



## Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 06:48 AM EST

PDB ID : 7K1N  
EMDB ID : EMD-22626  
Title : CryoEM structure of inactivated-form DNA-PK (Complex V)  
Authors : Chen, X.; Gellert, M.; Yang, W.  
Deposited on : 2020-09-08  
Resolution : 3.90 Å(reported)

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

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

---

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

EMDB validation analysis : 0.0.1.dev43  
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) : 2.31.2

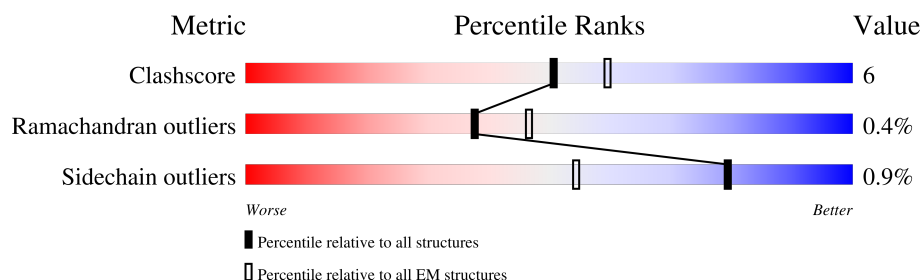
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	4128	
2	B	609	
3	C	732	
4	D	24	
4	F	24	
5	E	16	
5	G	16	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39521 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3634	Total	C	N	O	S	0	0
			28808	18485	4884	5252	187		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	490	Total	C	N	O	S	0	0
			3954	2533	671	733	17		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	655	Total	C	N	O	S	0	0
			5251	3359	877	989	26		

- Molecule 4 is a DNA chain called DNA (5'-D(P\*GP\*CP\*AP\*TP\*GP\*CP\*TP\*CP\*TP\*AP\*CP\*TP\*GP\*CP\*TP\*TP\*CP\*GP\*AP\*TP\*AP\*TP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	24	Total	C	N	O	P	0	0
			484	233	82	146	23		
4	F	21	Total	C	N	O	P	0	0
			425	204	69	131	21		

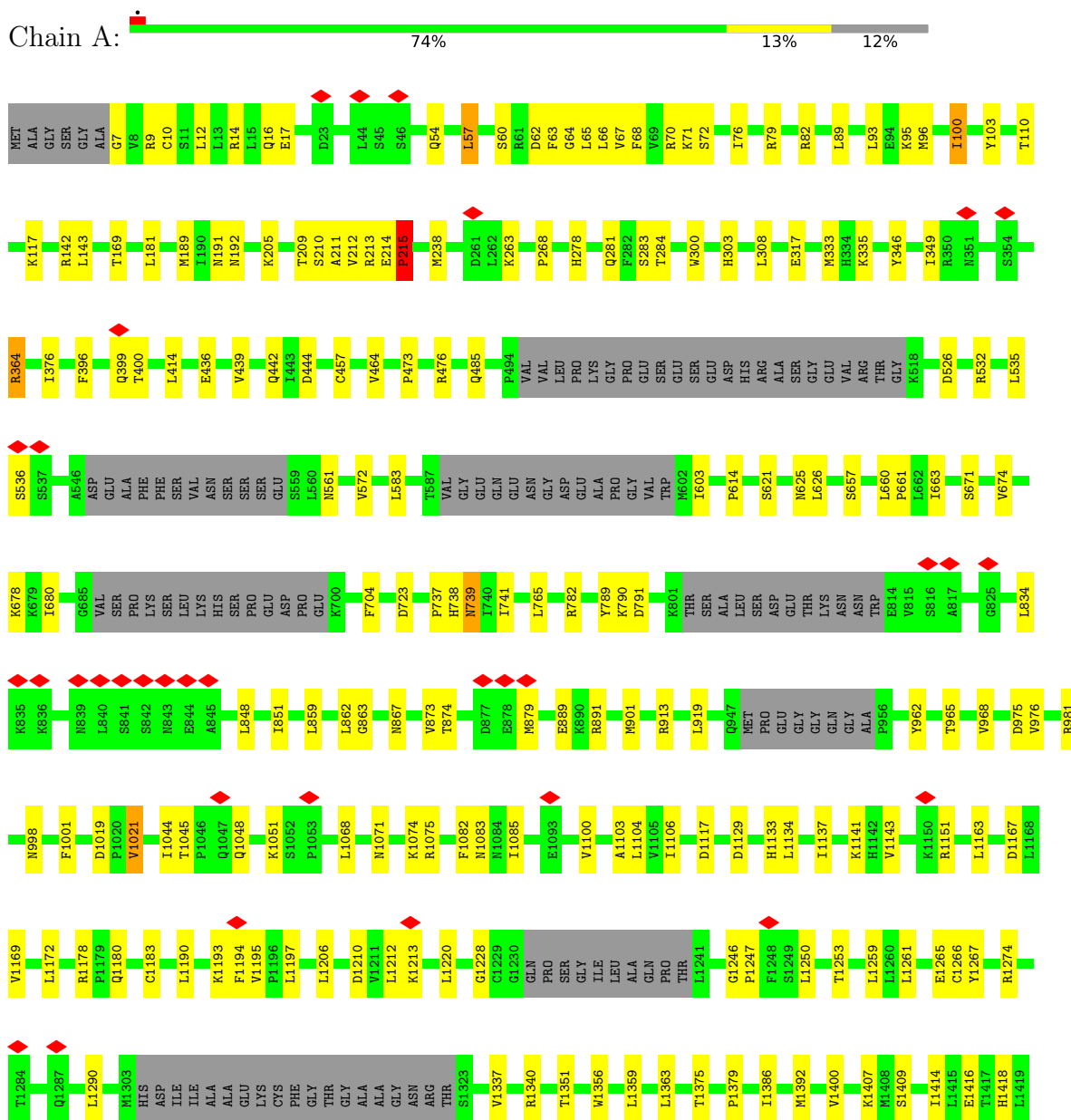
- Molecule 5 is a DNA chain called DNA (5'-D(P\*AP\*AP\*GP\*CP\*AP\*GP\*TP\*AP\*GP\*AP\*GP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	13	Total	C	N	O	P	0	0
			269	128	58	71	12		
5	G	16	Total	C	N	O	P	0	0
			330	157	68	90	15		

### 3 Residue-property plots

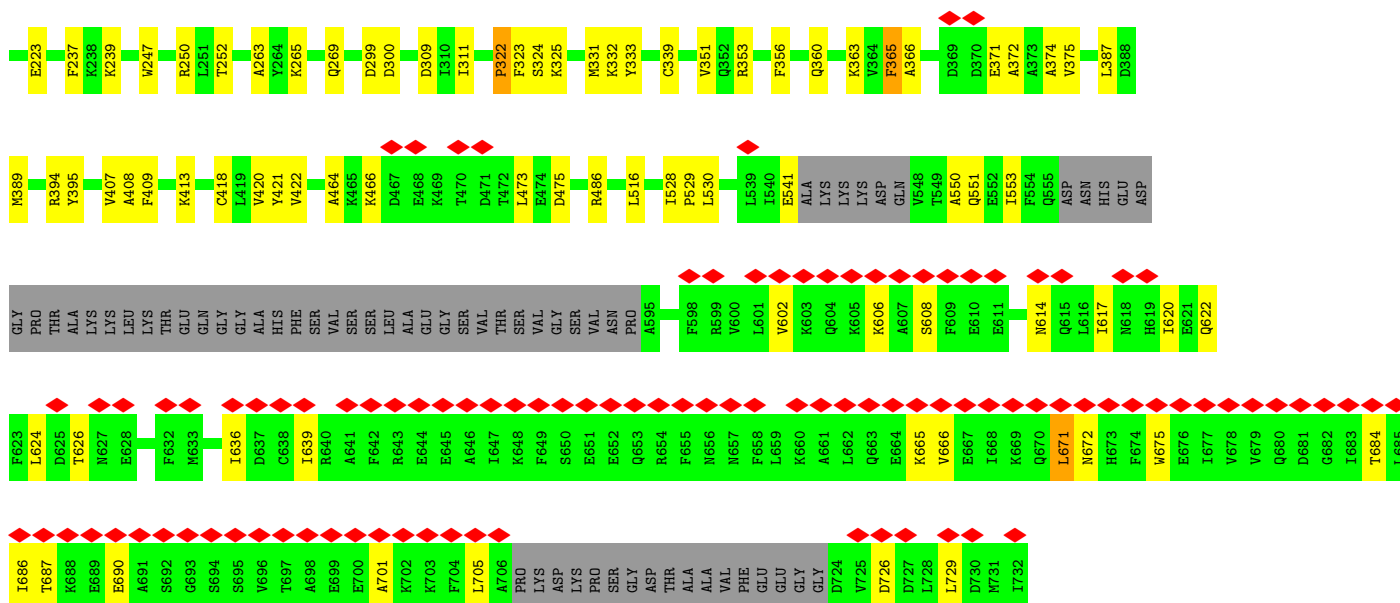
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

