



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 08:53 AM UTC

PDB ID : 8CPZ / pdb_00008cpz
EMDB ID : EMD-16791
Title : Photorhabdus luminescens TcdA1 prepore-to-pore intermediate, K1179W mutant
Authors : Nganga, P.N.; Roderer, D.; Belyy, A.; Prumbaum, D.; Raunser, S.
Deposited on : 2023-03-03
Resolution : 2.90 Å(reported)

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

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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

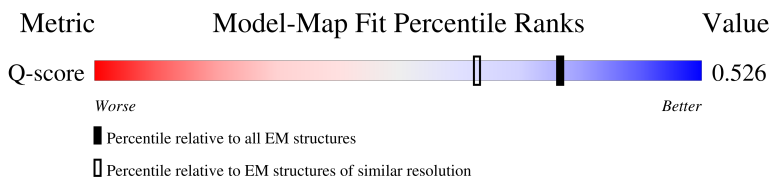
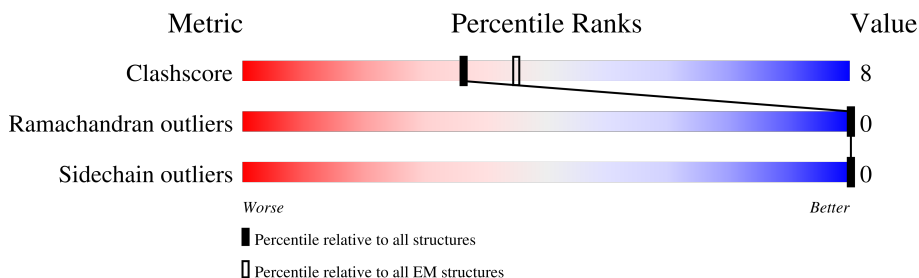
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	2535	 67% 16% 16%
1	B	2535	 67% 16% 16%
1	C	2535	 68% 16% 16%
1	D	2535	 68% 16% 16%

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Mol	Chain	Length	Quality of chain
1	E	2535	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 84420 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 TcdA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	B	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	C	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	D	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	E	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q9RN43
A	-17	ALA	-	expression tag	UNP Q9RN43
A	-16	HIS	-	expression tag	UNP Q9RN43
A	-15	HIS	-	expression tag	UNP Q9RN43
A	-14	HIS	-	expression tag	UNP Q9RN43
A	-13	HIS	-	expression tag	UNP Q9RN43
A	-12	HIS	-	expression tag	UNP Q9RN43
A	-11	HIS	-	expression tag	UNP Q9RN43
A	-10	SER	-	expression tag	UNP Q9RN43
A	-9	SER	-	expression tag	UNP Q9RN43
A	-8	GLY	-	expression tag	UNP Q9RN43
A	-7	LEU	-	expression tag	UNP Q9RN43
A	-6	GLU	-	expression tag	UNP Q9RN43
A	-5	VAL	-	expression tag	UNP Q9RN43
A	-4	LEU	-	expression tag	UNP Q9RN43
A	-3	PHE	-	expression tag	UNP Q9RN43
A	-2	GLN	-	expression tag	UNP Q9RN43
A	-1	GLY	-	expression tag	UNP Q9RN43
A	0	PRO	-	expression tag	UNP Q9RN43
A	1179	TRP	LYS	engineered mutation	UNP Q9RN43

