



## Full wwPDB EM Validation Report ⓘ

Apr 10, 2022 – 04:14 am BST

PDB ID : 7R03  
EMDB ID : EMD-14218  
Title : Neurofibromin occluded conformation  
Authors : Chaker-Margot, M.; Scheffzek, K.; Maier, T.  
Deposited on : 2022-02-01  
Resolution : 3.60 Å(reported)  
Based on initial models : 2E2X, 6V65

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.

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

EMDB validation analysis : 0.0.0.dev97  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

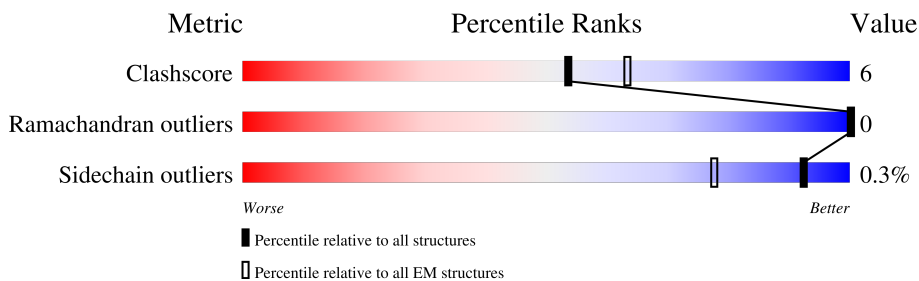
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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	2818	
1	B	2818	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 35621 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.

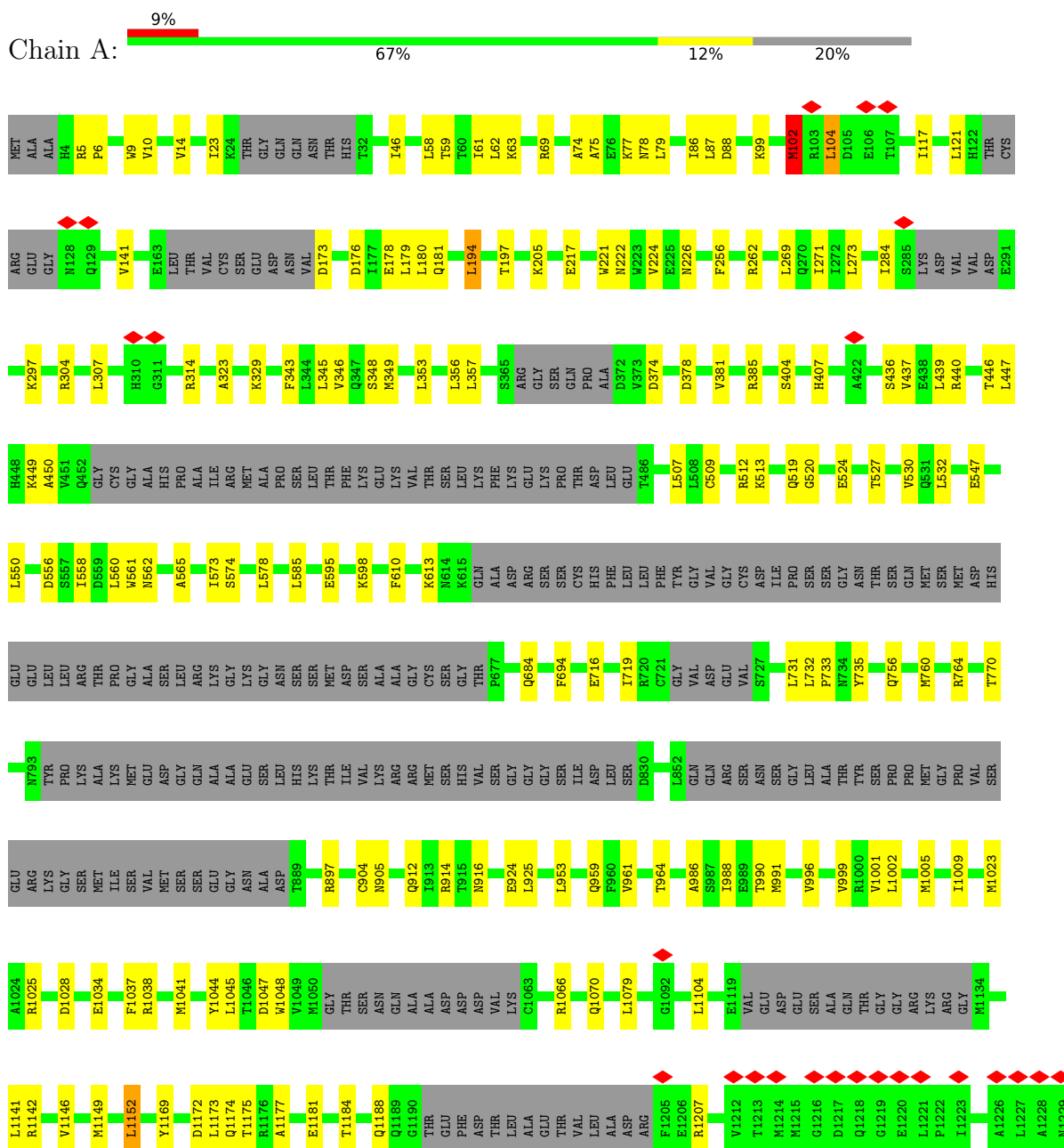
- Molecule 1 is a protein called Isoform I of Neurofibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2241	17792	11438	2996	3243	115	0	0
1	B	2246	17829	11459	3005	3250	115	0	0

### 3 Residue-property plots

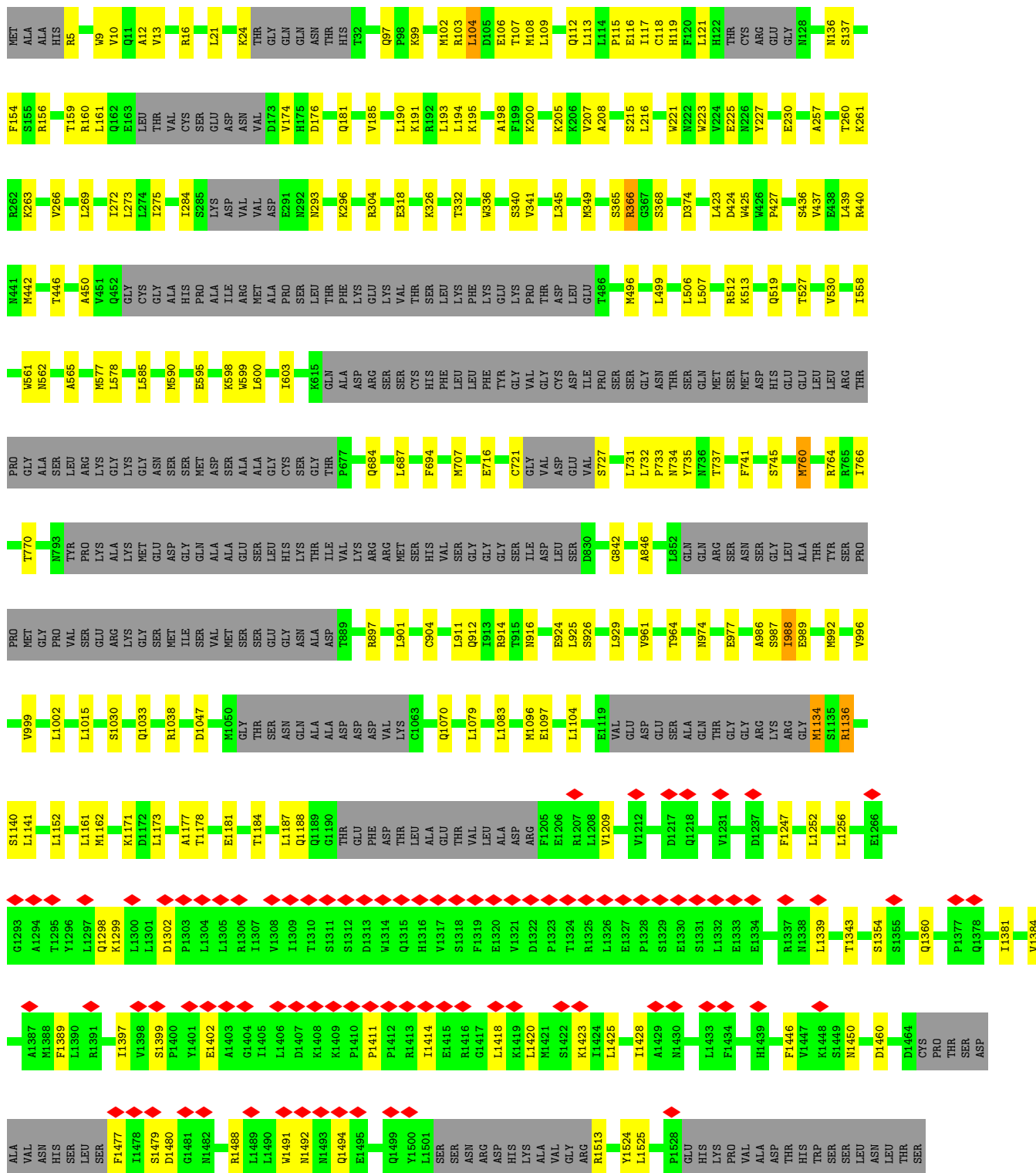
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





