C	35	ASN
3	C	42	ASN
3	C	56	ASN
3	C	57	ASN
3	C	88	GLN
3	C	140	ASN
3	C	189	ASN
3	C	238	GLN
4	D	44	GLN
4	D	48	GLN
5	E	91	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	66:GLU	C	67:ILE	N	2.58

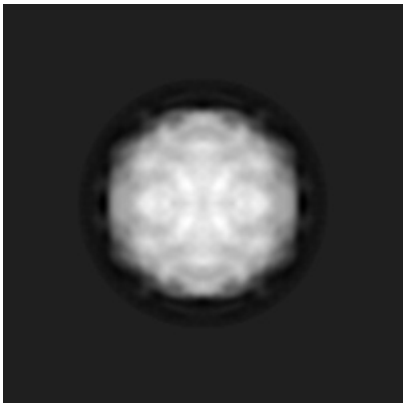
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1057. These allow visual inspection of the internal detail of the map and identification of artifacts.

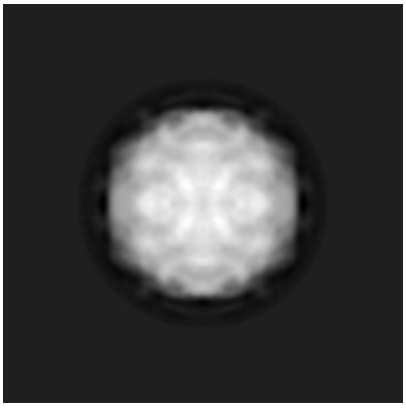
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

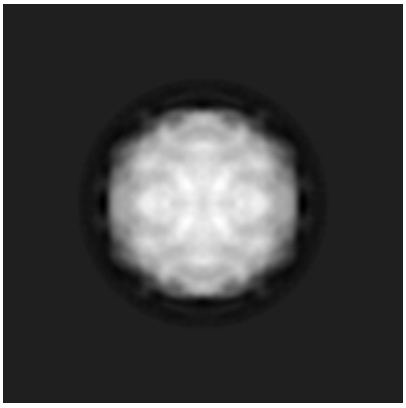
6.1.1 Primary map



X



Y

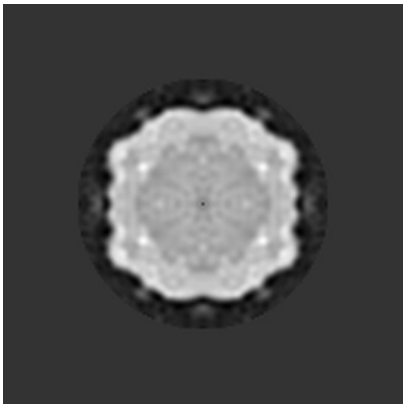


Z

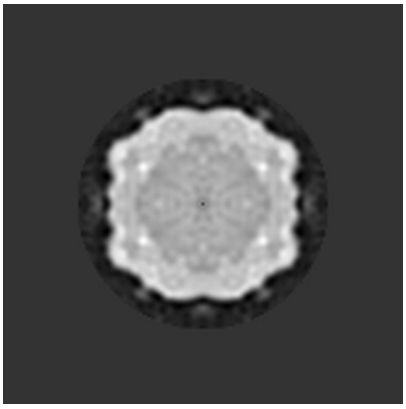
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

