



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:29 PM UTC

PDB ID : 9MLI / pdb_00009mli
EMDB ID : EMD-48373
Title : Xenorhabdus nematophilus XptA2 RBD C Chimera
Authors : Aller, S.G.; Martin, C.L.
Deposited on : 2024-12-19
Resolution : 3.40 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

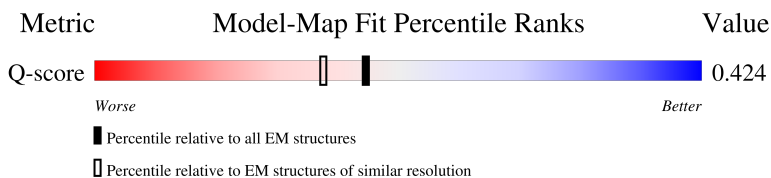
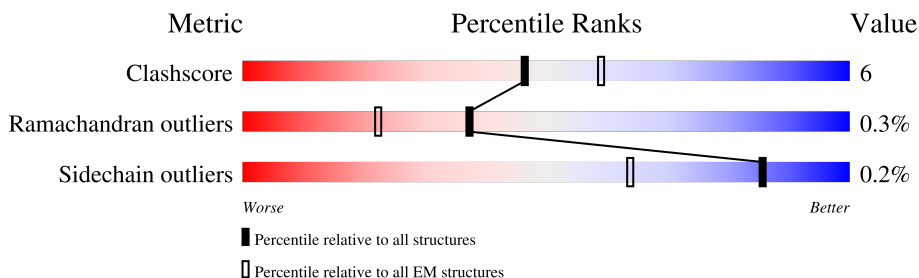
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	2543	 83% 16% .
1	B	2543	 85% 14% .
1	C	2543	 84% 15% .
1	D	2543	 86% 13% .

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Mol	Chain	Length	Quality of chain
1	E	2543	85% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 99395 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

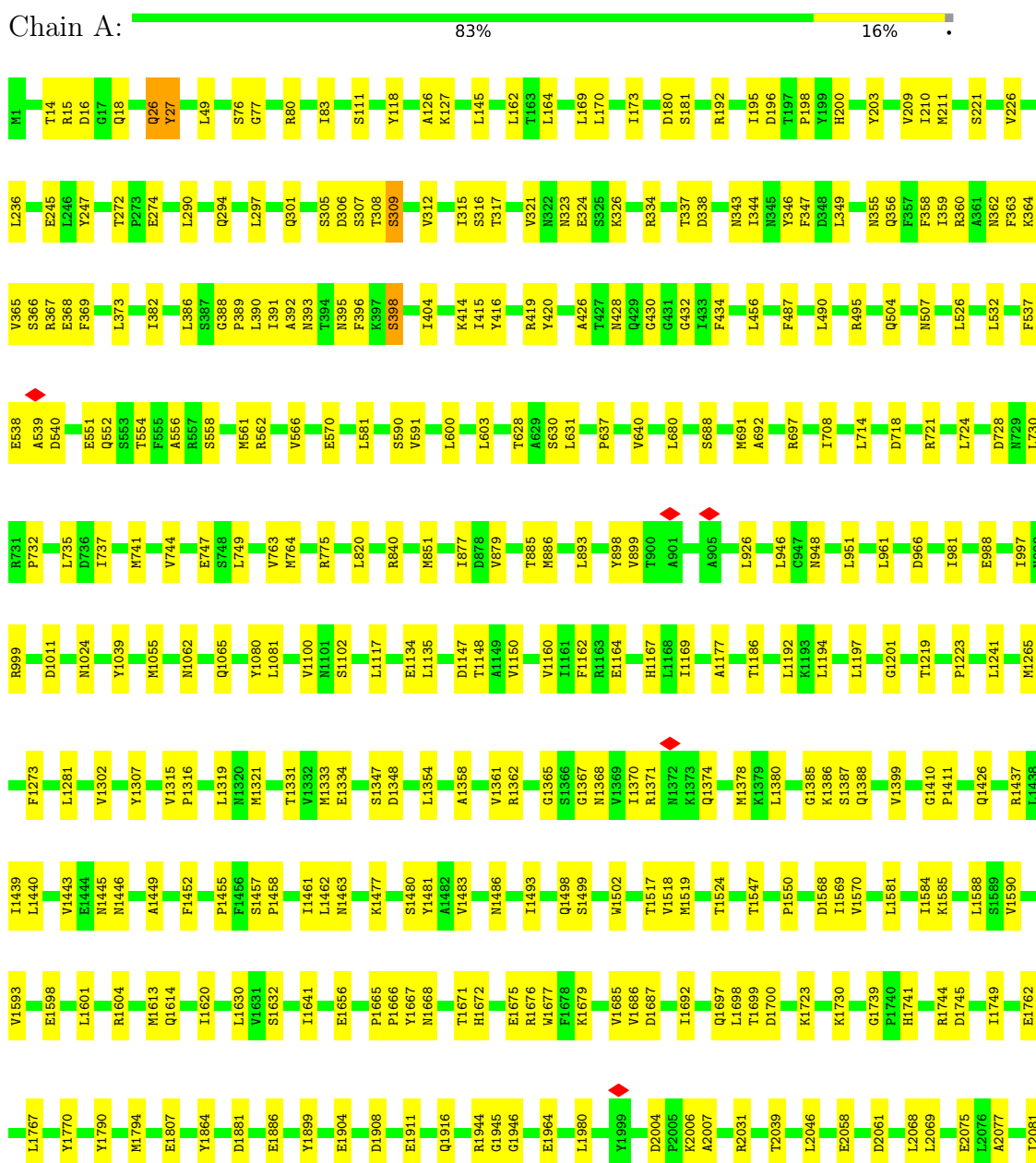
- Molecule 1 is a protein called A component of insecticidal toxin complex (Tc).

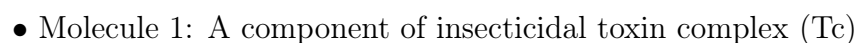
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2519	Total 19879	C 12549	N 3397	O 3863	S 70	0	0
1	B	2519	Total 19879	C 12549	N 3397	O 3863	S 70	0	0
1	C	2519	Total 19879	C 12549	N 3397	O 3863	S 70	0	0
1	D	2519	Total 19879	C 12549	N 3397	O 3863	S 70	0	0
1	E	2519	Total 19879	C 12549	N 3397	O 3863	S 70	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: A component of insecticidal toxin complex (Tc)





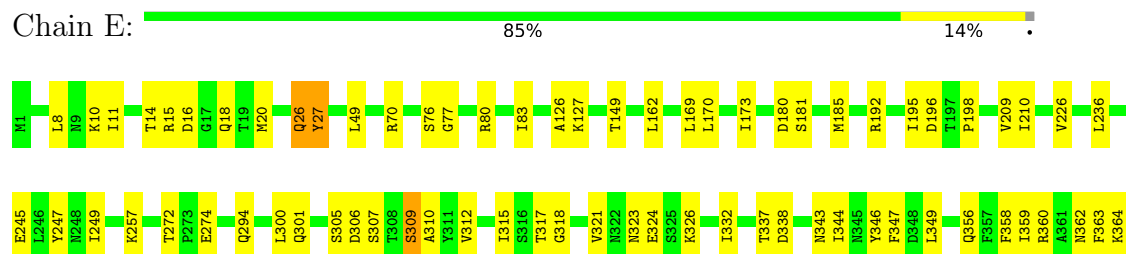
R2519
SER
GLU
ASN
LEU
TYR
PHE
GLN
GLY
ASP
TRP
ASP
LYS
LEU
GLU
HIS
HIS
HIS
HIS
HIS

- Molecule 1: A component of insecticidal toxin complex (Tc)

Chain C:  84% 15%

D2434	A2437	V2438	L2439	K2440	G2442	G2443	M2447	P2448	I2454	A2455	L2456	F2466	M2467	L2468	D2469	F2470	E2479	A2496	T2497	D2498	K2501	L2504	E2505	R2519	SER	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ASP	TRP	LYS	ASP	ASP	ASP	ASP	LYS	LEU	GLU	HIS	HIS	HIS	HIS	HIS	
W2205	E2231	V2237	H2246	T2247	Q2248	L2253	K2257	Y2264	K2270	L2271	L2281	T2282	F2285	C2286	L2287	R2294	T2303	W2318	L2323	E2329	E2343	V2344	T2345	L2372	K2376	S2382	R2398	Y2408	P2409	L2412	R2416	K2419	V2423															
Q1916	L1939	T1940	M1941	L1942	G1943	R1944	G1945	G1946	N1955	E1964	L1980	T2003	D2004	P2005	K2006	A2007	R2031	T2039	L2046	E2058	D2061	L2070	M2074	E2075	L2076	A2077	L2081	Q2084	Q2085	R2086	L2130	A2133	Q2137	V2143	A2173	V2177	R2201											
I1641	E1656	P1665	P1666	M1668	T1671	H1672	E1675	R1676	W1677	F1678	K1679	V1685	V1686	I1692	Q1697	L1698	T1699	D1700	L1711	K1730	R1744	D1745	I1749	E1762	Y1783	Y1784	E1807	D1860	P1861	M1862	R1871	D1881	D1890	Y1899	E1904	E1911	D1912											
F1456	S1457	P1458	I1461	L1462	V1483	N1486	I1493	Q1498	S1499	I1514	V1518	M1519	T1524	F1527	G1527	L1528	D1531	T1547	P1550	L1551	I1569	V1570	T1573	L1581	I1584	K1585	L1588	V1593	E1598	L1601	R1604	Q1614	L1622	N1623	T1624	S1632												
P1316	L1319	M1320	M1321	T1331	E1334	Q1340	S1347	D1348	L1354	H1355	A1358	R1362	G1365	S1366	G1367	N1368	V1369	M1372	K1373	Q1374	I1375	M1378	G1385	K1386	S1387	Q1388	V1399	Q1426	R1437	L1438	I1439	L1440	V1443	E1444	N1445	N1446	A1449	F1452	P1455									
I997	N998	R999	Y1039	M1055	M1056	R1070	E1074	Y1080	L1081	F1084	V1100	L1117	E1134	T1148	T1157	V1160	F1161	F1162	R1163	E1164	H1167	L1168	I1169	L1192	K1193	L1194	L1197	G1201	L946	C947	N948	L961	D966	V977	I981	R985	E988											
M741	T742	L743	V744	L745	K746	E747	M750	E753	T754	V763	M764	R775	L776	L820	R840	M851	C815	M816	L817	Y818	K626	T647	T660	W661	L680	I687	S688	M691	R697	I708	D718	R721	L724	D728	R729	L730	R731	P732	I737									
K364	V365	S366	F367	E368	F369	L373	R374	L386	S387	G388	F389	I391	A392	S398	L401	S402	M403	I404	S405	E408	K414	I415	Y416	Y420	A426	T427	N428	Q429	G430	G431	G432	L456	F487	R495	Q504	N507	L532	E538	L539	D540	E551	Q552						
S553	T554	F555	A556	R562	V566	G569	E570	L581	N585	L589	S590	V591	A604	L614	C615	M616	L617	Y618	K626	T647	T660	W661	L680	I687	S688	M691	R697	I708	D718	R721	L724	D728	R729	L730	R731	P732	I737											
L236	E245	L246	Y247	N248	I249	I271	W281	L297	Q301	S305	D306	S307	S308	S309	Y311	V312	T315	S316	T317	G318	V321	K322	N323	E324	S325	K326	L332	T337	D338	N343	I344	N345	Y346	F347	T197	P198	Y199	Y351	Q356	F357	F358	L359	R360	A361	N362	F363		
M1	T14	R15	D16	G17	Q18	Q26	Y27	R70	S76	G77	R80	S305	D306	S307	S91	K105	P115	A126	K127	T317	L145	M155	N322	N323	E324	S325	K326	L169	L170	I173	D180	S181	R192	N343	I344	N345	Y346	F347	T197	P198	Y199	H200	Y203	V209	I210	S221	N362	F363

- Molecule 1: A component of insecticidal toxin complex (Tc)



ASP	M2318	D2061	I11749	D1568	K1386	D1057	V763	M561	V365
TTR	L2324	L2069	I11757	I1569	S1387	E1061	R775	R562	S366
LYS	L2325	A2077	Y1784	L1581	Q1388	L1081	L776	V566	R367
ASP	E2329	T2081	Y1785	T1584	V1399	L1117	R796	E570	E368
ASP	K2332	Q2084	E1786	K1585	G1410	E1134	L820	L581	F369
LEU	L2372	Q2085	Y1790	L1588	P1411	H1167	M830	L589	L373
GLU	L2372	R2086	E1807	S1589	N1416	E1194	M840	S590	R374
HIS	S2382	L2115	D1860	V1590	N1421	A1177	R851	V591	K375
HIS	R2398	D2132	F1661	E1598	Y1437	T1186	M856	L600	I382
HIS	P2409	Q2137	M1862	T1624	L1438	L1194	T877	T601	L386
HIS	L2412	Q2137	D1881	T1624	L1440	A1195	D878	L602	S367
HIS	K2419	V2143	Y1899	S1632	V1443	F1196	V879	L603	G388
HIS	V2423	L2160	E1904	R1633	E1444	T1219	M886	A604	I391
HIS	A2437	A2173	L1905	T1640	N1445	T1219	M886	L614	A392
		S2174	D1908	T1664	F1452	P1223	L893	L617	N395
	Y2441	V2177	E1911	P1665	P1455	M1285	L893	S630	F396
	G2442	R2201	Q1916	P1666	F1456	F1273	Y898	L631	K414
	G2443	R2201	Q1916	N1667	S1457	F1273	Y899	P637	I415
	M2447	W2205	L1939	N1668	P1458	T900	T900	V640	Y416
	P2448	E2231	T1940	H1672	I1462	V1315	A901	N671	Y420
	L2456	E2231	M1941	R1676	N1463	L1319	I902	L680	A426
	F2466	V2237	R1944	K1679	K1477	M1321	I903	I687	T428
	M2467	E2252	G1946	K1679	V1483	T1331	A904	I687	M428
	F2470	L2253	A1954	V1685	N1486	E1334	L926	R697	Q429
	I2471	K2287	N1955	V1686	N1486	S1347	D936	L714	G430
	D2472	L2263	S1956	D1687	I1493	D1348	E940	L714	G431
	E2479	Y2264	Y1999	I1692	I1493	E940	L946	D718	G432
	T2497	W2267	D2004	Q1697	Y1497	L1354	L946	R721	L456
	D2498	K2270	P2005	L1698	Q1498	H1355	C947	L724	F487
	K2501	L2281	K2006	T1699	W1502	N1356	N948	N507	Q604
	L2504	T2282	A2007	D1700	W1518	R1362	L961	D728	N507
	E2505	Q2283	T2010	L1711	M1519	Y1363	D966	P732	L532
	R2519	S2284	R2031	M1726	T1524	G1365	Y977	L735	E538
SER	GLU	F2285	T2039	K1730	F1527	S1386	N981	D736	A539
GLU	ASN	M2288	T2039	G1739	D1531	N1368	I981	I737	D540
ASN	LEU	H1741	V2043	H1740	T1547	R1371	I997	M741	E551
LEU	TYR	R1744	L2046	H1741	T1547	N1372	I998	Q552	S553
TYR	PHE	T2303	L2046	H1741	T1547	L1380	R999	V744	T554
PHE	GLN	L2317	E2058	R1744	P1550	L1380	A1000	F555	F555
GLN	GLY			D1745	L1551	G1385	L1001	E747	A556
GLY				D1745	L1551	G1385	Q1052		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77025	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.962	Depositor
Minimum map value	-0.404	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.0894	Depositor
Map size (Å)	485.46, 485.46, 485.46	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3485, 1.3485, 1.3485	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/20285	0.34	6/27556 (0.0%)
1	B	0.18	0/20285	0.34	7/27556 (0.0%)
1	C	0.18	0/20285	0.34	6/27556 (0.0%)
1	D	0.18	0/20285	0.35	6/27556 (0.0%)
1	E	0.18	0/20285	0.35	6/27556 (0.0%)
All	All	0.18	0/101425	0.34	31/137780 (0.0%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2497	THR	CA-C-N	13.96	146.83	121.70
1	D	2497	THR	C-N-CA	13.96	146.83	121.70
1	B	2497	THR	CA-C-N	13.93	146.76	121.70
1	B	2497	THR	C-N-CA	13.93	146.76	121.70
1	C	2497	THR	CA-C-N	13.92	146.75	121.70
1	C	2497	THR	C-N-CA	13.92	146.75	121.70
1	E	26	GLN	CA-C-N	13.86	146.65	121.70
1	E	26	GLN	C-N-CA	13.86	146.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	GLN	CA-C-N	13.85	146.64	121.70
1	A	26	GLN	C-N-CA	13.85	146.64	121.70
1	E	2497	THR	CA-C-N	13.83	146.60	121.70
1	E	2497	THR	C-N-CA	13.83	146.60	121.70
1	A	2497	THR	CA-C-N	13.83	146.59	121.70
1	A	2497	THR	C-N-CA	13.83	146.59	121.70
1	B	26	GLN	CA-C-N	13.76	146.47	121.70
1	B	26	GLN	C-N-CA	13.76	146.47	121.70
1	C	26	GLN	CA-C-N	13.74	146.44	121.70
1	C	26	GLN	C-N-CA	13.74	146.44	121.70
1	D	26	GLN	CA-C-N	13.73	146.42	121.70
1	D	26	GLN	C-N-CA	13.73	146.42	121.70
1	B	312	VAL	CA-C-N	8.89	137.70	121.70
1	B	312	VAL	C-N-CA	8.89	137.70	121.70
1	A	312	VAL	CA-C-N	8.69	137.34	121.70
1	A	312	VAL	C-N-CA	8.69	137.34	121.70
1	D	312	VAL	CA-C-N	8.61	137.19	121.70
1	D	312	VAL	C-N-CA	8.61	137.19	121.70
1	C	312	VAL	CA-C-N	8.51	137.01	121.70
1	C	312	VAL	C-N-CA	8.51	137.01	121.70
1	E	312	VAL	CA-C-N	8.44	136.90	121.70
1	E	312	VAL	C-N-CA	8.44	136.90	121.70
1	B	1386	LYS	CB-CA-C	-5.07	109.75	115.79