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP Q9RN43
B	-17	ALA	-	expression tag	UNP Q9RN43
B	-16	HIS	-	expression tag	UNP Q9RN43
B	-15	HIS	-	expression tag	UNP Q9RN43
B	-14	HIS	-	expression tag	UNP Q9RN43
B	-13	HIS	-	expression tag	UNP Q9RN43
B	-12	HIS	-	expression tag	UNP Q9RN43
B	-11	HIS	-	expression tag	UNP Q9RN43
B	-10	SER	-	expression tag	UNP Q9RN43
B	-9	SER	-	expression tag	UNP Q9RN43
B	-8	GLY	-	expression tag	UNP Q9RN43
B	-7	LEU	-	expression tag	UNP Q9RN43
B	-6	GLU	-	expression tag	UNP Q9RN43
B	-5	VAL	-	expression tag	UNP Q9RN43
B	-4	LEU	-	expression tag	UNP Q9RN43
B	-3	PHE	-	expression tag	UNP Q9RN43
B	-2	GLN	-	expression tag	UNP Q9RN43
B	-1	GLY	-	expression tag	UNP Q9RN43
B	0	PRO	-	expression tag	UNP Q9RN43
B	1179	TRP	LYS	engineered mutation	UNP Q9RN43
C	-18	MET	-	initiating methionine	UNP Q9RN43
C	-17	ALA	-	expression tag	UNP Q9RN43
C	-16	HIS	-	expression tag	UNP Q9RN43
C	-15	HIS	-	expression tag	UNP Q9RN43
C	-14	HIS	-	expression tag	UNP Q9RN43
C	-13	HIS	-	expression tag	UNP Q9RN43
C	-12	HIS	-	expression tag	UNP Q9RN43
C	-11	HIS	-	expression tag	UNP Q9RN43
C	-10	SER	-	expression tag	UNP Q9RN43
C	-9	SER	-	expression tag	UNP Q9RN43
C	-8	GLY	-	expression tag	UNP Q9RN43
C	-7	LEU	-	expression tag	UNP Q9RN43
C	-6	GLU	-	expression tag	UNP Q9RN43
C	-5	VAL	-	expression tag	UNP Q9RN43
C	-4	LEU	-	expression tag	UNP Q9RN43
C	-3	PHE	-	expression tag	UNP Q9RN43
C	-2	GLN	-	expression tag	UNP Q9RN43
C	-1	GLY	-	expression tag	UNP Q9RN43
C	0	PRO	-	expression tag	UNP Q9RN43
C	1179	TRP	LYS	engineered mutation	UNP Q9RN43
D	-18	MET	-	initiating methionine	UNP Q9RN43
D	-17	ALA	-	expression tag	UNP Q9RN43