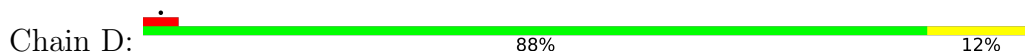


T3198	K2978	Q2979	Q2984	MET	HIS	GLY	L2327	S2124	F2043	E1969	F1782	N1589	R1420
D2980	Q2979	K2985	K2986	TYR	LYS	GLY	R328	W2125	D2044	K1973	I1785	T1590	E1421
E2985	L2837	L2836	L2837	ARG	ARG	SER	Y329	W2126	T2047	N1974	F1605	F1605	K1422
E2990	N2841	N2841	N2841	GLY	ARG	ALA	E2332	G2131	G2048	L1975	R1788	R1608	E1430
F2993	R2842	R2842	R2842	VAL	TRP	ARG	E2332	W2135	VAL	L1984	R1811	D1440	D1440
L3011	T2846	T2846	T2846	ALA	PRO	ARG	E2338	R2143	SER	K1985	R1816	L1623	R1445
D3026	S2849	S2849	S2849	PRO	ALA	ALA	C2342	L2149	TYR	R1987	V1920	W1626	C1455
L3027	F2854	F2854	F2854	ARG	LEU	GLY	V2345	T2153	SER	N1988	L1824	W1632	L1458
N3028	C2857	C2857	C2857	LYS	SER	ILE	H2352	K2162	GLN	V1994	W1929	W1633	H1459
S3047	L2858	L2858	L2858	VAL	ARG	ALA	H2352	H2163	ASP	GLU	L1639	A1634	R1460
K3048	Q2859	Q2859	Q2859	PRO	THR	THR	F2360	W2164	ARG	PRO	L1833	G1462	G1461
L3049	C2880	C2880	C2880	GLY	GLN	GLN	D2376	L2169	PRO	MET	L1836	K1642	L1463
K3050	P2887	P2887	P2887	GLY	GLN	GLN	F2383	L2171	ALA	GLU	L1837	V1645	D1474
Q3054	L2897	L2897	L2897	ARG	PHE	THR	F2384	Q2177	ARG	LYS	E1838	T1663	L1475
D3058	R2898	R2898	R2898	THR	THR	LEU	P2387	G2178	ARG	TYR	V1950	H1476	H1476
L3061	L2899	L2899	L2899	LEU	THR	THR	K2388	G2179	ARG	ILE	S1853	L1484	L1484
M3069	LEU	LEU	LEU	GLY	GLN	GLN	R2404	T2182	ARG	GLU	T1682	G1494	G1494
H3070	PRO	PRO	PRO	THR	THR	THR	R2404	H2183	GLU	ILE	T1682	L1684	GLU
S3083	ALA	ALA	ALA	ASP	ASP	ASP	M2408	H2184	ARG	ARG	T1857	L1686	ARG
D3095	GLY	GLY	GLY	GLY	GLY	GLY	D2428	V2187	ASP	ALA	L1858	H1687	GLN
R3098	ASP	ASP	ASP	ASP	ASP	ASP	H2464	V2187	PRO	ALA	D1864	L1688	CYS
Y3102	ARG	ARG	ARG	ARG	ARG	ARG	C2469	V2190	THR	ARG	T1865	P1697	LEU
V3119	LEU	LEU	LEU	LEU	LEU	LEU	C2469	V2190	VAL	GLU	Q1866	P1697	P1501
R3125	ILE	ILE	ILE	THR	THR	THR	L2476	T2193	ASP	ALA	I1867	G1704	S1502
E3137	Q2784	Q2784	Q2784	ASP	ASP	ASP	P2487	A2200	VAL	ASN	T1868	L1707	L1503
Q3139	I2785	I2785	I2785	PRO	PRO	PRO	E2488	R2214	LEU	GLY	K1869	C1507	C1507
E3140	S2788	S2788	S2788	LEU	LEU	LEU	E2488	R2214	ASP	ASP	R1883	Q1725	L1524
K3147	T2792	T2792	T2792	VAL	VAL	VAL	S2489	R2254	GLY	PRO	D1888	S1726	C1525
N3150	D2801	D2801	D2801	ARG	ARG	ARG	E2490	L2256	THR	TYR	K1892	E1728	L1532
W3164	F2802	F2802	F2802	THR	THR	THR	T2491	F2257	GLY	SER	I1896	R1735	A1541
T3165	S2810	S2810	S2810	ALA	ALA	ALA	D2492	P2265	PRO	LEU	I1896	F1736	SER
N3166	S2810	S2810	S2810	GLN	GLN	GLN	N2493	P2266	GLN	ALA	G1908	N1738	LEU
R3167	K2824	K2824	K2824	ASP	ASP	ASP	Q2496	P2290	GLY	ASP	I1905	E1751	SER
F3189	T2825	T2825	T2825	LEU	LEU	LEU	V2505	Q2295	GLY	T2034	G1908	L1752	GLY
L3190	L2826	L2826	L2826	THR	THR	THR	T2507	S2296	ASP	T2035	K1917	V1765	SER
L3197	Q2971	Q2971	Q2971	THR	THR	THR	D2512	F2309	VAL	S2037	F1956	M1774	H1552
	K2829	K2829	K2829	ALA	ALA	ALA	F2524		PRO	M2040	G1964	L1777	M1574
											S1968		D1588

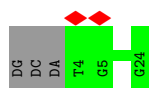
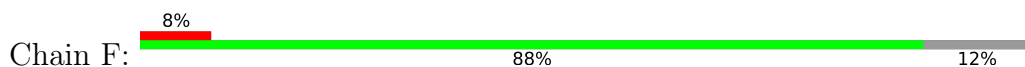




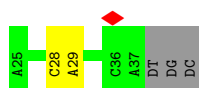
- Molecule 4: DNA (5'-D(P\*GP\*CP\*AP\*TP\*GP\*CP\*TP\*CP\*TP\*AP\*CP\*TP\*GP\*CP\*TP\*T  
P\*CP\*GP\*AP\*TP\*AP\*TP\*CP\*G)-3')



- Molecule 4: DNA (5'-D(P\*GP\*CP\*AP\*TP\*GP\*CP\*TP\*CP\*TP\*AP\*CP\*TP\*GP\*CP\*TP\*T  
P\*CP\*GP\*AP\*TP\*AP\*TP\*CP\*G)-3')



- Molecule 5: DNA (5'-D(P\*AP\*AP\*GP\*CP\*AP\*GP\*TP\*AP\*GP\*AP\*GP\*CP\*A)-3')



- Molecule 5: DNA (5'-D(P\*AP\*AP\*GP\*CP\*AP\*GP\*TP\*AP\*GP\*AP\*GP\*CP\*A)-3')



There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138985	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.055	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	408.31998, 408.31998, 408.31998	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	1/29394 (0.0%)	0.59	11/39755 (0.0%)
2	B	0.36	0/4031	0.60	2/5429 (0.0%)
3	C	0.32	0/5351	0.60	2/7213 (0.0%)
4	D	0.80	0/540	1.06	0/831
4	F	0.77	0/473	1.05	0/727
5	E	0.60	0/304	0.87	0/468
5	G	0.77	0/372	0.90	0/573
All	All	0.39	1/40465 (0.0%)	0.62	15/54996 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1195	VAL	C-N	5.33	1.44	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3311	ASN	N-CA-C	-8.40	88.33	111.00
3	C	671	LEU	CA-CB-CG	7.85	133.36	115.30
1	A	2887	PRO	CB-CA-C	7.76	131.41	112.00
1	A	1984	LEU	CA-CB-CG	6.89	131.15	115.30
2	B	497	LEU	N-CA-C	-5.85	95.20	111.00
1	A	2545	LEU	CA-CB-CG	5.58	128.13	115.30
2	B	356	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	1524	LEU	CA-CB-CG	5.53	128.03	115.30
3	C	194	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	765	LEU	CA-CB-CG	5.48	127.89	115.30
1	A	444	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	3918	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	975	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	2528	GLU	C-N-CA	5.12	134.50	121.70
1	A	1044	ILE	C-N-CA	5.06	134.36	121.70

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	28808	0	29022	330	0
2	B	3954	0	4042	66	0
3	C	5251	0	5269	78	0
4	D	484	0	274	2	0
4	F	425	0	240	0	0
5	E	269	0	146	1	0
5	G	330	0	180	0	0
All	All	39521	0	39173	460	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 6.

