



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:45 PM UTC

PDB ID : 3J4Q / pdb_00003j4q
EMDB ID : EMD-5755
Title : Pseudo-atomic model of the AKAP18-PKA complex in a bent conformation
derived from electron microscopy
Authors : Reichow, S.L.; Gonen, T.
Deposited on : 2013-09-25
Resolution : 35.00 Å (reported)
Based on initial models : 2VFL, 2IZX, 2QVS

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

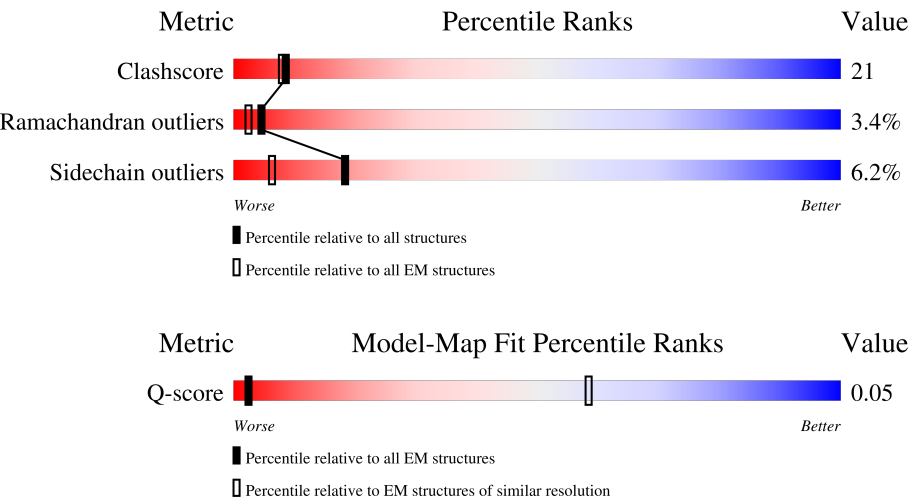
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 35.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12 (35.00 - 35.00)

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	353	53%11%35%
2	B	402	13% 57%32%5%5%
2	C	402	14% 57%33%5%
3	D	351	54%30%7%7%

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Mol	Chain	Length	Quality of chain
3	E	351	55% 29% 7% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12906 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 A-kinase anchor protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	1	0
			1836	1180	312	336	8		

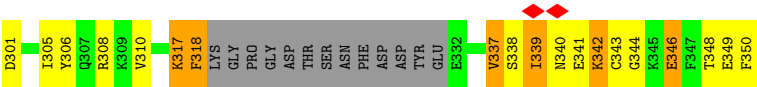
- Molecule 2 is a protein called cAMP-dependent protein kinase type II-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	382	Total	C	N	O	S	0	0
			3018	1888	514	601	15		
2	C	382	Total	C	N	O	S	0	0
			3018	1888	514	601	15		

- Molecule 3 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	325	Total	C	N	O	S	0	0
			2517	1632	430	450	5		
3	E	325	Total	C	N	O	S	0	0
			2517	1632	430	450	5		





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Each Micrograph	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	52000	Depositor
Image detector	GENERIC GATAN	Depositor
Maximum map value	12.970	Depositor
Minimum map value	-3.924	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.35	Depositor
Map size ($\text{\AA}$)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	4.2, 4.2, 4.2	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.60	0/1872	0.82	0/2518
2	B	0.58	3/3065 (0.1%)	1.04	20/4135 (0.5%)
2	C	0.56	2/3065 (0.1%)	1.04	19/4135 (0.5%)
3	D	0.46	1/2581 (0.0%)	1.17	24/3498 (0.7%)
3	E	0.46	1/2581 (0.0%)	1.17	24/3498 (0.7%)
All	All	0.53	7/13164 (0.1%)	1.07	87/17784 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	81	LYS	CA-C	-6.65	1.50	1.53
3	D	81	LYS	CA-C	-6.50	1.50	1.53
2	C	313	LYS	CA-CB	5.43	1.60	1.53
2	B	313	LYS	CA-CB	5.42	1.60	1.53
2	B	87	PRO	N-CD	5.24	1.55	1.47
2	B	86	VAL	C-N	5.20	1.41	1.34
2	C	26	PRO	CA-C	5.14	1.55	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	81	LYS	CA-C-O	22.00	130.70	117.94
3	D	81	LYS	CA-C-O	21.92	130.65	117.94
3	E	114	SER	CA-C-O	17.22	138.98	120.55
3	D	114	SER	CA-C-O	17.16	138.91	120.55
3	D	116	LEU	CA-C-O	15.99	143.37	120.51
3	E	116	LEU	CA-C-O	15.92	143.27	120.51
3	E	115	ASN	N-CA-C	11.28	134.83	110.80
3	D	115	ASN	N-CA-C	11.27	134.81	110.80
3	D	114	SER	N-CA-C	-10.68	98.37	111.40
3	E	114	SER	N-CA-C	-10.62	98.45	111.40
3	E	80	VAL	CB-CA-C	-10.33	94.35	111.29
3	D	80	VAL	CB-CA-C	-10.32	94.36	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	316	LYS	N-CA-C	9.83	131.73	110.80
2	B	316	LYS	N-CA-C	9.78	131.63	110.80
3	E	81	LYS	N-CA-CB	9.75	126.96	110.49
3	D	81	LYS	N-CA-CB	9.74	126.95	110.49
3	D	114	SER	CB-CA-C	8.71	125.42	110.79
3	E	114	SER	CB-CA-C	8.69	125.39	110.79
3	D	113	ASN	CB-CA-C	-7.59	95.32	110.42
3	E	113	ASN	CB-CA-C	-7.56	95.37	110.42
3	E	81	LYS	N-CA-C	-7.52	102.62	108.78
3	D	81	LYS	N-CA-C	-7.51	102.62	108.78
2	C	318	GLY	N-CA-C	7.35	126.08	112.77
2	B	318	GLY	N-CA-C	7.32	126.02	112.77
2	C	317	ASN	CA-C-O	7.17	130.76	120.51
2	B	317	ASN	CA-C-O	7.15	130.74	120.51
3	D	114	SER	N-CA-CB	7.06	120.58	110.13
3	E	114	SER	N-CA-CB	7.05	120.56	110.13
2	C	189	ASP	CB-CA-C	-6.77	106.86	116.34
2	C	311	LYS	N-CA-C	-6.76	104.19	113.18
2	B	311	LYS	N-CA-C	-6.75	104.20	113.18
2	B	316	LYS	CA-C-O	-6.74	110.87	120.51
2	C	316	LYS	CA-C-O	-6.73	110.89	120.51
2	B	189	ASP	CB-CA-C	-6.71	106.94	116.34
2	C	315	ASN	CA-C-O	-6.57	111.11	120.51
2	B	315	ASN	CA-C-O	-6.55	111.14	120.51
2	C	118	HIS	CA-C-N	6.55	126.58	119.90
2	C	118	HIS	C-N-CA	6.55	126.58	119.90
3	E	236	PRO	CA-C-N	6.51	126.44	119.28
3	E	236	PRO	C-N-CA	6.51	126.44	119.28
3	D	116	LEU	CB-CA-C	-6.51	97.47	110.42
2	B	118	HIS	CA-C-N	6.50	126.53	119.90
2	B	118	HIS	C-N-CA	6.50	126.53	119.90
3	E	116	LEU	CB-CA-C	-6.50	97.49	110.42
3	D	236	PRO	CA-C-N	6.49	126.42	119.28
3	D	236	PRO	C-N-CA	6.49	126.42	119.28
2	B	195	VAL	N-CA-C	6.47	120.11	111.44
2	C	195	VAL	N-CA-C	6.47	120.10	111.44
2	C	316	LYS	CB-CA-C	-6.42	97.65	110.42
2	B	316	LYS	CB-CA-C	-6.38	97.72	110.42
3	D	115	ASN	CB-CA-C	-6.28	97.91	110.42
3	E	115	ASN	CB-CA-C	-6.28	97.92	110.42
2	C	239	ILE	N-CA-C	5.78	115.96	110.53
2	B	239	ILE	N-CA-C	5.77	115.95	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	380	ILE	N-CA-C	5.75	118.24	111.05
2	B	380	ILE	N-CA-C	5.75	118.23	111.05
3	D	98	VAL	N-CA-C	5.71	117.83	108.97
2	B	136	LEU	N-CA-C	5.70	118.23	111.33
3	E	98	VAL	N-CA-C	5.69	117.79	108.97
2	C	136	LEU	N-CA-C	5.69	118.21	111.33
3	E	192	LYS	N-CA-C	-5.64	98.01	107.99
3	E	139	SER	N-CA-C	-5.59	103.15	110.53
3	D	139	SER	N-CA-C	-5.59	103.15	110.53
3	D	192	LYS	N-CA-C	-5.59	98.10	107.99
2	C	59	HIS	N-CA-C	5.58	117.37	111.28
2	C	318	GLY	CA-C-O	-5.54	114.12	122.71
2	B	318	GLY	CA-C-O	-5.51	114.17	122.71
2	C	314	SER	N-CA-C	5.42	122.34	110.80
2	B	314	SER	N-CA-C	5.41	122.33	110.80
3	D	105	LYS	N-CA-C	5.40	118.20	109.40
3	D	235	TYR	CA-C-N	5.39	123.54	119.66
3	D	235	TYR	C-N-CA	5.39	123.54	119.66
3	E	105	LYS	N-CA-C	5.38	118.17	109.40
3	E	196	TRP	N-CA-C	5.36	122.40	114.09
3	D	196	TRP	N-CA-C	5.33	122.35	114.09
3	E	235	TYR	CA-C-N	5.33	123.49	119.66
3	E	235	TYR	C-N-CA	5.33	123.49	119.66
2	B	86	VAL	CA-C-N	-5.32	113.15	119.05
2	B	86	VAL	C-N-CA	-5.32	113.15	119.05
2	B	224	GLU	N-CA-C	-5.30	102.02	109.96
2	C	224	GLU	N-CA-C	-5.25	102.08	109.96
2	B	89	PRO	CA-N-CD	-5.23	104.68	112.00
3	D	165	ARG	N-CA-C	5.20	119.57	113.23
3	E	165	ARG	N-CA-C	5.19	119.56	113.23
3	E	214	GLY	N-CA-C	-5.09	105.35	112.18
3	D	214	GLY	N-CA-C	-5.08	105.37	112.18
2	C	26	PRO	O-C-N	5.06	123.53	121.15

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1836	0	1893	57	0
2	B	3018	0	2929	131	0
2	C	3018	0	2929	127	0
3	D	2517	0	2349	122	0
3	E	2517	0	2349	126	0
All	All	12906	0	12449	541	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 21.

