Full wwPDB EM Validation Report

Nov 10, 2026 – 06:48 pm GMT

PDB ID	:	9T7B / pdb_00009t7b
EMDB ID	:	EMD-55632
Title	:	cryo-EM structure of LARP1 TOS peptide bound to human mTOR complex 1
Authors	:	Craigie, L.M.; Maier, T.
Deposited on	:	2025-11-10
Resolution	:	3.16 Å(reported)
Based on initial model	:	9F44

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 (i) 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 (1)) were used in the production of this report:

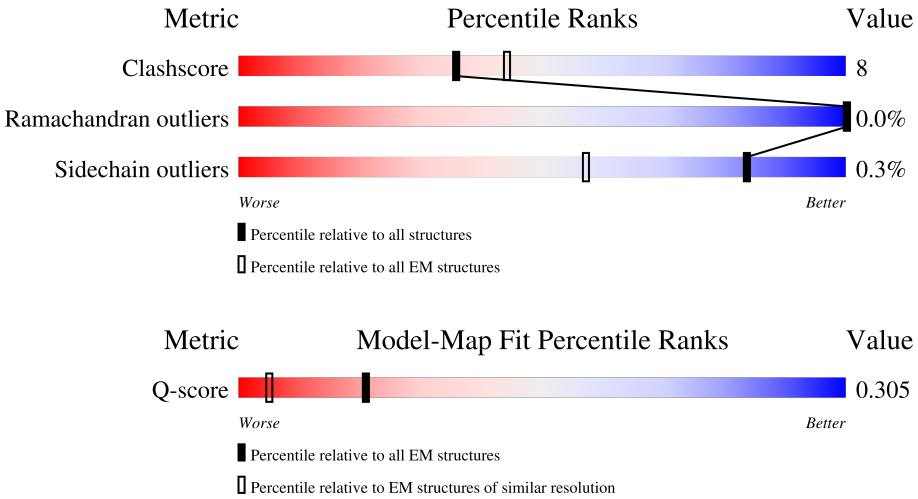
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

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 3.16 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	14474 (2.66 - 3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	326	85% 12%
1	D	326	85% 12%
2	G	16	19% 38% 6% 56%
2	H	16	19% 44% 56%

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Mol	Chain	Length	Quality of chain
3	A	2549	70% 16% 14%
3	B	2549	70% 16% 14%
4	E	1363	64% 13% 23%
4	F	1363	65% 12% 23%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 113464 atoms, of which 56648 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 Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	317	Total	C	H	N	O	S	0	0
			4797	1526	2341	436	476	18		
1	D	317	Total	C	H	N	O	S	0	0
			4797	1526	2341	436	476	18		

- Molecule 2 is a protein called La-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	7	Total	C	H	N	O	0	0
			113	42	49	7	15		
2	H	7	Total	C	H	N	O	0	0
			113	42	49	7	15		

- Molecule 3 is a protein called Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	2192	Total	C	H	N	O	S	0	0
			35020	11158	17553	3060	3137	112		
3	B	2192	Total	C	H	N	O	S	0	0
			35020	11158	17553	3060	3137	112		

- Molecule 4 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	1052	Total	C	H	N	O	S	0	0
			16760	5361	8375	1450	1518	56		
4	F	1052	Total	C	H	N	O	S	0	0
			16760	5361	8375	1450	1518	56		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-27	HIS	-	expression tag	UNP Q8N122

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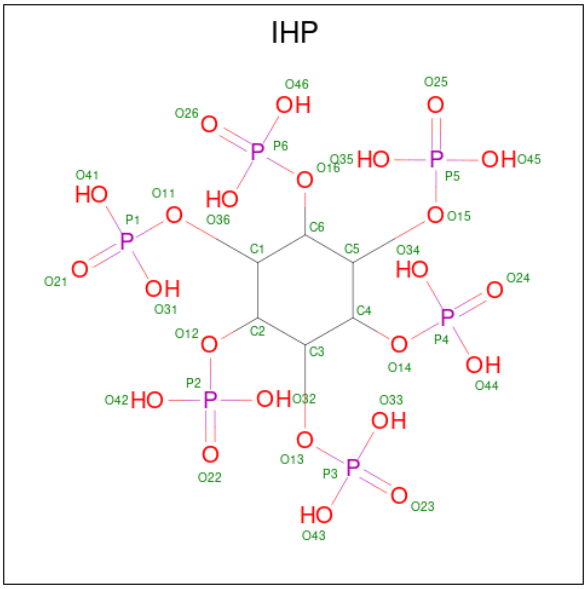
Chain	Residue	Modelled	Actual	Comment	Reference
E	-26	HIS	-	expression tag	UNP Q8N122
E	-25	HIS	-	expression tag	UNP Q8N122
E	-24	HIS	-	expression tag	UNP Q8N122
E	-23	HIS	-	expression tag	UNP Q8N122
E	-22	HIS	-	expression tag	UNP Q8N122
E	-21	HIS	-	expression tag	UNP Q8N122
E	-20	HIS	-	expression tag	UNP Q8N122
E	-19	HIS	-	expression tag	UNP Q8N122
E	-18	HIS	-	expression tag	UNP Q8N122
E	-17	GLU	-	expression tag	UNP Q8N122
E	-16	GLN	-	expression tag	UNP Q8N122
E	-15	LYS	-	expression tag	UNP Q8N122
E	-14	LEU	-	expression tag	UNP Q8N122
E	-13	ILE	-	expression tag	UNP Q8N122
E	-12	SER	-	expression tag	UNP Q8N122
E	-11	GLU	-	expression tag	UNP Q8N122
E	-10	GLU	-	expression tag	UNP Q8N122
E	-9	ASP	-	expression tag	UNP Q8N122
E	-8	LEU	-	expression tag	UNP Q8N122
E	-7	ASP	-	expression tag	UNP Q8N122
E	-6	TYR	-	expression tag	UNP Q8N122
E	-5	LYS	-	expression tag	UNP Q8N122
E	-4	ASP	-	expression tag	UNP Q8N122
E	-3	ASP	-	expression tag	UNP Q8N122
E	-2	ASP	-	expression tag	UNP Q8N122
E	-1	ASP	-	expression tag	UNP Q8N122
E	0	LYS	-	expression tag	UNP Q8N122
F	-27	HIS	-	expression tag	UNP Q8N122
F	-26	HIS	-	expression tag	UNP Q8N122
F	-25	HIS	-	expression tag	UNP Q8N122
F	-24	HIS	-	expression tag	UNP Q8N122
F	-23	HIS	-	expression tag	UNP Q8N122
F	-22	HIS	-	expression tag	UNP Q8N122
F	-21	HIS	-	expression tag	UNP Q8N122
F	-20	HIS	-	expression tag	UNP Q8N122
F	-19	HIS	-	expression tag	UNP Q8N122
F	-18	HIS	-	expression tag	UNP Q8N122
F	-17	GLU	-	expression tag	UNP Q8N122
F	-16	GLN	-	expression tag	UNP Q8N122
F	-15	LYS	-	expression tag	UNP Q8N122
F	-14	LEU	-	expression tag	UNP Q8N122
F	-13	ILE	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-12	SER	-	expression tag	UNP Q8N122
F	-11	GLU	-	expression tag	UNP Q8N122
F	-10	GLU	-	expression tag	UNP Q8N122
F	-9	ASP	-	expression tag	UNP Q8N122
F	-8	LEU	-	expression tag	UNP Q8N122
F	-7	ASP	-	expression tag	UNP Q8N122
F	-6	TYR	-	expression tag	UNP Q8N122
F	-5	LYS	-	expression tag	UNP Q8N122
F	-4	ASP	-	expression tag	UNP Q8N122
F	-3	ASP	-	expression tag	UNP Q8N122
F	-2	ASP	-	expression tag	UNP Q8N122
F	-1	ASP	-	expression tag	UNP Q8N122
F	0	LYS	-	expression tag	UNP Q8N122

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	O	P	0
			42	6	6	24	6	
5	B	1	Total	C	H	O	P	0
			42	6	6	24	6	

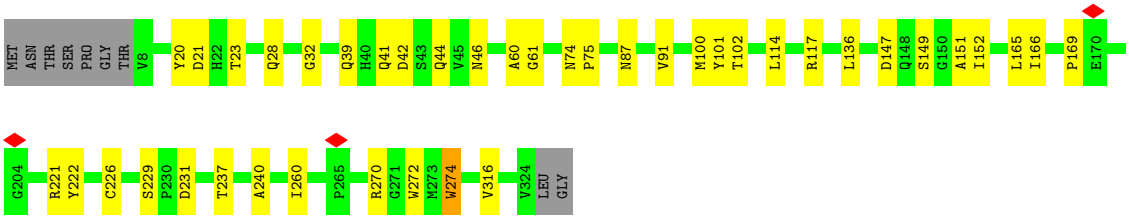
3 Residue-property plots (i)

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: Target of rapamycin complex subunit LST8

Chain C:

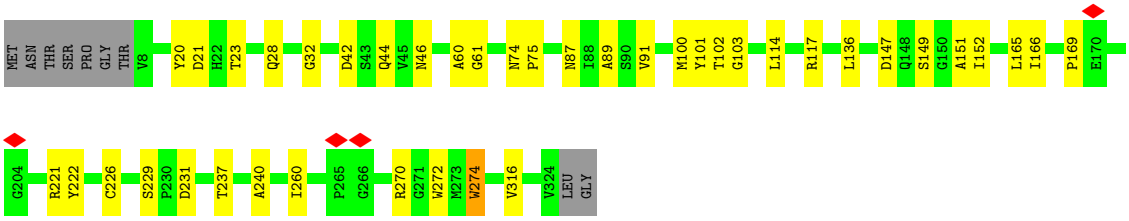




• Molecule 1: Target of rapamycin complex subunit LST8

Chain D:

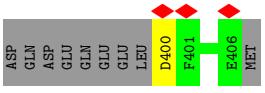




• Molecule 2: La-related protein 1

Chain G:

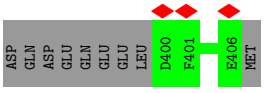




• Molecule 2: La-related protein 1

Chain H:

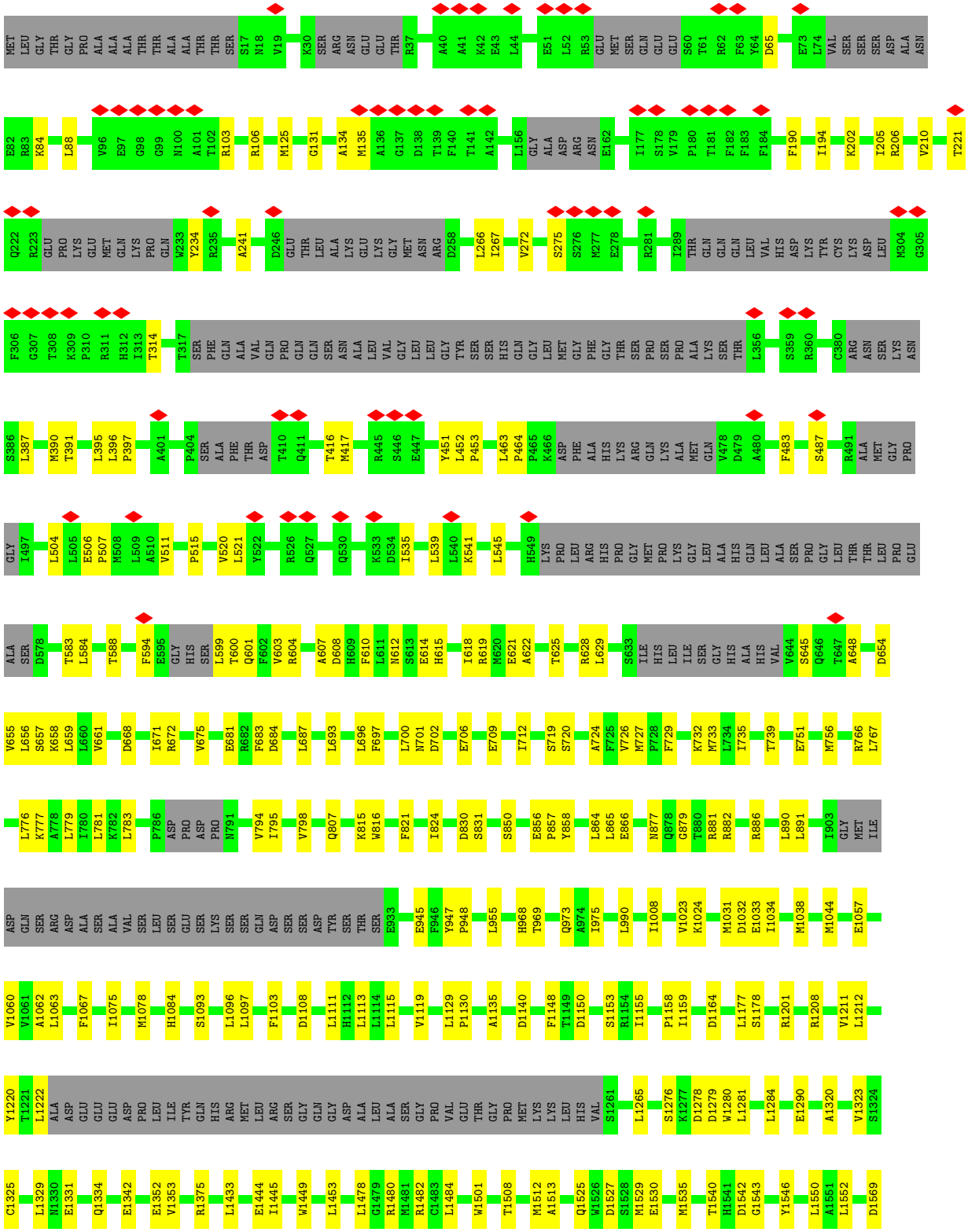


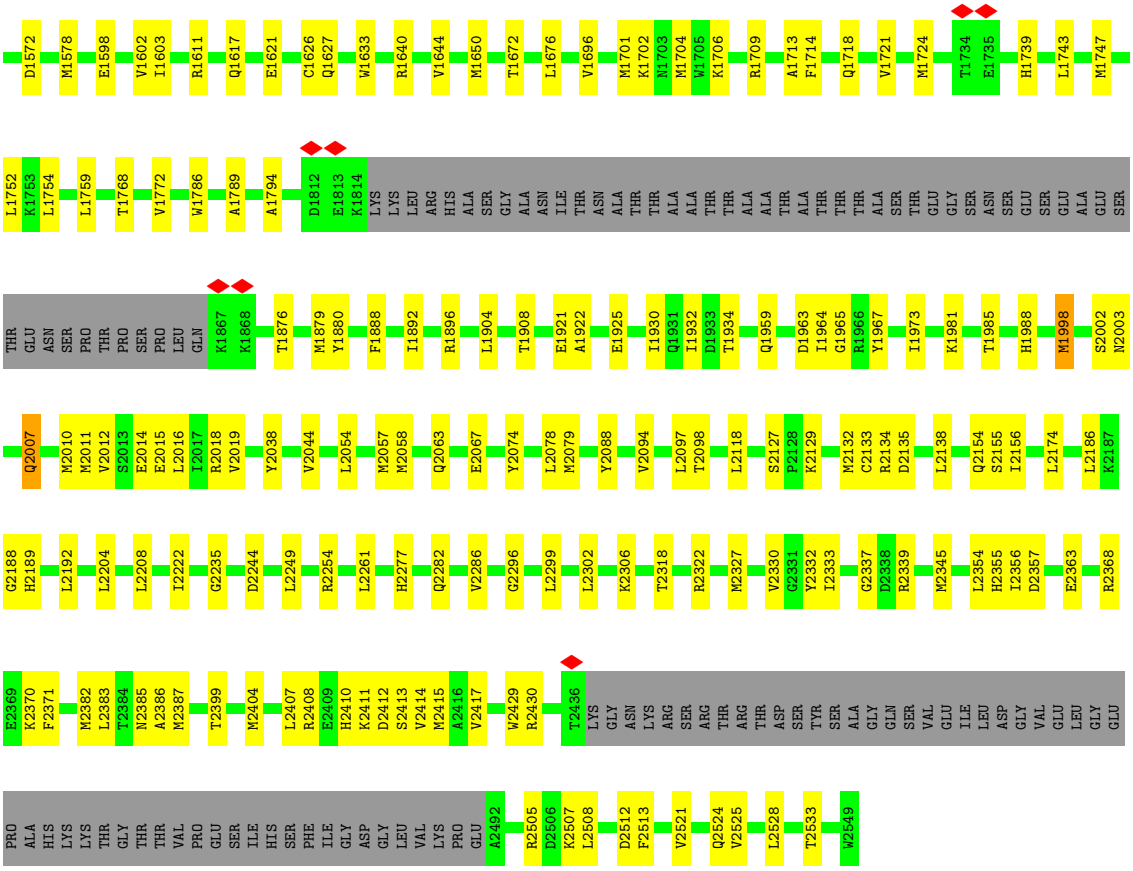


• Molecule 3: Serine/threonine-protein kinase mTOR

Chain A:



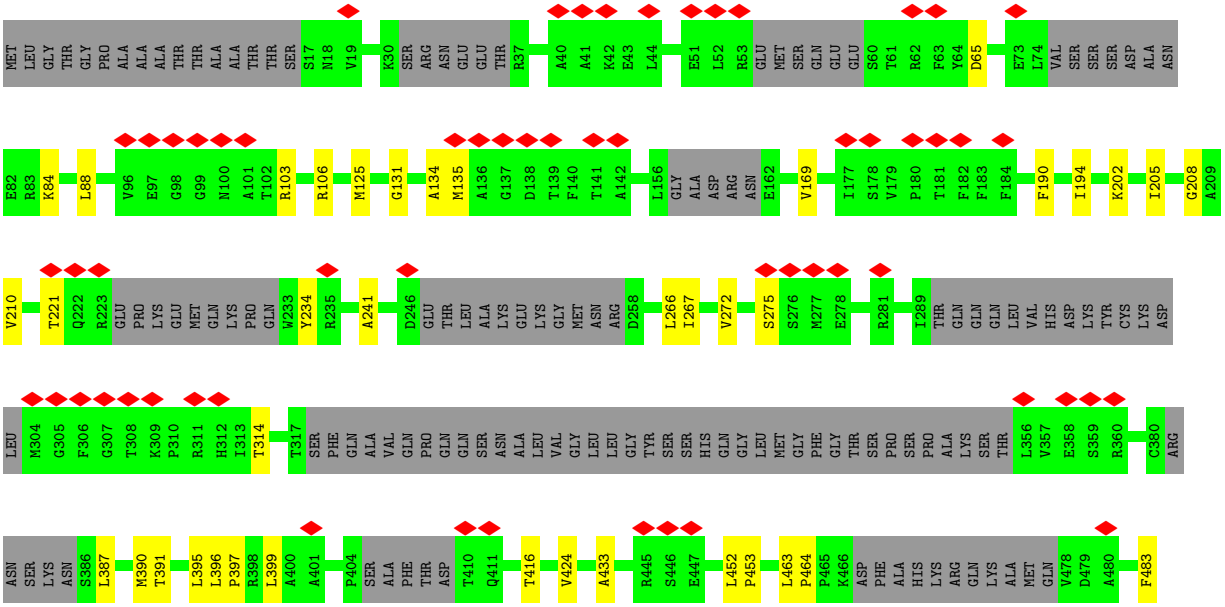


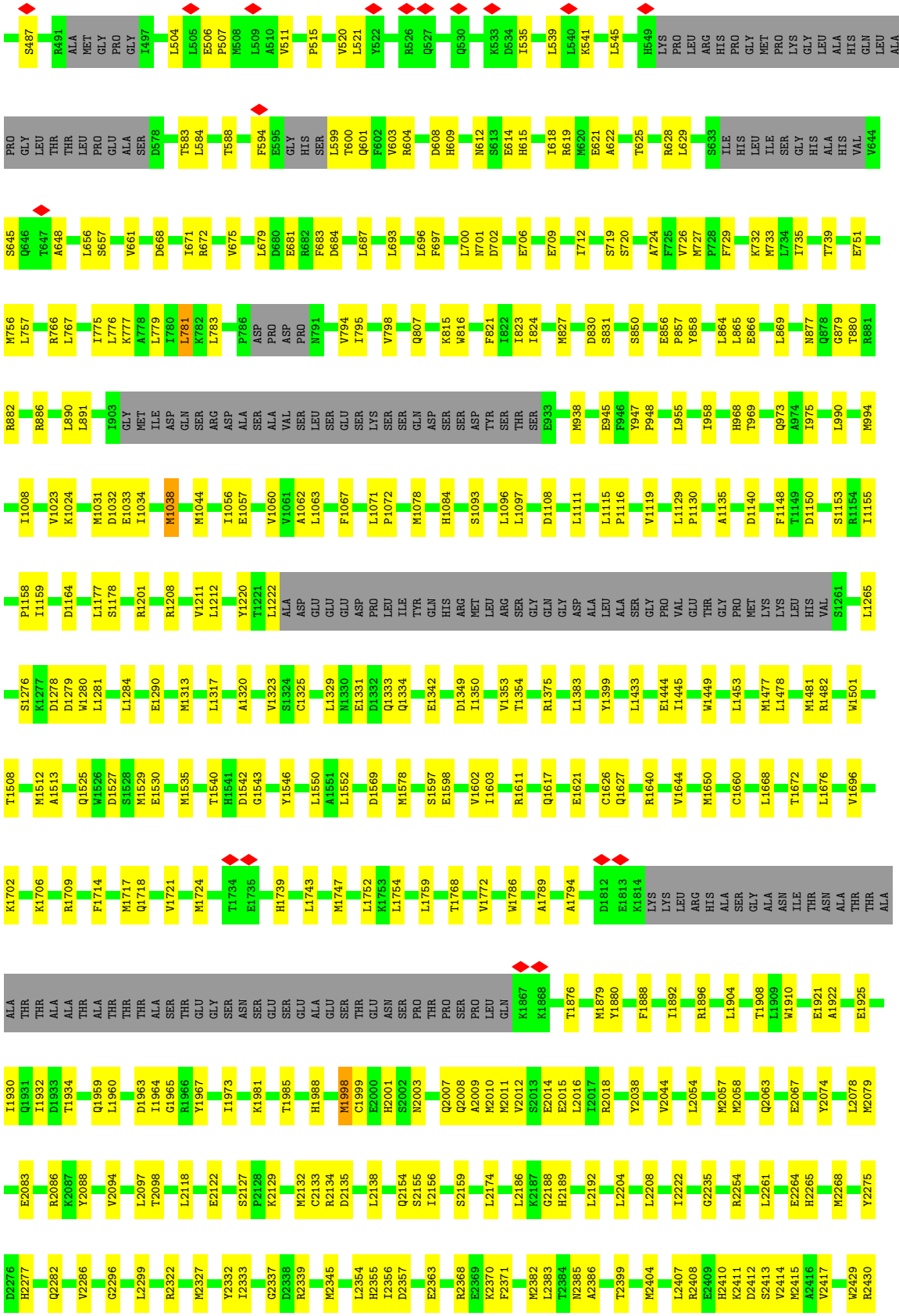


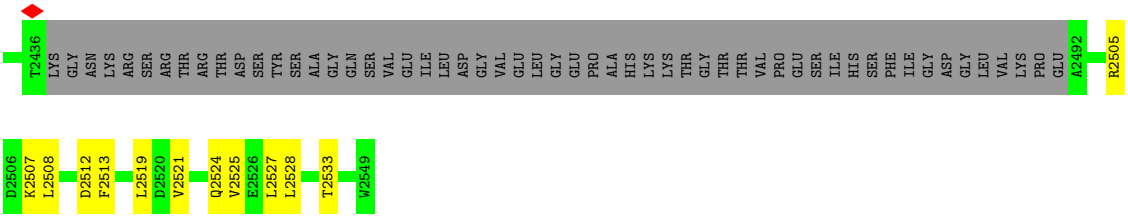
• Molecule 3: Serine/threonine-protein kinase mTOR

Chain B:





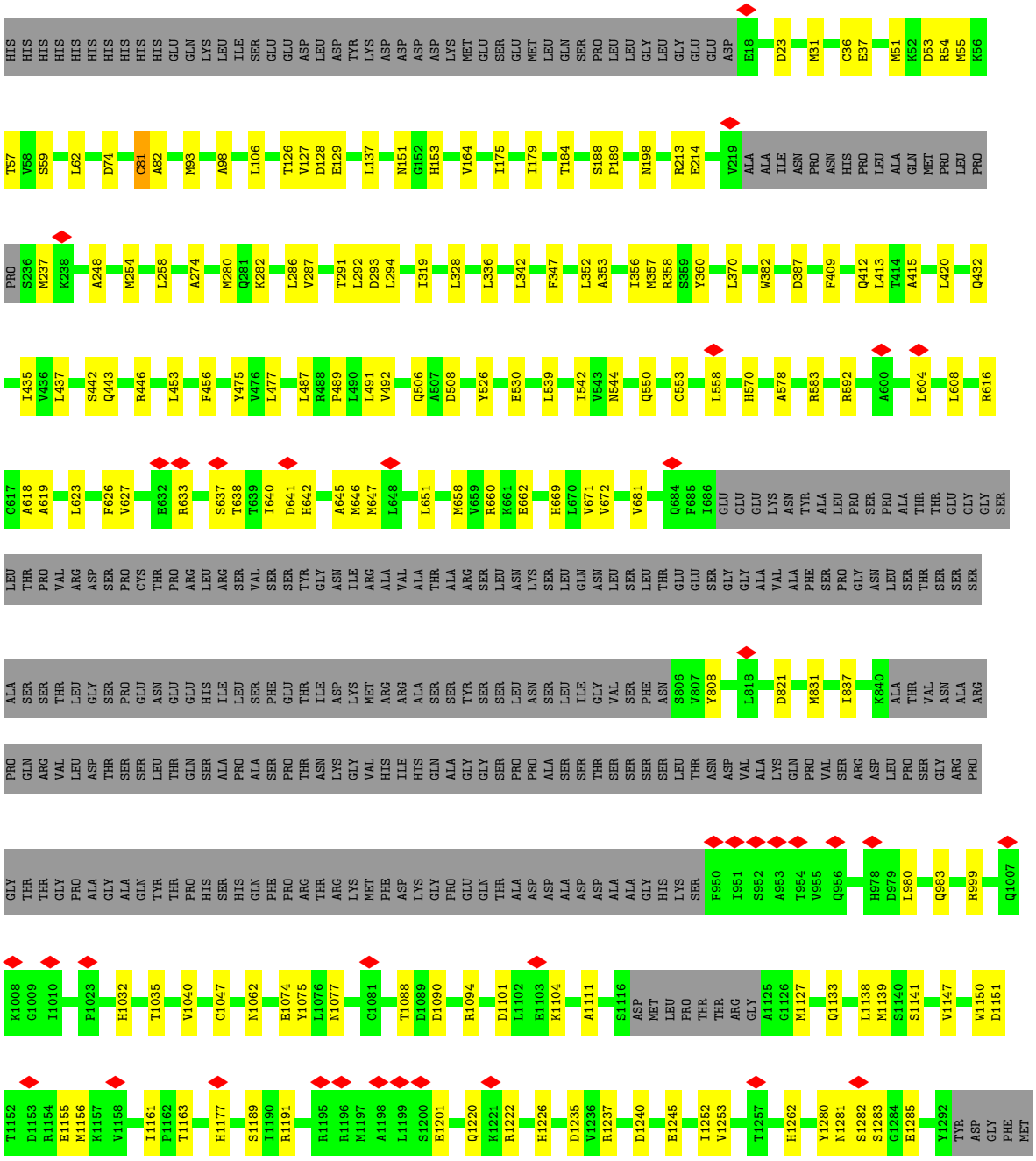

S487 R491 ALA MET GLY PRO GLY I497 L504 L505 E506 P507 M508 L509 A510 V511 P515 V520 L521 Y522 R526 Q527 Q530 K533 D534 I535 L539 L540 K541 L545 H549 LYS PRO LEU ARG HIS PRO GLY MET PRO LYS GLY LEU ALA ALA HIS GLN LEU ALA SER
PRO GLY LEU THR THR LEU PRO GLU ALA SER D578 T583 L584 T588 F594 E595 GLY HIS SER L599 T600 Q601 F602 V603 R604 D608 H609 N612 S613 E614 H615 I618 R619 W620 E621 A622 T625 R628 L629 S633 ILE HIS LEU ILE SER GLY HIS ALA HIS VAL V644
S645 Q646 T647 A648 L656 S657 V661 D668 I671 R672 V675 L679 D680 E681 R682 F683 D684 L687 L693 L696 F697 L700 N701 D702 E706 E709 I712 S719 S720 A724 F725 V726 M727 P728 F729 K732 M733 L734 I735 T739 E751
M756 L757 R766 L767 I775 L776 K777 A778 L779 T780 L781 K782 L783 P786 ASP PRO ASP PRO N791 V794 I795 V798 Q807 K815 W816 F821 I822 I823 I824 M827 D830 S831 S850 E856 P857 Y858 L864 L865 E866 L869 N877 Q878 G879 T880 R881
R882 R886 L890 L891 I903 GLY MET ILE ASP GLN SER ARG ASP ALA SER ALA VAL SER LEU SER GLU SER LYS SER SER GLN ASP SER SER ASP TYR SER THR SER E933 M938 E945 F946 Y947 P948 L955 I958 H968 T969 Q973 A974 I975 L990 M994
I1008 V1023 K1024 M1031 D1032 E1033 I1034 M1038 M1044 I1056 E1057 V1060 V1061 A1062 L1063 F1067 L1071 P1072 M1078 H1084 S1093 L1096 L1097 D1108 L1111 L1115 P1116 V1119 L1129 P1130 A1135 D1140 F1148 T1149 D1150 S1153 R1154 I1155
P1158 I1159 D1164 L1177 S1178 R1201 R1208 V1211 L1212 Y1220 T1221 L1222 ALA ASP GLU GLU GLU ASP PRO LEU ILE TYR GLN HIS ARG MET LEU ARG SER GLY GLN GLY ASP ALA LEU ALA SER GLY PRO VAL GLU THR GLY PRO MET LYS LYS LEU HIS VAL S1261 L1265
S1276 K1277 D1278 D1279 W1280 L1281 L1284 E1290 M1313 L1317 A1320 V1323 S1324 C1325 L1329 N1330 E1331 D1332 Q1333 Q1334 E1342 D1349 I1350 V1353 T1354 R1375 L1383 Y1399 L1433 E1444 I1445 W1449 L1453 M1477 L1478 M1481 R1482 W1501
T1508 M1512 A1513 Q1525 W1526 D1527 S1528 M1529 E1530 M1535 T1540 H1541 D1542 G1543 Y1546 L1550 A1551 L1552 D1569 M1578 S1597 E1598 V1602 I1603 R1611 Q1617 E1621 C1626 Q1627 R1640 V1644 M1650 C1660 L1668 T1672 L1676 V1696
K1702 K1706 R1709 F1714 M1717 Q1718 V1721 M1724 T1734 E1735 H1739 L1743 M1747 L1752 K1753 L1754 L1759 T1768 V1772 W1786 A1789 A1794 D1812 E1813 K1814 LYS LYS LEU ARG HIS ALA SER GLY ALA ASN ILE THR ASN ALA THR THR ALA
ALA THR THR ALA ALA THR ALA THR THR THR ALA SER THR GLU GLY SER ASN SER GLU SER GLU ALA GLU SER THR GLU ASN SER PRO THR PRO SER PRO LEU GLN K1867 K1868 T1876 M1879 Y1880 F1888 I1892 R1896 L1904 T1908 L1909 W1910 E1921 A1922 E1925
I1930 Q1931 I1932 D1933 T1934 Q1959 L1960 D1963 I1964 G1965 R1966 Y1967 I1973 K1981 T1985 H1988 M1998 C1999 E2000 H2001 S2002 N2003 Q2007 Q2008 A2009 M2010 M2011 V2012 S2013 E2014 E2015 L2016 I2017 R2018 Y2038 V2044 L2054 M2057 M2058 Q2063 E2067 Y2074 L2078 M2079
E2083 R2086 K2087 Y2088 V2094 L2097 T2098 L2118 E2122 S2127 P2128 K2129 M2132 C2133 R2134 D2135 L2138 Q2154 S2155 I2156 S2159 L2174 L2186 K2187 G2188 H2189 L2192 L2204 L2208 I2222 G2235 R2254 L2261 E2264 H2265 W2268 Y2275
D2276 H2277 Q2282 V2286 G2296 L2299 R2322 M2327 Y2332 I2333 G2337 D2338 R2339 M2345 L2354 H2355 I2356 D2357 E2363 R2368 E2369 K2370 F2371 M2382 L2383 T2384 N2385 A2386 T2399 M2404 L2407 R2408 E2409 H2410 K2411 D2412 S2413 V2414 M2415 A2416 V2417 W2429 R2430

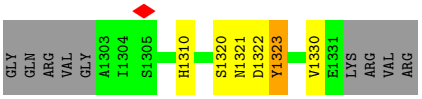


• Molecule 4: Regulatory-associated protein of mTOR

Chain E:



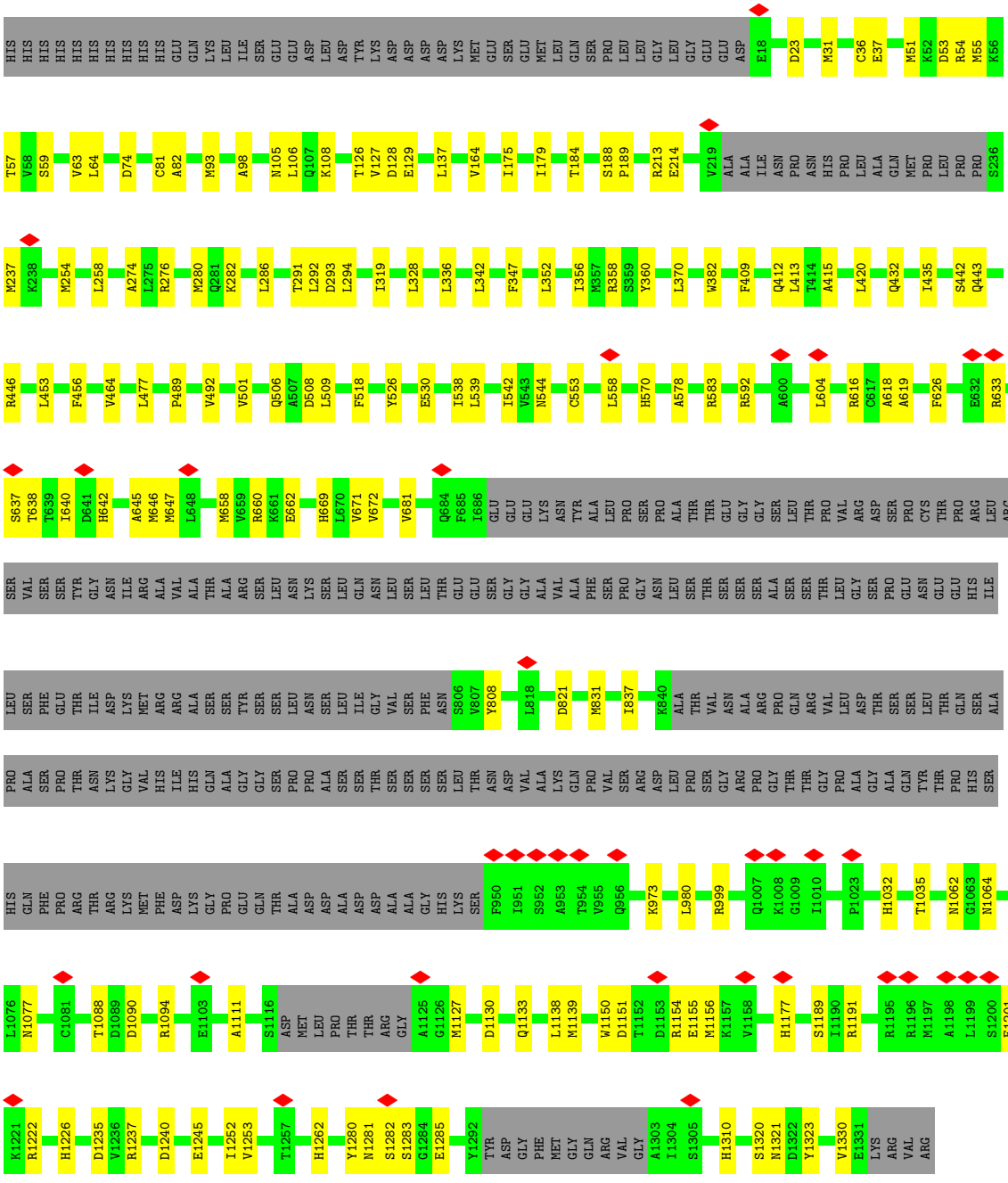




• Molecule 4: Regulatory-associated protein of mTOR

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	929719	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.555	Depositor
Minimum map value	-0.271	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	467.2, 467.2, 467.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97333336, 0.97333336, 0.97333336	Depositor

5 Model quality

5.1 Standard geometry

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

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	C	0.09	0/2514	0.25	0/3426
1	D	0.09	0/2514	0.25	0/3426
2	G	0.05	0/65	0.18	0/86
2	H	0.06	0/65	0.22	0/86
3	A	0.11	0/17814	0.27	0/24116
3	B	0.11	0/17814	0.27	0/24116
4	E	0.11	0/8585	0.26	0/11680
4	F	0.10	0/8585	0.26	0/11680
All	All	0.11	0/57956	0.27	0/78616

There are no bond length outliers.

There are no bond angle outliers.

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	C	2456	2341	2341	26	0
1	D	2456	2341	2341	26	0
2	G	64	49	48	1	0
2	H	64	49	48	0	0
3	A	17467	17553	17553	299	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17467	17553	17553	307	0
4	E	8385	8375	8375	131	0
4	F	8385	8375	8375	116	0
5	A	36	6	6	0	0
5	B	36	6	6	0	0
All	All	56816	56648	56646	888	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 8.