All (460) 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)
1:A:3352:GLU:HG3	1:A:3355:LYS:HG3	1.38	1.00
1:A:7:GLY:N	1:A:10:CYS:HG	1.69	0.90
1:A:3352:GLU:HG3	1:A:3355:LYS:CG	2.13	0.77
1:A:1416:GLU:O	1:A:1420:ARG:HB2	1.86	0.74
2:B:495:LEU:HB3	2:B:497:LEU:CD2	2.24	0.68
2:B:165:ARG:HA	2:B:199:PHE:O	1.94	0.68
2:B:495:LEU:HB3	2:B:497:LEU:HD23	1.76	0.68
1:A:1151:ARG:HD2	1:A:1163:LEU:H	1.60	0.66
1:A:3586:LYS:HG2	1:A:3667:LEU:HD21	1.78	0.66
3:C:387:LEU:HB3	3:C:389:MET:HG2	1.78	0.66
1:A:3647:GLY:HA2	1:A:3651:LEU:HB2	1.78	0.65
1:A:1206:LEU:O	1:A:1210:ASP:HB2	1.95	0.65
2:B:264:ASN:HD22	3:C:530:LEU:HD13	1.62	0.65
1:A:3630:ARG:HG2	1:A:3632:PHE:H	1.63	0.64
1:A:4028:ILE:HG22	1:A:4029:GLN:HG2	1.81	0.63
1:A:1356:TRP:HE1	1:A:1409:SER:HB2	1.63	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:408:ALA:HA	3:C:420:VAL:O	1.99	0.62
2:B:35:ARG:NH2	2:B:80:ARG:O	2.34	0.61
3:C:409:PHE:HB2	3:C:420:VAL:HG22	1.84	0.60
1:A:1178:ARG:NH1	1:A:1183:CYS:SG	2.75	0.60
1:A:54:GLN:HA	1:A:57:LEU:HB3	1.84	0.60
2:B:36:ASP:OD1	2:B:36:ASP:N	2.35	0.59
2:B:368:VAL:HG13	2:B:434:LEU:HD11	1.84	0.59
1:A:1375:THR:HA	1:A:1379:PRO:HB3	1.84	0.59
1:A:3648:GLY:O	1:A:3653:ARG:NH1	2.36	0.59
1:A:2524:PHE:O	1:A:2530:ARG:NH2	2.36	0.59
2:B:204:HIS:O	2:B:237:SER:N	2.36	0.59
1:A:215:PRO:HD3	3:C:550:ALA:HB2	1.85	0.59
1:A:1704:GLY:HA2	1:A:1707:LEU:HB3	1.85	0.59
1:A:859:LEU:O	1:A:867:ASN:ND2	2.36	0.59
1:A:791:ASP:OD1	1:A:791:ASP:N	2.36	0.59
3:C:466:LYS:HA	3:C:473:LEU:HA	1.85	0.59
3:C:684:THR:HG21	3:C:705:LEU:HD21	1.84	0.59
1:A:1266:CYS:SG	1:A:1267:TYR:N	2.75	0.58
1:A:3959:MET:SD	1:A:3959:MET:N	2.73	0.58
2:B:413:LEU:HB3	2:B:432:PHE:HD2	1.68	0.58
1:A:3755:GLY:HA2	1:A:3799:ARG:HB2	1.86	0.58
3:C:11:VAL:HB	3:C:132:ILE:HG12	1.85	0.58
2:B:241:ASP:OD1	2:B:241:ASP:N	2.37	0.58
1:A:3831:ASP:HB3	1:A:3834:ALA:HB2	1.86	0.58
1:A:1684:LEU:HB3	1:A:1688:LEU:HB2	1.86	0.58
1:A:1969:GLU:HB2	1:A:1975:LEU:HB3	1.85	0.58
1:A:3050:LYS:O	1:A:3054:GLN:NE2	2.37	0.57
1:A:3327:ASN:HB2	1:A:3388:ALA:HB2	1.86	0.57
1:A:72:SER:O	1:A:82:ARG:NH1	2.37	0.57
3:C:131:HIS:NE2	3:C:133:GLU:OE2	2.38	0.57
1:A:1274:ARG:NH1	1:A:1351:THR:OG1	2.38	0.57
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.38	0.57
3:C:407:VAL:O	3:C:421:TYR:HA	2.05	0.57
1:A:998:ASN:HA	1:A:1001:PHE:HB2	1.87	0.57
2:B:245:LYS:O	2:B:245:LYS:HG3	2.05	0.57
1:A:1190:LEU:O	1:A:1194:PHE:HB2	2.05	0.56
1:A:3119:VAL:O	1:A:3125:ARG:NH2	2.38	0.56
1:A:3289:ARG:NH1	1:A:3993:SER:OG	2.38	0.56
1:A:1261:LEU:HD13	1:A:1337:VAL:HG12	1.88	0.56
1:A:3595:GLU:OE2	1:A:3602:ASN:ND2	2.37	0.56
2:B:48:MET:SD	2:B:48:MET:N	2.77	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:ASN:ND2	3:C:103:GLN:O	2.38	0.56
1:A:1829:TRP:O	1:A:1883:ARG:NH2	2.38	0.56
1:A:2177:ASN:HB3	1:A:2182:ILE:HG12	1.86	0.56
1:A:3299:THR:HA	1:A:3302:LYS:HE3	1.87	0.56
1:A:2458:VAL:HG11	1:A:2476:ILE:HD11	1.86	0.56
3:C:265:LYS:NZ	3:C:360:GLN:OE1	2.37	0.56
1:A:1681:ASP:HB3	1:A:1683:LYS:HE3	1.87	0.56
1:A:1751:GLU:O	1:A:1788:ARG:NH2	2.39	0.56
1:A:2143:ARG:HG2	1:A:2171:LEU:HD21	1.88	0.56
1:A:3314:SER:O	1:A:3318:LYS:NZ	2.39	0.56
2:B:144:SER:HB3	2:B:186:ALA:HA	1.88	0.56
2:B:399:ARG:NH2	3:C:516:LEU:O	2.38	0.56
1:A:723:ASP:OD1	1:A:723:ASP:N	2.37	0.56
1:A:657:SER:HA	1:A:660:LEU:HB2	1.88	0.56
1:A:901:MET:SD	1:A:2535:THR:OG1	2.63	0.56
1:A:3190:LEU:HD22	1:A:3231:ILE:HG23	1.88	0.56
1:A:3352:GLU:HB3	1:A:3355:LYS:HB2	1.87	0.56
1:A:2963:SER:OG	1:A:3251:ASN:ND2	2.39	0.55
1:A:1104:LEU:HD12	1:A:1134:LEU:HD23	1.88	0.55
1:A:10:CYS:SG	1:A:14:ARG:NH2	2.73	0.55
1:A:4083:GLY:HA3	1:A:4091:ALA:HB2	1.87	0.55
1:A:210:SER:HB2	2:B:332:GLU:HG3	1.88	0.55
1:A:1021:VAL:O	1:A:1021:VAL:HG13	2.06	0.55
1:A:1833:LEU:HB3	1:A:1836:LEU:HB2	1.88	0.55
1:A:2810:SER:HG	1:A:2857:CYS:HG	1.53	0.55
1:A:3360:LEU:HG	1:A:3373:VAL:HG11	1.88	0.55
1:A:1129:ASP:O	1:A:1133:HIS:ND1	2.40	0.55
1:A:3573:ASN:HB3	1:A:3627:ALA:HB2	1.89	0.55
2:B:495:LEU:CB	2:B:497:LEU:HD21	2.37	0.55
3:C:137:ASP:HA	3:C:166:PRO:HD3	1.89	0.55
1:A:442:GLN:NE2	1:A:457:CYS:SG	2.79	0.55
1:A:2230:VAL:O	1:A:2234:ASN:ND2	2.40	0.55
1:A:3484:THR:HG22	1:A:3513:ALA:HA	1.88	0.55
3:C:66:ASN:ND2	3:C:68:LEU:O	2.38	0.55
1:A:1228:GLY:HA3	1:A:1259:LEU:HD13	1.89	0.55
3:C:371:GLU:HB2	3:C:374:ALA:HB3	1.87	0.55
1:A:3253:SER:O	1:A:3257:LYS:NZ	2.39	0.54
3:C:57:VAL:HG22	3:C:79:VAL:HG12	1.89	0.54
1:A:1071:ASN:O	1:A:1075:ARG:NH1	2.41	0.54
1:A:1075:ARG:NH2	1:A:1117:ASP:OD1	2.38	0.54
5:E:28:DC:H2"	5:E:29:DA:C8	2.42	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LYS:HE2	2:B:83:LEU:HD11	1.89	0.54
1:A:2376:ASP:OD1	1:A:2404:ARG:NH2	2.41	0.54
1:A:526:ASP:OD1	1:A:526:ASP:N	2.39	0.54
1:A:1590:THR:HG1	1:A:1632:TRP:HE1	1.54	0.54
1:A:3378:TYR:OH	1:A:3426:LYS:NZ	2.40	0.54
1:A:4088:ASN:ND2	1:A:4113:ASP:OD2	2.39	0.54
1:A:414:LEU:HD12	1:A:464:VAL:HG21	1.88	0.54
1:A:621:SER:O	1:A:625:ASN:ND2	2.40	0.54
2:B:219:ASP:OD1	2:B:219:ASP:N	2.40	0.54
1:A:7:GLY:N	1:A:10:CYS:SG	2.76	0.54
1:A:3813:LYS:HB2	1:A:3925:LEU:HB3	1.89	0.54
2:B:95:ASN:HD21	2:B:99:PHE:HB2	1.73	0.54
1:A:1400:VAL:HG11	1:A:1460:ARG:HG2	1.90	0.54
1:A:14:ARG:HA	1:A:17:GLU:HB2	1.90	0.54
1:A:1414:ILE:O	1:A:1418:HIS:ND1	2.36	0.54
3:C:219:ASP:OD1	3:C:219:ASP:N	2.35	0.54
1:A:212:VAL:HG12	1:A:213:ARG:HB2	1.88	0.53
1:A:3714:GLU:O	1:A:3718:ARG:NH1	2.42	0.53
1:A:76:ILE:O	1:A:79:ARG:NH1	2.42	0.53
2:B:249:LYS:NZ	2:B:250:GLU:O	2.42	0.53
1:A:1143:VAL:HG23	1:A:1197:LEU:HD21	1.90	0.53
1:A:4006:VAL:HA	1:A:4011:PHE:HZ	1.73	0.53
1:A:1100:VAL:HA	1:A:1103:ALA:HB3	1.90	0.53
1:A:2034:SER:N	1:A:2037:SER:HG	2.05	0.53
1:A:4049:ARG:NH2	1:A:4062:ASP:OD2	2.38	0.53
3:C:111:LEU:HD11	3:C:150:ILE:HD12	1.91	0.53
1:A:2962:ARG:NH1	1:A:4101:GLU:OE2	2.42	0.53
2:B:95:ASN:OD1	2:B:95:ASN:N	2.41	0.53
1:A:1267:TYR:HE2	1:A:1290:LEU:HD13	1.73	0.53
1:A:1820:VAL:HG23	1:A:1824:LEU:HD11	1.90	0.52
2:B:143:LEU:HD23	2:B:182:LYS:HE3	1.90	0.52
3:C:687:THR:HG22	3:C:701:ALA:HB2	1.90	0.52
1:A:2103:HIS:O	1:A:2107:SER:CB	2.58	0.52
1:A:572:VAL:HG23	1:A:626:LEU:HD11	1.92	0.52
1:A:2978:LYS:NZ	1:A:2985:GLU:OE2	2.43	0.52
2:B:49:PHE:O	2:B:128:GLN:NE2	2.42	0.52
1:A:1169:VAL:HA	1:A:1172:LEU:HD12	1.92	0.52
1:A:60:SER:OG	1:A:63:PHE:O	2.26	0.52
1:A:278:HIS:HB3	1:A:281:GLN:HG3	1.92	0.52
1:A:3652:LEU:HD22	1:A:3653:ARG:HH21	1.75	0.51
1:A:2384:PHE:O	1:A:2388:LYS:NZ	2.43	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4010:SER:O	1:A:4015:ASN:ND2	2.43	0.51
3:C:250:ARG:HH21	3:C:252:THR:HG21	1.75	0.51
1:A:9:ARG:HA	1:A:12:LEU:HD13	1.92	0.51
1:A:603:ILE:HG13	1:A:1083:ASN:HB3	1.91	0.51
1:A:2254:ARG:HA	1:A:2257:PHE:HB3	1.92	0.51
1:A:2493:ASN:HA	1:A:2496:GLN:HE21	1.74	0.51
1:A:3602:ASN:N	1:A:3602:ASN:OD1	2.42	0.51
2:B:55:ASP:OD1	2:B:55:ASP:N	2.43	0.51
1:A:142:ARG:HE	1:A:143:LEU:H	1.58	0.51
1:A:1634:ALA:O	1:A:1642:LYS:NZ	2.43	0.51
1:A:1440:ASP:OD1	1:A:1440:ASP:N	2.35	0.51
1:A:3048:LYS:HB3	1:A:3061:LEU:HD22	1.92	0.51
1:A:3147:LYS:HB3	1:A:3150:ASN:HB2	1.93	0.51
2:B:505:ASP:OD2	3:C:333:TYR:OH	2.28	0.51
1:A:739:ASN:OD1	1:A:739:ASN:N	2.44	0.51
1:A:3137:GLU:OE2	1:A:3167:ARG:NH2	2.42	0.51
