



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:08 AM UTC

PDB ID : 5A22 / pdb_00005a22
EMDB ID : EMD-6337
Title : Structure of the L protein of vesicular stomatitis virus from electron cryomicroscopy
Authors : Liang, B.; Li, Z.; Jenni, S.; Rameh, A.A.; Morin, B.M.; Grant, T.; Grigorieff, N.; Harrison, S.C.; Whelan, S.P.J.
Deposited on : 2015-05-06
Resolution : 3.80 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

A user guide is available at

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

The types of validation reports are described at

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

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

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

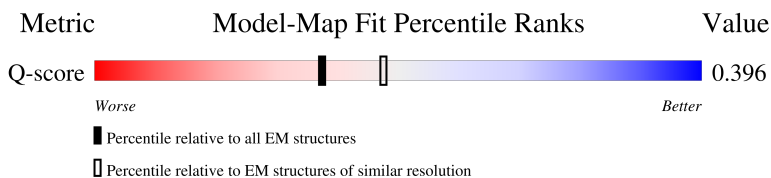
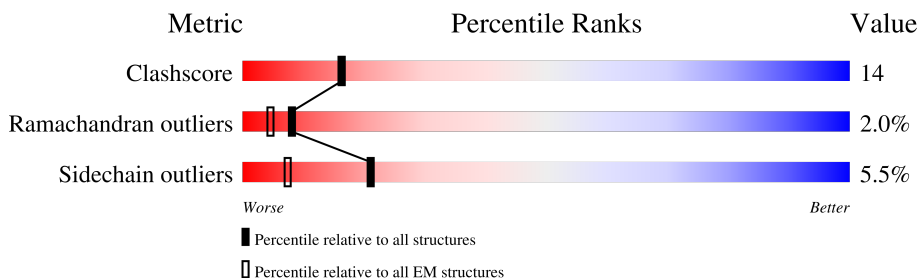
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2109	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32187 atoms, of which 16110 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 VESICULAR STOMATITIS VIRUS L POLYMERASE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	2002	32185	10249	16110	2803	2934	89	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ARG	PRO	conflict	UNP P03523
A	467	ASP	HIS	conflict	UNP P03523
A	548	LEU	PHE	conflict	UNP P03523
A	549	ARG	PRO	conflict	UNP P03523
A	670	ARG	PRO	conflict	UNP P03523
A	910	PHE	SER	conflict	UNP P03523
A	1026	ALA	PRO	conflict	UNP P03523
A	1348	GLY	ALA	conflict	UNP P03523
A	1589	ALA	PRO	conflict	UNP P03523

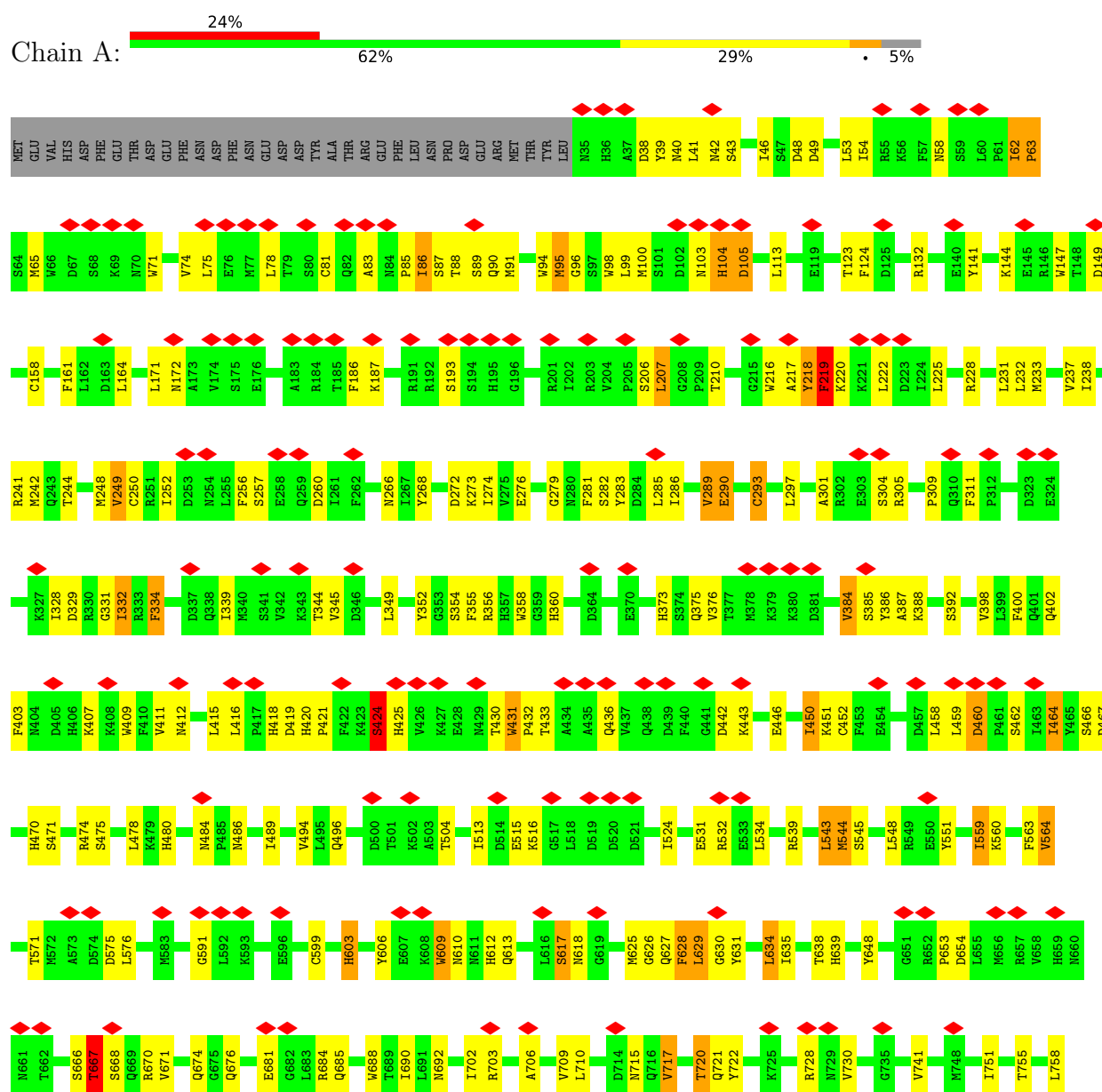
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Zn	0
			2	2	

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: VESICULAR STOMATITIS VIRUS L POLYMERASE





K2089	E2090	D2091	R2092	S2093	L2094	L2095	M2096	L2097	K2098	S2099	D2100	L2101	H2102	E2103	S2106	W2107	R2108	D2109	D2028	S2029	L2030	A2031	P2032	L2033	G2034	W2035	W2036	L2037	R2038	S2039	L2040	E2041	L2042	V2043	Q2046	V2047	R2048	L2049	M2050	P2051	F2052	N2053	E2054	L2055	L2056	F2057	W2058	Q2059	L2060	C2061	R2062	T2063	V2064	D2065	N2066	H2067	L2068	K2069	W2070	S2071	N2072	L2073	R2074	R2075	N2076	T2077	G2078	N2079	I2080	E2081	W2082	L2083	W2084	R2085	R2086	I2087	S2088																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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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	74940	Depositor
Resolution determination method	Not provided	
CTF correction method	INDIVIDUAL PARTICLES	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	40410	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	5.041	Depositor
Minimum map value	-2.928	Depositor
Average map value	0.052	Depositor
Map value standard deviation	0.385	Depositor
Recommended contour level	1.2	Depositor
Map size ($\text{\AA}$)	148.44, 148.44, 148.44	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.237, 1.237, 1.237	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.57	2/16456 (0.0%)	0.99	51/22270 (0.2%)

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	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	VAL	CA-CB	6.60	1.61	1.54
1	A	865	ILE	CA-CB	5.08	1.60	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1165	GLN	CA-C-N	-9.65	107.78	119.84
1	A	1165	GLN	C-N-CA	-9.65	107.78	119.84
1	A	1447	PRO	N-CA-C	8.12	120.60	110.70
1	A	1954	ASN	CA-C-N	-7.92	112.22	120.38
1	A	1954	ASN	C-N-CA	-7.92	112.22	120.38
1	A	62	ILE	CA-C-N	-7.48	110.49	119.84
1	A	62	ILE	C-N-CA	-7.48	110.49	119.84
1	A	332	ILE	N-CA-C	-7.23	103.24	110.62
1	A	1495	ILE	N-CA-C	7.06	117.16	110.53
1	A	217	ALA	N-CA-C	6.62	119.01	109.14
1	A	1456	GLY	CA-C-N	6.42	126.55	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1456	GLY	C-N-CA	6.42	126.55	119.87
1	A	2031	ALA	CA-C-N	-6.39	112.42	119.19
1	A	2031	ALA	C-N-CA	-6.39	112.42	119.19
1	A	591	GLY	N-CA-C	-6.26	106.90	114.66
1	A	249	VAL	N-CA-C	6.25	117.75	110.62
1	A	2078	GLY	N-CA-C	6.21	118.95	110.69
1	A	1105	HIS	CA-C-N	6.11	126.28	119.32
1	A	1105	HIS	C-N-CA	6.11	126.28	119.32
1	A	484	ASN	CA-C-N	5.94	127.26	119.84
1	A	484	ASN	C-N-CA	5.94	127.26	119.84
1	A	1949	GLY	CA-C-N	5.92	127.24	119.84
1	A	1949	GLY	C-N-CA	5.92	127.24	119.84
1	A	1823	GLN	N-CA-C	-5.82	106.57	113.38
1	A	1149	LEU	CA-C-N	-5.73	112.68	119.84
1	A	1149	LEU	C-N-CA	-5.73	112.68	119.84
1	A	1503	HIS	CB-CA-C	-5.61	109.12	115.79
1	A	1951	ILE	CA-C-N	5.57	126.12	120.38
1	A	1951	ILE	C-N-CA	5.57	126.12	120.38
1	A	1360	TYR	N-CA-C	-5.53	105.80	112.54
1	A	305	ARG	CA-C-N	5.50	125.59	119.32
1	A	305	ARG	C-N-CA	5.50	125.59	119.32
1	A	1622	PRO	N-CA-C	5.48	120.09	111.38
1	A	1199	THR	N-CA-C	-5.44	105.35	111.28
1	A	1515	SER	CB-CA-C	-5.38	108.79	115.89
1	A	83	ALA	N-CA-C	-5.36	101.28	108.19
1	A	609	TRP	N-CA-C	-5.35	105.53	111.36
1	A	1250	LEU	N-CA-C	5.33	118.35	110.46
1	A	628	PHE	CA-C-N	-5.30	113.86	122.34
1	A	628	PHE	C-N-CA	-5.30	113.86	122.34
1	A	38	ASP	N-CA-C	5.26	117.54	109.07
1	A	290	GLU	CA-C-N	-5.25	113.63	119.19
1	A	290	GLU	C-N-CA	-5.25	113.63	119.19
1	A	1080	THR	N-CA-C	-5.18	99.22	108.13
1	A	2009	TYR	N-CA-C	5.17	117.10	108.99
1	A	2101	LEU	N-CA-C	-5.14	99.84	110.80
1	A	790	GLU	N-CA-C	-5.13	105.77	112.23
1	A	464	ILE	CB-CA-C	-5.12	107.36	111.71
1	A	2014	SER	N-CA-C	5.04	114.90	108.24
1	A	1118	THR	CA-C-N	-5.00	113.77	118.97
1	A	1118	THR	C-N-CA	-5.00	113.77	118.97