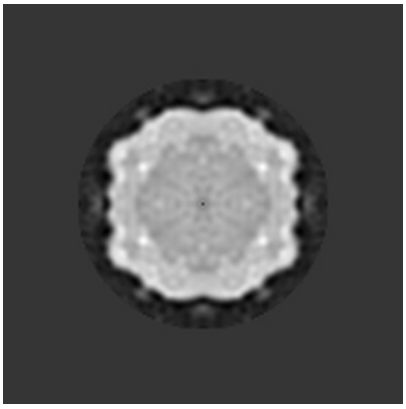
6.2.1 Primary map



X Index: 87



Y Index: 87

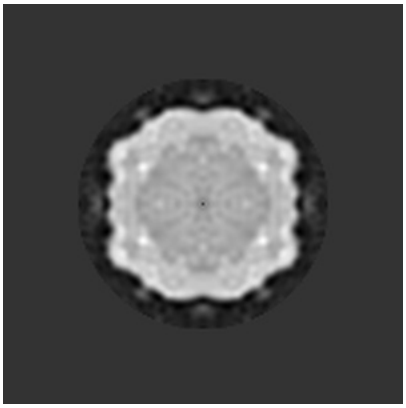


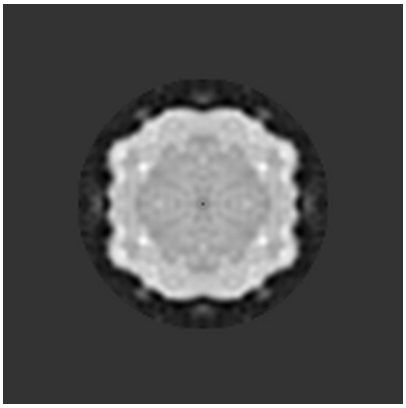
Z Index: 87

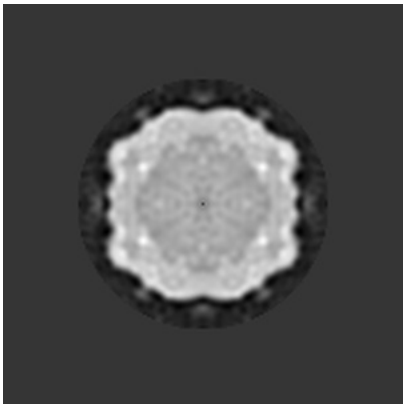
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 87

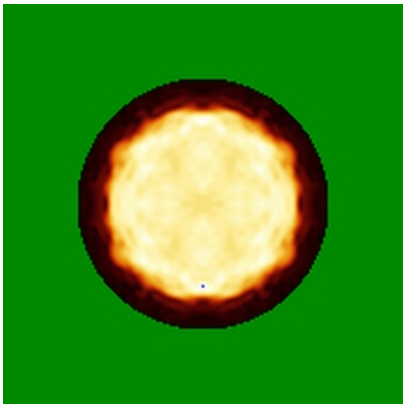

Y Index: 87

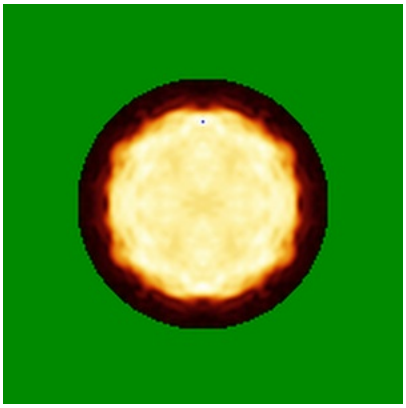

Z Index: 87

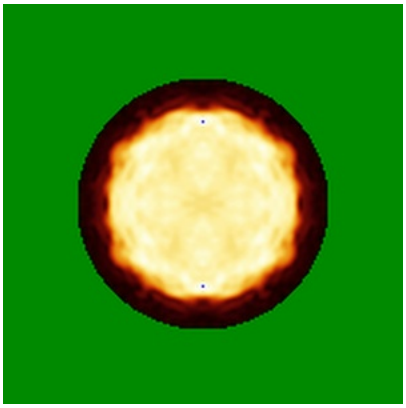
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