2:B:52:GLN:HE22	2:B:207:LYS:HA	1.74	0.51
3:C:624:LEU:HD12	3:C:665:LYS:HE2	1.92	0.51
1:A:3026:ASP:N	1:A:3026:ASP:OD1	2.44	0.51
1:A:1206:LEU:O	1:A:1210:ASP:CB	2.58	0.51
1:A:1685:ASP:H	1:A:1688:LEU:HD12	1.75	0.51
1:A:1726:SER:OG	1:A:1727:ARG:N	2.44	0.51
1:A:1986:ARG:NH2	1:A:1988:TYR:OH	2.43	0.51
2:B:480:ASN:O	2:B:484:GLN:HB2	2.11	0.51
3:C:223:GLU:OE2	3:C:239:LYS:NZ	2.43	0.50
1:A:1407:LYS:NZ	1:A:1462:GLY:O	2.44	0.50
1:A:2131:GLY:O	1:A:2135:ASN:ND2	2.44	0.50
3:C:6:ASN:ND2	3:C:128:GLU:OE1	2.43	0.50
1:A:1019:ASP:OD1	1:A:1019:ASP:N	2.43	0.50
1:A:2824:LYS:O	1:A:2829:LYS:NZ	2.38	0.50
1:A:3354:ASP:OD1	1:A:3354:ASP:N	2.44	0.50
1:A:1836:LEU:HD21	1:A:1839:PHE:HB3	1.93	0.50
3:C:17:GLY:O	3:C:20:MET:HB3	2.11	0.50
1:A:189:MET:HG2	1:A:192:ASN:HD21	1.77	0.50
1:A:738:HIS:ND1	1:A:741:ILE:O	2.44	0.50
1:A:2507:ILE:HG21	1:A:2547:SER:HB3	1.93	0.50
2:B:266:ASP:OD1	2:B:266:ASP:N	2.43	0.50
1:A:1418:HIS:O	1:A:1422:LYS:NZ	2.36	0.50
1:A:1888:ASP:OD1	1:A:1888:ASP:N	2.42	0.50
2:B:245:LYS:O	2:B:246:VAL:HG22	2.11	0.50
2:B:288:LEU:HB3	3:C:311:ILE:HG13	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLN:NE2	1:A:62:ASP:O	2.45	0.49
1:A:889:GLU:O	1:A:891:ARG:NH1	2.45	0.49
1:A:2897:LEU:HD11	1:A:2922:ARG:HB3	1.94	0.49
1:A:3588:TRP:NE1	1:A:3609:MET:SD	2.80	0.49
2:B:35:ARG:HH22	2:B:80:ARG:HB2	1.77	0.49
2:B:86:VAL:HG13	2:B:104:VAL:HG12	1.93	0.49
3:C:63:GLY:O	3:C:78:THR:OG1	2.30	0.49
1:A:66:LEU:HD11	1:A:110:THR:HG21	1.94	0.49
1:A:399:GLN:HG3	1:A:400:THR:HG23	1.94	0.49
1:A:2428:ASP:O	1:A:2432:GLN:NE2	2.44	0.49
1:A:3140:GLU:OE2	1:A:3164:TRP:NE1	2.45	0.49
2:B:194:ARG:NH1	2:B:219:ASP:O	2.46	0.49
2:B:202:LEU:HG	2:B:221:ILE:HD12	1.94	0.49
1:A:1068:LEU:HD21	1:A:1106:ILE:HD11	1.95	0.49
1:A:1178:ARG:HG2	1:A:1180:GLN:H	1.77	0.49
1:A:1588:ASP:N	1:A:1588:ASP:OD1	2.46	0.49
1:A:2290:PRO:HB3	1:A:2295:GLN:HA	1.94	0.49
1:A:1503:LEU:HD13	1:A:1508:LYS:HE2	1.94	0.48
2:B:507:THR:OG1	3:C:394:ARG:NH1	2.45	0.48
1:A:2551:GLU:OE2	1:A:2849:SER:OG	2.30	0.48
1:A:2990:GLU:HA	1:A:2993:PHE:HB3	1.95	0.48
1:A:3468:LEU:HA	1:A:3471:ILE:HG22	1.95	0.48
1:A:3700:GLU:OE2	1:A:3716:HIS:ND1	2.36	0.48
2:B:107:GLU:O	2:B:115:ARG:NH1	2.37	0.48
3:C:199:GLU:HA	3:C:202:LYS:HD2	1.95	0.48
1:A:1455:CYS:HA	1:A:1458:LEU:HD12	1.95	0.48
1:A:535:LEU:O	1:A:561:ASN:ND2	2.46	0.48
1:A:1440:ASP:O	1:A:1445:ARG:NH1	2.46	0.48
2:B:326:GLN:HE21	2:B:328:ILE:HD11	1.77	0.48
1:A:100:ILE:HG22	1:A:103:TYR:HB2	1.96	0.48
1:A:737:PRO:O	1:A:739:ASN:OD1	2.32	0.48
1:A:1853:SER:OG	1:A:1866:GLN:NE2	2.46	0.48
1:A:2859:GLN:NE2	1:A:2880:CYS:SG	2.77	0.48
1:A:333:MET:SD	1:A:333:MET:N	2.76	0.48
1:A:1045:THR:OG1	1:A:1048:GLN:NE2	2.46	0.48
1:A:1265:GLU:OE2	1:A:1340:ARG:NE	2.42	0.48
1:A:268:PRO:HB2	1:A:308:LEU:HD11	1.96	0.48
1:A:4011:PHE:HA	1:A:4015:ASN:HD22	1.78	0.48
1:A:1359:LEU:HB3	1:A:1363:LEU:HD21	1.95	0.48
1:A:2103:HIS:O	1:A:2107:SER:HB3	2.13	0.48
1:A:2265:PRO:HB3	1:A:2309:PHE:CG	2.49	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3590:ASN:HA	1:A:3593:ARG:HG2	1.94	0.48
1:A:2162:LYS:HA	1:A:2200:ALA:HB2	1.96	0.48
1:A:1167:ASP:OD1	1:A:1167:ASP:N	2.44	0.48
2:B:416:GLN:NE2	2:B:433:GLN:OE1	2.40	0.48
1:A:191:ASN:OD1	1:A:191:ASN:N	2.47	0.47
3:C:636:ILE:HA	3:C:639:ILE:HG12	1.95	0.47
1:A:1250:LEU:O	1:A:1253:THR:OG1	2.28	0.47
1:A:2290:PRO:HD3	1:A:2296:SER:HB3	1.95	0.47
1:A:2540:LEU:HD11	1:A:2835:LYS:HD2	1.95	0.47
1:A:2555:LEU:HD21	1:A:2854:PHE:HD1	1.79	0.47
1:A:3069:MET:O	1:A:3070:HIS:ND1	2.48	0.47
2:B:495:LEU:HD22	2:B:497:LEU:HD21	1.97	0.47
1:A:3448:GLU:HG2	1:A:3482:LEU:HD11	1.95	0.47
1:A:3471:ILE:O	1:A:3475:TYR:HB2	2.13	0.47
1:A:3751:LEU:HB3	1:A:3803:ILE:HG23	1.95	0.47
1:A:671:SER:HA	1:A:674:VAL:HG12	1.97	0.47
1:A:2149:LEU:O	1:A:2153:THR:OG1	2.29	0.47
1:A:3457:ASN:OD1	1:A:3494:GLN:NE2	2.47	0.47
1:A:2937:ASP:OD1	1:A:3784:ARG:NH2	2.46	0.47
1:A:3786:LEU:HD22	1:A:3910:LEU:HD22	1.97	0.47
3:C:351:VAL:HG21	3:C:407:VAL:HG21	1.97	0.47
1:A:2103:HIS:O	1:A:2107:SER:OG	2.32	0.47
1:A:2459:VAL:HB	1:A:2505:VAL:HG21	1.96	0.47
2:B:375:VAL:HG12	3:C:541:GLU:HB2	1.96	0.47
1:A:1407:LYS:HD3	1:A:1463:LEU:HD12	1.96	0.47
3:C:309:ASP:OD1	3:C:309:ASP:N	2.39	0.47
3:C:365:PHE:CD2	3:C:366:ALA:N	2.83	0.47
3:C:672:ASN:HA	3:C:675:TRP:HB2	1.96	0.47
1:A:583:LEU:HA	1:A:614:PRO:HA	1.97	0.46
1:A:1071:ASN:HD22	1:A:1074:LYS:HG3	1.80	0.46
1:A:1762:MET:HA	1:A:1765:VAL:HG12	1.97	0.46
1:A:2327:LEU:HD11	1:A:2345:VAL:HG11	1.96	0.46
1:A:3620:PRO:HG2	1:A:3621:LYS:HE2	1.96	0.46
1:A:3761:ASP:HA	1:A:3764:VAL:HG22	1.97	0.46
1:A:1782:PHE:HA	1:A:1785:ILE:HD12	1.96	0.46
1:A:3658:ASP:OD1	1:A:3658:ASP:N	2.47	0.46
1:A:4044:ILE:O	1:A:4048:LYS:HB2	2.15	0.46
3:C:11:VAL:O	3:C:132:ILE:HA	2.15	0.46
3:C:666:VAL:O	3:C:675:TRP:NE1	2.40	0.46
1:A:2184:TYR:HA	1:A:2187:VAL:HG22	1.97	0.46
1:A:4099:SER:O	1:A:4103:GLN:HB2	2.15	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:TYR:HA	1:A:965:THR:HG22	1.97	0.46
1:A:1686:LEU:HB3	1:A:1738:ASN:HD21	1.80	0.46
1:A:2837:LEU:O	1:A:2841:ASN:ND2	2.35	0.46
1:A:211:ALA:HB2	3:C:551:GLN:HE21	1.81	0.46
3:C:39:THR:O	3:C:43:GLN:HB2	2.15	0.46
1:A:96:MET:SD	1:A:96:MET:N	2.89	0.46
1:A:3492:CYS:SG	1:A:3524:ASN:ND2	2.88	0.46
1:A:704:PHE:HD1	1:A:704:PHE:O	1.99	0.46
1:A:873:VAL:HG13	1:A:874:THR:H	1.80	0.46
1:A:1896:ILE:HD12	1:A:1908:GLY:HA2	1.97	0.46
1:A:3508:LYS:NZ	1:A:3509:ASP:O	2.44	0.46
1:A:3289:ARG:NH1	1:A:3993:SER:O	2.49	0.46
3:C:6:ASN:HB3	3:C:7:LYS:H	1.58	0.46
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.76	0.46
1:A:2169:LEU:HD21	1:A:2193:ILE:HG21	1.98	0.46
2:B:140:ASP:OD1	2:B:140:ASP:N	2.42	0.46
2:B:263:LEU:HB2	2:B:267:ILE:HG13	1.97	0.46
2:B:407:PRO:HG2	3:C:486:ARG:HD2	1.97	0.46
1:A:3530:VAL:HG11	1:A:3568:ILE:HG21	1.99	0.45
1:A:3885:ARG:HA	1:A:3888:VAL:HG12	1.98	0.45
2:B:160:LYS:HB2	2:B:160:LYS:HE3	1.78	0.45
1:A:2927:ALA:HB2	1:A:2942:ILE:HD11	1.98	0.45
1:A:3883:LEU:HB3	1:A:3970:LEU:HD13	1.98	0.45
2:B:83:LEU:HD12	2:B:111:PRO:HD3	1.99	0.45
3:C:686:ILE:HD12	3:C:690:GLU:HB2	1.99	0.45
1:A:1917:LYS:O	1:A:1917:LYS:NZ	2.46	0.45
1:A:2126:MET:HG3	1:A:2164:TRP:HE1	1.80	0.45
1:A:976:VAL:O	1:A:981:ARG:NH1	2.49	0.45
1:A:300:TRP:HD1	1:A:303:HIS:HD2	1.64	0.45
3:C:528:ILE:HG23	3:C:529:PRO:HD3	1.98	0.45
3:C:666:VAL:HA	3:C:671:LEU:HD21	1.99	0.45
1:A:317:GLU:OE2	1:A:364:ARG:NE	2.42	0.45
1:A:1856:THR:HG22	1:A:1858:LEU:HD22	1.97	0.45
2:B:93:ASP:HB3	2:B:101:ASN:H	1.82	0.45
3:C:69:SER:HA	3:C:74:TYR:HB2	1.99	0.45
1:A:1507:CYS:SG	1:A:1508:LYS:N	2.90	0.45
1:A:2338:GLU:O	1:A:2342:CYS:CB	2.65	0.45
1:A:4115:ASN:OD1	1:A:4119:ARG:NH2	2.49	0.45
1:A:1623:LEU:HA	1:A:1626:TRP:HD1	1.82	0.45
3:C:464:ALA:HA	3:C:475:ASP:HA	1.99	0.45
2:B:495:LEU:CB	2:B:497:LEU:CD2	2.90	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:OG1	4:D:14:DC:OP1	2.30	0.44
1:A:532:ARG:O	1:A:536:SER:OG	2.32	0.44
1:A:704:PHE:O	1:A:704:PHE:CD1	2.70	0.44
1:A:1212:LEU:HD13	1:A:1220:LEU:HB2	1.99	0.44
1:A:1633:TRP:HA	1:A:1642:LYS:HZ2	1.81	0.44
1:A:3680:LEU:HD22	1:A:3724:GLU:HG2	1.99	0.44
1:A:3772:ASN:HA	1:A:3775:LEU:HB2	1.98	0.44
3:C:356:PHE:HD2	3:C:422:VAL:HG11	1.81	0.44