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	B	398	SER	Peptide
1	C	398	SER	Peptide
1	D	398	SER	Peptide
1	E	398	SER	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	19879	0	19498	276	0
1	B	19879	0	19498	251	0
1	C	19879	0	19498	266	0
1	D	19879	0	19498	237	0
1	E	19879	0	19498	253	0
All	All	99395	0	97490	1202	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1202) 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:E:2447:MET:HE3	1:E:2448:PRO:HD2	1.58	0.85
1:B:2056:MET:HE2	1:B:2267:MET:HE3	1.59	0.83
1:A:306:ASP:OD1	1:A:307:SER:N	2.14	0.81
1:D:2497:THR:H	1:D:2498:ASP:HB2	1.46	0.81
1:C:2497:THR:H	1:C:2498:ASP:HB2	1.47	0.79
1:B:369:PHE:HD2	1:B:388:GLY:H	1.30	0.79
1:A:369:PHE:HD2	1:A:388:GLY:H	1.32	0.78
1:A:2447:MET:HE3	1:A:2448:PRO:HD2	1.65	0.78
1:B:2497:THR:H	1:B:2498:ASP:HB2	1.47	0.77
1:D:2039:THR:HG22	1:D:2285:PHE:HB3	1.67	0.77
1:E:2497:THR:H	1:E:2498:ASP:HB2	1.49	0.76
1:A:2497:THR:H	1:A:2498:ASP:HB2	1.50	0.76
1:C:306:ASP:OD1	1:C:307:SER:N	2.19	0.76
1:E:306:ASP:OD1	1:E:307:SER:N	2.19	0.76
1:C:369:PHE:HD2	1:C:388:GLY:H	1.31	0.76
1:B:2039:THR:HG22	1:B:2285:PHE:HB3	1.67	0.75
1:D:369:PHE:HD2	1:D:388:GLY:H	1.31	0.75
1:B:365:VAL:HG13	1:B:391:ILE:HA	1.69	0.74
1:B:306:ASP:OD1	1:B:307:SER:N	2.21	0.74
1:E:369:PHE:HD2	1:E:388:GLY:H	1.33	0.73
1:A:2039:THR:HG22	1:A:2285:PHE:HB3	1.71	0.73
1:D:301:GLN:HB2	1:D:315:ILE:HD11	1.71	0.73
1:D:306:ASP:OD1	1:D:307:SER:N	2.22	0.73
1:A:1440:LEU:HB2	1:A:1452:PHE:HB2	1.71	0.72
1:A:365:VAL:HG22	1:A:392:ALA:H	1.54	0.72
1:A:1666:PRO:HG2	1:B:1386:LYS:HD2	1.72	0.72
1:D:1440:LEU:HB2	1:D:1452:PHE:HB2	1.71	0.72
1:C:365:VAL:HG22	1:C:392:ALA:H	1.54	0.72
1:C:2039:THR:HG22	1:C:2285:PHE:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLN:HB2	1:A:315:ILE:HD11	1.72	0.72
1:D:365:VAL:HG13	1:D:391:ILE:HA	1.71	0.71
1:D:977:VAL:HB	1:D:981:ILE:HD11	1.73	0.71
1:A:2075:GLU:OE2	1:B:2246:HIS:NE2	2.24	0.71
1:C:367:ARG:HH22	1:C:389:PRO:HB3	1.56	0.70
1:E:365:VAL:HG13	1:E:391:ILE:HA	1.71	0.70
1:B:301:GLN:HB2	1:B:315:ILE:HD11	1.73	0.70
1:E:1440:LEU:HB2	1:E:1452:PHE:HB2	1.73	0.70
1:C:1387:SER:OG	1:C:1388:GLN:N	2.22	0.69
1:B:2318:MET:HE1	1:C:2271:LEU:HB2	1.74	0.69
1:D:1387:SER:OG	1:D:1388:GLN:N	2.22	0.69
1:D:1666:PRO:HG2	1:E:1386:LYS:HD2	1.73	0.69
1:E:2039:THR:HG22	1:E:2285:PHE:HB3	1.72	0.69
1:B:1057:ASP:O	1:B:1061:GLU:HG3	1.92	0.69
1:B:1368:ASN:O	1:B:1372:ASN:ND2	2.25	0.69
1:B:1666:PRO:HG2	1:C:1386:LYS:HD2	1.75	0.69
1:A:1386:LYS:HD2	1:E:1666:PRO:HG2	1.75	0.69
1:E:1134:GLU:N	1:E:1134:GLU:OE1	2.26	0.69
1:B:1440:LEU:HB2	1:B:1452:PHE:HB2	1.75	0.69
1:C:343:ASN:HA	1:C:363:PHE:HB2	1.75	0.69
1:C:2470:PHE:HB2	1:D:2467:MET:HE1	1.75	0.69
1:E:364:LYS:NZ	1:E:366:SER:OG	2.23	0.69
1:C:1624:THR:HG1	1:C:1784:TYR:HH	1.38	0.68
1:B:346:TYR:HE1	1:B:359:ILE:HG22	1.59	0.68
1:D:885:THR:HG22	1:D:886:MET:H	1.57	0.68
1:B:1134:GLU:N	1:B:1134:GLU:OE2	2.26	0.68
1:D:1368:ASN:O	1:D:1372:ASN:ND2	2.27	0.68
1:D:343:ASN:HA	1:D:363:PHE:HB2	1.76	0.67
1:B:1319:LEU:HD22	1:B:1588:LEU:HD13	1.76	0.67
1:C:346:TYR:HE1	1:C:359:ILE:HG22	1.59	0.67
1:C:1666:PRO:HG2	1:D:1386:LYS:HD2	1.77	0.67
1:C:365:VAL:HG13	1:C:391:ILE:HA	1.77	0.66
1:B:343:ASN:HA	1:B:363:PHE:HB2	1.78	0.66
1:B:2470:PHE:HB2	1:C:2467:MET:HE1	1.78	0.66
1:C:1440:LEU:HB2	1:C:1452:PHE:HB2	1.76	0.66
1:E:226:VAL:HG11	1:E:879:VAL:HG21	1.76	0.66
1:E:1624:THR:HG1	1:E:1784:TYR:HH	1.39	0.66
1:A:365:VAL:HG13	1:A:391:ILE:HA	1.78	0.65
1:C:226:VAL:HG11	1:C:879:VAL:HG21	1.78	0.65
1:D:365:VAL:HG22	1:D:392:ALA:H	1.61	0.65
1:A:226:VAL:HG11	1:A:879:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1319:LEU:HD22	1:A:1588:LEU:HD13	1.79	0.65
1:C:697:ARG:NH1	1:C:728:ASP:OD2	2.30	0.65
1:C:1426:GLN:HB3	1:C:1462:LEU:HD22	1.79	0.65
1:D:226:VAL:HG11	1:D:879:VAL:HG21	1.79	0.65
1:D:346:TYR:HE1	1:D:359:ILE:HG22	1.60	0.65
1:E:343:ASN:HA	1:E:363:PHE:HB2	1.78	0.64
1:E:346:TYR:HE1	1:E:359:ILE:HG22	1.62	0.64
1:B:2084:GLN:HB3	1:B:2237:VAL:HG22	1.80	0.64
1:D:1916:GLN:HE22	1:E:294:GLN:HE22	1.45	0.64
1:A:1916:GLN:HE22	1:B:294:GLN:HE22	1.44	0.63
1:C:1385:GLY:HA2	1:C:1386:LYS:HZ3	1.61	0.63
1:E:1387:SER:OG	1:E:1388:GLN:N	2.23	0.63
1:A:338:ASP:OD2	1:A:428:ASN:ND2	2.31	0.63
1:B:180:ASP:OD1	1:B:181:SER:N	2.32	0.63
1:B:365:VAL:HG22	1:B:392:ALA:H	1.63	0.63
1:C:977:VAL:HB	1:C:981:ILE:HD11	1.80	0.63
1:A:1881:ASP:OD1	1:A:1899:TYR:OH	2.17	0.63
1:C:2447:MET:HE3	1:C:2448:PRO:HD2	1.81	0.63
1:A:2437:ALA:HB3	1:A:2456:LEU:HB2	1.80	0.63
1:E:697:ARG:NH1	1:E:728:ASP:OD2	2.32	0.63
1:C:1319:LEU:HD22	1:C:1588:LEU:HD13	1.81	0.63
1:C:1904:GLU:OE2	1:D:999:ARG:NH1	2.28	0.63
1:A:294:GLN:HE22	1:E:1916:GLN:HE22	1.45	0.62
1:B:2329:GLU:HG2	1:C:2281:LEU:HD11	1.81	0.62
1:D:1236:GLN:OE1	1:D:1308:ARG:NH1	2.32	0.62
1:B:2423:VAL:HG13	1:B:2456:LEU:HD11	1.80	0.62
1:D:1904:GLU:OE2	1:E:999:ARG:NH1	2.26	0.62
1:E:180:ASP:OD1	1:E:181:SER:N	2.32	0.62
1:C:236:LEU:HB2	1:C:487:PHE:HB2	1.81	0.62
1:A:2084:GLN:HB3	1:A:2237:VAL:HG22	1.81	0.62
1:A:718:ASP:OD1	1:A:721:ARG:NH2	2.33	0.62
1:E:1941:MET:SD	1:E:1944:ARG:NH2	2.73	0.62
1:D:192:ARG:NH1	1:D:245:GLU:OE2	2.33	0.61
1:C:1519:MET:SD	1:C:1524:THR:OG1	2.55	0.61
1:D:1624:THR:OG1	1:D:1784:TYR:OH	2.17	0.61
1:B:2042:LEU:HB3	1:B:2282:THR:HG22	1.83	0.61
1:D:1385:GLY:HA2	1:D:1386:LYS:HZ3	1.65	0.61
1:B:236:LEU:HB2	1:B:487:PHE:HB2	1.82	0.61
1:E:192:ARG:NH1	1:E:245:GLU:OE2	2.33	0.61
1:A:343:ASN:HA	1:A:363:PHE:HB2	1.82	0.61
1:A:1679:LYS:HD3	1:A:1692:ILE:HD12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:ASP:OD1	1:B:721:ARG:NH2	2.34	0.61
1:C:1667:TYR:HB2	1:C:1698:LEU:HB3	1.83	0.61
1:D:1457:SER:OG	1:D:1458:PRO:HD3	2.00	0.61
1:E:1385:GLY:HA2	1:E:1386:LYS:HZ3	1.63	0.61
1:A:1668:ASN:ND2	1:A:1671:THR:OG1	2.33	0.60
1:C:196:ASP:OD2	1:C:948:ASN:ND2	2.34	0.60
1:E:718:ASP:OD1	1:E:721:ARG:NH2	2.34	0.60
1:D:196:ASP:OD2	1:D:948:ASN:ND2	2.34	0.60
1:A:1790:TYR:HH	1:A:1864:TYR:HH	1.48	0.60
1:B:1881:ASP:OD1	1:B:1899:TYR:OH	2.19	0.60
1:D:236:LEU:HB2	1:D:487:PHE:HB2	1.83	0.60
1:E:196:ASP:OD2	1:E:948:ASN:ND2	2.35	0.60
1:E:236:LEU:HB2	1:E:487:PHE:HB2	1.84	0.60
1:A:1426:GLN:HB3	1:A:1462:LEU:HD22	1.82	0.60
1:B:196:ASP:OD2	1:B:948:ASN:ND2	2.35	0.60
1:B:1387:SER:OG	1:B:1388:GLN:N	2.21	0.60
1:A:2470:PHE:HB2	1:B:2467:MET:HE1	1.84	0.60
1:C:1399:VAL:HA	1:C:1498:GLN:O	2.02	0.60
1:E:1667:TYR:HB2	1:E:1698:LEU:HB3	1.84	0.60
1:E:1668:ASN:ND2	1:E:1671:THR:OG1	2.34	0.60
1:A:367:ARG:HH22	1:A:389:PRO:HB3	1.65	0.60
1:A:373:LEU:HB2	1:A:416:TYR:HB3	1.84	0.59
1:D:1668:ASN:ND2	1:D:1671:THR:OG1	2.31	0.59
1:E:1598:GLU:OE1	1:E:1598:GLU:N	2.31	0.59
1:C:310:ALA:HB1	1:C:315:ILE:HD13	1.84	0.59
1:C:1668:ASN:ND2	1:C:1671:THR:OG1	2.32	0.59
1:A:1399:VAL:HA	1:A:1498:GLN:O	2.02	0.59
1:B:1668:ASN:ND2	1:B:1671:THR:OG1	2.34	0.59
1:C:1916:GLN:HE22	1:D:294:GLN:HE22	1.48	0.59
1:A:1697:GLN:NE2	1:A:1944:ARG:O	2.35	0.59
1:D:2084:GLN:HB3	1:D:2237:VAL:HG22	1.84	0.59
1:C:1458:PRO:HG2	1:C:1461:ILE:HD12	1.85	0.59
1:C:2086:ARG:NH1	1:D:2231:GLU:OE2	2.36	0.59
1:A:196:ASP:OD2	1:A:948:ASN:ND2	2.36	0.59
1:B:1334:GLU:OE2	1:B:1362:ARG:NH2	2.35	0.59
1:E:2084:GLN:HB3	1:E:2237:VAL:HG22	1.84	0.59
1:D:1881:ASP:OD1	1:D:1899:TYR:OH	2.19	0.59
1:A:1321:MET:HB3	1:A:1584:ILE:HG21	1.85	0.59
1:C:338:ASP:OD2	1:C:428:ASN:ND2	2.35	0.59
1:D:708:ILE:HD12	1:D:764:MET:HE1	1.85	0.59
1:E:1457:SER:HB3	1:E:1458:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:718:ASP:OD1	1:D:721:ARG:NH2	2.35	0.58
1:A:210:ILE:HD11	1:A:893:LEU:HD21	1.86	0.58
1:A:1457:SER:HB3	1:A:1458:PRO:HD3	1.85	0.58
1:C:2084:GLN:HB3	1:C:2237:VAL:HG22	1.84	0.58
1:B:1667:TYR:HB2	1:B:1698:LEU:HB3	1.84	0.58
1:B:338:ASP:OD2	1:B:428:ASN:ND2	2.36	0.58
1:C:1697:GLN:NE2	1:C:1944:ARG:O	2.36	0.58
1:C:1881:ASP:OD1	1:C:1899:TYR:OH	2.21	0.58
1:B:226:VAL:HG11	1:B:879:VAL:HG21	1.84	0.58
1:C:708:ILE:HD12	1:C:764:MET:HE1	1.86	0.58
1:A:80:ARG:HH11	1:A:83:ILE:HG13	1.68	0.58
1:A:2086:ARG:NH1	1:B:2231:GLU:OE2	2.37	0.58
1:A:2372:LEU:HD11	1:A:2504:LEU:HB3	1.86	0.58
1:B:2086:ARG:NH1	1:C:2231:GLU:OE2	2.37	0.58
1:D:1519:MET:SD	1:D:1524:THR:OG1	2.61	0.58
1:B:697:ARG:NH1	1:B:728:ASP:OD2	2.36	0.58
1:B:1519:MET:SD	1:B:1524:THR:OG1	2.59	0.58
1:C:347:PHE:HD1	1:C:360:ARG:HG3	1.68	0.58
1:D:2086:ARG:NH1	1:E:2231:GLU:OE2	2.37	0.58
1:A:1062:ASN:O	1:A:1065:GLN:NE2	2.37	0.57
1:B:1697:GLN:NE2	1:B:1944:ARG:O	2.37	0.57
1:E:338:ASP:OD2	1:E:428:ASN:ND2	2.37	0.57
1:E:1697:GLN:NE2	1:E:1944:ARG:O	2.36	0.57
1:A:1601:LEU:HD12	1:A:1613:MET:HE1	1.86	0.57
1:C:1340:GLN:HB2	1:C:1355:HIS:HB2	1.86	0.57
1:D:338:ASP:OD2	1:D:428:ASN:ND2	2.37	0.57
1:A:180:ASP:OD1	1:A:181:SER:N	2.35	0.57
1:A:192:ARG:NH1	1:A:245:GLU:OE2	2.37	0.57
1:A:236:LEU:HB2	1:A:487:PHE:HB2	1.85	0.57
1:B:1457:SER:HB3	1:B:1458:PRO:HD3	1.86	0.57
1:C:851:MET:HG2	1:C:877:ILE:HD13	1.86	0.57
1:D:2329:GLU:HG2	1:E:2281:LEU:HD11	1.85	0.57
1:E:301:GLN:O	1:E:317:THR:HG21	2.04	0.57
1:A:2408:TYR:HB2	1:A:2416:ARG:HH12	1.70	0.57
1:B:1385:GLY:HA2	1:B:1386:LYS:HZ3	1.70	0.57
1:B:2497:THR:N	1:B:2498:ASP:HB2	2.19	0.57
1:A:2231:GLU:OE2	1:E:2086:ARG:NH1	2.37	0.57
1:D:1667:TYR:HB2	1:D:1698:LEU:HB3	1.86	0.57
1:E:724:LEU:HD22	1:E:737:ILE:HD11	1.87	0.57
1:A:1519:MET:SD	1:A:1524:THR:OG1	2.59	0.57
1:A:2329:GLU:HG2	1:B:2281:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2437:ALA:HB3	1:B:2456:LEU:HB2	1.87	0.57
1:A:697:ARG:NH1	1:A:728:ASP:OD2	2.38	0.56
1:C:2497:THR:N	1:C:2498:ASP:HB2	2.18	0.56
1:D:306:ASP:OD1	1:D:307:SER:OG	2.23	0.56
1:D:2497:THR:N	1:D:2498:ASP:HB2	2.18	0.56
1:B:1624:THR:OG1	1:B:1784:TYR:OH	2.15	0.56
1:A:886:MET:HE3	1:B:569:GLY:H	1.70	0.56
1:C:2318:MET:HE1	1:D:2267:MET:HA	1.86	0.56
1:B:1904:GLU:OE2	1:C:999:ARG:NH1	2.30	0.56
1:C:1457:SER:HB3	1:C:1458:PRO:HD3	1.86	0.56
1:B:1147:ASP:N	1:B:1147:ASP:OD1	2.38	0.56
1:B:1380:LEU:HD11	1:B:1463:ASN:HB3	1.88	0.56
1:D:1679:LYS:HD3	1:D:1692:ILE:HD12	1.88	0.56
1:E:1881:ASP:OD1	1:E:1899:TYR:OH	2.22	0.56
1:C:192:ARG:NH1	1:C:245:GLU:OE2	2.39	0.56
1:E:2497:THR:N	1:E:2498:ASP:HB2	2.20	0.56
1:A:1011:ASP:OD1	1:A:1011:ASP:N	2.36	0.56
1:B:886:MET:HE3	1:C:569:GLY:H	1.70	0.56
1:B:1679:LYS:HD3	1:B:1692:ILE:HD12	1.87	0.56
1:E:830:MET:HE1	1:E:840:ARG:HG2	1.88	0.56
1:A:364:LYS:NZ	1:A:366:SER:OG	2.38	0.55
1:A:1387:SER:OG	1:A:1388:GLN:N	2.22	0.55
1:D:1941:MET:HE1	1:D:1944:ARG:HH21	1.71	0.55
1:D:1656:GLU:OE2	1:D:1744:ARG:NH2	2.39	0.55
1:E:1570:VAL:HG22	1:E:1585:LYS:HG2	1.88	0.55
1:E:365:VAL:HG22	1:E:392:ALA:H	1.70	0.55
1:B:1676:ARG:HD2	1:B:1946:GLY:HA3	1.89	0.55
1:D:1399:VAL:HA	1:D:1498:GLN:O	2.07	0.55
1:E:11:ILE:HG22	1:E:20:MET:HE3	1.87	0.55
1:C:1679:LYS:HD3	1:C:1692:ILE:HD12	1.88	0.55
1:D:2437:ALA:HB3	1:D:2456:LEU:HB2	1.87	0.55
1:A:1399:VAL:HG12	1:A:1499:SER:HA	1.88	0.55
1:C:718:ASP:OD1	1:C:721:ARG:NH2	2.40	0.55
1:D:1769:ASN:HB2	1:E:1547:THR:HG21	1.89	0.55
1:C:2075:GLU:OE2	1:D:2246:HIS:NE2	2.35	0.55
1:D:2419:LYS:HG2	1:E:2466:PHE:CZ	2.42	0.55
1:A:1944:ARG:HG2	1:A:1944:ARG:HH11	1.72	0.55
1:B:1790:TYR:HH	1:B:1864:TYR:HH	1.55	0.55
1:A:1676:ARG:HD2	1:A:1946:GLY:HA3	1.89	0.54
1:C:1399:VAL:HG12	1:C:1499:SER:HA	1.87	0.54
1:B:347:PHE:CD1	1:B:360:ARG:HG3	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1645:GLU:OE1	1:B:1645:GLU:N	2.27	0.54
1:C:347:PHE:CD1	1:C:360:ARG:HG3	2.42	0.54
1:E:851:MET:HG2	1:E:877:ILE:HD13	1.89	0.54
1:A:732:PRO:HB3	1:A:763:VAL:HG21	1.89	0.54
1:A:1117:LEU:HD11	1:C:2143:VAL:HG23	1.87	0.54
1:B:2382:SER:O	1:B:2398:ARG:NH2	2.41	0.54
1:D:2423:VAL:HG13	1:D:2456:LEU:HD11	1.89	0.54
1:E:1679:LYS:HD3	1:E:1692:ILE:HD12	1.90	0.54
1:B:1726:MET:HE2	1:B:1760:HIS:HB3	1.87	0.54
1:B:2408:TYR:HB2	1:B:2416:ARG:HH12	1.72	0.54
1:D:724:LEU:HD22	1:D:737:ILE:HD11	1.89	0.54
1:B:961:LEU:HB2	1:B:966:ASP:HB3	1.90	0.54
1:A:2501:LYS:NZ	1:A:2505:GLU:OE2	2.39	0.54
1:B:732:PRO:HB3	1:B:763:VAL:HG21	1.89	0.54
1:B:1370:ILE:HA	1:B:1374:GLN:HG3	1.90	0.54
1:C:750:ASN:HB3	1:C:754:THR:HG22	1.88	0.54
1:E:300:LEU:HG	1:E:317:THR:HG23	1.90	0.54
1:A:1667:TYR:HB2	1:A:1698:LEU:HB3	1.89	0.54
1:B:192:ARG:NH1	1:B:245:GLU:OE2	2.40	0.54
1:C:1941:MET:SD	1:C:1944:ARG:NH2	2.80	0.54
1:C:2006:LYS:HE2	1:C:2006:LYS:HA	1.90	0.54
1:C:732:PRO:HB3	1:C:763:VAL:HG21	1.90	0.53
1:D:126:ALA:HB2	1:D:997:ILE:HD11	1.89	0.53
1:C:1676:ARG:HD2	1:C:1946:GLY:HA3	1.89	0.53
1:E:2263:LEU:O	1:E:2267:MET:HG3	2.09	0.53
1:A:1134:GLU:OE2	1:A:1134:GLU:N	2.41	0.53
1:D:91:SER:HB3	1:D:1942:LEU:HD11	1.90	0.53
1:C:2294:ARG:NH2	1:C:2303:THR:OG1	2.41	0.53
1:D:732:PRO:HB3	1:D:763:VAL:HG21	1.90	0.53
1:D:1636:THR:HG22	1:D:1637:GLY:H	1.71	0.53
1:E:1697:GLN:NE2	1:E:1945:GLY:O	2.42	0.53
1:A:1334:GLU:OE2	1:A:1362:ARG:NH2	2.42	0.53
1:B:347:PHE:HD1	1:B:360:ARG:HG3	1.73	0.53
1:B:2075:GLU:OE2	1:C:2246:HIS:NE2	2.36	0.53
1:D:1443:VAL:HG23	1:D:1445:ASN:H	1.73	0.53
1:B:2419:LYS:HG2	1:C:2466:PHE:CZ	2.43	0.53
1:D:198:PRO:HG3	1:D:245:GLU:HB3	1.91	0.53
1:C:2046:LEU:HD22	1:C:2282:THR:HG21	1.90	0.53
1:B:15:ARG:O	1:B:15:ARG:HG2	2.09	0.53
1:B:373:LEU:HB2	1:B:416:TYR:HB3	1.90	0.53
1:A:306:ASP:OD1	1:A:307:SER:OG	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2046:LEU:HD22	1:A:2282:THR:HG21	1.91	0.53
1:E:538:GLU:HG2	1:E:591:VAL:HG23	1.90	0.53
1:B:210:ILE:HD11	1:B:893:LEU:HD21	1.90	0.52
1:E:538:GLU:O	1:E:540:ASP:N	2.38	0.52
1:B:1367:GLY:HA2	1:B:1371:ARG:HH22	1.73	0.52
1:D:1321:MET:HA	1:D:1321:MET:HE3	1.90	0.52
1:E:1676:ARG:HD2	1:E:1946:GLY:HA3	1.90	0.52
1:A:2130:LEU:HD11	1:E:1061:GLU:OE1	2.09	0.52
1:B:1331:THR:HG21	1:B:1581:LEU:HG	1.90	0.52
1:C:1374:GLN:O	1:C:1378:MET:HG3	2.09	0.52
1:D:1334:GLU:OE2	1:D:1362:ARG:NH2	2.42	0.52
1:E:1399:VAL:HA	1:E:1498:GLN:O	2.10	0.52
1:A:1443:VAL:HG23	1:A:1445:ASN:H	1.74	0.52
1:A:1632:SER:N	1:B:1164:GLU:OE1	2.42	0.52
1:A:2281:LEU:HD11	1:E:2329:GLU:HG2	1.91	0.52
1:B:535:LYS:HE2	1:B:535:LYS:HA	1.92	0.52
1:A:305:SER:OG	1:A:306:ASP:N	2.41	0.52
1:A:1331:THR:HG21	1:A:1581:LEU:HG	1.92	0.52
1:C:961:LEU:HB2	1:C:966:ASP:HB3	1.92	0.52
1:D:1134:GLU:OE1	1:D:1134:GLU:N	2.38	0.52
1:E:775:ARG:HH12	1:E:2253:LEU:HD12	1.73	0.52
1:A:2466:PHE:CZ	1:E:2419:LYS:HG2	2.44	0.52
1:C:15:ARG:O	1:C:15:ARG:HG2	2.09	0.52
1:D:15:ARG:O	1:D:15:ARG:HG2	2.09	0.52
1:D:358:PHE:HD2	1:D:401:LEU:HD11	1.75	0.52
1:B:1443:VAL:HG23	1:B:1445:ASN:H	1.74	0.52
1:B:1483:VAL:HG13	1:B:1493:ILE:HG23	1.92	0.52
1:B:554:THR:HG22	1:B:556:ALA:H	1.75	0.52
1:C:538:GLU:O	1:C:540:ASP:N	2.41	0.52
1:D:961:LEU:HB2	1:D:966:ASP:HB3	1.91	0.52
1:A:15:ARG:O	1:A:15:ARG:HG2	2.09	0.52
1:C:1656:GLU:OE2	1:C:1744:ARG:NH2	2.41	0.52
1:C:2201:ARG:HD3	1:C:2205:TRP:CH2	2.45	0.52
1:E:732:PRO:HB3	1:E:763:VAL:HG21	1.92	0.52
1:E:2501:LYS:NZ	1:E:2505:GLU:OE2	2.41	0.52
1:A:708:ILE:HD12	1:A:764:MET:HE1	1.91	0.52
1:A:2467:MET:HE1	1:E:2470:PHE:HB2	1.92	0.52
1:C:554:THR:HG22	1:C:556:ALA:H	1.75	0.52
1:D:2470:PHE:HB2	1:E:2467:MET:HE1	1.92	0.51
1:E:126:ALA:HB2	1:E:997:ILE:HD11	1.91	0.51
1:E:210:ILE:HD11	1:E:893:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:ARG:HH11	1:E:83:ILE:HG13	1.75	0.51
1:A:2497:THR:N	1:A:2498:ASP:HB2	2.20	0.51
1:B:1399:VAL:HA	1:B:1498:GLN:O	2.11	0.51
1:C:2133:ALA:O	1:C:2137:GLN:HG3	2.10	0.51
1:D:155:MET:HG3	1:D:986:LEU:HD12	1.91	0.51
1:D:200:HIS:HB3	1:D:203:TYR:HB3	1.92	0.51
1:B:630:SER:O	1:B:630:SER:OG	2.28	0.51
1:A:851:MET:HG2	1:A:877:ILE:HD13	1.92	0.51
1:A:1517:THR:HG23	1:A:1570:VAL:HB	1.92	0.51
1:A:2263:LEU:O	1:A:2267:MET:HG3	2.10	0.51
1:B:80:ARG:HH11	1:B:83:ILE:HG21	1.76	0.51
1:B:2113:GLN:OE1	1:B:2209:ARG:NH1	2.39	0.51
1:C:2501:LYS:NZ	1:C:2505:GLU:OE2	2.39	0.51
1:D:26:GLN:N	1:D:27:TYR:HB3	2.25	0.51
1:A:1380:LEU:HD11	1:A:1463:ASN:HB3	1.93	0.51
1:D:1380:LEU:HD11	1:D:1463:ASN:HB3	1.93	0.51
1:D:1399:VAL:HG12	1:D:1499:SER:HA	1.92	0.51
1:E:15:ARG:O	1:E:15:ARG:HG2	2.08	0.51
1:E:1367:GLY:HA2	1:E:1371:ARG:HH22	1.76	0.51
1:A:26:GLN:N	1:A:27:TYR:HB3	2.26	0.51
1:A:1613:MET:HG2	1:A:1620:ILE:HB	1.93	0.51
1:B:1315:VAL:HG12	1:B:1590:VAL:HG22	1.91	0.51
1:D:697:ARG:NH1	1:D:728:ASP:OD2	2.43	0.51
1:E:26:GLN:N	1:E:27:TYR:HB3	2.24	0.51
1:A:360:ARG:HH22	1:A:419:ARG:HD2	1.76	0.51
1:A:885:THR:HG22	1:A:886:MET:H	1.74	0.51
1:B:126:ALA:HB2	1:B:997:ILE:HD11	1.92	0.51
1:C:404:ILE:HD13	1:C:414:LYS:HD2	1.91	0.51
1:E:1519:MET:SD	1:E:1524:THR:OG1	2.60	0.51
1:E:2382:SER:O	1:E:2398:ARG:NH2	2.44	0.51
1:C:1697:GLN:NE2	1:C:1945:GLY:O	2.44	0.51
1:E:1443:VAL:HG23	1:E:1445:ASN:H	1.76	0.51
1:B:1656:GLU:OE2	1:B:1744:ARG:NH2	2.43	0.51
1:D:2201:ARG:HD3	1:D:2205:TRP:CH2	2.46	0.51
1:A:346:TYR:HE1	1:A:359:ILE:HG22	1.77	0.50
1:C:1483:VAL:HG13	1:C:1493:ILE:HG23	1.93	0.50
1:D:2419:LYS:HG2	1:E:2466:PHE:HZ	1.76	0.50
1:E:401:LEU:HD13	1:E:414:LYS:HZ1	1.75	0.50
1:A:358:PHE:HB2	1:A:398:SER:HB3	1.92	0.50
1:A:2173:ALA:O	1:A:2177:VAL:HG13	2.12	0.50
1:B:209:VAL:HG22	1:B:926:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1331:THR:HG21	1:D:1581:LEU:HG	1.93	0.50
1:A:2252:GLU:HG2	1:E:2010:THR:HG21	1.93	0.50
1:A:221:SER:OG	1:A:495:ARG:NH2	2.45	0.50
1:A:1385:GLY:HA2	1:A:1386:LYS:HZ3	1.75	0.50
1:D:830:MET:HG3	1:E:671:ASN:HD22	1.77	0.50
1:E:1057:ASP:O	1:E:1061:GLU:HG3	2.12	0.50
1:D:2343:GLU:OE2	1:E:2466:PHE:HE2	1.94	0.50
1:C:1167:HIS:HD2	1:C:1194:LEU:HD11	1.76	0.50
1:A:532:LEU:HD11	1:A:562:ARG:HD3	1.94	0.50
1:B:2441:TYR:CZ	1:B:2443:GLY:HA3	2.47	0.50
1:C:405:SER:N	1:C:408:GLU:OE2	2.42	0.50
1:D:209:VAL:HG22	1:D:926:LEU:HD11	1.94	0.50
1:A:2031:ARG:NH2	1:A:2479:GLU:OE2	2.45	0.50
1:B:26:GLN:N	1:B:27:TYR:HB3	2.25	0.50
1:D:2173:ALA:O	1:D:2177:VAL:HG13	2.12	0.50
1:E:1321:MET:HE3	1:E:1584:ILE:HG22	1.93	0.50
1:A:2058:GLU:OE2	1:B:2264:TYR:OH	2.30	0.50
1:D:1886:GLU:OE1	1:D:1886:GLU:HA	2.12	0.50
1:E:1319:LEU:HD22	1:E:1588:LEU:HD13	1.93	0.50
1:E:1331:THR:HG21	1:E:1581:LEU:HG	1.93	0.50
1:A:1570:VAL:HG22	1:A:1585:LYS:HG2	1.92	0.49
1:B:775:ARG:HH12	1:B:2253:LEU:HD12	1.77	0.49
1:B:1134:GLU:H	1:B:1134:GLU:CD	2.19	0.49
1:B:1100:VAL:HB	1:B:1593:VAL:HG22	1.94	0.49
1:C:91:SER:HB3	1:C:1942:LEU:HD11	1.94	0.49
1:C:2408:TYR:HB2	1:C:2416:ARG:HH12	1.76	0.49
1:D:252:GLU:O	1:D:450:LYS:NZ	2.41	0.49
1:A:1367:GLY:HA2	1:A:1371:ARG:HH22	1.76	0.49
1:B:404:ILE:HD13	1:B:414:LYS:HD2	1.94	0.49
1:B:2503:LEU:HD23	1:B:2504:LEU:HD23	1.94	0.49
1:D:1483:VAL:HG13	1:D:1493:ILE:HG23	1.95	0.49
1:E:2173:ALA:O	1:E:2177:VAL:HG13	2.12	0.49
1:A:537:PHE:CE2	1:A:539:ALA:HB3	2.47	0.49
1:B:1316:PRO:HG2	1:B:1588:LEU:HD11	1.93	0.49
1:C:209:VAL:HG22	1:C:926:LEU:HD11	1.93	0.49
1:D:324:GLU:HG3	1:D:326:LYS:HG2	1.95	0.49
1:D:420:TYR:CD1	1:D:426:ALA:HB2	2.48	0.49
1:D:1458:PRO:HD2	1:D:1461:ILE:HG21	1.94	0.49
1:D:1570:VAL:HG22	1:D:1585:LYS:HG2	1.94	0.49