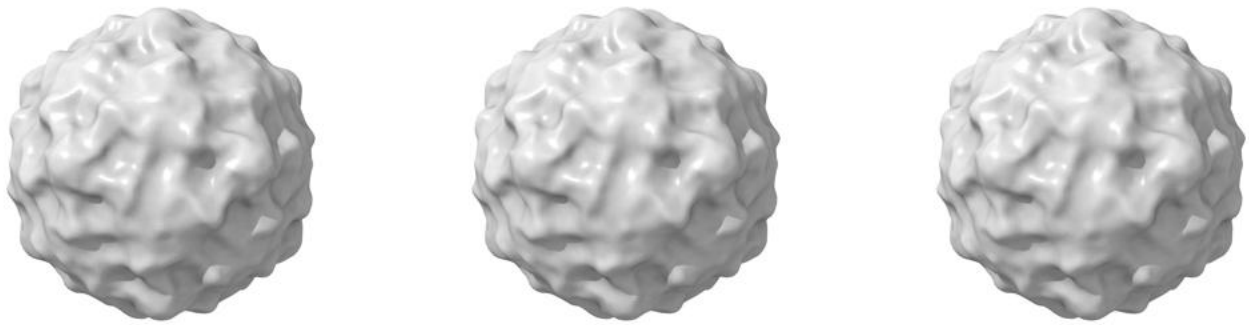

Y


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

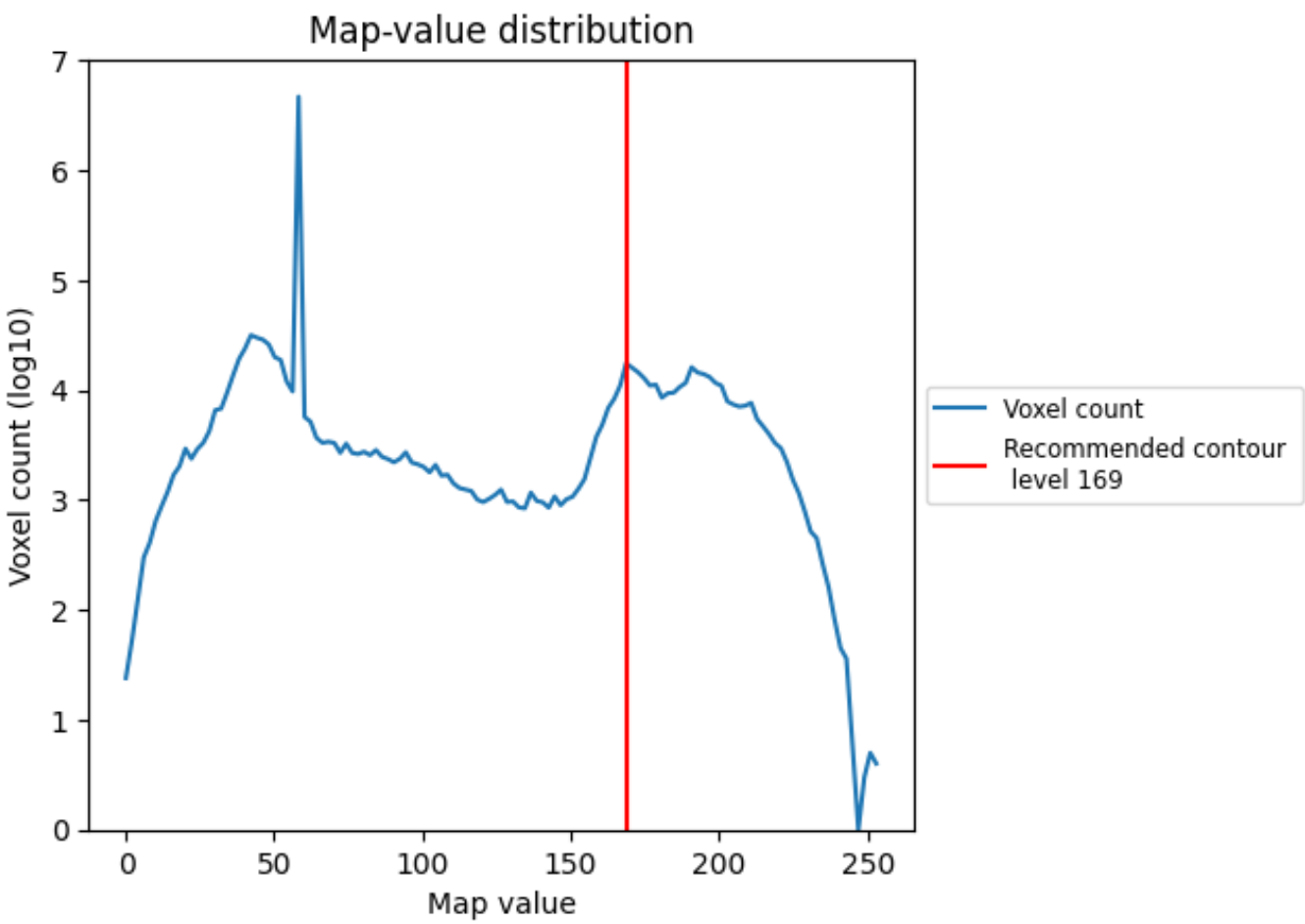
6.6 Mask visualisation (i)

