



## Full wwPDB EM Validation Report ⓘ

Feb 12, 2024 – 08:35 PM EST

PDB ID : 3J4Q  
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 : 2QVS, 2VFL, 2IZX

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

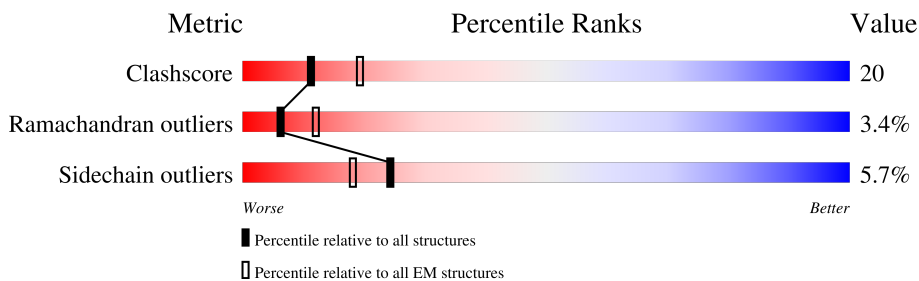
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	353	
2	B	402	
2	C	402	
3	D	351	
3	E	351	

## 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
			Total	C	N	O	S		
1	A	230	1836	1180	312	336	8	1	0

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

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

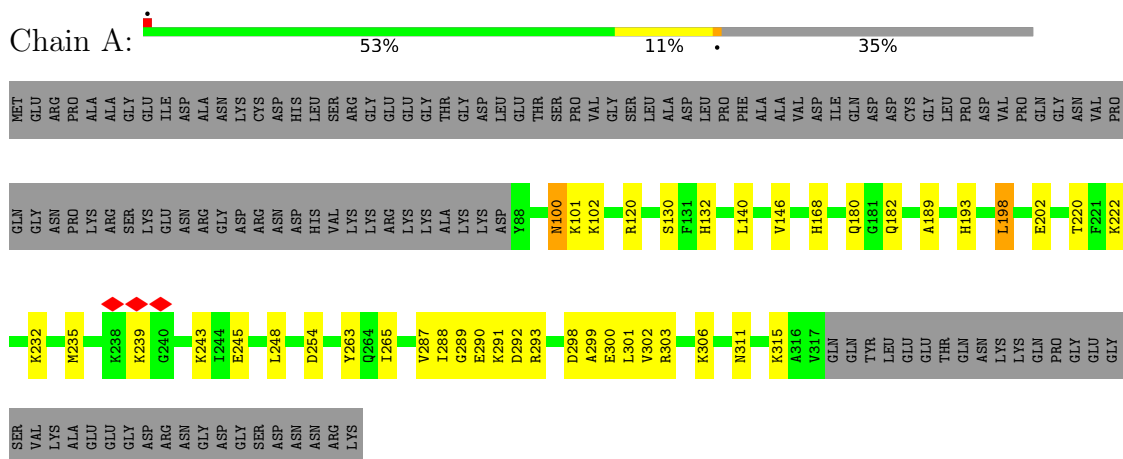
- Molecule 3 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

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

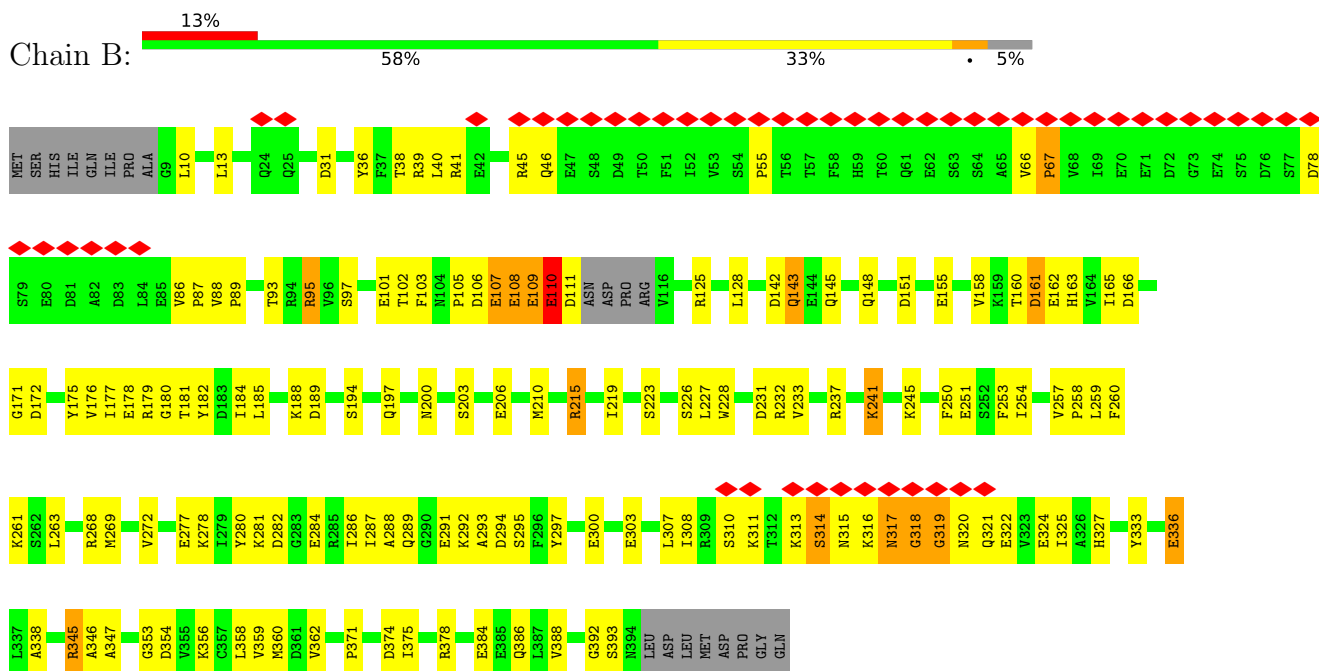
### 3 Residue-property plots

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.