1:D:1167:HIS:HD2	1:D:1194:LEU:HD11	1.77	0.49
1:A:420:TYR:CD1	1:A:426:ALA:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2318:MET:HE1	1:B:2271:LEU:HB2	1.94	0.49
1:B:367:ARG:HD2	1:B:367:ARG:O	2.13	0.49
1:B:1911:GLU:OE1	1:B:1911:GLU:N	2.46	0.49
1:D:1426:GLN:HB3	1:D:1462:LEU:HD22	1.94	0.49
1:E:2046:LEU:HD22	1:E:2282:THR:HG21	1.93	0.49
1:C:2441:TYR:CZ	1:C:2443:GLY:HA3	2.47	0.49
1:D:554:THR:HG22	1:D:556:ALA:H	1.77	0.49
1:A:551:GLU:O	1:A:552:GLN:HG3	2.12	0.49
1:C:221:SER:OG	1:C:495:ARG:NH2	2.45	0.49
1:C:324:GLU:HG3	1:C:326:LYS:HG2	1.95	0.49
1:C:1570:VAL:HG22	1:C:1585:LYS:HG2	1.94	0.49
1:E:2294:ARG:NH2	1:E:2303:THR:OG1	2.46	0.49
1:B:1807:GLU:N	1:B:1807:GLU:OE1	2.45	0.49
1:C:26:GLN:N	1:C:27:TYR:HB3	2.27	0.49
1:B:1300:ASP:OD2	1:B:1604:ARG:NH2	2.38	0.48
1:D:551:GLU:O	1:D:552:GLN:HG3	2.12	0.48
1:E:899:VAL:HG12	1:E:899:VAL:O	2.13	0.48
1:A:538:GLU:O	1:A:540:ASP:N	2.39	0.48
1:A:2264:TYR:OH	1:E:2058:GLU:OE2	2.29	0.48
1:B:2173:ALA:O	1:B:2177:VAL:HG13	2.12	0.48
1:C:420:TYR:CD1	1:C:426:ALA:HB2	2.49	0.48
1:D:373:LEU:HB2	1:D:416:TYR:HB3	1.95	0.48
1:A:321:VAL:HG22	1:A:323:ASN:H	1.78	0.48
1:B:2204:GLU:OE1	1:B:2204:GLU:HA	2.14	0.48
1:C:724:LEU:HD22	1:C:737:ILE:HD11	1.95	0.48
1:C:1443:VAL:HG23	1:C:1445:ASN:H	1.77	0.48
1:C:2372:LEU:HD11	1:C:2504:LEU:HB3	1.95	0.48
1:C:2419:LYS:HG2	1:D:2466:PHE:CE1	2.48	0.48
1:E:306:ASP:OD1	1:E:307:SER:OG	2.26	0.48
1:E:324:GLU:HG3	1:E:326:LYS:HG2	1.95	0.48
1:E:2441:TYR:CZ	1:E:2443:GLY:HA3	2.48	0.48
1:A:1316:PRO:HG2	1:A:1588:LEU:HD11	1.95	0.48
1:C:70:ARG:NH1	1:C:1860:ASP:OD2	2.43	0.48
1:C:2173:ALA:O	1:C:2177:VAL:HG13	2.13	0.48
1:C:2329:GLU:HG2	1:D:2281:LEU:HD11	1.94	0.48
1:C:2409:PRO:HG2	1:C:2412:LEU:HD13	1.96	0.48
1:D:1676:ARG:HD2	1:D:1946:GLY:HA3	1.95	0.48
1:D:347:PHE:CD1	1:D:360:ARG:HG3	2.48	0.48
1:A:1219:THR:HG21	1:A:1223:PRO:HA	1.95	0.48
1:A:1483:VAL:HG13	1:A:1493:ILE:HG23	1.96	0.48
1:B:1358:ALA:HB2	1:B:1547:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ARG:NH1	1:C:367:ARG:HA	2.28	0.48
1:C:551:GLU:O	1:C:552:GLN:HG3	2.13	0.48
1:D:386:LEU:HG	1:D:398:SER:HB2	1.96	0.48
1:E:310:ALA:HB1	1:E:315:ILE:HD13	1.95	0.48
1:B:899:VAL:HG12	1:B:899:VAL:O	2.14	0.48
1:D:532:LEU:HD11	1:D:562:ARG:HD3	1.96	0.48
1:D:1354:LEU:O	1:D:1550:PRO:HA	2.14	0.48
1:D:2441:TYR:CZ	1:D:2443:GLY:HA3	2.48	0.48
1:E:551:GLU:O	1:E:552:GLN:HG3	2.13	0.48
1:A:404:ILE:HG21	1:A:414:LYS:HZ3	1.79	0.48
1:A:692:ALA:HA	1:A:741:MET:HE3	1.94	0.48
1:B:170:LEU:HD13	1:B:946:LEU:HD11	1.96	0.48
1:B:551:GLU:O	1:B:552:GLN:HG3	2.13	0.48
1:D:1300:ASP:OD2	1:D:1604:ARG:NH2	2.39	0.48
1:A:2068:LEU:HD22	1:B:2253:LEU:HD13	1.95	0.48
1:A:2201:ARG:HD3	1:A:2205:TRP:CH2	2.49	0.48
1:C:2058:GLU:OE2	1:D:2264:TYR:OH	2.29	0.48
1:D:1941:MET:HE2	1:D:1941:MET:HA	1.95	0.48
1:A:324:GLU:HG3	1:A:326:LYS:HG2	1.94	0.48
1:C:1890:ASP:OD1	1:C:1890:ASP:N	2.47	0.48
1:C:899:VAL:O	1:C:899:VAL:HG12	2.14	0.47
1:C:1134:GLU:N	1:C:1134:GLU:OE2	2.47	0.47
1:C:1219:THR:HG21	1:C:1223:PRO:HA	1.96	0.47
1:D:680:LEU:HD22	1:D:744:VAL:HG22	1.96	0.47
1:D:1050:ILE:H	1:D:1050:ILE:HD12	1.79	0.47
1:E:977:VAL:HB	1:E:981:ILE:HD11	1.95	0.47
1:E:1219:THR:HG21	1:E:1223:PRO:HA	1.96	0.47
1:D:307:SER:O	1:D:309:SER:N	2.47	0.47
1:E:321:VAL:HG22	1:E:323:ASN:H	1.79	0.47
1:E:1315:VAL:HG12	1:E:1590:VAL:HG22	1.95	0.47
1:A:554:THR:HG22	1:A:556:ALA:H	1.79	0.47
1:A:961:LEU:HB2	1:A:966:ASP:HB3	1.95	0.47
1:A:1672:HIS:O	1:A:1730:LYS:HG2	2.14	0.47
1:A:2497:THR:H	1:A:2498:ASP:CB	2.24	0.47
1:B:272:THR:OG1	1:B:274:GLU:OE1	2.33	0.47
1:B:1167:HIS:HD2	1:B:1194:LEU:HD11	1.79	0.47
1:C:2248:GLN:O	1:C:2248:GLN:NE2	2.47	0.47
1:D:2058:GLU:OE2	1:E:2264:TYR:OH	2.30	0.47
1:E:14:THR:C	1:E:16:ASP:H	2.23	0.47
1:E:630:SER:O	1:E:630:SER:OG	2.28	0.47
1:E:1911:GLU:N	1:E:1911:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2437:ALA:HB3	1:E:2456:LEU:HB2	1.95	0.47
1:A:346:TYR:OH	1:A:395:ASN:OD1	2.32	0.47
1:A:1911:GLU:N	1:A:1911:GLU:OE1	2.47	0.47
1:A:2491:LEU:HD23	1:A:2510:ILE:HD13	1.97	0.47
1:C:2423:VAL:HG13	1:C:2456:LEU:HD11	1.97	0.47
1:D:2409:PRO:HG2	1:D:2412:LEU:HD13	1.96	0.47
1:A:1458:PRO:HD2	1:A:1461:ILE:HG21	1.97	0.47
1:A:1656:GLU:OE2	1:A:1744:ARG:NH2	2.46	0.47
1:C:776:LEU:HD12	1:C:776:LEU:HA	1.79	0.47
1:D:1807:GLU:OE1	1:D:1807:GLU:N	2.45	0.47
1:E:181:SER:O	1:E:185:MET:HG2	2.15	0.47
1:A:349:LEU:HD11	1:A:356:GLN:HB3	1.95	0.47
1:A:414:LYS:HB2	1:A:434:PHE:CD2	2.49	0.47
1:A:724:LEU:HD22	1:A:737:ILE:HD11	1.96	0.47
1:A:1148:THR:O	1:A:1148:THR:OG1	2.30	0.47
1:B:2006:LYS:HD3	1:B:2007:ALA:N	2.29	0.47
1:B:2143:VAL:HG23	1:E:1117:LEU:HD11	1.96	0.47
1:C:358:PHE:HB2	1:C:398:SER:HB3	1.97	0.47
1:C:1367:GLY:HA2	1:C:1371:ARG:HH22	1.80	0.47
1:D:210:ILE:HD11	1:D:893:LEU:HD21	1.96	0.47
1:D:504:GLN:HA	1:D:507:ASN:HD22	1.79	0.47
1:D:2278:PHE:O	1:D:2282:THR:HG23	2.15	0.47
1:E:198:PRO:HG3	1:E:245:GLU:HB3	1.96	0.47
1:E:307:SER:O	1:E:309:SER:N	2.48	0.47
1:E:1364:ASP:OD1	1:E:1365:GLY:N	2.48	0.47
1:E:1757:ILE:H	1:E:1757:ILE:HD12	1.79	0.47
1:A:899:VAL:HG12	1:A:899:VAL:O	2.14	0.47
1:C:2497:THR:H	1:C:2498:ASP:CB	2.24	0.47
1:E:820:LEU:HD12	1:E:820:LEU:HA	1.77	0.47
1:A:164:LEU:HD13	1:A:988:GLU:HG2	1.95	0.47
1:B:1908:ASP:OD1	1:B:1908:ASP:N	2.38	0.47
1:E:856:MET:HB3	1:E:856:MET:HE3	1.74	0.47
1:A:126:ALA:HB2	1:A:997:ILE:HD11	1.96	0.47
1:B:324:GLU:HG3	1:B:326:LYS:HG2	1.96	0.47
1:B:358:PHE:HB2	1:B:398:SER:HB3	1.96	0.47
1:B:1219:THR:HG21	1:B:1223:PRO:HA	1.97	0.47
1:B:1570:VAL:HG22	1:B:1585:LYS:HG2	1.95	0.47
1:B:1672:HIS:O	1:B:1730:LYS:HG2	2.15	0.47
1:C:566:VAL:HB	1:C:570:GLU:HB2	1.97	0.47
1:D:2501:LYS:NZ	1:D:2505:GLU:OE2	2.44	0.47
1:D:380:SER:O	1:D:403:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:ILE:HD13	1:D:414:LYS:HD2	1.97	0.46
1:D:1130:MET:HE1	1:D:1620:ILE:HD11	1.97	0.46
1:E:209:VAL:HG22	1:E:926:LEU:HD11	1.97	0.46
1:E:368:GLU:N	1:E:368:GLU:OE1	2.48	0.46
1:B:1368:ASN:OD1	1:B:1368:ASN:N	2.48	0.46
1:B:1374:GLN:O	1:B:1378:MET:HG2	2.14	0.46
1:C:1955:ASN:C	1:C:1955:ASN:OD1	2.59	0.46
1:D:364:LYS:NZ	1:D:366:SER:OG	2.31	0.46
1:D:899:VAL:HG12	1:D:899:VAL:O	2.15	0.46
1:E:1483:VAL:HG13	1:E:1493:ILE:HG23	1.97	0.46
1:E:1699:THR:OG1	1:E:1700:ASP:N	2.48	0.46
1:E:2409:PRO:HG2	1:E:2412:LEU:HD13	1.98	0.46
1:A:334:ARG:NH1	1:A:347:PHE:O	2.43	0.46
1:A:414:LYS:HB2	1:A:434:PHE:HD2	1.80	0.46
1:B:724:LEU:HD22	1:B:737:ILE:HD11	1.96	0.46
1:B:1050:ILE:HD12	1:B:1050:ILE:H	1.79	0.46
1:B:2409:PRO:HG2	1:B:2412:LEU:HD13	1.97	0.46
1:C:1437:ARG:HB3	1:C:1455:PRO:HA	1.97	0.46
1:A:775:ARG:HH12	1:A:2253:LEU:HD12	1.80	0.46
1:A:1730:LYS:HD2	1:A:1730:LYS:HA	1.72	0.46
1:B:2201:ARG:HD3	1:B:2205:TRP:CH2	2.51	0.46
1:C:247:TYR:CZ	1:C:898:TYR:HB3	2.50	0.46
1:C:604:ALA:HB2	1:C:614:LEU:HD22	1.96	0.46
1:C:1730:LYS:HA	1:C:1730:LYS:HD2	1.74	0.46
1:E:603:LEU:HD21	1:E:640:VAL:HG23	1.98	0.46
1:B:1157:ILE:HD11	1:B:1168:LEU:HD21	1.97	0.46
1:B:2112:TYR:CZ	1:B:2208:GLN:HG2	2.51	0.46
1:B:2376:LYS:HE2	1:B:2376:LYS:HB2	1.85	0.46
1:C:1911:GLU:OE1	1:C:1911:GLU:N	2.49	0.46
1:E:162:LEU:HD23	1:E:162:LEU:HA	1.83	0.46
1:E:2497:THR:H	1:E:2498:ASP:CB	2.25	0.46
1:E:192:ARG:HG2	1:E:249:ILE:HD11	1.97	0.46
1:E:1672:HIS:O	1:E:1730:LYS:HG2	2.16	0.46
1:E:2201:ARG:HD3	1:E:2205:TRP:CH2	2.50	0.46
1:A:1169:ILE:HD11	1:A:1192:LEU:HD11	1.97	0.46
1:A:1723:LYS:HD2	1:A:1741:HIS:CE1	2.51	0.46
1:B:1431:ASN:OD1	1:B:1434:TYR:N	2.47	0.46
1:C:80:ARG:HH11	1:C:83:ILE:HG13	1.81	0.46
1:C:373:LEU:HB2	1:C:416:TYR:HB3	1.97	0.46
1:D:557:ARG:O	1:D:561:MET:HG3	2.15	0.46
1:E:170:LEU:HD13	1:E:946:LEU:HD11	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:936:ASP:O	1:E:940:GLU:HG3	2.16	0.46
1:D:1219:THR:HG21	1:D:1223:PRO:HA	1.97	0.46
1:E:305:SER:OG	1:E:306:ASP:N	2.49	0.46
1:E:554:THR:HG22	1:E:556:ALA:H	1.80	0.46
1:A:504:GLN:HA	1:A:507:ASN:HD22	1.80	0.46
1:A:688:SER:OG	1:A:691:MET:HE3	2.16	0.46
1:A:1601:LEU:HA	1:A:1614:GLN:O	2.16	0.46
1:A:2077:ALA:O	1:A:2081:ILE:HG12	2.16	0.46
1:A:2382:SER:O	1:A:2398:ARG:NH2	2.48	0.46
1:A:2409:PRO:HG2	1:A:2412:LEU:HD13	1.97	0.46
1:B:1601:LEU:HA	1:B:1614:GLN:O	2.15	0.46
1:C:538:GLU:CD	1:C:591:VAL:HG23	2.41	0.46
1:C:2343:GLU:OE2	1:C:2345:THR:OG1	2.30	0.46
1:D:1081:LEU:HD23	1:D:1081:LEU:HA	1.83	0.46
1:D:1774:MET:HE3	1:D:1774:MET:HB3	1.84	0.46
1:E:1334:GLU:OE2	1:E:1362:ARG:NH2	2.49	0.46
1:B:2061:ASP:HB3	1:C:2257:LYS:HD3	1.98	0.46
1:C:532:LEU:HD11	1:C:562:ARG:HD3	1.98	0.46
1:C:1368:ASN:OD1	1:C:1368:ASN:N	2.49	0.46
1:D:346:TYR:OH	1:D:395:ASN:OD1	2.33	0.46
1:E:358:PHE:HB2	1:E:398:SER:HB3	1.97	0.46
1:A:1385:GLY:HA2	1:A:1386:LYS:NZ	2.31	0.45
1:B:70:ARG:NH1	1:B:1860:ASP:OD2	2.49	0.45
1:C:2031:ARG:NH2	1:C:2479:GLU:OE2	2.49	0.45
1:E:420:TYR:CD1	1:E:426:ALA:HB2	2.50	0.45
1:E:1167:HIS:HD2	1:E:1194:LEU:HD11	1.81	0.45
1:E:2006:LYS:HD3	1:E:2007:ALA:N	2.31	0.45
1:A:200:HIS:HB3	1:A:203:TYR:HB3	1.98	0.45
1:A:338:ASP:O	1:A:430:GLY:HA2	2.15	0.45
1:A:393:ASN:OD1	1:E:149:THR:OG1	2.30	0.45
1:A:2332:LYS:HD2	1:B:2281:LEU:HD22	1.98	0.45
1:B:420:TYR:CD1	1:B:426:ALA:HB2	2.50	0.45
1:B:776:LEU:HD12	1:B:776:LEU:HA	1.77	0.45
1:C:581:LEU:HA	1:C:581:LEU:HD23	1.81	0.45
1:C:1148:THR:O	1:C:1148:THR:OG1	2.32	0.45
1:D:221:SER:OG	1:D:495:ARG:NH2	2.49	0.45
1:E:1730:LYS:HA	1:E:1730:LYS:HD2	1.73	0.45
1:A:2201:ARG:HD3	1:A:2205:TRP:CZ2	2.51	0.45
1:A:2284:SER:O	1:A:2288:MET:HG2	2.15	0.45
1:B:15:ARG:NH2	1:B:16:ASP:HB2	2.31	0.45
1:B:1437:ARG:HB3	1:B:1455:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:ARG:NH2	1:C:403:ASN:O	2.49	0.45
1:C:504:GLN:HA	1:C:507:ASN:HD22	1.81	0.45
1:C:660:ILE:HD12	1:C:660:ILE:HA	1.80	0.45
1:C:2437:ALA:HB3	1:C:2456:LEU:HB2	1.97	0.45
1:E:10:LYS:HB3	1:E:10:LYS:HE3	1.86	0.45
1:A:272:THR:OG1	1:A:274:GLU:OE1	2.32	0.45
1:A:1164:GLU:OE1	1:E:1632:SER:N	2.49	0.45
1:B:91:SER:HB3	1:B:1942:LEU:HD11	1.99	0.45
1:B:1417:LYS:HB2	1:B:1417:LYS:HE2	1.71	0.45
1:B:1518:VAL:HG12	1:B:1569:ILE:HG12	1.98	0.45
1:B:1666:PRO:HB3	1:B:1700:ASP:C	2.42	0.45
1:D:775:ARG:HH12	1:D:2253:LEU:HD12	1.82	0.45
1:E:504:GLN:HA	1:E:507:ASN:ND2	2.32	0.45
1:A:566:VAL:HB	1:A:570:GLU:HB2	1.98	0.45
1:A:2281:LEU:HD22	1:E:2332:LYS:HD2	1.97	0.45
1:A:2496:ALA:HB1	1:A:2504:LEU:HD22	1.99	0.45
1:B:198:PRO:HG3	1:B:245:GLU:HB3	1.98	0.45
1:B:687:ILE:HD11	1:B:741:MET:SD	2.55	0.45
1:B:1117:LEU:HD11	1:D:2143:VAL:HG23	1.97	0.45
1:B:1399:VAL:HG12	1:B:1497:TYR:HD2	1.82	0.45
1:B:2058:GLU:OE2	1:C:2264:TYR:OH	2.32	0.45
1:B:2201:ARG:HD3	1:B:2205:TRP:CZ2	2.52	0.45
1:C:195:ILE:HG22	1:C:948:ASN:HD21	1.81	0.45
1:C:1316:PRO:HG2	1:C:1588:LEU:HD11	1.97	0.45
1:C:1632:SER:N	1:D:1164:GLU:OE2	2.49	0.45
1:B:747:GLU:H	1:B:747:GLU:CD	2.25	0.45
1:B:2270:LYS:HB3	1:B:2270:LYS:HE3	1.78	0.45
1:C:169:LEU:O	1:C:173:ILE:HG12	2.16	0.45
1:C:589:LEU:HD23	1:C:589:LEU:HA	1.83	0.45
1:C:936:ASP:O	1:C:940:GLU:HG3	2.17	0.45
1:C:1672:HIS:O	1:C:1730:LYS:HG2	2.16	0.45
1:D:80:ARG:HH11	1:D:83:ILE:HG13	1.81	0.45
1:D:347:PHE:CE2	1:D:415:ILE:HG12	2.52	0.45
1:D:1601:LEU:HA	1:D:1614:GLN:O	2.16	0.45
1:E:1380:LEU:HD11	1:E:1463:ASN:HB3	1.98	0.45
1:A:127:LYS:HB3	1:A:127:LYS:HE2	1.66	0.45
1:A:169:LEU:O	1:A:173:ILE:HG12	2.17	0.45
1:A:2006:LYS:HD3	1:A:2007:ALA:N	2.31	0.45
1:B:169:LEU:O	1:B:173:ILE:HG12	2.17	0.45
1:C:307:SER:O	1:C:309:SER:N	2.49	0.45
1:C:315:ILE:HG22	1:C:332:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1039:TYR:OH	1:C:1964:GLU:O	2.23	0.45
1:C:1197:LEU:HD11	1:C:1201:GLY:HA2	1.98	0.45
1:D:566:VAL:HB	1:D:570:GLU:HB2	1.98	0.45
1:E:70:ARG:NH1	1:E:1860:ASP:OD2	2.50	0.45
1:E:338:ASP:O	1:E:430:GLY:HA2	2.16	0.45
1:E:532:LEU:HD11	1:E:562:ARG:HD3	1.99	0.45
1:E:1368:ASN:OD1	1:E:1368:ASN:N	2.48	0.45
1:E:2372:LEU:HD11	1:E:2504:LEU:HB3	1.99	0.45
1:A:1439:ILE:HG13	1:A:1486:ASN:CB	2.47	0.45
1:A:1568:ASP:OD1	1:A:1568:ASP:N	2.50	0.45
1:A:2318:MET:SD	1:B:2267:MET:HG2	2.56	0.45
1:A:2497:THR:HB	1:A:2498:ASP:HB2	1.99	0.45
1:B:386:LEU:HG	1:B:398:SER:HB2	1.98	0.45
1:B:1049:ARG:HH21	1:B:1056:MET:HE2	1.82	0.45
1:C:301:GLN:HB3	1:C:317:THR:HG21	1.99	0.45
1:C:1439:ILE:HG13	1:C:1486:ASN:CB	2.47	0.45
1:D:2171:LEU:HD12	1:D:2171:LEU:H	1.82	0.45
1:D:2294:ARG:NH2	1:D:2303:THR:OG1	2.49	0.45
1:E:2447:MET:HE3	1:E:2447:MET:HA	1.99	0.45
1:E:2497:THR:HB	1:E:2498:ASP:HB2	1.99	0.45
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.78	0.45
1:A:80:ARG:HA	1:A:80:ARG:HD3	1.83	0.45
1:B:532:LEU:HD11	1:B:562:ARG:HD3	1.98	0.45
1:B:1632:SER:N	1:C:1164:GLU:OE1	2.49	0.45
1:C:321:VAL:HG22	1:C:323:ASN:H	1.81	0.45
1:C:338:ASP:O	1:C:430:GLY:HA2	2.16	0.45
1:C:2270:LYS:HE3	1:C:2270:LYS:HB3	1.77	0.45
1:D:1461:ILE:HG13	1:D:1462:LEU:N	2.31	0.45
1:D:1711:LEU:HD23	1:D:1711:LEU:HA	1.86	0.45
1:E:1439:ILE:HG13	1:E:1486:ASN:CB	2.47	0.45
1:A:76:SER:N	1:A:77:GLY:HA3	2.32	0.45
1:A:386:LEU:HG	1:A:398:SER:HB2	1.99	0.45
1:A:2160:LEU:HD13	1:E:2160:LEU:HD21	1.99	0.45
1:B:936:ASP:O	1:B:940:GLU:HG3	2.17	0.45
1:C:1601:LEU:HA	1:C:1614:GLN:O	2.17	0.45
1:D:1127:ILE:HD12	1:D:1127:ILE:HA	1.84	0.45
1:D:1744:ARG:HD2	1:D:1745:ASP:O	2.17	0.45
1:E:886:MET:HE3	1:E:886:MET:HB3	1.87	0.45
1:E:1862:MET:HE2	1:E:1862:MET:HB2	1.79	0.45
1:A:1148:THR:HG23	1:A:1150:VAL:HG13	1.99	0.44
1:B:2419:LYS:HG2	1:C:2466:PHE:HZ	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:936:ASP:O	1:D:940:GLU:HG3	2.17	0.44
1:D:1911:GLU:OE1	1:D:1911:GLU:N	2.48	0.44
1:E:1385:GLY:HA2	1:E:1386:LYS:NZ	2.32	0.44
1:E:2077:ALA:O	1:E:2081:ILE:HG12	2.18	0.44
1:A:630:SER:O	1:A:630:SER:OG	2.30	0.44
1:B:127:LYS:HB3	1:B:127:LYS:HE2	1.71	0.44
1:B:367:ARG:CZ	1:B:368:GLU:HG3	2.47	0.44
1:C:305:SER:OG	1:C:306:ASP:N	2.50	0.44
1:C:1624:THR:OG1	1:C:1784:TYR:OH	2.19	0.44
1:C:1807:GLU:OE1	1:C:1807:GLU:N	2.47	0.44
1:D:2503:LEU:HD23	1:D:2504:LEU:HD23	2.00	0.44
1:E:247:TYR:CZ	1:E:898:TYR:HB3	2.52	0.44
1:E:367:ARG:NH1	1:E:368:GLU:HG3	2.32	0.44
1:E:2270:LYS:HE3	1:E:2270:LYS:HB3	1.78	0.44
1:A:631:LEU:HD23	1:A:631:LEU:HA	1.86	0.44
1:A:301:GLN:HB3	1:A:317:THR:HG21	2.00	0.44
1:A:414:LYS:HE3	1:A:414:LYS:HA	1.99	0.44
1:A:581:LEU:HD23	1:A:581:LEU:HA	1.86	0.44
1:A:1739:GLY:O	1:A:1741:HIS:HD2	1.99	0.44
1:A:1744:ARG:HD2	1:A:1745:ASP:O	2.18	0.44
1:A:2441:TYR:CZ	1:A:2443:GLY:HA3	2.53	0.44
1:B:181:SER:O	1:B:185:MET:HG2	2.17	0.44
1:B:1697:GLN:NE2	1:B:1945:GLY:O	2.50	0.44
1:C:1365:GLY:HA3	1:C:1371:ARG:HB2	2.00	0.44
1:D:747:GLU:CD	1:D:747:GLU:H	2.25	0.44
1:D:1315:VAL:HG12	1:D:1590:VAL:HG22	1.99	0.44
1:D:1439:ILE:HG13	1:D:1486:ASN:CB	2.47	0.44
1:E:360:ARG:CZ	1:E:362:ASN:HD21	2.30	0.44
1:E:566:VAL:HB	1:E:570:GLU:HB2	1.99	0.44
1:E:1081:LEU:HD23	1:E:1081:LEU:HA	1.83	0.44
1:E:2317:LEU:O	1:E:2318:MET:HG2	2.17	0.44
1:A:1147:ASP:OD1	1:A:1147:ASP:N	2.49	0.44
1:A:1904:GLU:OE2	1:B:999:ARG:NH1	2.35	0.44
1:B:2174:SER:O	1:B:2177:VAL:HG22	2.18	0.44
1:D:951:LEU:HA	1:D:951:LEU:HD23	1.88	0.44
1:B:902:LEU:HB3	1:B:903:ASN:H	1.70	0.44
1:C:76:SER:N	1:C:77:GLY:HA3	2.33	0.44
1:C:210:ILE:HD11	1:C:893:LEU:HD21	1.99	0.44
1:C:753:GLU:OE1	1:C:753:GLU:N	2.46	0.44
1:C:1055:MET:HE2	1:C:1055:MET:HB3	1.77	0.44
1:C:1519:MET:HE3	1:C:1519:MET:HB3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:LEU:HG	1:D:382:ILE:HD13	2.00	0.44
1:D:1100:VAL:HB	1:D:1593:VAL:HG22	1.98	0.44
1:D:2010:THR:HG21	1:E:2252:GLU:HG2	1.99	0.44
1:E:76:SER:N	1:E:77:GLY:HA3	2.32	0.44
1:E:349:LEU:HD11	1:E:356:GLN:HB3	1.99	0.44
1:A:209:VAL:HG22	1:A:926:LEU:HD11	1.98	0.44
1:A:600:LEU:HD21	1:A:628:THR:HG21	1.99	0.44
1:A:1767:LEU:HB3	1:A:1770:TYR:HB2	2.00	0.44
1:A:2257:LYS:HD3	1:E:2061:ASP:HB3	2.00	0.44
1:B:504:GLN:HA	1:B:507:ASN:ND2	2.32	0.44
1:B:1730:LYS:HD2	1:B:1730:LYS:HA	1.74	0.44
1:C:15:ARG:NH2	1:C:16:ASP:HB2	2.33	0.44
1:C:360:ARG:NH2	1:C:362:ASN:OD1	2.50	0.44
1:C:367:ARG:HA	1:C:367:ARG:CZ	2.48	0.44
1:C:1167:HIS:CD2	1:C:1194:LEU:HD11	2.52	0.44
1:D:14:THR:C	1:D:16:ASP:H	2.26	0.44
1:D:338:ASP:O	1:D:430:GLY:HA2	2.18	0.44
1:D:401:LEU:HD12	1:D:401:LEU:H	1.82	0.44
1:E:1177:ALA:HB2	1:E:1186:THR:HG22	1.99	0.44
1:E:1639:ASP:OD2	1:E:1640:THR:N	2.51	0.44
1:A:170:LEU:HD13	1:A:946:LEU:HD11	2.00	0.44
1:A:747:GLU:CD	1:A:747:GLU:H	2.25	0.44
1:A:1518:VAL:HG12	1:A:1569:ILE:HG12	1.99	0.44
1:B:321:VAL:HG22	1:B:323:ASN:H	1.82	0.44
1:B:360:ARG:NH1	1:B:362:ASN:HD21	2.15	0.44
1:B:691:MET:HE2	1:B:691:MET:HB3	1.75	0.44
1:B:1177:ALA:HB2	1:B:1186:THR:HG22	2.00	0.44
1:B:1699:THR:HG22	1:B:1703:ILE:HD11	2.00	0.44
1:B:2501:LYS:NZ	1:B:2505:GLU:OE2	2.43	0.44
1:C:200:HIS:HB3	1:C:203:TYR:HB3	1.99	0.44
1:C:618:TYR:OH	1:C:626:LYS:O	2.28	0.44
1:E:538:GLU:OE2	1:E:590:SER:HA	2.18	0.44
1:A:14:THR:C	1:A:16:ASP:H	2.26	0.44
1:A:1039:TYR:OH	1:A:1964:GLU:O	2.31	0.44
1:A:1347:SER:OG	1:A:1348:ASP:N	2.50	0.44
1:C:1685:VAL:HG12	1:C:1686:VAL:HG23	1.99	0.44
1:C:2382:SER:O	1:C:2398:ARG:NH2	2.51	0.44
1:D:15:ARG:NH2	1:D:16:ASP:HB2	2.33	0.44
1:D:1672:HIS:O	1:D:1730:LYS:HG2	2.17	0.44
1:D:2115:LEU:HD23	1:D:2115:LEU:HA	1.85	0.44
1:E:80:ARG:HH11	1:E:83:ILE:HG21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:ARG:HA	1:E:80:ARG:HD3	1.86	0.44
1:E:1458:PRO:HD2	1:E:1461:ILE:HG21	2.00	0.44
1:E:1744:ARG:HD2	1:E:1745:ASP:O	2.18	0.44
1:A:15:ARG:NH2	1:A:16:ASP:HB2	2.33	0.43
1:A:840:ARG:HA	1:A:840:ARG:HD2	1.79	0.43
1:A:1980:LEU:HD23	1:A:1980:LEU:HA	1.85	0.43
1:B:145:LEU:HD23	1:B:145:LEU:HA	1.88	0.43
1:B:840:ARG:HD2	1:B:840:ARG:HA	1.81	0.43
1:C:14:THR:C	1:C:16:ASP:H	2.26	0.43
1:C:126:ALA:HB2	1:C:997:ILE:HD11	1.99	0.43
1:C:687:ILE:HD11	1:C:741:MET:HE2	2.00	0.43
1:C:1699:THR:OG1	1:C:1700:ASP:N	2.51	0.43
1:D:169:LEU:O	1:D:173:ILE:HG12	2.18	0.43
1:D:375:LYS:HE3	1:D:381:GLY:N	2.33	0.43
1:E:195:ILE:HG22	1:E:948:ASN:HD21	1.81	0.43
1:E:1518:VAL:HG12	1:E:1569:ILE:HG12	2.00	0.43
1:E:1905:LEU:HD23	1:E:1905:LEU:HA	1.85	0.43
1:E:2284:SER:O	1:E:2288:MET:HG2	2.18	0.43
1:A:297:LEU:O	1:A:316:SER:OG	2.31	0.43
1:B:307:SER:O	1:B:309:SER:N	2.51	0.43
1:B:1378:MET:HG2	1:B:1378:MET:H	1.67	0.43
1:C:1070:ARG:O	1:C:1074:GLU:HG2	2.18	0.43
1:D:1039:TYR:OH	1:D:1964:GLU:O	2.29	0.43
1:E:1477:LYS:O	1:E:1502:TRP:NE1	2.51	0.43
1:E:1527:PHE:CG	1:E:1551:LEU:HD23	2.53	0.43
1:A:1437:ARG:HB3	1:A:1455:PRO:HA	2.00	0.43
1:A:1598:GLU:OE1	1:A:1598:GLU:N	2.49	0.43
1:A:2419:LYS:HG2	1:B:2466:PHE:CZ	2.53	0.43
1:B:1439:ILE:HG13	1:B:1486:ASN:CB	2.48	0.43
1:B:1633:ARG:HD2	1:B:1640:THR:HG22	1.99	0.43
1:B:2069:LEU:HD23	1:B:2069:LEU:HA	1.87	0.43
1:D:305:SER:OG	1:D:306:ASP:N	2.49	0.43
1:E:1664:ILE:HG23	1:E:1726:MET:HE1	1.99	0.43
1:B:1127:ILE:HD12	1:B:1127:ILE:HA	1.86	0.43
1:C:14:THR:HG22	1:C:18:GLN:O	2.19	0.43
1:C:162:LEU:HA	1:C:162:LEU:HD23	1.80	0.43
1:C:747:GLU:CD	1:C:747:GLU:H	2.25	0.43
1:C:820:LEU:HD12	1:C:820:LEU:HA	1.76	0.43