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

7 Map analysis (i)

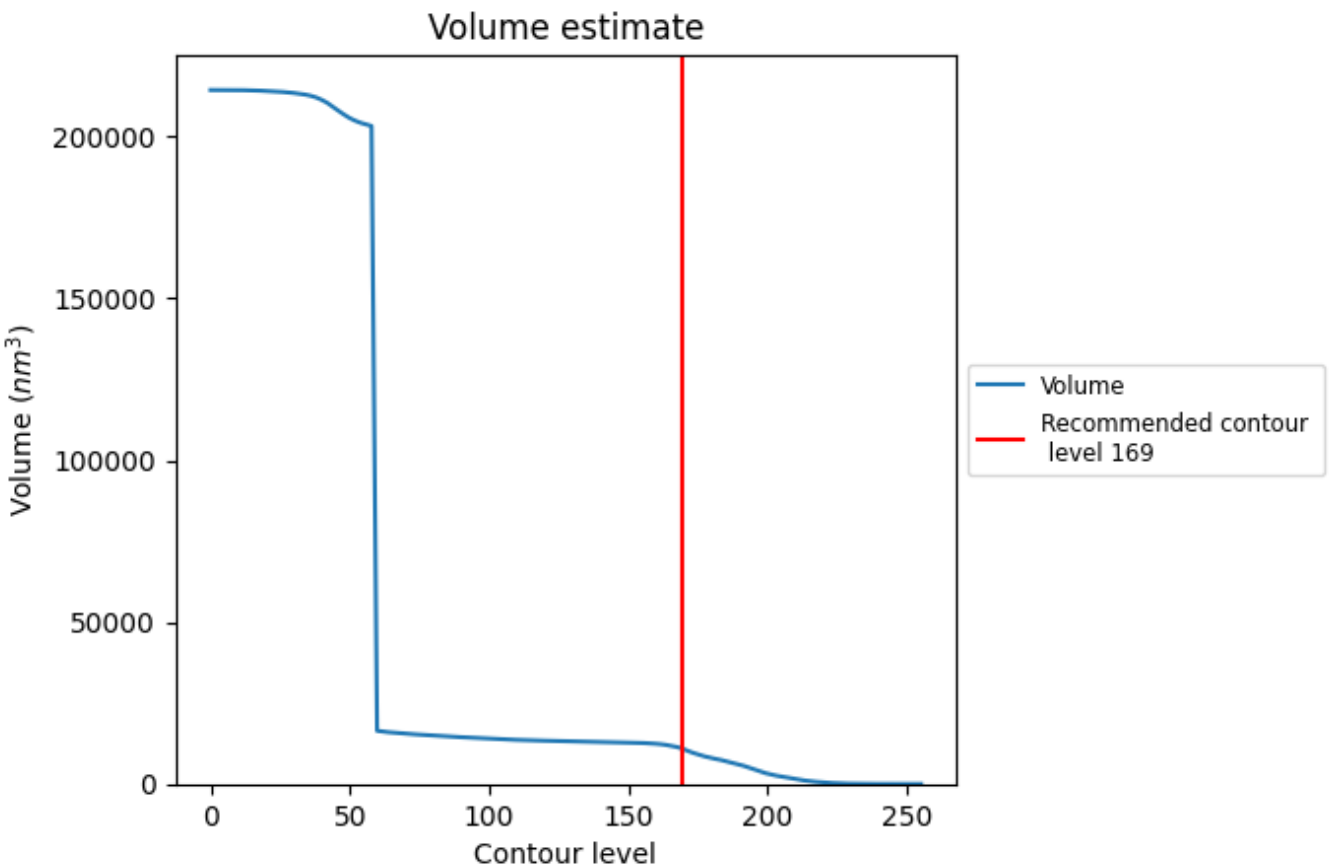
This section contains the results of statistical analysis of the map.