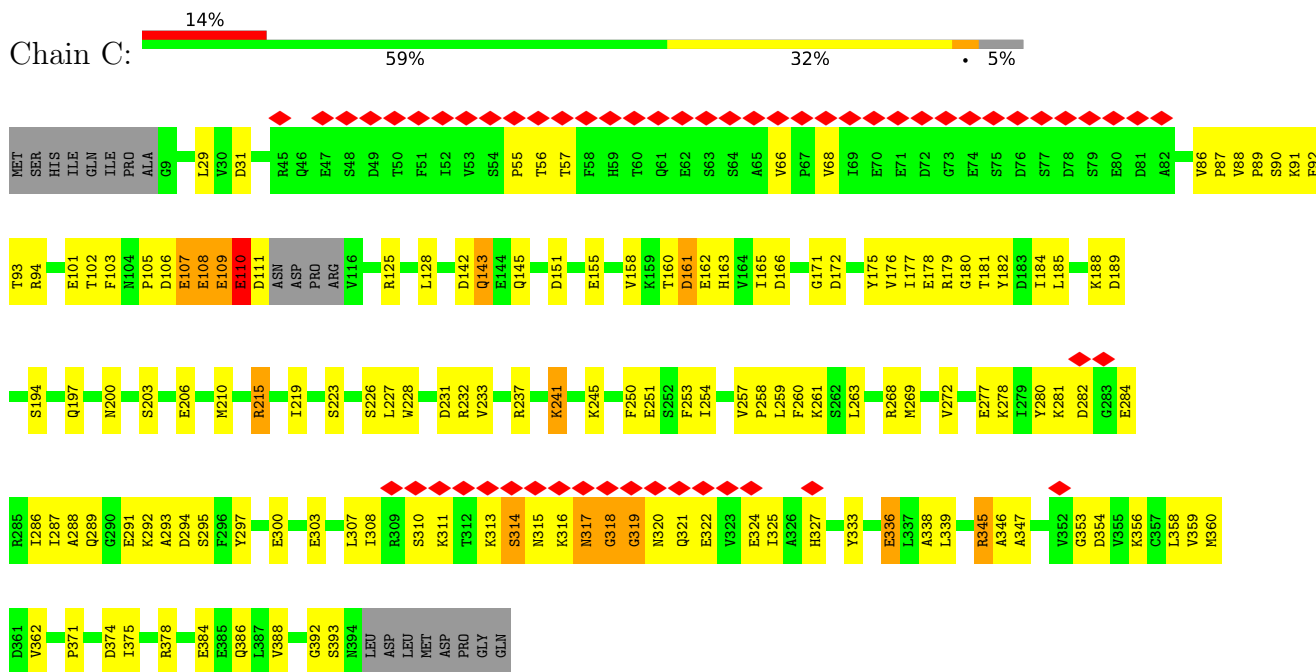
- Molecule 1: A-kinase anchor protein 18



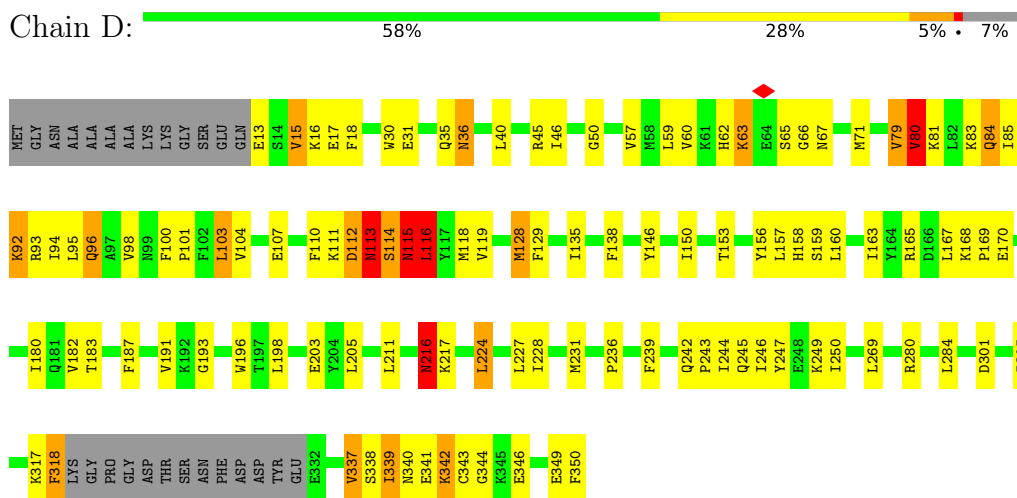
- Molecule 2: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 2: cAMP-dependent protein kinase type II-alpha regulatory subunit



• Molecule 3: cAMP-dependent protein kinase catalytic subunit alpha



• Molecule 3: cAMP-dependent protein kinase catalytic subunit alpha



K317	F318	LYS	GLY	PRO	GLY	ASP	THR	SER	ASN	PHE	ASP	ASP	TYR	GLU	E332	V337	S338	I339	N340	E341	K342	C343	G344	K345	E346	E349	F350
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## 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 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	0.50	0/1872	0.58	0/2518
2	B	0.51	1/3065 (0.0%)	0.72	9/4135 (0.2%)
2	C	0.48	0/3065	0.70	6/4135 (0.1%)
3	D	0.38	0/2581	0.80	14/3498 (0.4%)
3	E	0.38	0/2581	0.80	14/3498 (0.4%)
All	All	0.46	1/13164 (0.0%)	0.73	43/17784 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	87	PRO	N-CD	5.16	1.55	1.47

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	116	LEU	CA-C-O	11.08	143.37	120.10
3	E	116	LEU	CA-C-O	11.03	143.27	120.10
3	D	116	LEU	CA-C-N	-10.76	93.53	117.20
3	E	116	LEU	CA-C-N	-10.74	93.57	117.20
3	D	114	SER	CA-C-N	-9.82	95.59	117.20
3	E	114	SER	CA-C-N	-9.81	95.62	117.20
3	E	81	LYS	N-CA-CB	9.09	126.96	110.60
3	D	81	LYS	N-CA-CB	9.08	126.95	110.60
3	E	114	SER	CA-C-O	8.99	138.98	120.10
3	E	80	VAL	CB-CA-C	-8.97	94.35	111.40
3	D	80	VAL	CB-CA-C	-8.97	94.36	111.40
3	D	114	SER	CA-C-O	8.96	138.91	120.10
3	E	115	ASN	N-CA-C	8.83	134.83	111.00
3	D	115	ASN	N-CA-C	8.82	134.81	111.00
3	D	114	SER	CB-CA-C	8.06	125.42	110.10
3	E	114	SER	CB-CA-C	8.05	125.39	110.10
2	C	316	LYS	N-CA-C	7.68	131.73	111.00
2	B	316	LYS	N-CA-C	7.64	131.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	113	ASN	CB-CA-C	-7.54	95.32	110.40
3	E	113	ASN	CB-CA-C	-7.51	95.37	110.40
3	D	114	SER	N-CA-CB	6.72	120.58	110.50
3	E	114	SER	N-CA-CB	6.71	120.56	110.50
3	D	116	LEU	CB-CA-C	-6.70	97.47	110.20
3	E	116	LEU	CB-CA-C	-6.69	97.49	110.20
2	C	316	LYS	CB-CA-C	-6.38	97.65	110.40
2	B	316	LYS	CB-CA-C	-6.34	97.72	110.40
3	D	115	ASN	CB-CA-C	-6.24	97.91	110.40
3	E	115	ASN	CB-CA-C	-6.24	97.92	110.40
2	B	88	VAL	C-N-CD	6.19	141.41	128.40
3	D	81	LYS	CA-C-N	-6.15	103.67	117.20
3	E	81	LYS	CA-C-N	-6.15	103.68	117.20
2	B	86	VAL	C-N-CD	5.68	140.34	128.40
2	C	317	ASN	CA-C-N	-5.35	105.51	116.20
2	B	317	ASN	CA-C-N	-5.33	105.54	116.20
2	C	318	GLY	N-CA-C	5.19	126.08	113.10
2	B	31	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	318	GLY	N-CA-C	5.17	126.02	113.10
2	B	39	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	C	31	ASP	CB-CG-OD2	5.15	122.93	118.30
2	C	317	ASN	CA-C-O	5.08	130.76	120.10
2	B	317	ASN	CA-C-O	5.07	130.74	120.10
3	E	81	LYS	CA-C-O	5.05	130.70	120.10
3	D	81	LYS	CA-C-O	5.03	130.65	120.10