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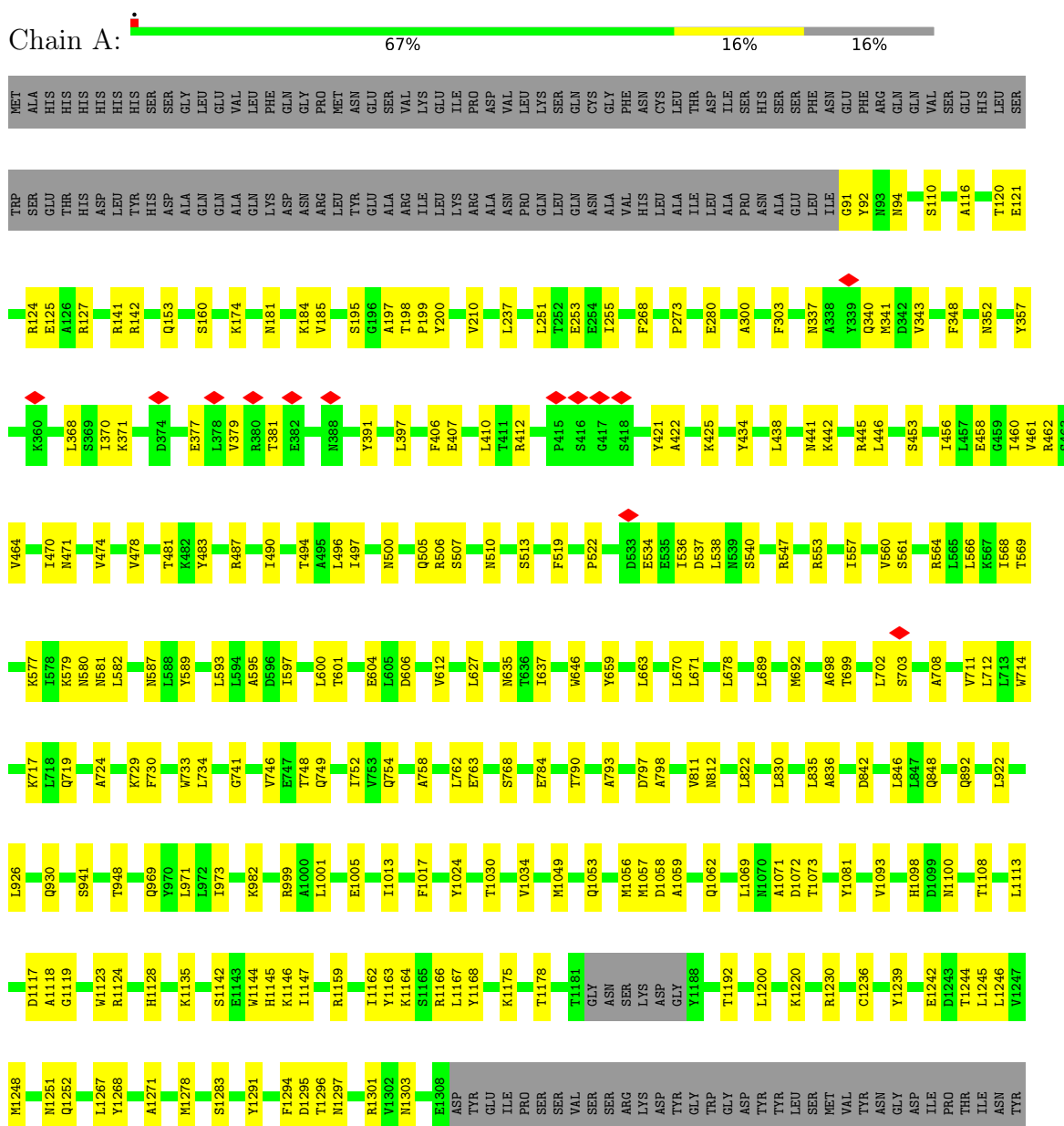
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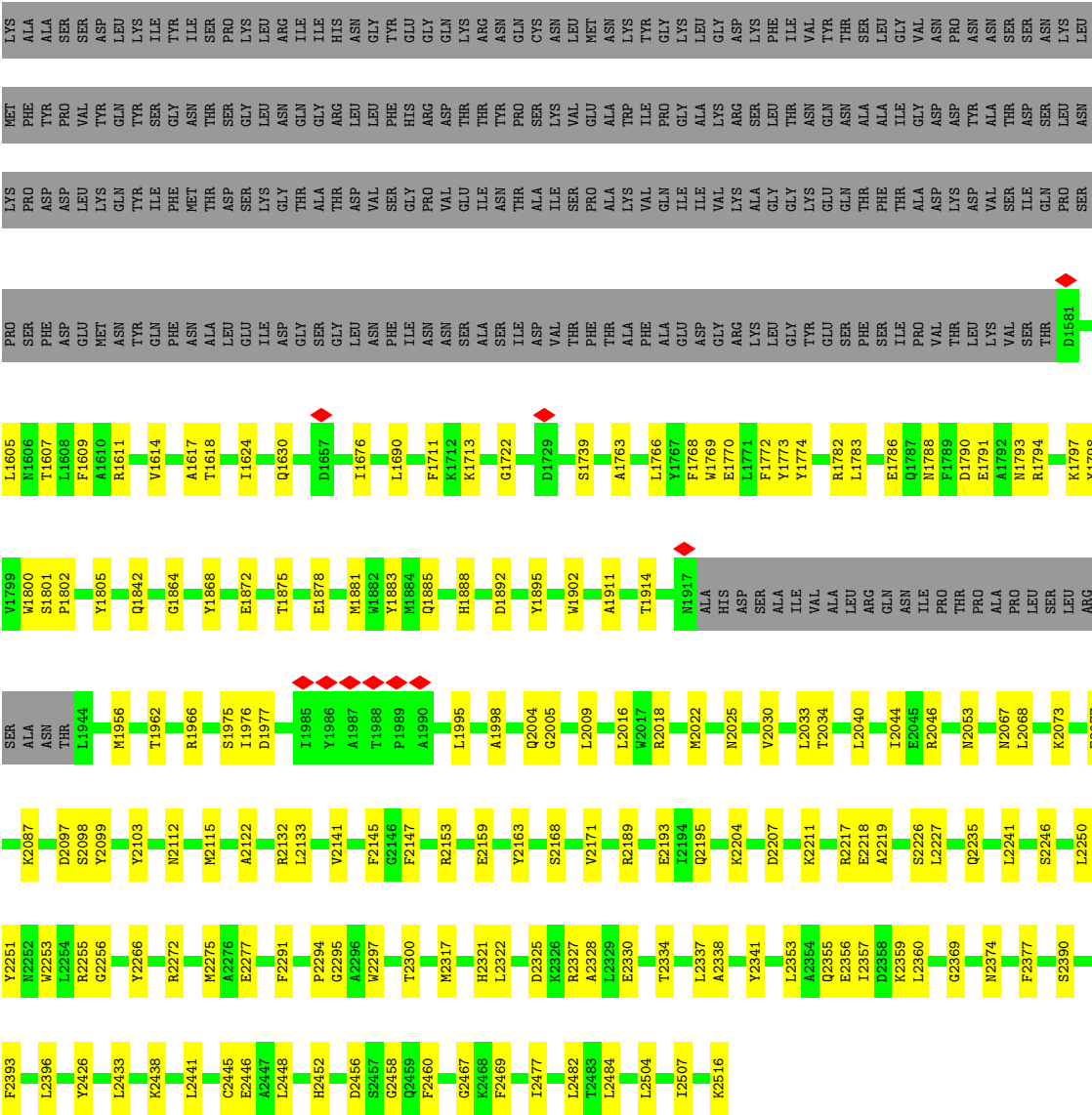
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	HIS	-	expression tag	UNP Q9RN43
D	-15	HIS	-	expression tag	UNP Q9RN43
D	-14	HIS	-	expression tag	UNP Q9RN43
D	-13	HIS	-	expression tag	UNP Q9RN43
D	-12	HIS	-	expression tag	UNP Q9RN43
D	-11	HIS	-	expression tag	UNP Q9RN43
D	-10	SER	-	expression tag	UNP Q9RN43
D	-9	SER	-	expression tag	UNP Q9RN43
D	-8	GLY	-	expression tag	UNP Q9RN43
D	-7	LEU	-	expression tag	UNP Q9RN43
D	-6	GLU	-	expression tag	UNP Q9RN43
D	-5	VAL	-	expression tag	UNP Q9RN43
D	-4	LEU	-	expression tag	UNP Q9RN43
D	-3	PHE	-	expression tag	UNP Q9RN43
D	-2	GLN	-	expression tag	UNP Q9RN43
D	-1	GLY	-	expression tag	UNP Q9RN43