● Molecule 1: Isoform I of Neurofibromin





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	360000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	52.359	Depositor
Minimum map value	-21.262	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.935	Depositor
Recommended contour level	6.0	Depositor
Map size ( $\text{\AA}$ )	541.696, 541.696, 541.696	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.058, 1.058, 1.058	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	0.31	0/18149	0.63	17/24597 (0.1%)
1	B	0.32	0/18188	0.66	18/24651 (0.1%)
All	All	0.32	0/36337	0.64	35/49248 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
All	All	0	9

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	2012	ASP	CB-CG-OD1	8.54	125.99	118.30
1	A	1141	LEU	CA-CB-CG	8.18	134.12	115.30
1	B	2715	ASP	CB-CG-OD1	8.09	125.58	118.30
1	A	102	MET	CA-CB-CG	7.71	126.41	113.30
1	A	988	ILE	CG1-CB-CG2	-7.62	94.64	111.40
1	A	356	LEU	CA-CB-CG	7.46	132.45	115.30
1	B	988	ILE	CG1-CB-CG2	-7.23	95.49	111.40
1	A	273	LEU	CA-CB-CG	7.06	131.54	115.30
1	B	423	LEU	CA-CB-CG	6.76	130.86	115.30
1	A	88	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	1152	LEU	CA-CB-CG	6.48	130.20	115.30
1	A	1152	LEU	CA-CB-CG	6.46	130.16	115.30
1	B	104	LEU	CA-CB-CG	6.28	129.74	115.30
1	B	216	LEU	CA-CB-CG	6.16	129.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	104	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	225	GLU	CA-CB-CG	5.77	126.10	113.40
1	B	161	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	2089	LEU	CA-CB-CG	5.76	128.55	115.30
1	B	1252	LEU	CA-CB-CG	5.57	128.10	115.30
1	B	1932	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	2422	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	760	MET	CB-CG-SD	5.46	128.79	112.40
1	A	1967	MET	CA-CB-CG	5.41	122.50	113.30
1	B	225	GLU	N-CA-CB	5.35	120.23	110.60
1	B	1935	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	1829	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	B	2089	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	1967	MET	CA-CB-CG	5.24	122.20	113.30
1	A	2422	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	194	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	2033	MET	CA-CB-CG	5.19	122.12	113.30
1	B	1141	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	2060	LEU	CB-CG-CD2	5.11	119.69	111.00
1	A	2067	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	MET	Peptide
1	A	1070	GLN	Peptide
1	A	986	ALA	Peptide
1	B	102	MET	Peptide
1	B	1134	MET	Peptide
1	B	366	ARG	Peptide
1	B	368	SER	Peptide
1	B	424	ASP	Peptide
1	B	986	ALA	Peptide