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	1836	0	1893	56	0
2	B	3018	0	2929	127	0
2	C	3018	0	2929	122	0
3	D	2517	0	2349	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2517	0	2349	116	0
All	All	12906	0	12449	511	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 20.

All (511) 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
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
1:A:289:GLY:C	1:A:291:LYS:HA	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:113:ASN:HA	3:D:341:GLU:HA	1.74	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:E:135:ILE:HD11	3:E:138:PHE:CE1	2.29	0.67
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
3:E:86:GLU:C	3:E:88:THR:H	1.99	0.66
1:A:263:TYR:CE1	1:A:287:VAL:CG1	2.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:GLU:C	3:D:88:THR:H	1.99	0.65
3:D:62:HIS:HB3	3:D:67:ASN:H	1.61	0.65
3:E:112:ASP:C	3:E:114:SER:H	1.99	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
3:D:112:ASP:C	3:D:114:SER:H	1.99	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:C:103:PHE:HZ	2:C:241:LYS:HZ3	1.46	0.64
3:E:128:MET:HA	3:E:128:MET:HE3	1.79	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
1:A:168:HIS:CE1	1:A:292:ASP:HB3	2.34	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:18:PHE:HE2	3:D:306:TYR:HH	1.48	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
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
2:C:109:GLU:O	2:C:110:GLU:C	2.40	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
2:B:109:GLU:O	2:B:110:GLU:C	2.40	0.59
2:C:237:ARG:HH21	2:C:237:ARG:CB	2.15	0.59
1:A:100:ASN:C	1:A:100:ASN:HD22	2.06	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
3:D:156:TYR:CD2	3:D:157:LEU:HD12	2.38	0.59
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
3:E:85:ILE:C	3:E:85:ILE:HD12	2.24	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:D:85:ILE:HD12	3:D:85:ILE:C	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
2:C:102:THR:HG22	2:C:103:PHE:N	2.21	0.56
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
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
1:A:290:GLU:H	1:A:292:ASP:CG	2.09	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: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
3:D:86:GLU:C	3:D:88:THR:N	2.60	0.55
3:D:224:LEU:HD22	3:D:228:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:94:ARG:HG3	3:E:129:PHE:CE2	2.42	0.54
3:D:50:GLY:HA3	3:D:57:VAL:O	2.08	0.54
3:E:35:GLN:O	3:E:36:ASN:C	2.46	0.54
3:E:18:PHE:HE2	3:E:306:TYR:HH	1.56	0.54
2:C:278:LYS:HZ3	2:C:359:VAL:HG21	1.72	0.54
3:D:35:GLN:O	3:D:36:ASN:C	2.46	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
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
3:D:318:PHE:HD1	3:D:318:PHE:O	1.90	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:342:LYS:C	3:D:344:GLY:H	2.11	0.53
3:E:86:GLU:C	3:E:88:THR:N	2.60	0.53
3:E:342:LYS:C	3:E:344:GLY:H	2.11	0.53
3:D:227:LEU:O	3:D:231:MET:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:184:ILE:C	2:C:185:LEU:HD12	2.30	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:281:LYS:O	2:C:284:GLU:HG2	2.10	0.52
2:B:184:ILE:C	2:B:185:LEU:HD12	2.30	0.52
2:B:281:LYS:O	2:B:284:GLU:HG2	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:E:112:ASP:C	3:E:114:SER:N	2.65	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:318:GLY:O	2:C:319:GLY:C	2.51	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
3:D:111:LYS:CB	3:D:116:LEU:H	2.26	0.49
2:B:278:LYS:HZ3	2:B:359:VAL:HG21	1.78	0.48
3:D:84:GLN:HG3	3:D:85:ILE:N	2.28	0.48
2:B:318:GLY:O	2:B:319:GLY:C	2.51	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:311:LYS:C	2:C:313:LYS:H	2.17	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
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
2:C:110:GLU:O	2:C:111:ASP:CG	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:191:VAL:HG13	3:D:216:ASN:ND2	2.29	0.47
2:B:110:GLU:O	2:B:111:ASP:CG	2.53	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: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
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
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:H	2.17	0.46
3:D:112:ASP:C	3:D:114:SER:N	2.65	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: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:B:210:MET:HE2	3:D:198:LEU:HD11	1.98	0.46
2:B:163:HIS:ND1	2:B:166:ASP:OD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:210:MET:HE3	3:E:210:ILE:HG23	1.98	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
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
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:110:GLU:H	2:B:110:GLU:CD	2.18	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: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
2:B:206:GLU:OE1	3:D:244:ILE:HD13	2.16	0.45
2:B:107:GLU:O	2:B:107:GLU:CG	2.62	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
2:C:110:GLU:H	2:C:110:GLU:CD	2.18	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:90:ASN:C	3:D:90:ASN:HD22	2.19	0.44
2:B:297:TYR:O	2:B:333:TYR:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
2:C:181:THR:C	2:C:182:TYR:CD1	2.93	0.43
2:C:107:GLU:O	2:C:107:GLU:CG	2.62	0.42
2:C:210:MET:HE2	3:E:198:LEU:HD11	2.01	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
3:E:90:ASN:C	3:E:90:ASN:HD22	2.19	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:C:88:VAL:O	2:C:89:PRO:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:THR:C	2:B:182:TYR:CD1	2.93	0.42
2:B:322:GLU:HA	2:B:322:GLU:OE1	2.20	0.42
1:A:100:ASN:C	1:A:100:ASN:ND2	2.71	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
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
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
2:C:319:GLY:O	2:C:320:ASN:C	2.58	0.42
3:D:156:TYR:HD2	3:D:157:LEU:CD1	2.33	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:B:311:LYS:C	2:B:313:LYS:N	2.73	0.41
2:C:105:PRO:HG2	2:C:106:ASP:H	1.85	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:91:GLU:O	3:E:95:LEU:HD23	2.19	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: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
2:C:311:LYS:C	2:C:313:LYS:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:GLY:O	2:B:320:ASN:C	2.58	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
3:E:236:PRO:HG2	3:E:239:PHE:HB2	2.02	0.41
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:D:338:SER:C	3:D:340:ASN:H	2.25	0.41
3:E:305:ILE:CD1	3:E:310:VAL:HG21	2.50	0.41
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: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:E:338:SER:C	3:E:340:ASN:N	2.74	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:338:SER:C	3:E:340:ASN:H	2.25	0.40
2:B:109:GLU:O	2:B:111:ASP:CG	2.60	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: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%)	4	26
2	C	378/402 (94%)	351 (93%)	16 (4%)	11 (3%)	4	29
3	D	321/351 (92%)	277 (86%)	28 (9%)	16 (5%)	2	20
3	E	321/351 (92%)	277 (86%)	28 (9%)	16 (5%)	2	20
All	All	1627/1859 (88%)	1477 (91%)	95 (6%)	55 (3%)	6	26