1:C:840:ARG:HA	1:C:840:ARG:HD2	1.80	0.43
1:C:1347:SER:OG	1:C:1348:ASP:N	2.50	0.43
1:C:1666:PRO:HB3	1:C:1700:ASP:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1939:LEU:HD23	1:C:1939:LEU:HA	1.88	0.43
1:E:347:PHE:HD1	1:E:360:ARG:HG3	1.83	0.43
1:A:538:GLU:OE1	1:A:590:SER:HA	2.17	0.43
1:A:1358:ALA:HB2	1:A:1547:THR:HG23	2.01	0.43
1:B:1744:ARG:HD2	1:B:1745:ASP:O	2.18	0.43
1:C:730:LEU:HD23	1:C:730:LEU:HA	1.89	0.43
1:C:1117:LEU:HD11	1:E:2143:VAL:HG23	2.00	0.43
1:D:272:THR:OG1	1:D:274:GLU:OE1	2.36	0.43
1:D:1955:ASN:OD1	1:D:1955:ASN:C	2.61	0.43
1:D:2201:ARG:HD3	1:D:2205:TRP:CZ2	2.53	0.43
1:D:2501:LYS:HB3	1:D:2501:LYS:HE3	1.81	0.43
1:E:127:LYS:HB3	1:E:127:LYS:HE2	1.69	0.43
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.86	0.43
1:A:1601:LEU:HD12	1:A:1613:MET:CE	2.48	0.43
1:B:1169:ILE:HD11	1:B:1192:LEU:HD11	1.99	0.43
1:B:1385:GLY:HA2	1:B:1386:LYS:NZ	2.33	0.43
1:C:350:MET:HE3	1:C:350:MET:HB3	1.87	0.43
1:C:1265:MET:HE3	1:C:1273:PHE:CD2	2.54	0.43
1:C:1744:ARG:HD2	1:C:1745:ASP:O	2.19	0.43
1:C:2074:MET:HE1	1:C:2248:GLN:OE1	2.18	0.43
1:D:2332:LYS:HD2	1:E:2281:LEU:HD22	2.01	0.43
1:E:315:ILE:HG22	1:E:332:ILE:HB	2.00	0.43
1:E:2031:ARG:NH2	1:E:2479:GLU:OE2	2.52	0.43
1:A:111:SER:OG	1:A:1964:GLU:OE1	2.30	0.43
1:A:1177:ALA:HB2	1:A:1186:THR:HG22	2.01	0.43
1:A:1807:GLU:OE1	1:A:1807:GLU:N	2.49	0.43
1:B:76:SER:N	1:B:77:GLY:HA3	2.33	0.43
1:C:1100:VAL:HB	1:C:1593:VAL:HG22	2.01	0.43
1:C:1302:VAL:HG12	1:C:1604:ARG:HG2	2.01	0.43
1:C:2376:LYS:HE2	1:C:2376:LYS:HB2	1.85	0.43
1:C:2501:LYS:HE3	1:C:2501:LYS:HB3	1.80	0.43
1:D:80:ARG:HA	1:D:80:ARG:HD3	1.86	0.43
1:D:364:LYS:HZ3	1:D:366:SER:HG	1.57	0.43
1:D:1319:LEU:HD22	1:D:1588:LEU:HD13	2.01	0.43
1:D:1368:ASN:N	1:D:1368:ASN:OD1	2.49	0.43
1:D:1633:ARG:HB2	1:D:1641:ILE:HG12	2.00	0.43
1:D:2031:ARG:NH2	1:D:2479:GLU:OE2	2.52	0.43
1:E:346:TYR:OH	1:E:395:ASN:OD1	2.37	0.43
1:A:1055:MET:HG3	1:A:1080:TYR:CE1	2.53	0.43
1:A:1100:VAL:HB	1:A:1593:VAL:HG22	2.01	0.43
1:A:1302:VAL:HG12	1:A:1604:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1477:LYS:O	1:A:1502:TRP:NE1	2.51	0.43
1:A:1908:ASP:OD1	1:A:1908:ASP:N	2.42	0.43
1:B:338:ASP:O	1:B:430:GLY:HA2	2.19	0.43
1:B:1354:LEU:O	1:B:1550:PRO:HA	2.18	0.43
1:B:2350:LEU:HD12	1:B:2510:ILE:HD12	2.01	0.43
1:B:2497:THR:HB	1:B:2498:ASP:HB2	2.00	0.43
1:C:105:LYS:HG3	1:C:1912:ASP:HB2	2.01	0.43
1:C:364:LYS:NZ	1:C:366:SER:OG	2.37	0.43
1:C:1081:LEU:HD11	1:C:1641:ILE:HD13	2.00	0.43
1:D:1167:HIS:CD2	1:D:1194:LEU:HD11	2.53	0.43
1:D:1753:ASN:O	1:D:1756:SER:OG	2.29	0.43
1:E:1437:ARG:HB3	1:E:1455:PRO:HA	2.00	0.43
1:E:1711:LEU:HD23	1:E:1711:LEU:HA	1.85	0.43
1:A:211:MET:HE2	1:A:211:MET:HA	2.00	0.43
1:B:405:SER:N	1:B:408:GLU:OE2	2.47	0.43
1:B:1531:ASP:OD1	1:B:1531:ASP:N	2.51	0.43
1:B:2077:ALA:O	1:B:2081:ILE:HG12	2.19	0.43
1:C:2497:THR:HB	1:C:2498:ASP:HB2	2.01	0.43
1:D:76:SER:N	1:D:77:GLY:HA3	2.32	0.43
1:D:1527:PHE:CG	1:D:1551:LEU:HD23	2.53	0.43
1:D:1902:THR:HG22	1:D:1976:LEU:HD11	2.00	0.43
1:D:2061:ASP:HB3	1:E:2257:LYS:HD3	2.00	0.43
1:D:2112:TYR:CZ	1:D:2208:GLN:HG2	2.54	0.43
1:D:2408:TYR:HB2	1:D:2416:ARG:HH12	1.83	0.43
1:E:1167:HIS:CD2	1:E:1196:PHE:HB3	2.54	0.43
1:E:1354:LEU:O	1:E:1550:PRO:HA	2.19	0.43
1:A:680:LEU:HD22	1:A:744:VAL:HG22	2.00	0.43
1:A:1135:LEU:HD23	1:A:1135:LEU:HA	1.88	0.43
1:A:1374:GLN:O	1:A:1378:MET:HG2	2.19	0.43
1:A:1886:GLU:OE1	1:A:1886:GLU:HA	2.19	0.43
1:A:2143:VAL:HG23	1:D:1117:LEU:HD11	2.00	0.43
1:B:305:SER:OG	1:B:306:ASP:N	2.51	0.43
1:B:2390:ASN:OD1	1:B:2391:ARG:NH1	2.52	0.43
1:C:985:ARG:O	1:C:988:GLU:HG3	2.18	0.43
1:D:630:SER:O	1:D:630:SER:OG	2.31	0.43
1:E:1685:VAL:O	1:E:1687:ASP:N	2.52	0.43
1:A:637:PRO:O	1:A:640:VAL:HG12	2.19	0.42
1:A:2350:LEU:HD23	1:A:2350:LEU:HA	1.87	0.42
1:B:414:LYS:HE3	1:B:414:LYS:HB3	1.78	0.42
1:C:2077:ALA:O	1:C:2081:ILE:HG12	2.19	0.42
1:C:2287:LEU:HD23	1:C:2287:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:PHE:HB2	1:D:398:SER:HB3	2.01	0.42
1:D:1162:PHE:HB2	1:D:1241:LEU:HD13	2.01	0.42
1:D:1347:SER:OG	1:D:1348:ASP:N	2.49	0.42
1:D:1437:ARG:HB3	1:D:1455:PRO:HA	2.01	0.42
1:D:2342:LEU:O	1:D:2517:THR:HA	2.18	0.42
1:D:2382:SER:O	1:D:2398:ARG:NH2	2.50	0.42
1:E:374:ARG:HD2	1:E:375:LYS:HD3	2.01	0.42
1:E:1399:VAL:HG22	1:E:1497:TYR:HD2	1.84	0.42
1:E:1666:PRO:HB3	1:E:1700:ASP:C	2.44	0.42
1:E:2501:LYS:O	1:E:2505:GLU:HG3	2.19	0.42
1:A:1368:ASN:N	1:A:1368:ASN:OD1	2.49	0.42
1:A:1697:GLN:NE2	1:A:1945:GLY:O	2.52	0.42
1:B:345:ASN:ND2	1:B:362:ASN:O	2.52	0.42
1:B:2345:THR:HG23	1:B:2515:ARG:HG2	2.01	0.42
1:C:127:LYS:HB3	1:C:127:LYS:HE2	1.68	0.42
1:C:745:LEU:HA	1:C:745:LEU:HD23	1.78	0.42
1:C:1055:MET:HG3	1:C:1080:TYR:CE1	2.54	0.42
1:C:1056:MET:HE2	1:C:1056:MET:HB3	1.76	0.42
1:C:1169:ILE:HD11	1:C:1192:LEU:HD11	2.01	0.42
1:D:1177:ALA:HB2	1:D:1186:THR:HG22	2.01	0.42
1:D:1385:GLY:HA2	1:D:1386:LYS:NZ	2.34	0.42
1:D:1699:THR:OG1	1:D:1700:ASP:N	2.52	0.42
1:E:602:LEU:HD23	1:E:602:LEU:HA	1.85	0.42
1:E:1807:GLU:OE1	1:E:1807:GLU:N	2.48	0.42
1:A:247:TYR:CZ	1:A:898:TYR:HB3	2.54	0.42
1:A:2501:LYS:O	1:A:2505:GLU:HG3	2.20	0.42
1:B:247:TYR:CZ	1:B:898:TYR:HB3	2.55	0.42
1:C:80:ARG:HH11	1:C:83:ILE:HG21	1.84	0.42
1:D:14:THR:HG22	1:D:18:GLN:O	2.18	0.42
1:D:538:GLU:O	1:D:540:ASP:N	2.46	0.42
1:E:581:LEU:HD23	1:E:581:LEU:HA	1.88	0.42
1:B:195:ILE:HG22	1:B:948:ASN:HD21	1.83	0.42
1:C:145:LEU:HD23	1:C:145:LEU:HA	1.84	0.42
1:C:198:PRO:HG3	1:C:245:GLU:HB3	2.01	0.42
1:C:1527:PHE:CG	1:C:1551:LEU:HD23	2.55	0.42
1:C:2318:MET:HE2	1:C:2318:MET:HB2	1.65	0.42
1:C:2496:ALA:HB1	1:C:2504:LEU:HD22	2.01	0.42
1:E:631:LEU:HD23	1:E:631:LEU:HA	1.90	0.42
1:E:747:GLU:H	1:E:747:GLU:CD	2.26	0.42
1:E:776:LEU:HD12	1:E:776:LEU:HA	1.79	0.42
1:E:1639:ASP:OD2	1:E:1639:ASP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1939:LEU:HD23	1:E:1939:LEU:HA	1.86	0.42
1:E:2043:VAL:HG11	1:E:2324:LEU:HG	2.01	0.42
1:B:566:VAL:HB	1:B:570:GLU:HB2	2.01	0.42
1:B:2031:ARG:NH2	1:B:2479:GLU:OE2	2.53	0.42
1:B:2263:LEU:O	1:B:2267:MET:HB2	2.19	0.42
1:B:2501:LYS:HE3	1:B:2501:LYS:HB3	1.82	0.42
1:C:1514:ILE:HG12	1:C:1573:THR:HG23	2.02	0.42
1:D:49:LEU:HA	1:D:49:LEU:HD12	1.79	0.42
1:D:1666:PRO:HB3	1:D:1700:ASP:C	2.45	0.42
1:E:1347:SER:OG	1:E:1348:ASP:N	2.49	0.42
1:E:1633:ARG:HD2	1:E:1640:THR:HG22	2.02	0.42
1:D:1944:ARG:O	1:D:1944:ARG:NH1	2.53	0.42
1:E:272:THR:OG1	1:E:274:GLU:OE1	2.34	0.42
1:E:589:LEU:HD23	1:E:589:LEU:HA	1.87	0.42
1:A:198:PRO:HG3	1:A:245:GLU:HB3	2.00	0.42
1:A:367:ARG:HA	1:A:367:ARG:NH1	2.35	0.42
1:B:2286:CYS:SG	1:B:2323:LEU:HD12	2.60	0.42
1:C:337:THR:HG22	1:C:432:GLY:HA2	2.02	0.42
1:C:2070:LEU:HD23	1:C:2070:LEU:HA	1.90	0.42
1:D:581:LEU:HD23	1:D:581:LEU:HA	1.81	0.42
1:D:724:LEU:HD23	1:D:724:LEU:HA	1.83	0.42
1:D:902:LEU:HB3	1:D:903:ASN:H	1.71	0.42
1:D:1265:MET:HE3	1:D:1273:PHE:CD2	2.54	0.42
1:E:337:THR:HG22	1:E:432:GLY:HA2	2.01	0.42
1:E:1265:MET:HE3	1:E:1273:PHE:CD2	2.54	0.42
1:E:2115:LEU:HD23	1:E:2115:LEU:HA	1.84	0.42
1:B:14:THR:C	1:B:16:ASP:H	2.28	0.42
1:B:301:GLN:HB3	1:B:317:THR:HG21	2.01	0.42
1:B:728:ASP:HB2	1:B:737:ILE:HG12	2.02	0.42
1:B:1081:LEU:HD11	1:B:1641:ILE:HD13	2.02	0.42
1:B:1347:SER:OG	1:B:1348:ASP:N	2.51	0.42
1:C:1665:PRO:HG3	1:C:1762:GLU:HB2	2.02	0.42
1:C:2501:LYS:O	1:C:2505:GLU:HG3	2.20	0.42
1:D:307:SER:C	1:D:309:SER:H	2.28	0.42
1:E:14:THR:HG22	1:E:18:GLN:O	2.20	0.42
1:E:49:LEU:HD12	1:E:49:LEU:HA	1.80	0.42
1:E:637:PRO:HA	1:E:640:VAL:HG12	2.02	0.42
1:E:2031:ARG:NH1	1:E:2472:ASP:O	2.50	0.42
1:E:2069:LEU:HD23	1:E:2069:LEU:HA	1.88	0.42
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.84	0.42
1:A:820:LEU:HD12	1:A:820:LEU:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:MET:HE3	1:A:1273:PHE:CD2	2.55	0.42
1:A:1378:MET:HG2	1:A:1378:MET:H	1.67	0.42
1:B:349:LEU:HD11	1:B:356:GLN:HB3	2.02	0.42
1:B:1980:LEU:HD23	1:B:1980:LEU:HA	1.84	0.42
1:C:180:ASP:OD1	1:C:181:SER:N	2.51	0.42
1:C:688:SER:OG	1:C:691:MET:HE3	2.19	0.42
1:C:1321:MET:HB3	1:C:1584:ILE:HG21	2.02	0.42
1:C:1331:THR:HG21	1:C:1581:LEU:HD11	2.01	0.42
1:D:1411:PRO:HA	1:D:1425:VAL:O	2.19	0.42
1:D:2204:GLU:OE2	1:D:2204:GLU:HA	2.20	0.42
1:E:317:THR:HG22	1:E:318:GLY:H	1.84	0.42
1:E:735:LEU:HD23	1:E:735:LEU:HA	1.85	0.42
1:E:1167:HIS:CD2	1:E:1194:LEU:HD11	2.55	0.42
1:E:2174:SER:O	1:E:2177:VAL:HG22	2.20	0.42
1:A:526:LEU:HD23	1:A:526:LEU:HA	1.92	0.42
1:A:999:ARG:NH1	1:E:1904:GLU:OE1	2.35	0.42
1:A:1281:LEU:HD12	1:A:1281:LEU:HA	1.86	0.42
1:A:1446:ASN:OD1	1:A:1449:ALA:N	2.53	0.42
1:A:2270:LYS:HE3	1:A:2270:LYS:HB3	1.78	0.42
1:B:1411:PRO:HA	1:B:1425:VAL:O	2.20	0.42
1:B:1519:MET:HE3	1:B:1519:MET:HB3	1.81	0.42
1:C:192:ARG:HG2	1:C:249:ILE:HD11	2.02	0.42
1:C:902:LEU:HD23	1:C:902:LEU:HA	1.94	0.42
1:C:1084:PHE:HE1	1:C:1783:TYR:HB3	1.85	0.42
1:D:306:ASP:OD1	1:D:306:ASP:C	2.63	0.42
1:E:373:LEU:HG	1:E:382:ILE:HD13	2.02	0.42
1:E:687:ILE:HD11	1:E:741:MET:SD	2.60	0.42
1:E:2325:LEU:O	1:E:2329:GLU:HG3	2.19	0.42
1:A:360:ARG:NH1	1:A:362:ASN:HD21	2.18	0.41
1:A:747:GLU:HG2	1:A:749:LEU:HG	2.01	0.41
1:A:2503:LEU:HD23	1:A:2504:LEU:HD12	2.02	0.41
1:C:680:LEU:HD22	1:C:744:VAL:HG22	2.01	0.41
1:C:1358:ALA:HB2	1:C:1547:THR:HG23	2.01	0.41
1:C:1598:GLU:OE1	1:C:1598:GLU:N	2.43	0.41
1:D:80:ARG:HH11	1:D:83:ILE:HG21	1.84	0.41
1:D:195:ILE:HG22	1:D:948:ASN:HD21	1.85	0.41
1:D:1699:THR:HG22	1:D:1703:ILE:HD11	2.02	0.41
1:E:373:LEU:HB2	1:E:416:TYR:HB3	2.02	0.41
1:E:1519:MET:HB2	1:E:1568:ASP:HB2	2.02	0.41
1:E:2132:ASP:C	1:E:2132:ASP:OD2	2.63	0.41
1:A:1370:ILE:HA	1:A:1374:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HD13	1:B:988:GLU:HG2	2.01	0.41
1:B:415:ILE:CG2	1:B:432:GLY:H	2.32	0.41
1:B:735:LEU:HD23	1:B:735:LEU:HA	1.86	0.41
1:B:1446:ASN:OD1	1:B:1449:ALA:N	2.53	0.41
1:C:1375:ILE:HA	1:C:1378:MET:HE3	2.01	0.41
1:C:1518:VAL:HG12	1:C:1569:ILE:HG12	2.01	0.41
1:D:301:GLN:HB3	1:D:317:THR:HG21	2.03	0.41
1:D:688:SER:OG	1:D:691:MET:HE3	2.20	0.41
1:E:561:MET:HE3	1:E:561:MET:HB3	1.86	0.41
1:E:1052:GLN:NE2	1:E:1057:ASP:OD1	2.49	0.41
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.88	0.41
1:A:714:LEU:HD23	1:A:714:LEU:HA	1.84	0.41
1:B:373:LEU:HG	1:B:382:ILE:HD13	2.02	0.41
1:B:1071:ASP:N	1:B:1071:ASP:OD1	2.52	0.41
1:B:1365:GLY:HA3	1:B:1371:ARG:HB2	2.02	0.41
1:B:1699:THR:OG1	1:B:1700:ASP:N	2.51	0.41
1:C:1160:VAL:HG12	1:C:1167:HIS:HB2	2.02	0.41
1:E:680:LEU:HD22	1:E:744:VAL:HG22	2.01	0.41
1:E:2318:MET:HB3	1:E:2318:MET:HE2	1.61	0.41
1:A:307:SER:O	1:A:309:SER:N	2.53	0.41
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.90	0.41
1:A:603:LEU:HD23	1:A:603:LEU:HA	1.83	0.41
1:A:1160:VAL:HG21	1:A:1241:LEU:HD11	2.02	0.41
1:A:1333:MET:HG2	1:A:1361:VAL:HG22	2.01	0.41
1:A:2174:SER:O	1:A:2177:VAL:HG22	2.21	0.41
1:B:456:LEU:HD23	1:B:456:LEU:HA	1.88	0.41
1:C:306:ASP:OD1	1:C:307:SER:OG	2.26	0.41
1:C:1162:PHE:HB2	1:C:1241:LEU:HD13	2.02	0.41
1:C:1531:ASP:OD1	1:C:1531:ASP:N	2.52	0.41
1:D:2501:LYS:O	1:D:2505:GLU:HG3	2.21	0.41
1:A:337:THR:HG22	1:A:432:GLY:HA2	2.01	0.41
1:A:538:GLU:HG3	1:A:591:VAL:HG22	2.02	0.41
1:A:730:LEU:HD23	1:A:730:LEU:HA	1.93	0.41
1:A:1315:VAL:HG12	1:A:1590:VAL:HG22	2.02	0.41
1:A:1630:LEU:HD23	1:A:1630:LEU:HA	1.87	0.41
1:A:1699:THR:OG1	1:A:1700:ASP:N	2.54	0.41
1:A:2069:LEU:HD23	1:A:2069:LEU:HA	1.86	0.41
1:A:2081:ILE:HD13	1:A:2240:GLN:HB3	2.03	0.41
1:A:2318:MET:HB3	1:A:2318:MET:HE2	1.73	0.41
1:C:297:LEU:O	1:C:316:SER:OG	2.29	0.41
1:C:456:LEU:HD23	1:C:456:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2468:LEU:HD12	1:C:2468:LEU:HA	1.89	0.41
1:D:840:ARG:HD2	1:D:840:ARG:HA	1.81	0.41
1:E:1739:GLY:O	1:E:1741:HIS:ND1	2.52	0.41
1:E:1908:ASP:OD1	1:E:1908:ASP:N	2.39	0.41
1:A:195:ILE:HG22	1:A:948:ASN:HD21	1.83	0.41
1:A:368:GLU:HB2	1:A:420:TYR:HB2	2.02	0.41
1:A:558:SER:HA	1:A:561:MET:HE2	2.03	0.41
1:A:1365:GLY:HA3	1:A:1371:ARG:HB2	2.03	0.41
1:A:1480:SER:OG	1:A:1481:TYR:N	2.54	0.41
1:A:1666:PRO:HB3	1:A:1700:ASP:C	2.45	0.41
1:A:1675:GLU:HB3	1:A:1677:TRP:HD1	1.86	0.41
1:B:1726:MET:HE3	1:B:1728:PHE:CE2	2.55	0.41
1:B:2098:LEU:HD11	1:B:2219:MET:HG2	2.02	0.41
1:B:2501:LYS:O	1:B:2505:GLU:HG3	2.21	0.41
1:C:358:PHE:CE2	1:C:401:LEU:HD21	2.56	0.41
1:C:1370:ILE:HA	1:C:1374:GLN:HG3	2.03	0.41
1:C:1871:ARG:HD3	1:C:1871:ARG:HA	1.83	0.41
1:D:360:ARG:HH12	1:D:390:LEU:HD13	1.85	0.41
1:D:2467:MET:SD	1:D:2467:MET:N	2.93	0.41
1:D:2497:THR:HB	1:D:2498:ASP:HB2	2.03	0.41
1:E:1531:ASP:OD1	1:E:1531:ASP:N	2.52	0.41
1:E:1954:ALA:O	1:E:1956:SER:N	2.54	0.41
1:A:415:ILE:CG2	1:A:432:GLY:H	2.34	0.41
1:A:2285:PHE:O	1:A:2288:MET:HG3	2.21	0.41
1:B:401:LEU:H	1:B:401:LEU:HD12	1.84	0.41
1:B:1416:ASN:HB3	1:B:1421:TYR:HB2	2.01	0.41
1:B:1711:LEU:HA	1:B:1711:LEU:HD23	1.86	0.41
1:B:2224:GLU:HA	1:B:2227:LYS:HG2	2.03	0.41
1:C:271:ILE:HD13	1:C:281:TRP:HZ2	1.86	0.41
1:D:1685:VAL:HG12	1:D:1686:VAL:HG23	2.03	0.41
1:D:1848:LEU:HD23	1:D:1848:LEU:HA	1.92	0.41
1:D:1942:LEU:HD12	1:D:1942:LEU:HA	1.89	0.41
1:E:8:LEU:HD22	1:E:20:MET:HB3	2.03	0.41
1:E:169:LEU:O	1:E:173:ILE:HG12	2.20	0.41
1:E:386:LEU:HG	1:E:398:SER:HB2	2.03	0.41
1:E:617:LEU:HD23	1:E:617:LEU:HA	1.89	0.41
1:A:373:LEU:HG	1:A:382:ILE:HD13	2.02	0.41
1:A:951:LEU:HD23	1:A:951:LEU:HA	1.93	0.41
1:B:1235:PHE:HB3	1:B:1240:THR:HG22	2.03	0.41
1:B:2498:ASP:HB3	1:B:2499:ARG:H	1.75	0.41
1:C:401:LEU:H	1:C:401:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1446:ASN:OD1	1:C:1449:ALA:N	2.53	0.41
1:D:145:LEU:HD23	1:D:145:LEU:HA	1.84	0.41
1:D:180:ASP:OD1	1:D:181:SER:N	2.50	0.41
1:D:2077:ALA:O	1:D:2081:ILE:HG12	2.21	0.41
1:E:359:ILE:HA	1:E:396:PHE:O	2.20	0.41
1:A:359:ILE:HA	1:A:396:PHE:O	2.21	0.41
1:A:735:LEU:HD23	1:A:735:LEU:HA	1.85	0.41
1:A:1081:LEU:HD11	1:A:1641:ILE:HD13	2.03	0.41
1:A:1665:PRO:HG3	1:A:1762:GLU:HB2	2.03	0.41
1:A:2061:ASP:HB3	1:B:2257:LYS:HD3	2.03	0.41
1:A:2115:LEU:HD23	1:A:2115:LEU:HA	1.84	0.41
1:A:2372:LEU:HD23	1:A:2372:LEU:HA	1.88	0.41
1:B:922:MET:HE3	1:B:922:MET:HB3	1.87	0.41
1:B:1081:LEU:HA	1:B:1081:LEU:HD23	1.84	0.41
1:B:1287:LEU:HD23	1:B:1287:LEU:HA	1.93	0.41
1:C:115:PRO:HD2	1:C:155:MET:HE1	2.03	0.41
1:C:386:LEU:HG	1:C:398:SER:HB2	2.02	0.41
1:C:1354:LEU:O	1:C:1550:PRO:HA	2.20	0.41
1:D:271:ILE:HD13	1:D:281:TRP:HZ2	1.86	0.41
1:D:506:LEU:HD12	1:D:506:LEU:HA	1.90	0.41
1:D:1001:LEU:HD23	1:D:1001:LEU:HA	1.91	0.41
1:D:1446:ASN:OD1	1:D:1449:ALA:N	2.53	0.41
1:D:1519:MET:HE3	1:D:1519:MET:HB3	1.90	0.41
1:D:1769:ASN:ND2	1:E:1356:ASN:OD1	2.53	0.41
1:D:1871:ARG:HD3	1:D:1871:ARG:HA	1.85	0.41
1:D:2350:LEU:HD12	1:D:2510:ILE:HD12	2.02	0.41
1:D:2392:GLN:HB2	1:D:2494:PRO:HA	2.03	0.41
1:D:2416:ARG:O	1:D:2483:VAL:HG23	2.21	0.41
1:E:637:PRO:O	1:E:640:VAL:HG12	2.21	0.41
1:E:1001:LEU:HD23	1:E:1001:LEU:HA	1.90	0.41
1:E:1410:GLY:HA2	1:E:1411:PRO:HD3	1.95	0.41
1:A:360:ARG:HH12	1:A:390:LEU:HD13	1.86	0.41
1:A:504:GLN:HA	1:A:507:ASN:ND2	2.36	0.41
1:B:602:LEU:HD23	1:B:602:LEU:HA	1.84	0.41
1:B:2318:MET:HE1	1:C:2271:LEU:CB	2.48	0.41
1:C:317:THR:OG1	1:C:318:GLY:N	2.53	0.41
1:C:1862:MET:HE2	1:C:1862:MET:HB2	1.80	0.41
1:D:239:LEU:HD23	1:D:239:LEU:HA	1.90	0.41
1:D:414:LYS:HE3	1:D:414:LYS:HB3	1.80	0.41
1:D:504:GLN:O	1:D:507:ASN:ND2	2.54	0.41
1:D:817:ILE:HD13	1:D:817:ILE:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:LYS:HE3	1:E:257:LYS:HB3	1.94	0.41
1:E:307:SER:C	1:E:309:SER:H	2.28	0.41
1:E:714:LEU:HD23	1:E:714:LEU:HA	1.87	0.41
1:E:1117:LEU:HD23	1:E:1117:LEU:HA	1.91	0.41
1:E:1786:GLU:HA	1:E:1790:TYR:HB2	2.03	0.41
1:A:404:ILE:HD13	1:A:414:LYS:NZ	2.36	0.40
1:A:490:LEU:HD23	1:A:490:LEU:HA	1.92	0.40
1:A:1410:GLY:HA2	1:A:1411:PRO:HD3	1.95	0.40
1:B:14:THR:HG22	1:B:18:GLN:O	2.20	0.40
1:B:321:VAL:HG13	1:B:324:GLU:H	1.85	0.40
1:C:170:LEU:HD13	1:C:946:LEU:HD11	2.04	0.40
1:C:351:TYR:HA	1:C:356:GLN:HG3	2.03	0.40
1:C:581:LEU:HD22	1:C:585:ASN:HA	2.03	0.40
1:C:616:MET:HE3	1:C:661:TRP:HB2	2.03	0.40
1:C:743:LEU:HD23	1:C:743:LEU:HA	1.87	0.40
1:C:775:ARG:HH12	1:C:2253:LEU:HD12	1.85	0.40
1:E:14:THR:C	1:E:16:ASP:N	2.80	0.40
1:E:2501:LYS:HB3	1:E:2501:LYS:HE3	1.81	0.40
1:A:1944:ARG:HG2	1:A:1944:ARG:NH1	2.34	0.40
1:B:200:HIS:HB3	1:B:203:TYR:HB3	2.02	0.40
1:B:1517:THR:HG23	1:B:1570:VAL:HB	2.03	0.40
1:B:1882:MET:HE2	1:B:1882:MET:HB2	1.86	0.40
1:B:2347:THR:N	1:C:2434:ASP:OD2	2.54	0.40
1:C:415:ILE:CG2	1:C:432:GLY:H	2.34	0.40
1:C:1157:ILE:HD11	1:C:1168:LEU:HD21	2.03	0.40
1:C:1675:GLU:HB3	1:C:1677:TRP:HD1	1.86	0.40
1:C:1980:LEU:HD23	1:C:1980:LEU:HA	1.87	0.40
1:C:2006:LYS:HD3	1:C:2007:ALA:N	2.36	0.40
1:C:2061:ASP:HB3	1:D:2257:LYS:HD3	2.02	0.40
1:C:2439:LEU:HB3	1:C:2454:ILE:HG12	2.02	0.40
1:D:743:LEU:HD23	1:D:743:LEU:HA	1.87	0.40
1:D:1952:ARG:HD2	1:D:1952:ARG:HA	1.81	0.40
1:E:2201:ARG:HD3	1:E:2205:TRP:CZ2	2.56	0.40
1:A:118:TYR:OH	1:A:1024:ASN:O	2.31	0.40
1:A:899:VAL:O	1:A:899:VAL:CG1	2.69	0.40
1:A:1354:LEU:O	1:A:1550:PRO:HA	2.20	0.40
1:B:1954:ALA:O	1:B:1956:SER:N	2.54	0.40
1:C:899:VAL:O	1:C:899:VAL:CG1	2.70	0.40
1:C:1622:LEU:HD23	1:C:1622:LEU:HA	1.90	0.40
1:E:1416:ASN:HB3	1:E:1421:TYR:HB2	2.03	0.40
1:A:14:THR:HG22	1:A:18:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:LEU:HD11	1:A:1201:GLY:HA2	2.02	0.40
1:B:49:LEU:HA	1:B:49:LEU:HD12	1.90	0.40
1:B:660:ILE:HD12	1:B:660:ILE:HA	1.89	0.40
1:B:1061:GLU:OE1	1:C:2130:LEU:HD11	2.22	0.40
1:B:1809:THR:OG1	1:B:1875:GLN:NE2	2.50	0.40
1:B:1866:ILE:O	1:B:1870:MET:HG3	2.21	0.40
1:B:1983:LEU:HD23	1:B:1983:LEU:HA	1.92	0.40
1:B:2115:LEU:HD23	1:B:2115:LEU:HA	1.87	0.40
1:B:2508:SER:OG	1:B:2509:ASP:N	2.54	0.40
1:C:1334:GLU:OE2	1:C:1362:ARG:NH2	2.55	0.40
1:C:2286:CYS:SG	1:C:2323:LEU:HD12	2.62	0.40
1:C:2419:LYS:HG2	1:D:2466:PHE:HE1	1.86	0.40
1:D:321:VAL:HG22	1:D:323:ASN:H	1.86	0.40
1:D:957:GLU:HA	1:D:957:GLU:OE2	2.22	0.40
1:D:1531:ASP:N	1:D:1531:ASP:OD1	2.54	0.40
1:E:600:LEU:HD23	1:E:600:LEU:HA	1.94	0.40
1:A:1102:SER:OG	1:A:1307:TYR:OH	2.34	0.40
1:A:1167:HIS:HD2	1:A:1194:LEU:HD11	1.86	0.40
1:A:1685:VAL:O	1:A:1687:ASP:N	2.55	0.40
1:B:1630:LEU:HD23	1:B:1630:LEU:HA	1.91	0.40
1:C:1711:LEU:HA	1:C:1711:LEU:HD23	1.85	0.40
1:D:321:VAL:HG13	1:D:324:GLU:H	1.86	0.40
1:E:456:LEU:HD23	1:E:456:LEU:HA	1.88	0.40
1:E:604:ALA:HB2	1:E:614:LEU:HD22	2.03	0.40
1:E:961:LEU:HB2	1:E:966:ASP:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2517/2543 (99%)	2388 (95%)	121 (5%)	8 (0%)	36 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	2517/2543 (99%)	2392 (95%)	118 (5%)	7 (0%)	36	65
1	C	2517/2543 (99%)	2391 (95%)	119 (5%)	7 (0%)	36	65
1	D	2517/2543 (99%)	2390 (95%)	120 (5%)	7 (0%)	36	65
1	E	2517/2543 (99%)	2384 (95%)	126 (5%)	7 (0%)	36	65
All	All	12585/12715 (99%)	11945 (95%)	604 (5%)	36 (0%)	37	65