## 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	17792	0	18031	193	0
1	B	17829	0	18071	211	0
All	All	35621	0	36102	397	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 (397) 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:117:ILE:O	1:A:121:LEU:HB2	1.70	0.90
1:B:109:LEU:O	1:B:113:LEU:HB2	1.83	0.77
1:B:1742:GLN:HG2	1:B:1761:ILE:HG12	1.77	0.65
1:A:353:LEU:O	1:A:357:LEU:HB2	1.97	0.64
1:A:1748:ARG:HA	1:A:1756:VAL:O	1.99	0.63
1:B:1177:ALA:HB2	1:B:1848:LEU:HD23	1.78	0.63
1:B:904:CYS:HB3	1:B:914:ARG:HE	1.63	0.63
1:B:760:MET:HG3	1:B:846:ALA:HB2	1.80	0.63
1:A:217:GLU:HB2	1:A:269:LEU:HD21	1.80	0.62
1:A:2274:VAL:O	1:A:2277:LEU:HB2	1.99	0.62
1:B:195:LYS:O	1:B:198:ALA:HB3	2.00	0.62
1:A:1925:LEU:HA	1:A:1928:MET:HG2	1.82	0.61
1:B:2250:LEU:HB2	1:B:2273:THR:HG21	1.81	0.61
1:A:1689:ASP:HB3	1:A:1757:PHE:HB2	1.83	0.61
1:B:1177:ALA:O	1:B:1181:GLU:N	2.34	0.61
1:B:2267:GLN:O	1:B:2270:ILE:HB	2.01	0.61
1:B:425:TRP:HB3	1:B:427:PRO:HD2	1.83	0.60
1:A:1146:VAL:HA	1:A:1149:MET:HG2	1.84	0.60
1:B:996:VAL:HG12	1:B:1015:LEU:HD21	1.82	0.60
1:A:62:LEU:HB3	1:A:86:ILE:HG21	1.84	0.59
1:B:284:ILE:HD11	1:B:296:LYS:HE3	1.83	0.59
1:B:595:GLU:HA	1:B:598:LYS:HD2	1.83	0.59
1:A:1742:GLN:HG2	1:A:1761:ILE:HG12	1.83	0.59
1:B:269:LEU:O	1:B:273:LEU:HB2	2.03	0.59
1:A:2607:LYS:HA	1:A:2643:LYS:HD2	1.85	0.58
1:B:2030:ILE:HD11	1:B:2073:LEU:HD12	1.84	0.58
1:B:2274:VAL:O	1:B:2277:LEU:HB2	2.04	0.58
1:A:329:LYS:NZ	1:A:378:ASP:O	2.36	0.58
1:A:764:ARG:NH1	1:A:924:GLU:OE1	2.36	0.58
1:A:507:LEU:HG	1:A:512:ARG:HH22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ALA:O	1:A:79:LEU:HB2	2.04	0.58
1:A:1038:ARG:NH1	1:A:1079:LEU:O	2.38	0.57
1:A:1688:ILE:HG13	1:A:1694:LEU:HD12	1.85	0.57
1:B:1689:ASP:HB3	1:B:1757:PHE:HB2	1.87	0.57
1:B:737:THR:HG21	1:B:766:ILE:HA	1.87	0.57
1:B:1748:ARG:HA	1:B:1756:VAL:O	2.04	0.56
1:A:58:LEU:HA	1:A:61:ILE:HD12	1.86	0.56
1:B:1488:ARG:O	1:B:1492:ASN:ND2	2.38	0.56
1:A:2366:ASN:ND2	1:A:2413:GLN:O	2.39	0.56
1:B:205:LYS:HD3	1:B:208:ALA:HB2	1.87	0.56
1:A:1399:SER:HB3	1:A:1402:GLU:HB2	1.88	0.56
1:A:2182:GLU:OE2	1:A:2279:LYS:NZ	2.37	0.56
1:B:2267:GLN:HA	1:B:2270:ILE:HD12	1.88	0.56
1:B:507:LEU:HG	1:B:512:ARG:HH22	1.70	0.56
1:B:1660:ASN:OD1	1:B:1759:ASN:ND2	2.36	0.56
1:B:513:LYS:NZ	1:B:519:GLN:O	2.39	0.56
1:B:1446:PHE:O	1:B:1450:ASN:ND2	2.39	0.56
1:B:2710:ILE:O	1:B:2713:PHE:HB3	2.06	0.56
1:A:904:CYS:O	1:A:914:ARG:NH2	2.38	0.55
1:A:14:VAL:HG13	1:A:61:ILE:HD11	1.87	0.55
1:A:732:LEU:HG	1:A:770:THR:HG23	1.87	0.55
1:A:2080:PRO:HB3	1:A:2208:TRP:HB2	1.89	0.55
1:A:2422:LEU:HD21	1:A:2602:LEU:HD21	1.88	0.55
1:A:2064:MET:O	1:A:2068:SER:HB2	2.07	0.55
1:B:257:ALA:HB1	1:B:263:LYS:HG2	1.88	0.55
1:A:1181:GLU:O	1:A:1184:THR:HB	2.07	0.55
1:B:156:ARG:O	1:B:159:THR:HB	2.06	0.55
1:A:450:ALA:HB1	1:A:532:LEU:HD21	1.89	0.55
1:B:1590:ARG:NH1	1:B:1625:THR:OG1	2.40	0.54
1:B:117:ILE:O	1:B:121:LEU:N	2.41	0.54
1:A:574:SER:O	1:A:578:LEU:HB2	2.07	0.54
1:A:2419:ALA:HA	1:A:2422:LEU:HD23	1.89	0.54
1:B:115:PRO:O	1:B:119:HIS:ND1	2.39	0.54
1:B:721:CYS:HG	1:B:727:SER:N	2.06	0.54
1:B:2080:PRO:HB3	1:B:2208:TRP:HB2	1.89	0.54
1:B:221:TRP:HZ2	1:B:326:LYS:HG3	1.73	0.54
1:A:1446:PHE:O	1:A:1450:ASN:ND2	2.40	0.54
1:A:1958:ILE:HG21	1:A:1996:THR:HG21	1.89	0.54
1:B:1399:SER:HB3	1:B:1402:GLU:HB2	1.89	0.54
1:A:513:LYS:NZ	1:A:519:GLN:O	2.40	0.53
1:A:2030:ILE:HD11	1:A:2073:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2033:MET:HB2	1:A:2060:LEU:HD22	1.90	0.53
1:A:304:ARG:HE	1:A:307:LEU:HD12	1.73	0.53
1:B:437:VAL:HG22	1:B:440:ARG:HH21	1.74	0.53
1:B:1491:TRP:HA	1:B:1494:GLN:HB2	1.89	0.53
1:B:2292:LYS:HB2	1:B:2342:ILE:HG13	1.90	0.53
1:A:1411:PRO:HD2	1:A:1414:ILE:HD12	1.91	0.53
1:A:1177:ALA:HB2	1:A:1848:LEU:HD23	1.90	0.53
1:B:2607:LYS:HA	1:B:2643:LYS:HD2	1.91	0.53
1:A:1483:VAL:HG21	1:A:1636:ASP:HB3	1.90	0.53
1:A:2348:TRP:O	1:A:2352:GLN:NE2	2.42	0.53
1:B:2373:LEU:HD12	1:B:2388:THR:HG23	1.91	0.53
1:A:2710:ILE:O	1:A:2713:PHE:HB3	2.08	0.53
1:B:764:ARG:NH1	1:B:924:GLU:OE1	2.38	0.53
1:A:87:LEU:HD22	1:A:141:VAL:HG21	1.90	0.52
1:A:2683:GLN:HA	1:A:2688:ASN:HB2	1.92	0.52
1:B:10:VAL:O	1:B:13:VAL:HB	2.08	0.52
1:A:1360:GLN:HE21	1:A:1477:PHE:HB2	1.74	0.52
1:B:1688:ILE:HG13	1:B:1694:LEU:HD12	1.89	0.52
1:B:2033:MET:HB2	1:B:2060:LEU:HD22	1.92	0.52
1:A:1725:LEU:HB2	1:A:1790:THR:HG23	1.90	0.52
1:B:911:LEU:HA	1:B:914:ARG:HD3	1.92	0.52
1:A:2038:ASP:OD1	1:A:2214:ARG:NH1	2.42	0.52
1:B:1679:LEU:HB3	1:B:1685:LEU:HD11	1.91	0.52
1:A:595:GLU:HA	1:A:598:LYS:HD2	1.91	0.52
1:A:1238:GLU:O	1:A:1241:ARG:HB3	2.10	0.52
1:A:1967:MET:O	1:A:1970:SER:OG	2.27	0.52
1:B:190:LEU:O	1:B:193:LEU:HB2	2.11	0.51
1:B:926:SER:HB3	1:B:929:LEU:HB2	1.92	0.51
1:A:912:GLN:O	1:A:916:ASN:ND2	2.44	0.51
1:B:2607:LYS:HE2	1:B:2639:LEU:HD12	1.92	0.51
1:A:2281:GLN:OE1	1:A:2319:GLN:NE2	2.43	0.51
1:B:2589:LEU:HD12	1:B:2591:ASP:H	1.74	0.51
1:A:117:ILE:O	1:A:121:LEU:CB	2.52	0.51
1:B:600:LEU:HA	1:B:603:ILE:HD12	1.91	0.51
1:A:1298:GLN:O	1:A:1302:ASP:HB2	2.10	0.51
1:B:446:THR:O	1:B:450:ALA:N	2.44	0.51
1:B:1209:VAL:HG21	1:B:1525:LEU:HD11	1.92	0.51
1:A:1023:MET:SD	1:A:1038:ARG:NH2	2.84	0.51
1:A:1173:LEU:HB3	1:A:1848:LEU:HD11	1.93	0.51
1:B:332:THR:O	1:B:425:TRP:NE1	2.38	0.51
1:A:343:PHE:HA	1:A:346:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1590:ARG:NH1	1:A:1625:THR:OG1	2.44	0.51
1:B:988:ILE:HG22	1:B:992:MET:HG2	1.93	0.51
1:B:2038:ASP:OD1	1:B:2214:ARG:NH1	2.43	0.51
1:A:77:LYS:NZ	1:A:78:ASN:OD1	2.44	0.51
1:A:404:SER:HA	1:A:407:HIS:HD2	1.76	0.51
1:B:1178:THR:O	1:B:1181:GLU:HB2	2.10	0.51
1:B:1725:LEU:HB2	1:B:1790:THR:HG23	1.93	0.51
1:B:2600:THR:HG21	1:B:2682:LEU:HD21	1.93	0.51
1:B:1732:VAL:HG12	1:B:1745:SER:HA	1.93	0.50
1:A:2065:LEU:HD22	1:A:2100:SER:HB2	1.94	0.50
1:A:74:ALA:O	1:A:78:ASN:HB2	2.12	0.50
1:A:684:GLN:NE2	1:A:716:GLU:OE2	2.45	0.50
1:A:1142:ARG:HH22	1:A:1174:GLN:HB3	1.76	0.50
1:A:2216:ALA:O	1:A:2224:GLN:NE2	2.38	0.50
1:B:996:VAL:HA	1:B:999:VAL:HG12	1.93	0.50
1:B:1360:GLN:HE21	1:B:1477:PHE:HB2	1.76	0.50
1:A:1679:LEU:HB3	1:A:1685:LEU:HD11	1.92	0.50
1:A:1972:GLN:OE1	1:B:1882:ASN:ND2	2.44	0.50
1:A:1849:ARG:HD3	1:A:1879:ILE:HB	1.92	0.50