1:A:65:LEU:HD11	1:A:89:LEU:HD21	1.98	0.44
1:A:1816:ARG:HA	1:A:1816:ARG:HD2	1.80	0.44
1:A:1892:LYS:HD2	1:A:1896:ILE:HD11	1.99	0.44
1:A:3095:ASP:N	1:A:3095:ASP:OD1	2.50	0.44
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	1.99	0.44
1:A:3958:LEU:O	1:A:4110:GLN:NE2	2.50	0.44
1:A:4029:GLN:HB3	1:A:4030:GLU:H	1.47	0.44
2:B:363:ARG:HH11	3:C:269:GLN:HE22	1.65	0.44
1:A:1697:PRO:HG3	1:A:1752:LEU:HD21	2.00	0.44
2:B:342:ASP:OD1	2:B:342:ASP:N	2.50	0.44
1:A:2043:PHE:O	1:A:2047:THR:OG1	2.31	0.44
1:A:238:MET:SD	1:A:283:SER:N	2.91	0.44
1:A:1386:ILE:HG23	1:A:1392:MET:HG3	2.00	0.44
1:A:2842:ARG:O	1:A:2846:THR:OG1	2.31	0.44
1:A:215:PRO:HG2	3:C:553:ILE:HG21	2.00	0.44
1:A:678:LYS:HD2	1:A:737:PRO:HA	1.99	0.44
1:A:1850:VAL:HA	1:A:1853:SER:HB3	1.98	0.44
1:A:9:ARG:HB3	1:A:63:PHE:HE2	1.83	0.44
1:A:68:PHE:HA	1:A:71:LYS:HG2	2.00	0.44
1:A:1869:LYS:HE3	1:A:1869:LYS:HB2	1.87	0.44
1:A:1964:GLY:O	1:A:1968:SER:OG	2.36	0.44
3:C:365:PHE:HB3	3:C:418:CYS:SG	2.57	0.44
1:A:2492:ASP:O	1:A:2496:GLN:NE2	2.51	0.43
1:A:2788:SER:O	1:A:2792:THR:OG1	2.34	0.43
1:A:3531:TYR:HB3	1:A:3796:MET:HA	2.00	0.43
2:B:207:LYS:HB2	2:B:213:ILE:HD11	2.00	0.43
2:B:237:SER:OG	2:B:238:LYS:N	2.51	0.43
1:A:436:GLU:HA	1:A:439:VAL:HG12	2.00	0.43
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.48	0.43
1:A:3629:ARG:HH12	1:A:3634:GLN:HG3	1.84	0.43
1:A:3767:LEU:HD13	1:A:3918:LEU:HD22	2.00	0.43
3:C:363:LYS:HG2	3:C:420:VAL:HG12	1.99	0.43
2:B:485:GLN:NE2	3:C:332:LYS:O	2.39	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:VAL:HG13	3:C:58:LEU:HD11	2.01	0.43
3:C:602:VAL:HA	3:C:606:LYS:HD2	2.00	0.43
1:A:93:LEU:HD12	1:A:100:ILE:HD13	2.00	0.43
1:A:335:LYS:HE2	1:A:376:ILE:HD11	1.99	0.43
1:A:913:ARG:HH22	1:A:2803:ILE:HG13	1.83	0.43
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.91	0.43
1:A:1989:ASN:OD1	1:A:1989:ASN:N	2.45	0.43
1:A:2383:PHE:HE2	1:A:2408:MET:HE1	1.84	0.43
1:A:67:VAL:HA	1:A:70:ARG:HB2	2.00	0.43
1:A:485:GLN:HE22	1:A:2040:MET:HA	1.84	0.43
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	2.01	0.43
1:A:1632:TRP:HB3	1:A:1645:VAL:HG21	2.00	0.43
1:A:3876:SER:O	1:A:3876:SER:OG	2.35	0.43
1:A:1729:PHE:HB2	1:A:1736:PHE:HB2	1.99	0.43
1:A:2784:GLN:HB3	1:A:2785:ILE:H	1.61	0.43
2:B:410:PHE:HB2	2:B:439:PHE:HE1	1.84	0.43
2:B:497:LEU:H	2:B:497:LEU:HG	1.59	0.43
3:C:61:THR:OG1	3:C:62:ASP:N	2.50	0.43
1:A:851:ILE:HD13	1:A:851:ILE:HA	1.89	0.42
1:A:1190:LEU:HA	1:A:1193:LYS:HG2	2.00	0.42
1:A:2387:PRO:O	2:B:158:GLN:NE2	2.46	0.42
1:A:3098:ARG:HE	1:A:3102:TYR:HE2	1.65	0.42
1:A:3138:ILE:HG12	1:A:3189:PHE:HZ	1.84	0.42
1:A:3686:TRP:HH2	1:A:3699:LEU:HD11	1.84	0.42
2:B:143:LEU:O	2:B:145:GLU:N	2.52	0.42
1:A:95:LYS:HA	1:A:834:LEU:HD11	2.00	0.42
1:A:782:ARG:NH1	1:A:3166:ASN:OD1	2.52	0.42
1:A:3011:LEU:HD23	1:A:3047:SER:HB2	2.01	0.42
1:A:3554:PHE:HD1	1:A:3557:ARG:HH21	1.66	0.42
1:A:3829:LEU:HD23	1:A:3829:LEU:HA	1.87	0.42
1:A:346:TYR:HA	1:A:349:ILE:HG22	2.01	0.42
1:A:3623:PRO:HG3	1:A:3633:ILE:HG12	2.02	0.42
2:B:240:GLU:HA	2:B:243:LEU:HD12	2.01	0.42
2:B:245:LYS:O	2:B:246:VAL:CG2	2.67	0.42
1:A:2980:ASP:OD1	1:A:2980:ASP:N	2.46	0.42
2:B:262:LYS:HA	2:B:268:VAL:HG12	2.01	0.42
3:C:116:ASP:O	3:C:120:HIS:ND1	2.49	0.42
1:A:2036:LEU:O	1:A:2040:MET:HB2	2.19	0.42
2:B:51:SER:O	2:B:51:SER:OG	2.38	0.42
3:C:12:LEU:HD13	3:C:38:ILE:HD11	2.02	0.42
1:A:485:GLN:HE21	1:A:2040:MET:HG3	1.85	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1900:PHE:HD1	1:A:1900:PHE:HA	1.76	0.42
1:A:1864:ASP:HA	1:A:1867:ILE:HD12	2.01	0.42
1:A:2190:VAL:HA	1:A:2193:ILE:HG22	2.02	0.42
1:A:3883:LEU:HD13	1:A:3970:LEU:HD22	2.01	0.42
3:C:413:LYS:HD3	3:C:413:LYS:HA	1.87	0.42
3:C:606:LYS:NZ	3:C:608:SER:O	2.53	0.42
1:A:2955:SER:O	1:A:2971:GLN:NE2	2.52	0.42
1:A:3733:ARG:HH22	1:A:4022:LYS:HD2	1.85	0.41
3:C:331:MET:HE3	3:C:331:MET:HB2	1.81	0.41
1:A:3351:ILE:O	1:A:3352:GLU:HB2	2.19	0.41
3:C:353:ARG:HA	3:C:356:PHE:HE1	1.85	0.41
3:C:726:ASP:HA	3:C:729:LEU:HG	2.01	0.41
1:A:205:LYS:O	1:A:209:THR:OG1	2.34	0.41
1:A:680:ILE:HD12	1:A:680:ILE:HA	1.95	0.41
1:A:2286:PRO:HB3	1:A:2329:TYR:CE2	2.56	0.41
1:A:2464:HIS:ND1	1:A:2469:CYS:SG	2.93	0.41
3:C:45:GLN:HE21	3:C:237:PHE:HE1	1.68	0.41
3:C:132:ILE:O	3:C:161:LEU:HA	2.21	0.41
1:A:848:LEU:HD12	1:A:848:LEU:HA	1.91	0.41
1:A:863:GLY:HA2	1:A:3167:ARG:HG3	2.01	0.41
1:A:1137:ILE:HD12	1:A:1137:ILE:HA	1.94	0.41
1:A:1590:THR:OG1	1:A:1632:TRP:NE1	2.46	0.41
1:A:1811:ARG:HE	3:C:626:THR:HG23	1.86	0.41
2:B:346:MET:HB2	2:B:346:MET:HE3	1.66	0.41
3:C:108:LEU:HD13	3:C:147:LEU:HD21	2.03	0.41
3:C:372:ALA:HA	3:C:375:VAL:HG12	2.02	0.41
1:A:12:LEU:HD23	1:A:64:GLY:HA2	2.01	0.41
1:A:473:PRO:HA	1:A:476:ARG:HG2	2.01	0.41
1:A:1532:LEU:HD23	1:A:1532:LEU:HA	1.86	0.41
2:B:422:ASP:N	2:B:422:ASP:OD2	2.53	0.41
3:C:155:LYS:NZ	3:C:215:LEU:O	2.49	0.41
3:C:614:ASN:OD1	3:C:614:ASN:N	2.53	0.41
1:A:214:GLU:HA	1:A:215:PRO:HD2	1.73	0.41
1:A:1141:LYS:HD3	1:A:1141:LYS:HA	1.93	0.41
3:C:339:CYS:O	3:C:395:TYR:HA	2.21	0.41
1:A:117:LYS:HE2	1:A:117:LYS:HB2	1.80	0.41
1:A:862:LEU:HD12	1:A:862:LEU:HA	1.94	0.41
1:A:1605:PHE:O	1:A:1608:ARG:NH2	2.45	0.41
1:A:3489:SER:O	1:A:3489:SER:OG	2.34	0.41
3:C:617:ILE:HA	3:C:620:ILE:HG12	2.01	0.41
1:A:790:LYS:HE2	1:A:790:LYS:HB3	1.88	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:MET:H	1:A:879:MET:HG2	1.66	0.41
1:A:1774:MET:HB3	1:A:1777:LEU:HD21	2.02	0.41
1:A:2801:ASP:N	1:A:2801:ASP:OD1	2.54	0.41
1:A:3620:PRO:HG3	1:A:3638:LYS:HD3	2.03	0.41
1:A:3753:LYS:HE2	1:A:3803:ILE:HG21	2.01	0.41
3:C:247:TRP:HB3	3:C:263:ALA:HB3	2.03	0.41
1:A:1246:GLY:HA2	1:A:1247:PRO:HD3	1.95	0.41
1:A:1474:ASP:OD1	1:A:1474:ASP:N	2.52	0.41
1:A:2256:ILE:H	1:A:2256:ILE:HG12	1.64	0.41
1:A:2352:HIS:HB3	1:A:2360:PHE:HB2	2.03	0.41
3:C:324:SER:OG	3:C:325:LYS:N	2.53	0.41
1:A:2328:ARG:NH1	1:A:2332:GLU:OE2	2.55	0.40
3:C:138:LEU:HD23	3:C:138:LEU:HA	1.95	0.40
1:A:96:MET:HB2	1:A:100:ILE:HD11	2.04	0.40
1:A:3582:GLU:OE2	1:A:3671:ASN:ND2	2.55	0.40
1:A:3975:LYS:HA	1:A:3975:LYS:HD3	1.89	0.40
4:D:19:DA:H2'	4:D:20:DT:H71	2.04	0.40
1:A:76:ILE:HD13	1:A:76:ILE:HA	1.96	0.40
1:A:2834:GLN:HE21	1:A:2834:GLN:HB2	1.59	0.40
1:A:3714:GLU:H	1:A:3714:GLU:HG2	1.79	0.40
1:A:3772:ASN:HD22	1:A:3788:LEU:HB2	1.86	0.40
1:A:3972:LEU:HD23	1:A:3972:LEU:HA	1.91	0.40
2:B:94:LYS:HB3	2:B:103:TYR:CD1	2.57	0.40
3:C:322:PRO:HB2	3:C:323:PHE:H	1.65	0.40
1:A:919:LEU:HD11	1:A:968:VAL:HG23	2.03	0.40
1:A:1484:LEU:HD22	1:A:1524:LEU:HD21	2.03	0.40
1:A:1725:GLN:HG2	3:C:622:GLN:HG3	2.04	0.40
1:A:3962:ARG:NH1	1:A:4128:MET:O	2.55	0.40
2:B:238:LYS:HZ3	2:B:238:LYS:HG2	1.75	0.40
1:A:181:LEU:HB3	1:A:189:MET:HE1	2.03	0.40
1:A:663:ILE:HD13	1:A:663:ILE:HA	1.93	0.40
2:B:358:LYS:HD2	2:B:358:LYS:HA	1.84	0.40
2:B:510:LYS:HE2	2:B:510:LYS:HB2	1.97	0.40
3:C:666:VAL:HB	3:C:675:TRP:CD1	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3594/4128 (87%)	3123 (87%)	459 (13%)	12 (0%)	41	75
2	B	486/609 (80%)	409 (84%)	74 (15%)	3 (1%)	25	63
3	C	645/732 (88%)	549 (85%)	92 (14%)	4 (1%)	25	63
All	All	4725/5469 (86%)	4081 (86%)	625 (13%)	19 (0%)	38	71