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	TYR
1	A	2498	ASP
1	B	27	TYR
1	B	2498	ASP
1	C	27	TYR
1	C	2498	ASP
1	D	27	TYR
1	D	2498	ASP
1	E	27	TYR
1	E	2498	ASP
1	A	309	SER
1	A	344	ILE
1	B	309	SER
1	B	344	ILE
1	C	309	SER
1	C	344	ILE
1	D	309	SER
1	D	344	ILE
1	E	309	SER
1	E	344	ILE
1	A	308	THR
1	A	1749	ILE
1	C	1749	ILE
1	D	1749	ILE
1	E	1749	ILE
1	B	1686	VAL
1	B	1749	ILE
1	C	1686	VAL
1	A	1686	VAL
1	A	2004	ASP
1	B	2004	ASP
1	C	2004	ASP

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Mol	Chain	Res	Type
1	D	1686	VAL
1	D	2004	ASP
1	E	1686	VAL
1	E	2004	ASP

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	2167/2192 (99%)	2159 (100%)	8 (0%)	84	83
1	B	2167/2192 (99%)	2161 (100%)	6 (0%)	86	84
1	C	2167/2192 (99%)	2164 (100%)	3 (0%)	88	89
1	D	2167/2192 (99%)	2164 (100%)	3 (0%)	88	89
1	E	2167/2192 (99%)	2165 (100%)	2 (0%)	88	89
All	All	10835/10960 (99%)	10813 (100%)	22 (0%)	85	85