1:A:2378:ARG:HH22	1:A:2609:THR:HG22	1.76	0.50
1:B:260:THR:HA	1:B:263:LYS:HB2	1.94	0.50
1:B:272:ILE:HA	1:B:275:ILE:HD12	1.93	0.50
1:A:2088:PHE:O	1:A:2226:ARG:NH1	2.45	0.49
1:B:223:TRP:NE1	1:B:227:TYR:OH	2.45	0.49
1:B:732:LEU:HG	1:B:770:THR:HG23	1.94	0.49
1:A:562:ASN:ND2	1:A:565:ALA:O	2.45	0.49
1:A:1860:THR:HG22	1:A:1865:LEU:HD11	1.94	0.49
1:A:1996:THR:HG22	1:A:2006:LYS:HD3	1.93	0.49
1:B:374:ASP:OD2	1:B:374:ASP:N	2.46	0.49
1:B:999:VAL:HG23	1:B:1002:LEU:HD12	1.94	0.49
1:A:1987:ASP:OD1	1:A:1987:ASP:N	2.43	0.49
1:B:103:ARG:HH22	1:B:106:GLU:H	1.60	0.49
1:A:374:ASP:OD2	1:A:374:ASP:N	2.45	0.49
1:A:446:THR:O	1:A:450:ALA:N	2.46	0.49
1:B:341:VAL:O	1:B:345:LEU:N	2.45	0.49
1:A:1732:VAL:HG12	1:A:1745:SER:HA	1.95	0.49
1:B:1718:VAL:HG13	1:B:1735:LYS:HG2	1.95	0.49
1:A:23:ILE:O	1:A:69:ARG:NH1	2.45	0.48
1:A:999:VAL:HG23	1:A:1002:LEU:HD12	1.94	0.48
1:B:1038:ARG:HD2	1:B:1083:LEU:HD13	1.95	0.48
1:A:2316:LEU:HD12	1:A:2319:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:VAL:HG21	1:B:190:LEU:HB3	1.95	0.48
1:B:599:TRP:CE2	1:B:603:ILE:HD11	2.48	0.48
1:B:174:VAL:HG22	1:B:176:ASP:H	1.79	0.48
1:B:1411:PRO:HD2	1:B:1414:ILE:HD12	1.94	0.48
1:B:558:ILE:HA	1:B:561:TRP:HB2	1.95	0.48
1:B:2281:GLN:OE1	1:B:2319:GLN:NE2	2.45	0.48
1:A:1169:TYR:OH	1:A:1835:ASN:OD1	2.31	0.48
1:A:1744:THR:HG23	1:A:1759:ASN:HB2	1.94	0.48
1:B:2644:ILE:HD13	1:B:2647:LEU:HD12	1.95	0.48
1:A:345:LEU:O	1:A:348:SER:OG	2.32	0.48
1:B:12:ALA:O	1:B:16:ARG:N	2.46	0.48
1:B:897:ARG:O	1:B:901:LEU:HB2	2.13	0.48
1:B:2088:PHE:O	1:B:2226:ARG:NH1	2.46	0.48
1:B:2303:GLN:O	1:B:2706:TYR:OH	2.30	0.48
1:A:1047:ASP:OD1	1:A:1047:ASP:N	2.47	0.47
1:B:2316:LEU:HD12	1:B:2319:GLN:HE21	1.79	0.47
1:A:6:PRO:HB2	1:B:2637:HIS:CE1	2.49	0.47
1:A:1845:ASP:OD2	1:A:1847:SER:OG	2.33	0.47
1:B:2644:ILE:HD12	1:B:2660:ILE:HG23	1.95	0.47
1:B:446:THR:HG21	1:B:496:MET:HE1	1.96	0.47
1:B:2422:LEU:HD21	1:B:2602:LEU:HD21	1.96	0.47
1:A:284:ILE:O	1:A:297:LYS:NZ	2.46	0.47
1:A:1582:ASN:ND2	1:A:1619:GLU:OE2	2.45	0.47
1:B:2178:LEU:HD12	1:B:2229:VAL:HG21	1.97	0.47
1:A:256:PHE:O	1:A:262:ARG:NH1	2.48	0.47
1:A:1977:GLY:O	1:A:1981:GLN:HB2	2.14	0.47
1:B:1946:LYS:HA	1:B:1949:ARG:HD3	1.96	0.47
1:A:271:ILE:HD13	1:A:323:ALA:HA	1.96	0.47
1:A:897:ARG:HA	1:A:897:ARG:HD2	1.72	0.47
1:B:989:GLU:OE2	1:B:1033:GLN:NE2	2.48	0.47
1:B:1173:LEU:HB3	1:B:1848:LEU:HD11	1.95	0.47
1:B:1298:GLN:O	1:B:1302:ASP:HB2	2.15	0.47
1:A:1582:ASN:HB3	1:A:1618:TYR:HA	1.97	0.47
1:A:1846:PRO:HB3	1:B:2157:PHE:HD2	1.80	0.47
1:A:59:THR:HA	1:A:62:LEU:HG	1.96	0.47
1:A:1938:PHE:O	1:A:1941:HIS:ND1	2.48	0.47
1:A:2239:SER:HB2	1:A:2242:GLN:HB2	1.97	0.47
1:B:2238:VAL:HG11	1:B:2284:LEU:HA	1.96	0.47
1:B:21:LEU:HD23	1:B:24:LYS:HG3	1.97	0.46
1:B:1134:MET:SD	1:B:1136:ARG:NH1	2.88	0.46
1:B:1932:LEU:HD21	1:B:1979:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:HB2	1:B:108:MET:HB2	1.97	0.46
1:A:1958:ILE:HD12	1:A:2010:MET:HE1	1.97	0.46
1:B:1389:PHE:HE1	1:B:1425:LEU:HD13	1.81	0.46
1:B:1420:LEU:HD23	1:B:1423:LYS:HD3	1.98	0.46
1:B:2236:LYS:HA	1:B:2236:LYS:HD3	1.79	0.46
1:A:2155:ILE:HD12	1:A:2158:ARG:HE	1.81	0.46
1:A:2193:GLU:HA	1:A:2196:MET:HG2	1.97	0.46
1:B:436:SER:O	1:B:439:LEU:HB2	2.16	0.46
1:B:1582:ASN:HB3	1:B:1618:TYR:HA	1.97	0.46
1:B:1584:ILE:HA	1:B:1619:GLU:O	2.15	0.46
1:B:2193:GLU:HA	1:B:2196:MET:HG2	1.98	0.46
1:A:1843:SER:O	1:A:1849:ARG:NH2	2.49	0.46
1:B:1381:ILE:HD12	1:B:1384:VAL:HB	1.98	0.46
1:B:2708:GLU:O	1:B:2711:VAL:HB	2.15	0.46
1:A:953:LEU:HD11	1:A:1001:VAL:HG12	1.96	0.46
1:A:2157:PHE:HD2	1:B:1846:PRO:HB3	1.81	0.46
1:B:1570:SER:O	1:B:1591:ARG:NH1	2.39	0.46
1:A:314:ARG:HD2	1:A:314:ARG:HA	1.73	0.46
1:A:990:THR:OG1	1:A:991:MET:SD	2.74	0.46
1:B:190:LEU:O	1:B:194:LEU:N	2.46	0.46
1:B:1339:LEU:O	1:B:1343:THR:OG1	2.22	0.46
1:A:556:ASP:OD1	1:A:556:ASP:N	2.45	0.46
1:B:263:LYS:HA	1:B:266:VAL:HG22	1.98	0.46
1:B:897:ARG:HH22	1:B:901:LEU:HD13	1.81	0.46
1:B:2033:MET:HG3	1:B:2064:MET:HE3	1.97	0.46
1:B:2657:LEU:HA	1:B:2660:ILE:HD12	1.98	0.46
1:B:1397:ILE:HG23	1:B:1418:LEU:HD22	1.97	0.45
1:A:527:THR:HA	1:A:530:VAL:HG12	1.98	0.45
1:A:558:ILE:HA	1:A:561:TRP:HB2	1.99	0.45
1:A:2373:LEU:HD12	1:A:2388:THR:HG23	1.98	0.45
1:B:707:MET:HG3	1:B:741:PHE:HD1	1.80	0.45
1:B:1670:LYS:NZ	1:B:1750:LYS:O	2.42	0.45
1:A:610:PHE:HA	1:A:613:LYS:HD2	1.98	0.45
1:B:191:LYS:HA	1:B:194:LEU:HD12	1.99	0.45
1:B:227:TYR:HE1	1:B:230:GLU:HB2	1.81	0.45
1:A:2583:LEU:HG	1:A:2584:LEU:HD12	1.98	0.45
1:A:2683:GLN:OE1	1:A:2688:ASN:ND2	2.50	0.45
1:A:509:CYS:HA	1:A:560:LEU:HD12	1.98	0.45
1:A:1343:THR:HA	1:A:1421:MET:HE1	1.99	0.45
1:B:578:LEU:HD11	1:B:687:LEU:HD12	1.98	0.45
1:B:999:VAL:HG11	1:B:1015:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:VAL:HA	1:A:999:VAL:HG12	1.99	0.45
1:A:1913:PHE:O	1:A:1921:LYS:NZ	2.43	0.45
1:B:1247:PHE:HD2	1:B:1256:LEU:HD22	1.81	0.45
1:B:1958:ILE:HG21	1:B:1996:THR:HG21	1.97	0.45
1:B:1997:SER:OG	1:B:2063:TYR:OH	2.32	0.45
1:B:2037:ILE:HD11	1:B:2057:ILE:HG12	1.98	0.45
1:B:154:PHE:O	1:B:200:LYS:NZ	2.50	0.45
1:B:269:LEU:HA	1:B:272:ILE:HB	1.99	0.45
1:B:585:LEU:HA	1:B:590:MET:HE1	1.98	0.45
1:B:1184:THR:HG22	1:B:1188:GLN:HE22	1.82	0.45
1:B:1425:LEU:HD23	1:B:1428:ILE:HD12	1.99	0.45
1:B:684:GLN:NE2	1:B:716:GLU:OE2	2.50	0.45
1:B:1972:GLN:HA	1:B:1976:TRP:HD1	1.81	0.45
1:B:1974:LYS:HD2	1:B:1974:LYS:HA	1.69	0.45
1:A:1184:THR:HG22	1:A:1188:GLN:HE22	1.82	0.45
1:A:1893:THR:O	1:A:1897:ASN:HB2	2.17	0.45
1:B:741:PHE:O	1:B:745:SER:HB3	2.17	0.45
1:A:1339:LEU:O	1:A:1343:THR:OG1	2.25	0.44
1:A:2236:LYS:HA	1:A:2236:LYS:HD3	1.79	0.44
1:B:181:GLN:HE21	1:B:215:SER:HA	1.81	0.44
1:B:318:GLU:HG2	1:B:365:SER:HB3	1.98	0.44
1:A:437:VAL:HG22	1:A:440:ARG:HH21	1.82	0.44
1:A:585:LEU:HD22	1:A:694:PHE:HZ	1.82	0.44
1:A:1944:ASP:HA	1:A:1947:ARG:HE	1.82	0.44
1:B:439:LEU:O	1:B:442:MET:HB3	2.16	0.44
1:A:9:TRP:HZ2	1:B:2641:ASP:HA	1.83	0.44
1:B:97:GLN:HG2	1:B:99:LYS:HG2	1.99	0.44
1:B:115:PRO:HA	1:B:118:CYS:HB3	2.00	0.44
1:B:1162:MET:HB3	1:B:1824:ILE:HB	1.99	0.44
1:B:1161:LEU:HD22	1:B:1826:PRO:HA	2.00	0.44
1:A:1584:ILE:HA	1:A:1619:GLU:O	2.17	0.44
1:A:2189:LEU:HD12	1:A:2234:ILE:HD13	1.98	0.44
1:B:1070:GLN:NE2	1:B:1140:SER:OG	2.50	0.44