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1476	HIS
1	A	2826	LEU
1	A	3352	GLU
2	B	144	SER
1	A	215	PRO
1	A	3058	ASP
1	A	3311	ASN
2	B	245	LYS
3	C	299	ASP
3	C	322	PRO
1	A	1021	VAL
1	A	3028	ASN
1	A	3083	SER
3	C	300	ASP
1	A	661	PRO
1	A	2548	PRO
1	A	2547	SER
3	C	193	PRO
2	B	499	GLU

### 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	3174/3671 (86%)	3146 (99%)	28 (1%)	78	87
2	B	444/548 (81%)	436 (98%)	8 (2%)	59	77
3	C	587/649 (90%)	586 (100%)	1 (0%)	93	96
All	All	4205/4868 (86%)	4168 (99%)	37 (1%)	79	87

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	100	ILE
1	A	215	PRO
1	A	284	THR
1	A	364	ARG
1	A	396	PHE
1	A	739	ASN
1	A	789	TYR
1	A	1051	LYS
1	A	1213	LYS
1	A	1639	LEU
1	A	1735	ARG
1	A	1752	LEU
1	A	1837	ARG
1	A	2183	HIS
1	A	2214	ARG
1	A	3058	ASP
1	A	3301	LEU
1	A	3310	ASN
1	A	3335	ARG
1	A	3352	GLU
1	A	3642	LYS
1	A	3650	LYS
1	A	3653	ARG
1	A	3696	ARG
1	A	3743	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	4023	LYS
1	A	4036	LYS
2	B	36	ASP
2	B	217	TYR
2	B	292	THR
2	B	368	VAL
2	B	409	TYR
2	B	470	ARG
2	B	493	LEU
2	B	497	LEU
3	C	365	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	192	ASN
1	A	303	HIS
1	A	442	GLN
1	A	485	GLN
1	A	720	GLN
1	A	867	ASN
1	A	1048	GLN
1	A	1115	HIS
1	A	1598	ASN
1	A	1610	ASN
1	A	1624	GLN
1	A	1772	HIS
1	A	1866	GLN
1	A	2103	HIS
1	A	2135	ASN
1	A	2222	HIS
1	A	2283	ASN
1	A	2365	ASN
1	A	2432	GLN
1	A	2496	GLN
1	A	2834	GLN
1	A	2885	GLN
1	A	3112	GLN
1	A	3122	HIS
1	A	3251	ASN
1	A	3379	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	3383	GLN
1	A	3524	ASN
1	A	3573	ASN
1	A	3760	GLN
1	A	3772	ASN
1	A	3822	GLN
1	A	4110	GLN
2	B	52	GLN
2	B	152	ASN
2	B	264	ASN
2	B	326	GLN
2	B	360	HIS
3	C	269	GLN
3	C	411	HIS
3	C	511	HIS
3	C	551	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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 ⓘ

There are no chain breaks in this entry.

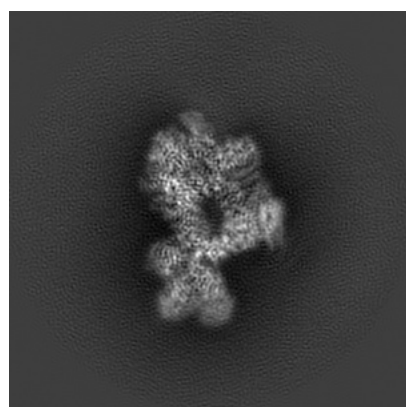
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22626. These allow visual inspection of the internal detail of the map and identification of artifacts.

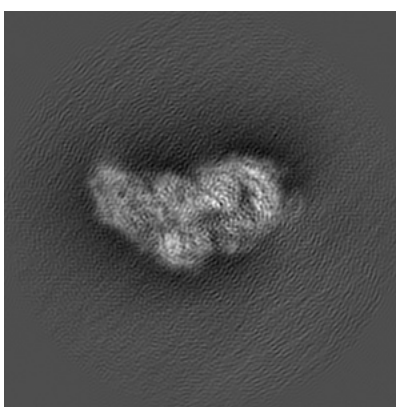
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

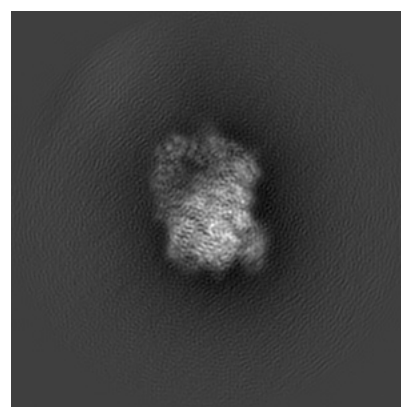
#### 6.1.1 Primary map



X



Y

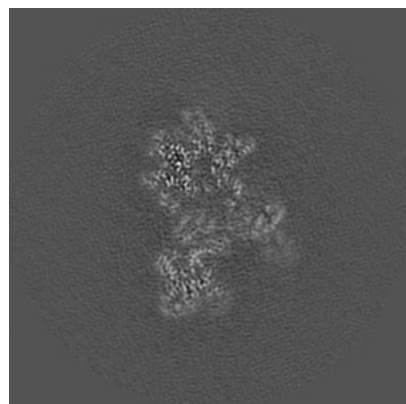


Z

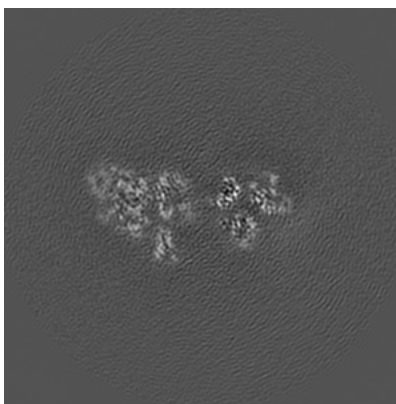
The images above show the map projected in three orthogonal directions.

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

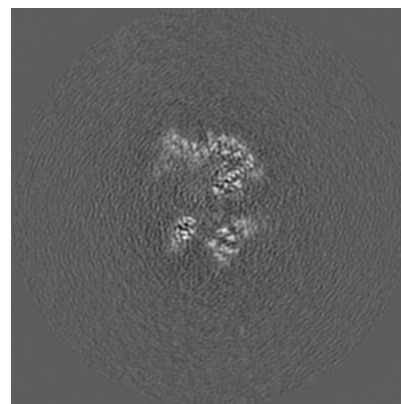
#### 6.2.1 Primary map



X Index: 176



Y Index: 176

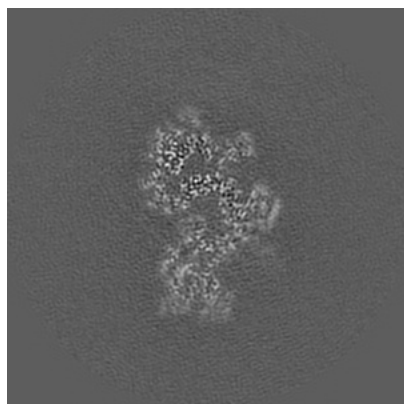


Z Index: 176

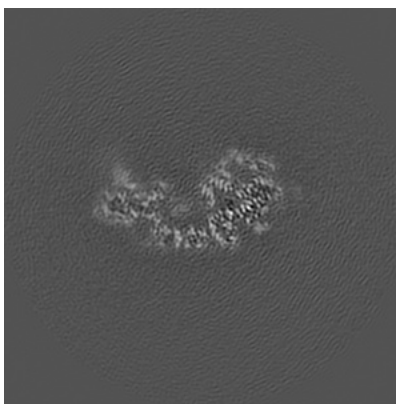
The images above show central slices of the map in three orthogonal directions.