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	LEU
1	A	355	ASN
1	A	981	ILE
1	A	1162	PHE
1	A	1794	MET
1	A	2137	GLN
1	A	2323	LEU
1	A	2423	VAL
1	B	504	GLN
1	B	1135	LEU
1	B	1162	PHE
1	B	1428	HIS
1	B	2130	LEU
1	B	2508	SER
1	C	317	THR

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Mol	Chain	Res	Type
1	C	647	THR
1	C	1315	VAL
1	D	1061	GLU
1	D	1168	LEU
1	D	1397	ASN
1	E	2137	GLN
1	E	2423	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	507	ASN
1	A	624	ASN
1	A	682	ASN
1	A	822	ASN
1	A	863	GLN
1	A	921	ASN
1	A	962	HIS
1	A	975	ASN
1	A	1002	ASN
1	A	1138	ASN
1	A	1320	ASN
1	A	1337	ASN
1	A	1388	GLN
1	A	1420	ASN
1	A	1562	ASN
1	A	1596	ASN
1	A	1741	HIS
1	A	2107	ASN
1	A	2208	GLN
1	A	2222	GLN
1	A	2248	GLN
1	A	2311	ASN
1	A	2384	ASN
1	A	2417	GLN
1	B	275	ASN
1	B	294	GLN
1	B	428	ASN
1	B	507	ASN
1	B	624	ASN
1	B	671	ASN
1	B	682	ASN

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Mol	Chain	Res	Type
1	B	863	GLN
1	B	921	ASN
1	B	975	ASN
1	B	1138	ASN
1	B	1320	ASN
1	B	1337	ASN
1	B	1372	ASN
1	B	1388	GLN
1	B	1420	ASN
1	B	1562	ASN
1	B	1596	ASN
1	B	1697	GLN
1	B	1760	HIS
1	B	1916	GLN
1	B	2106	GLN
1	B	2384	ASN
1	C	60	ASN
1	C	172	HIS
1	C	275	ASN
1	C	294	GLN
1	C	428	ASN
1	C	507	ASN
1	C	585	ASN
1	C	682	ASN
1	C	863	GLN
1	C	884	HIS
1	C	921	ASN
1	C	962	HIS
1	C	975	ASN
1	C	1002	ASN
1	C	1138	ASN
1	C	1320	ASN
1	C	1337	ASN
1	C	1388	GLN
1	C	1562	ASN
1	C	1596	ASN
1	C	1916	GLN
1	C	1936	GLN
1	C	2107	ASN
1	C	2222	GLN
1	C	2311	ASN
1	C	2370	GLN

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Mol	Chain	Res	Type
1	C	2417	GLN
1	D	60	ASN
1	D	275	ASN
1	D	428	ASN
1	D	507	ASN
1	D	822	ASN
1	D	863	GLN
1	D	975	ASN
1	D	1048	GLN
1	D	1103	ASN
1	D	1320	ASN
1	D	1337	ASN
1	D	1420	ASN
1	D	1596	ASN
1	D	1769	ASN
1	D	1916	GLN
1	D	1936	GLN
1	D	2106	GLN
1	D	2107	ASN
1	D	2121	ASN
1	D	2250	GLN
1	D	2311	ASN
1	D	2384	ASN
1	D	2465	GLN
1	E	60	ASN
1	E	200	HIS
1	E	275	ASN
1	E	322	ASN
1	E	323	ASN
1	E	354	ASN
1	E	411	ASN
1	E	494	HIS
1	E	507	ASN
1	E	512	ASN
1	E	585	ASN
1	E	682	ASN
1	E	863	GLN
1	E	921	ASN
1	E	975	ASN
1	E	1002	ASN
1	E	1138	ASN
1	E	1320	ASN

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Mol	Chain	Res	Type
1	E	1337	ASN
1	E	1420	ASN
1	E	1562	ASN
1	E	1596	ASN
1	E	1697	GLN
1	E	1863	HIS
1	E	1916	GLN
1	E	1936	GLN
1	E	2107	ASN
1	E	2222	GLN
1	E	2311	ASN
1	E	2384	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

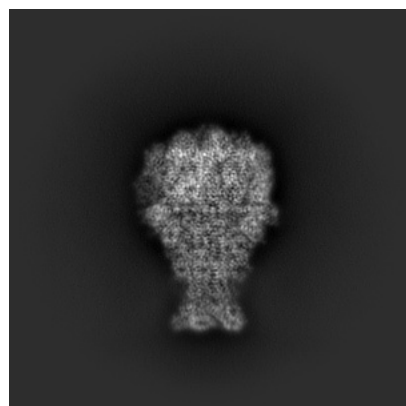
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48373. These allow visual inspection of the internal detail of the map and identification of artifacts.