1:A:178:GLU:O	1:A:181:GLN:HB2	2.18	0.44
1:A:1044:TYR:O	1:A:1048:TRP:NE1	2.47	0.44
1:A:1172:ASP:O	1:A:1175:THR:OG1	2.35	0.44
1:A:1779:THR:HA	1:A:1789:LEU:O	2.17	0.44
1:B:732:LEU:O	1:B:734:ASN:N	2.44	0.44
1:B:1299:LYS:HA	1:B:1299:LYS:HD3	1.82	0.44
1:B:112:GLN:NE2	1:B:116:GLU:OE2	2.51	0.44
1:B:1621:VAL:HG22	1:B:1657:TYR:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2064:MET:O	1:B:2068:SER:HB3	2.18	0.44
1:B:2089:LEU:O	1:B:2092:THR:OG1	2.30	0.44
1:A:348:SER:OG	1:A:349:MET:SD	2.68	0.43
1:A:1810:TRP:CD1	1:A:1811:GLU:HG2	2.53	0.43
1:A:2133:THR:HG21	1:B:1524:TYR:HD1	1.83	0.43
1:A:2350:CYS:HA	1:A:2353:MET:HG3	2.00	0.43
1:A:2657:LEU:HA	1:A:2660:ILE:HD12	1.99	0.43
1:B:293:ASN:HA	1:B:296:LYS:HE2	1.99	0.43
1:B:912:GLN:O	1:B:916:ASN:ND2	2.50	0.43
1:B:1047:ASP:N	1:B:1047:ASP:OD1	2.50	0.43
1:B:2250:LEU:HD11	1:B:2270:ILE:HG23	2.00	0.43
1:B:2379:HIS:CE1	1:B:2384:ILE:HG13	2.54	0.43
1:A:436:SER:O	1:A:439:LEU:HB2	2.18	0.43
1:B:925:LEU:HD12	1:B:925:LEU:HA	1.91	0.43
1:A:194:LEU:HA	1:A:197:THR:HG22	2.01	0.43
1:A:446:THR:HA	1:A:449:LYS:HD2	2.00	0.43
1:A:2644:ILE:HD12	1:A:2660:ILE:HG23	1.99	0.43
1:B:974:ASN:HD21	1:B:977:GLU:HG2	1.84	0.43
1:B:336:TRP:NE1	1:B:340:SER:O	2.49	0.43
1:B:2708:GLU:OE2	1:B:2712:LYS:NZ	2.45	0.43
1:A:1025:ARG:NH2	1:A:1028:ASP:OD2	2.52	0.43
1:A:1642:PHE:HZ	1:A:1676:LEU:HD23	1.84	0.43
1:A:1810:TRP:HD1	1:A:1811:GLU:HG2	1.84	0.43
1:A:2713:PHE:O	1:A:2716:ALA:HB3	2.18	0.43
1:B:205:LYS:HE2	1:B:207:VAL:HG23	2.00	0.43
1:B:842:GLY:O	1:B:846:ALA:HB2	2.18	0.43
1:B:1769:GLU:H	1:B:1781:THR:HB	1.83	0.43
1:B:2366:ASN:ND2	1:B:2413:GLN:O	2.51	0.43
1:A:1843:SER:OG	1:A:1844:SER:N	2.51	0.43
1:A:1954:LEU:O	1:A:1958:ILE:HG12	2.19	0.43
1:B:136:ASN:OD1	1:B:137:SER:N	2.51	0.43
1:B:160:ARG:HG2	1:B:174:VAL:HB	2.00	0.43
1:B:562:ASN:ND2	1:B:565:ALA:O	2.52	0.43
1:B:1744:THR:HG23	1:B:1759:ASN:HB2	2.01	0.43
1:B:2062:ARG:HA	1:B:2062:ARG:HD3	1.86	0.43
1:A:173:ASP:OD1	1:A:205:LYS:NZ	2.46	0.42
1:B:304:ARG:NE	1:B:349:MET:HG3	2.32	0.42
1:A:1149:MET:HA	1:A:1152:LEU:HD23	1.99	0.42
1:A:2346:LEU:HD13	1:A:2713:PHE:HE1	1.84	0.42
1:A:905:ASN:OD1	1:A:959:GLN:NE2	2.52	0.42
1:A:1575:ALA:HB1	1:A:1704:LYS:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:LEU:HD23	1:B:735:TYR:HB2	2.00	0.42
1:B:577:MET:HE2	1:B:577:MET:HB3	1.84	0.42
1:B:1184:THR:O	1:B:1187:LEU:HB3	2.20	0.42
1:B:1771:CYS:HB3	1:B:1779:THR:HB	2.01	0.42
1:B:1835:ASN:OD1	1:B:1927:TYR:OH	2.38	0.42
1:A:1104:LEU:HD23	1:A:1104:LEU:HA	1.89	0.42
1:B:2314:THR:OG1	1:B:2387:ARG:NH2	2.50	0.42
1:A:1005:MET:O	1:A:1009:ILE:N	2.40	0.42
1:B:99:LYS:HD2	1:B:99:LYS:HA	1.75	0.42
1:B:1626:HIS:NE2	1:B:1766:GLU:OE1	2.49	0.42
1:A:1041:MET:O	1:A:1045:LEU:HB2	2.20	0.42
1:A:1248:ASP:HB2	1:A:1253:LEU:HD22	2.02	0.42
1:B:1803:ILE:HA	1:B:1806:ILE:HG12	2.02	0.42
1:B:1104:LEU:HD23	1:B:1104:LEU:HA	1.92	0.42
1:A:1889:SER:O	1:A:1893:THR:OG1	2.35	0.42
1:A:1744:THR:HA	1:A:1759:ASN:HA	2.02	0.41
1:B:527:THR:HA	1:B:530:VAL:HG12	2.02	0.41
1:A:176:ASP:HA	1:A:179:LEU:HD23	2.01	0.41
1:A:547:GLU:HA	1:A:550:LEU:HG	2.02	0.41
1:A:716:GLU:HA	1:A:719:ILE:HG12	2.01	0.41
1:A:756:GLN:O	1:A:760:MET:HG2	2.20	0.41
1:A:2044:PRO:HB2	1:A:2221:PRO:HD2	2.03	0.41
1:B:732:LEU:HA	1:B:733:PRO:HD3	1.90	0.41
1:A:221:TRP:HA	1:A:224:VAL:HG22	2.02	0.41
1:A:447:LEU:O	1:A:450:ALA:HB3	2.20	0.41
1:A:1358:PRO:HA	1:A:1359:PRO:HD3	1.88	0.41
1:A:1645:PHE:HB2	1:A:1650:TYR:CZ	2.54	0.41
1:B:103:ARG:HH22	1:B:107:THR:H	1.68	0.41
1:B:961:VAL:HA	1:B:964:THR:HG22	2.02	0.41
1:B:1967:MET:O	1:B:1970:SER:OG	2.35	0.41
1:B:1979:LEU:HD23	1:B:1979:LEU:HA	1.84	0.41
1:A:1745:SER:OG	1:A:1758:LEU:N	2.53	0.41
1:B:1479:SER:OG	1:B:1480:ASP:N	2.54	0.41
1:B:1768:GLU:O	1:B:1807:ARG:NH2	2.41	0.41
1:A:2177:ALA:O	1:A:2180:SER:OG	2.27	0.41
1:A:1034:GLU:HA	1:A:1037:PHE:HB3	2.03	0.41
1:A:2248:ARG:HE	1:A:2718:ILE:HD12	1.85	0.41
1:B:1096:MET:SD	1:B:1097:GLU:N	2.94	0.41
1:B:2044:PRO:HB2	1:B:2221:PRO:HD2	2.02	0.41
1:A:1397:ILE:HG23	1:A:1418:LEU:HD22	2.03	0.41
1:A:1769:GLU:H	1:A:1781:THR:HB	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2176:PHE:HZ	1:A:2181:LEU:HB2	1.85	0.41
1:B:2124:THR:HA	1:B:2127:VAL:HG12	2.02	0.41
1:B:2643:LYS:HE2	1:B:2643:LYS:HB3	1.90	0.41
1:A:63:LYS:HD2	1:A:63:LYS:HA	1.96	0.41
1:A:222:ASN:O	1:A:226:ASN:ND2	2.54	0.41
1:B:499:LEU:HD21	1:B:506:LEU:HD23	2.02	0.41
1:B:2230:VAL:O	1:B:2234:ILE:HG12	2.21	0.41
1:A:10:VAL:HG12	1:A:46:ILE:HD13	2.02	0.41
1:A:102:MET:HG2	1:A:104:LEU:HD23	2.02	0.41
1:A:732:LEU:HA	1:A:733:PRO:HD3	1.90	0.41
1:A:961:VAL:HA	1:A:964:THR:HG22	2.02	0.41
1:A:1621:VAL:HG22	1:A:1657:TYR:HB2	2.03	0.41
1:A:1806:ILE:HA	1:A:1809:ARG:HB3	2.03	0.41
1:B:987:SER:OG	1:B:1030:SER:O	2.32	0.41
1:B:1585:PHE:HE2	1:B:1609:THR:HG22	1.86	0.41
1:B:1606:VAL:O	1:B:1610:LEU:HB2	2.20	0.41
1:B:1898:GLU:HA	1:B:1899:PRO:HD3	1.94	0.41
1:B:2129:ARG:HE	1:B:2129:ARG:HB2	1.65	0.41
1:B:2634:PRO:HA	1:B:2637:HIS:HB2	2.03	0.41
1:B:1038:ARG:NH1	1:B:1079:LEU:O	2.54	0.41
1:B:1958:ILE:HD11	1:B:1993:PHE:HE1	1.86	0.41
1:A:731:LEU:HD23	1:A:735:TYR:HD1	1.86	0.40
1:A:1411:PRO:HA	1:A:1412:PRO:HD3	1.95	0.40
1:A:2292:LYS:HD2	1:A:2342:ILE:HD11	2.04	0.40
1:B:191:LYS:O	1:B:194:LEU:HB2	2.22	0.40
1:B:585:LEU:HD22	1:B:694:PHE:HZ	1.86	0.40
1:A:381:VAL:O	1:A:385:ARG:HG2	2.20	0.40
1:B:1354:SER:OG	1:B:1460:ASP:OD1	2.38	0.40
1:A:99:LYS:HD2	1:A:99:LYS:HA	1.85	0.40
1:A:520:GLY:O	1:A:524:GLU:N	2.48	0.40
1:A:1207:ARG:H	1:A:1207:ARG:HD2	1.86	0.40
1:B:734:ASN:OD1	1:B:770:THR:OG1	2.40	0.40
1:A:573:ILE:HD12	1:A:573:ILE:HA	1.99	0.40
1:A:1286:THR:HA	1:A:1289:PHE:HD2	1.86	0.40
1:A:1400:PRO:HB2	1:A:1406:LEU:HD12	2.04	0.40
1:A:1488:ARG:O	1:A:1492:ASN:ND2	2.39	0.40
1:A:2641:ASP:HA	1:B:9:TRP:HZ2	1.87	0.40
1:A:925:LEU:HD12	1:A:925:LEU:HA	1.96	0.40
1:B:2185:THR:HG21	1:B:2230:VAL:HG22	2.03	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	2201/2818 (78%)	2111 (96%)	90 (4%)	0	100	100
1	B	2208/2818 (78%)	2113 (96%)	95 (4%)	0	100	100
All	All	4409/5636 (78%)	4224 (96%)	185 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1993/2512 (79%)	1990 (100%)	3 (0%)	93	98
1	B	1997/2512 (80%)	1989 (100%)	8 (0%)	91	97
All	All	3990/5024 (79%)	3979 (100%)	11 (0%)	92	97