All (888) 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)
3:A:1284:LEU:HD11	3:A:1353:VAL:HG22	1.40	1.00
3:B:1284:LEU:HD11	3:B:1353:VAL:HG22	1.48	0.91
4:E:93:MET:HE2	4:E:93:MET:O	1.74	0.86
3:A:1724:MET:HE1	3:A:1743:LEU:HD22	1.59	0.84
4:F:93:MET:HE2	4:F:93:MET:O	1.78	0.83
3:B:1540:THR:OG1	3:B:1542:ASP:OD1	1.99	0.80
3:A:2011:MET:SD	3:A:2012:VAL:N	2.54	0.80
3:A:2408:ARG:NH2	3:A:2524:GLN:OE1	2.15	0.80
3:B:2408:ARG:NH2	3:B:2524:GLN:OE1	2.15	0.79
3:A:1540:THR:OG1	3:A:1542:ASP:OD1	2.00	0.78
3:B:2011:MET:SD	3:B:2012:VAL:N	2.56	0.78
4:F:93:MET:HE1	4:F:98:ALA:N	1.98	0.78
4:E:93:MET:HE1	4:E:98:ALA:N	2.00	0.77
3:A:2282:GLN:O	3:A:2286:VAL:HG23	1.84	0.77
4:E:592:ARG:NH1	4:E:626:PHE:O	2.17	0.77
3:A:1108:ASP:OD1	4:E:358:ARG:NH2	2.18	0.77
3:B:1159:ILE:HG21	3:B:1177:LEU:HD13	1.66	0.77
3:A:672:ARG:NH1	3:A:702:ASP:OD2	2.19	0.76
3:B:1108:ASP:OD1	4:F:358:ARG:NH2	2.19	0.76
4:F:592:ARG:NH1	4:F:626:PHE:O	2.18	0.76
3:B:2282:GLN:O	3:B:2286:VAL:HG23	1.85	0.76
4:E:184:THR:OG1	4:E:213:ARG:NH2	2.19	0.76
4:F:184:THR:OG1	4:F:213:ARG:NH2	2.19	0.76
3:A:1159:ILE:HG21	3:A:1177:LEU:HD13	1.66	0.75
3:B:1724:MET:HE1	3:B:1743:LEU:HD22	1.66	0.75
3:B:672:ARG:NH1	3:B:702:ASP:OD1	2.19	0.75
3:B:1904:LEU:O	3:B:1908:THR:HG23	1.87	0.75
3:A:1904:LEU:O	3:A:1908:THR:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:657:SER:O	3:B:661:VAL:HG13	1.87	0.74
3:A:1032:ASP:OD1	3:A:1033:GLU:N	2.21	0.73
3:A:657:SER:O	3:A:661:VAL:HG13	1.89	0.73
3:B:777:LYS:O	3:B:781:LEU:HD22	1.87	0.73
3:A:1111:LEU:HD21	3:A:1148:PHE:HE1	1.51	0.73
3:A:1342:GLU:OE2	3:A:1375:ARG:N	2.22	0.73
1:C:39:GLN:NE2	1:C:41:GLN:OE1	2.21	0.72
3:A:601:GLN:N	3:A:601:GLN:OE1	2.22	0.72
3:A:2299:LEU:HD22	3:A:2386:ALA:HB2	1.72	0.72
3:B:1111:LEU:HD21	3:B:1148:PHE:HE1	1.54	0.72
3:A:719:SER:OG	3:A:766:ARG:NH2	2.22	0.72
3:B:1342:GLU:OE2	3:B:1375:ARG:N	2.22	0.72
3:B:1032:ASP:OD1	3:B:1033:GLU:N	2.21	0.72
3:B:1896:ARG:NH2	3:B:1934:THR:OG1	2.23	0.72
3:A:1896:ARG:NH2	3:A:1934:THR:OG1	2.23	0.71
3:B:601:GLN:N	3:B:601:GLN:OE1	2.22	0.71
4:E:553:CYS:SG	4:E:558:LEU:HD13	2.31	0.71
3:B:2299:LEU:HD22	3:B:2386:ALA:HB2	1.72	0.71
3:B:719:SER:OG	3:B:766:ARG:NH2	2.24	0.71
3:B:2088:TYR:CE1	3:B:2097:LEU:HD23	2.26	0.71
1:C:229:SER:OG	1:C:231:ASP:OD1	2.04	0.71
3:B:2265:HIS:ND1	3:B:2268:MET:SD	2.63	0.70
3:A:777:LYS:O	3:A:781:LEU:HD13	1.91	0.70
3:A:2088:TYR:CE1	3:A:2097:LEU:HD23	2.27	0.70
3:B:877:ASN:OD1	3:B:879:GLY:N	2.25	0.70
3:A:877:ASN:OD1	3:A:879:GLY:N	2.25	0.70
3:A:2368:ARG:NH1	3:A:2370:LYS:O	2.25	0.70
3:B:727:MET:HE3	3:B:767:LEU:HD23	1.74	0.70
3:A:619:ARG:NH2	3:A:668:ASP:OD2	2.26	0.69
3:B:2368:ARG:NH1	3:B:2370:LYS:O	2.26	0.69
4:F:553:CYS:SG	4:F:558:LEU:HD13	2.32	0.69
3:A:727:MET:HE3	3:A:767:LEU:HD23	1.74	0.69
4:E:660:ARG:NH2	4:E:1111:ALA:O	2.25	0.69
3:A:739:THR:HG21	4:F:282:LYS:NZ	2.07	0.69
3:B:1650:MET:SD	3:B:1676:LEU:HD12	2.33	0.69
3:B:619:ARG:NH2	3:B:668:ASP:OD2	2.26	0.68
3:B:1965:GLY:HA3	3:B:1998:MET:HE2	1.76	0.68
4:F:1138:LEU:O	4:F:1150:TRP:N	2.26	0.68
3:B:706:GLU:OE1	3:B:706:GLU:N	2.26	0.68
3:B:739:THR:HG21	4:E:282:LYS:NZ	2.08	0.68
1:C:21:ASP:OD2	1:C:23:THR:OG1	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1650:MET:SD	3:A:1676:LEU:HD12	2.33	0.68
3:A:706:GLU:N	3:A:706:GLU:OE1	2.26	0.68
1:C:87:ASN:ND2	3:A:2277:HIS:O	2.27	0.68
3:A:2521:VAL:O	3:A:2525:VAL:HG23	1.94	0.68
3:A:2363:GLU:OE2	3:A:2363:GLU:N	2.27	0.68
3:B:2521:VAL:O	3:B:2525:VAL:HG23	1.94	0.67
3:B:2363:GLU:OE1	3:B:2363:GLU:N	2.28	0.67
4:F:660:ARG:NH1	4:F:821:ASP:OD2	2.28	0.67
4:E:660:ARG:NH1	4:E:821:ASP:OD2	2.27	0.67
4:F:660:ARG:NH2	4:F:1111:ALA:O	2.26	0.67
3:A:968:HIS:CE1	3:A:1008:ILE:HD13	2.30	0.67
4:F:1088:THR:OG1	4:F:1090:ASP:OD1	2.11	0.67
1:D:87:ASN:ND2	3:B:2277:HIS:O	2.27	0.66
1:D:21:ASP:OD2	1:D:23:THR:OG1	2.12	0.66
3:B:1998:MET:SD	3:B:1998:MET:N	2.69	0.66
3:A:1111:LEU:HD21	3:A:1148:PHE:CE1	2.29	0.66
3:A:1542:ASP:OD1	3:A:1543:GLY:N	2.29	0.66
3:A:2337:GLY:O	3:A:2339:ARG:NH1	2.29	0.65
3:B:584:LEU:O	3:B:588:THR:HG23	1.96	0.65
3:B:1284:LEU:HD21	3:B:1353:VAL:HG13	1.78	0.65
3:B:2016:LEU:HD12	3:B:2186:LEU:HD21	1.78	0.65
3:B:1444:GLU:OE1	3:B:1444:GLU:N	2.30	0.65
3:A:2016:LEU:HD12	3:A:2186:LEU:HD21	1.77	0.65
4:E:1138:LEU:O	4:E:1150:TRP:N	2.30	0.65
3:A:584:LEU:O	3:A:588:THR:HG23	1.96	0.65
3:A:1284:LEU:HD21	3:A:1353:VAL:HG13	1.78	0.65
3:B:850:SER:O	3:B:1611:ARG:NH2	2.29	0.65
3:B:2337:GLY:O	3:B:2339:ARG:NH1	2.30	0.64
4:E:1189:SER:OG	4:E:1191:ARG:NH1	2.31	0.64
3:A:1965:GLY:HA3	3:A:1998:MET:HE2	1.77	0.64
3:A:2204:LEU:HD13	3:A:2417:VAL:HG21	1.78	0.64
4:E:1088:THR:OG1	4:E:1090:ASP:OD1	2.16	0.64
3:B:1542:ASP:OD1	3:B:1543:GLY:N	2.30	0.64
3:A:1444:GLU:N	3:A:1444:GLU:OE1	2.30	0.64
4:F:1189:SER:OG	4:F:1191:ARG:NH1	2.31	0.64
1:D:100:MET:SD	1:D:114:LEU:HD21	2.39	0.63
3:A:1701:MET:HE3	3:A:1701:MET:HA	1.81	0.63
4:E:1139:MET:CE	4:E:1147:VAL:HG13	2.29	0.63
3:A:732:LYS:NZ	3:B:1150:ASP:OD1	2.32	0.62
4:F:980:LEU:HD12	4:F:980:LEU:O	2.00	0.62
3:A:2118:LEU:HD23	3:A:2118:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2204:LEU:HD13	3:B:2417:VAL:HG21	1.79	0.62
3:B:1276:SER:OG	3:B:1278:ASP:OD1	2.05	0.62
3:B:2038:TYR:OH	3:B:2097:LEU:HD22	1.99	0.62
1:C:100:MET:SD	1:C:114:LEU:HD21	2.40	0.62
3:A:850:SER:O	3:A:1611:ARG:NH2	2.32	0.61
3:A:2038:TYR:OH	3:A:2097:LEU:HD22	2.01	0.61
3:A:1276:SER:OG	3:A:1278:ASP:OD1	2.10	0.61
3:B:2079:MET:HE2	3:B:2079:MET:HA	1.81	0.61
3:B:2333:ILE:HD12	3:B:2508:LEU:HD22	1.83	0.61
3:A:2299:LEU:HD22	3:A:2386:ALA:CB	2.31	0.61
3:B:712:ILE:HG21	3:B:756:MET:HE1	1.82	0.60
1:D:229:SER:OG	1:D:231:ASP:OD1	2.09	0.60
3:A:2333:ILE:HD12	3:A:2508:LEU:HD22	1.83	0.60
3:B:2129:LYS:O	3:B:2132:MET:HE3	2.01	0.60
3:A:2063:GLN:N	3:A:2067:GLU:OE1	2.34	0.60
3:B:969:THR:OG1	3:B:973:GLN:OE1	2.17	0.60
3:B:2063:GLN:N	3:B:2067:GLU:OE1	2.34	0.60
4:E:128:ASP:OD1	4:E:129:GLU:N	2.35	0.60
4:E:980:LEU:HD12	4:E:980:LEU:O	2.00	0.60
4:F:128:ASP:OD1	4:F:129:GLU:N	2.35	0.60
3:B:882:ARG:NH2	3:B:1569:ASP:OD2	2.35	0.59
3:B:1034:ILE:O	3:B:1038:MET:HG3	2.02	0.59
3:A:1998:MET:HA	3:A:1998:MET:HE3	1.84	0.59
3:A:700:LEU:HD23	3:A:700:LEU:O	2.03	0.59
3:A:1075:ILE:HG21	3:A:1113:LEU:HD23	1.85	0.59
3:B:882:ARG:NE	3:B:1569:ASP:OD1	2.35	0.59
3:A:608:ASP:OD1	3:A:612:ASN:ND2	2.36	0.59
4:E:638:THR:HG22	4:E:642:HIS:NE2	2.18	0.59
3:A:2129:LYS:O	3:A:2132:MET:HE3	2.03	0.59
3:B:890:LEU:HD22	3:B:1597:SER:HB3	1.85	0.59
3:B:2412:ASP:OD1	3:B:2413:SER:N	2.35	0.59
3:B:1265:LEU:N	3:B:1290:GLU:OE2	2.36	0.58
3:A:882:ARG:NH2	3:A:1569:ASP:OD2	2.37	0.58
3:A:1998:MET:SD	3:A:1998:MET:N	2.76	0.58
3:A:131:GLY:O	3:A:134:ALA:N	2.37	0.58
3:A:2412:ASP:OD1	3:A:2413:SER:N	2.35	0.58
3:B:1721:VAL:HG21	3:B:1754:LEU:HD11	1.85	0.58
3:B:2015:GLU:OE1	3:B:2127:SER:OG	2.14	0.58
3:B:131:GLY:O	3:B:134:ALA:N	2.37	0.58
3:B:756:MET:HE3	3:B:756:MET:HA	1.86	0.58
3:B:1932:ILE:HD13	3:B:1967:TYR:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1959:GLN:NE2	3:B:1963:ASP:OD2	2.37	0.58
4:E:1330:VAL:O	4:E:1330:VAL:HG13	2.04	0.58
3:A:1759:LEU:CD2	3:A:1772:VAL:HG21	2.34	0.58
3:B:621:GLU:O	3:B:625:THR:HG22	2.04	0.58
3:B:645:SER:HB3	3:B:648:ALA:HB3	1.86	0.58
3:B:751:GLU:HG3	3:B:794:VAL:HG13	1.86	0.58
3:B:1759:LEU:CD2	3:B:1772:VAL:HG21	2.34	0.58
3:A:1701:MET:HE3	3:A:1701:MET:CA	2.34	0.57
3:B:681:GLU:OE1	3:B:681:GLU:N	2.35	0.57
4:F:1330:VAL:O	4:F:1330:VAL:HG13	2.04	0.57
3:A:645:SER:HB3	3:A:648:ALA:HB3	1.87	0.57
3:A:1265:LEU:N	3:A:1290:GLU:OE2	2.36	0.57
4:E:57:THR:HG23	4:E:57:THR:O	2.03	0.57
1:D:42:ASP:O	1:D:42:ASP:OD2	2.22	0.57
4:F:57:THR:HG23	4:F:57:THR:O	2.03	0.57
1:C:46:ASN:N	1:C:60:ALA:O	2.35	0.57
1:D:274:TRP:CZ2	1:D:316:VAL:HG12	2.40	0.57
4:E:1074:GLU:OE1	4:E:1075:TYR:N	2.37	0.57
4:F:645:ALA:HB3	4:F:646:MET:HE2	1.86	0.57
3:A:712:ILE:HG21	3:A:756:MET:CE	2.34	0.57
3:A:751:GLU:HG3	3:A:794:VAL:HG13	1.86	0.57
3:B:603:VAL:CG1	3:B:629:LEU:HD22	2.35	0.57
3:B:700:LEU:HD23	3:B:700:LEU:O	2.03	0.57
4:E:831:MET:HE3	4:E:831:MET:O	2.05	0.57
3:A:2322:ARG:HD3	3:A:2399:THR:HG21	1.86	0.57
4:E:412:GLN:OE1	4:E:432:GLN:NE2	2.35	0.57
1:C:42:ASP:O	1:C:42:ASP:OD2	2.23	0.57
3:B:1998:MET:HE3	3:B:1998:MET:HA	1.86	0.57
3:A:712:ILE:HG21	3:A:756:MET:HE1	1.86	0.56
4:F:1074:GLU:OE1	4:F:1075:TYR:N	2.37	0.56
4:F:1151:ASP:OD2	4:F:1154:ARG:NE	2.37	0.56
3:A:1932:ILE:HD13	3:A:1967:TYR:HD2	1.68	0.56
3:A:2079:MET:HE2	3:A:2079:MET:HA	1.87	0.56
3:B:1752:LEU:HD11	3:B:1789:ALA:HA	1.87	0.56
4:E:93:MET:HE2	4:E:93:MET:C	2.30	0.56
1:C:274:TRP:CZ2	1:C:316:VAL:HG12	2.41	0.56
3:B:712:ILE:HG21	3:B:756:MET:CE	2.34	0.56
4:E:151:ASN:OD1	4:E:153:HIS:ND1	2.37	0.56
3:A:1598:GLU:O	3:A:1602:VAL:HG23	2.06	0.56
3:A:1752:LEU:HD11	3:A:1789:ALA:HA	1.88	0.56
3:A:603:VAL:CG1	3:A:629:LEU:HD22	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1721:VAL:HG21	3:A:1754:LEU:HD11	1.88	0.56
3:A:2097:LEU:HD12	3:A:2098:THR:N	2.21	0.56
3:B:2097:LEU:HD12	3:B:2098:THR:N	2.21	0.56
4:F:1062:ASN:ND2	4:F:1064:ASN:OD1	2.39	0.56
4:F:831:MET:O	4:F:831:MET:HE3	2.05	0.56
4:F:604:LEU:HD21	4:F:619:ALA:HB1	1.88	0.56
4:F:1127:MET:HA	4:F:1127:MET:HE3	1.86	0.56
3:B:709:GLU:O	3:B:712:ILE:HG22	2.05	0.56
3:B:1598:GLU:O	3:B:1602:VAL:HG23	2.05	0.56
4:F:57:THR:HG21	4:F:342:LEU:CD2	2.36	0.56
1:C:117:ARG:O	1:C:117:ARG:NE	2.31	0.55
3:B:1721:VAL:HG21	3:B:1754:LEU:CD1	2.36	0.55
4:E:353:ALA:O	4:E:357:MET:HG3	2.06	0.55
3:A:969:THR:OG1	3:A:973:GLN:OE1	2.22	0.55
3:A:2363:GLU:OE1	3:A:2507:LYS:NZ	2.31	0.55
3:B:314:THR:OG1	3:B:807:GLN:NE2	2.39	0.55
3:A:621:GLU:O	3:A:625:THR:HG22	2.05	0.55
4:E:57:THR:HG21	4:E:342:LEU:CD2	2.36	0.55
4:E:608:LEU:HD23	4:E:651:LEU:HD11	1.87	0.55
4:F:319:ILE:HD13	4:F:382:TRP:HB2	1.87	0.55
1:C:147:ASP:OD2	1:C:149:SER:OG	2.25	0.55
1:D:152:ILE:N	1:D:165:LEU:O	2.39	0.55
4:F:1235:ASP:OD2	4:F:1237:ARG:NH2	2.40	0.55
3:A:314:THR:OG1	3:A:807:GLN:NE2	2.39	0.55
3:A:882:ARG:NE	3:A:1569:ASP:OD1	2.40	0.55
4:E:1127:MET:HE3	4:E:1127:MET:HA	1.88	0.55
3:A:2254:ARG:NH1	3:A:2261:LEU:O	2.40	0.55
3:B:1999:CYS:O	3:B:2003:ASN:OD1	2.25	0.55
4:F:412:GLN:OE1	4:F:432:GLN:NE2	2.36	0.55
1:D:46:ASN:N	1:D:60:ALA:O	2.34	0.55
3:A:1721:VAL:HG21	3:A:1754:LEU:CD1	2.36	0.55
3:B:2332:TYR:OH	3:B:2512:ASP:OD2	2.25	0.55
4:E:319:ILE:HD13	4:E:382:TRP:HB2	1.87	0.55
4:E:645:ALA:HB3	4:E:646:MET:HE2	1.89	0.55
3:A:739:THR:HG21	4:F:282:LYS:HZ3	1.71	0.55
3:B:779:LEU:HD22	3:B:798:VAL:HG23	1.89	0.55
4:F:638:THR:HG22	4:F:642:HIS:NE2	2.22	0.54
3:A:2015:GLU:OE1	3:A:2127:SER:OG	2.13	0.54
1:D:147:ASP:OD2	1:D:149:SER:OG	2.25	0.54
3:A:2345:MET:SD	3:A:2354:LEU:HD22	2.46	0.54
4:F:1283:SER:OG	4:F:1285:GLU:OE1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:615:HIS:ND1	3:A:618:ILE:HD12	2.22	0.54
3:A:779:LEU:HD22	3:A:798:VAL:HG23	1.90	0.54
3:B:739:THR:HG21	4:E:282:LYS:HZ2	1.71	0.54
1:C:152:ILE:N	1:C:165:LEU:O	2.39	0.54
4:E:1139:MET:HE1	4:E:1141:SER:HB3	1.90	0.54
4:E:1235:ASP:OD2	4:E:1237:ARG:NH2	2.41	0.54
1:C:166:ILE:HD11	1:C:169:PRO:HA	1.90	0.54
3:A:2332:TYR:OH	3:A:2512:ASP:OD2	2.25	0.54
3:B:487:SER:HB3	3:B:520:VAL:HG13	1.90	0.54
1:D:166:ILE:HD11	1:D:169:PRO:HA	1.90	0.53
1:D:240:ALA:HB1	1:D:272:TRP:NE1	2.23	0.53
4:E:530:GLU:OE2	4:E:570:HIS:NE2	2.41	0.53
3:A:487:SER:HB3	3:A:520:VAL:HG13	1.90	0.53
3:A:387:LEU:O	3:A:390:MET:HE3	2.07	0.53
3:A:864:LEU:HD21	3:A:891:LEU:HD21	1.90	0.53
3:B:615:HIS:ND1	3:B:618:ILE:HD12	2.23	0.53
3:A:1626:CYS:SG	3:A:1627:GLN:N	2.82	0.53
3:A:1879:MET:C	3:A:1879:MET:HE2	2.34	0.53
3:B:1111:LEU:HD21	3:B:1148:PHE:CE1	2.38	0.53
3:A:1115:LEU:HD11	3:A:1155:ILE:HD11	1.90	0.53
3:B:1879:MET:C	3:B:1879:MET:HE2	2.34	0.53
3:B:864:LEU:HD21	3:B:891:LEU:HD21	1.90	0.53
3:B:2345:MET:SD	3:B:2354:LEU:HD22	2.48	0.53
3:A:1084:HIS:O	3:A:1084:HIS:ND1	2.42	0.53
3:A:2512:ASP:OD1	3:A:2513:PHE:N	2.41	0.53
4:F:1130:ASP:O	4:F:1139:MET:HE1	2.09	0.53
3:B:608:ASP:OD1	3:B:612:ASN:ND2	2.42	0.53
3:B:1084:HIS:O	3:B:1084:HIS:ND1	2.42	0.53
3:B:2512:ASP:OD1	3:B:2513:PHE:N	2.41	0.53
4:E:1283:SER:OG	4:E:1285:GLU:OE1	2.26	0.53
3:A:684:ASP:C	3:A:684:ASP:OD1	2.52	0.53
3:A:739:THR:HG21	4:F:282:LYS:HZ2	1.74	0.53
3:A:1034:ILE:O	3:A:1038:MET:HG3	2.08	0.53
1:D:44:GLN:NE2	1:D:46:ASN:OD1	2.41	0.52
3:A:65:ASP:OD2	3:A:106:ARG:NH1	2.42	0.52
3:A:659:LEU:HD11	3:A:675:VAL:HG23	1.90	0.52
3:A:1164:ASP:OD1	3:A:1201:ARG:NH1	2.42	0.52
3:B:684:ASP:C	3:B:684:ASP:OD1	2.53	0.52
4:E:126:THR:OG1	4:E:128:ASP:OD1	2.24	0.52
4:F:36:CYS:SG	4:F:37:GLU:N	2.82	0.52
3:B:1164:ASP:OD1	3:B:1201:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1626:CYS:SG	3:B:1627:GLN:N	2.82	0.52
4:F:530:GLU:OE2	4:F:570:HIS:NE2	2.43	0.52
1:C:240:ALA:HB1	1:C:272:TRP:NE1	2.24	0.52
3:A:756:MET:HE3	3:A:756:MET:HA	1.91	0.52
3:B:387:LEU:O	3:B:390:MET:HE3	2.08	0.52
3:A:1709:ARG:HA	3:A:1709:ARG:NE	2.25	0.52
3:A:2299:LEU:H	3:A:2382:MET:HE2	1.75	0.52
3:A:1060:VAL:HG12	3:A:1067:PHE:CD2	2.45	0.52
3:B:1115:LEU:HD11	3:B:1155:ILE:HD11	1.91	0.52
3:A:2188:GLY:O	3:A:2189:HIS:ND1	2.43	0.52
3:B:656:LEU:HD21	3:B:683:PHE:CD1	2.44	0.52
3:B:521:LEU:HD22	3:B:539:LEU:HD12	1.92	0.52
4:E:293:ASP:OD1	4:E:294:LEU:N	2.43	0.52
4:E:1151:ASP:O	4:E:1155:GLU:N	2.43	0.52
4:F:671:VAL:HG21	4:F:837:ILE:HD11	1.91	0.52
1:C:44:GLN:NE2	1:C:46:ASN:OD1	2.43	0.52
3:A:735:ILE:O	3:A:739:THR:HG23	2.10	0.52
3:B:1752:LEU:HD12	3:B:1786:TRP:CZ3	2.45	0.52
3:B:2188:GLY:O	3:B:2189:HIS:ND1	2.43	0.52
3:A:210:VAL:HG21	3:A:266:LEU:HD13	1.92	0.52
3:B:968:HIS:CG	3:B:969:THR:N	2.78	0.52
3:A:2383:LEU:HD12	3:A:2383:LEU:H	1.76	0.51
3:B:131:GLY:O	3:B:135:MET:SD	2.69	0.51
3:B:1449:TRP:O	3:B:1453:LEU:HG	2.10	0.51
3:B:1501:TRP:CZ3	3:B:1535:MET:HE1	2.46	0.51
3:B:2368:ARG:NH1	3:B:2371:PHE:O	2.44	0.51
3:B:2383:LEU:HD12	3:B:2383:LEU:H	1.74	0.51
4:E:671:VAL:HG21	4:E:837:ILE:HD11	1.92	0.51
3:B:65:ASP:OD2	3:B:106:ARG:NH1	2.41	0.51
3:B:210:VAL:HG21	3:B:266:LEU:HD13	1.93	0.51
3:B:712:ILE:CG2	3:B:756:MET:HE1	2.40	0.51
3:B:2254:ARG:NH1	3:B:2261:LEU:O	2.43	0.51
3:B:1060:VAL:HG12	3:B:1067:PHE:CD2	2.45	0.51
4:E:36:CYS:SG	4:E:37:GLU:N	2.83	0.51
4:E:55:MET:HE2	4:E:55:MET:HA	1.92	0.51
3:B:968:HIS:CE1	3:B:1008:ILE:HD13	2.44	0.51
3:B:1879:MET:HE2	3:B:1879:MET:O	2.10	0.51
3:A:1752:LEU:HD12	3:A:1786:TRP:CZ3	2.46	0.51
3:A:1879:MET:HE2	3:A:1879:MET:O	2.11	0.51
4:E:409:PHE:O	4:E:413:LEU:HD23	2.11	0.51
4:E:477:LEU:HD22	4:E:508:ASP:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:131:GLY:O	3:A:135:MET:SD	2.69	0.51
3:A:1449:TRP:O	3:A:1453:LEU:HG	2.10	0.51
3:A:1530:GLU:HA	3:A:1550:LEU:HD11	1.93	0.51
3:A:2368:ARG:NH1	3:A:2371:PHE:O	2.44	0.51
3:B:2345:MET:CE	3:B:2354:LEU:HD22	2.41	0.51
4:F:31:MET:SD	4:F:31:MET:N	2.84	0.51
4:F:293:ASP:OD1	4:F:294:LEU:N	2.43	0.51
3:A:1552:LEU:HD13	3:A:1603:ILE:HG13	1.93	0.50
3:B:945:GLU:OE1	3:B:945:GLU:N	2.44	0.50
3:B:2192:LEU:HD12	3:B:2235:GLY:HA3	1.92	0.50
4:E:31:MET:SD	4:E:31:MET:N	2.83	0.50
4:F:409:PHE:O	4:F:413:LEU:HD23	2.11	0.50
3:B:776:LEU:HD23	3:B:816:TRP:CD1	2.46	0.50
3:B:1530:GLU:HA	3:B:1550:LEU:HD11	1.94	0.50
3:B:2010:MET:HE3	3:B:2010:MET:HA	1.93	0.50
4:E:646:MET:HE2	4:E:646:MET:N	2.26	0.50
3:A:735:ILE:HD11	4:F:286:LEU:HD22	1.93	0.50
3:A:1959:GLN:NE2	3:A:1963:ASP:OD2	2.44	0.50
3:A:1876:THR:O	3:A:1879:MET:SD	2.70	0.50
3:A:681:GLU:OE1	3:A:681:GLU:N	2.43	0.50
4:E:669:HIS:O	4:E:672:VAL:HG12	2.12	0.50
3:A:221:THR:OG1	3:A:234:TYR:OH	2.25	0.50
3:A:656:LEU:HD21	3:A:683:PHE:CD1	2.47	0.50
3:A:2208:LEU:HD21	3:A:2410:HIS:HB2	1.93	0.50
3:B:1876:THR:O	3:B:1879:MET:SD	2.69	0.50
3:B:2118:LEU:HD23	3:B:2118:LEU:O	2.11	0.50
4:F:1077:ASN:OD1	4:F:1133:GLN:NE2	2.43	0.50
4:E:604:LEU:HD21	4:E:619:ALA:HB1	1.92	0.50
4:F:352:LEU:HD21	4:F:356:ILE:HD12	1.94	0.50
1:D:117:ARG:O	1:D:117:ARG:NE	2.31	0.50
3:A:272:VAL:O	3:A:275:SER:OG	2.27	0.50
3:A:2192:LEU:HD12	3:A:2235:GLY:HA3	1.92	0.50
4:E:1281:ASN:OD1	4:E:1282:SER:N	2.42	0.50
3:A:521:LEU:HD22	3:A:539:LEU:HD12	1.93	0.49
3:A:990:LEU:HD21	3:A:1023:VAL:HG21	1.94	0.49
3:B:1525:GLN:N	3:B:1525:GLN:OE1	2.45	0.49
3:B:1552:LEU:HD13	3:B:1603:ILE:HG13	1.94	0.49
4:F:55:MET:HA	4:F:55:MET:HE2	1.92	0.49
4:F:477:LEU:HD22	4:F:508:ASP:OD1	2.12	0.49
3:A:1278:ASP:OD1	3:A:1279:ASP:N	2.45	0.49
3:A:1752:LEU:HD12	3:A:1786:TRP:CH2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:669:HIS:O	4:F:672:VAL:HG12	2.12	0.49
3:A:858:TYR:CE1	3:A:865:LEU:HD13	2.48	0.49
3:A:2003:ASN:OD1	3:A:2007:GLN:NE2	2.46	0.49
3:B:221:THR:OG1	3:B:234:TYR:OH	2.24	0.49
3:B:990:LEU:HD21	3:B:1023:VAL:HG21	1.94	0.49
3:B:2264:GLU:O	3:B:2268:MET:HG3	2.13	0.49
3:B:2299:LEU:H	3:B:2382:MET:HE2	1.78	0.49
3:A:2018:ARG:NH1	3:A:2067:GLU:OE2	2.46	0.49
3:B:739:THR:HG21	4:E:282:LYS:HZ3	1.76	0.49
4:F:164:VAL:HG23	4:F:179:ILE:HD11	1.95	0.49
4:F:443:GLN:OE1	4:F:446:ARG:NE	2.41	0.49
3:A:2011:MET:SD	3:A:2011:MET:C	2.95	0.49
3:B:858:TYR:CE1	3:B:865:LEU:HD13	2.47	0.49
3:B:1331:GLU:HA	3:B:1334:GLN:HB2	1.94	0.49
4:F:1151:ASP:O	4:F:1155:GLU:N	2.42	0.49
3:A:968:HIS:ND1	3:A:1008:ILE:HD13	2.28	0.49
3:A:1525:GLN:OE1	3:A:1525:GLN:N	2.46	0.49
3:B:515:PRO:HD3	3:B:584:LEU:HD11	1.95	0.49
3:B:1512:MET:O	3:B:1513:ALA:C	2.56	0.49
3:B:2018:ARG:NH1	3:B:2067:GLU:OE2	2.46	0.49
4:E:453:LEU:HD23	4:E:453:LEU:O	2.12	0.49
4:F:638:THR:HG22	4:F:642:HIS:CE1	2.48	0.49
3:A:521:LEU:HD21	3:A:535:ILE:CG2	2.43	0.49
3:B:521:LEU:HD21	3:B:535:ILE:CG2	2.43	0.49
4:E:164:VAL:HG23	4:E:179:ILE:HD11	1.95	0.49
4:E:637:SER:HA	4:E:640:ILE:HG22	1.95	0.49
4:E:1139:MET:SD	4:E:1139:MET:C	2.96	0.49
3:A:1178:SER:OG	3:A:1208:ARG:NH2	2.46	0.49
3:B:1208:ARG:O	3:B:1212:LEU:HG	2.13	0.49
3:B:1278:ASP:OD1	3:B:1279:ASP:N	2.46	0.49
4:E:336:LEU:HD21	4:E:347:PHE:CE2	2.48	0.49
3:A:720:SER:OG	3:A:766:ARG:NH2	2.45	0.48
3:A:1331:GLU:HA	3:A:1334:GLN:HB2	1.94	0.48
3:A:2222:ILE:HG23	3:A:2327:MET:SD	2.53	0.48
3:A:2299:LEU:C	3:A:2299:LEU:HD23	2.38	0.48
3:B:720:SER:OG	3:B:766:ARG:NH2	2.44	0.48
3:B:2208:LEU:HD21	3:B:2410:HIS:HB2	1.94	0.48
4:F:412:GLN:HB3	4:F:435:ILE:HG21	1.95	0.48
3:A:654:ASP:O	3:A:658:LYS:HG3	2.13	0.48
3:A:1208:ARG:O	3:A:1212:LEU:HG	2.13	0.48
3:A:1714:PHE:O	3:A:1718:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:735:ILE:O	3:B:739:THR:HG23	2.13	0.48
4:F:336:LEU:HD21	4:F:347:PHE:CE2	2.48	0.48
4:F:518:PHE:CE1	4:F:538:ILE:HG21	2.48	0.48
3:B:1178:SER:OG	3:B:1208:ARG:NH2	2.46	0.48
3:A:515:PRO:HD3	3:A:584:LEU:HD11	1.95	0.48
3:B:1752:LEU:HD12	3:B:1786:TRP:CH2	2.48	0.48
4:F:1062:ASN:O	4:F:1094:ARG:NH1	2.46	0.48
3:A:1501:TRP:CZ3	3:A:1535:MET:HE1	2.49	0.48
3:A:2054:LEU:O	3:A:2058:MET:SD	2.71	0.48
4:F:126:THR:OG1	4:F:128:ASP:OD1	2.24	0.48
3:B:1739:HIS:O	3:B:1743:LEU:HG	2.13	0.48
3:B:2054:LEU:O	3:B:2058:MET:SD	2.72	0.48
3:A:776:LEU:HD23	3:A:816:TRP:CD1	2.49	0.48
4:E:23:ASP:OD2	4:E:999:ARG:NH2	2.44	0.48
3:B:2299:LEU:HD22	3:B:2386:ALA:CB	2.42	0.48
4:F:506:GLN:NE2	4:F:542:ILE:O	2.46	0.48
3:A:88:LEU:HG	3:A:125:MET:HE2	1.96	0.48
4:F:93:MET:HE1	4:F:98:ALA:CA	2.42	0.48
3:B:735:ILE:HD11	4:E:286:LEU:HD22	1.96	0.48
3:B:1031:MET:HG3	3:B:1063:LEU:HD11	1.95	0.48
3:B:1097:LEU:HD13	3:B:1135:ALA:HA	1.96	0.48
3:B:2222:ILE:HG23	3:B:2327:MET:SD	2.53	0.48
4:E:59:SER:CB	4:E:137:LEU:HD22	2.44	0.48
1:D:42:ASP:OD2	1:D:42:ASP:C	2.57	0.47
3:A:2345:MET:CE	3:A:2354:LEU:HD22	2.44	0.47
3:A:2354:LEU:HD23	3:A:2355:HIS:N	2.29	0.47
3:B:506:GLU:HG3	3:B:507:PRO:HD3	1.96	0.47
3:B:1281:LEU:HA	3:B:1284:LEU:HD12	1.95	0.47
4:E:412:GLN:HB3	4:E:435:ILE:HG21	1.96	0.47
3:A:1031:MET:HG3	3:A:1063:LEU:HD11	1.95	0.47
3:B:1508:THR:O	3:B:1512:MET:HG3	2.14	0.47
3:A:945:GLU:N	3:A:945:GLU:OE1	2.44	0.47
3:A:968:HIS:CG	3:A:969:THR:N	2.82	0.47
3:B:424:VAL:HG23	3:B:433:ALA:HB1	1.96	0.47
3:B:1208:ARG:O	3:B:1211:VAL:HG12	2.15	0.47
3:B:2354:LEU:HD23	3:B:2355:HIS:N	2.28	0.47
4:E:1245:GLU:N	4:E:1245:GLU:OE1	2.48	0.47
4:F:336:LEU:HD21	4:F:347:PHE:CD2	2.50	0.47
3:A:1739:HIS:O	3:A:1743:LEU:HG	2.14	0.47
3:B:2011:MET:SD	3:B:2011:MET:C	2.97	0.47
3:B:2057:MET:HG3	3:B:2058:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2354:LEU:HD21	3:B:2356:ILE:HG23	1.96	0.47
4:E:662:GLU:O	4:E:662:GLU:OE2	2.32	0.47
4:F:637:SER:HA	4:F:640:ILE:HG22	1.96	0.47
1:C:260:ILE:O	1:C:270:ARG:NH1	2.47	0.47
3:A:1527:ASP:N	3:A:1527:ASP:OD1	2.48	0.47
3:B:614:GLU:N	3:B:614:GLU:OE2	2.47	0.47
4:E:336:LEU:HD21	4:E:347:PHE:CD2	2.50	0.47
4:E:420:LEU:HD21	4:E:456:PHE:HA	1.96	0.47
4:E:1101:ASP:OD2	4:E:1104:LYS:NZ	2.41	0.47
4:F:59:SER:CB	4:F:137:LEU:HD22	2.43	0.47