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1071	LEU	Peptide
1	A	1125	THR	Peptide
1	A	1151	ALA	Peptide
1	A	1167	TRP	Peptide
1	A	1285	ASP	Peptide
1	A	1380	HIS	Peptide
1	A	1621	TYR	Peptide
1	A	1789	GLN	Peptide
1	A	1955	PRO	Peptide
1	A	2066	ASN	Peptide
1	A	2106	SER	Peptide
1	A	431	TRP	Peptide
1	A	63	PRO	Peptide
1	A	766	GLU	Peptide

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	16075	16110	16109	458	0
2	A	2	0	0	0	0
All	All	16077	16110	16109	458	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 14.

All (458) 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:100:MET:SD	1:A:241:ARG:NH1	2.51	0.84
1:A:88:THR:O	1:A:91:MET:N	2.21	0.73
1:A:977:ARG:O	1:A:986:LYS:NZ	2.22	0.72
1:A:419:ASP:HB2	1:A:421:PRO:HD2	1.71	0.71
1:A:1361:GLN:OE1	1:A:1364:ARG:NH2	2.23	0.70
1:A:147:TRP:NE1	1:A:250:CYS:SG	2.65	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:SER:N	1:A:544:MET:O	2.25	0.69
1:A:1637:SER:O	1:A:2038:ARG:NH1	2.27	0.68
1:A:354:SER:O	1:A:356:ARG:N	2.26	0.68
1:A:301:ALA:O	1:A:304:SER:OG	2.13	0.67
1:A:1128:PHE:O	1:A:1130:TYR:N	2.28	0.67
1:A:767:THR:OG1	1:A:768:MET:N	2.22	0.67
1:A:1117:GLU:OE1	1:A:1740:ARG:NH2	2.28	0.66
1:A:384:VAL:O	1:A:387:ALA:N	2.31	0.64
1:A:354:SER:C	1:A:356:ARG:H	2.05	0.63
1:A:474:ARG:NH2	1:A:674:GLN:OE1	2.32	0.62
1:A:375:GLN:OE1	1:A:612:HIS:NE2	2.33	0.62
1:A:424:SER:OG	1:A:425:HIS:N	2.28	0.62
1:A:1254:THR:O	1:A:1257:MET:N	2.31	0.61
1:A:132:ARG:NH2	1:A:917:HIS:O	2.33	0.61
1:A:571:THR:HG1	1:A:776:TYR:HH	1.48	0.60
1:A:1838:CYS:SG	1:A:1839:LYS:N	2.75	0.60
1:A:1290:SER:OG	1:A:1291:CYS:N	2.30	0.60
1:A:629:LEU:O	1:A:631:TYR:N	2.31	0.59
1:A:940:ILE:HA	1:A:943:ILE:HG22	1.84	0.58
1:A:1963:ASN:HA	1:A:1966:ILE:HG22	1.86	0.58
1:A:228:ARG:HG2	1:A:232:LEU:HD12	1.84	0.58
1:A:1945:HIS:HB2	1:A:2077:THR:HG23	1.84	0.58
1:A:467:ASP:OD1	1:A:1041:ASN:ND2	2.34	0.58
1:A:1798:GLY:HA2	1:A:1859:TRP:HH2	1.69	0.58
1:A:2074:ARG:HA	1:A:2080:ILE:HG13	1.86	0.58
1:A:902:ASP:OD2	1:A:1103:VAL:N	2.37	0.57
1:A:206:SER:OG	1:A:207:LEU:N	2.38	0.57
1:A:74:VAL:HG21	1:A:216:TRP:CD1	2.39	0.57
1:A:1822:VAL:HG11	1:A:1863:TYR:CE2	2.39	0.57
1:A:1973:PHE:CE1	1:A:1988:CYS:HB3	2.40	0.57
1:A:1551:LEU:O	1:A:1555:LEU:N	2.38	0.57
1:A:486:ASN:OD1	1:A:486:ASN:N	2.38	0.57
1:A:286:ILE:O	1:A:289:VAL:N	2.38	0.57
1:A:309:PRO:HG2	1:A:741:VAL:HG21	1.86	0.56
1:A:1906:PHE:CD1	1:A:1963:ASN:HB2	2.39	0.56
1:A:1198:MET:HE2	1:A:1198:MET:HA	1.87	0.56
1:A:2016:ARG:HA	1:A:2087:ILE:CG1	2.35	0.56
1:A:880:LEU:HD11	1:A:886:GLY:HA3	1.87	0.56
1:A:1206:SER:OG	1:A:1211:GLU:OE2	2.23	0.56
1:A:613:GLN:HG3	1:A:688:TRP:CD2	2.41	0.56
1:A:1822:VAL:C	1:A:1824:THR:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:LEU:HB2	1:A:1094:TRP:HH2	1.70	0.56
1:A:419:ASP:CB	1:A:421:PRO:HD2	2.34	0.55
1:A:1495:ILE:O	1:A:1533:TYR:OH	2.23	0.55
1:A:1949:GLY:O	1:A:2009:TYR:N	2.38	0.55
1:A:1537:LEU:HG	1:A:1538:SER:H	1.70	0.55
1:A:2080:ILE:O	1:A:2083:ILE:N	2.35	0.55
1:A:1186:ILE:HG22	1:A:1187:SER:N	2.21	0.55
1:A:432:PRO:HB3	1:A:436:GLN:HB2	1.89	0.55
1:A:42:ASN:ND2	1:A:802:ASN:OD1	2.39	0.55
1:A:409:TRP:CZ2	1:A:431:TRP:HE3	2.25	0.55
1:A:1006:ILE:HG22	1:A:1008:PRO:HD2	1.88	0.54
1:A:1079:TRP:CD1	1:A:1085:HIS:CG	2.95	0.54
1:A:1130:TYR:HB2	1:A:1296:HIS:CE1	2.42	0.54
1:A:1187:SER:HA	1:A:1191:GLU:HA	1.90	0.54
1:A:443:LYS:O	1:A:446:GLU:N	2.35	0.54
1:A:943:ILE:CD1	1:A:1004:TRP:CE3	2.90	0.54
1:A:1982:ILE:O	1:A:1985:TYR:N	2.40	0.54
1:A:880:LEU:CD1	1:A:886:GLY:HA3	2.37	0.53
1:A:403:PHE:CE2	1:A:431:TRP:HB2	2.43	0.53
1:A:88:THR:OG1	1:A:89:SER:N	2.41	0.53
1:A:1894:ASP:O	1:A:1896:PHE:N	2.40	0.53
1:A:286:ILE:O	1:A:289:VAL:HG12	2.08	0.53
1:A:1627:MET:HE1	1:A:1803:GLU:HA	1.90	0.53
1:A:1976:SER:OG	1:A:1981:ASP:O	2.26	0.53
1:A:1503:HIS:HB2	1:A:1504:TYR:HD2	1.74	0.53
1:A:1682:ARG:HE	1:A:1715:THR:HG21	1.72	0.53
1:A:1943:ILE:O	1:A:2011:GLN:NE2	2.37	0.53
1:A:416:LEU:O	1:A:418:HIS:N	2.39	0.53
1:A:1641:LEU:HB3	1:A:1883:THR:HB	1.91	0.52
1:A:755:THR:HG22	1:A:760:LEU:HB2	1.92	0.52
1:A:219:PHE:N	1:A:219:PHE:CD1	2.77	0.52
1:A:420:HIS:N	1:A:421:PRO:HD2	2.24	0.52
1:A:450:ILE:HG23	1:A:451:LYS:N	2.23	0.52
1:A:2031:ALA:HB3	1:A:2032:PRO:HD3	1.92	0.52
1:A:706:ALA:HB3	1:A:721:GLN:HB2	1.92	0.52
1:A:1923:ARG:HB2	1:A:1930:ILE:HD11	1.92	0.52
1:A:1934:TYR:HA	1:A:1937:ILE:HG22	1.91	0.52
1:A:2000:TRP:CH2	1:A:2011:GLN:HB2	2.45	0.52
1:A:1950:PRO:HA	1:A:2008:GLY:HA3	1.92	0.52
1:A:2012:LYS:NZ	1:A:2076:ASN:O	2.43	0.51
1:A:460:ASP:OD1	1:A:462:SER:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:GLY:HA3	1:A:1079:TRP:CZ2	2.45	0.51
1:A:1091:TYR:CD1	1:A:1091:TYR:C	2.87	0.51
1:A:43:SER:C	1:A:531:GLU:HB3	2.35	0.51
1:A:1943:ILE:HG21	1:A:2013:TRP:CD1	2.46	0.51
1:A:2016:ARG:HA	1:A:2087:ILE:HG12	1.93	0.51
1:A:1417:ILE:CD1	1:A:1549:ALA:HB2	2.41	0.51
1:A:1974:TRP:CE2	1:A:2040:LEU:HB3	2.46	0.51
1:A:1038:THR:O	1:A:1042:SER:N	2.44	0.51
1:A:931:GLY:HA3	1:A:1079:TRP:HZ2	1.76	0.50
1:A:1473:TYR:CD1	1:A:1473:TYR:C	2.89	0.50
1:A:78:LEU:HG	1:A:219:PHE:CZ	2.45	0.50
1:A:158:CYS:HA	1:A:242:MET:HE3	1.93	0.50
1:A:124:PHE:HD2	1:A:141:TYR:HB2	1.76	0.50
1:A:470:HIS:HA	1:A:543:LEU:HB2	1.93	0.50
1:A:1231:THR:C	1:A:1233:ARG:H	2.19	0.50
1:A:797:VAL:HG12	1:A:798:THR:N	2.26	0.50
1:A:1450:LEU:HG	1:A:1480:MET:HB3	1.94	0.50
1:A:1644:LEU:CB	1:A:1645:PRO:CD	2.89	0.50