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

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Mol	Chain	Res	Type
2	C	110	GLU
2	C	315	ASN
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 [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	202/302 (67%)	196 (97%)	6 (3%)	41	63
2	B	330/357 (92%)	311 (94%)	19 (6%)	20	45
2	C	330/357 (92%)	313 (95%)	17 (5%)	23	48
3	D	240/306 (78%)	223 (93%)	17 (7%)	14	39
3	E	240/306 (78%)	223 (93%)	17 (7%)	14	39
All	All	1342/1628 (82%)	1266 (94%)	76 (6%)	24	45



All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	120	ARG
1	A	198	LEU
1	A	232	LYS
1	A	243	LYS
1	A	254	ASP
2	B	78	ASP
2	B	95	ARG
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	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	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	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
2	C	384	GLU
2	C	386	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	D	15	VAL
3	D	17	GLU
3	D	31	GLU
3	D	84	GLN
3	D	87	HIS
3	D	90	ASN
3	D	92	LYS
3	D	96	GLN
3	D	103	LEU
3	D	128	MET
3	D	160	LEU
3	D	211	LEU
3	D	216	ASN
3	D	224	LEU
3	D	269	LEU
3	D	318	PHE
3	D	342	LYS
3	E	15	VAL
3	E	17	GLU
3	E	31	GLU
3	E	84	GLN
3	E	87	HIS
3	E	90	ASN
3	E	92	LYS
3	E	96	GLN
3	E	103	LEU
3	E	128	MET
3	E	160	LEU
3	E	211	LEU
3	E	216	ASN
3	E	224	LEU
3	E	269	LEU
3	E	318	PHE
3	E	342	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	100	ASN
1	A	112	ASN
1	A	132	HIS
1	A	139	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	174	HIS
1	A	193	HIS
1	A	311	ASN
2	B	46	GLN
2	B	124	GLN
2	B	129	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	B	386	GLN
2	C	25	GLN
2	C	124	GLN
2	C	129	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
2	C	386	GLN
3	D	35	GLN
3	D	36	ASN
3	D	39	GLN
3	D	62	HIS
3	D	67	ASN
3	D	90	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	289	ASN
3	D	293	ASN
3	E	35	GLN
3	E	36	ASN
3	E	39	GLN
3	E	62	HIS
3	E	67	ASN

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Mol	Chain	Res	Type
3	E	90	ASN
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	289	ASN
3	E	293	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 monosaccharides 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.

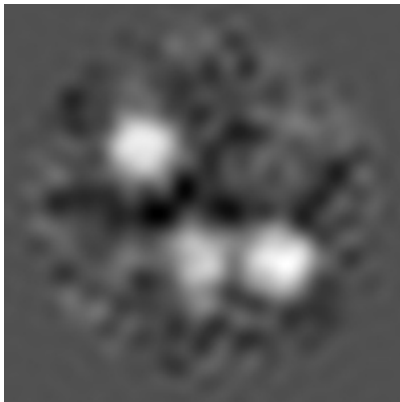
## 6 Map visualisation [i](#)

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.

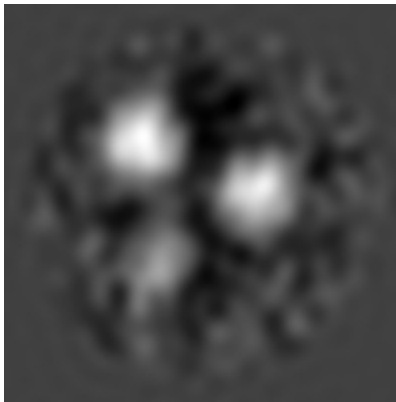
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

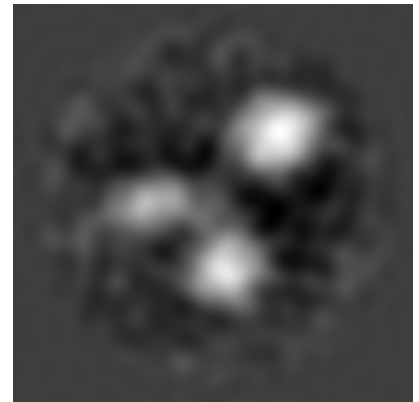
#### 6.1.1 Primary map



X



Y

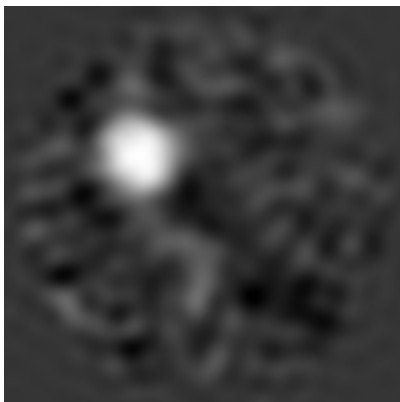


Z

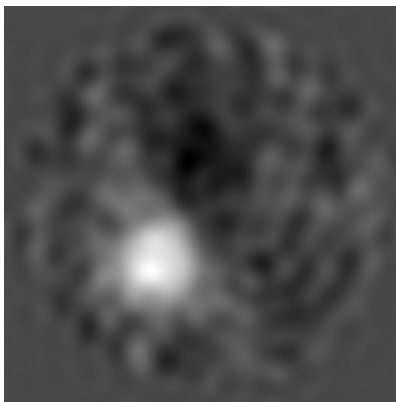
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