1:C:42:ASP:OD2	1:C:42:ASP:C	2.57	0.47
3:A:417:MET:HE3	3:A:451:TYR:CD2	2.50	0.47
3:A:614:GLU:OE2	3:A:614:GLU:N	2.47	0.47
3:B:886:ARG:O	3:B:890:LEU:HD23	2.14	0.47
3:B:1794:ALA:HB1	3:B:1888:PHE:CD1	2.50	0.47
3:B:2133:CYS:O	3:B:2134:ARG:NE	2.48	0.47
3:B:2299:LEU:HD23	3:B:2299:LEU:C	2.40	0.47
4:E:287:VAL:HG21	4:E:387:ASP:OD2	2.14	0.47
4:E:1077:ASN:OD1	4:E:1133:GLN:NE2	2.42	0.47
4:F:420:LEU:HD21	4:F:456:PHE:HA	1.97	0.47
4:F:646:MET:HE2	4:F:646:MET:N	2.30	0.47
1:D:260:ILE:O	1:D:270:ARG:NH1	2.47	0.47
3:B:2132:MET:SD	3:B:2132:MET:C	2.98	0.47
3:B:2354:LEU:HD23	3:B:2354:LEU:C	2.40	0.47
4:E:1252:ILE:HG23	4:E:1280:TYR:CE2	2.50	0.47
4:F:662:GLU:OE2	4:F:662:GLU:O	2.32	0.47
3:A:1752:LEU:HD11	3:A:1789:ALA:CA	2.45	0.47
3:A:2354:LEU:HD23	3:A:2354:LEU:C	2.40	0.47
3:A:2357:ASP:OD2	3:A:2357:ASP:C	2.58	0.47
3:B:1752:LEU:HD11	3:B:1789:ALA:CA	2.45	0.47
3:A:241:ALA:HB2	3:A:267:ILE:HG21	1.97	0.47
3:A:1097:LEU:HD13	3:A:1135:ALA:HA	1.96	0.47
3:A:1150:ASP:OD2	3:B:732:LYS:NZ	2.48	0.47
3:B:88:LEU:HG	3:B:125:MET:HE2	1.96	0.47
3:B:241:ALA:HB2	3:B:267:ILE:HG21	1.97	0.47
3:B:2357:ASP:C	3:B:2357:ASP:OD2	2.58	0.47
4:F:53:ASP:OD1	4:F:53:ASP:N	2.48	0.47
4:F:1252:ILE:HG23	4:F:1280:TYR:CE2	2.50	0.47
3:A:396:LEU:HB3	3:A:416:THR:HG23	1.96	0.46
3:A:506:GLU:HG3	3:A:507:PRO:HD3	1.96	0.46
3:A:1542:ASP:O	3:A:1546:TYR:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2058:MET:SD	3:A:2058:MET:N	2.88	0.46
3:A:2411:LYS:HA	3:A:2414:VAL:HG12	1.98	0.46
3:B:541:LYS:O	3:B:545:LEU:HG	2.15	0.46
3:B:1477:MET:O	3:B:1481:MET:HG3	2.15	0.46
4:E:506:GLN:NE2	4:E:542:ILE:O	2.46	0.46
3:A:65:ASP:OD1	3:A:103:ARG:NH1	2.48	0.46
3:A:1512:MET:O	3:A:1513:ALA:C	2.57	0.46
3:A:2002:SER:O	3:A:2003:ASN:HB3	2.15	0.46
3:B:1542:ASP:O	3:B:1546:TYR:HD2	1.98	0.46
1:D:147:ASP:OD1	1:D:151:ALA:N	2.48	0.46
3:A:1478:LEU:O	3:A:1482:ARG:HG3	2.15	0.46
3:A:2038:TYR:CE2	3:A:2044:VAL:HG22	2.50	0.46
3:B:687:LEU:HD21	3:B:696:LEU:HD22	1.97	0.46
3:B:1093:SER:O	3:B:1097:LEU:HG	2.15	0.46
3:B:2038:TYR:CE2	3:B:2044:VAL:HG22	2.50	0.46
4:F:23:ASP:OD2	4:F:999:ARG:NH2	2.44	0.46
4:F:1245:GLU:N	4:F:1245:GLU:OE1	2.47	0.46
1:D:28:GLN:O	1:D:32:GLY:N	2.49	0.46
3:A:709:GLU:O	3:A:712:ILE:HG22	2.15	0.46
3:A:1208:ARG:O	3:A:1211:VAL:HG12	2.15	0.46
3:A:1281:LEU:HA	3:A:1284:LEU:HD12	1.96	0.46
3:A:1627:GLN:O	3:A:1633:TRP:NE1	2.46	0.46
3:A:2244:ASP:OD1	3:A:2249:LEU:HD21	2.15	0.46
3:B:2058:MET:SD	3:B:2058:MET:N	2.88	0.46
4:E:1062:ASN:O	4:E:1094:ARG:NH1	2.49	0.46
4:F:604:LEU:C	4:F:604:LEU:HD23	2.41	0.46
3:A:1724:MET:CE	3:A:1743:LEU:HB3	2.45	0.46
3:A:1879:MET:SD	3:A:1880:TYR:N	2.89	0.46
3:A:2354:LEU:HD21	3:A:2356:ILE:HG23	1.97	0.46
3:B:947:TYR:HB2	3:B:948:PRO:HD3	1.96	0.46
4:E:328:LEU:HD11	4:E:370:LEU:HD22	1.97	0.46
4:E:1201:GLU:N	4:E:1201:GLU:OE1	2.48	0.46
4:F:214:GLU:CD	4:F:237:MET:HE2	2.40	0.46
1:C:91:VAL:HG23	1:C:102:THR:HG22	1.97	0.46
3:A:947:TYR:HB2	3:A:948:PRO:HD3	1.96	0.46
3:A:1598:GLU:OE2	3:A:1640:ARG:NE	2.45	0.46
3:A:1672:THR:O	3:A:1676:LEU:HD23	2.16	0.46
3:A:1985:THR:O	3:A:1988:HIS:ND1	2.49	0.46
3:B:2411:LYS:HA	3:B:2414:VAL:HG12	1.98	0.46
4:E:51:MET:O	4:E:54:ARG:NH1	2.49	0.46
4:E:53:ASP:N	4:E:53:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:57:THR:HG21	4:E:342:LEU:HD22	1.96	0.46
4:E:214:GLU:CD	4:E:237:MET:HE2	2.40	0.46
3:A:700:LEU:HD13	3:A:733:MET:SD	2.56	0.46
3:A:607:ALA:HA	3:A:610:PHE:CE2	2.51	0.46
3:A:1794:ALA:HB1	3:A:1888:PHE:CD1	2.50	0.46
3:A:2327:MET:HA	3:A:2327:MET:HE3	1.97	0.46
3:A:2357:ASP:OD2	3:A:2357:ASP:O	2.34	0.46
3:B:1433:LEU:HD22	3:B:1453:LEU:HD12	1.98	0.46
3:B:1598:GLU:OE2	3:B:1640:ARG:NE	2.43	0.46
4:E:1147:VAL:HB	4:E:1161:ILE:HG13	1.97	0.46
4:F:1226:HIS:ND1	4:F:1240:ASP:OD1	2.49	0.46
3:B:1672:THR:O	3:B:1676:LEU:HD23	2.16	0.46
4:F:51:MET:O	4:F:54:ARG:NH1	2.49	0.46
4:F:1281:ASN:OD1	4:F:1282:SER:N	2.42	0.46
1:D:20:TYR:CE2	1:D:316:VAL:HG11	2.51	0.46
3:A:541:LYS:O	3:A:545:LEU:HG	2.15	0.46
3:A:1093:SER:O	3:A:1097:LEU:HG	2.15	0.46
3:A:2057:MET:HG3	3:A:2058:MET:SD	2.55	0.46
3:B:821:PHE:HA	3:B:824:ILE:HG22	1.98	0.46
3:B:1445:ILE:HG23	3:B:1449:TRP:CE3	2.50	0.46
3:B:2429:TRP:CE3	3:B:2430:ARG:N	2.84	0.46
1:C:28:GLN:O	1:C:32:GLY:N	2.49	0.45
3:A:2429:TRP:CE3	3:A:2430:ARG:N	2.84	0.45
3:B:1527:ASP:OD1	3:B:1527:ASP:N	2.47	0.45
3:B:2122:GLU:OE1	3:B:2159:SER:OG	2.18	0.45
3:B:2204:LEU:C	3:B:2204:LEU:HD23	2.41	0.45
4:E:647:MET:HE3	4:E:647:MET:HA	1.97	0.45
4:F:57:THR:HG21	4:F:342:LEU:HD22	1.97	0.45
4:F:328:LEU:HD11	4:F:370:LEU:HD22	1.97	0.45
1:C:147:ASP:OD1	1:C:151:ALA:N	2.48	0.45
3:A:1578:MET:HA	3:A:1578:MET:HE2	1.98	0.45
3:B:2357:ASP:OD2	3:B:2357:ASP:O	2.34	0.45
4:E:539:LEU:HD13	4:E:558:LEU:HD12	1.97	0.45
4:F:93:MET:HE2	4:F:93:MET:C	2.40	0.45
3:A:687:LEU:HD21	3:A:696:LEU:HD22	1.97	0.45
3:A:1702:LYS:O	3:A:1706:LYS:HG3	2.16	0.45
3:B:2008:GLN:O	3:B:2012:VAL:HG12	2.17	0.45
4:E:1127:MET:HE3	4:E:1141:SER:O	2.16	0.45
1:D:226:CYS:SG	1:D:237:THR:HG23	2.57	0.45
3:A:1445:ILE:HG23	3:A:1449:TRP:CE3	2.50	0.45
3:A:1932:ILE:HD11	3:A:1964:ILE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:700:LEU:HD13	3:B:733:MET:SD	2.56	0.45
3:B:1985:THR:O	3:B:1988:HIS:ND1	2.49	0.45
1:C:226:CYS:SG	1:C:237:THR:HG23	2.56	0.45
3:A:2010:MET:HE3	3:A:2010:MET:HA	1.98	0.45
3:B:396:LEU:HB3	3:B:416:THR:HG23	1.97	0.45
3:B:1433:LEU:HD22	3:B:1453:LEU:CD1	2.46	0.45
4:E:352:LEU:HD21	4:E:356:ILE:HD12	1.99	0.45
4:F:105:ASN:OD1	4:F:108:LYS:NZ	2.45	0.45
1:C:20:TYR:CE1	1:C:316:VAL:HG11	2.51	0.45
3:A:390:MET:SD	3:A:391:THR:N	2.90	0.45
3:A:1024:LYS:HA	3:A:1062:ALA:HB1	1.98	0.45
3:A:2204:LEU:HD23	3:A:2204:LEU:C	2.41	0.45
3:B:2155:SER:C	3:B:2156:ILE:HD12	2.42	0.45
3:B:2327:MET:HE3	3:B:2327:MET:HA	1.97	0.45
3:B:1879:MET:SD	3:B:1880:TYR:N	2.90	0.45
3:A:603:VAL:HG11	3:A:629:LEU:HD22	1.98	0.45
3:A:1044:MET:HE3	3:A:1044:MET:O	2.16	0.45
3:A:1433:LEU:HD22	3:A:1453:LEU:CD1	2.47	0.45
3:A:2208:LEU:HD21	3:A:2410:HIS:CB	2.47	0.45
4:E:93:MET:HE1	4:E:98:ALA:CA	2.46	0.45
4:E:604:LEU:HD23	4:E:604:LEU:C	2.41	0.45
1:D:46:ASN:ND2	1:D:61:GLY:O	2.49	0.45
3:B:483:PHE:HZ	3:B:511:VAL:HG11	1.82	0.45
3:B:1714:PHE:O	3:B:1718:GLN:HG3	2.17	0.45
4:F:127:VAL:HG23	4:F:175:ILE:HD12	1.99	0.45
4:F:1177:HIS:O	4:F:1177:HIS:CG	2.70	0.45
3:A:504:LEU:O	3:A:507:PRO:HD2	2.17	0.44
3:B:65:ASP:OD1	3:B:103:ARG:NH1	2.50	0.44
3:B:1024:LYS:HA	3:B:1062:ALA:HB1	1.98	0.44
3:B:1578:MET:HE2	3:B:1578:MET:HA	1.99	0.44
4:F:453:LEU:O	4:F:453:LEU:HD23	2.16	0.44
1:C:46:ASN:ND2	1:C:61:GLY:O	2.50	0.44
3:A:1552:LEU:HD13	3:A:1603:ILE:CG1	2.47	0.44
3:B:603:VAL:HG11	3:B:629:LEU:HD22	1.98	0.44
3:B:1721:VAL:HA	3:B:1747:MET:HE1	1.99	0.44
3:B:1768:THR:O	3:B:1772:VAL:HG23	2.18	0.44
3:B:2296:GLY:O	3:B:2385:ASN:ND2	2.50	0.44
4:E:127:VAL:HG23	4:E:175:ILE:HD12	1.99	0.44
4:E:608:LEU:CD2	4:E:651:LEU:HD11	2.46	0.44
4:E:658:MET:SD	4:E:658:MET:C	3.00	0.44
4:E:1226:HIS:ND1	4:E:1240:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:63:VAL:C	4:F:64:LEU:HD12	2.41	0.44
4:F:291:THR:HG22	4:F:292:LEU:N	2.32	0.44
3:B:1932:ILE:HD11	3:B:1964:ILE:HA	1.99	0.44
4:F:1320:SER:OG	4:F:1321:ASN:N	2.50	0.44
3:A:1768:THR:O	3:A:1772:VAL:HG23	2.17	0.44
3:A:2133:CYS:O	3:A:2134:ARG:NE	2.50	0.44
3:B:955:LEU:HD13	3:B:975:ILE:HG13	1.98	0.44
3:B:1038:MET:HE1	3:B:1056:ILE:HG12	1.98	0.44
3:B:1617:GLN:O	3:B:1621:GLU:HG3	2.17	0.44
4:E:1156:MET:SD	4:E:1156:MET:N	2.90	0.44
3:A:821:PHE:HA	3:A:824:ILE:HG22	1.98	0.44
3:A:1433:LEU:HD22	3:A:1453:LEU:HD12	1.99	0.44
3:A:1964:ILE:O	3:A:1967:TYR:O	2.36	0.44
3:A:2174:LEU:HD12	3:A:2174:LEU:N	2.33	0.44
4:E:681:VAL:HG21	4:E:808:TYR:HB2	2.00	0.44
4:E:1252:ILE:HG23	4:E:1280:TYR:HE2	1.83	0.44
4:F:658:MET:SD	4:F:658:MET:C	3.00	0.44
4:F:1156:MET:SD	4:F:1156:MET:N	2.91	0.44
4:F:1252:ILE:HG22	4:F:1253:VAL:HG23	2.00	0.44
3:A:483:PHE:HZ	3:A:511:VAL:HG11	1.81	0.44
3:B:1478:LEU:O	3:B:1482:ARG:HG3	2.17	0.44
4:E:291:THR:HG22	4:E:292:LEU:N	2.32	0.44
3:A:599:LEU:HD22	3:A:629:LEU:HD11	2.00	0.44
3:A:1650:MET:HA	3:A:1650:MET:HE3	1.99	0.44
3:A:1701:MET:HE1	3:A:1713:ALA:HA	1.99	0.44
3:B:504:LEU:O	3:B:507:PRO:HD2	2.18	0.44
3:B:583:THR:HG23	3:B:621:GLU:HG3	2.00	0.44
3:B:2174:LEU:N	3:B:2174:LEU:HD12	2.33	0.44
3:B:2268:MET:HE2	3:B:2275:TYR:CD2	2.53	0.44
4:E:62:LEU:HD22	4:E:106:LEU:CD2	2.47	0.44
3:A:1617:GLN:O	3:A:1621:GLU:HG3	2.17	0.44
3:A:2135:ASP:OD2	3:A:2154:GLN:NE2	2.51	0.44
3:B:815:LYS:HD3	3:B:815:LYS:N	2.33	0.44
3:B:2208:LEU:HD21	3:B:2410:HIS:CB	2.48	0.44
4:E:55:MET:HE2	4:E:55:MET:CA	2.48	0.44
4:E:453:LEU:HD23	4:E:453:LEU:C	2.43	0.44
3:A:622:ALA:HA	3:A:625:THR:HG22	2.00	0.44
3:A:2155:SER:C	3:A:2156:ILE:HD12	2.43	0.44
3:B:390:MET:SD	3:B:391:THR:N	2.91	0.44
4:F:544:ASN:OD1	4:F:583:ARG:NH1	2.51	0.44
4:F:1201:GLU:N	4:F:1201:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:400:ASP:N	2:G:400:ASP:OD2	2.49	0.43
3:A:2296:GLY:O	3:A:2385:ASN:ND2	2.51	0.43
3:B:539:LEU:HD22	3:B:594:PHE:HE1	1.83	0.43
3:B:783:LEU:HD23	3:B:795:ILE:HD11	2.00	0.43
3:B:1552:LEU:HD13	3:B:1603:ILE:CG1	2.48	0.43
3:B:1910:TRP:CH2	3:B:1960:LEU:HD12	2.53	0.43
4:E:274:ALA:HB2	4:E:352:LEU:HD11	1.99	0.43
4:E:578:ALA:HB3	4:E:618:ALA:HB1	2.00	0.43
4:F:681:VAL:HG21	4:F:808:TYR:HB2	2.00	0.43
3:A:202:LYS:HG3	3:A:205:ILE:HD12	2.01	0.43
3:A:1981:LYS:NZ	3:A:2014:GLU:OE2	2.52	0.43
3:B:1999:CYS:C	3:B:2001:HIS:N	2.76	0.43
4:E:487:LEU:HB3	4:E:491:LEU:CD1	2.48	0.43
4:E:1139:MET:HE3	4:E:1147:VAL:HG13	1.98	0.43
4:F:81:CYS:SG	4:F:82:ALA:N	2.91	0.43
3:A:955:LEU:HD13	3:A:975:ILE:HG13	2.00	0.43
4:E:188:SER:OG	4:E:189:PRO:HD3	2.18	0.43
4:E:437:LEU:HD21	4:E:475:TYR:CE2	2.53	0.43
4:E:544:ASN:OD1	4:E:583:ARG:NH1	2.51	0.43
4:F:1252:ILE:HG23	4:F:1280:TYR:HE2	1.83	0.43
3:A:1892:ILE:HG21	3:A:1930:ILE:HD11	2.00	0.43
3:A:2382:MET:HE3	3:A:2382:MET:HA	2.00	0.43
4:E:1262:HIS:NE2	4:E:1310:HIS:O	2.51	0.43
3:A:712:ILE:CG2	3:A:756:MET:HE1	2.49	0.43
3:A:1721:VAL:HA	3:A:1747:MET:HE1	2.00	0.43
3:B:396:LEU:N	3:B:397:PRO:HD2	2.34	0.43
3:B:599:LEU:HD22	3:B:629:LEU:HD11	2.01	0.43
4:E:1252:ILE:HG22	4:E:1253:VAL:HG23	2.00	0.43
3:B:1325:CYS:O	3:B:1329:LEU:HG	2.19	0.43
3:B:1349:ASP:OD1	3:B:1354:THR:OG1	2.32	0.43
3:B:1964:ILE:O	3:B:1967:TYR:O	2.36	0.43
3:B:2135:ASP:OD2	3:B:2154:GLN:NE2	2.51	0.43
3:B:2333:ILE:HG13	3:B:2407:LEU:HD23	2.01	0.43
3:B:2382:MET:HA	3:B:2382:MET:HE3	2.01	0.43
4:E:443:GLN:OE1	4:E:446:ARG:NE	2.41	0.43
4:E:1177:HIS:O	4:E:1177:HIS:CG	2.70	0.43
4:F:55:MET:HE2	4:F:55:MET:CA	2.48	0.43
4:F:274:ALA:HB2	4:F:352:LEU:HD11	2.01	0.43
1:D:89:ALA:N	1:D:103:GLY:O	2.52	0.43
3:A:1650:MET:HE3	3:A:1650:MET:CA	2.49	0.43
3:B:272:VAL:O	3:B:275:SER:OG	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:622:ALA:HA	3:B:625:THR:HG22	2.01	0.43
4:E:1320:SER:OG	4:E:1321:ASN:N	2.52	0.43
1:C:221:ARG:HG2	1:C:240:ALA:HB3	2.01	0.43
3:A:396:LEU:N	3:A:397:PRO:HD2	2.34	0.43
3:A:815:LYS:HD3	3:A:815:LYS:N	2.33	0.43
3:A:1325:CYS:O	3:A:1329:LEU:HG	2.19	0.43
3:A:1921:GLU:O	3:A:1925:GLU:HG2	2.19	0.43
3:B:968:HIS:ND1	3:B:969:THR:N	2.66	0.43
4:F:1220:GLN:OE1	4:F:1222:ARG:NH1	2.52	0.43
3:B:675:VAL:O	3:B:679:LEU:HD23	2.19	0.43
3:B:719:SER:HA	3:B:726:VAL:HG11	2.00	0.43
3:B:994:MET:HE3	3:B:994:MET:HA	2.00	0.43
4:F:74:ASP:OD1	4:F:74:ASP:N	2.52	0.43
4:F:442:SER:OG	4:F:443:GLN:N	2.52	0.43
4:F:647:MET:HE3	4:F:647:MET:HA	2.00	0.43
4:F:1262:HIS:NE2	4:F:1310:HIS:O	2.51	0.43
3:A:600:THR:HG22	3:A:604:ARG:CZ	2.49	0.43
3:A:1973:ILE:HD12	3:A:2138:LEU:CD1	2.49	0.43
3:B:1280:TRP:O	3:B:1284:LEU:HG	2.19	0.43
3:B:1650:MET:HE3	3:B:1650:MET:HA	2.01	0.43
4:E:1040:VAL:O	4:E:1047:CYS:N	2.47	0.43
3:B:84:LYS:HA	3:B:125:MET:HE1	2.01	0.42
3:B:958:ILE:HD11	3:B:1313:MET:HB2	2.01	0.42
3:B:1702:LYS:O	3:B:1706:LYS:HG3	2.19	0.42
4:E:616:ARG:NH1	4:E:1156:MET:SD	2.92	0.42
4:E:1220:GLN:OE1	4:E:1222:ARG:NH1	2.52	0.42
3:A:1922:ALA:O	3:A:1925:GLU:HG3	2.18	0.42
3:B:1140:ASP:OD1	3:B:1140:ASP:C	2.62	0.42
3:B:1650:MET:HE3	3:B:1650:MET:CA	2.50	0.42
3:B:1921:GLU:O	3:B:1925:GLU:HG2	2.19	0.42
4:E:550:GLN:NE2	4:E:583:ARG:O	2.48	0.42
3:B:767:LEU:HD13	3:B:767:LEU:C	2.44	0.42
3:A:539:LEU:HD22	3:A:594:PHE:HE1	1.85	0.42
3:A:866:GLU:OE1	3:A:866:GLU:N	2.46	0.42
3:B:1044:MET:HE3	3:B:1044:MET:O	2.19	0.42
3:B:1922:ALA:O	3:B:1925:GLU:HG3	2.20	0.42
4:F:276:ARG:O	4:F:280:MET:HG3	2.19	0.42
4:F:291:THR:HG22	4:F:292:LEU:H	1.83	0.42
3:A:881:ARG:NH1	3:A:1572:ASP:OD1	2.53	0.42
3:A:886:ARG:O	3:A:890:LEU:HD23	2.20	0.42
3:A:2333:ILE:HG13	3:A:2407:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:600:THR:HG22	3:B:604:ARG:CZ	2.49	0.42
3:B:724:ALA:HB3	4:E:415:ALA:HB2	2.00	0.42
3:B:1529:MET:HE1	3:B:1546:TYR:HD1	1.85	0.42
3:B:1892:ILE:HG21	3:B:1930:ILE:HD11	2.01	0.42
4:F:633:ARG:HB3	4:F:637:SER:CB	2.50	0.42
3:A:390:MET:SD	3:A:390:MET:C	3.03	0.42
3:A:654:ASP:OD1	3:A:655:VAL:N	2.53	0.42
3:A:1140:ASP:OD1	3:A:1140:ASP:C	2.62	0.42
3:B:202:LYS:HG3	3:B:205:ILE:HD12	2.00	0.42
3:B:390:MET:SD	3:B:390:MET:C	3.03	0.42
3:B:2345:MET:HE1	3:B:2354:LEU:HD22	2.02	0.42
1:D:101:TYR:HE2	1:D:136:LEU:HD13	1.85	0.42
3:A:190:PHE:CZ	3:A:194:ILE:HD12	2.55	0.42
3:A:693:LEU:HD22	3:A:697:PHE:CZ	2.55	0.42
3:B:1115:LEU:N	3:B:1116:PRO:HD2	2.35	0.42
3:B:2009:ALA:HA	3:B:2012:VAL:HG12	2.01	0.42
3:A:767:LEU:HD13	3:A:767:LEU:C	2.45	0.42
3:A:783:LEU:HD23	3:A:795:ILE:HD11	2.02	0.42
3:A:1650:MET:HE2	3:A:1696:VAL:CG2	2.49	0.42
3:A:2404:MET:CG	3:A:2521:VAL:HG13	2.50	0.42
3:B:1220:TYR:OH	3:B:1222:LEU:HD22	2.20	0.42
3:B:1721:VAL:HG13	3:B:1747:MET:CE	2.50	0.42
3:B:2296:GLY:C	3:B:2382:MET:HE1	2.45	0.42
4:E:74:ASP:OD2	4:E:74:ASP:N	2.53	0.42
4:E:604:LEU:HD22	4:E:623:LEU:HD21	2.02	0.42
4:E:1032:HIS:CG	4:E:1035:THR:HG22	2.55	0.42
3:A:463:LEU:N	3:A:464:PRO:HD2	2.35	0.42
3:A:701:ASN:O	3:B:1153:SER:OG	2.37	0.42
3:B:1973:ILE:HD12	3:B:2138:LEU:CD1	2.48	0.42
4:F:578:ALA:HB3	4:F:618:ALA:HB1	2.01	0.42
3:B:463:LEU:N	3:B:464:PRO:HD2	2.35	0.42
3:B:2415:MET:HE2	3:B:2505:ARG:CZ	2.50	0.42
4:E:258:LEU:HD11	4:E:360:TYR:CZ	2.54	0.42
4:F:59:SER:HB2	4:F:137:LEU:HD22	2.02	0.42
4:F:106:LEU:O	4:F:106:LEU:HD23	2.19	0.42
4:F:509:LEU:HD23	4:F:509:LEU:C	2.45	0.42
4:F:1032:HIS:CG	4:F:1035:THR:HG22	2.55	0.42
3:A:583:THR:HG23	3:A:621:GLU:HG3	2.02	0.41
3:A:719:SER:HA	3:A:726:VAL:HG11	2.01	0.41
3:A:968:HIS:ND1	3:A:969:THR:N	2.68	0.41
3:A:1220:TYR:OH	3:A:1222:LEU:HD22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1320:ALA:O	3:A:1323:VAL:HG12	2.19	0.41
3:A:1352:GLU:OE1	3:A:1352:GLU:N	2.48	0.41
3:B:2074:TYR:O	3:B:2078:LEU:HD23	2.20	0.41
4:E:291:THR:HG22	4:E:292:LEU:H	1.83	0.41
4:E:604:LEU:HD23	4:E:604:LEU:O	2.20	0.41
3:A:84:LYS:HA	3:A:125:MET:HE1	2.01	0.41
3:A:1280:TRP:O	3:A:1284:LEU:HG	2.20	0.41
3:A:1721:VAL:HG13	3:A:1747:MET:CE	2.50	0.41
3:A:2094:VAL:HA	3:A:2097:LEU:HG	2.02	0.41
3:B:1313:MET:SD	3:B:1317:LEU:HD11	2.60	0.41
3:B:1320:ALA:O	3:B:1323:VAL:HG12	2.19	0.41
3:B:2404:MET:CG	3:B:2521:VAL:HG13	2.50	0.41
4:F:973:LYS:C	4:F:973:LYS:HD2	2.45	0.41
3:A:1078:MET:HG2	3:A:1096:LEU:HD11	2.03	0.41
3:B:622:ALA:HA	3:B:625:THR:CG2	2.51	0.41
4:E:442:SER:OG	4:E:443:GLN:N	2.51	0.41
4:E:1322:ASP:OD1	4:E:1323:TYR:N	2.52	0.41
1:D:221:ARG:HG2	1:D:240:ALA:HB3	2.01	0.41
3:A:610:PHE:CD1	3:A:610:PHE:C	2.97	0.41
3:A:1508:THR:O	3:A:1512:MET:HG3	2.21	0.41
3:B:757:LEU:HD11	3:B:775:ILE:HD11	2.02	0.41
4:E:638:THR:HG22	4:E:642:HIS:CE1	2.55	0.41
4:F:489:PRO:HA	4:F:492:VAL:HG12	2.02	0.41
3:A:1060:VAL:HG12	3:A:1067:PHE:CE2	2.56	0.41
3:B:1060:VAL:HG12	3:B:1067:PHE:CE2	2.56	0.41
4:E:254:MET:O	4:E:254:MET:CG	2.68	0.41
4:E:633:ARG:HB3	4:E:637:SER:CB	2.50	0.41
4:F:188:SER:OG	4:F:189:PRO:HD3	2.20	0.41
4:F:980:LEU:HD12	4:F:980:LEU:C	2.46	0.41
3:A:856:GLU:N	3:A:857:PRO:HD2	2.36	0.41
3:A:1119:VAL:HG13	3:A:1158:PRO:HG2	2.02	0.41
3:A:1153:SER:OG	3:B:701:ASN:O	2.39	0.41
3:B:938:MET:HE3	3:B:938:MET:HB3	1.99	0.41
4:E:54:ARG:C	4:E:55:MET:HE2	2.46	0.41
4:E:81:CYS:SG	4:E:82:ALA:N	2.92	0.41
4:E:1147:VAL:HG23	4:E:1163:THR:HG22	2.03	0.41
4:F:539:LEU:HD13	4:F:558:LEU:HD12	2.01	0.41
1:D:74:ASN:N	1:D:75:PRO:HD3	2.35	0.41
3:B:823:ILE:O	3:B:827:MET:HE3	2.21	0.41
3:B:830:ASP:OD1	3:B:831:SER:N	2.54	0.41
3:B:1350:ILE:O	3:B:1354:THR:OG1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2094:VAL:HA	3:B:2097:LEU:HG	2.02	0.41
4:E:198:ASN:ND2	4:E:248:ALA:O	2.54	0.41
4:E:258:LEU:HD21	4:E:280:MET:SD	2.61	0.41
4:E:627:VAL:HG13	4:E:641:ASP:OD1	2.21	0.41
1:C:101:TYR:HE2	1:C:136:LEU:HD13	1.86	0.41
1:C:221:ARG:O	1:C:222:TYR:C	2.63	0.41
3:A:266:LEU:HD23	3:A:395:LEU:HD21	2.03	0.41
3:A:830:ASP:OD2	3:A:831:SER:N	2.54	0.41
3:A:1129:LEU:N	3:A:1130:PRO:HD2	2.36	0.41
3:A:2074:TYR:O	3:A:2078:LEU:HD23	2.21	0.41
3:A:2318:THR:O	3:A:2322:ARG:HG2	2.21	0.41
3:B:693:LEU:HD12	3:B:697:PHE:CZ	2.55	0.41
3:B:1071:LEU:N	3:B:1072:PRO:HD2	2.36	0.41
3:B:1078:MET:HG2	3:B:1096:LEU:HD11	2.03	0.41
3:B:1329:LEU:HD13	3:B:1333:GLN:HB2	2.03	0.41
3:B:1709:ARG:HA	3:B:1709:ARG:CZ	2.51	0.41
3:B:1981:LYS:NZ	3:B:2014:GLU:OE2	2.53	0.41
3:B:2332:TYR:CZ	3:B:2528:LEU:HD21	2.56	0.41
3:B:2404:MET:HG2	3:B:2521:VAL:HG13	2.02	0.41
1:D:91:VAL:HG23	1:D:102:THR:HG22	2.03	0.41
1:D:221:ARG:O	1:D:222:TYR:C	2.63	0.41
3:A:1529:MET:HE1	3:A:1546:TYR:HD1	1.85	0.41
3:A:2132:MET:SD	3:A:2132:MET:C	3.04	0.41
3:A:2222:ILE:HD11	3:A:2330:VAL:HG21	2.03	0.41
3:A:2332:TYR:CZ	3:A:2528:LEU:HD21	2.56	0.41
3:A:2415:MET:HE2	3:A:2505:ARG:CZ	2.51	0.41
3:B:272:VAL:HG11	3:B:399:LEU:HD23	2.02	0.41
3:B:729:PHE:CZ	3:B:733:MET:HE3	2.56	0.41
3:B:856:GLU:N	3:B:857:PRO:HD2	2.35	0.41
3:B:1057:GLU:O	3:B:1060:VAL:HG22	2.21	0.41
3:B:1129:LEU:N	3:B:1130:PRO:HD2	2.36	0.41
3:B:1717:MET:HG3	3:B:1754:LEU:HG	2.03	0.41
3:B:2322:ARG:HG2	3:B:2399:THR:HG21	2.03	0.41
3:B:2363:GLU:OE2	3:B:2507:LYS:NZ	2.32	0.41
4:F:188:SER:N	4:F:189:PRO:CD	2.84	0.41
4:F:258:LEU:HD11	4:F:360:TYR:CZ	2.55	0.41
3:A:724:ALA:HB3	4:F:415:ALA:HB2	2.02	0.41
3:A:729:PHE:CZ	3:A:733:MET:HE3	2.56	0.41
3:B:1119:VAL:HG13	3:B:1158:PRO:HG2	2.02	0.41
4:F:412:GLN:CB	4:F:435:ILE:HG21	2.51	0.41
1:C:74:ASN:N	1:C:75:PRO:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2533:THR:O	3:B:2533:THR:HG22	2.21	0.40
4:E:198:ASN:CG	4:E:248:ALA:O	2.64	0.40
4:F:616:ARG:NH1	4:F:1156:MET:SD	2.94	0.40
3:A:1640:ARG:O	3:A:1644:VAL:HG12	2.21	0.40
3:A:2016:LEU:HA	3:A:2019:VAL:HG22	2.03	0.40
3:A:2302:LEU:HD12	3:A:2306:LYS:HD3	2.03	0.40
3:A:2387:MET:HE2	3:A:2387:MET:HB3	1.98	0.40
3:A:2415:MET:HE3	3:A:2415:MET:HB3	1.97	0.40
3:B:452:LEU:N	3:B:453:PRO:HD2	2.36	0.40
3:B:866:GLU:OE1	3:B:866:GLU:N	2.45	0.40
3:B:1650:MET:HE2	3:B:1696:VAL:CG2	2.51	0.40
4:F:254:MET:O	4:F:254:MET:CG	2.68	0.40
3:A:622:ALA:HA	3:A:625:THR:CG2	2.51	0.40
3:A:1060:VAL:HG11	3:A:1103:PHE:CD2	2.56	0.40
3:A:1644:VAL:O	3:A:1644:VAL:HG13	2.21	0.40
3:B:169:VAL:HG11	3:B:208:GLY:HA3	2.04	0.40
3:B:190:PHE:CZ	3:B:194:ILE:HD12	2.55	0.40
3:B:628:ARG:HA	3:B:628:ARG:NE	2.37	0.40
3:B:877:ASN:HB3	3:B:880:THR:HG22	2.04	0.40
3:B:1759:LEU:HD22	3:B:1772:VAL:HG21	2.03	0.40
4:E:188:SER:N	4:E:189:PRO:CD	2.85	0.40
4:E:983:GLN:CD	4:E:983:GLN:C	2.89	0.40
4:F:464:VAL:CG1	4:F:501:VAL:HG11	2.51	0.40
3:A:452:LEU:N	3:A:453:PRO:HD2	2.36	0.40
3:A:1057:GLU:O	3:A:1060:VAL:HG22	2.22	0.40
3:A:2533:THR:HG22	3:A:2533:THR:O	2.21	0.40
3:B:1383:LEU:HD22	3:B:1399:TYR:OH	2.21	0.40
3:B:1660:CYS:SG	3:B:1668:LEU:HD22	2.62	0.40
3:B:2083:GLU:OE1	3:B:2086:ARG:NH2	2.54	0.40
3:B:2519:LEU:HD21	3:B:2527:LEU:HD12	2.04	0.40
4:E:489:PRO:HA	4:E:492:VAL:HG12	2.03	0.40
4:E:647:MET:HE3	4:E:647:MET:CA	2.50	0.40
4:F:258:LEU:HD21	4:F:280:MET:SD	2.61	0.40
3:A:206:ARG:O	3:A:210:VAL:HG23	2.22	0.40
3:A:628:ARG:NE	3:A:628:ARG:HA	2.37	0.40
3:A:1480:ARG:O	3:A:1484:LEU:HD23	2.22	0.40
3:A:2404:MET:HG2	3:A:2521:VAL:HG13	2.02	0.40
3:B:266:LEU:HD23	3:B:395:LEU:HD21	2.03	0.40
3:B:1644:VAL:O	3:B:1644:VAL:HG13	2.21	0.40
4:E:59:SER:HB2	4:E:137:LEU:HD22	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	C	315/326 (97%)	304 (96%)	11 (4%)	0	100	100
1	D	315/326 (97%)	304 (96%)	11 (4%)	0	100	100
2	G	5/16 (31%)	5 (100%)	0	0	100	100
2	H	5/16 (31%)	5 (100%)	0	0	100	100
3	A	2150/2549 (84%)	2104 (98%)	46 (2%)	0	100	100
3	B	2150/2549 (84%)	2101 (98%)	49 (2%)	0	100	100
4	E	1040/1363 (76%)	1015 (98%)	24 (2%)	1 (0%)	48	76
4	F	1040/1363 (76%)	1015 (98%)	25 (2%)	0	100	100
All	All	7020/8508 (82%)	6853 (98%)	166 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	81	CYS