1:A:1732:TYR:HB3	1:A:1733:PRO:HD2	1.94	0.50
1:A:1804:SER:OG	1:A:1805:GLU:N	2.44	0.50
1:A:1896:PHE:O	1:A:1899:ILE:N	2.45	0.50
1:A:1123:CYS:SG	1:A:1296:HIS:CD2	3.04	0.50
1:A:1644:LEU:HB3	1:A:1645:PRO:CD	2.42	0.50
1:A:2040:LEU:HA	1:A:2043:VAL:HG22	1.94	0.50
1:A:2096:MET:C	1:A:2097:LEU:HG	2.37	0.50
1:A:244:THR:CG2	1:A:791:THR:HG23	2.41	0.50
1:A:782:PHE:CD1	1:A:783:ARG:HG3	2.47	0.50
1:A:54:ILE:HD12	1:A:85:PRO:HG3	1.94	0.49
1:A:147:TRP:NE1	1:A:250:CYS:HG	2.10	0.49
1:A:1291:CYS:SG	1:A:1292:THR:N	2.85	0.49
1:A:1703:ARG:HA	1:A:2107:TRP:CZ2	2.47	0.49
1:A:2081:GLU:O	1:A:2085:ARG:N	2.43	0.49
1:A:78:LEU:HD23	1:A:219:PHE:HE2	1.77	0.49
1:A:911:TRP:HA	1:A:914:ILE:HG22	1.93	0.49
1:A:1234:MET:HB2	1:A:1236:HIS:ND1	2.28	0.49
1:A:104:HIS:CD2	1:A:206:SER:HA	2.47	0.49
1:A:575:ASP:CG	1:A:576:LEU:H	2.20	0.49
1:A:1636:LEU:CD1	1:A:1875:ALA:HA	2.42	0.49
1:A:311:PHE:CD2	1:A:768:MET:HG3	2.47	0.49
1:A:420:HIS:N	1:A:421:PRO:CD	2.76	0.49
1:A:1742:TRP:HB3	1:A:1781:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:HIS:ND1	1:A:1106:PRO:HD2	2.27	0.49
1:A:1152:TYR:HB3	1:A:1277:GLN:HE22	1.77	0.49
1:A:1128:PHE:HB2	1:A:1259:ASP:CG	2.38	0.49
1:A:272:ASP:O	1:A:276:GLU:N	2.46	0.49
1:A:1190:VAL:HG11	1:A:1198:MET:HE3	1.94	0.49
1:A:1636:LEU:HD22	1:A:1874:ARG:NH2	2.28	0.49
1:A:430:THR:O	1:A:431:TRP:C	2.56	0.49
1:A:147:TRP:CD1	1:A:250:CYS:SG	3.06	0.49
1:A:617:SER:OG	1:A:618:ASN:N	2.45	0.49
1:A:1779:ARG:NH1	1:A:1810:THR:O	2.45	0.48
1:A:1998:ILE:HG22	1:A:2023:ASP:HA	1.94	0.48
1:A:53:LEU:HD13	1:A:71:TRP:CG	2.47	0.48
1:A:430:THR:O	1:A:430:THR:HG22	2.13	0.48
1:A:904:VAL:HG12	1:A:908:LEU:HD12	1.94	0.48
1:A:1644:LEU:O	1:A:1645:PRO:C	2.54	0.48
1:A:376:VAL:HG11	1:A:676:GLN:CG	2.43	0.48
1:A:900:PHE:CZ	1:A:1105:HIS:HB2	2.48	0.48
1:A:964:LEU:HB3	1:A:1054:LEU:HD11	1.96	0.48
1:A:1203:ASN:HA	1:A:1206:SER:HB3	1.94	0.48
1:A:297:LEU:HB3	1:A:773:TYR:CE1	2.48	0.48
1:A:1409:MET:CE	1:A:1495:ILE:HD13	2.42	0.48
1:A:1644:LEU:CB	1:A:1645:PRO:HD2	2.43	0.48
1:A:373:HIS:CG	1:A:670:ARG:HD3	2.48	0.48
1:A:1956:PRO:CG	1:A:2022:LYS:HG3	2.43	0.48
1:A:48:ASP:OD1	1:A:49:ASP:N	2.46	0.48
1:A:99:LEU:HD13	1:A:241:ARG:NH2	2.29	0.48
1:A:1388:PRO:HD3	1:A:1396:ARG:CZ	2.44	0.48
1:A:1823:GLN:HA	1:A:1878:VAL:HG22	1.94	0.48
1:A:1954:ASN:C	1:A:1956:PRO:HD2	2.39	0.47
1:A:432:PRO:CB	1:A:436:GLN:HB2	2.44	0.47
1:A:638:THR:OG1	1:A:639:HIS:N	2.47	0.47
1:A:466:SER:HB3	1:A:1167:TRP:HB3	1.96	0.47
1:A:702:ILE:HD12	1:A:703:ARG:HB2	1.96	0.47
1:A:1079:TRP:HD1	1:A:1085:HIS:CG	2.33	0.47
1:A:1916:ALA:HB1	1:A:1934:TYR:HE1	1.78	0.47
1:A:872:THR:HG23	1:A:1069:LEU:HD23	1.96	0.47
1:A:880:LEU:C	1:A:880:LEU:HD12	2.39	0.47
1:A:1076:CYS:SG	1:A:1077:LYS:N	2.81	0.47
1:A:164:LEU:HD12	1:A:238:ILE:HG21	1.97	0.47
1:A:770:SER:C	1:A:772:ASP:N	2.72	0.47
1:A:1387:PHE:HB3	1:A:1388:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2070:TRP:O	1:A:2074:ARG:N	2.48	0.47
1:A:524:ILE:HG22	1:A:648:TYR:HE1	1.78	0.47
1:A:1667:LEU:HB3	1:A:1759:ILE:HD13	1.96	0.47
1:A:666:SER:OG	1:A:667:THR:N	2.48	0.47
1:A:915:HIS:CG	1:A:1078:MET:HE2	2.49	0.47
1:A:1397:GLY:C	1:A:1461:GLU:HG3	2.39	0.47
1:A:409:TRP:CZ2	1:A:431:TRP:CE3	3.02	0.47
1:A:576:LEU:HD21	1:A:824:HIS:CE1	2.49	0.47
1:A:1895:PRO:HB3	1:A:2042:LEU:HG	1.97	0.47
1:A:571:THR:OG1	1:A:776:TYR:OH	2.24	0.47
1:A:1487:TYR:CD1	1:A:1487:TYR:C	2.93	0.47
1:A:123:THR:HG23	1:A:879:TYR:CE1	2.50	0.46
1:A:1387:PHE:HB3	1:A:1388:PRO:HD2	1.97	0.46
1:A:1075:SER:OG	1:A:1076:CYS:N	2.48	0.46
1:A:1090:ARG:HD2	1:A:1098:VAL:HG21	1.98	0.46
1:A:864:LYS:O	1:A:865:ILE:HG23	2.16	0.46
1:A:945:LYS:HB3	1:A:946:LEU:HD12	1.97	0.46
1:A:1021:THR:HG22	1:A:1022:PHE:N	2.30	0.46
1:A:2040:LEU:N	1:A:2040:LEU:HD12	2.30	0.46
1:A:81:CYS:SG	1:A:220:LYS:HD2	2.56	0.46
1:A:560:LYS:HA	1:A:564:VAL:CG2	2.45	0.46
1:A:1823:GLN:HG2	1:A:1881:TYR:CE2	2.50	0.46
1:A:95:MET:HG3	1:A:96:GLY:N	2.30	0.46
1:A:1135:CYS:SG	1:A:1291:CYS:HB3	2.56	0.46
1:A:354:SER:C	1:A:356:ARG:N	2.72	0.46
1:A:458:LEU:HD23	1:A:464:ILE:HG12	1.96	0.46
1:A:1022:PHE:CE1	1:A:1326:LEU:HD22	2.51	0.46
1:A:1503:HIS:HB2	1:A:1504:TYR:CD2	2.51	0.46
1:A:1827:SER:HA	1:A:1874:ARG:HH22	1.81	0.46
1:A:1955:PRO:HD2	1:A:2000:TRP:CZ2	2.50	0.46
1:A:219:PHE:N	1:A:219:PHE:HD1	2.14	0.46
1:A:241:ARG:HH21	1:A:358:TRP:HB3	1.81	0.46
1:A:400:PHE:HD2	1:A:431:TRP:HZ2	1.64	0.46
1:A:770:SER:C	1:A:772:ASP:H	2.23	0.46
1:A:920:SER:OG	1:A:921:GLU:N	2.46	0.46
1:A:1627:MET:HE2	1:A:1802:CYS:CB	2.46	0.46
1:A:415:LEU:HD23	1:A:421:PRO:HB2	1.98	0.46
1:A:94:TRP:CE3	1:A:222:LEU:HD13	2.52	0.46
1:A:1151:ALA:CB	1:A:2106:SER:HB3	2.46	0.46
1:A:360:HIS:NE2	1:A:532:ARG:HD3	2.31	0.45
1:A:878:LEU:C	1:A:879:TYR:CD1	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:PHE:CD2	1:A:1099:ILE:HG21	2.51	0.45
1:A:147:TRP:CD1	1:A:250:CYS:HG	2.34	0.45
1:A:915:HIS:NE2	1:A:1078:MET:HG3	2.31	0.45
1:A:1782:VAL:HG12	1:A:1783:HIS:N	2.31	0.45
1:A:1066:LEU:N	1:A:1066:LEU:HD23	2.31	0.45
1:A:1739:PRO:O	1:A:1740:ARG:HB3	2.16	0.45
1:A:1922:ASP:C	1:A:1924:PRO:HD3	2.40	0.45
1:A:283:TYR:CD1	1:A:283:TYR:N	2.85	0.45
1:A:1142:VAL:HG23	1:A:1249:ARG:HE	1.82	0.45
1:A:1646:THR:HG22	1:A:1647:GLY:N	2.31	0.45
1:A:1958:ASP:OD1	1:A:1959:GLY:N	2.50	0.45
1:A:2100:ASP:CG	1:A:2101:LEU:H	2.25	0.45
1:A:720:THR:HG22	1:A:722:TYR:CE2	2.52	0.45