D	0	PRO	-	expression tag	UNP Q9RN43
D	1179	TRP	LYS	engineered mutation	UNP Q9RN43
E	-18	MET	-	initiating methionine	UNP Q9RN43
E	-17	ALA	-	expression tag	UNP Q9RN43
E	-16	HIS	-	expression tag	UNP Q9RN43
E	-15	HIS	-	expression tag	UNP Q9RN43
E	-14	HIS	-	expression tag	UNP Q9RN43
E	-13	HIS	-	expression tag	UNP Q9RN43
E	-12	HIS	-	expression tag	UNP Q9RN43
E	-11	HIS	-	expression tag	UNP Q9RN43
E	-10	SER	-	expression tag	UNP Q9RN43
E	-9	SER	-	expression tag	UNP Q9RN43
E	-8	GLY	-	expression tag	UNP Q9RN43
E	-7	LEU	-	expression tag	UNP Q9RN43
E	-6	GLU	-	expression tag	UNP Q9RN43
E	-5	VAL	-	expression tag	UNP Q9RN43
E	-4	LEU	-	expression tag	UNP Q9RN43
E	-3	PHE	-	expression tag	UNP Q9RN43
E	-2	GLN	-	expression tag	UNP Q9RN43
E	-1	GLY	-	expression tag	UNP Q9RN43
E	0	PRO	-	expression tag	UNP Q9RN43
E	1179	TRP	LYS	engineered mutation	UNP Q9RN43