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	C	269/276 (98%)	268 (100%)	1 (0%)	84	84
1	D	269/276 (98%)	268 (100%)	1 (0%)	84	84
2	G	7/16 (44%)	7 (100%)	0	100	100
2	H	7/16 (44%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	1876/2220 (84%)	1872 (100%)	4 (0%)	87	87
3	B	1876/2220 (84%)	1869 (100%)	7 (0%)	84	84
4	E	928/1191 (78%)	926 (100%)	2 (0%)	87	87
4	F	928/1191 (78%)	926 (100%)	2 (0%)	87	87
All	All	6160/7406 (83%)	6143 (100%)	17 (0%)	84	85

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	274	TRP
1	D	274	TRP
3	A	671	ILE
3	A	1704	MET
3	A	1998	MET
3	A	2007	GLN
3	B	609	HIS
3	B	671	ILE
3	B	781	LEU
3	B	869	LEU
3	B	1038	MET
3	B	1998	MET
3	B	2007	GLN
4	E	526	TYR
4	E	1323	TYR
4	F	526	TYR
4	F	1323	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	536	GLN
3	A	612	ASN
3	A	701	ASN
3	A	1077	HIS
3	A	1157	HIS
3	A	1398	HIS
3	A	1405	GLN
3	A	1446	GLN
3	A	1739	HIS
3	A	1808	ASN