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.

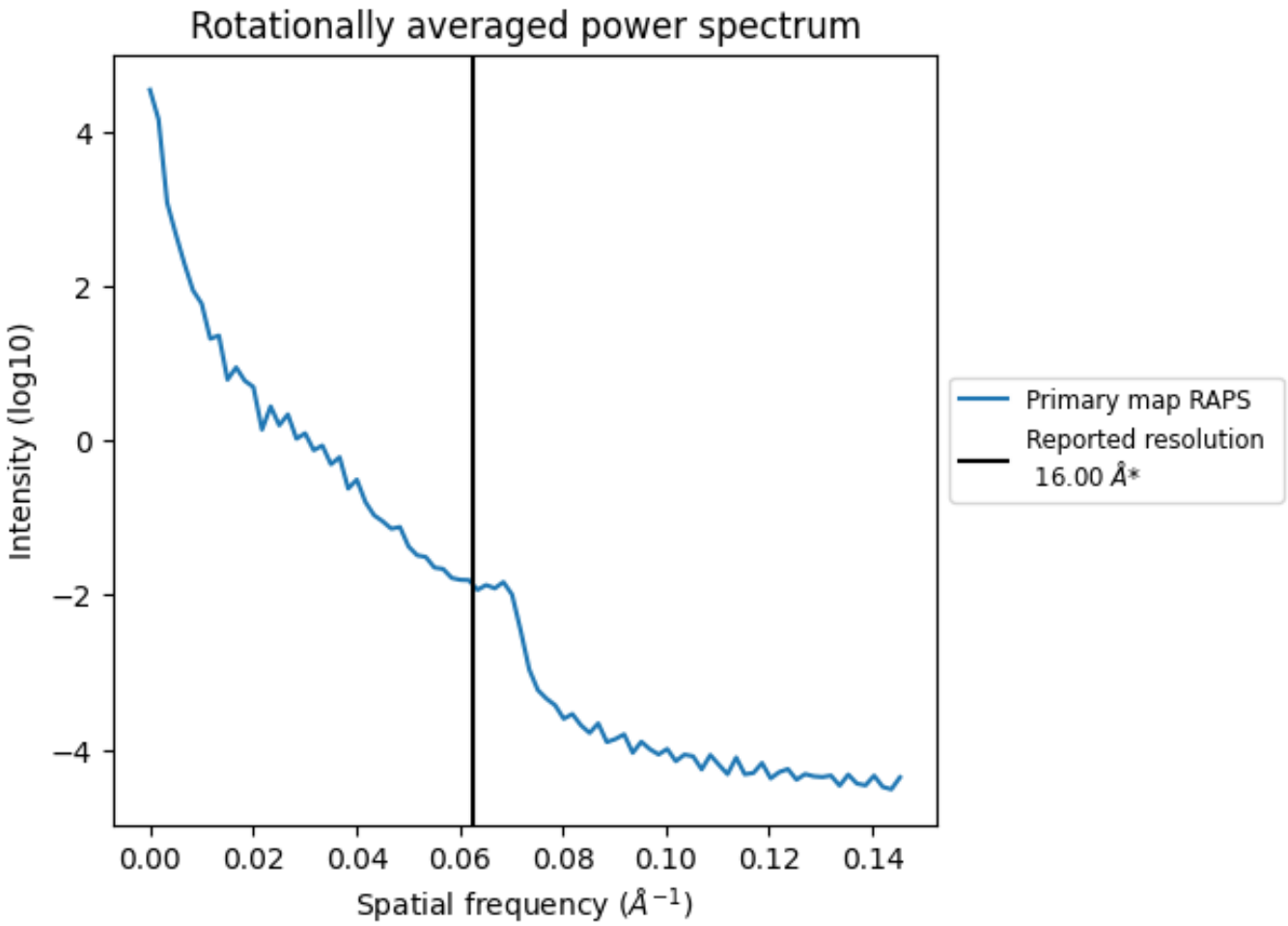
7.2 Volume estimate (i)