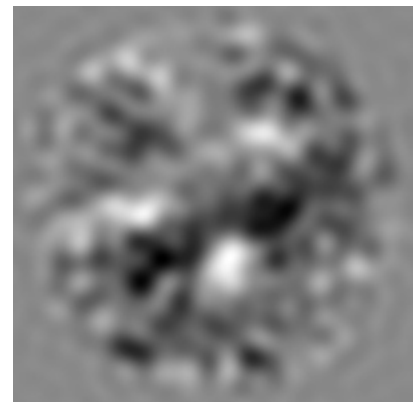
#### 6.2.1 Primary map



X Index: 60



Y Index: 60

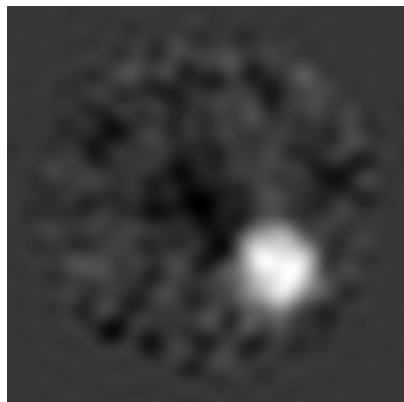


Z Index: 60

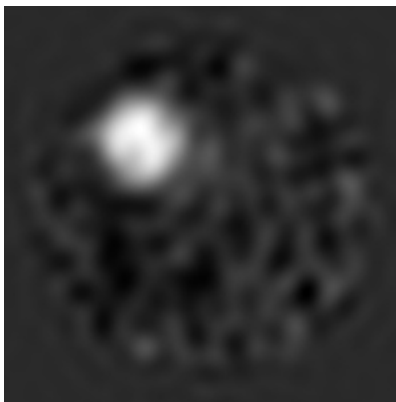
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

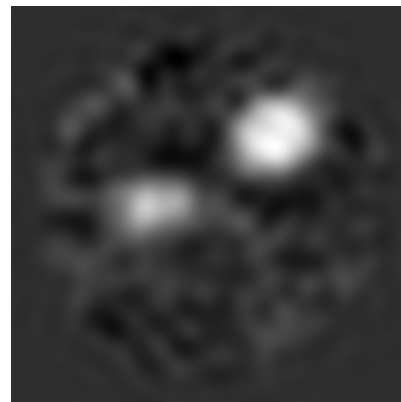
### 6.3.1 Primary map



X Index: 80



Y Index: 81

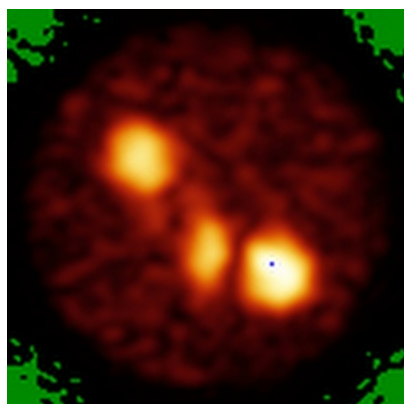


Z Index: 43

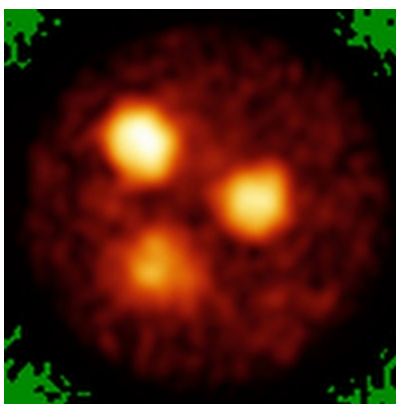
The images above show the largest variance slices of the map in three orthogonal directions.

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

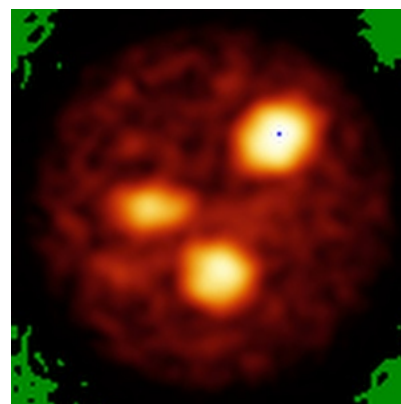
### 6.4.1 Primary map



X



Y

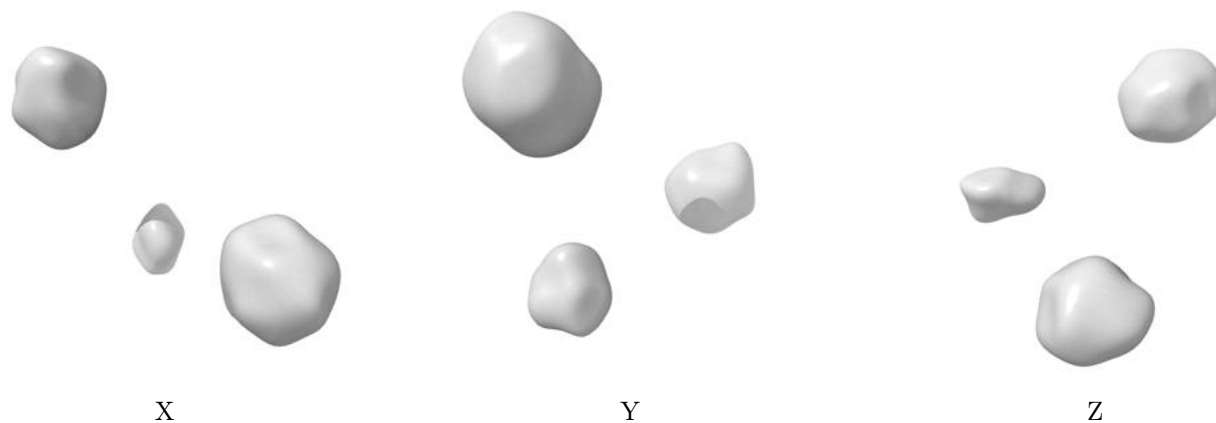


Z

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 [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