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	1066	ARG
1	A	1683	LYS
1	B	5	ARG
1	B	261	LYS
1	B	366	ARG
1	B	1136	ARG
1	B	1171	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1513	ARG
1	B	1940	LYS
1	B	2328	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	B	1070	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 [i](#)

There are no chain breaks in this entry.

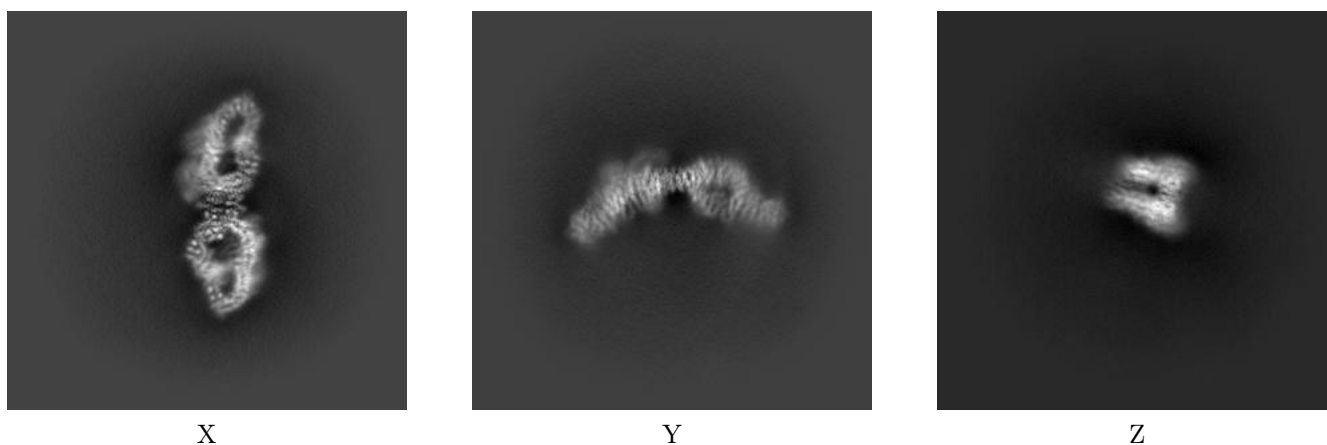
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14218. 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](#)

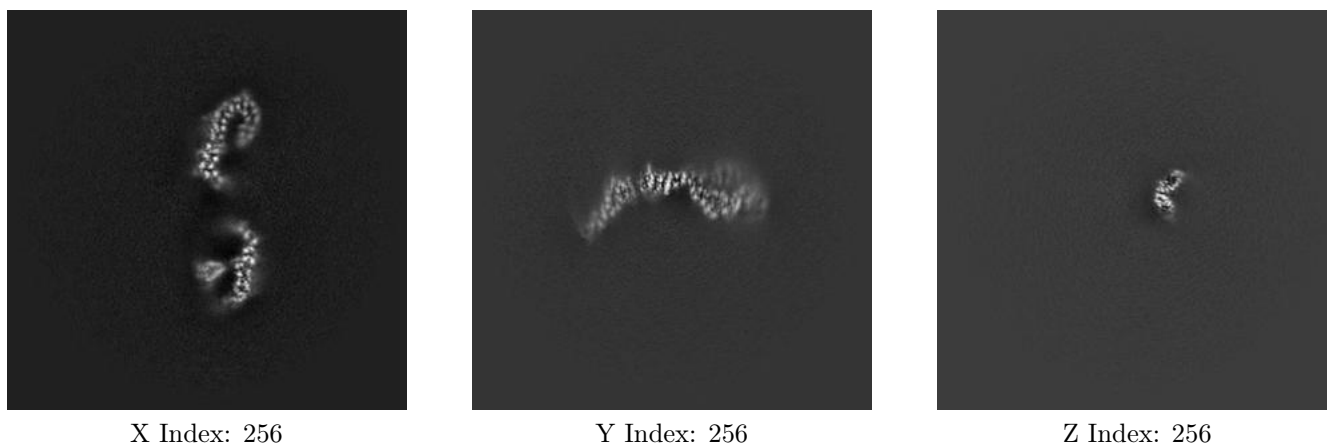
#### 6.1.1 Primary map



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

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

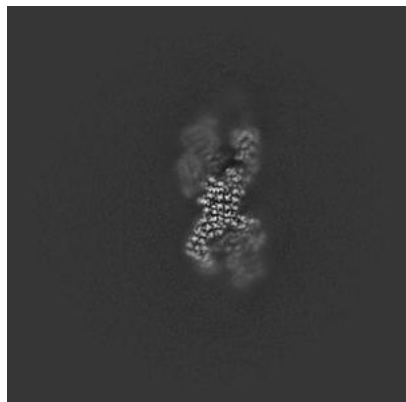
#### 6.2.1 Primary map



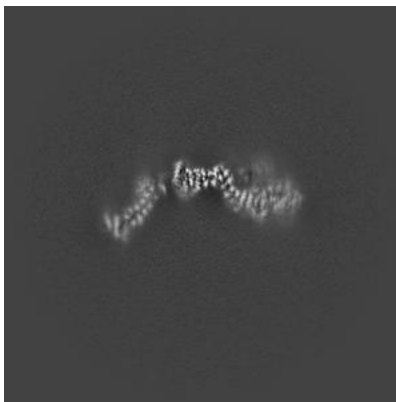
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 290



Y Index: 263



Z Index: 238

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

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

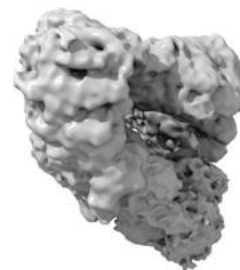
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