3 Residue-property plots

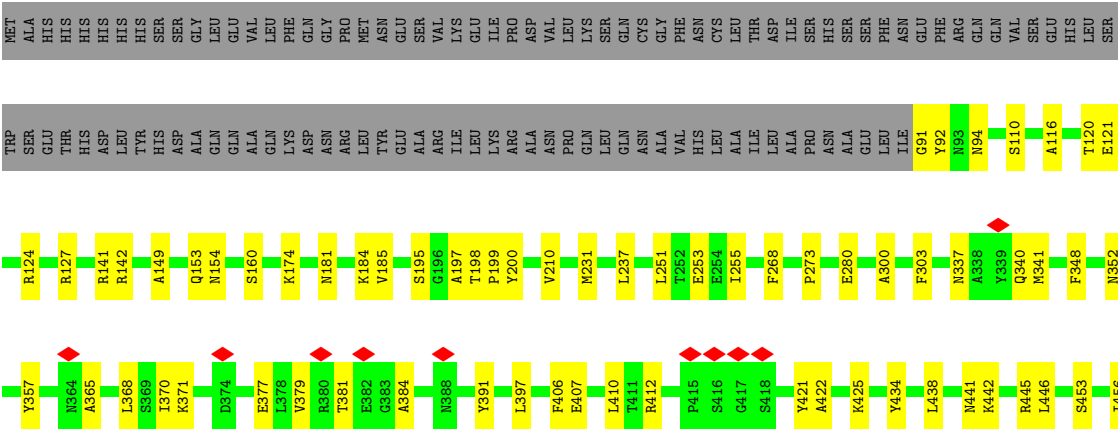
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: TcdA1