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Mol	Chain	Res	Type
3	A	2055	HIS
3	A	2117	GLN
3	A	2154	GLN
3	A	2265	HIS
3	A	2515	HIS
3	B	536	GLN
3	B	701	ASN
3	B	1077	HIS
3	B	1106	ASN
3	B	1157	HIS
3	B	1405	GLN
3	B	1446	GLN
3	B	1454	HIS
3	B	1703	ASN
3	B	1729	GLN
3	B	1739	HIS
3	B	1758	GLN
3	B	1808	ASN
3	B	1886	GLN
3	B	2055	HIS
3	B	2117	GLN
3	B	2154	GLN
3	B	2502	ASN
3	B	2515	HIS
4	E	67	ASN
4	E	140	ASN
4	E	149	HIS
4	E	547	HIS
4	F	149	HIS
4	F	547	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	IHP	A	2601	-	36,36,36	0.75	1 (2%)	54,60,60	0.35	0
5	IHP	B	2601	-	36,36,36	0.75	1 (2%)	54,60,60	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IHP	A	2601	-	-	1/30/54/54	0/1/1/1
5	IHP	B	2601	-	-	1/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2601	IHP	P3-O13	2.88	1.64	1.59
5	A	2601	IHP	P3-O13	2.88	1.64	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

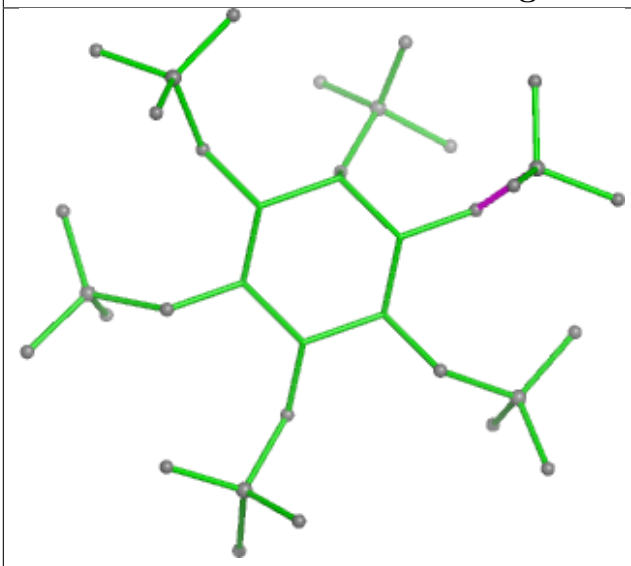
Mol	Chain	Res	Type	Atoms
5	A	2601	IHP	C3-O13-P3-O23
5	B	2601	IHP	C3-O13-P3-O23

There are no ring outliers.

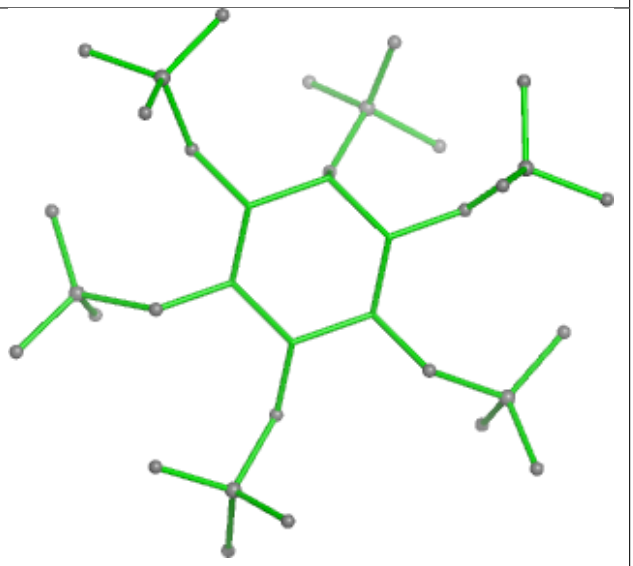
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