1:A:1599:PRO:HD3	1:A:1716:LEU:C	2.42	0.45
1:A:1999:ARG:NH1	1:A:2018:ASP:OD1	2.48	0.45
1:A:1891:PHE:N	1:A:1891:PHE:CD1	2.83	0.45
1:A:304:SER:HB2	1:A:783:ARG:CZ	2.47	0.45
1:A:551:TYR:OH	1:A:684:ARG:NH2	2.50	0.45
1:A:610:ASN:HB3	1:A:681:GLU:H	1.82	0.45
1:A:1454:ARG:HG3	1:A:1480:MET:HG3	1.99	0.45
1:A:609:TRP:HH2	1:A:692:ASN:HB2	1.82	0.45
1:A:983:GLN:HB2	1:A:1329:TRP:CZ3	2.52	0.45
1:A:1121:ALA:N	1:A:1122:PRO:HD2	2.32	0.45
1:A:1156:LYS:HA	1:A:2108:ARG:HB3	1.99	0.45
1:A:1416:VAL:HA	1:A:1419:ARG:HB3	1.99	0.45
1:A:75:LEU:HA	1:A:78:LEU:HD12	1.99	0.44
1:A:331:GLY:HA2	1:A:334:PHE:CD2	2.51	0.44
1:A:460:ASP:OD1	1:A:460:ASP:C	2.61	0.44
1:A:1189:PHE:HD1	1:A:1189:PHE:H	1.66	0.44
1:A:392:SER:OG	1:A:442:ASP:HB3	2.18	0.44
1:A:995:GLU:HG2	1:A:1320:PRO:HG2	1.98	0.44
1:A:334:PHE:N	1:A:334:PHE:CD1	2.85	0.44
1:A:419:ASP:C	1:A:421:PRO:HD2	2.42	0.44
1:A:496:GLN:NE2	1:A:1043:PHE:CE1	2.85	0.44
1:A:710:LEU:HB3	1:A:776:TYR:CE2	2.52	0.44
1:A:1010:PHE:HD1	1:A:1013:PHE:H	1.65	0.44
1:A:1118:THR:HB	1:A:1119:PRO:HD2	2.00	0.44
1:A:803:ASP:HB2	1:A:1036:SER:HB2	1.99	0.44
1:A:865:ILE:HD11	1:A:868:LEU:HD21	1.99	0.44
1:A:915:HIS:CG	1:A:1078:MET:SD	3.11	0.44
1:A:1081:CYS:SG	1:A:1299:CYS:HB2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:HIS:CG	1:A:1141:ASP:H	2.36	0.44
1:A:1284:ARG:O	1:A:1286:GLY:N	2.43	0.44
1:A:1227:HIS:HB3	1:A:1268:LEU:HD21	1.99	0.44
1:A:1231:THR:O	1:A:1233:ARG:N	2.51	0.44
1:A:424:SER:HA	1:A:430:THR:CB	2.48	0.44
1:A:545:SER:O	1:A:548:LEU:N	2.51	0.44
1:A:938:PHE:CD1	1:A:938:PHE:C	2.96	0.44
1:A:1081:CYS:HB3	1:A:1302:CYS:HB3	1.99	0.44
1:A:1190:VAL:HB	1:A:1198:MET:SD	2.58	0.44
1:A:1834:VAL:CG1	1:A:1835:TYR:N	2.80	0.44
1:A:1951:ILE:HA	1:A:2009:TYR:CZ	2.53	0.44
1:A:376:VAL:HG11	1:A:676:GLN:HG3	1.98	0.44
1:A:789:LEU:HB2	1:A:792:LYS:HB2	2.00	0.44
1:A:1443:LEU:HD21	1:A:1449:PHE:CE2	2.53	0.44
1:A:1894:ASP:C	1:A:1896:PHE:H	2.25	0.44
1:A:812:MET:HA	1:A:815:VAL:HG12	1.99	0.44
1:A:1967:ALA:HA	1:A:2036:TRP:NE1	2.33	0.44
1:A:1389:LEU:HD23	1:A:1391:ILE:CD1	2.48	0.43
1:A:1822:VAL:C	1:A:1824:THR:N	2.71	0.43
1:A:1943:ILE:HG21	1:A:2013:TRP:NE1	2.32	0.43
1:A:1992:ILE:HG13	1:A:1993:GLN:N	2.32	0.43
1:A:774:LEU:HD12	1:A:775:ASN:H	1.82	0.43
1:A:1002:PHE:CZ	1:A:1200:ILE:HD13	2.53	0.43
1:A:419:ASP:HB2	1:A:421:PRO:CD	2.42	0.43
1:A:563:PHE:CG	1:A:625:MET:HE1	2.54	0.43
1:A:861:VAL:HG13	1:A:864:LYS:HB3	1.98	0.43
1:A:946:LEU:HB2	1:A:1094:TRP:CH2	2.52	0.43
1:A:186:PHE:O	1:A:187:LYS:HB3	2.17	0.43
1:A:1895:PRO:O	1:A:2043:VAL:HG12	2.18	0.43
1:A:2100:ASP:OD1	1:A:2100:ASP:N	2.52	0.43
1:A:710:LEU:HB2	1:A:717:VAL:HG22	2.00	0.43
1:A:911:TRP:CE3	1:A:914:ILE:HG21	2.53	0.43
1:A:1119:PRO:C	1:A:1121:ALA:H	2.26	0.43
1:A:1872:PHE:CZ	1:A:1977:LEU:HA	2.53	0.43
1:A:1912:VAL:HG13	1:A:2064:VAL:HG11	2.01	0.43
1:A:1992:ILE:HA	1:A:2026:ILE:HD11	2.00	0.43
1:A:915:HIS:ND1	1:A:1078:MET:SD	2.92	0.43
1:A:1188:TRP:CE3	1:A:1189:PHE:HB3	2.54	0.43
1:A:1652:ILE:HD13	1:A:1652:ILE:HA	1.89	0.43
1:A:1440:ILE:HD13	1:A:1440:ILE:HA	1.92	0.43
1:A:1730:TRP:H	1:A:1730:TRP:CD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:CG2	1:A:879:TYR:CE1	3.02	0.43
1:A:403:PHE:O	1:A:407:LYS:HA	2.19	0.43
1:A:40:ASN:O	1:A:232:LEU:HD13	2.19	0.43
1:A:515:GLU:HG3	1:A:516:LYS:N	2.33	0.43
1:A:1178:ARG:HA	1:A:1231:THR:HG21	2.00	0.43
1:A:86:ILE:HG22	1:A:90:GLN:CB	2.48	0.43
1:A:603:HIS:CD2	1:A:767:THR:HG23	2.53	0.43
1:A:794:TRP:HA	1:A:797:VAL:HG23	2.00	0.43
1:A:969:VAL:HG21	1:A:1033:PHE:CD2	2.54	0.43
1:A:983:GLN:HB2	1:A:1329:TRP:HZ3	1.83	0.43
1:A:2080:ILE:C	1:A:2082:TRP:N	2.76	0.43
1:A:65:MET:HB3	1:A:486:ASN:HB3	2.01	0.42
1:A:784:GLY:HA3	1:A:1146:ARG:HD2	2.01	0.42
1:A:854:LEU:C	1:A:856:GLN:H	2.26	0.42
1:A:1078:MET:C	1:A:1079:TRP:HE3	2.27	0.42
1:A:1453:THR:OG1	1:A:1462:LEU:HD12	2.19	0.42
1:A:87:SER:C	1:A:88:THR:HG1	2.24	0.42
1:A:983:GLN:HG3	1:A:1329:TRP:HZ3	1.84	0.42
1:A:1189:PHE:O	1:A:1310:THR:HA	2.19	0.42
1:A:2028:ASP:OD1	1:A:2028:ASP:N	2.52	0.42
1:A:241:ARG:HD2	1:A:268:TYR:CE2	2.54	0.42
1:A:398:VAL:CG2	1:A:628:PHE:CZ	3.02	0.42
1:A:1330:ARG:HG3	1:A:1331:ASN:N	2.34	0.42
1:A:1946:ILE:HG21	1:A:2068:LEU:HB3	2.00	0.42
1:A:887:VAL:HG23	1:A:1066:LEU:HD21	2.02	0.42
1:A:1090:ARG:NH1	1:A:1102:THR:OG1	2.53	0.42
1:A:1149:LEU:CD2	1:A:1251:MET:HB2	2.49	0.42
1:A:1251:MET:SD	1:A:1697:LEU:HD21	2.59	0.42
1:A:1898:ASN:HA	1:A:1901:THR:HG22	2.01	0.42
1:A:1951:ILE:HA	1:A:2009:TYR:CE1	2.55	0.42
1:A:515:GLU:CG	1:A:516:LYS:N	2.82	0.42
1:A:1601:TRP:CZ3	1:A:1682:ARG:HD3	2.55	0.42
1:A:2065:ASP:HB3	1:A:2068:LEU:HD21	2.02	0.42
1:A:293:CYS:SG	1:A:352:TYR:HB2	2.58	0.42
1:A:467:ASP:CG	1:A:1037:ARG:HB3	2.45	0.42
1:A:666:SER:O	1:A:668:SER:N	2.53	0.42
1:A:599:CYS:O	1:A:771:ALA:HA	2.20	0.42
1:A:685:GLN:NE2	1:A:685:GLN:HA	2.35	0.42
1:A:880:LEU:HD12	1:A:880:LEU:O	2.19	0.42
1:A:2021:PRO:C	1:A:2023:ASP:H	2.27	0.42
1:A:2057:PHE:CE2	1:A:2070:TRP:HE3	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:HG21	1:A:216:TRP:CG	2.54	0.42
1:A:626:GLY:O	1:A:627:GLN:C	2.63	0.42
1:A:796:ARG:HB3	1:A:799:CYS:SG	2.60	0.42
1:A:1199:THR:O	1:A:1203:ASN:ND2	2.48	0.42
1:A:1319:PRO:HA	1:A:1320:PRO:HD3	1.85	0.42
1:A:1943:ILE:HD13	1:A:2013:TRP:CG	2.54	0.42
1:A:2052:PHE:HE1	1:A:2057:PHE:HB2	1.84	0.42
1:A:634:LEU:HG	1:A:635:ILE:N	2.35	0.42
1:A:834:ILE:N	1:A:834:ILE:HD12	2.34	0.42