All (541) 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:36:TYR:CE1	2:B:40:LEU:HD11	1.83	1.12
1:A:289:GLY:HA2	1:A:292:ASP:HB2	1.30	1.11
1:A:298:ASP:HB3	1:A:300:GLU:HB2	1.37	1.07
2:B:110:GLU:OE2	2:B:110:GLU:N	1.95	0.99
2:C:110:GLU:OE2	2:C:110:GLU:N	1.95	0.99
1:A:298:ASP:HB3	1:A:300:GLU:CB	1.94	0.98
3:D:15:VAL:HG23	3:D:16:LYS:HD2	1.46	0.96
1:A:289:GLY:CA	1:A:292:ASP:HB2	1.95	0.95
3:E:15:VAL:HG23	3:E:16:LYS:HD2	1.46	0.95
2:C:86:VAL:HG12	2:C:89:PRO:HG3	1.50	0.93
2:C:86:VAL:CG1	2:C:89:PRO:HG3	1.98	0.93
1:A:299:ALA:N	1:A:300:GLU:HA	1.85	0.91
2:C:92:PHE:HD1	3:E:133:ARG:HD2	1.33	0.90
1:A:290:GLU:N	1:A:291:LYS:HA	1.86	0.90
2:C:177:ILE:HA	2:C:227:LEU:HD23	1.54	0.90
1:A:298:ASP:HB3	1:A:300:GLU:CG	2.02	0.90
1:A:289:GLY:C	1:A:291:LYS:HA	1.97	0.89
2:B:110:GLU:OE2	2:B:110:GLU:CA	2.22	0.88
2:B:177:ILE:HA	2:B:227:LEU:HD23	1.54	0.87
3:D:104:VAL:HG11	3:D:183:THR:HG22	1.57	0.86
3:E:104:VAL:HG11	3:E:183:THR:HG22	1.57	0.86
2:C:110:GLU:OE2	2:C:110:GLU:CA	2.22	0.85
3:E:59:LEU:HD12	3:E:60:VAL:H	1.42	0.84
3:D:59:LEU:HD12	3:D:60:VAL:H	1.42	0.83
2:B:93:THR:O	3:D:129:PHE:CE2	2.31	0.82
1:A:298:ASP:CB	1:A:300:GLU:HB2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:16:LYS:HD2	3:D:16:LYS:H	1.48	0.78
1:A:290:GLU:N	1:A:292:ASP:HA	1.98	0.78
1:A:289:GLY:HA2	1:A:292:ASP:CB	2.13	0.78
3:E:16:LYS:HD2	3:E:16:LYS:H	1.48	0.77
3:E:153:THR:O	3:E:157:LEU:HD13	1.85	0.76
2:B:36:TYR:CE1	2:B:40:LEU:CD1	2.68	0.76
3:D:153:THR:O	3:D:157:LEU:HD13	1.85	0.76
2:B:45:ARG:HG2	2:B:46:GLN:HG3	1.67	0.76
1:A:290:GLU:H	1:A:292:ASP:HA	1.51	0.75
2:B:178:GLU:HG3	2:B:179:ARG:HG3	1.68	0.75
2:B:107:GLU:O	2:B:107:GLU:HG2	1.87	0.74
3:D:112:ASP:O	3:D:114:SER:N	2.21	0.74
3:D:13:GLU:HB2	3:D:15:VAL:HG22	1.70	0.74
2:C:178:GLU:HG3	2:C:179:ARG:HG3	1.68	0.73
2:C:307:LEU:O	2:C:347:ALA:HB1	1.88	0.73
2:B:307:LEU:O	2:B:347:ALA:HB1	1.88	0.73
2:B:45:ARG:HB3	2:B:46:GLN:CB	2.19	0.73
2:C:107:GLU:O	2:C:107:GLU:HG2	1.87	0.72
3:E:13:GLU:HB2	3:E:15:VAL:HG22	1.70	0.72
2:B:66:VAL:HB	2:B:67:PRO:HD3	1.70	0.72
3:E:112:ASP:O	3:E:114:SER:N	2.21	0.72
3:E:80:VAL:H	3:E:85:ILE:HG21	1.57	0.70
3:E:113:ASN:HA	3:E:341:GLU:HA	1.74	0.70
3:E:112:ASP:C	3:E:114:SER:H	1.99	0.70
3:D:80:VAL:H	3:D:85:ILE:HG21	1.57	0.69
3:E:115:ASN:O	3:E:116:LEU:CB	2.40	0.69
3:D:112:ASP:C	3:D:114:SER:H	1.99	0.69
2:C:92:PHE:CD1	3:E:133:ARG:HB3	2.28	0.69
3:D:100:PHE:CD1	3:D:101:PRO:HD2	2.28	0.69
3:D:115:ASN:O	3:D:116:LEU:CB	2.40	0.69
1:A:311:ASN:HD21	1:A:315:LYS:HE3	1.57	0.68
2:B:282:ASP:HB2	2:B:353:GLY:HA2	1.75	0.68
3:E:100:PHE:CD1	3:E:101:PRO:HD2	2.28	0.68
3:D:86:GLU:C	3:D:88:THR:H	1.99	0.68
3:D:113:ASN:HA	3:D:341:GLU:HA	1.74	0.68
3:E:86:GLU:C	3:E:88:THR:H	1.99	0.68
2:C:92:PHE:CD1	3:E:133:ARG:HD2	2.24	0.68
2:B:45:ARG:HB3	2:B:46:GLN:CG	2.23	0.68
2:C:282:ASP:HB2	2:C:353:GLY:HA2	1.75	0.68
3:D:227:LEU:HD13	3:D:231:MET:HE2	1.76	0.68
3:E:135:ILE:HD11	3:E:138:PHE:CE1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:62:HIS:O	3:D:66:GLY:HA2	1.94	0.67
1:A:290:GLU:H	1:A:292:ASP:CB	2.07	0.67
3:E:62:HIS:O	3:E:66:GLY:HA2	1.94	0.67
3:D:135:ILE:HD11	3:D:138:PHE:CE1	2.29	0.66
3:E:337:VAL:HG23	3:E:339:ILE:H	1.60	0.66
2:C:142:ASP:OD1	2:C:145:GLN:HG3	1.96	0.66
2:B:142:ASP:OD1	2:B:145:GLN:HG3	1.95	0.66
2:C:237:ARG:HB3	2:C:237:ARG:NH2	2.11	0.66
3:D:337:VAL:HG23	3:D:339:ILE:H	1.60	0.66
1:A:263:TYR:CE1	1:A:287:VAL:CG1	2.78	0.66
3:E:227:LEU:HD13	3:E:231:MET:HE2	1.76	0.66
3:E:62:HIS:HB3	3:E:67:ASN:H	1.61	0.65
2:B:45:ARG:NH1	2:B:46:GLN:HE22	1.94	0.65
3:E:40:LEU:HB2	3:E:110:PHE:CE2	2.31	0.65
3:D:62:HIS:HB3	3:D:67:ASN:H	1.61	0.65
2:B:184:ILE:HG23	2:B:219:ILE:CD1	2.27	0.65
3:D:80:VAL:H	3:D:85:ILE:CG2	2.10	0.65
3:E:80:VAL:H	3:E:85:ILE:CG2	2.10	0.65
3:D:40:LEU:HB2	3:D:110:PHE:CE2	2.31	0.65
1:A:290:GLU:H	1:A:292:ASP:CA	2.10	0.64
2:B:237:ARG:NH2	2:B:237:ARG:HB3	2.11	0.64
2:C:109:GLU:O	2:C:110:GLU:C	2.40	0.64
2:B:36:TYR:CZ	2:B:40:LEU:HD11	2.31	0.64
3:D:35:GLN:HB3	3:D:350:PHE:OXT	1.98	0.64
2:B:109:GLU:O	2:B:110:GLU:C	2.40	0.64
1:A:100:ASN:C	1:A:100:ASN:HD22	2.06	0.64
1:A:263:TYR:CZ	1:A:287:VAL:HG11	2.32	0.64
2:B:45:ARG:CZ	2:B:46:GLN:NE2	2.60	0.64
2:C:184:ILE:HG23	2:C:219:ILE:CD1	2.27	0.64
3:E:35:GLN:HB3	3:E:350:PHE:OXT	1.98	0.64
2:C:110:GLU:OE2	2:C:110:GLU:HA	1.98	0.64
2:B:313:LYS:O	2:B:314:SER:CB	2.46	0.64
2:B:333:TYR:CE2	2:B:336:GLU:HG2	2.33	0.64
2:C:258:PRO:HA	2:C:261:LYS:HG2	1.80	0.63
2:C:313:LYS:O	2:C:314:SER:CB	2.46	0.63
2:B:258:PRO:HA	2:B:261:LYS:HG2	1.80	0.63
3:E:85:ILE:C	3:E:85:ILE:HD12	2.24	0.63
1:A:168:HIS:CE1	1:A:292:ASP:HB3	2.34	0.63
3:D:85:ILE:HD12	3:D:85:ILE:C	2.24	0.63
2:B:110:GLU:OE2	2:B:110:GLU:HA	1.98	0.62
3:D:146:TYR:HB3	3:D:180:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:333:TYR:CE2	2:C:336:GLU:HG2	2.33	0.62
3:D:128:MET:HE3	3:D:128:MET:HA	1.81	0.62
3:E:146:TYR:HB3	3:E:180:ILE:HD11	1.80	0.62
1:A:289:GLY:O	1:A:291:LYS:HG2	2.00	0.62
2:C:293:ALA:HB1	2:C:338:ALA:HB2	1.81	0.62
3:D:13:GLU:HB2	3:D:15:VAL:CG2	2.29	0.62
3:E:128:MET:HA	3:E:128:MET:HE3	1.81	0.62
3:E:13:GLU:HB2	3:E:15:VAL:CG2	2.29	0.62
1:A:189:ALA:O	1:A:193:HIS:HE1	1.82	0.62
2:B:293:ALA:HB1	2:B:338:ALA:HB2	1.81	0.62
2:C:86:VAL:HG11	2:C:89:PRO:HG3	1.78	0.62
2:C:308:ILE:HB	2:C:325:ILE:HD11	1.82	0.62
2:B:38:THR:HG23	2:B:41:ARG:HH21	1.63	0.62
2:B:308:ILE:HB	2:B:325:ILE:HD11	1.82	0.61
3:E:71:MET:HA	3:E:118:MET:O	1.99	0.61
2:C:237:ARG:HB3	2:C:237:ARG:HH21	1.66	0.61
3:E:104:VAL:CG1	3:E:183:THR:HG22	2.28	0.61
3:D:71:MET:HA	3:D:118:MET:O	1.99	0.61
3:D:100:PHE:CG	3:D:101:PRO:HD2	2.35	0.61
2:B:45:ARG:HB3	2:B:46:GLN:HB2	1.83	0.61
3:E:100:PHE:CG	3:E:101:PRO:HD2	2.35	0.61
3:D:227:LEU:CD1	3:D:231:MET:HE2	2.31	0.61
1:A:298:ASP:HB3	1:A:300:GLU:HG3	1.83	0.61
2:B:237:ARG:HB3	2:B:237:ARG:HH21	1.66	0.61
3:D:104:VAL:CG1	3:D:183:THR:HG22	2.28	0.61
1:A:290:GLU:H	1:A:292:ASP:CG	2.09	0.60
2:C:278:LYS:HZ3	2:C:359:VAL:HG21	1.67	0.60
2:B:13:LEU:HD13	2:C:29:LEU:HB3	1.83	0.60
2:B:345:ARG:HG3	2:B:345:ARG:HH11	1.65	0.60
2:C:269:MET:SD	3:E:193:GLY:HA2	2.42	0.60
3:E:113:ASN:CA	3:E:341:GLU:HA	2.32	0.60
3:D:107:GLU:HB2	3:D:119:VAL:O	2.02	0.60
1:A:263:TYR:CE1	1:A:287:VAL:HG13	2.36	0.60
3:E:86:GLU:C	3:E:88:THR:N	2.60	0.60
2:C:237:ARG:HH21	2:C:237:ARG:CB	2.15	0.59
3:E:227:LEU:CD1	3:E:231:MET:HE2	2.31	0.59
2:C:345:ARG:HG3	2:C:345:ARG:HH11	1.65	0.59
2:B:237:ARG:HH21	2:B:237:ARG:CB	2.15	0.59
1:A:299:ALA:N	1:A:300:GLU:CA	2.63	0.59
3:D:113:ASN:CA	3:D:341:GLU:HA	2.32	0.59
2:B:269:MET:SD	3:D:193:GLY:HA2	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:156:TYR:CD2	3:D:157:LEU:HD12	2.38	0.59
3:E:35:GLN:O	3:E:36:ASN:C	2.46	0.59
3:D:35:GLN:O	3:D:36:ASN:C	2.46	0.58
1:A:189:ALA:O	1:A:193:HIS:CE1	2.55	0.58
3:D:342:LYS:O	3:D:344:GLY:N	2.34	0.58
3:E:156:TYR:CD2	3:E:157:LEU:HD12	2.38	0.58
3:E:107:GLU:HB2	3:E:119:VAL:O	2.02	0.58
2:B:103:PHE:HZ	2:B:241:LYS:HZ3	1.51	0.58
2:B:110:GLU:O	2:B:111:ASP:OD1	2.22	0.58
2:B:45:ARG:CG	2:B:46:GLN:HG3	2.34	0.58
3:D:62:HIS:CD2	3:D:63:LYS:H	2.22	0.58
3:E:62:HIS:CD2	3:E:63:LYS:H	2.21	0.58
2:B:165:ILE:HB	2:B:215:ARG:HG2	1.86	0.58
3:D:342:LYS:C	3:D:344:GLY:H	2.11	0.58
3:E:156:TYR:O	3:E:159:SER:HB3	2.04	0.58
3:E:163:ILE:HD12	3:E:165:ARG:HD3	1.85	0.58
3:E:342:LYS:C	3:E:344:GLY:H	2.11	0.58
2:B:178:GLU:HB3	2:B:226:SER:O	2.04	0.57
2:B:277:GLU:OE2	2:B:356:LYS:HE2	2.03	0.57
2:C:277:GLU:OE2	2:C:356:LYS:HE2	2.03	0.57
2:C:178:GLU:HB3	2:C:226:SER:O	2.04	0.57
3:D:150:ILE:HD13	3:D:167:LEU:HD11	1.86	0.57
3:D:243:PRO:HA	3:D:246:ILE:HD12	1.85	0.57
2:C:110:GLU:O	2:C:111:ASP:OD1	2.22	0.57
2:C:184:ILE:C	2:C:185:LEU:HD12	2.30	0.57
2:B:268:ARG:O	2:B:272:VAL:HG23	2.04	0.57
2:C:128:LEU:HD23	2:C:176:VAL:HG11	1.86	0.57
2:C:165:ILE:HB	2:C:215:ARG:HG2	1.86	0.57
3:D:163:ILE:HD12	3:D:165:ARG:HD3	1.85	0.57
3:E:342:LYS:O	3:E:344:GLY:N	2.34	0.57
2:B:184:ILE:C	2:B:185:LEU:HD12	2.30	0.57
3:D:135:ILE:HD11	3:D:138:PHE:HE1	1.69	0.57
2:C:268:ARG:O	2:C:272:VAL:HG23	2.04	0.57