The volume at the recommended contour level is 11015 nm^3; this corresponds to an approximate mass of 9950 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 (i)



*Reported resolution corresponds to spatial frequency of 0.062 Å^{-1}

8 Fourier-Shell correlation (i)

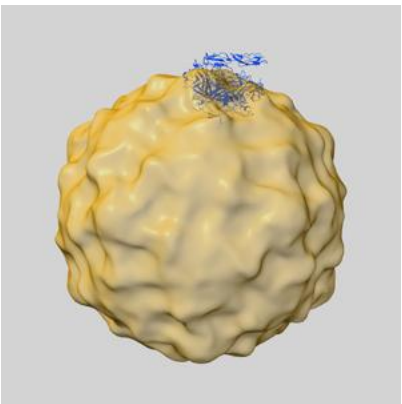
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

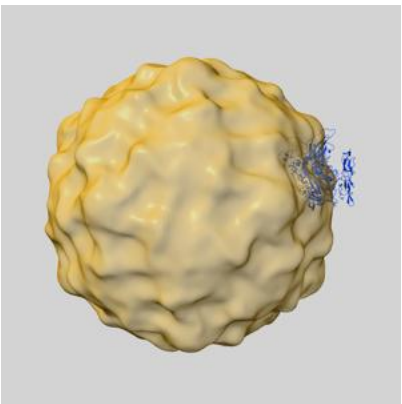
This section contains information regarding the fit between EMDB map EMD-1057 and PDB model 1UPN. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

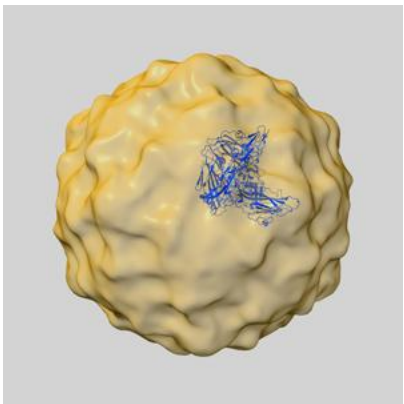
9.1.1 Map-model overlay (i)