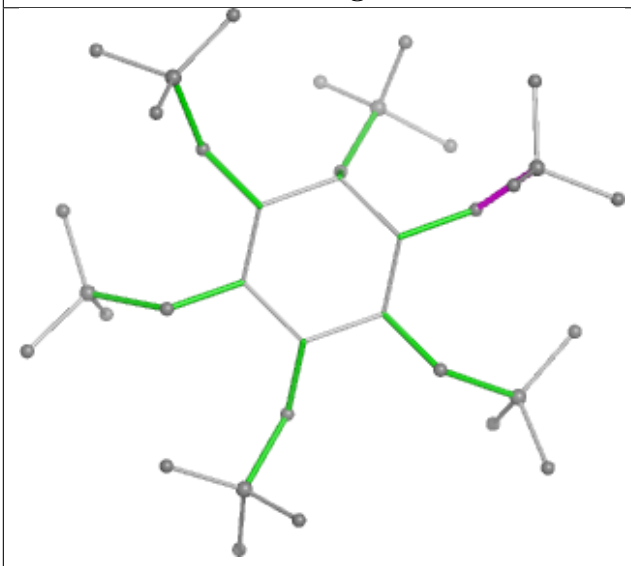
Ligand IHP A 2601



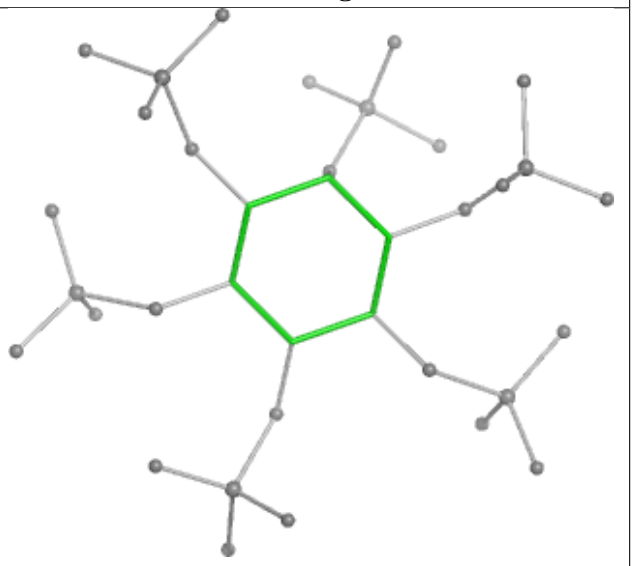
Bond lengths



Bond angles

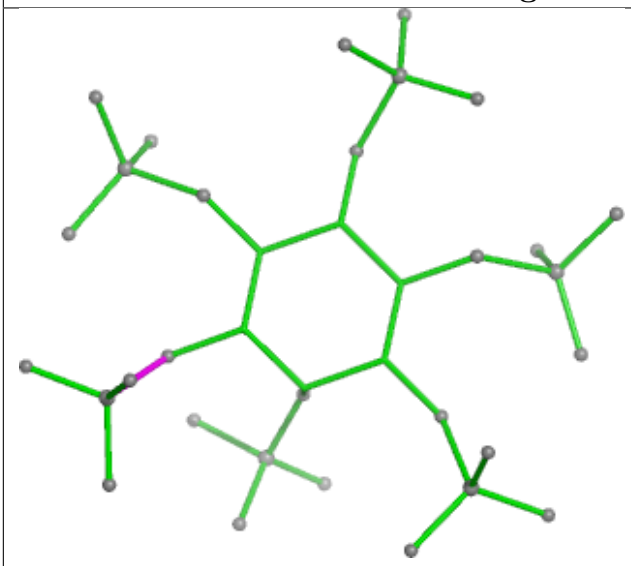


Torsions

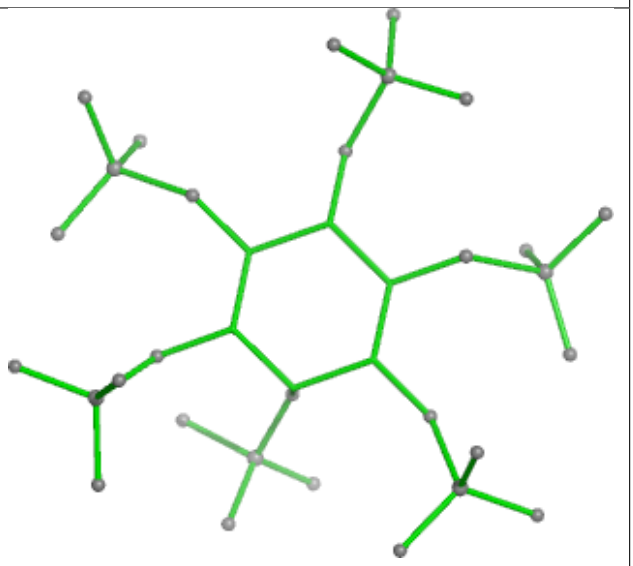


Rings

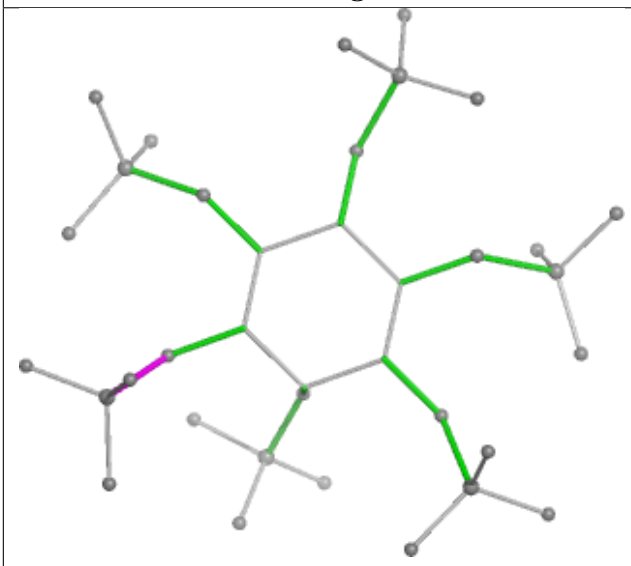
Ligand IHP B 2601



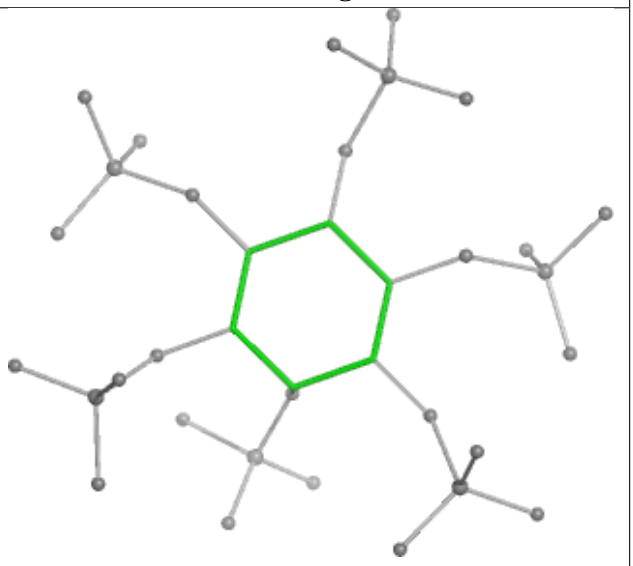
Bond lengths



Bond angles



Torsions



Rings

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.

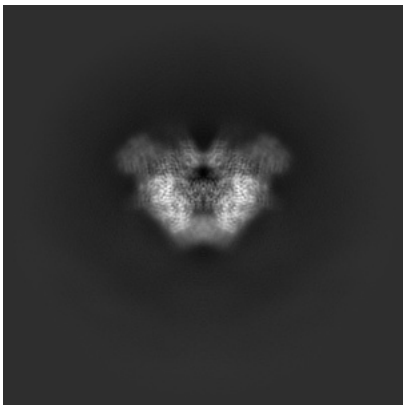
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55632. These allow visual inspection of the internal detail of the map and identification of artifacts.

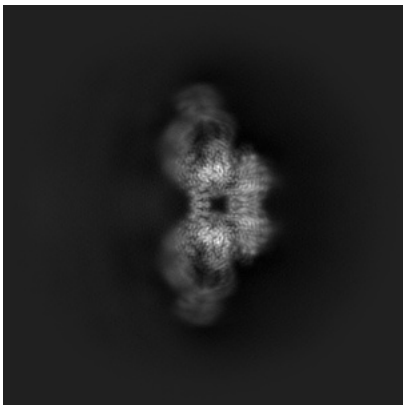
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

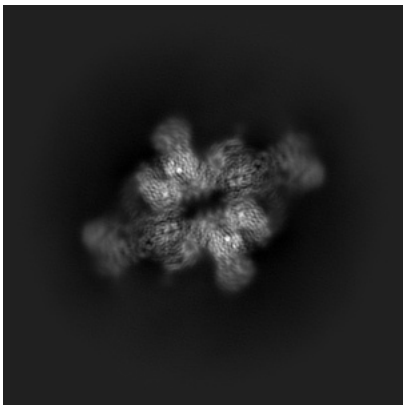
6.1.1 Primary map



X

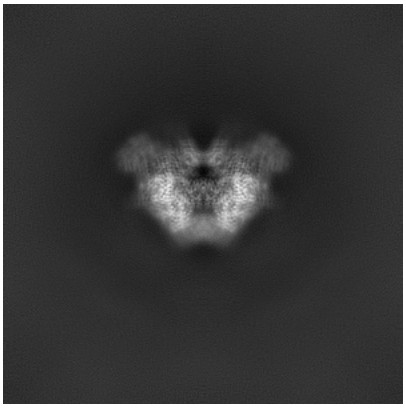


Y

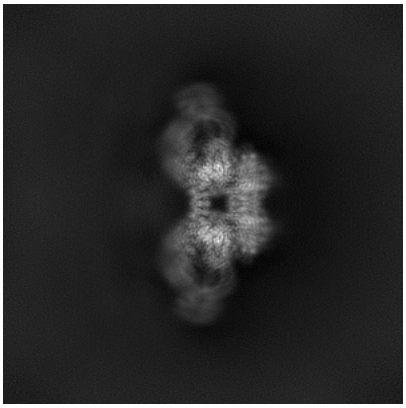


Z

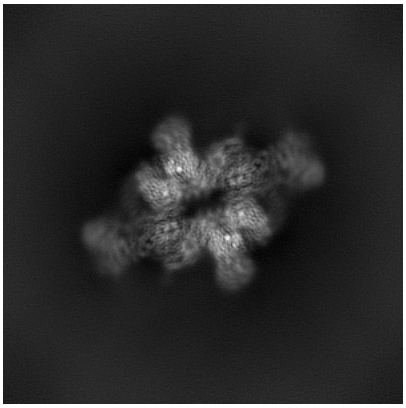
6.1.2 Raw map



X



Y



Z

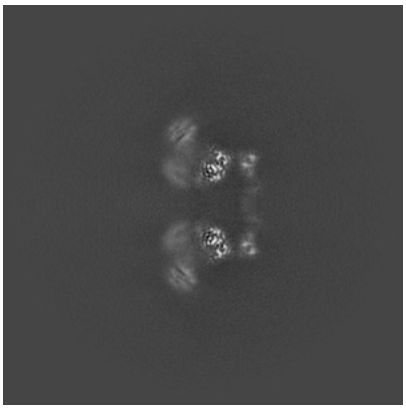
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

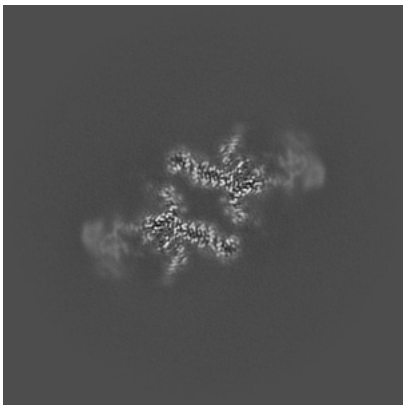
6.2.1 Primary map



X Index: 240



Y Index: 240

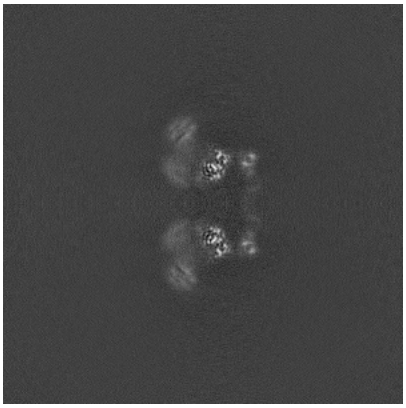


Z Index: 240

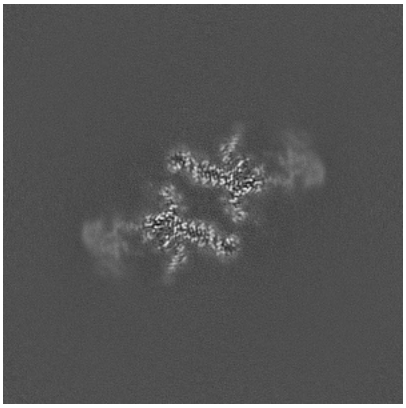
6.2.2 Raw map



X Index: 240



Y Index: 240

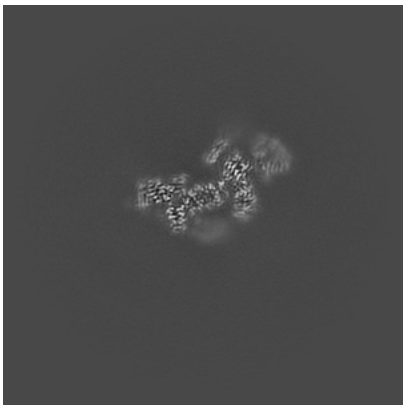


Z Index: 240

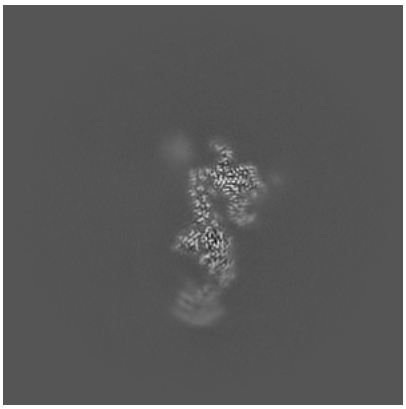
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

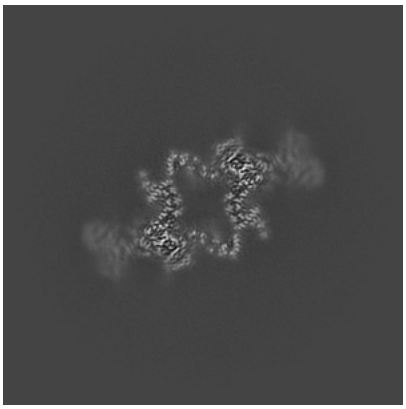
6.3.1 Primary map



X Index: 204

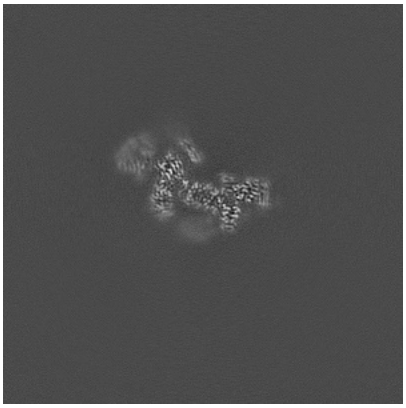


Y Index: 199

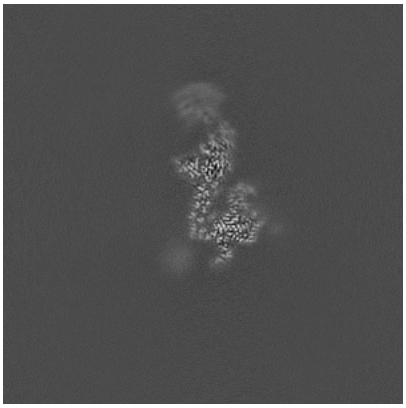


Z Index: 248

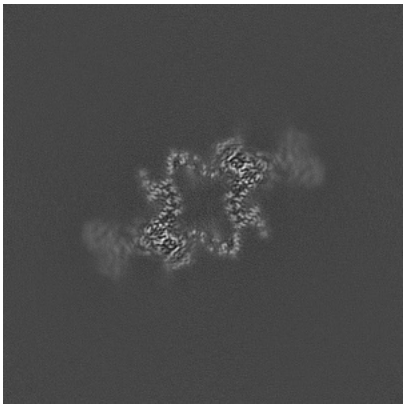
6.3.2 Raw map



X Index: 276



Y Index: 281



Z Index: 248

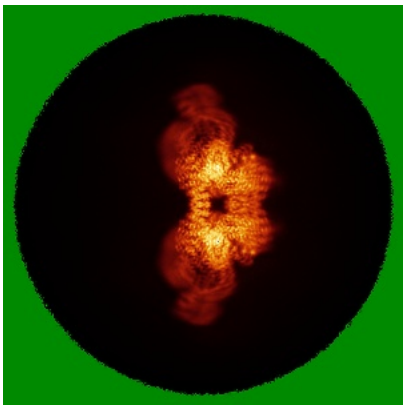
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

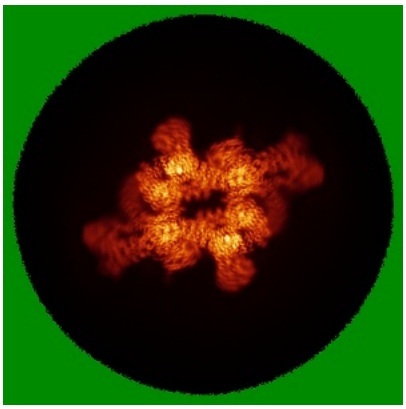
6.4.1 Primary map



X

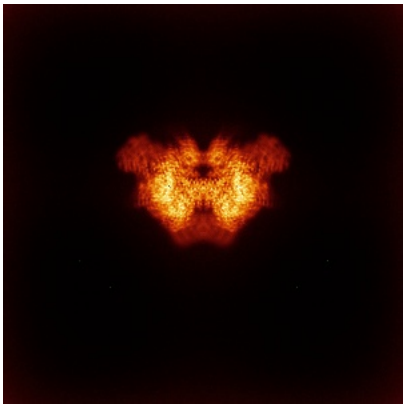


Y

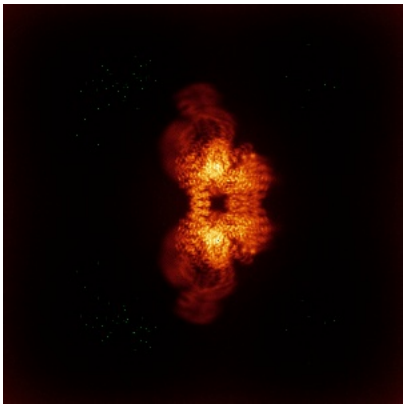


Z

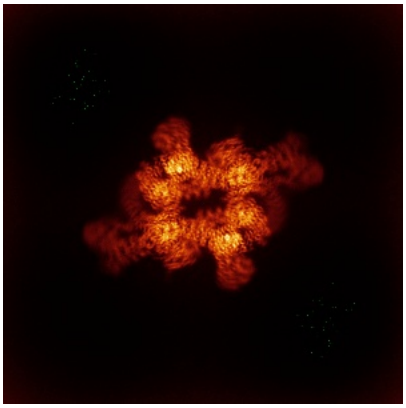
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

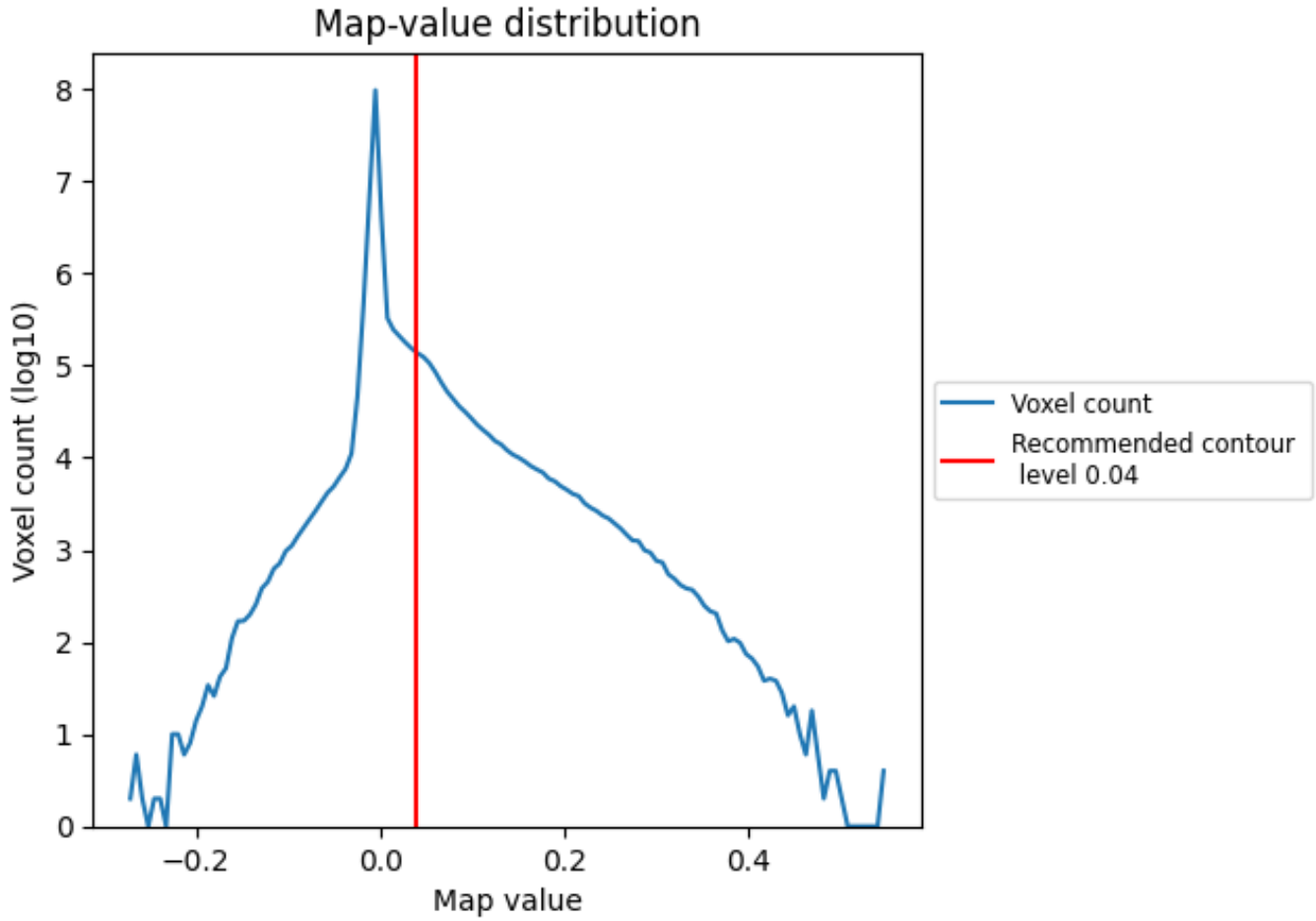
6.6 Mask visualisation (i)