3:E:135:ILE:HD11	3:E:138:PHE:HE1	1.69	0.56
2:C:280:TYR:CD2	2:C:286:ILE:HG12	2.39	0.56
2:C:160:THR:O	2:C:161:ASP:HB2	2.05	0.56
3:D:16:LYS:HD2	3:D:16:LYS:N	2.17	0.56
3:E:89:LEU:HD11	3:E:349:GLU:O	2.05	0.56
2:B:102:THR:HG22	2:B:103:PHE:N	2.21	0.56
2:B:160:THR:O	2:B:161:ASP:HB2	2.06	0.56
3:E:243:PRO:HA	3:E:246:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:89:LEU:HD11	3:D:349:GLU:O	2.05	0.56
3:D:156:TYR:O	3:D:159:SER:HB3	2.04	0.56
3:E:16:LYS:HD2	3:E:16:LYS:N	2.17	0.56
1:A:300:GLU:O	1:A:301:LEU:HB2	2.05	0.56
2:B:128:LEU:HD23	2:B:176:VAL:HG11	1.86	0.56
2:B:278:LYS:HZ2	2:B:359:VAL:HG21	1.70	0.56
3:D:107:GLU:HA	3:D:107:GLU:OE1	2.06	0.56
3:E:150:ILE:HD13	3:E:167:LEU:HD11	1.86	0.56
2:B:95:ARG:NH2	3:D:170:GLU:OE1	2.38	0.56
2:B:280:TYR:CD2	2:B:286:ILE:HG12	2.39	0.56
3:E:107:GLU:OE1	3:E:107:GLU:HA	2.06	0.56
2:B:307:LEU:HD23	2:B:324:GLU:HA	1.88	0.56
3:D:86:GLU:C	3:D:88:THR:N	2.60	0.56
3:E:59:LEU:HD12	3:E:60:VAL:N	2.18	0.56
3:D:305:ILE:HD12	3:D:310:VAL:HG21	1.87	0.55
2:C:102:THR:HG22	2:C:103:PHE:N	2.21	0.55
3:D:224:LEU:HD22	3:D:228:ILE:HG13	1.88	0.55
3:E:113:ASN:N	3:E:341:GLU:HG3	2.21	0.55
1:A:311:ASN:ND2	1:A:315:LYS:HE3	2.22	0.55
3:E:305:ILE:HD12	3:E:310:VAL:HG21	1.87	0.55
2:C:307:LEU:HD23	2:C:324:GLU:HA	1.88	0.55
2:C:253:PHE:O	2:C:257:VAL:HG23	2.07	0.55
2:C:287:ILE:CG2	2:C:345:ARG:HG2	2.37	0.55
3:E:18:PHE:HE2	3:E:306:TYR:HH	1.55	0.55
2:B:375:ILE:HA	2:B:378:ARG:HG3	1.89	0.55
2:C:375:ILE:HA	2:C:378:ARG:HG3	1.89	0.55
3:D:18:PHE:HE2	3:D:306:TYR:HH	1.55	0.55
3:E:224:LEU:HD22	3:E:228:ILE:HG13	1.88	0.55
1:A:303:ARG:O	1:A:306:LYS:N	2.39	0.54
2:B:158:VAL:HG13	2:B:162:GLU:OE1	2.07	0.54
3:E:15:VAL:HG23	3:E:16:LYS:CD	2.29	0.54
3:D:113:ASN:N	3:D:341:GLU:HG3	2.22	0.54
3:E:318:PHE:HD1	3:E:318:PHE:O	1.90	0.54
2:C:303:GLU:OE1	2:C:327:HIS:HE1	1.90	0.54
2:B:253:PHE:O	2:B:257:VAL:HG23	2.07	0.54
2:C:158:VAL:HG13	2:C:162:GLU:OE1	2.07	0.54
2:B:125:ARG:NH1	2:B:151:ASP:OD1	2.39	0.54
3:E:50:GLY:HA3	3:E:57:VAL:O	2.08	0.54
2:B:210:MET:HE1	3:D:210:ILE:HG23	1.89	0.54
2:C:94:ARG:HG3	3:E:129:PHE:CE2	2.42	0.54
2:C:210:MET:HE1	3:E:210:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:50:GLY:HA3	3:D:57:VAL:O	2.08	0.54
3:D:59:LEU:HD12	3:D:60:VAL:N	2.18	0.54
2:B:287:ILE:CG2	2:B:345:ARG:HG2	2.37	0.54
2:C:318:GLY:O	2:C:319:GLY:C	2.51	0.54
3:E:40:LEU:HD12	3:E:40:LEU:O	2.08	0.54
2:B:303:GLU:OE1	2:B:327:HIS:HE1	1.90	0.53
2:C:101:GLU:HG3	2:C:233:VAL:HG22	1.90	0.53
2:B:45:ARG:CB	2:B:46:GLN:HG3	2.39	0.53
3:D:15:VAL:HG23	3:D:16:LYS:CD	2.29	0.53
1:A:299:ALA:H	1:A:300:GLU:HA	1.72	0.53
2:B:278:LYS:HD2	2:B:280:TYR:OH	2.08	0.53
2:C:311:LYS:C	2:C:313:LYS:H	2.17	0.53
3:D:318:PHE:HD1	3:D:318:PHE:O	1.90	0.53
2:B:318:GLY:O	2:B:319:GLY:C	2.51	0.53
3:D:40:LEU:O	3:D:40:LEU:HD12	2.08	0.53
2:C:388:VAL:O	2:C:392:GLY:HA3	2.08	0.53
3:D:227:LEU:O	3:D:231:MET:HG3	2.09	0.53
2:C:278:LYS:HD2	2:C:280:TYR:OH	2.08	0.53
3:E:227:LEU:O	3:E:231:MET:HG3	2.09	0.53
2:B:101:GLU:HG3	2:B:233:VAL:HG22	1.90	0.52
2:B:388:VAL:O	2:B:392:GLY:HA3	2.08	0.52
3:D:245:GLN:O	3:D:249:LYS:HG3	2.10	0.52
3:E:245:GLN:O	3:E:249:LYS:HG3	2.10	0.52
2:C:110:GLU:O	2:C:111:ASP:CG	2.53	0.52
2:C:281:LYS:O	2:C:284:GLU:HG2	2.10	0.52
2:B:281:LYS:O	2:B:284:GLU:HG2	2.10	0.52
2:B:110:GLU:O	2:B:111:ASP:CG	2.53	0.52
2:C:318:GLY:O	2:C:320:ASN:N	2.43	0.52
1:A:198:LEU:O	1:A:202:GLU:HG2	2.10	0.52
1:A:300:GLU:HG2	1:A:301:LEU:HG	1.92	0.52
2:C:125:ARG:NH1	2:C:151:ASP:OD1	2.39	0.52
2:B:155:GLU:HB2	2:B:228:TRP:CZ3	2.45	0.52
1:A:263:TYR:CZ	1:A:287:VAL:CG1	2.92	0.52
1:A:263:TYR:OH	1:A:291:LYS:HD3	2.10	0.52
2:C:108:GLU:O	2:C:109:GLU:HB2	2.09	0.51
2:C:295:SER:HB2	2:C:360:MET:O	2.09	0.51
2:B:45:ARG:HB3	2:B:46:GLN:HG3	1.90	0.51
2:B:318:GLY:O	2:B:320:ASN:N	2.43	0.51
2:B:295:SER:HB2	2:B:360:MET:O	2.09	0.51
3:D:103:LEU:HD21	3:D:157:LEU:HD11	1.93	0.51
2:B:288:ALA:O	2:B:291:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:LYS:C	2:B:313:LYS:H	2.17	0.51
2:C:250:PHE:CE1	2:C:358:LEU:HD21	2.45	0.51
3:D:191:VAL:HG13	3:D:216:ASN:HD21	1.76	0.51
3:E:103:LEU:HD21	3:E:157:LEU:HD11	1.93	0.51
3:E:191:VAL:HG13	3:E:216:ASN:HD21	1.76	0.51
2:B:45:ARG:NH1	2:B:46:GLN:NE2	2.57	0.51
2:B:311:LYS:O	2:B:313:LYS:N	2.37	0.51
3:D:203:GLU:HG2	3:D:236:PRO:HG3	1.93	0.51
2:B:250:PHE:CE1	2:B:358:LEU:HD21	2.45	0.51
2:C:171:GLY:HA2	2:C:215:ARG:HH11	1.76	0.51
2:B:108:GLU:O	2:B:109:GLU:HB2	2.09	0.51
2:B:171:GLY:HA2	2:B:215:ARG:HH11	1.76	0.51
2:C:155:GLU:HB2	2:C:228:TRP:CZ3	2.45	0.51
2:C:288:ALA:O	2:C:291:GLU:HG2	2.11	0.51
2:B:45:ARG:CZ	2:B:46:GLN:HE22	2.23	0.51
2:B:160:THR:HB	2:B:223:SER:HA	1.94	0.50
1:A:311:ASN:HD21	1:A:315:LYS:CE	2.23	0.50
3:D:92:LYS:HD2	3:D:92:LYS:O	2.11	0.50
3:E:90:ASN:C	3:E:90:ASN:HD22	2.19	0.50
1:A:130:SER:O	1:A:132:HIS:HD2	1.95	0.50
3:E:92:LYS:HD2	3:E:92:LYS:O	2.11	0.50
3:E:203:GLU:HG2	3:E:236:PRO:HG3	1.93	0.50
2:B:110:GLU:H	2:B:110:GLU:CD	2.18	0.50
2:B:177:ILE:HG12	2:B:227:LEU:HD21	1.94	0.50
2:C:160:THR:HB	2:C:223:SER:HA	1.94	0.50
2:B:237:ARG:O	2:B:241:LYS:HB2	2.12	0.49
3:E:246:ILE:O	3:E:250:ILE:HG13	2.12	0.49
2:B:109:GLU:O	2:B:111:ASP:OD2	2.30	0.49
2:C:237:ARG:O	2:C:241:LYS:HB2	2.12	0.49
2:B:97:SER:HB3	3:D:187:PHE:HE2	1.77	0.49
3:D:111:LYS:CB	3:D:116:LEU:N	2.76	0.49
3:E:135:ILE:HD11	3:E:138:PHE:CD1	2.47	0.49
2:B:250:PHE:O	2:B:254:ILE:HG12	2.13	0.49
2:C:109:GLU:O	2:C:111:ASP:OD2	2.30	0.49
3:D:246:ILE:O	3:D:250:ILE:HG13	2.12	0.49
2:C:110:GLU:H	2:C:110:GLU:CD	2.18	0.49
3:D:135:ILE:HD11	3:D:138:PHE:CD1	2.47	0.49
3:E:84:GLN:HG3	3:E:85:ILE:N	2.28	0.49
3:E:111:LYS:CB	3:E:116:LEU:N	2.76	0.49
2:B:282:ASP:HB2	2:B:353:GLY:CA	2.42	0.49
2:C:311:LYS:O	2:C:313:LYS:N	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:111:LYS:CB	3:D:116:LEU:H	2.26	0.49
3:D:84:GLN:HG3	3:D:85:ILE:N	2.28	0.48
2:C:103:PHE:HZ	2:C:241:LYS:HZ3	1.59	0.48
2:C:177:ILE:HG12	2:C:227:LEU:HD21	1.94	0.48
2:C:282:ASP:HB2	2:C:353:GLY:CA	2.42	0.48
2:C:107:GLU:OE1	2:C:245:LYS:HE2	2.13	0.48
2:C:171:GLY:HA2	2:C:215:ARG:NH1	2.29	0.48
3:D:90:ASN:C	3:D:90:ASN:HD22	2.19	0.48
2:B:287:ILE:HG21	2:B:345:ARG:HG2	1.95	0.48
2:C:250:PHE:O	2:C:254:ILE:HG12	2.13	0.48
2:C:287:ILE:HG21	2:C:345:ARG:HG2	1.95	0.48
2:B:107:GLU:OE1	2:B:245:LYS:HE2	2.14	0.48
2:B:171:GLY:HA2	2:B:215:ARG:NH1	2.29	0.48
2:C:93:THR:HG22	2:C:94:ARG:O	2.14	0.48
2:C:297:TYR:CD1	2:C:297:TYR:N	2.81	0.48
3:E:79:VAL:O	3:E:80:VAL:CB	2.62	0.48
2:B:297:TYR:CD1	2:B:297:TYR:N	2.81	0.47
3:D:79:VAL:O	3:D:80:VAL:CB	2.61	0.47
3:E:84:GLN:HG3	3:E:86:GLU:H	1.79	0.47
2:C:271:ILE:HD12	2:C:360:MET:HE2	1.96	0.47
2:C:181:THR:C	2:C:182:TYR:CD1	2.93	0.47
3:D:191:VAL:HG13	3:D:216:ASN:ND2	2.29	0.47
2:B:181:THR:C	2:B:182:TYR:CD1	2.93	0.47
2:C:177:ILE:HG12	2:C:227:LEU:CD2	2.44	0.47
2:B:177:ILE:HG12	2:B:227:LEU:CD2	2.44	0.47
3:E:93:ARG:O	3:E:96:GLN:HG3	2.15	0.47
3:E:111:LYS:CB	3:E:116:LEU:H	2.26	0.47
1:A:180:GLN:O	1:A:182:GLN:NE2	2.47	0.47
3:D:84:GLN:HG3	3:D:86:GLU:H	1.80	0.47
3:E:191:VAL:HG13	3:E:216:ASN:ND2	2.29	0.47
1:A:235:MET:O	1:A:239:LYS:HG2	2.14	0.47
2:B:93:THR:OG1	3:D:129:PHE:HE2	1.98	0.47
2:C:88:VAL:O	2:C:89:PRO:C	2.58	0.47
2:C:185:LEU:HD12	2:C:185:LEU:N	2.30	0.47
3:D:80:VAL:N	3:D:85:ILE:HG21	2.29	0.47
3:D:175:ASP:OD2	3:D:308:ARG:NH2	2.45	0.47
3:E:301:ASP:O	3:E:305:ILE:HD13	2.14	0.47
1:A:290:GLU:HB2	1:A:292:ASP:OD1	2.15	0.47
2:C:88:VAL:N	2:C:89:PRO:HD3	2.29	0.47
3:D:104:VAL:HG13	3:D:182:VAL:O	2.15	0.47
3:E:158:HIS:HB3	3:E:217:LYS:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:93:ARG:O	3:D:96:GLN:HG3	2.15	0.47
3:E:86:GLU:O	3:E:88:THR:N	2.48	0.47
3:E:104:VAL:HG13	3:E:182:VAL:O	2.15	0.47
1:A:100:ASN:C	1:A:100:ASN:ND2	2.71	0.47
2:B:271:ILE:HD12	2:B:360:MET:HE2	1.96	0.47
2:B:210:MET:HE2	3:D:198:LEU:HD11	1.96	0.46
2:C:319:GLY:O	2:C:320:ASN:C	2.58	0.46
3:D:36:ASN:HA	3:D:110:PHE:HA	1.97	0.46
3:D:86:GLU:O	3:D:88:THR:N	2.48	0.46
3:D:158:HIS:HB3	3:D:217:LYS:HD3	1.96	0.46
3:E:36:ASN:HA	3:E:110:PHE:HA	1.98	0.46