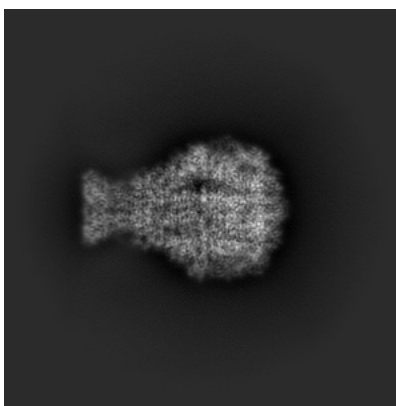
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

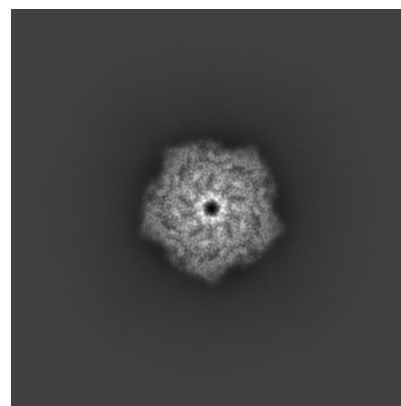
6.1.1 Primary map



X

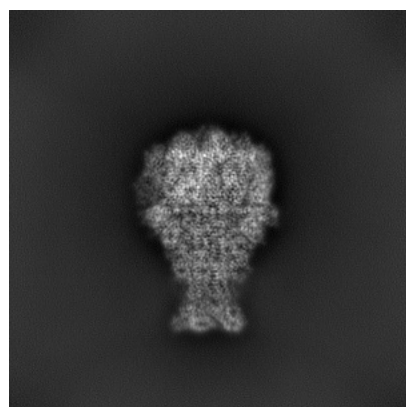


Y

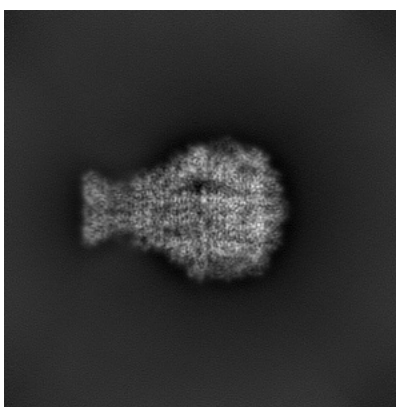


Z

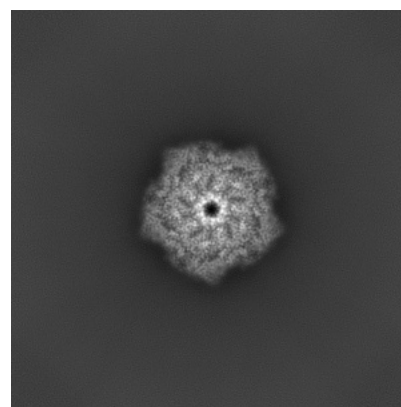
6.1.2 Raw map



X



Y

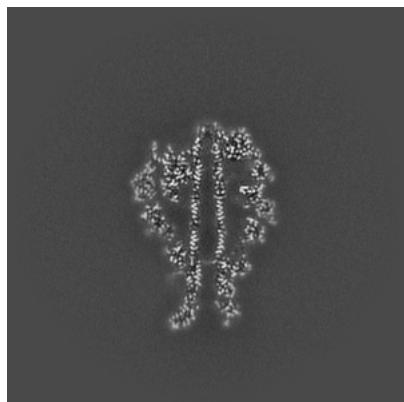


Z

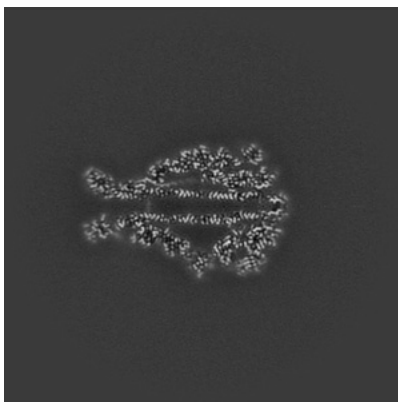
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

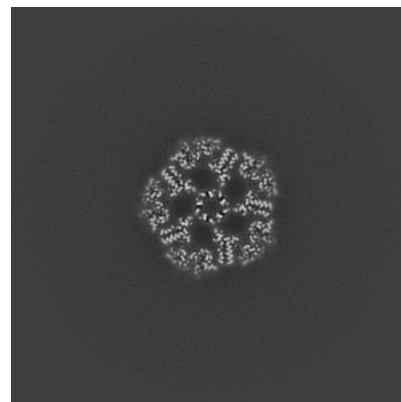
6.2.1 Primary map



X Index: 180

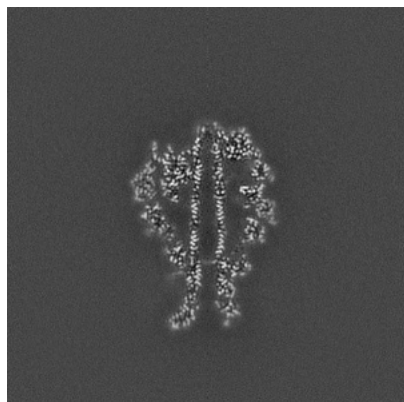


Y Index: 180

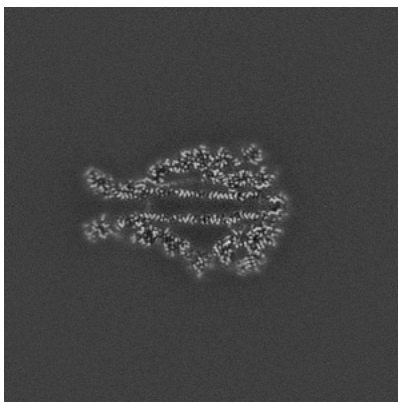


Z Index: 180

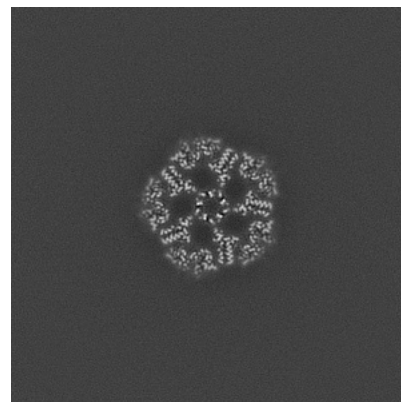
6.2.2 Raw map



X Index: 180



Y Index: 180

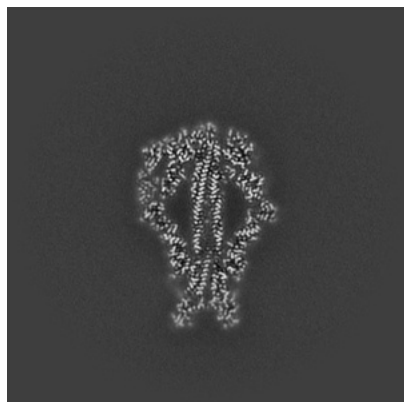


Z Index: 180

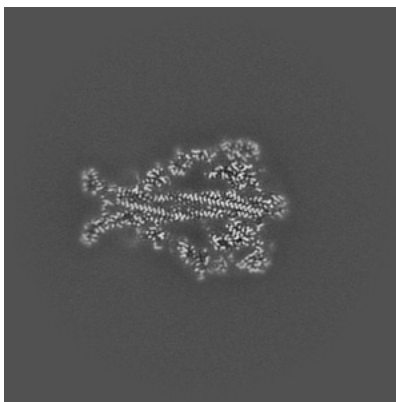
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

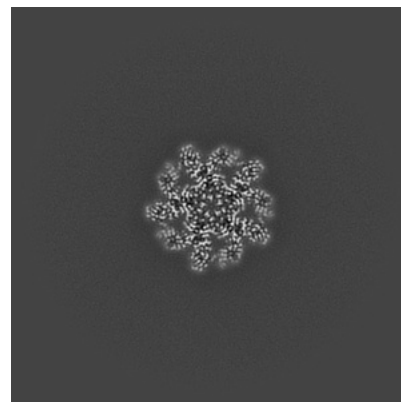
6.3.1 Primary map



X Index: 173

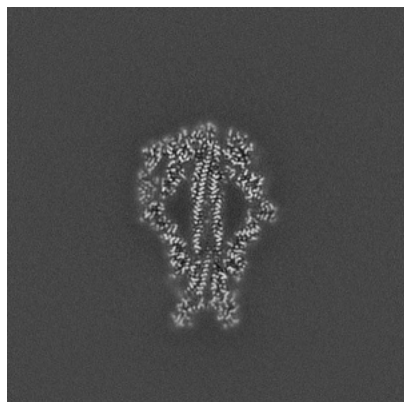


Y Index: 172

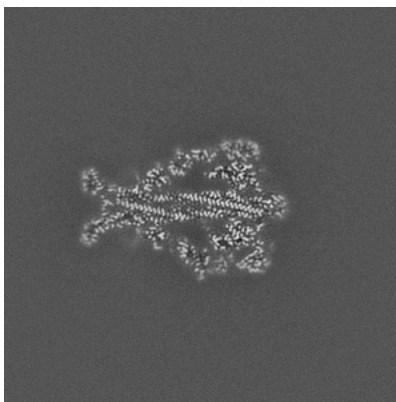


Z Index: 228

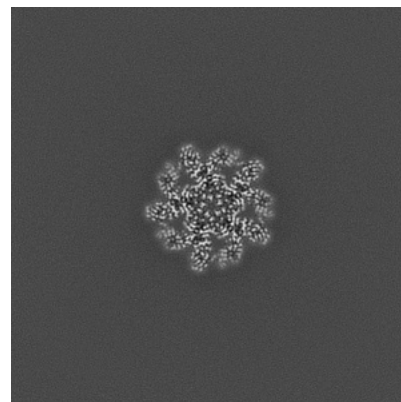
6.3.2 Raw map



X Index: 173



Y Index: 172

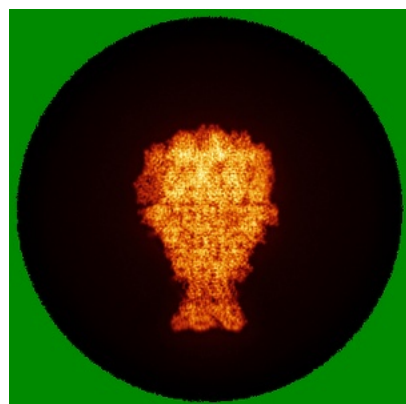


Z Index: 228

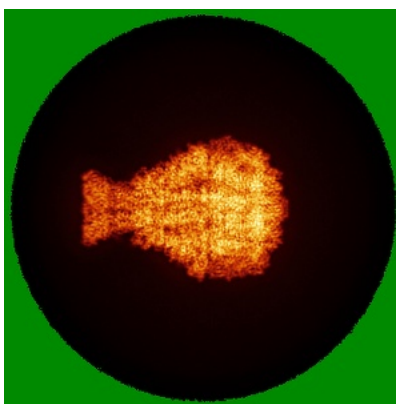
The images above show the largest variance slices of the map in three orthogonal directions.

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

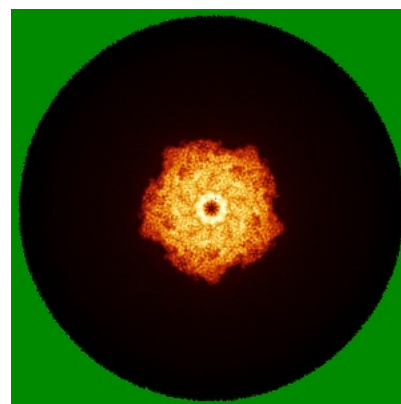
6.4.1 Primary map



X

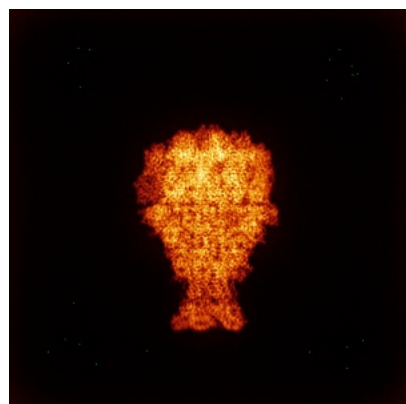


Y

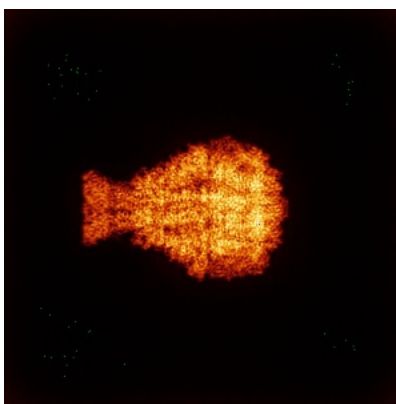


Z

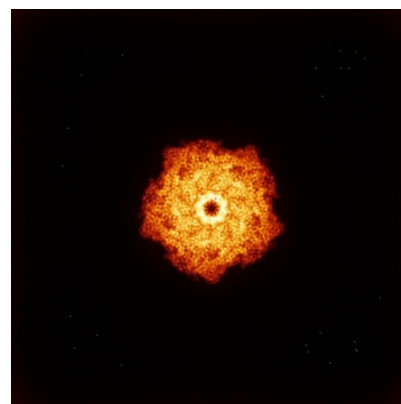
6.4.2 Raw map



X



Y

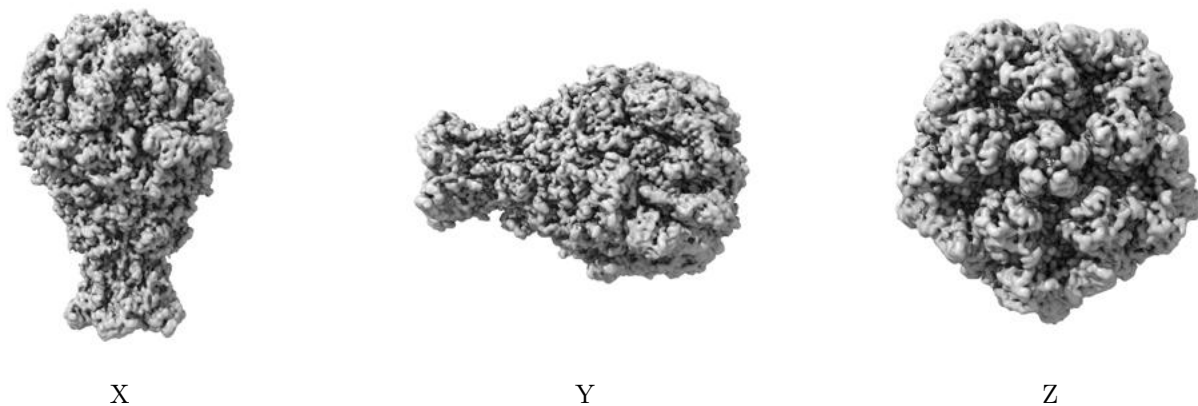


Z

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.

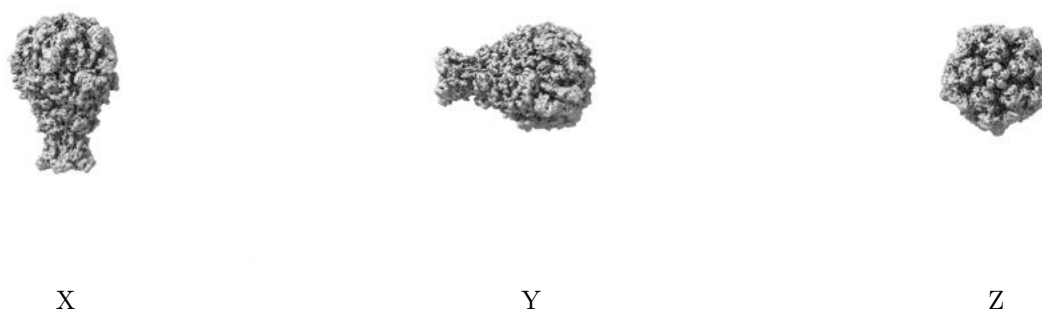
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0894. 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



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.

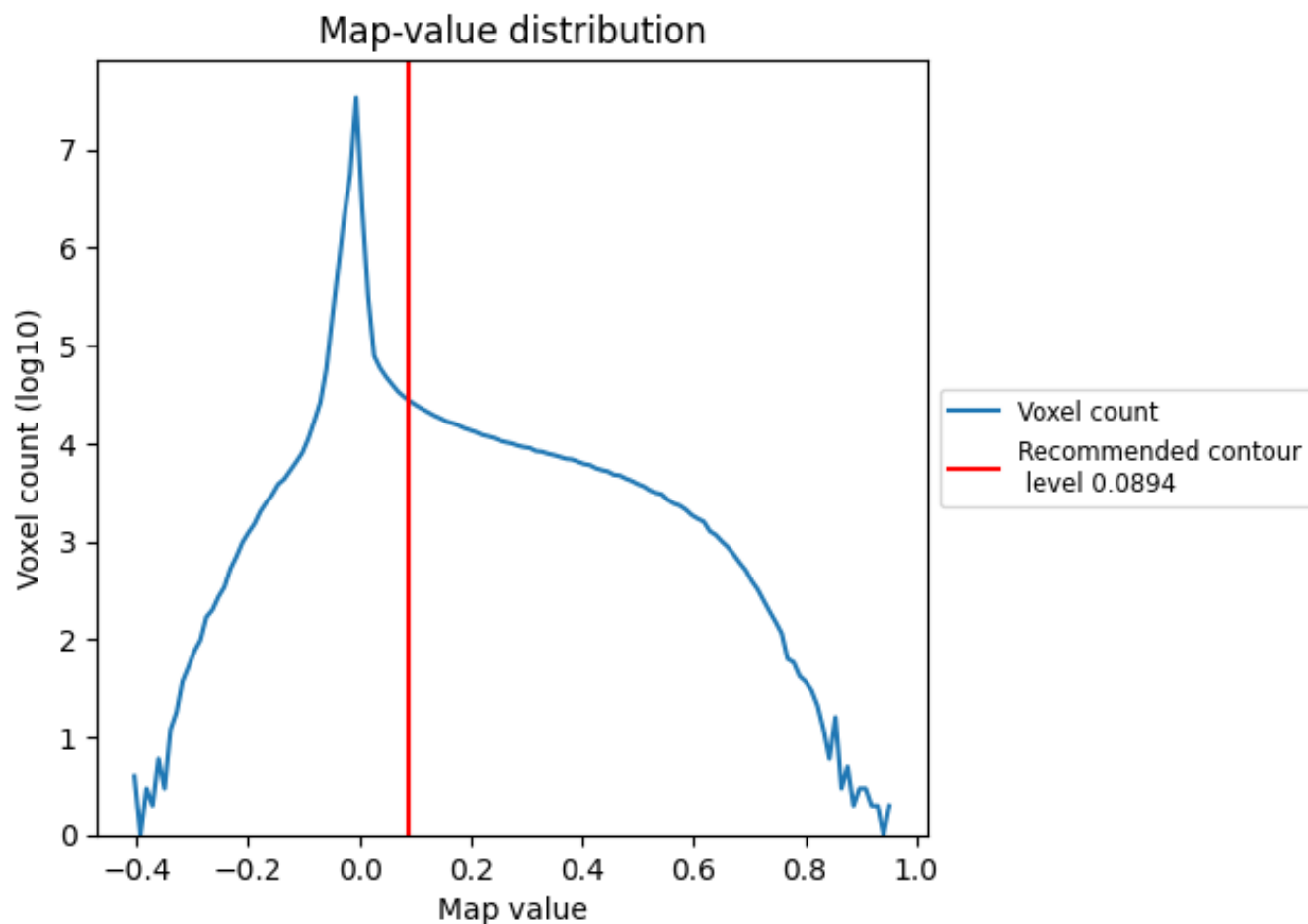
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