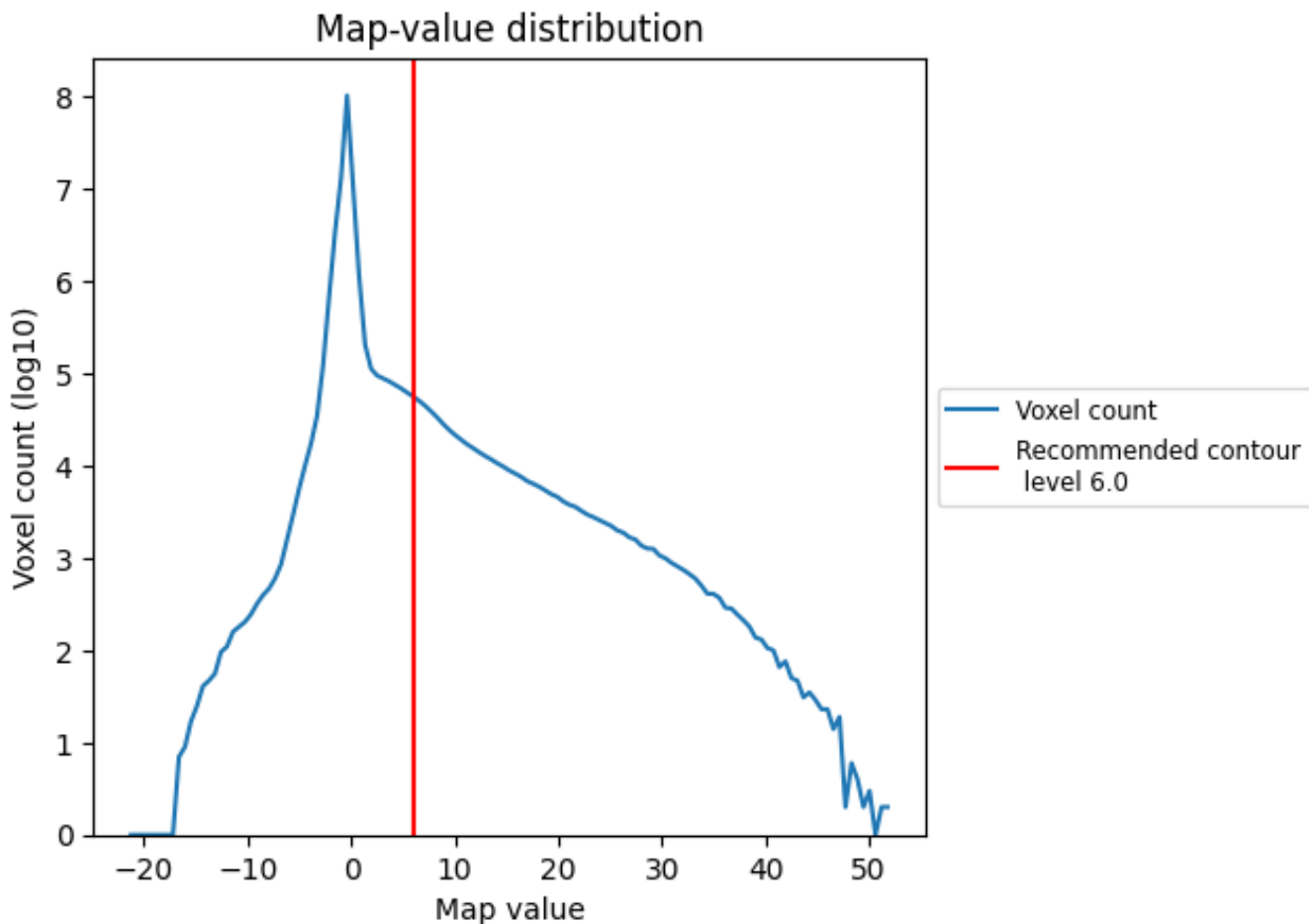
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

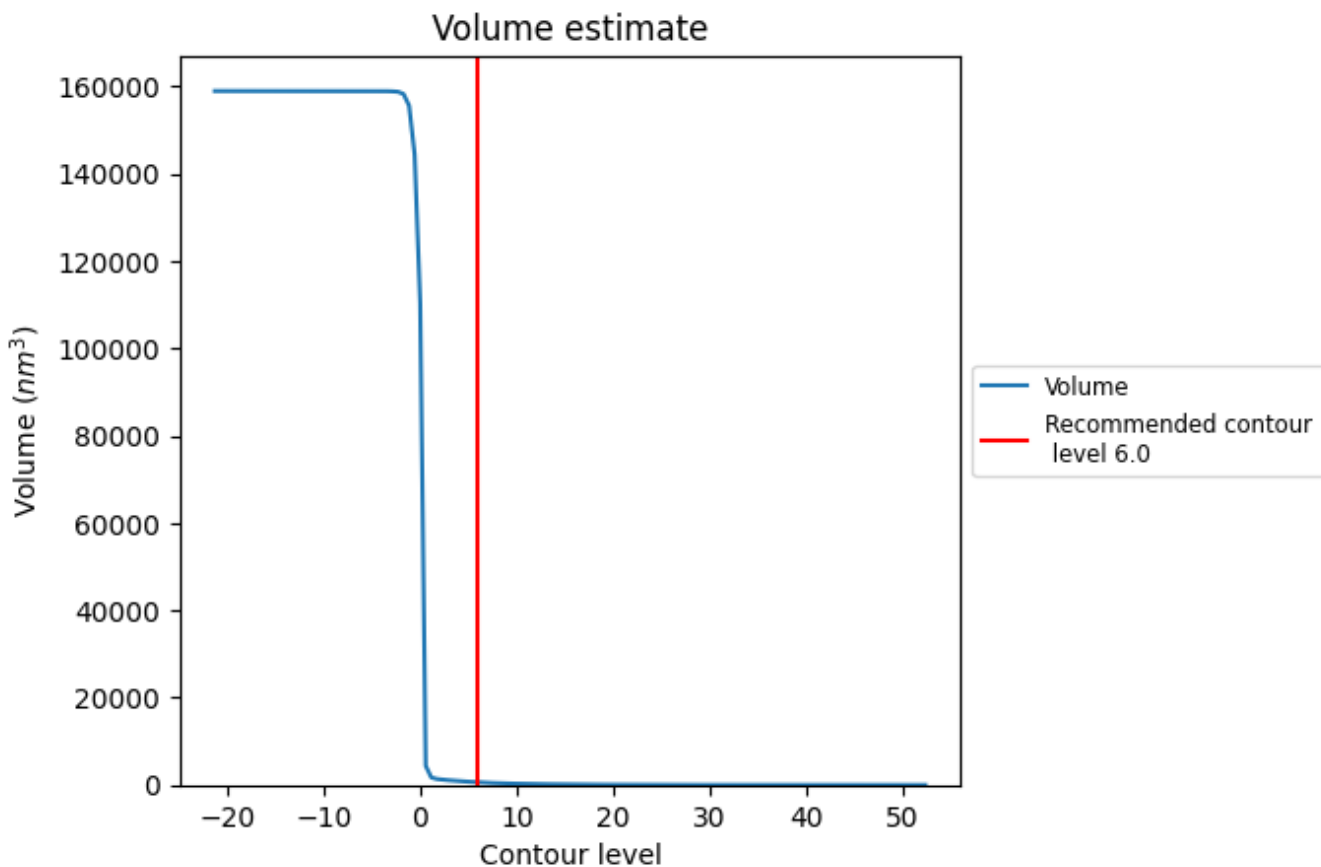
This section contains the results of statistical analysis of the map.