2:B:282:ASP:HA	2:B:353:GLY:O	2.16	0.46
2:B:311:LYS:C	2:B:313:LYS:N	2.73	0.46
2:B:185:LEU:HD12	2:B:185:LEU:N	2.30	0.46
2:C:280:TYR:HA	2:C:284:GLU:OE2	2.16	0.46
2:C:210:MET:HE2	3:E:198:LEU:HD11	1.96	0.46
2:C:260:PHE:HB3	2:C:263:LEU:HD12	1.97	0.46
3:E:177:GLN:NE2	3:E:308:ARG:NH1	2.64	0.46
2:C:92:PHE:HD1	3:E:133:ARG:CD	2.18	0.46
3:D:301:ASP:O	3:D:305:ILE:HD13	2.14	0.46
1:A:265:ILE:HD12	1:A:288:ILE:HD11	1.98	0.46
2:B:66:VAL:N	2:B:67:PRO:CD	2.78	0.46
2:C:311:LYS:C	2:C:313:LYS:N	2.73	0.46
2:B:163:HIS:ND1	2:B:166:ASP:OD1	2.46	0.46
2:B:319:GLY:O	2:B:320:ASN:C	2.58	0.46
2:B:260:PHE:HB3	2:B:263:LEU:HD12	1.97	0.45
2:B:280:TYR:HA	2:B:284:GLU:OE2	2.16	0.45
2:C:66:VAL:HG12	2:C:68:VAL:H	1.80	0.45
2:C:163:HIS:ND1	2:C:166:ASP:OD1	2.46	0.45
2:C:282:ASP:HA	2:C:353:GLY:O	2.16	0.45
3:D:84:GLN:HG3	3:D:85:ILE:H	1.81	0.45
3:D:177:GLN:NE2	3:D:308:ARG:NH1	2.64	0.45
3:E:280:ARG:O	3:E:284:LEU:HD13	2.17	0.45
3:E:317:LYS:HB2	3:E:317:LYS:NZ	2.31	0.45
2:B:251:GLU:OE2	2:B:251:GLU:HA	2.16	0.45
2:C:90:SER:O	2:C:91:LYS:CB	2.65	0.45
3:D:338:SER:C	3:D:340:ASN:H	2.25	0.45
1:A:168:HIS:HE1	1:A:292:ASP:HB3	1.81	0.45
1:A:299:ALA:HB1	1:A:302:VAL:HB	1.98	0.45
2:B:13:LEU:CD1	2:C:29:LEU:HB3	2.45	0.45
2:B:295:SER:HA	2:B:362:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:295:SER:HA	2:C:362:VAL:HG23	1.98	0.45
2:C:297:TYR:O	2:C:333:TYR:HB2	2.17	0.45
3:D:317:LYS:HB2	3:D:317:LYS:NZ	2.31	0.45
2:B:143:GLN:HE21	2:B:143:GLN:HB2	1.58	0.45
3:D:156:TYR:HD2	3:D:157:LEU:HD12	1.80	0.45
3:E:84:GLN:HG3	3:E:85:ILE:H	1.81	0.45
2:B:109:GLU:O	2:B:111:ASP:CG	2.60	0.45
2:C:206:GLU:OE1	3:E:244:ILE:HD13	2.16	0.45
3:D:94:ILE:O	3:D:98:VAL:HG22	2.17	0.45
1:A:100:ASN:ND2	1:A:102:LYS:H	2.14	0.45
1:A:263:TYR:CE1	1:A:287:VAL:HG11	2.48	0.45
2:C:345:ARG:HG3	2:C:345:ARG:NH1	2.30	0.45
3:E:35:GLN:HA	3:E:350:PHE:O	2.16	0.45
3:E:338:SER:C	3:E:340:ASN:N	2.74	0.45
2:B:206:GLU:OE1	3:D:244:ILE:HD13	2.16	0.45
2:C:109:GLU:O	2:C:111:ASP:CG	2.60	0.45
2:B:107:GLU:O	2:B:107:GLU:CG	2.62	0.45
3:E:338:SER:C	3:E:340:ASN:H	2.25	0.45
2:B:300:GLU:HG2	2:B:356:LYS:O	2.17	0.44
2:B:345:ARG:HG3	2:B:345:ARG:NH1	2.30	0.44
3:E:80:VAL:N	3:E:85:ILE:HG21	2.29	0.44
2:C:251:GLU:HA	2:C:251:GLU:OE2	2.16	0.44
3:E:65:SER:CB	3:E:67:ASN:ND2	2.81	0.44
2:C:300:GLU:HG2	2:C:356:LYS:O	2.17	0.44
2:B:175:TYR:O	2:B:203:SER:HA	2.18	0.44
3:D:338:SER:C	3:D:340:ASN:N	2.75	0.44
3:D:342:LYS:C	3:D:344:GLY:N	2.76	0.44
2:B:297:TYR:O	2:B:333:TYR:HB2	2.17	0.44
3:D:128:MET:HG2	3:D:169:PRO:HA	2.00	0.44
1:A:220:THR:OG1	1:A:222:LYS:HE3	2.18	0.44
1:A:263:TYR:HE1	1:A:291:LYS:HB3	1.83	0.44
2:C:177:ILE:HA	2:C:227:LEU:CD2	2.37	0.44
2:C:308:ILE:HG23	2:C:308:ILE:O	2.18	0.44
3:D:35:GLN:HA	3:D:350:PHE:O	2.16	0.44
3:D:65:SER:CB	3:D:67:ASN:ND2	2.81	0.44
3:D:112:ASP:C	3:D:114:SER:N	2.65	0.43
3:E:167:LEU:O	3:E:168:LYS:HB3	2.18	0.43
2:C:289:GLN:HG3	2:C:346:ALA:O	2.18	0.43
3:E:16:LYS:H	3:E:16:LYS:CD	2.26	0.43
3:E:156:TYR:HD2	3:E:157:LEU:HD12	1.80	0.43
1:A:100:ASN:HD21	1:A:102:LYS:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:THR:HB	2:B:223:SER:CA	2.49	0.43
2:C:175:TYR:O	2:C:203:SER:HA	2.18	0.43
3:D:103:LEU:HD12	3:D:182:VAL:HB	2.01	0.43
3:D:195:THR:C	3:D:196:TRP:CD1	2.96	0.43
3:E:195:THR:C	3:E:196:TRP:CD1	2.96	0.43
2:B:289:GLN:HG3	2:B:346:ALA:O	2.18	0.43
2:C:92:PHE:CE1	3:E:133:ARG:O	2.71	0.43
3:E:94:ILE:O	3:E:98:VAL:HG22	2.17	0.43
1:A:245:GLU:HB2	1:A:248:LEU:HG	1.99	0.43
3:D:280:ARG:O	3:D:284:LEU:HD13	2.17	0.43
3:E:128:MET:HG2	3:E:169:PRO:HA	2.00	0.43
1:A:303:ARG:O	1:A:306:LYS:HB3	2.19	0.43
2:B:308:ILE:O	2:B:308:ILE:HG23	2.18	0.43
3:E:83:LYS:O	3:E:83:LYS:HD3	2.19	0.43
2:B:66:VAL:N	2:B:67:PRO:HD2	2.34	0.43
2:B:180:GLY:N	2:B:200:ASN:OD1	2.50	0.43
2:B:294:ASP:O	2:B:362:VAL:HG23	2.18	0.43
2:C:294:ASP:O	2:C:362:VAL:HG23	2.18	0.43
3:D:90:ASN:C	3:D:90:ASN:ND2	2.77	0.43
2:C:107:GLU:O	2:C:107:GLU:CG	2.62	0.42
2:C:180:GLY:N	2:C:200:ASN:OD1	2.50	0.42
3:D:91:GLU:O	3:D:95:LEU:HD23	2.20	0.42
2:C:172:ASP:HA	2:C:232:ARG:HH12	1.84	0.42
3:D:167:LEU:O	3:D:168:LYS:HB3	2.19	0.42
3:E:91:GLU:O	3:E:95:LEU:CD2	2.67	0.42
2:B:308:ILE:CB	2:B:325:ILE:HD11	2.48	0.42
2:B:142:ASP:OD2	2:B:145:GLN:NE2	2.52	0.42
2:B:172:ASP:HA	2:B:232:ARG:HH12	1.84	0.42
2:B:322:GLU:HA	2:B:322:GLU:OE1	2.20	0.42
3:D:346:GLU:C	3:D:348:THR:H	2.27	0.42
3:D:36:ASN:HD22	3:D:111:LYS:H	1.67	0.42
1:A:290:GLU:N	1:A:292:ASP:CA	2.73	0.42
2:C:160:THR:HB	2:C:223:SER:CA	2.49	0.42
3:D:13:GLU:N	3:D:16:LYS:HD3	2.35	0.42
3:D:83:LYS:O	3:D:83:LYS:HD3	2.19	0.42
3:E:175:ASP:OD2	3:E:308:ARG:NH2	2.45	0.42
3:E:341:GLU:CD	3:E:341:GLU:N	2.78	0.42
3:E:346:GLU:C	3:E:348:THR:H	2.27	0.42
2:B:148:GLN:HE21	2:B:148:GLN:HB3	1.65	0.42
3:E:36:ASN:HD22	3:E:111:LYS:H	1.67	0.42
3:E:203:GLU:OE2	3:E:239:PHE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:PRO:HG2	2:B:106:ASP:H	1.85	0.42
2:B:245:LYS:HE3	2:B:245:LYS:HB2	1.95	0.42
3:D:156:TYR:HD2	3:D:157:LEU:CD1	2.33	0.42
3:E:90:ASN:C	3:E:90:ASN:ND2	2.77	0.42
1:A:293:ARG:NH1	1:A:298:ASP:OD1	2.50	0.42
2:C:322:GLU:OE1	2:C:322:GLU:HA	2.20	0.42
3:D:91:GLU:O	3:D:95:LEU:CD2	2.68	0.42
2:C:105:PRO:HG2	2:C:106:ASP:H	1.85	0.41
2:C:278:LYS:C	2:C:279:ILE:HD12	2.45	0.41
3:D:229:TYR:CD1	3:D:229:TYR:C	2.98	0.41
2:B:206:GLU:CD	2:B:206:GLU:H	2.28	0.41
2:C:142:ASP:OD2	2:C:145:GLN:NE2	2.52	0.41
3:D:305:ILE:CD1	3:D:310:VAL:HG21	2.50	0.41
3:E:103:LEU:HD12	3:E:182:VAL:HB	2.01	0.41
3:E:156:TYR:HD2	3:E:157:LEU:CD1	2.33	0.41
3:E:173:LEU:HD13	3:E:183:THR:CG2	2.51	0.41
2:C:108:GLU:H	2:C:108:GLU:HG3	1.45	0.41
3:D:203:GLU:OE2	3:D:239:PHE:HA	2.19	0.41
3:E:92:LYS:HD2	3:E:92:LYS:C	2.45	0.41
3:D:341:GLU:N	3:D:341:GLU:CD	2.78	0.41
3:E:91:GLU:O	3:E:95:LEU:HD23	2.19	0.41
1:A:298:ASP:HB3	1:A:300:GLU:CD	2.45	0.41
2:B:95:ARG:NE	3:D:170:GLU:OE1	2.53	0.41
2:C:308:ILE:CB	2:C:325:ILE:HD11	2.48	0.41
3:D:92:LYS:HD2	3:D:92:LYS:C	2.45	0.41
3:E:13:GLU:N	3:E:16:LYS:HD3	2.35	0.41
2:B:371:PRO:HG2	2:B:374:ASP:OD2	2.21	0.41
3:D:236:PRO:HG2	3:D:239:PHE:HB2	2.02	0.41
3:E:317:LYS:HB2	3:E:317:LYS:HZ2	1.85	0.41
2:B:10:LEU:HA	2:C:29:LEU:CD1	2.51	0.41
2:B:177:ILE:HA	2:B:227:LEU:CD2	2.37	0.41
3:D:16:LYS:H	3:D:16:LYS:CD	2.26	0.41
3:E:96:GLN:HE21	3:E:96:GLN:HB2	1.67	0.41
3:E:288:VAL:HG22	3:E:288:VAL:O	2.21	0.41
2:C:143:GLN:HE21	2:C:143:GLN:HB2	1.58	0.41
1:A:100:ASN:HD22	1:A:101:LYS:N	2.18	0.41
1:A:140:LEU:HD13	1:A:146:VAL:HA	2.02	0.41
1:A:263:TYR:CE1	1:A:291:LYS:HB3	2.56	0.41
2:C:206:GLU:CD	2:C:206:GLU:H	2.28	0.41
3:E:229:TYR:CD1	3:E:229:TYR:C	2.98	0.41
3:E:236:PRO:HG2	3:E:239:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:173:LEU:HD13	3:D:183:THR:CG2	2.51	0.41
3:D:242:GLN:HA	3:D:243:PRO:HD3	1.95	0.41
3:E:305:ILE:CD1	3:E:310:VAL:HG21	2.50	0.41
2:B:278:LYS:C	2:B:279:ILE:HD12	2.45	0.40
2:C:56:THR:O	2:C:57:THR:HG23	2.20	0.40
2:C:171:GLY:CA	2:C:215:ARG:NH1	2.84	0.40
2:C:336:GLU:CD	2:C:336:GLU:H	2.28	0.40
2:C:339:LEU:HD23	2:C:362:VAL:HG13	2.03	0.40
2:C:371:PRO:HG2	2:C:374:ASP:OD2	2.21	0.40
3:D:30:TRP:HZ3	3:D:94:ILE:HG12	1.86	0.40
3:D:205:LEU:HD12	3:D:247:TYR:CE1	2.56	0.40
3:D:196:TRP:CD1	3:D:196:TRP:N	2.90	0.40
3:E:317:LYS:NZ	3:E:317:LYS:CB	2.85	0.40
1:A:290:GLU:N	1:A:292:ASP:CB	2.82	0.40
2:C:188:LYS:O	2:C:189:ASP:HB2	2.20	0.40
3:E:103:LEU:HG	3:E:185:PHE:HZ	1.86	0.40
3:E:112:ASP:C	3:E:114:SER:N	2.65	0.40
3:E:342:LYS:C	3:E:344:GLY:N	2.76	0.40
2:B:188:LYS:O	2:B:189:ASP:HB2	2.21	0.40
2:C:245:LYS:HE3	2:C:245:LYS:HB2	1.95	0.40
2:C:277:GLU:HG2	2:C:358:LEU:HD23	2.04	0.40
3:E:85:ILE:C	3:E:85:ILE:CD1	2.91	0.40
3:E:196:TRP:CD1	3:E:196:TRP:N	2.90	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	229/353 (65%)	223 (97%)	6 (3%)	0	100	100
2	B	378/402 (94%)	349 (92%)	17 (4%)	12 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	378/402 (94%)	351 (93%)	16 (4%)	11 (3%)	3	23
3	D	321/351 (92%)	277 (86%)	28 (9%)	16 (5%)	1	16
3	E	321/351 (92%)	277 (86%)	28 (9%)	16 (5%)	1	16
All	All	1627/1859 (88%)	1477 (91%)	95 (6%)	55 (3%)	4	21