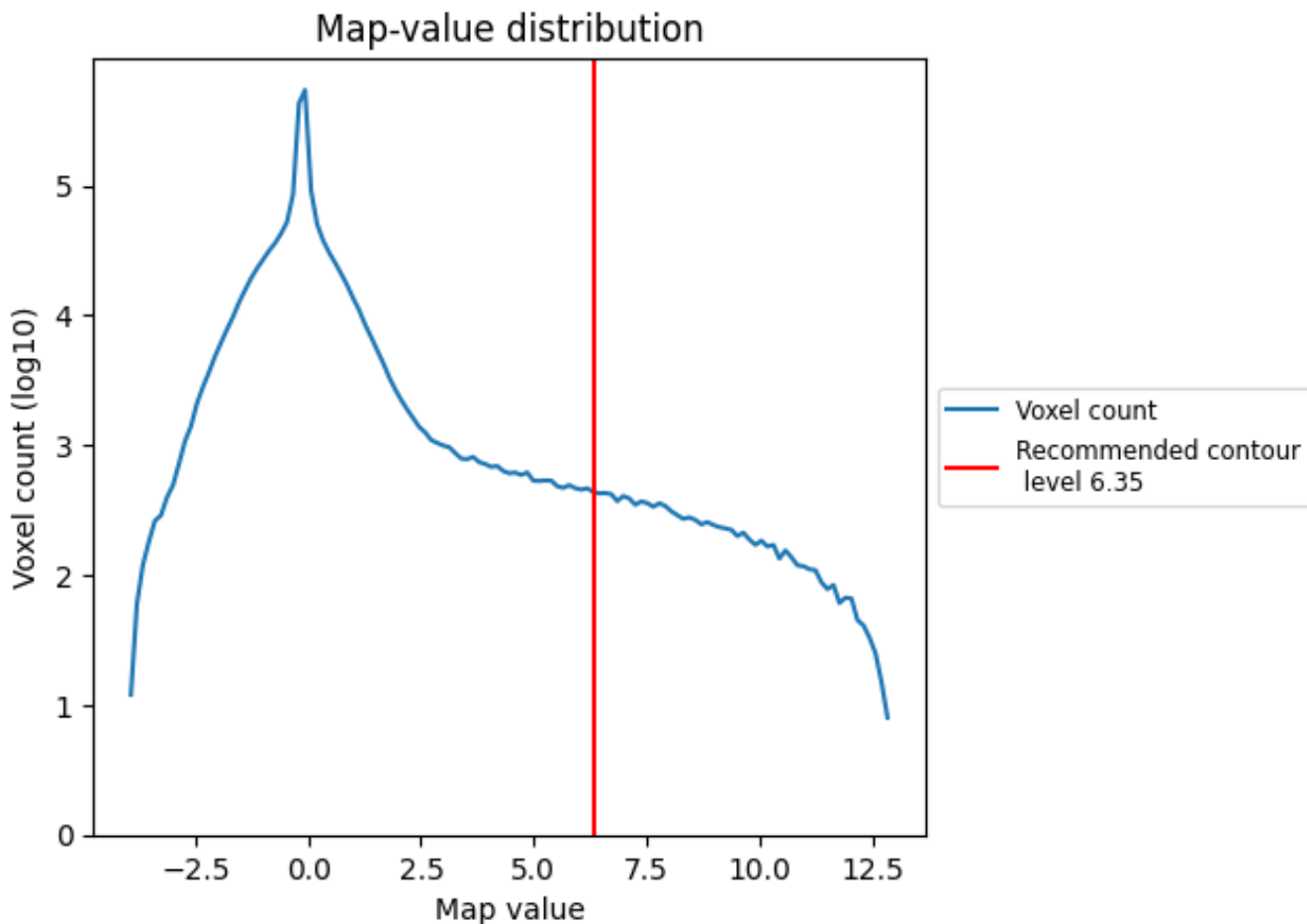
## 6.6 Mask visualisation [i](#)

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.

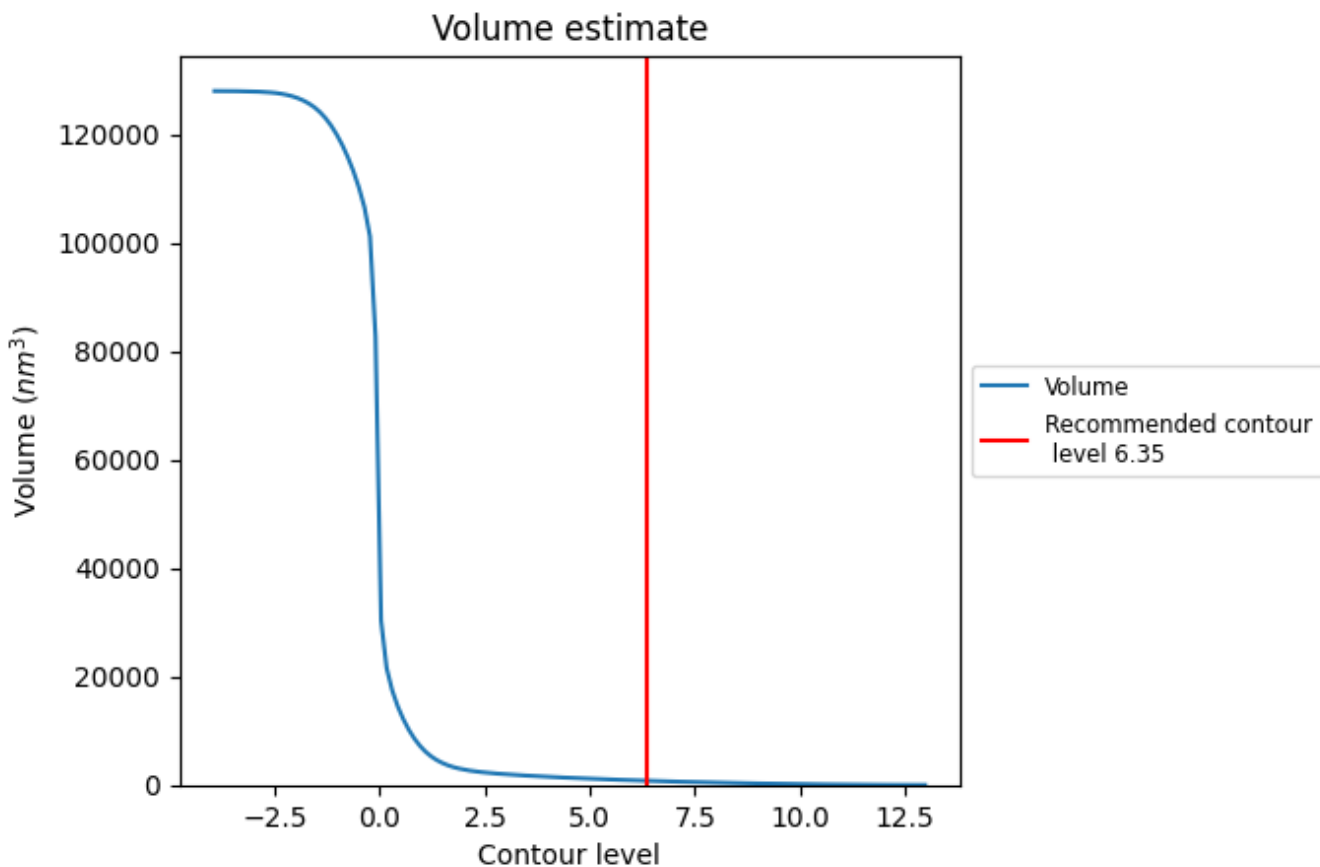
### 7.1 Map-value distribution [i](#)



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.