1:A:913:PHE:CD1	1:A:913:PHE:C	2.98	0.42
1:A:1206:SER:HB2	1:A:1211:GLU:HG3	2.01	0.42
1:A:1945:HIS:HE1	1:A:2068:LEU:HB2	1.84	0.42
1:A:629:LEU:C	1:A:631:TYR:H	2.21	0.42
1:A:864:LYS:C	1:A:865:ILE:HG23	2.44	0.42
1:A:865:ILE:HD11	1:A:868:LEU:HG	2.01	0.42
1:A:1140:HIS:CG	1:A:1141:ASP:N	2.88	0.42
1:A:1330:ARG:CG	1:A:1331:ASN:N	2.82	0.42
1:A:1671:ASP:HB3	1:A:1674:GLY:HA2	2.02	0.42
1:A:1974:TRP:HE1	1:A:2040:LEU:CD2	2.33	0.42
1:A:164:LEU:HD22	1:A:231:LEU:HD11	2.02	0.41
1:A:249:VAL:HG13	1:A:250:CYS:N	2.34	0.41
1:A:1425:LEU:HD23	1:A:1538:SER:CB	2.49	0.41
1:A:1425:LEU:HD23	1:A:1538:SER:HA	2.02	0.41
1:A:1651:LYS:CB	1:A:1824:THR:HG21	2.50	0.41
1:A:99:LEU:HD11	1:A:237:VAL:HG11	2.02	0.41
1:A:386:TYR:CD2	1:A:758:LEU:HD21	2.55	0.41
1:A:720:THR:CG2	1:A:722:TYR:CE2	3.03	0.41
1:A:1401:LEU:HD23	1:A:1487:TYR:CE1	2.55	0.41
1:A:1436:LEU:HD23	1:A:1437:ILE:HD13	2.02	0.41
1:A:2009:TYR:N	1:A:2009:TYR:CD1	2.87	0.41
1:A:274:ILE:HG22	1:A:282:SER:HB3	2.02	0.41
1:A:279:GLY:O	1:A:281:PHE:N	2.53	0.41
1:A:402:GLN:HE21	1:A:452:CYS:HB3	1.86	0.41
1:A:609:TRP:CH2	1:A:692:ASN:HB2	2.55	0.41
1:A:794:TRP:O	1:A:797:VAL:HG23	2.21	0.41
1:A:1149:LEU:HD23	1:A:1251:MET:HB2	2.02	0.41
1:A:1669:CYS:HB2	1:A:1736:LEU:HD13	2.02	0.41
1:A:257:SER:O	1:A:260:ASP:N	2.53	0.41
1:A:728:ARG:HB2	1:A:2025:ARG:HH12	1.85	0.41
1:A:865:ILE:HG13	1:A:866:PRO:N	2.35	0.41
1:A:915:HIS:CG	1:A:1078:MET:CE	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:THR:HB	1:A:1119:PRO:CD	2.51	0.41
1:A:1732:TYR:O	1:A:1734:SER:N	2.54	0.41
1:A:1765:VAL:HG11	1:A:1771:SER:HB2	2.02	0.41
1:A:1778:VAL:CG2	1:A:1811:ILE:HD11	2.50	0.41
1:A:1789:GLN:OE1	1:A:1789:GLN:N	2.53	0.41
1:A:1827:SER:CA	1:A:1874:ARG:HH22	2.34	0.41
1:A:2047:VAL:HG12	1:A:2048:ARG:N	2.35	0.41
1:A:606:TYR:HD2	1:A:609:TRP:HB2	1.86	0.41
1:A:1647:GLY:C	1:A:1649:HIS:N	2.75	0.41
1:A:1665:ASP:OD1	1:A:1688:ARG:N	2.43	0.41
1:A:559:ILE:CD1	1:A:625:MET:CE	2.98	0.41
1:A:946:LEU:HD22	1:A:1094:TRP:CH2	2.55	0.41
1:A:1106:PRO:HB2	1:A:1275:TYR:CD1	2.56	0.41
1:A:1862:LEU:HG	1:A:1863:TYR:N	2.36	0.41
1:A:1885:THR:HG22	1:A:1886:GLY:N	2.35	0.41
1:A:1961:ALA:HA	1:A:1964:VAL:HG12	2.03	0.41
1:A:248:MET:HE3	1:A:256:PHE:CZ	2.56	0.41
1:A:411:VAL:HG12	1:A:412:ASN:N	2.35	0.41
1:A:915:HIS:CD2	1:A:915:HIS:C	2.96	0.41
1:A:1627:MET:HE2	1:A:1802:CYS:HB2	2.02	0.41
1:A:1656:LEU:HD23	1:A:1663:TYR:HE1	1.86	0.41
1:A:1822:VAL:CB	1:A:1874:ARG:HD2	2.51	0.41
1:A:104:HIS:ND1	1:A:105:ASP:O	2.54	0.41
1:A:328:ILE:HG22	1:A:329:ASP:N	2.36	0.41
1:A:344:THR:HG22	1:A:345:VAL:N	2.36	0.41
1:A:865:ILE:HD11	1:A:868:LEU:CG	2.50	0.41
1:A:1447:PRO:HG2	1:A:1448:PRO:HD3	2.01	0.41
1:A:1813:GLY:HA3	1:A:1836:MET:SD	2.61	0.41
1:A:1945:HIS:CB	1:A:2077:THR:HG23	2.49	0.41
1:A:2010:LYS:CG	1:A:2011:GLN:N	2.84	0.41
1:A:88:THR:O	1:A:89:SER:C	2.63	0.41
1:A:252:ILE:HD12	1:A:830:ILE:CG2	2.51	0.41
1:A:285:LEU:HB3	1:A:332:ILE:HD12	2.02	0.41
1:A:496:GLN:HE22	1:A:1044:LYS:HB3	1.85	0.41
1:A:654:ASP:OD1	1:A:654:ASP:N	2.54	0.41
1:A:782:PHE:O	1:A:783:ARG:C	2.64	0.41
1:A:801:THR:HG22	1:A:802:ASN:H	1.86	0.41
1:A:955:ILE:HG22	1:A:956:ALA:N	2.35	0.41
1:A:970:LYS:HB2	1:A:1030:ILE:CD1	2.51	0.41
1:A:1136:PRO:C	1:A:1138:GLY:H	2.29	0.41
1:A:1636:LEU:HA	1:A:1639:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1884:LEU:HD11	1:A:1892:ILE:HG12	2.03	0.41
1:A:1888:PRO:HG2	1:A:1891:PHE:CE2	2.56	0.41
1:A:1901:THR:O	1:A:1905:ILE:N	2.53	0.41
1:A:2075:ARG:O	1:A:2076:ASN:C	2.64	0.41
1:A:1078:MET:HE3	1:A:1078:MET:HA	2.02	0.41
1:A:218:TYR:C	1:A:219:PHE:HD1	2.28	0.40
1:A:459:LEU:HD23	1:A:459:LEU:HA	1.99	0.40
1:A:1387:PHE:CB	1:A:1388:PRO:HD2	2.51	0.40
1:A:1627:MET:HG3	1:A:1628:PRO:HD2	2.03	0.40
1:A:385:SER:HA	1:A:388:LYS:HB2	2.03	0.40
1:A:875:TYR:O	1:A:879:TYR:HB2	2.21	0.40
1:A:1106:PRO:HB2	1:A:1275:TYR:CG	2.56	0.40
1:A:1409:MET:HG3	1:A:1529:LEU:HD21	2.04	0.40
1:A:1460:ASP:O	1:A:1463:GLU:N	2.50	0.40
1:A:1599:PRO:HD3	1:A:1717:GLY:HA3	2.02	0.40
1:A:1636:LEU:HB3	1:A:1826:PHE:HA	2.03	0.40
1:A:1643:GLN:O	1:A:1643:GLN:HG3	2.21	0.40
1:A:1860:LYS:HA	1:A:1865:PHE:CD2	2.56	0.40
1:A:39:TYR:CE1	1:A:172:ASN:HB3	2.56	0.40
1:A:78:LEU:HD23	1:A:219:PHE:CE2	2.56	0.40
1:A:252:ILE:HD12	1:A:830:ILE:HG22	2.03	0.40
1:A:781:ILE:HG23	1:A:785:VAL:O	2.21	0.40
1:A:830:ILE:O	1:A:833:MET:N	2.53	0.40
1:A:1215:ARG:C	1:A:1216:GLN:HG3	2.47	0.40
1:A:1414:CYS:O	1:A:1417:ILE:HG22	2.20	0.40
1:A:1781:TYR:HB3	1:A:1785:ILE:HD12	2.04	0.40
1:A:1963:ASN:HA	1:A:1966:ILE:CG2	2.51	0.40
1:A:2010:LYS:HG2	1:A:2011:GLN:N	2.34	0.40
1:A:403:PHE:HE2	1:A:431:TRP:CB	2.35	0.40
1:A:480:HIS:O	1:A:480:HIS:ND1	2.52	0.40
1:A:1188:TRP:CH2	1:A:1225:ALA:HA	2.57	0.40
1:A:1284:ARG:NH2	1:A:1293:ASP:OD1	2.54	0.40
1:A:1375:TYR:CD1	1:A:1415:GLN:HG2	2.56	0.40
1:A:1450:LEU:HA	1:A:1453:THR:HG22	2.03	0.40
1:A:2013:TRP:O	1:A:2077:THR:OG1	2.31	0.40
1:A:94:TRP:HZ3	1:A:98:TRP:CG	2.39	0.40
1:A:161:PHE:CD1	1:A:161:PHE:C	2.99	0.40
1:A:349:LEU:HD11	1:A:780:PRO:HG3	2.04	0.40
1:A:489:ILE:HD11	1:A:653:PRO:HB3	2.04	0.40
1:A:1872:PHE:CD2	1:A:1876:LYS:HE3	2.56	0.40
1:A:1951:ILE:O	1:A:1953:PRO:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1978:MET:HB3	1:A:2049:LEU:HD13	2.04	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	1994/2109 (94%)	1678 (84%)	277 (14%)	39 (2%)	6	32