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

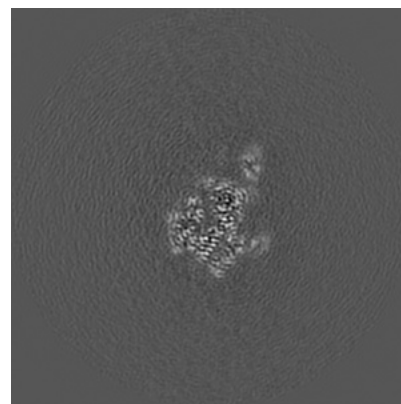
### 6.3.1 Primary map



X Index: 187



Y Index: 149



Z Index: 199

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

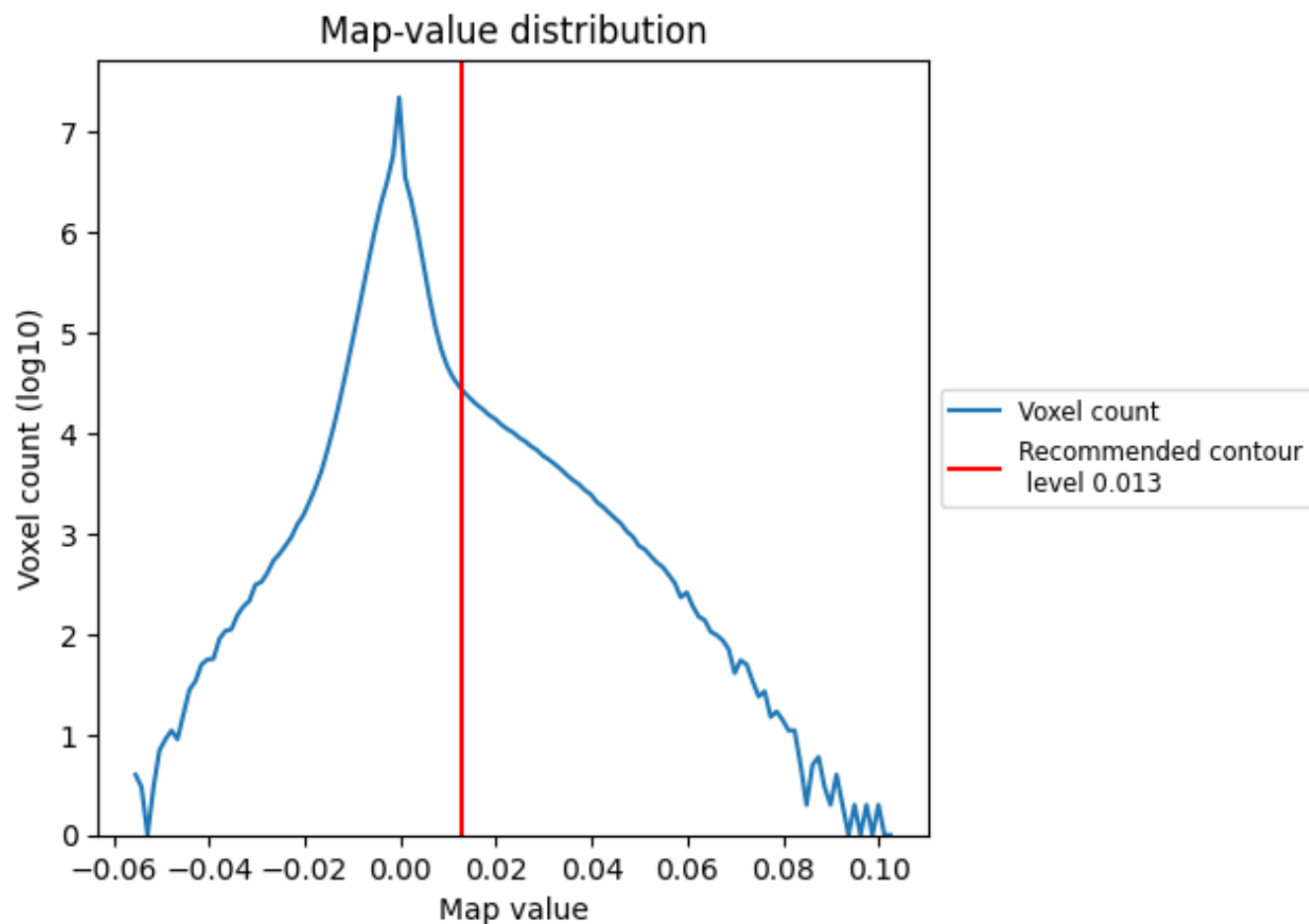
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

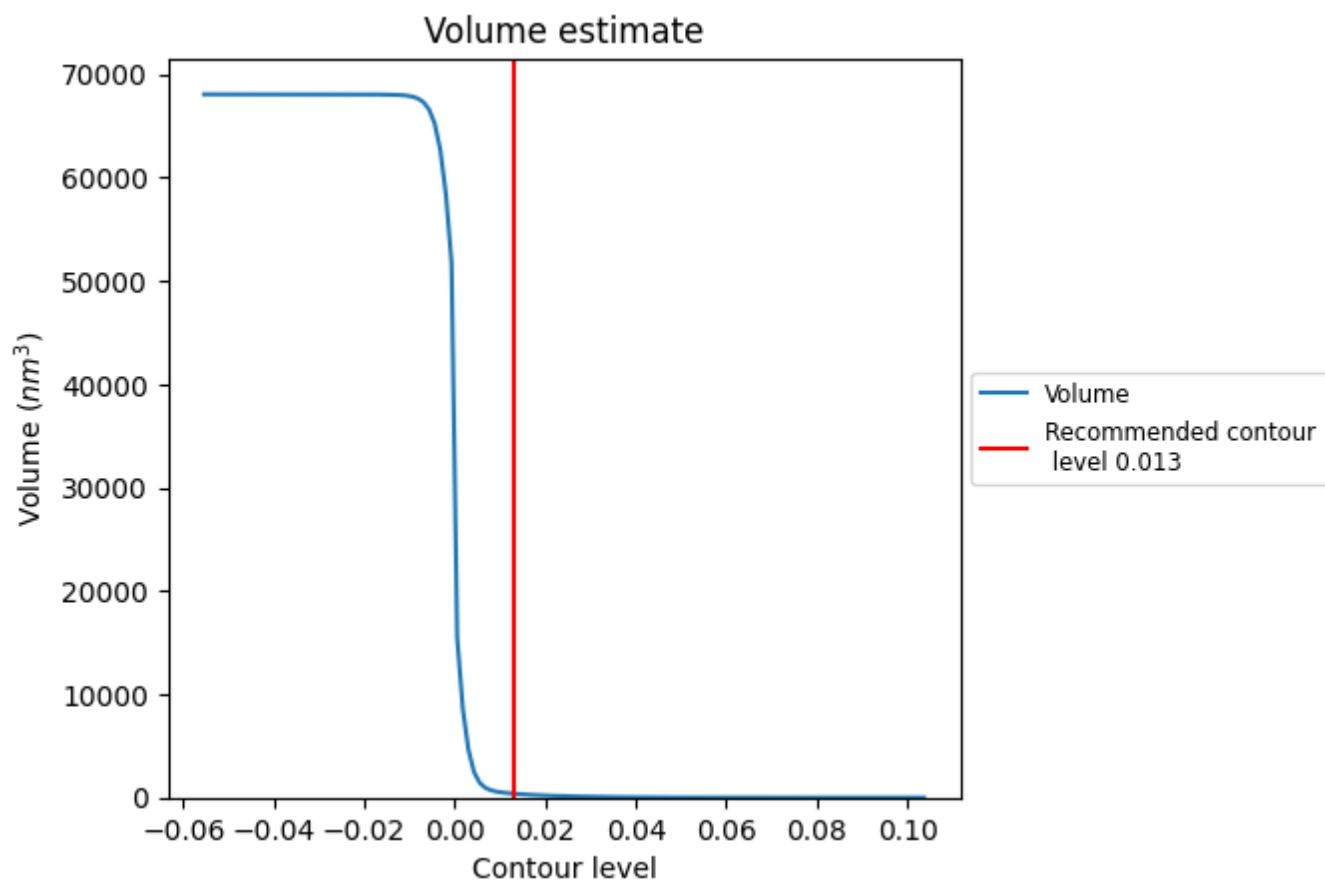
This section contains the results of statistical analysis of the map.

### 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.

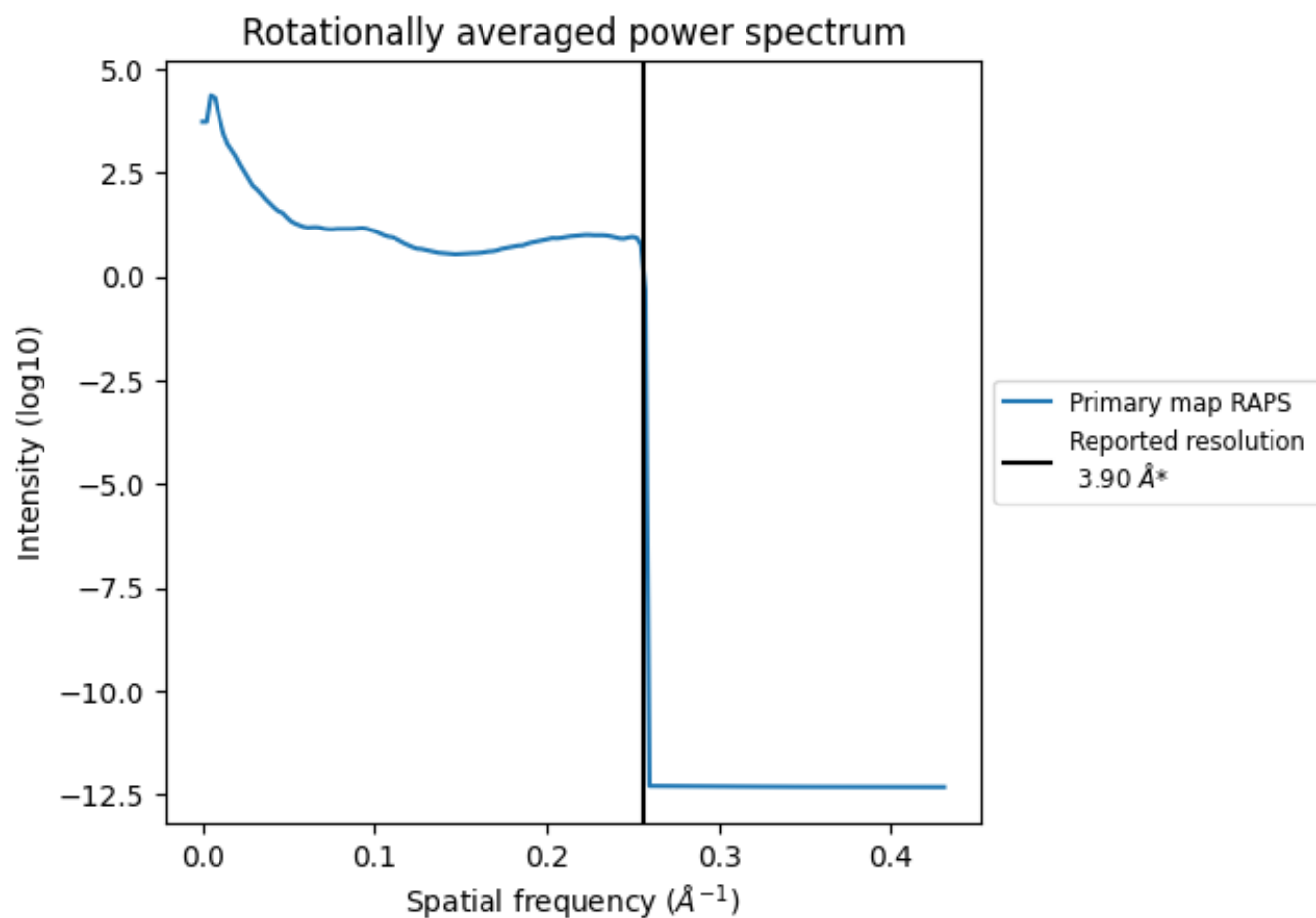
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm<sup>3</sup>; this corresponds to an approximate mass of 341 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 0.256 Å<sup>-1</sup>