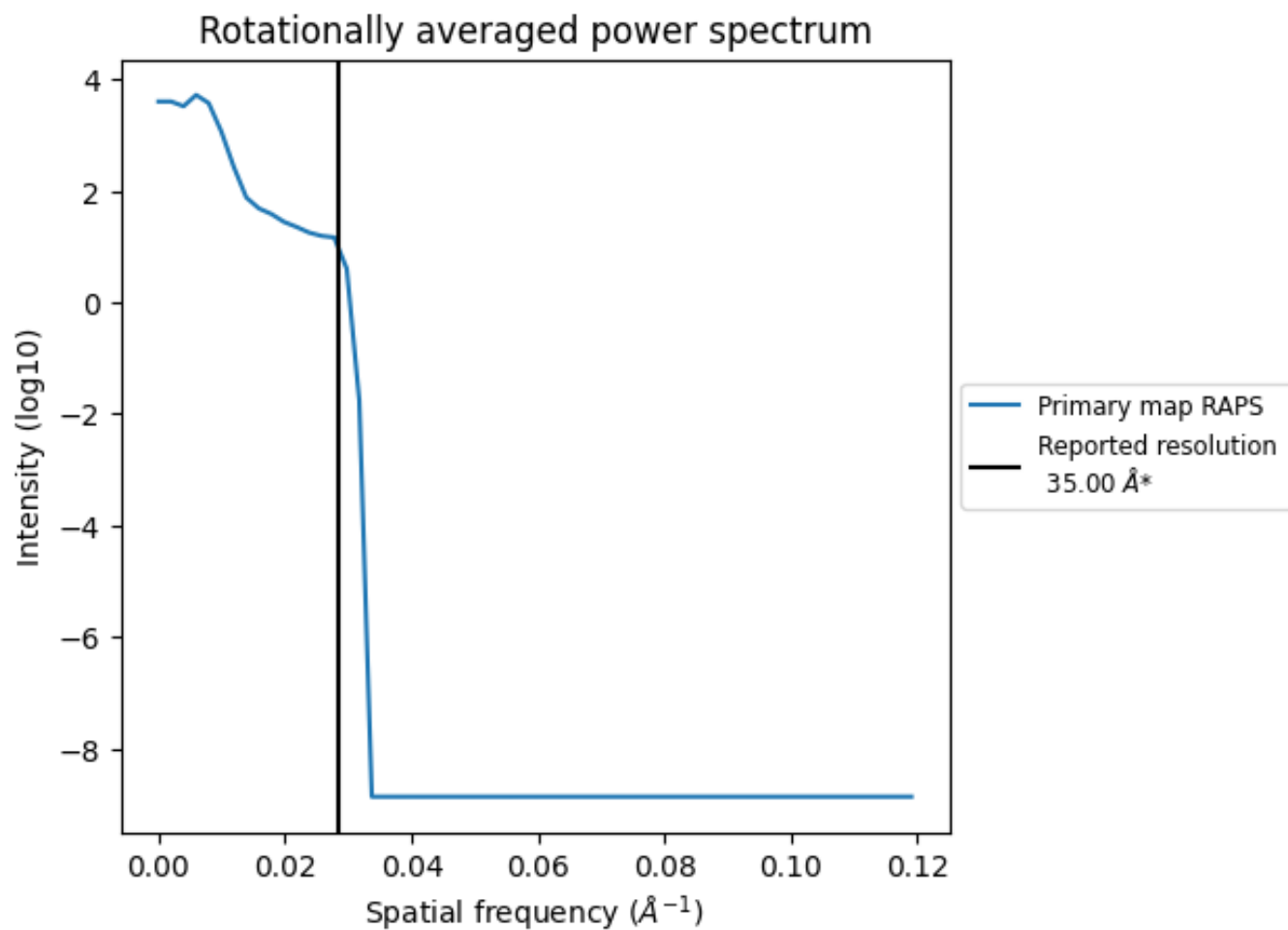
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 779  $\text{nm}^3$ ; 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 i



\*Reported resolution corresponds to spatial frequency of 0.029 Å<sup>-1</sup>

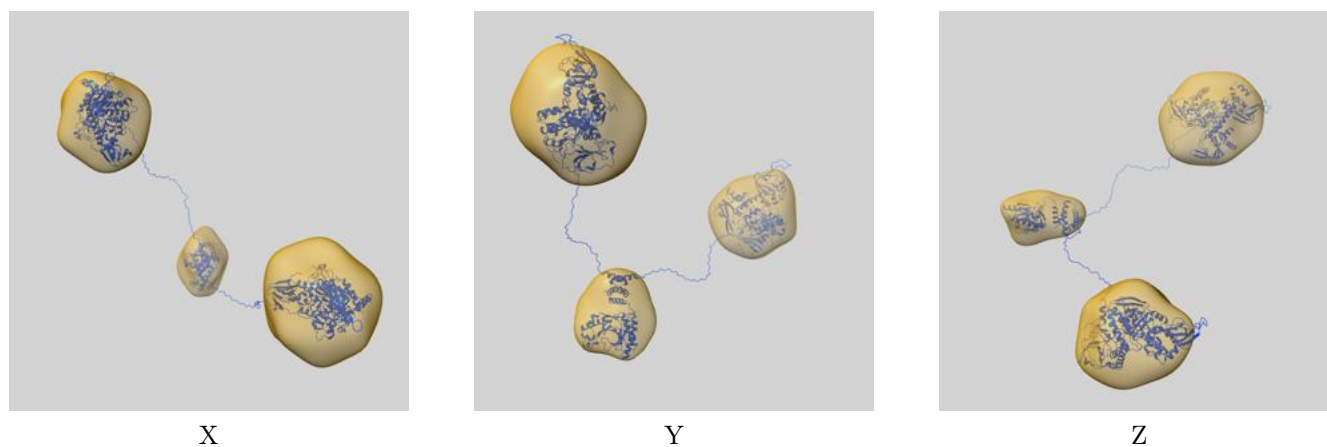
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

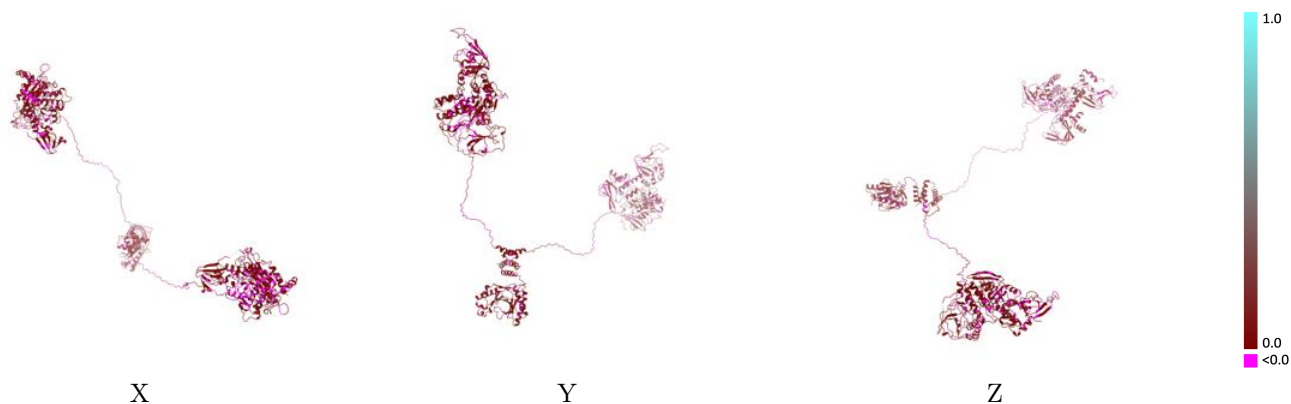
This section contains information regarding the fit between EMDB map EMD-5755 and PDB model 3J4Q. Per-residue inclusion information can be found in section 3 on page 4.