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO
1	A	355	PHE
1	A	730	VAL
1	A	1381	ALA
1	A	2066	ASN
1	A	384	VAL
1	A	1166	PRO
1	A	1232	SER
1	A	1803	GLU
1	A	58	ASN
1	A	218	TYR
1	A	667	THR
1	A	797	VAL
1	A	1186	ILE
1	A	219	PHE
1	A	539	ARG
1	A	901	PRO
1	A	1314	SER
1	A	1644	LEU
1	A	424	SER

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Mol	Chain	Res	Type
1	A	774	LEU
1	A	1081	CYS
1	A	1151	ALA
1	A	1387	PHE
1	A	1468	LYS
1	A	1635	LEU
1	A	2083	ILE
1	A	2107	TRP
1	A	62	ILE
1	A	104	HIS
1	A	630	GLY
1	A	1285	ASP
1	A	2101	LEU
1	A	46	ILE
1	A	559	ILE
1	A	900	PHE
1	A	1756	ILE
1	A	1519	ILE
1	A	1150	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	1794/1890 (95%)	1695 (94%)	99 (6%)	19 45

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	86	ILE
1	A	95	MET
1	A	103	ASN
1	A	105	ASP
1	A	113	LEU
1	A	144	LYS

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Mol	Chain	Res	Type
1	A	149	ASP
1	A	171	LEU
1	A	193	SER
1	A	207	LEU
1	A	210	THR
1	A	219	PHE
1	A	225	LEU
1	A	233	MET
1	A	266	ASN
1	A	273	LYS
1	A	290	GLU
1	A	293	CYS
1	A	334	PHE
1	A	339	ILE
1	A	424	SER
1	A	433	THR
1	A	450	ILE
1	A	460	ASP
1	A	475	SER
1	A	478	LEU
1	A	494	VAL
1	A	504	THR
1	A	513	ILE
1	A	534	LEU
1	A	543	LEU
1	A	544	MET
1	A	564	VAL
1	A	603	HIS
1	A	617	SER
1	A	629	LEU
1	A	634	LEU
1	A	667	THR
1	A	671	VAL
1	A	690	ILE
1	A	709	VAL
1	A	715	ASN
1	A	717	VAL
1	A	720	THR
1	A	751	ILE
1	A	766	GLU
1	A	767	THR
1	A	798	THR

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Mol	Chain	Res	Type
1	A	801	THR
1	A	812	MET
1	A	865	ILE
1	A	905	THR
1	A	929	VAL
1	A	952	SER
1	A	953	LEU
1	A	1030	ILE
1	A	1072	ARG
1	A	1088	THR
1	A	1105	HIS
1	A	1123	CYS
1	A	1142	VAL
1	A	1167	TRP
1	A	1189	PHE
1	A	1222	THR
1	A	1257	MET
1	A	1278	ILE
1	A	1290	SER
1	A	1302	CYS
1	A	1384	SER
1	A	1401	LEU
1	A	1408	LEU
1	A	1437	ILE
1	A	1440	ILE
1	A	1443	LEU
1	A	1452	LEU
1	A	1467	HIS
1	A	1471	THR
1	A	1476	SER
1	A	1491	GLN
1	A	1495	ILE
1	A	1502	SER
1	A	1609	ILE
1	A	1615	TYR
1	A	1655	ILE
1	A	1681	LEU
1	A	1728	THR
1	A	1754	LEU
1	A	1761	MET
1	A	1772	LEU
1	A	1782	VAL

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Mol	Chain	Res	Type
1	A	1820	ASP
1	A	1926	ASP
1	A	1927	LEU
1	A	2029	SER
1	A	2036	TRP
1	A	2071	SER
1	A	2072	ASN
1	A	2077	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	420	HIS
1	A	425	HIS
1	A	496	GLN
1	A	602	ASN
1	A	716	GLN
1	A	744	ASN
1	A	862	GLN
1	A	932	ASN
1	A	1277	GLN
1	A	1503	HIS
1	A	1643	GLN
1	A	1783	HIS
1	A	1914	HIS
1	A	2050	ASN
1	A	2053	ASN
1	A	2076	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

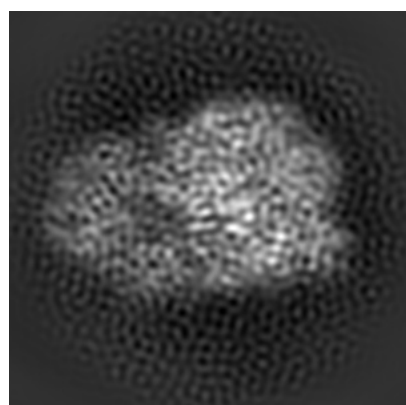
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6337. These allow visual inspection of the internal detail of the map and identification of artifacts.

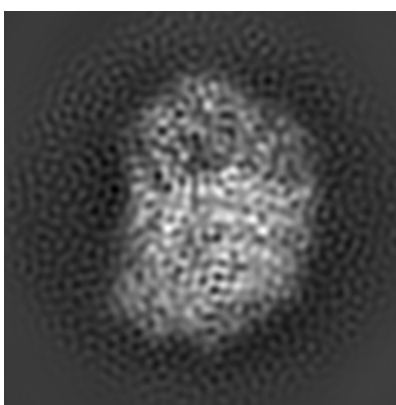
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

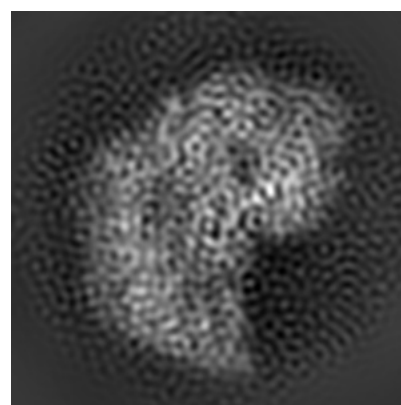
6.1.1 Primary map



X



Y

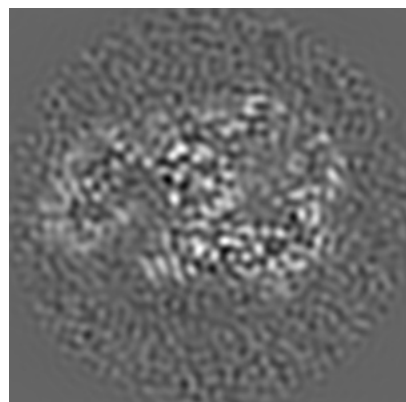


Z

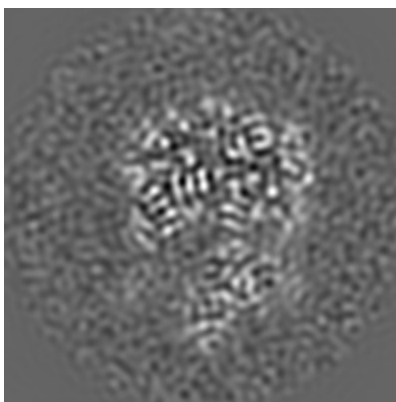
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

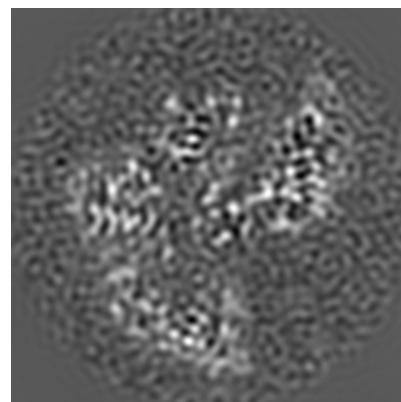
6.2.1 Primary map



X Index: 60



Y Index: 60

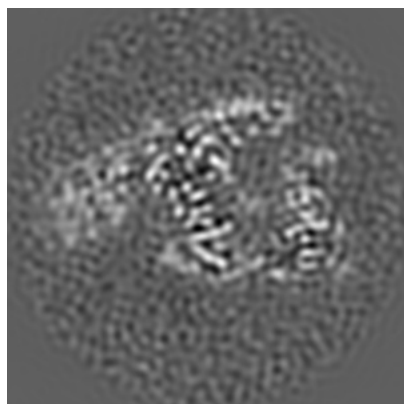


Z Index: 60

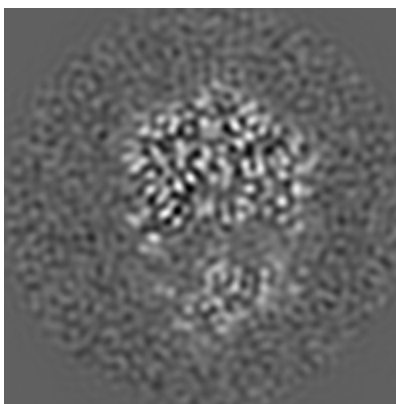
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

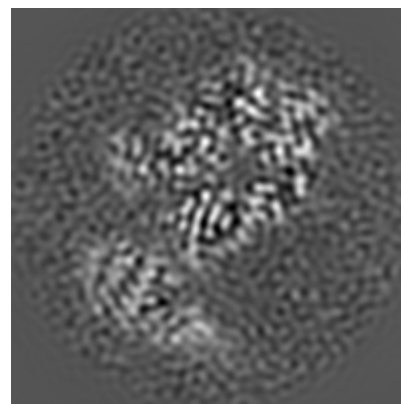
6.3.1 Primary map



X Index: 65



Y Index: 63

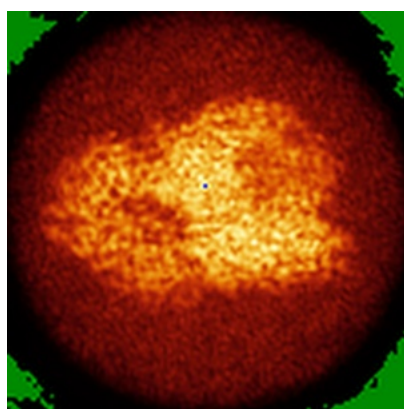


Z Index: 48

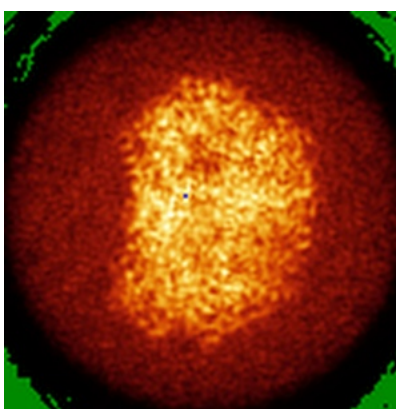
The images above show the largest variance slices of the map in three orthogonal directions.