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	109	GLU
2	B	310	SER
2	B	314	SER
2	B	317	ASN
2	B	319	GLY
2	C	109	GLU
2	C	310	SER
2	C	314	SER
2	C	317	ASN
2	C	319	GLY
3	D	79	VAL
3	D	112	ASP
3	D	115	ASN
3	D	343	CYS
3	E	79	VAL
3	E	112	ASP
3	E	115	ASN
3	E	343	CYS
2	B	393	SER
2	C	393	SER
3	D	36	ASN
3	D	80	VAL
3	D	113	ASN
3	D	337	VAL
3	E	36	ASN
3	E	80	VAL
3	E	113	ASN
3	E	337	VAL
2	B	110	GLU
2	B	315	ASN
2	B	321	GLN
2	C	110	GLU
2	C	315	ASN

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Mol	Chain	Res	Type
2	C	321	GLN
3	D	46	ILE
3	D	116	LEU
3	E	46	ILE
3	E	116	LEU
3	D	45	ARG
3	D	63	LYS
3	D	87	HIS
3	D	216	ASN
3	D	346	GLU
3	E	45	ARG
3	E	63	LYS
3	E	87	HIS
3	E	216	ASN
3	E	346	GLU
2	B	89	PRO
2	C	55	PRO
3	D	339	ILE
3	E	339	ILE
2	B	55	PRO
2	C	87	PRO
2	B	67	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	202/302 (67%)	196 (97%)	6 (3%)	36	57
2	B	330/357 (92%)	310 (94%)	20 (6%)	17	38
2	C	330/357 (92%)	311 (94%)	19 (6%)	18	40
3	D	240/306 (78%)	221 (92%)	19 (8%)	11	32
3	E	240/306 (78%)	221 (92%)	19 (8%)	11	32
All	All	1342/1628 (82%)	1259 (94%)	83 (6%)	18	38