### 9.1 Map-model overlay [i](#)



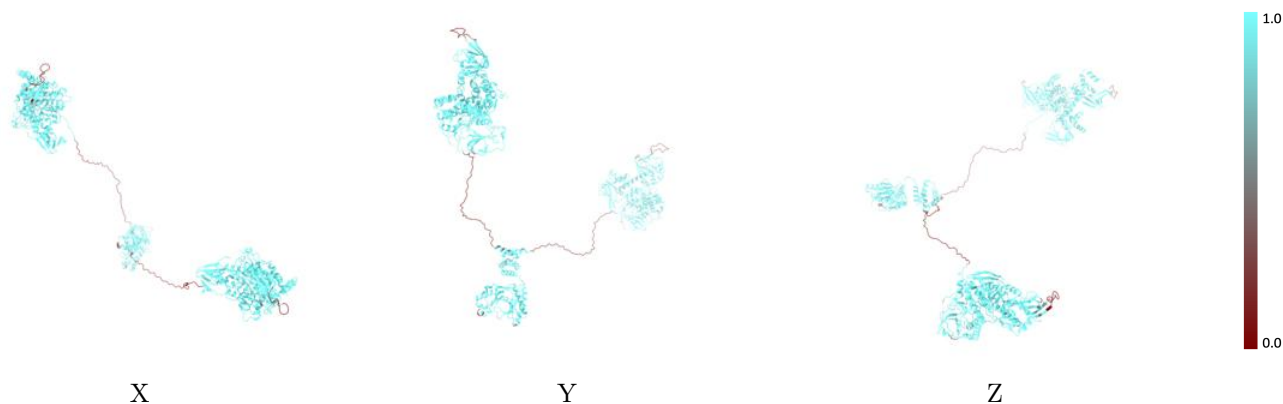
The images above show the 3D surface view of the map at the recommended contour level 6.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



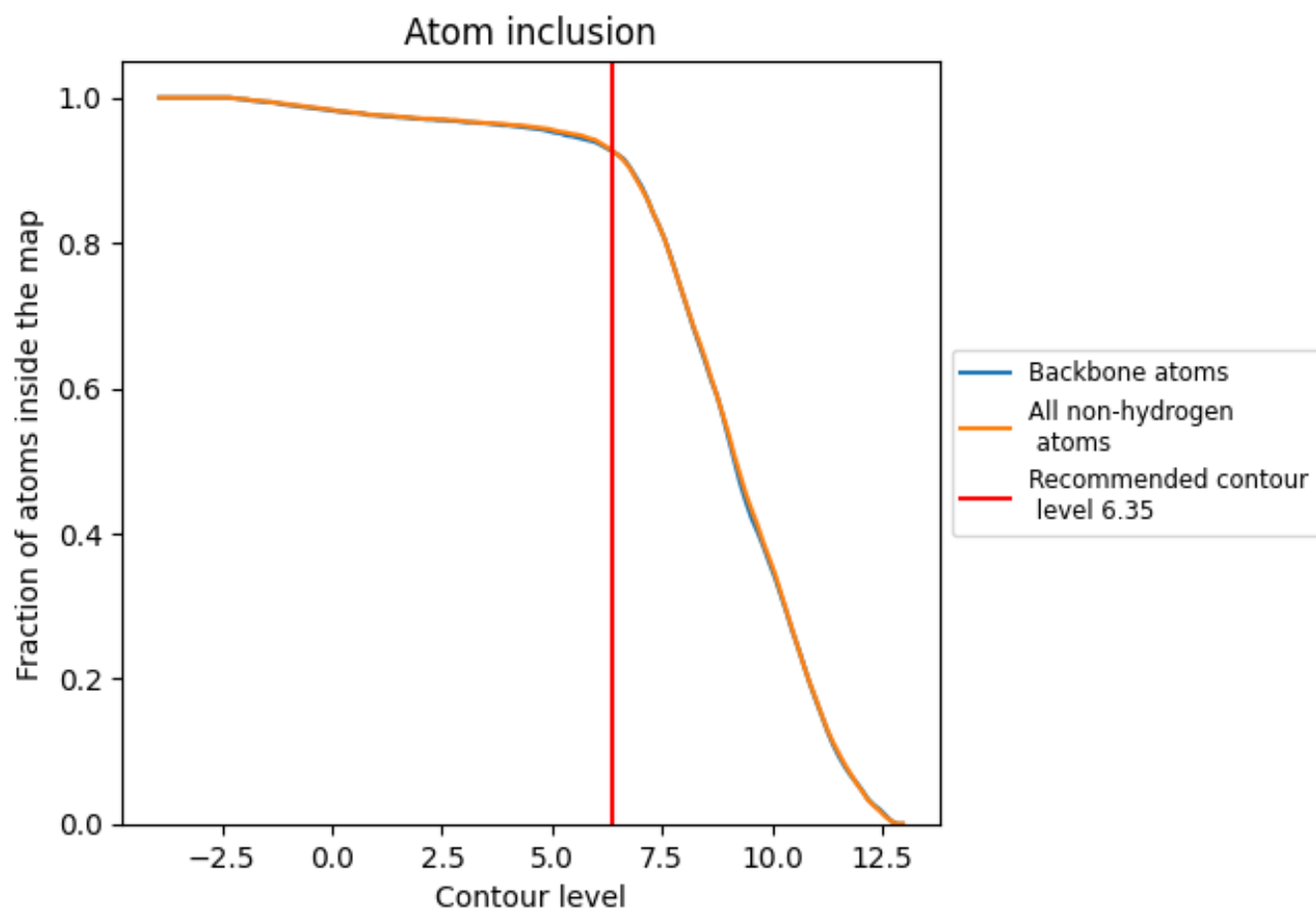
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (6.35).













## 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 [i](#)

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