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

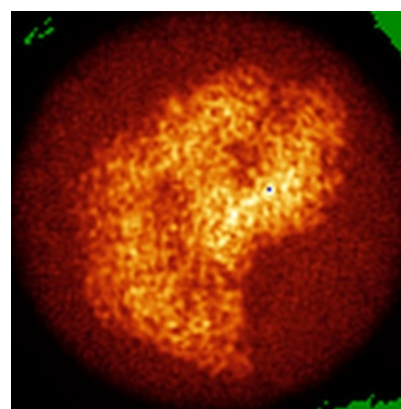
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

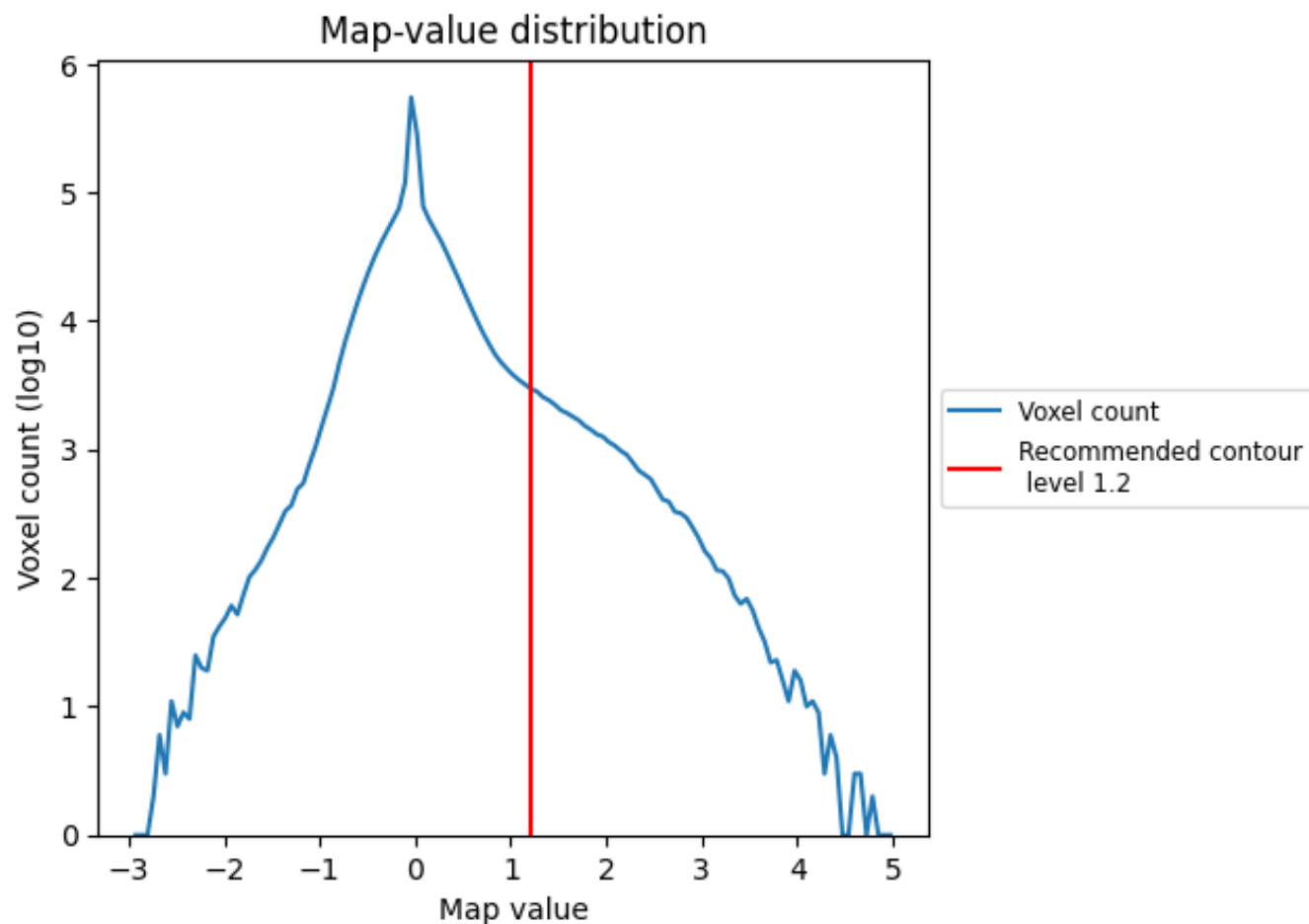
6.6 Mask visualisation

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

7 Map analysis [i](#)

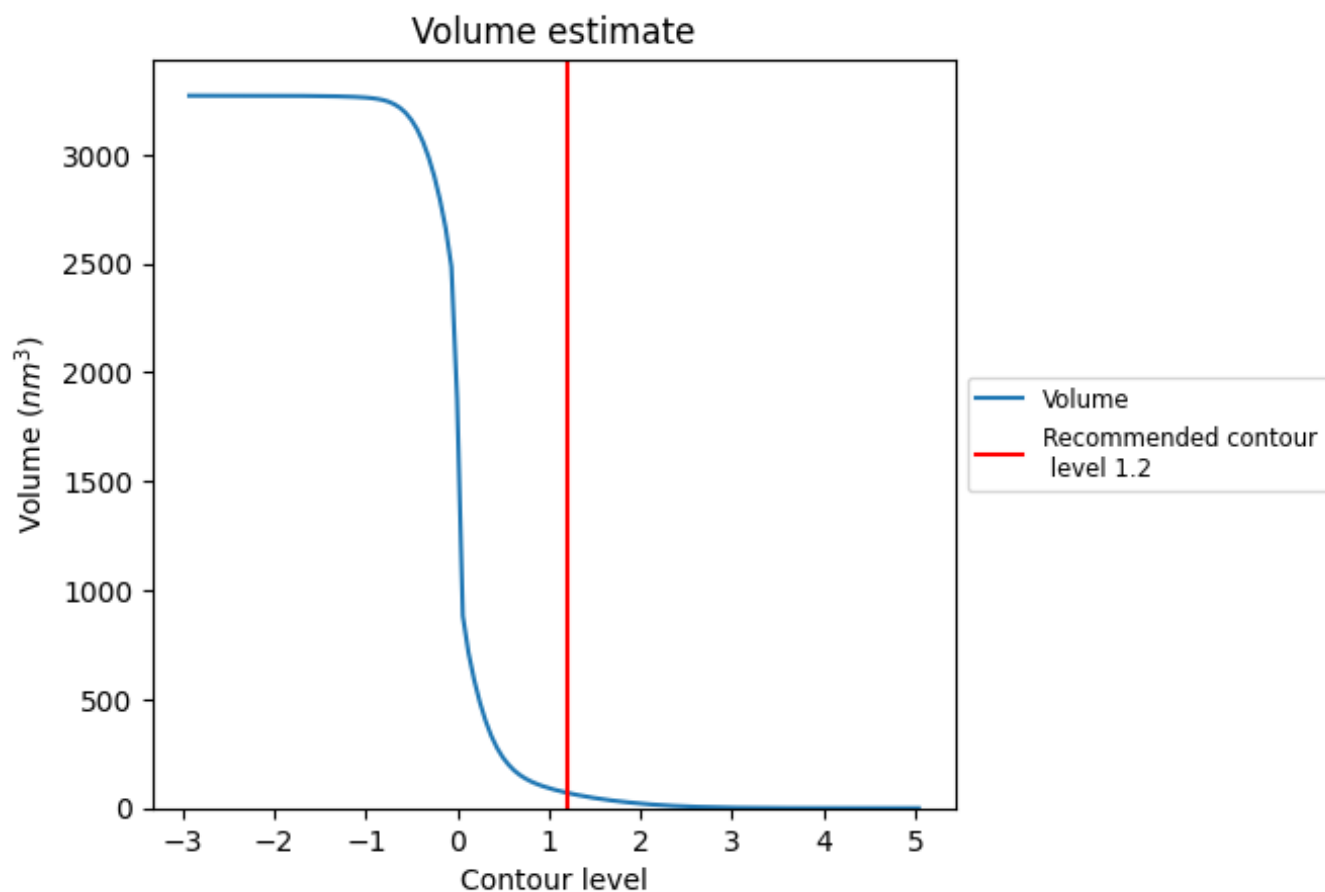
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