X

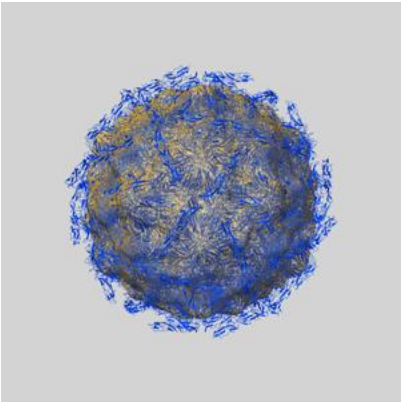


Y

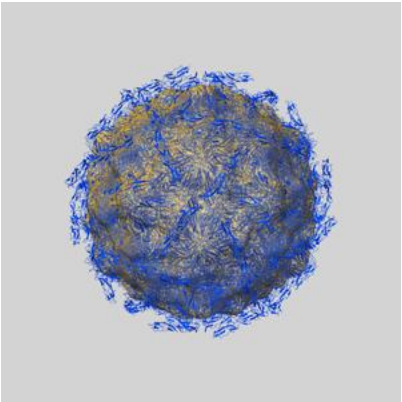


Z

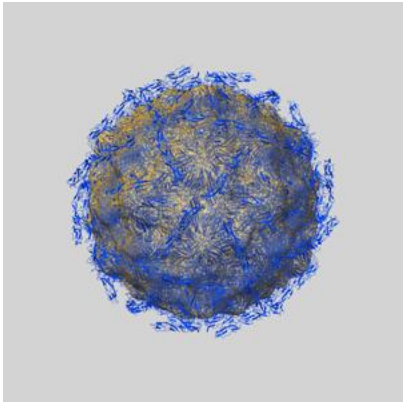
9.1.2 Map-model assembly overlay (i)



X



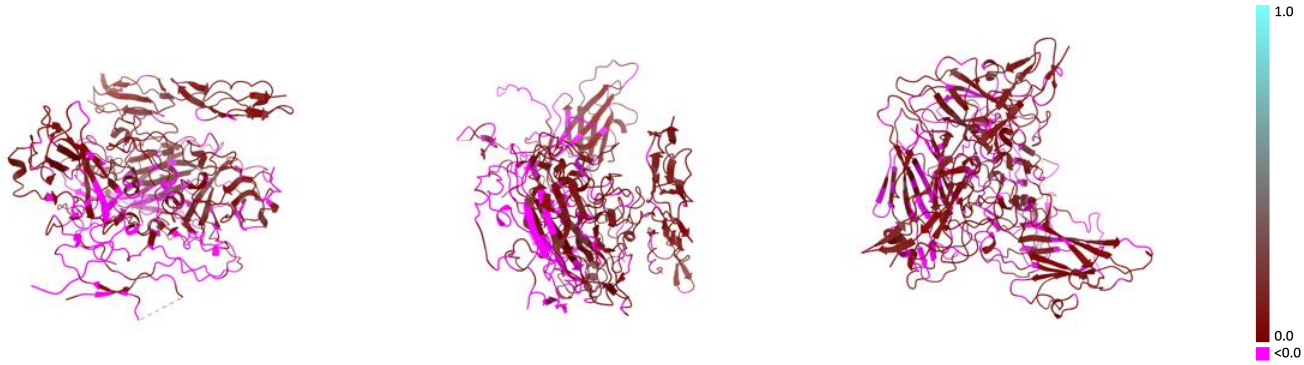
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 169.0 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.

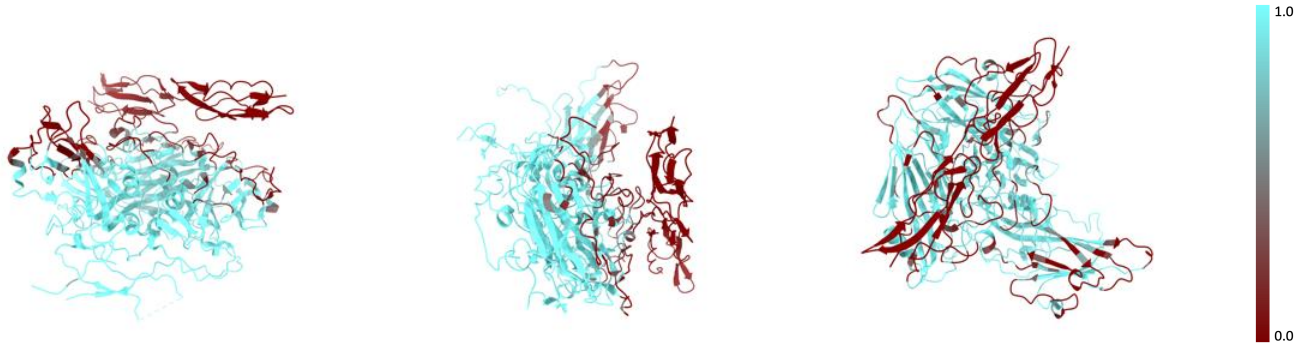
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