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	198	LEU
1	A	232	LYS
1	A	243	LYS
1	A	254	ASP
1	A	304	LEU
2	B	95	ARG
2	B	101	GLU
2	B	107	GLU
2	B	108	GLU
2	B	110	GLU
2	B	143	GLN
2	B	161	ASP
2	B	194	SER
2	B	197	GLN
2	B	206	GLU
2	B	215	ARG
2	B	231	ASP
2	B	241	LYS
2	B	259	LEU
2	B	292	LYS
2	B	336	GLU
2	B	345	ARG
2	B	354	ASP
2	B	384	GLU
2	B	386	GLN
2	C	101	GLU
2	C	107	GLU
2	C	108	GLU
2	C	110	GLU
2	C	143	GLN
2	C	161	ASP
2	C	194	SER
2	C	197	GLN
2	C	206	GLU
2	C	215	ARG
2	C	231	ASP
2	C	241	LYS
2	C	259	LEU
2	C	292	LYS
2	C	336	GLU
2	C	345	ARG
2	C	354	ASP

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Mol	Chain	Res	Type
2	C	384	GLU
2	C	386	GLN
3	D	15	VAL
3	D	17	GLU
3	D	31	GLU
3	D	87	HIS
3	D	95	LEU
3	D	96	GLN
3	D	103	LEU
3	D	128	MET
3	D	160	LEU
3	D	181	GLN
3	D	191	VAL
3	D	211	LEU
3	D	224	LEU
3	D	269	LEU
3	D	274	GLN
3	D	284	LEU
3	D	317	LYS
3	D	318	PHE
3	D	342	LYS
3	E	15	VAL
3	E	17	GLU
3	E	31	GLU
3	E	87	HIS
3	E	95	LEU
3	E	96	GLN
3	E	103	LEU
3	E	128	MET
3	E	160	LEU
3	E	181	GLN
3	E	191	VAL
3	E	211	LEU
3	E	224	LEU
3	E	269	LEU
3	E	274	GLN
3	E	284	LEU
3	E	317	LYS
3	E	318	PHE
3	E	342	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	112	ASN
1	A	132	HIS
1	A	174	HIS
1	A	182	GLN
1	A	193	HIS
1	A	277	ASN
1	A	311	ASN
2	B	46	GLN
2	B	59	HIS
2	B	124	GLN
2	B	143	GLN
2	B	145	GLN
2	B	148	GLN
2	B	173	ASN
2	B	197	GLN
2	B	327	HIS
2	C	15	GLN
2	C	25	GLN
2	C	124	GLN
2	C	143	GLN
2	C	145	GLN
2	C	148	GLN
2	C	173	ASN
2	C	197	GLN
2	C	327	HIS
3	D	35	GLN
3	D	36	ASN
3	D	39	GLN
3	D	62	HIS
3	D	67	ASN
3	D	96	GLN
3	D	171	ASN
3	D	176	GLN
3	D	177	GLN
3	D	181	GLN
3	D	216	ASN
3	D	245	GLN
3	D	289	ASN
3	D	293	ASN
3	D	340	ASN
3	E	35	GLN
3	E	36	ASN

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Mol	Chain	Res	Type
3	E	39	GLN
3	E	62	HIS
3	E	67	ASN
3	E	68	HIS
3	E	96	GLN
3	E	171	ASN
3	E	176	GLN
3	E	177	GLN
3	E	181	GLN
3	E	216	ASN
3	E	245	GLN
3	E	289	ASN
3	E	293	ASN
3	E	340	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

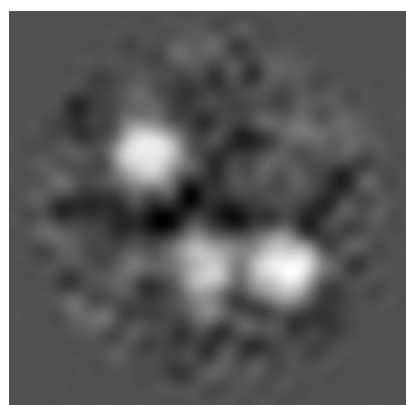
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5755. These allow visual inspection of the internal detail of the map and identification of artifacts.

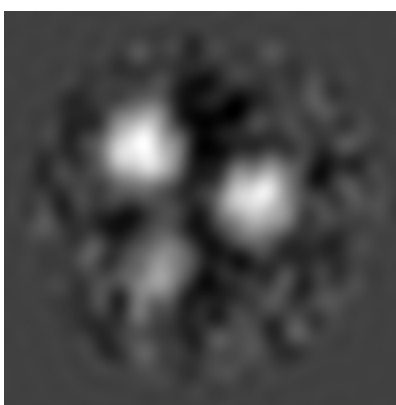
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

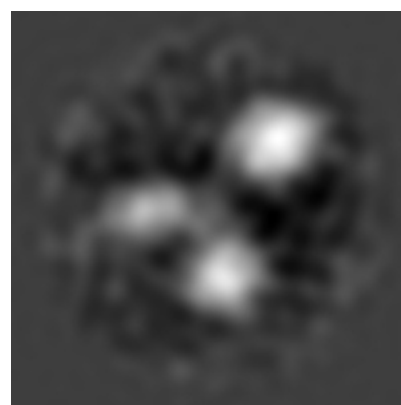
6.1.1 Primary map



X



Y

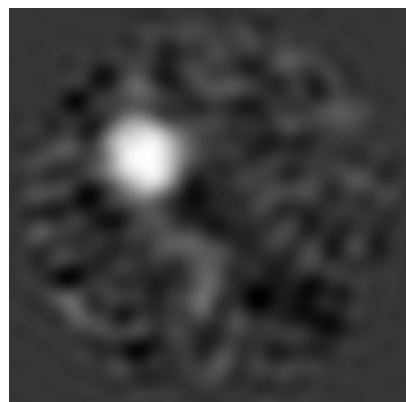


Z

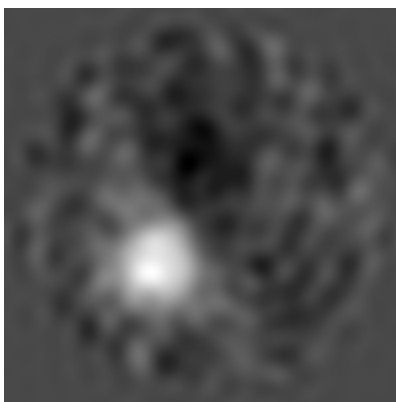
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

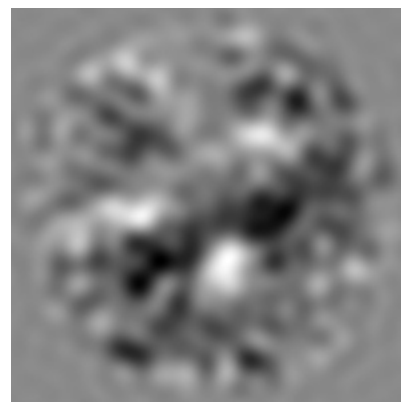
6.2.1 Primary map



X Index: 60



Y Index: 60

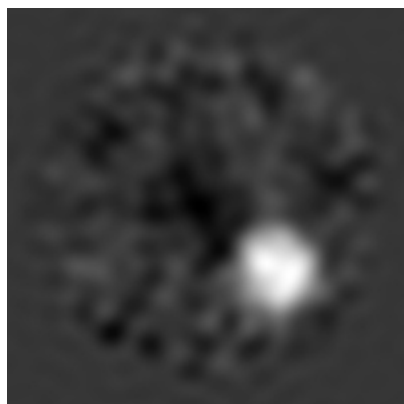


Z Index: 60

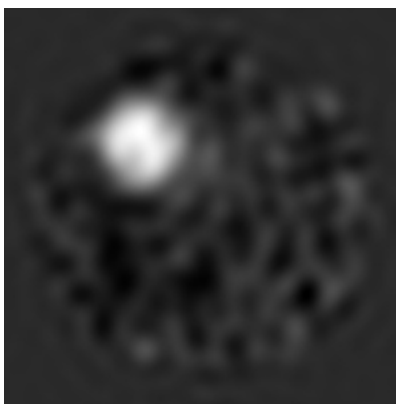
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