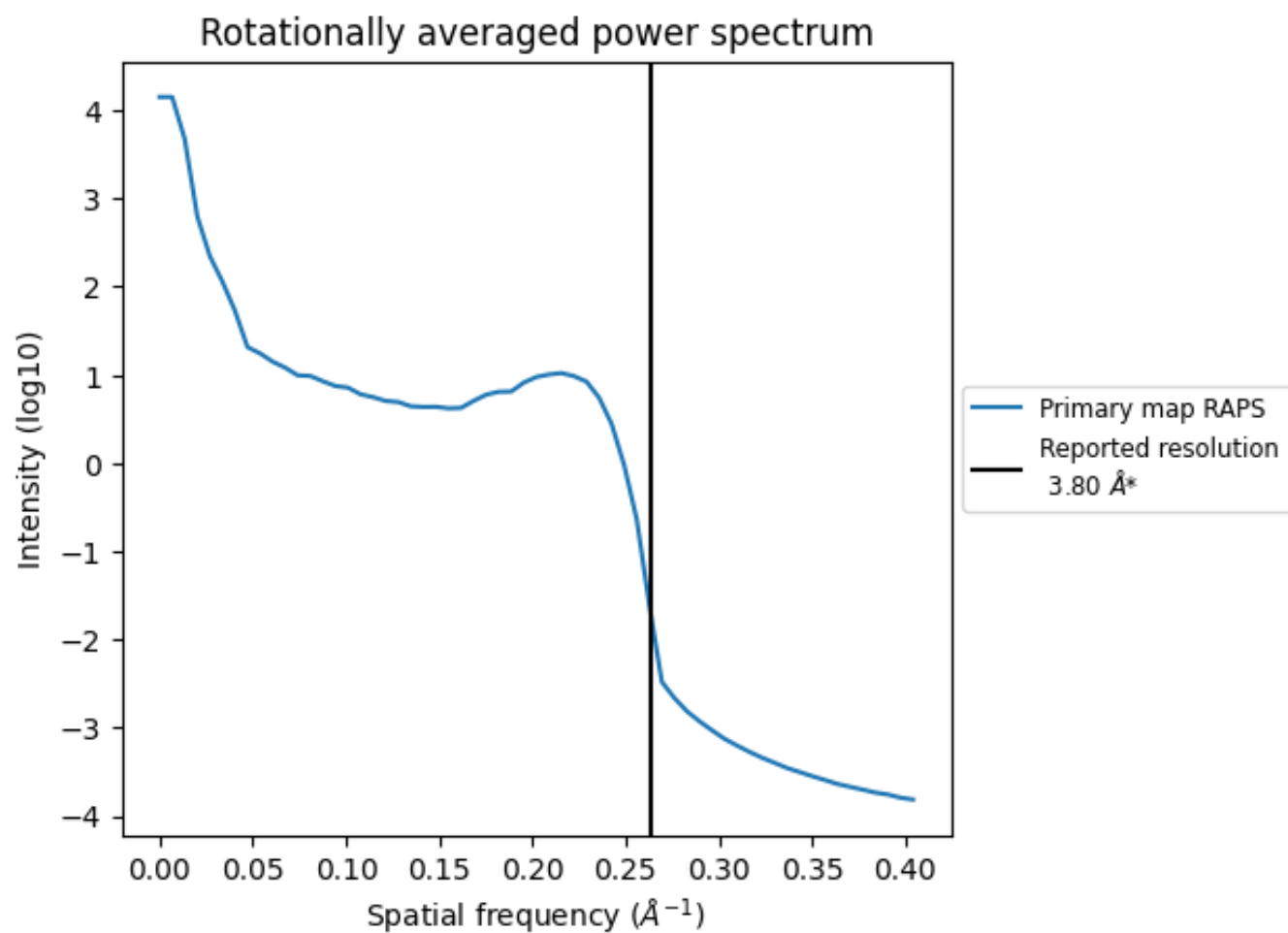
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm^3 ; this corresponds to an approximate mass of 64 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 0.263 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

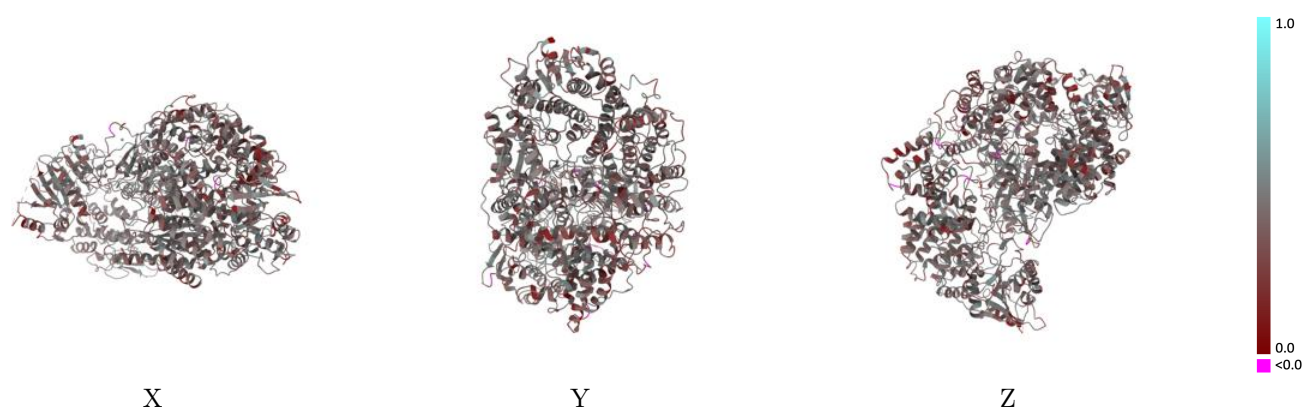
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6337 and PDB model 5A22. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

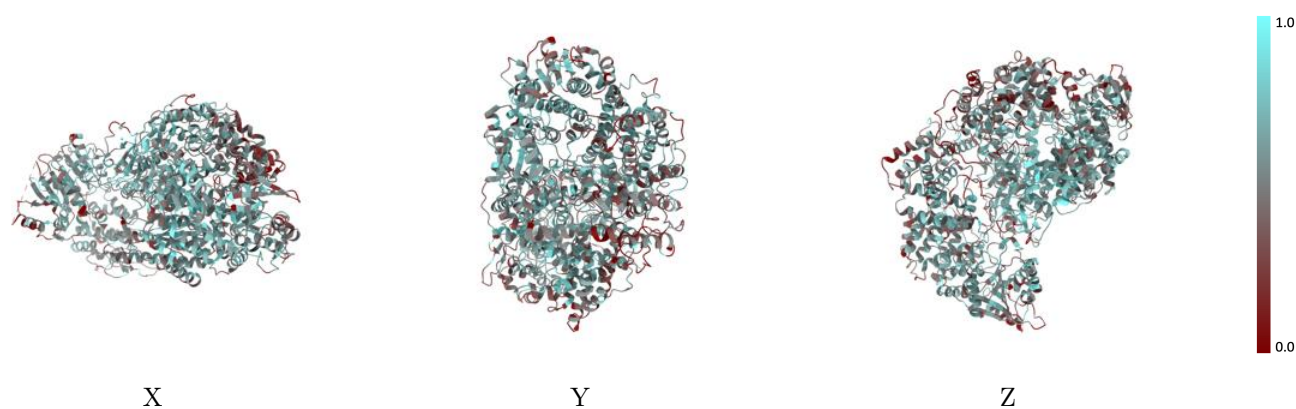
This section was not generated.

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



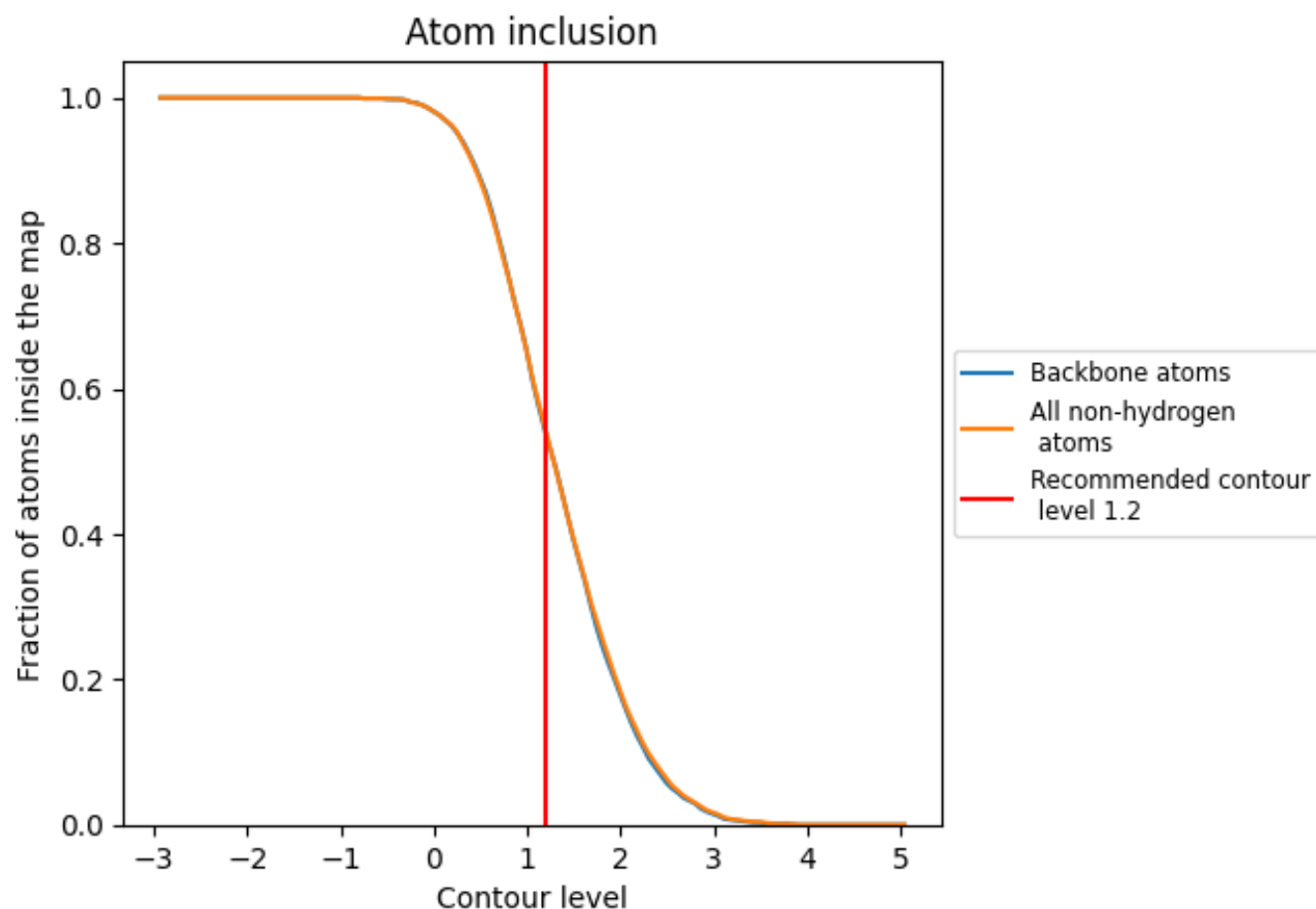
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5410	0.3960
A	0.5510	0.3960