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

7 Map analysis

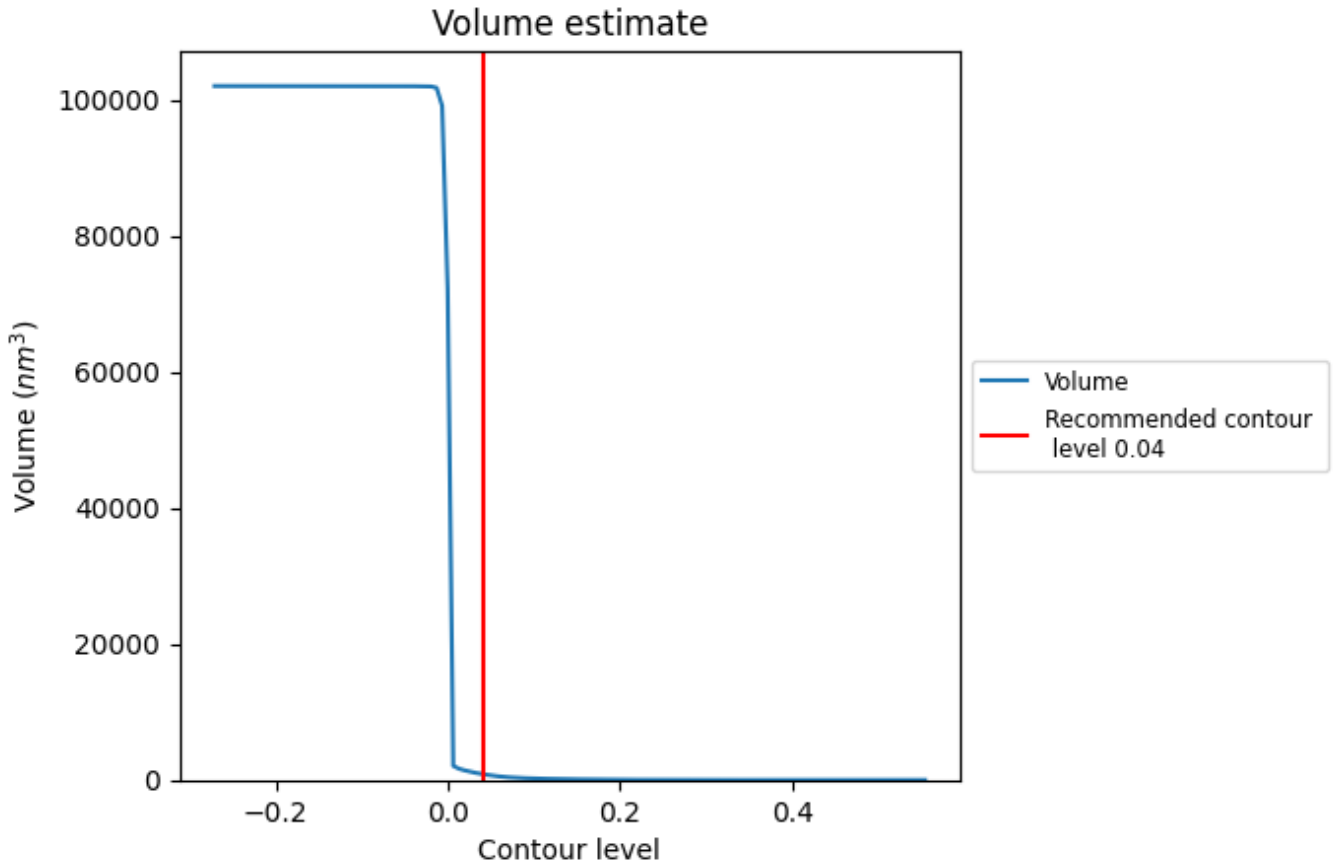
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

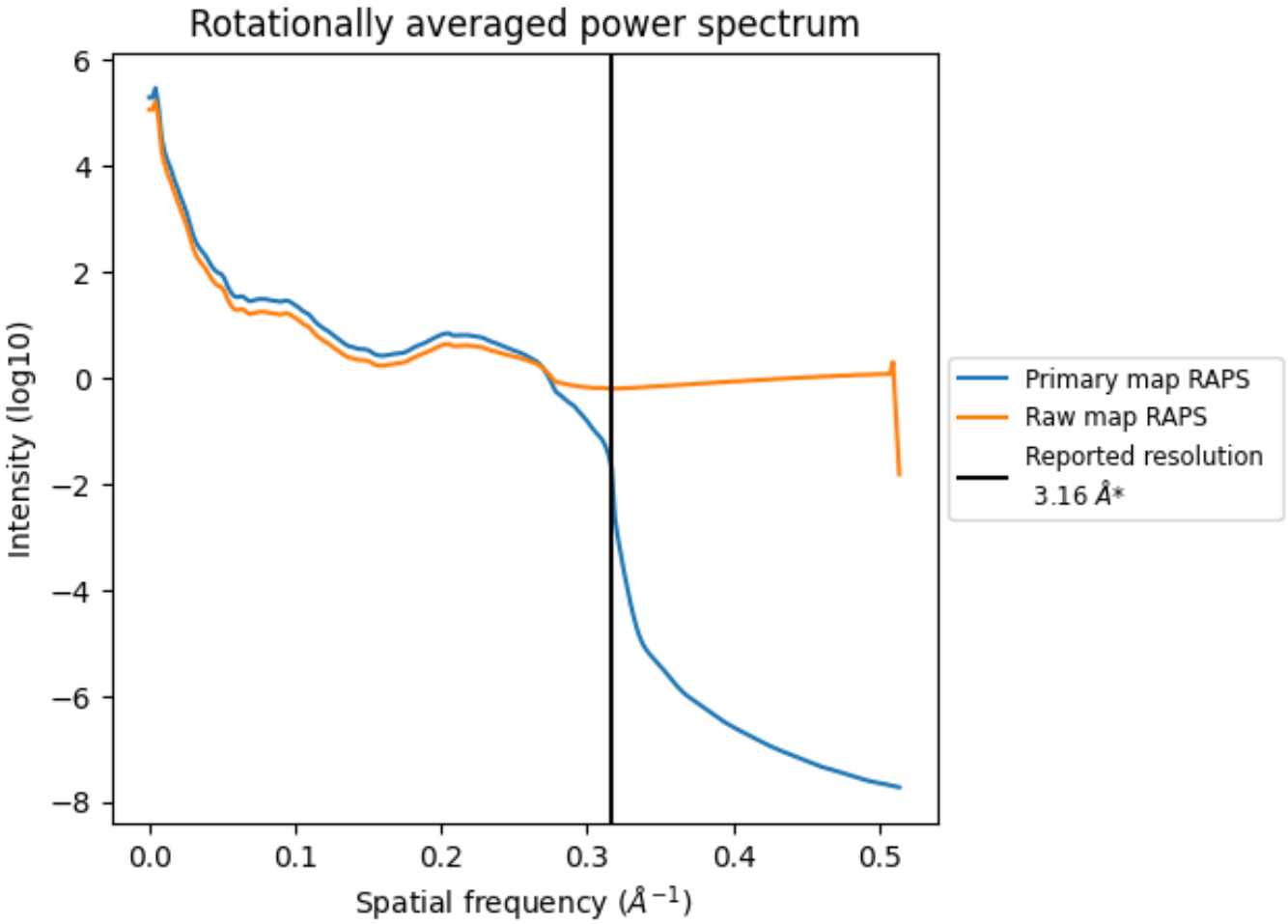
7.2 Volume estimate



The volume at the recommended contour level is 866 nm^3; this corresponds to an approximate mass of 782 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)

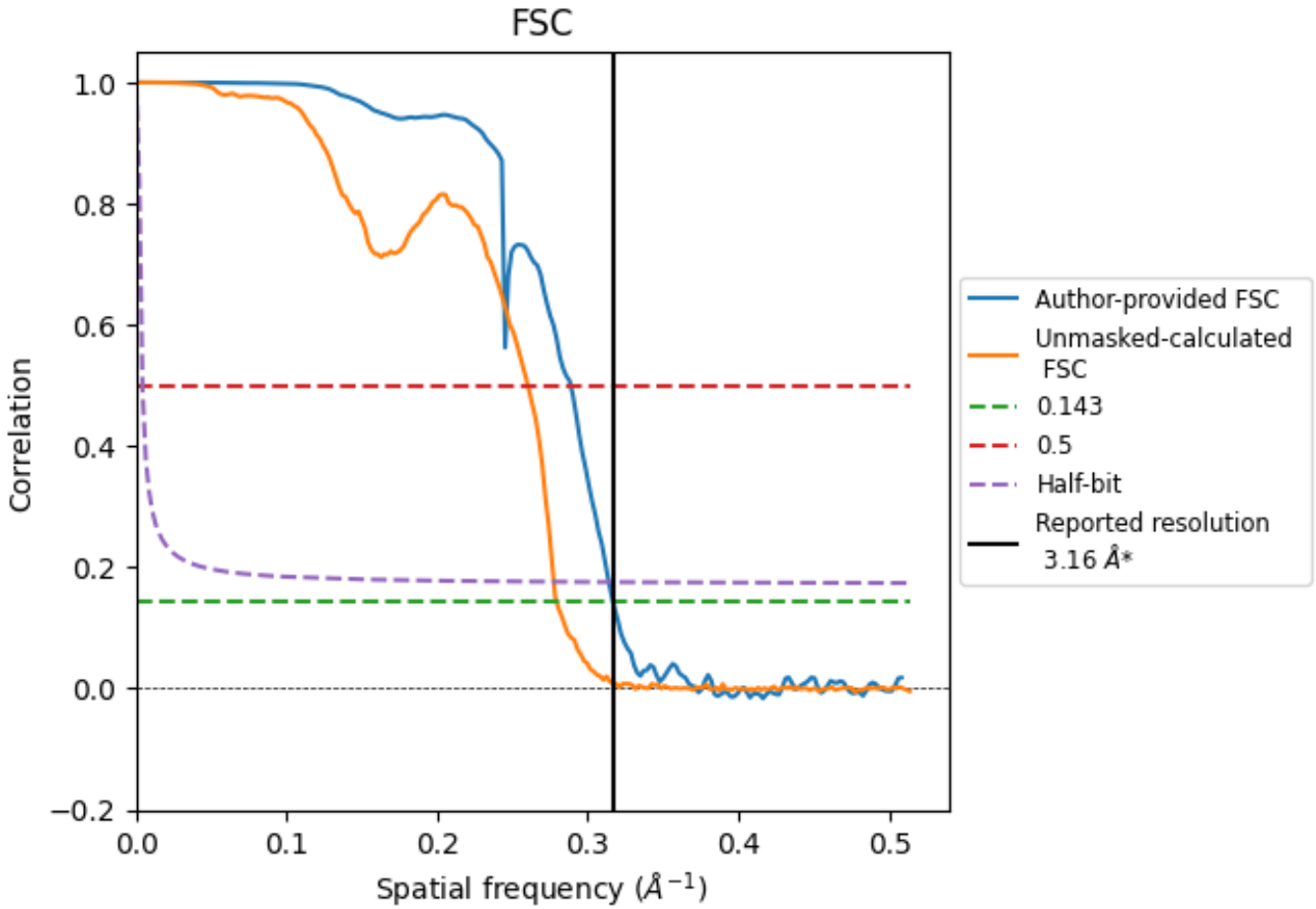


*Reported resolution corresponds to spatial frequency of 0.316 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8.2 Resolution estimates (i)

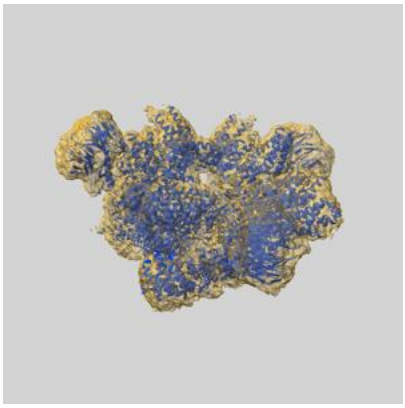
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.47	3.19
Unmasked-calculated*	3.58	3.84	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.58 differs from the reported value 3.16 by more than 10 %

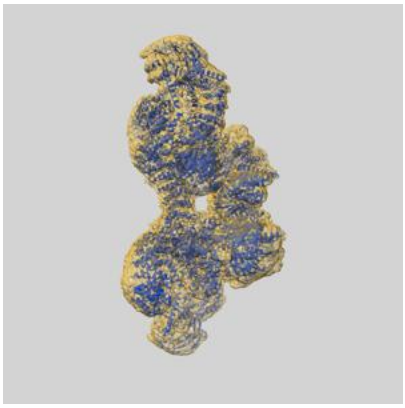
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55632 and PDB model 9T7B. Per-residue inclusion information can be found in section 3 on page 7.

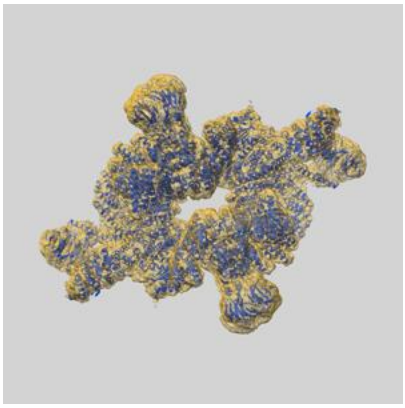
9.1 Map-model overlay



X



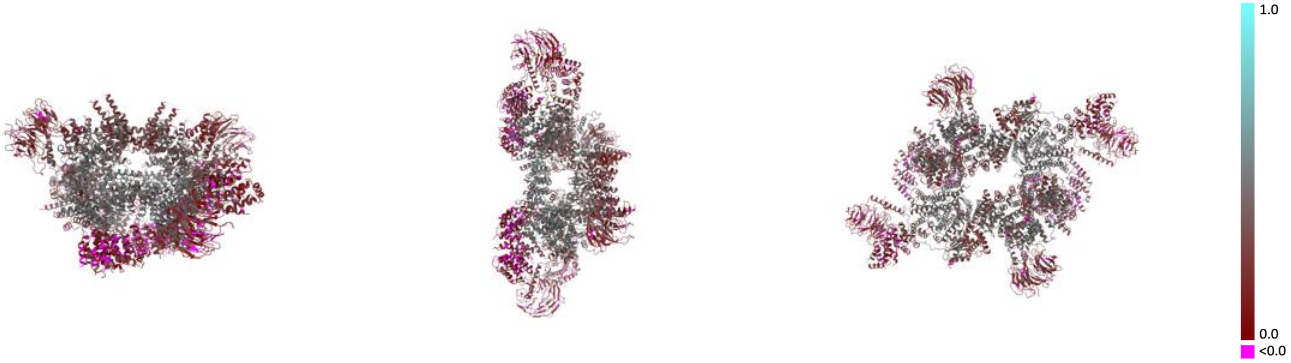
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

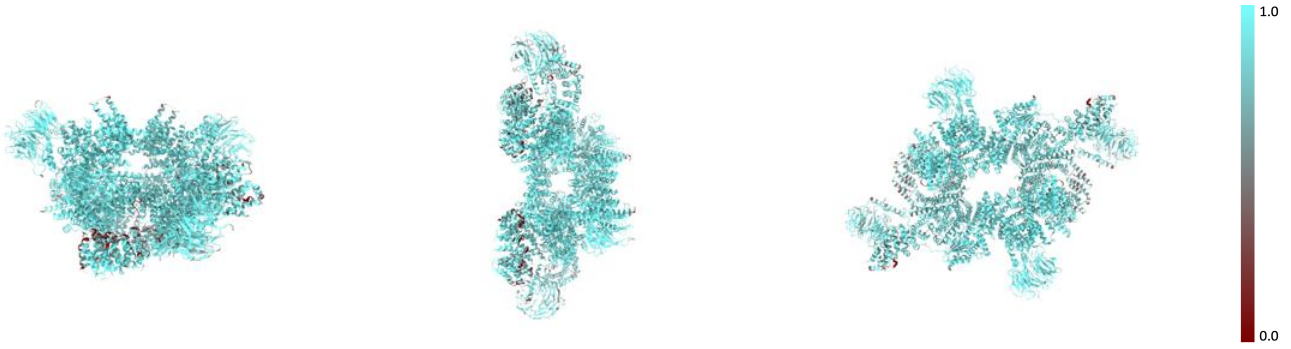
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

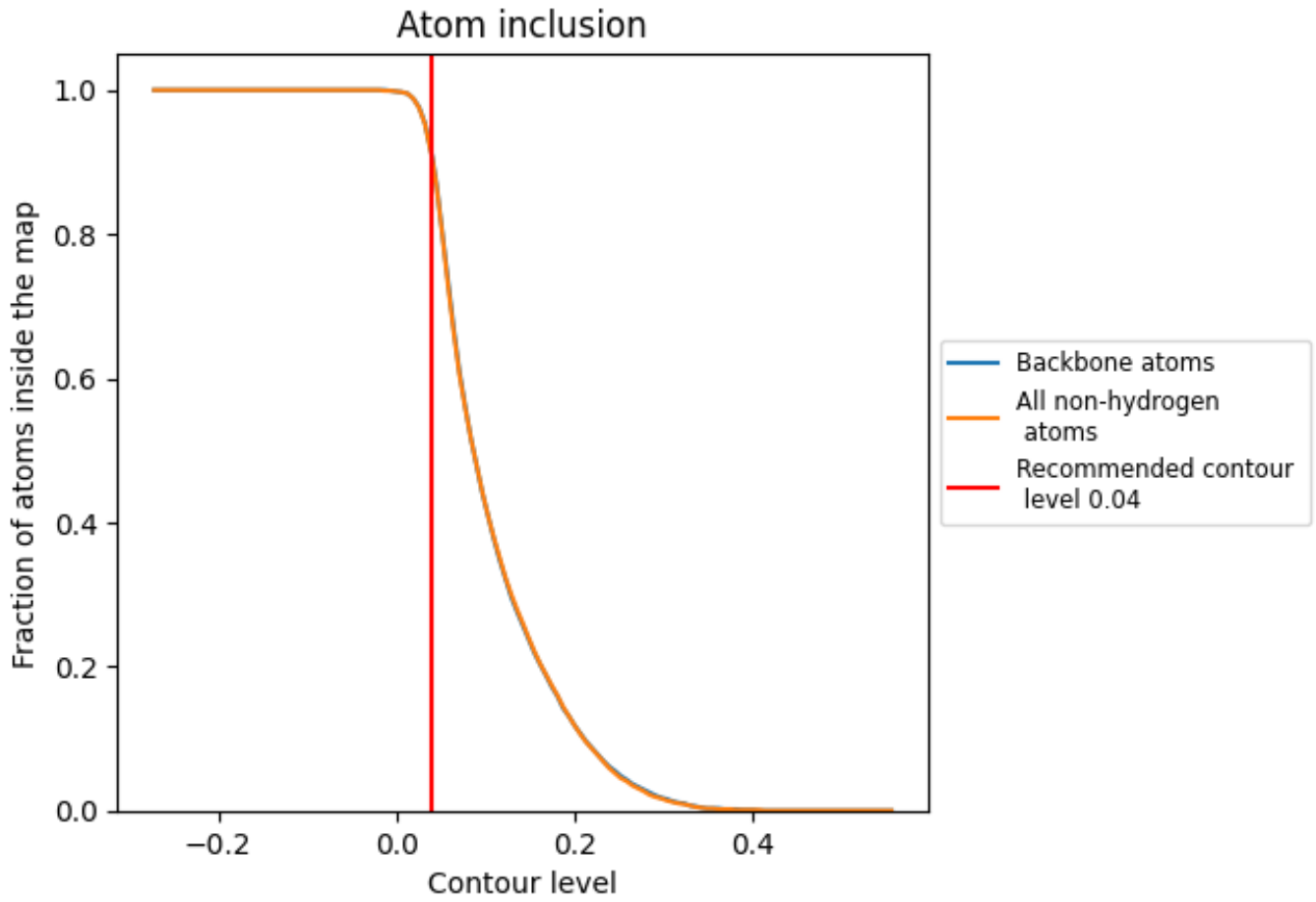
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9060	0.3050
A	0.9270	0.3430
B	0.9270	0.3430
C	0.9440	0.2010
D	0.9440	0.2000
E	0.8690	0.2570
F	0.8700	0.2550
G	0.3750	0.1860
H	0.3910	0.1700