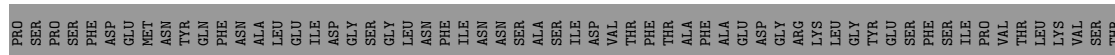




• Molecule 1: TcdA1



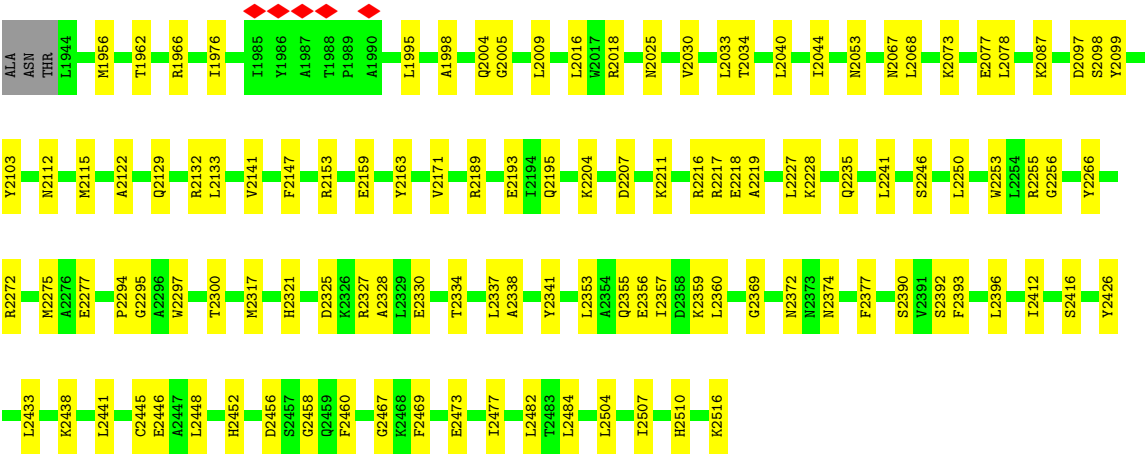
W2252	D2097	THR	K1797	L1605	SER	D1243	T1108	L926	V711	L566	G459
W2253	S2098	L1944	Y1798	N1606	PRO	T1244	L1113	Q930	L712	K567	I460
R2254	Y2099	M1956	P1799	T1607	PHE	L1245	D1117	S941	L713	I568	R461
G2256	Y2103	T1962	Y1800	F1608	ASP	L1246	A1118	T948	W714	T569	S463
Y2266	W2112	R1966	P1802	F1609	LEU	Q1252	G1119	N969	Q719	K577	V464
W2272	W2115	Y1805	Y1802	A1610	GLN	Y1268	G1120	Y970	A724	I578	I470
M2275	A2122	S1975	Y1805	Q1612	TYR	L1267	A1118	L971	F730	K579	M471
M2276	I1976	L1613	L1613	Y1614	ILE	Y1268	G1119	L972	A724	N581	V474
G2277	D1977	PHE	PHE	Y1614	GLY	Y1268	R1124	Y973	F730	L582	V474
I1985	G1864	ASN	ASN	A1617	ASN	A1271	R1124	K982	F730	M587	V478
Y1986	Y1868	ALA	ALA	T1618	THR	M1278	H1128	L971	W733	L588	V478
A1987	Y1868	LEU	LEU	Y1624	PRO	Y1291	S1129	L973	L734	Y589	Y483
T1988	E1878	GLY	GLY	Y1630	LYS	Y1291	K1130	Y973	G741	L593	R487
P1989	Y1881	ASP	ASP	Q1630	ARG	F1294	N1139	K982	V746	I597	I490
A1990	Y1882	THR	THR	Y1650	ILE	D1295	S1142	R999	E747	I597	I490
L1995	Y1883	GLY	GLY	G1656	GLY	T1296	E1143	A1000	T748	T601	E493
L1998	Q1885	ASN	ASN	D1657	LEU	N1297	W1144	L1001	Q749	T494	T494
Q2004	Q1885	ILE	ILE	I1676	PHE	R1301	H1145	E1005	H751	E604	A495
C2005	H1888	GLY	GLY	I1676	GLY	V1302	K1146	E1005	I752	L605	L496
L2009	D1892	ASN	ASN	L1690	PRO	N1303	I1147	T1013	Q754	D606	I497
L2016	Y1895	ASN	ASN	L1690	VAL	E1308	L1162	T1013	A758	V612	Q505
S2168	Y1902	ALA	ALA	F1711	THR	ASP	K1163	Y1024	T748	N635	R506
W2171	A1911	THR	THR	K1712	THR	TYR	K1164	T1030	Q749	I637	S507
R2189	N1917	PHE	PHE	K1712	ALA	ILE	R1166	Y1034	L762	N635	N510
E2193	ALA	ALA	ALA	K1712	ILE	PRO	H1167	T1048	E763	I637	N510
T2194	HIS	ALA	ALA	K1712	VAL	SER	L1167	M1049	S768	W466	S513
Q2195	ASP	ALA	ALA	K1712	VAL	SER	L1169	R1050	E784	Y659	R517
K2204	SER	ALA	ALA	S1739	GLN	ARG	T1178	Q1053	T790	N660	L518
D2207	ALA	ALA	ALA	Y1766	ILE	LYS	T1181	M1056	D797	K661	F519
L2040	ILE	ALA	ALA	Y1767	GLY	LYS	GLY	M1057	A798	L663	P522
K2211	LEU	ALA	ALA	F1768	LEU	ASP	ASN	D1058	L670	L670	D533
E2218	GLN	ALA	ALA	W1769	GLY	TYR	SER	A1059	V811	L671	E534
A2219	ASN	ALA	ALA	E1770	LYS	THR	LYS	L1059	N812	L678	E535
L2227	ILE	ALA	ALA	L1771	GLY	ASP	ASP	L1060	L822	L689	I536
Q2235	PRO	ALA	ALA	F1772	TYR	TYR	GLY	Q1062	L830	L689	D537
L2241	THR	ALA	ALA	Y1773	GLY	TYR	Y1188	L1069	L835	M692	L538
S2246	LEU	ALA	ALA	Y1774	GLY	THR	Y1188	A1070	A836	P694	S540
L2250	ARG	ALA	ALA	R1782	THR	VAL	T1192	D1072	D842	R547	R547
Y2251	SER	ALA	ALA	L1783	THR	VAL	L1200	T1073	A698	T699	R553
F2393	ASN	ALA	ALA	E1786	THR	VAL	K1220	Y1081	L846	I557	I557
W2325	THR	ALA	ALA	Q1787	THR	VAL	R1230	Y1081	L846	L702	V560
Y2326	ASN	ALA	ALA	F1788	THR	VAL	Q1236	Y1081	L846	S703	S611
Y2327	ASN	ALA	ALA	F1789	THR	VAL	Y1239	H1098	L846	E705	R564
Y2328	ASN	ALA	ALA	E1791	THR	VAL	E1242	N1100	L846	A708	A708
Y2329	ASN	ALA	ALA	E1792	THR	VAL	E1242	N1100	L846	A708	A708
Y2330	ASN	ALA	ALA	E1793	THR	VAL	E1242	N1100	L846	A708	A708
Y2331	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2332	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2333	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2334	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2335	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2336	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2337	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2338	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2339	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2340	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2341	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2342	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2343	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2344	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2345	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2346	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2347	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2348	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2349	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2350	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2351	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2352	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2353	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2354	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2355	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2356	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2357	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2358	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2359	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2360	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2361	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2362	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2363	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2364	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
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Y2366	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
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Y2368	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2369	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2370	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2371	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
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Y2373	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2374	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2375	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2376	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2377	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2378	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2379	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2380	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2381	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2382	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2383	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2384	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2385	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2386	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2387	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2388	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2389	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2390	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2391	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2392	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2393	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2394	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2395	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2396	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2397	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2398	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2399	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2400	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2401	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2402	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2403	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2404	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2405	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2406	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2407	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2408	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2409	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2410	ASN	ALA	ALA	E1794	THR	VAL	E1242	N1100	L846	A708	A708
Y2411	ASN	ALA	ALA	E1794	THR	VAL	E1242				