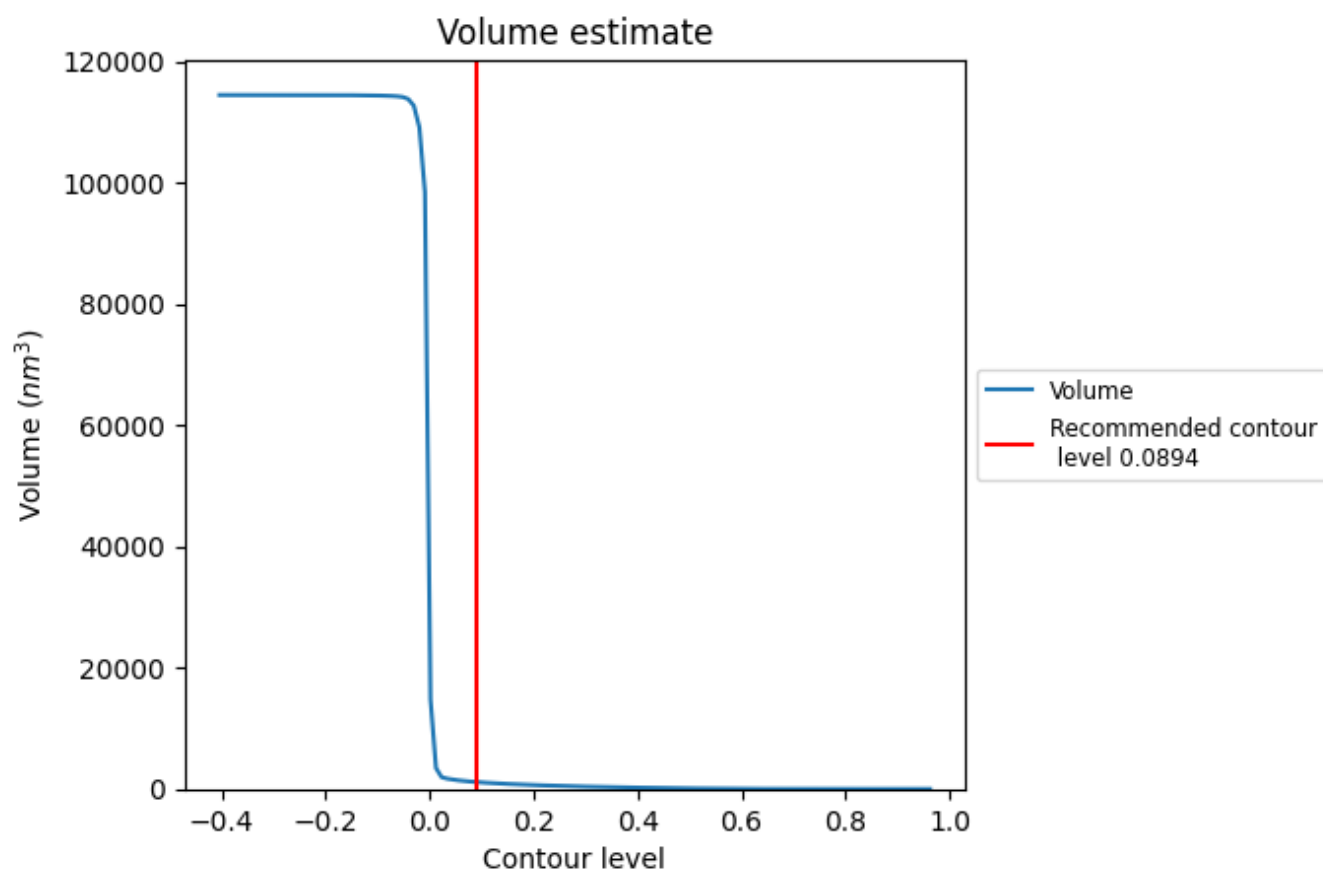
This section contains the results of statistical analysis of the map.

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.

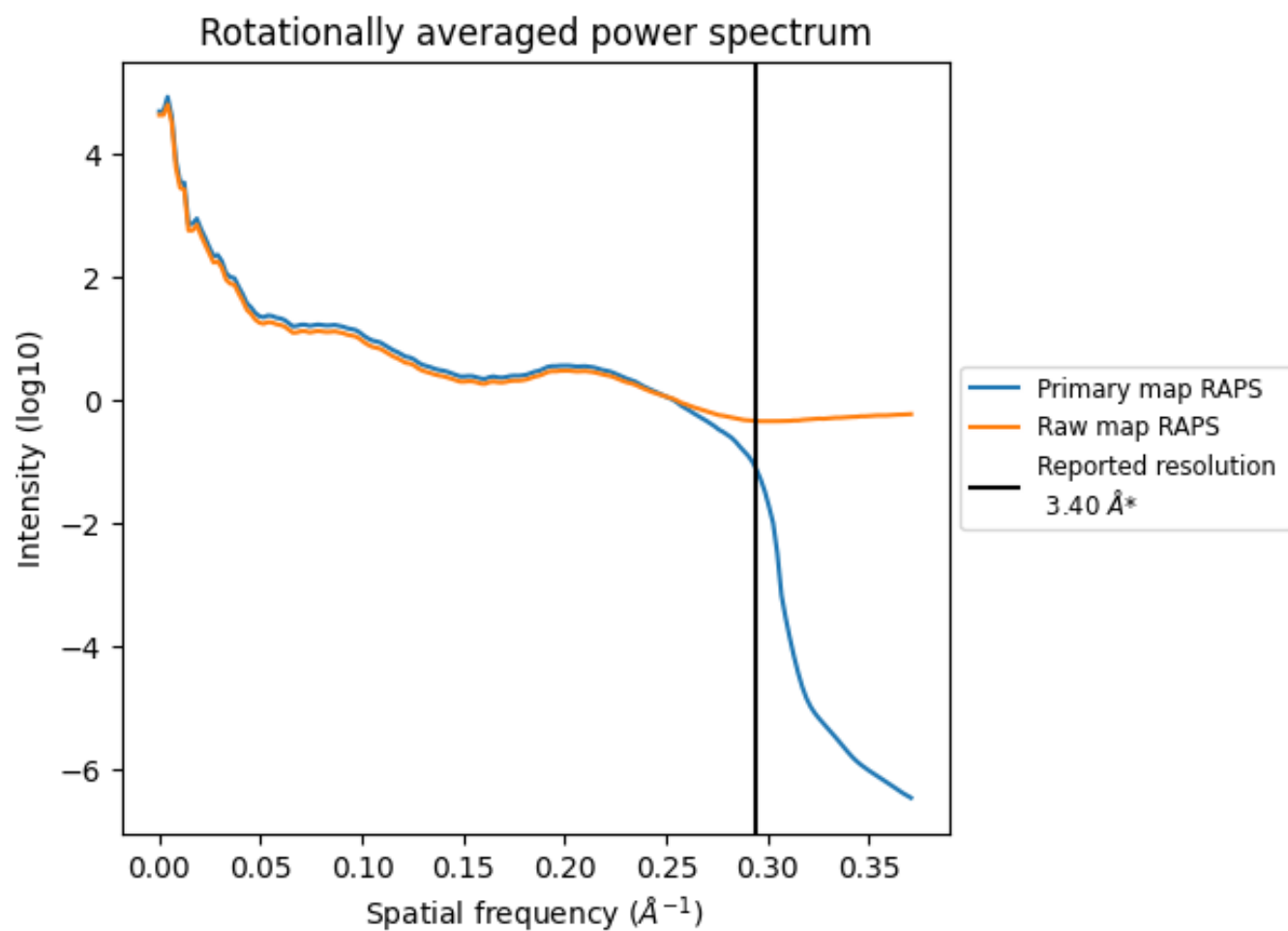
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1142 nm³; this corresponds to an approximate mass of 1031 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 ⓘ

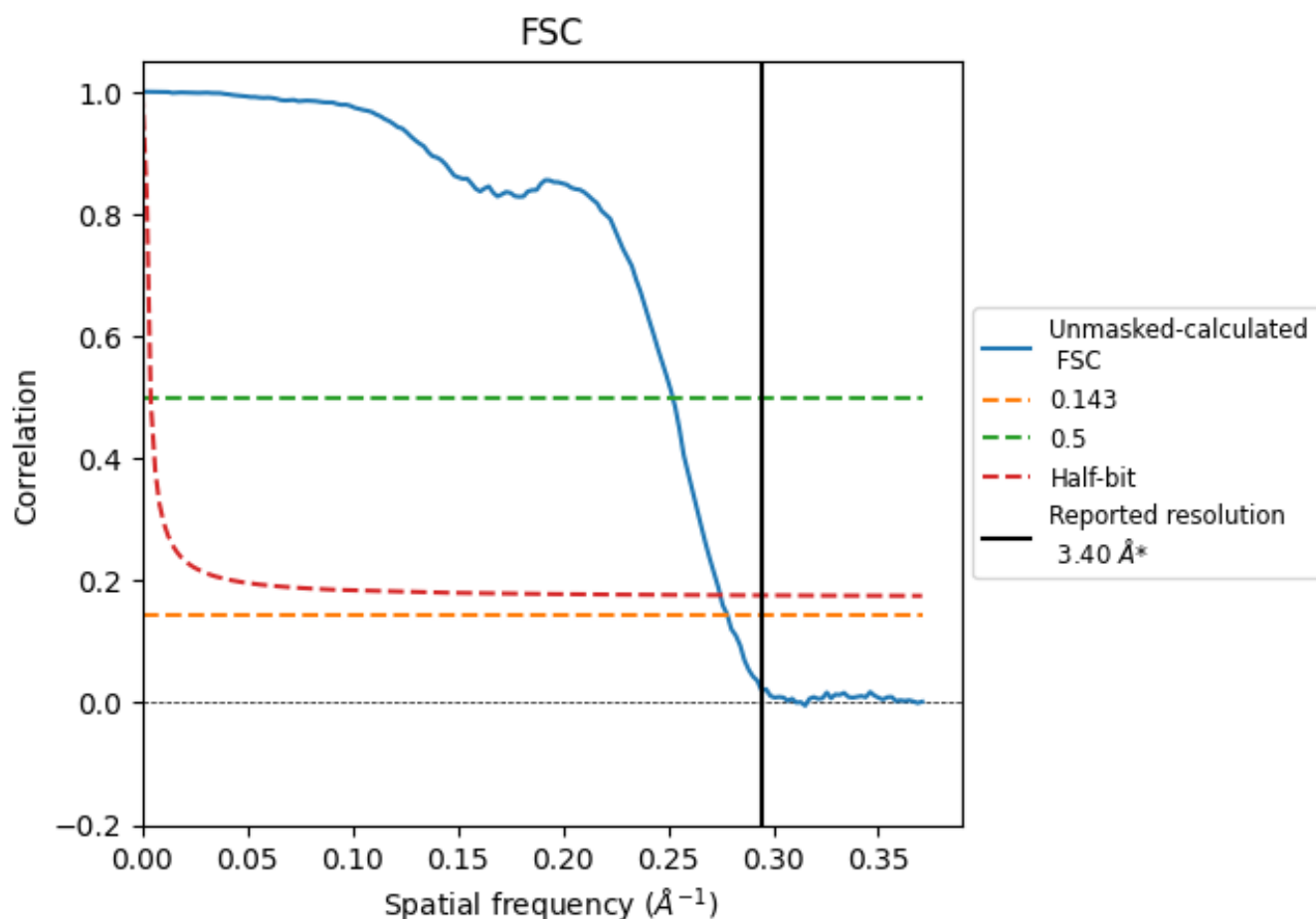


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

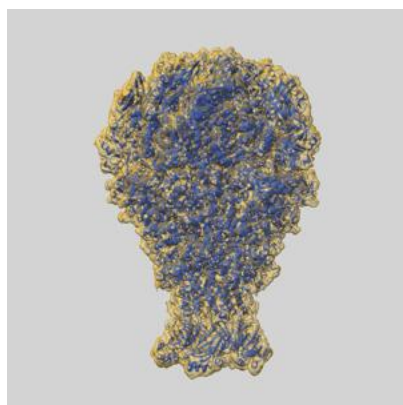
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.59	3.97	3.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

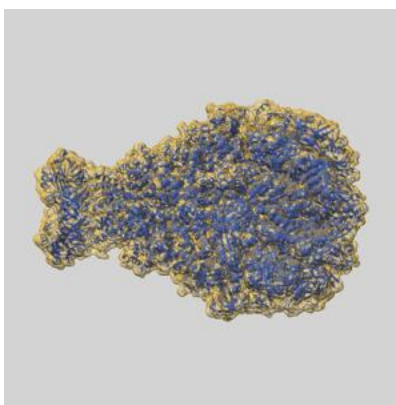
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48373 and PDB model 9MLI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

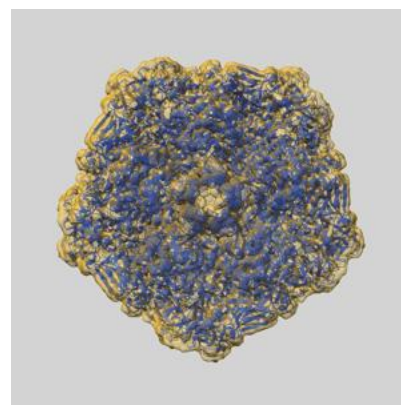
9.1 Map-model overlay [i](#)



X



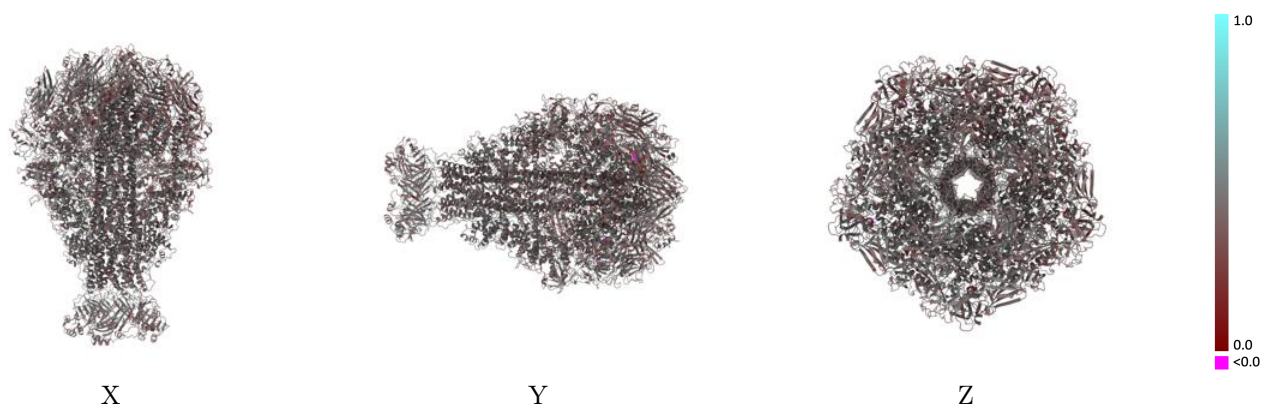
Y



Z

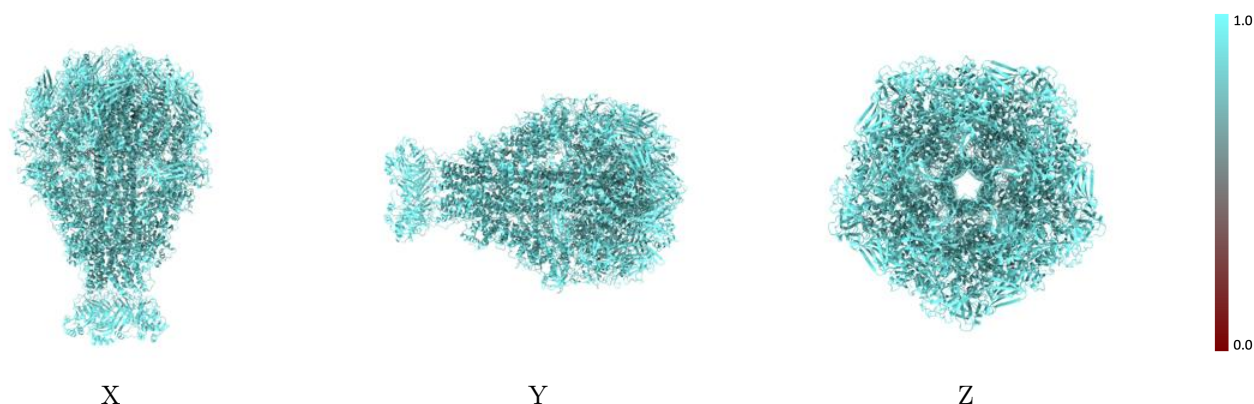
The images above show the 3D surface view of the map at the recommended contour level 0.0894 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



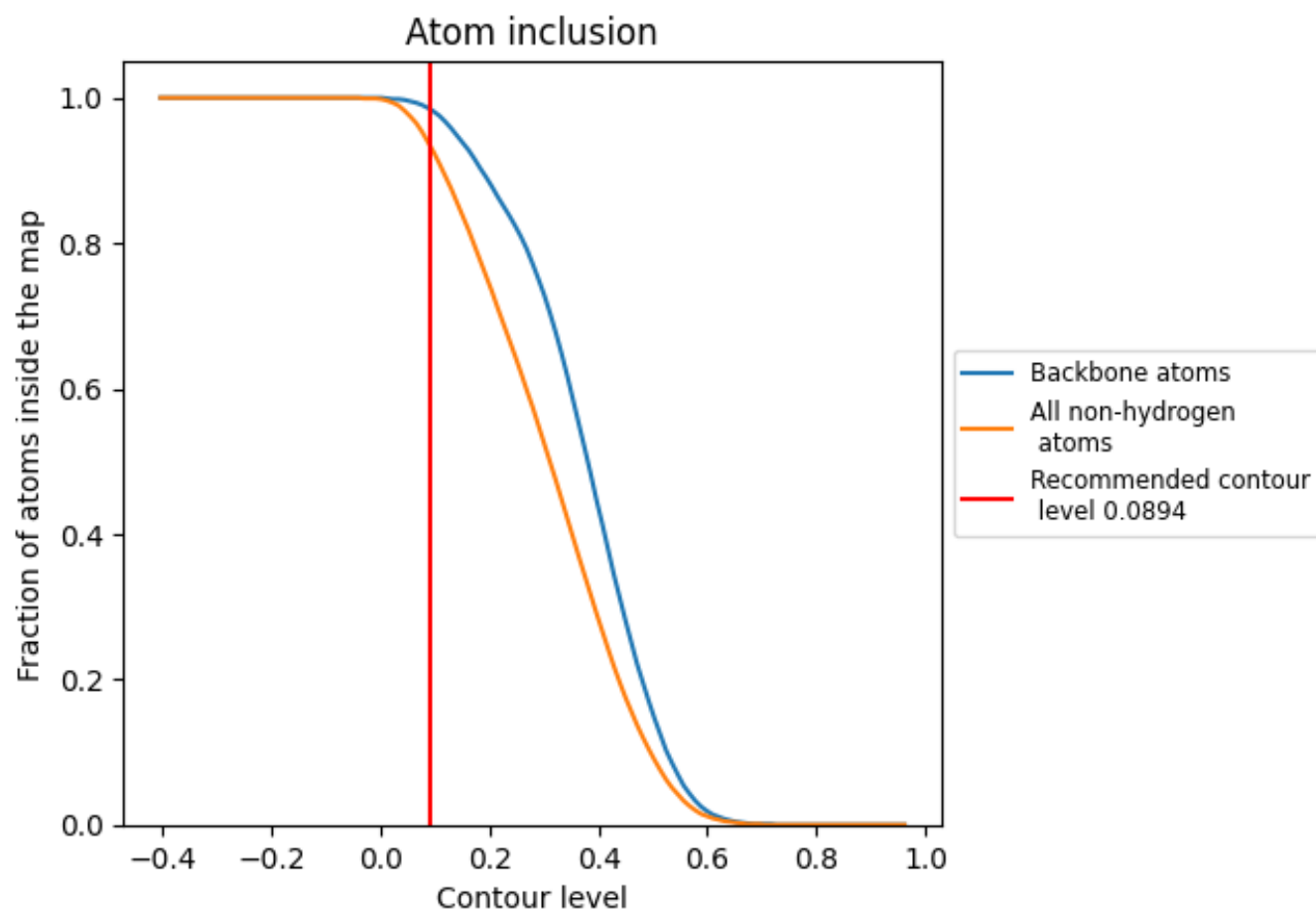
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0894).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0894) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9360	0.4240
A	0.9350	0.4230
B	0.9410	0.4400
C	0.9400	0.4310
D	0.9330	0.4160
E	0.9330	0.4110