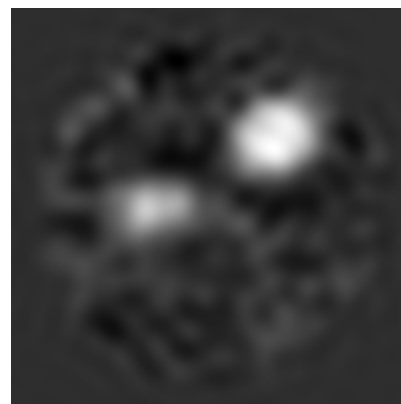
6.3.1 Primary map



X Index: 80



Y Index: 81

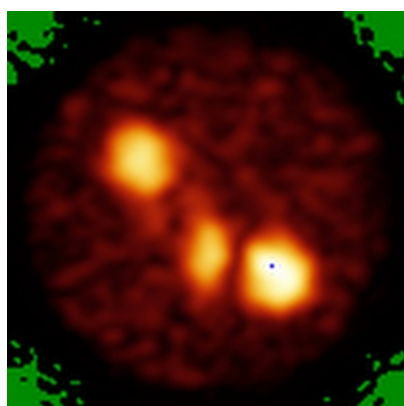


Z Index: 43

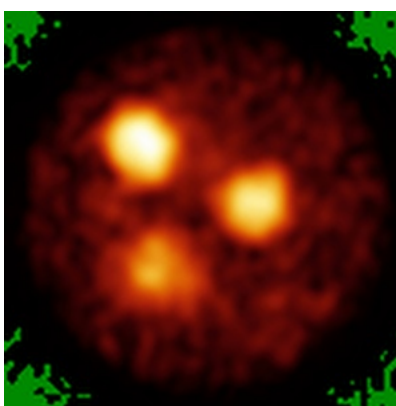
The images above show the largest variance slices of the map in three orthogonal directions.

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

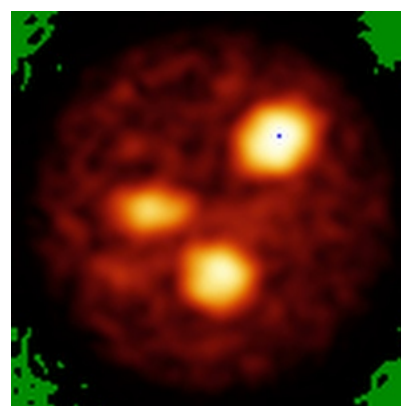
6.4.1 Primary map



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

This section was not generated.

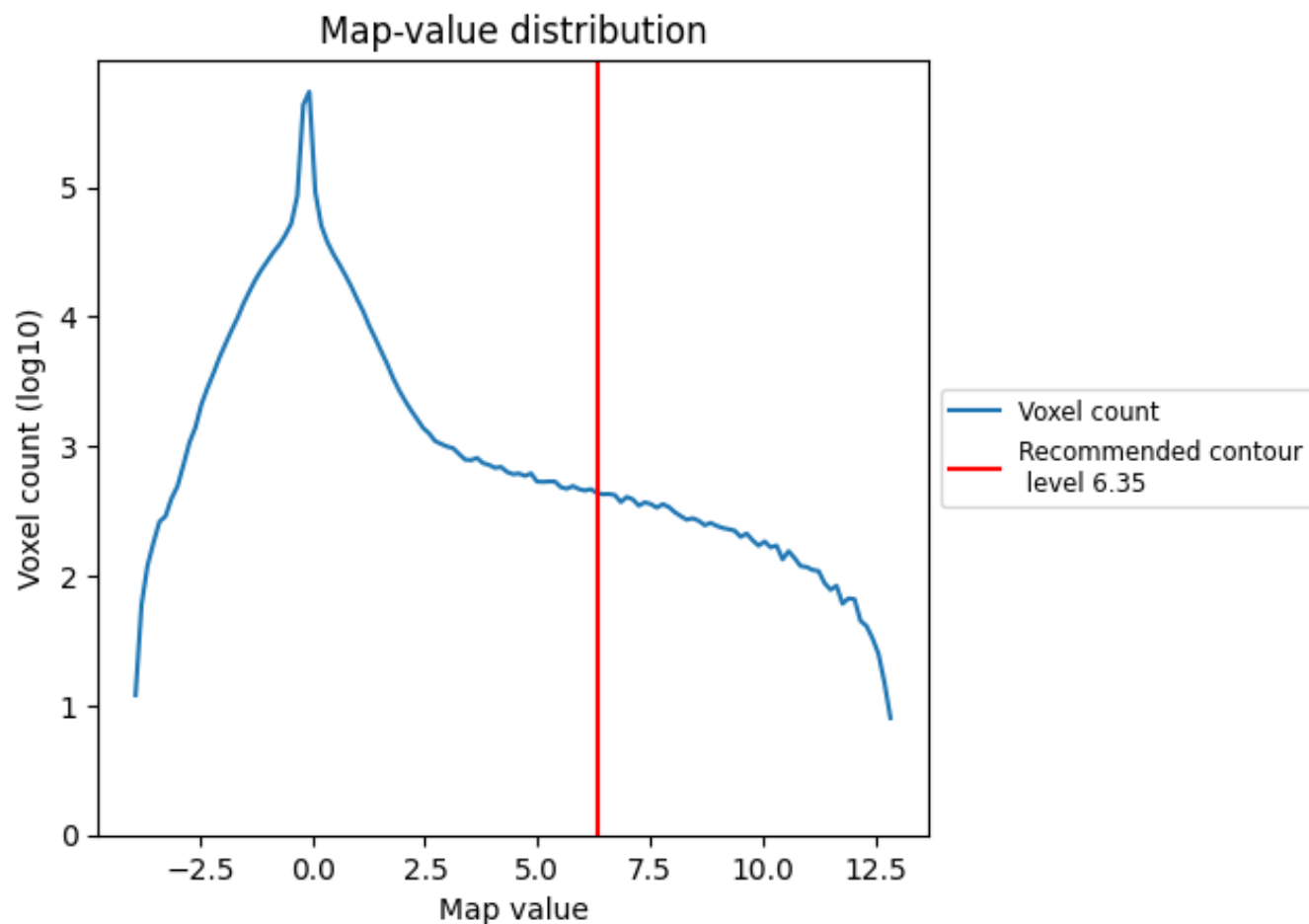
6.6 Mask visualisation

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

7 Map analysis [i](#)

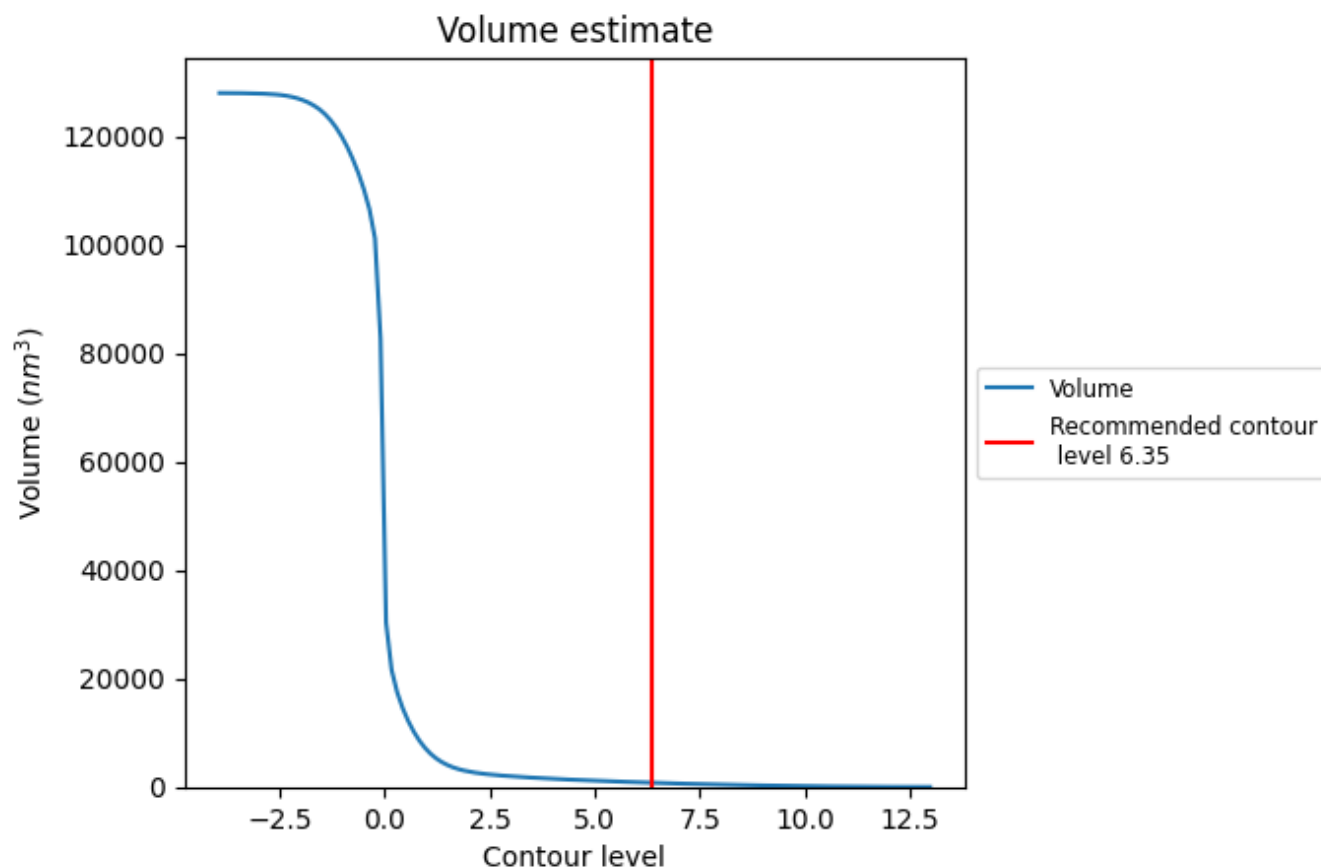
This section contains the results of statistical analysis of the map.

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.