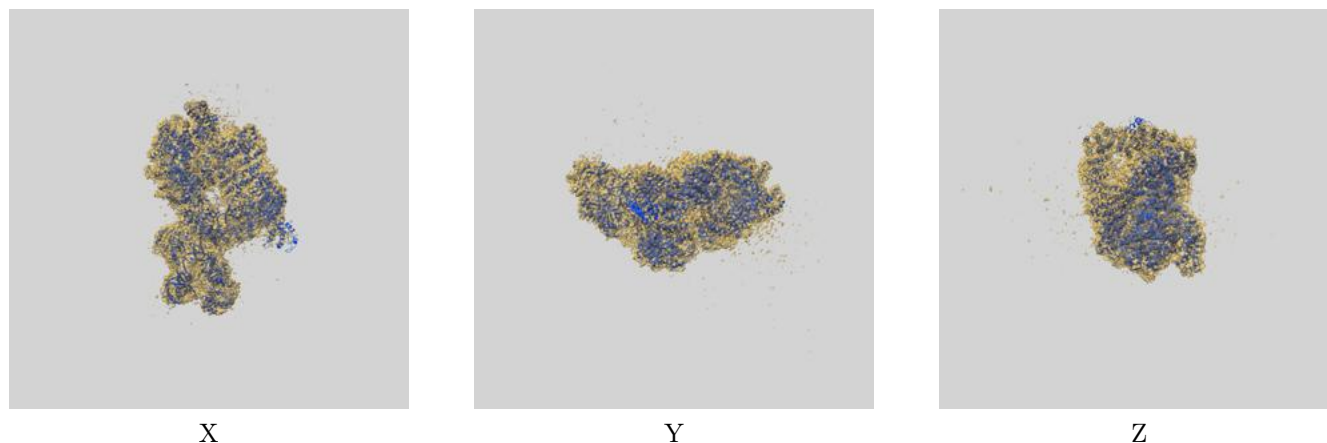
## 8 Fourier-Shell correlation

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

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

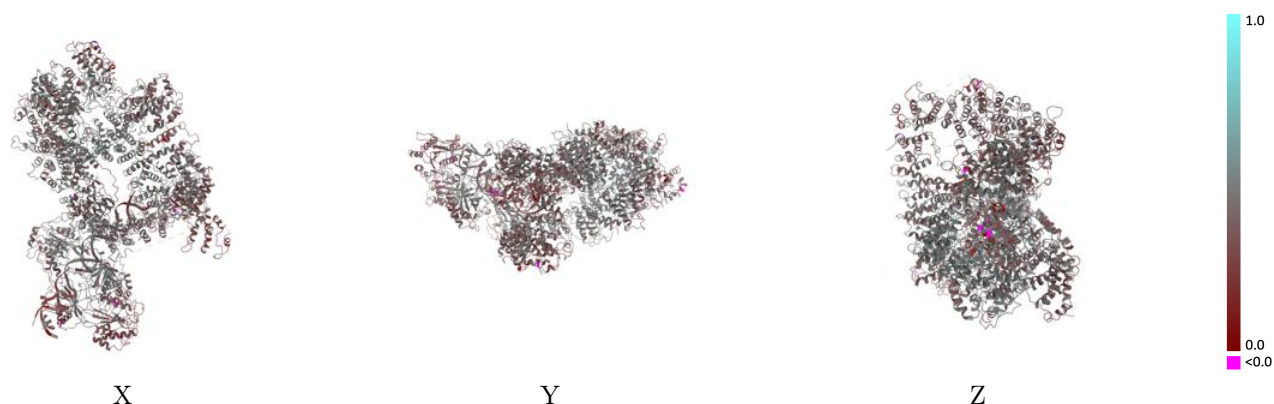
This section contains information regarding the fit between EMDB map EMD-22626 and PDB model 7K1N. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

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



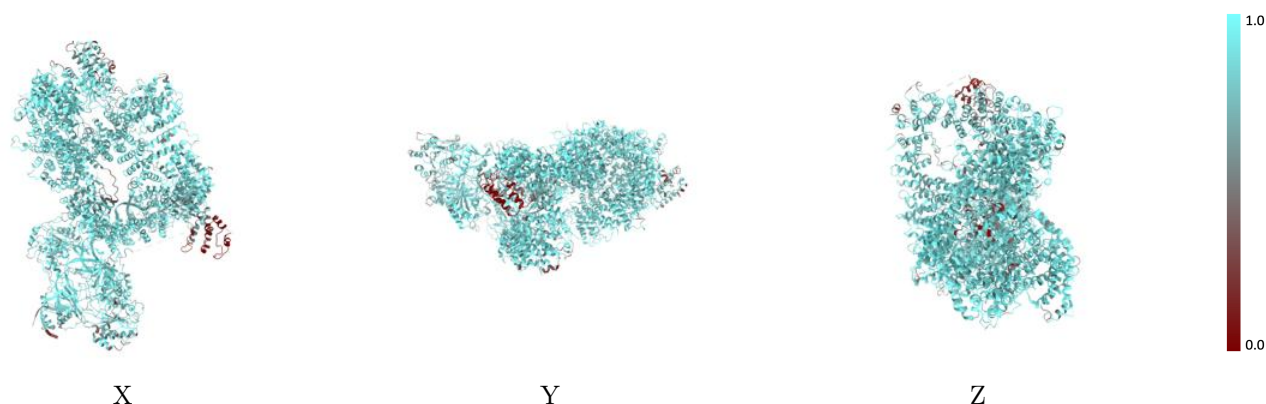
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



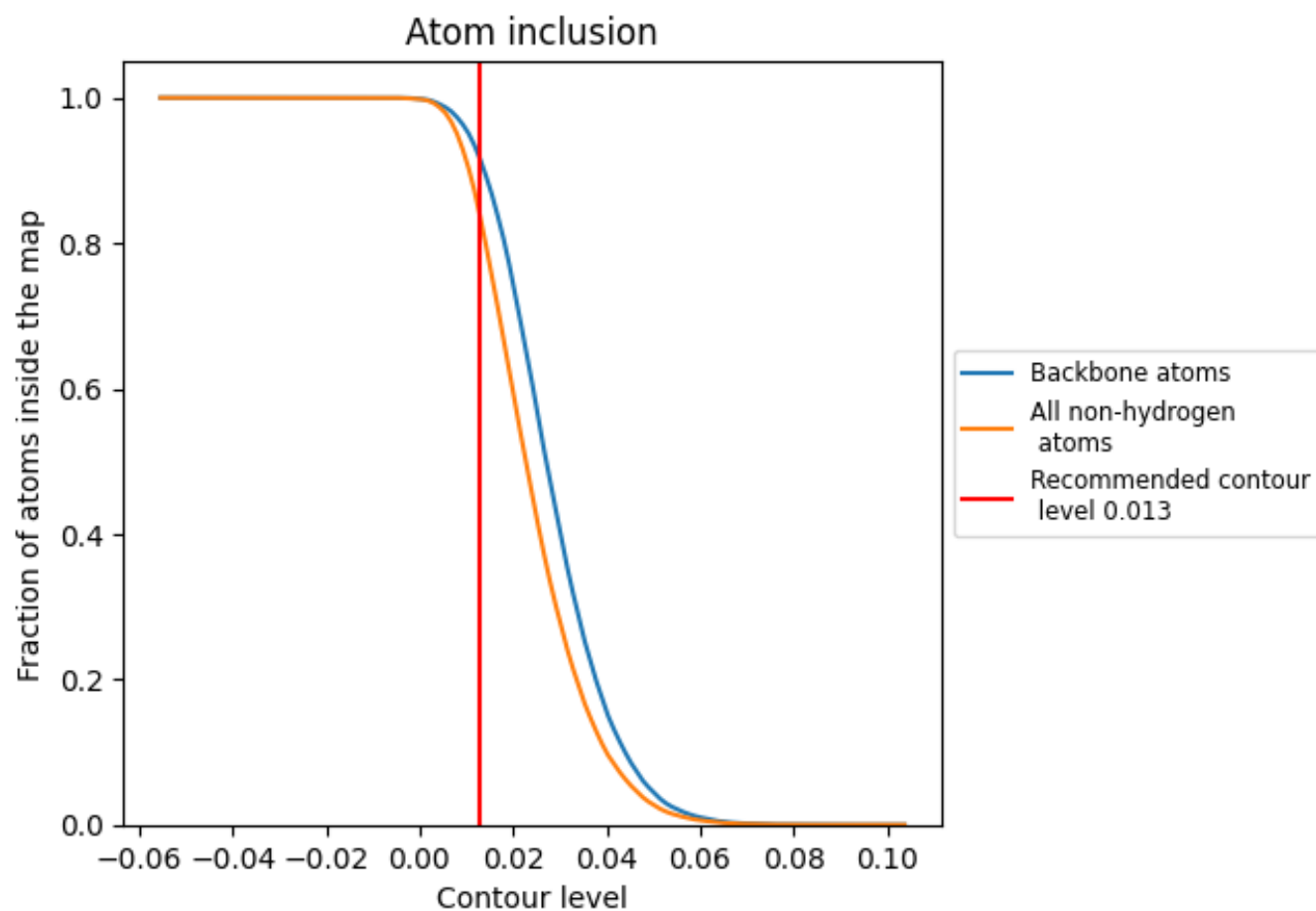
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8351	<div><div></div></div> 0.4170
A	<div><div></div></div> 0.8594	<div><div></div></div> 0.4300
B	<div><div></div></div> 0.8488	<div><div></div></div> 0.4160
C	<div><div></div></div> 0.6847	<div><div></div></div> 0.3710
D	<div><div></div></div> 0.8926	<div><div></div></div> 0.3510
E	<div><div></div></div> 0.7584	<div><div></div></div> 0.2840
F	<div><div></div></div> 0.8588	<div><div></div></div> 0.3510
G	<div><div></div></div> 0.9000	<div><div></div></div> 0.3430

1.0

0.0

<0.0