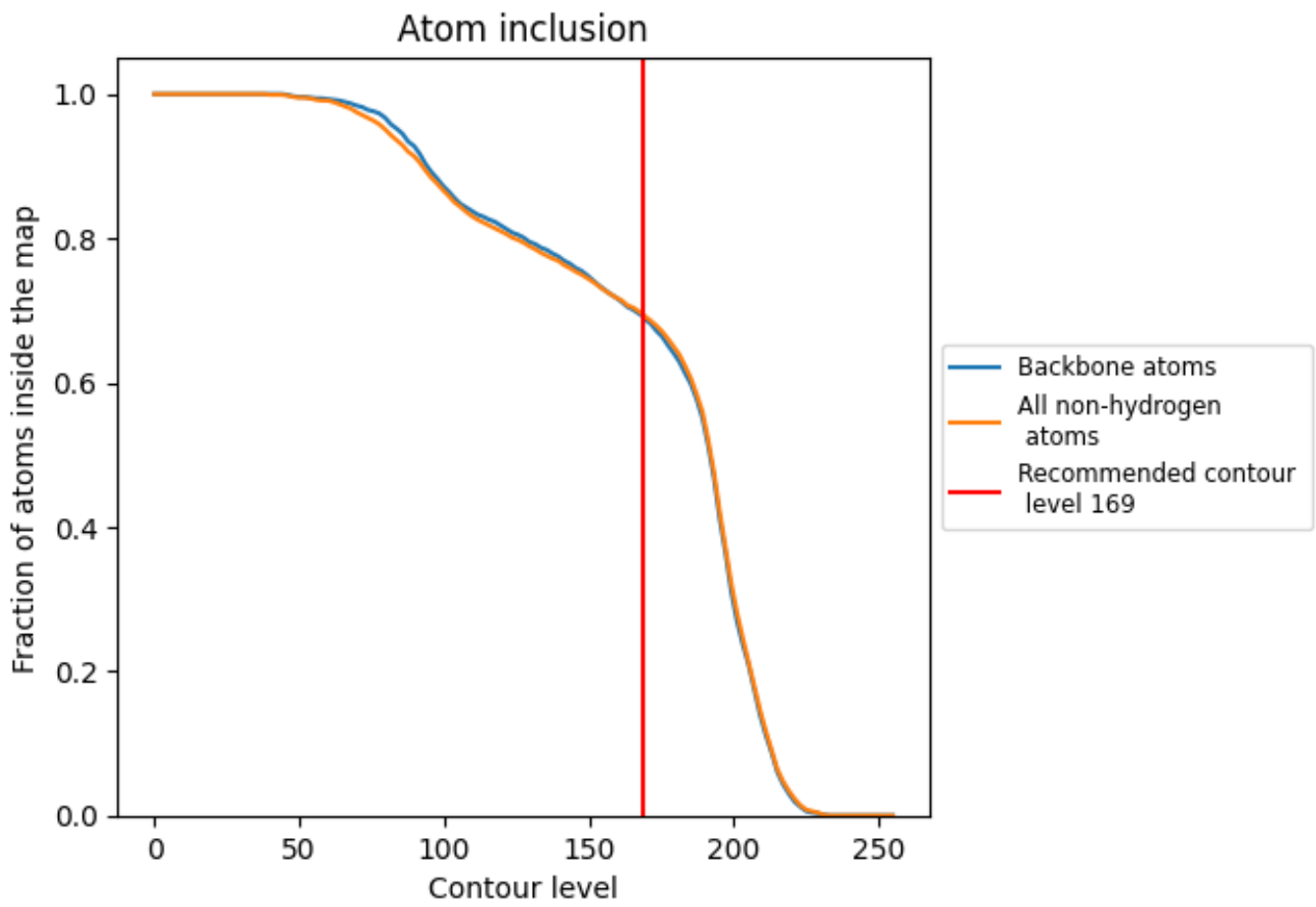
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (169).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6940	0.0320
A	0.7030	0.0210
B	0.8160	0.0290
C	0.8280	0.0320
D	1.0000	-0.0130
E	0.0000	0.0880