### 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.

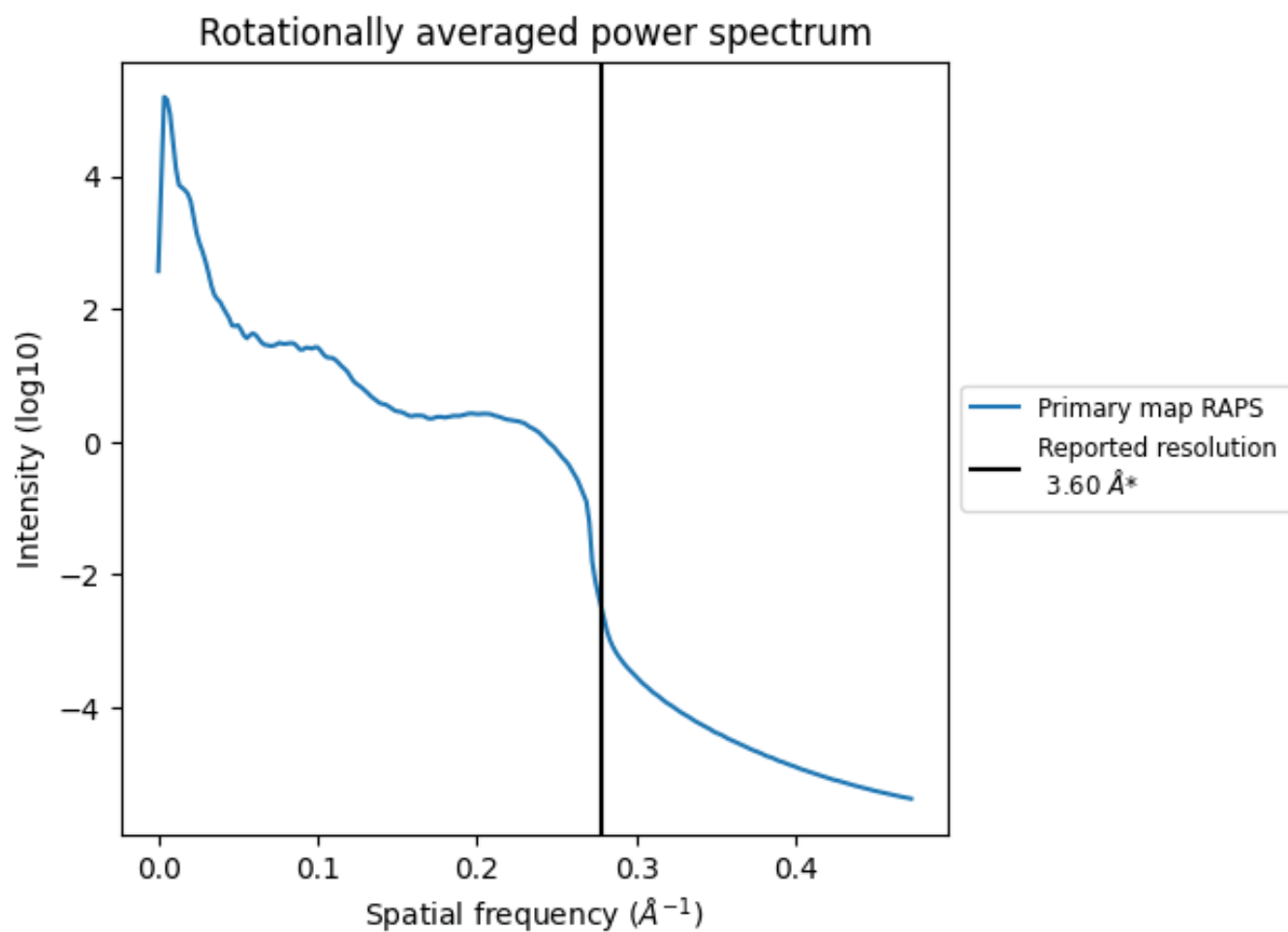
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 611 nm<sup>3</sup>; this corresponds to an approximate mass of 552 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 0.278 Å<sup>-1</sup>

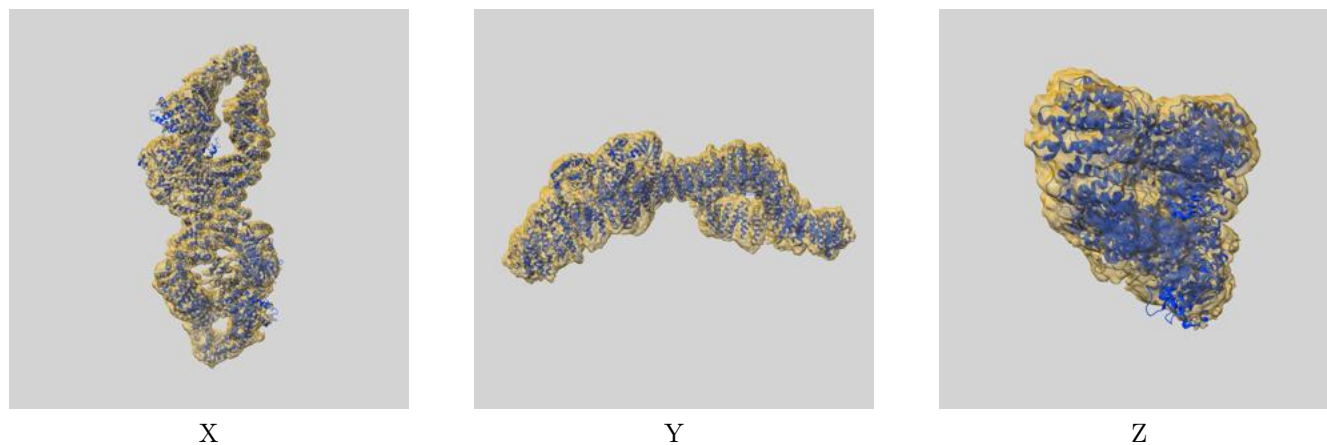
## 8 Fourier-Shell correlation

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

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

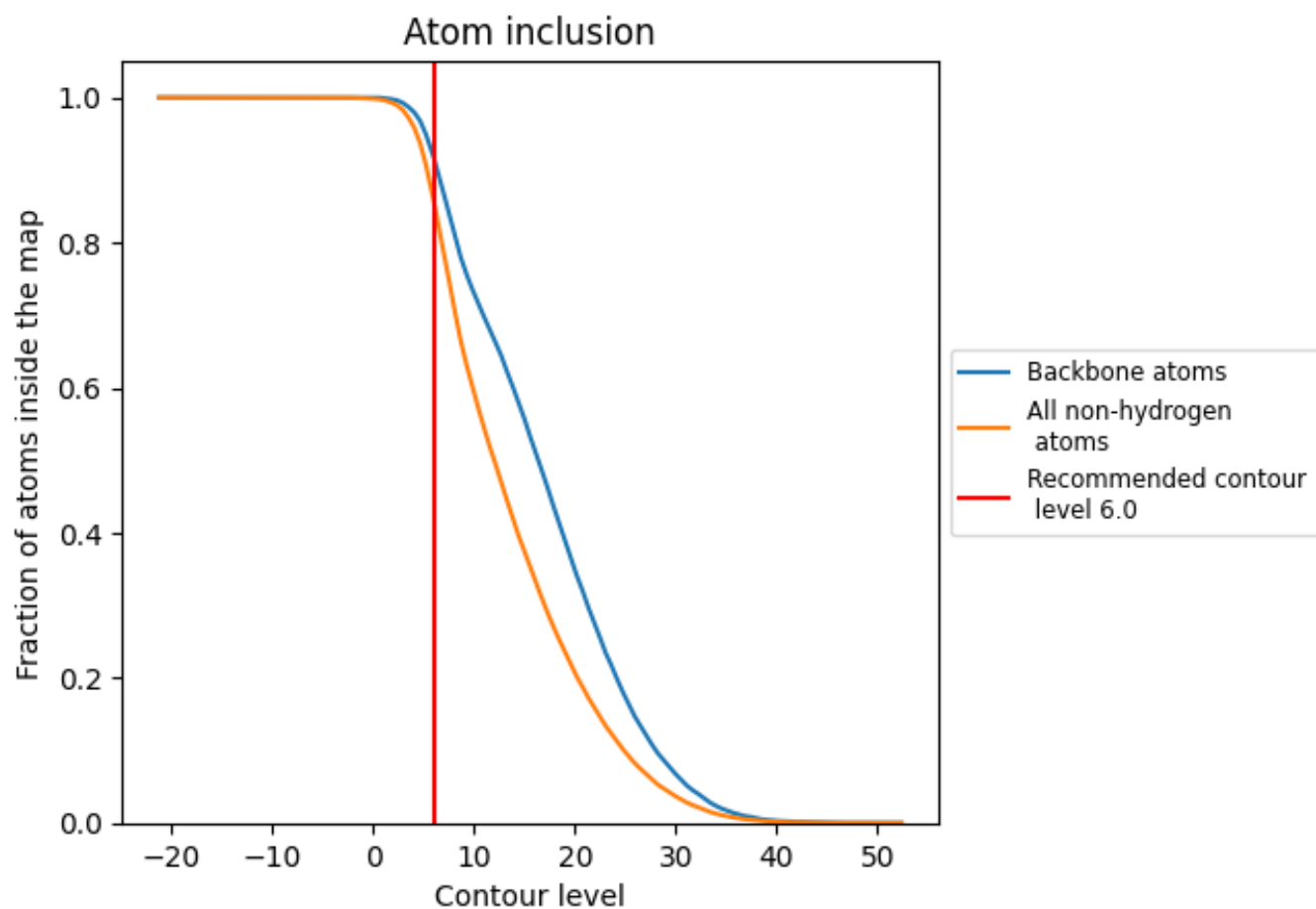
This section contains information regarding the fit between EMDB map EMD-14218 and PDB model 7R03. Per-residue inclusion information can be found in section 3 on page 4.

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



The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.