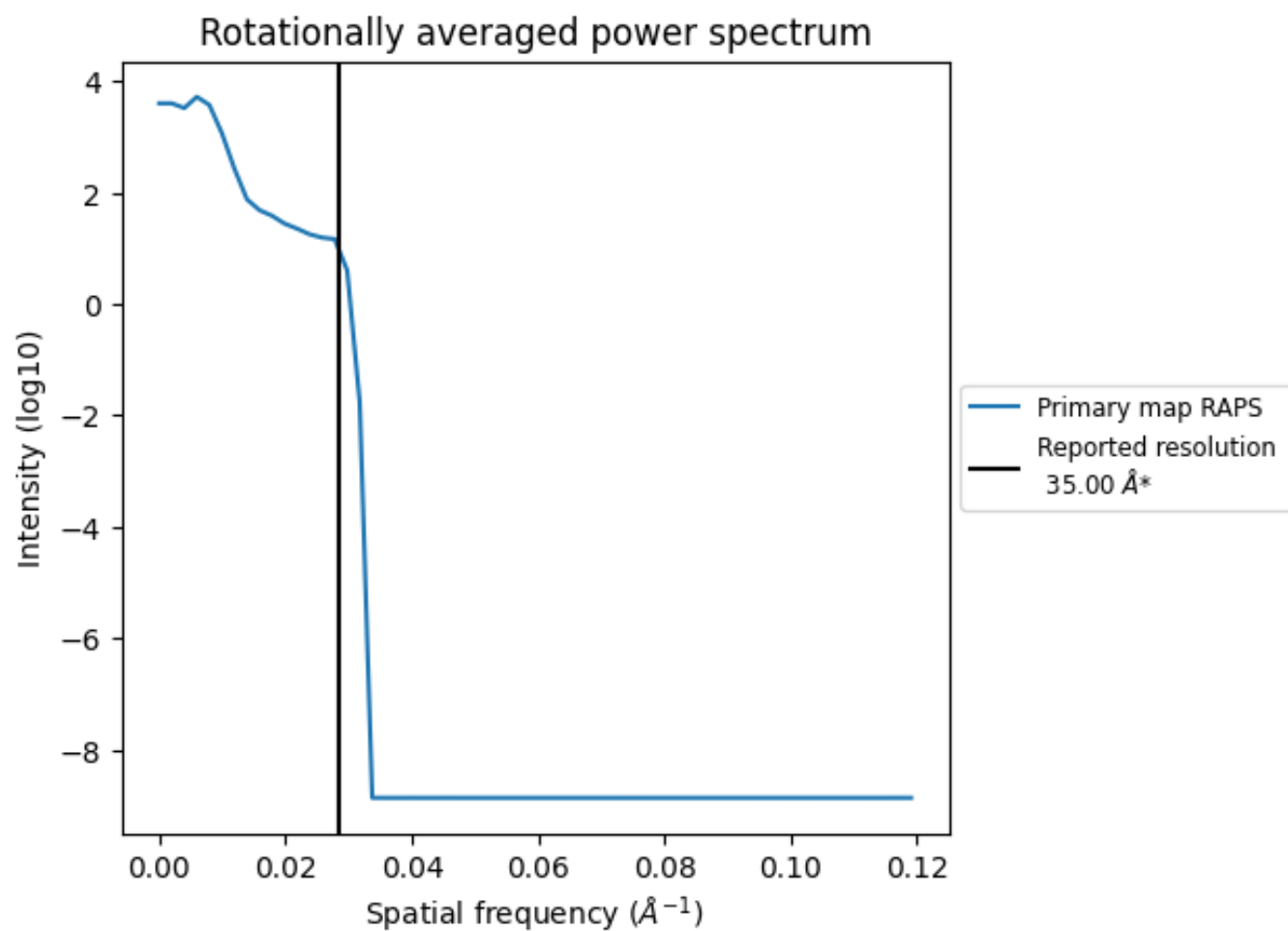
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 779 nm³; this corresponds to an approximate mass of 704 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 0.029 Å⁻¹

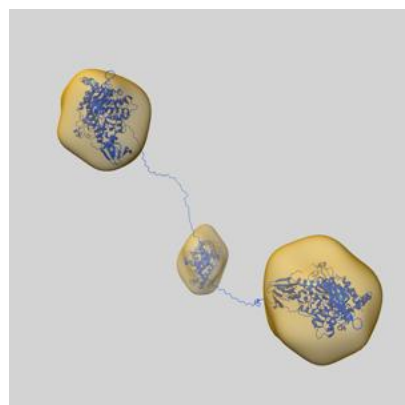
8 Fourier-Shell correlation ⓘ

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

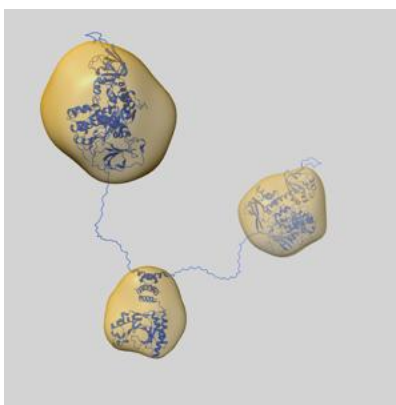
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5755 and PDB model 3J4Q. Per-residue inclusion information can be found in section [3](#) on page [5](#).

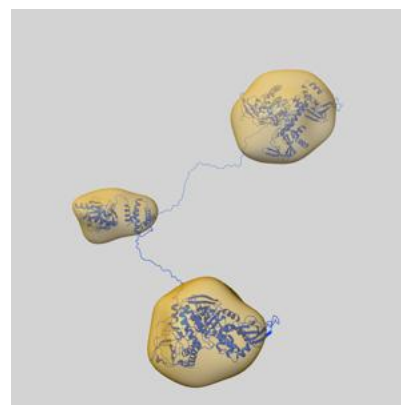
9.1 Map-model overlay [i](#)



X



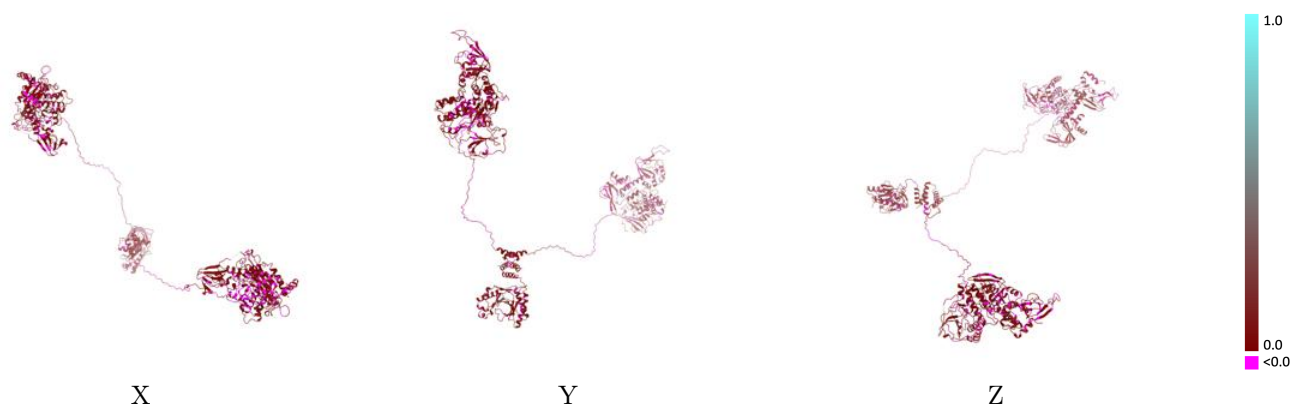
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

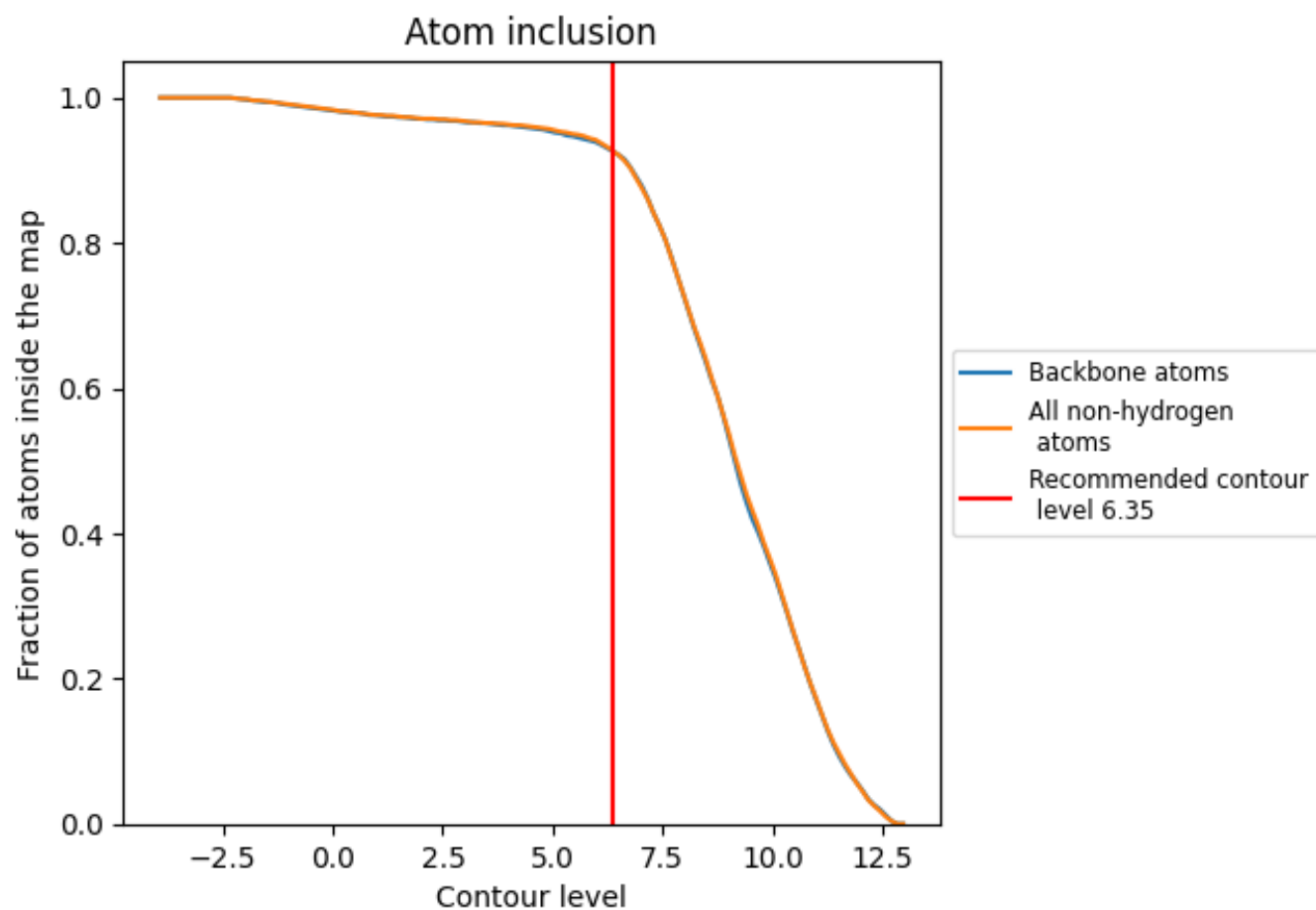


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (6.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9280	0.0500
A	0.9710	0.0680
B	0.8630	0.0440
C	0.8550	0.0410
D	0.9970	0.0400
E	0.9910	0.0630