TRP	Y1798	D1581	PRO	LEU	LYS	ASN	L1245	L1113	E705	I568	V464	Y357	R124	TRP
SER	Y1799	L1605	SER	ASN	LEU	TYR	M1248	D1117	A708	I569	I470	N364	R127	SER
GLU	W1800	L1606	PRO	LYS	PHE	ALA	N1251	A1118	V711	K577	M471	R129	R130	GLU
THR	S1801	T1607	PHE	PRO	TYR	ALA	Q1252	G1119	L712	L368	N474	S369	R141	THR
HIS	P1802	L1608	ASP	ASP	VAL	SER	Q1257	E1120	L713	N579	V478	N581	R142	HIS
ASP	Y1805	F1609	GLU	LEU	VAL	SER	L1267	W1123	W714	N580	V478	K371	Q153	ASP
LEU	Y1806	A1610	MET	LYS	GLN	ASP	Y1268	R1124	Q719	N581	T481	D374	Q154	LEU
THR	Q1842	G1611	TYR	ASN	THR	LEU	A1271	H1128	A724	N582	Y483	E377	S160	THR
GLN	Q1864	L1612	GLN	ILE	GLY	ILE	H1278	K1135	F730	N587	Y483	L379	K174	GLN
ASN	D1865	V1614	THR	ASN	ASN	ILE	H1278	K1135	F730	N588	Y483	L379	K174	ASN
ASP	Y1868	A1617	ALA	THR	THR	SER	S1283	K1135	F730	N589	Y483	L379	K174	ASP
LEU	E1878	T1618	LEU	ASP	SER	PRO	Y1291	S1142	L734	N593	R487	V379	N181	LEU
GLY	I1881	I1624	ILE	LYS	GLY	LYS	F1294	E1143	L734	N594	R487	V379	N181	GLY
THR	Q1882	Q1630	GLY	GLY	ASN	ARG	F1294	E1143	G741	N595	E493	T381	K184	THR
GLY	Y1883	Q1630	THR	THR	GLN	ILE	D1295	H1144	V746	N596	T494	E382	V185	GLY
SER	M1884	D1657	ARG	ALA	GLY	ILE	T1296	H1145	V746	N597	A495	N388	S195	SER
LEU	Q1885	L1657	THR	VAL	LEU	HIS	N1297	K1146	Q749	L600	L496	G196	G196	LEU
ASN	A1886	I1676	ASN	VAL	LEU	ASN	M1297	I1147	T801	L601	I497	Y391	T198	ASN
PHE	L1887	L1676	PHE	VAL	PHE	GLY	R1159	I1147	Q749	T801	I497	Y391	P199	PHE
GLY	H1888	L1690	GLY	GLY	THR	TYR	Y1163	K1164	V752	E604	N500	L397	Y200	GLY
PRO	D1892	F1711	PRO	PRO	ARG	GLY	N1303	K1164	Q754	L605	Q505	F406	V210	PRO
VAL	K1712	K1712	VAL	VAL	ASP	GLN	E1308	S1165	A758	L606	R506	E407	V210	VAL
THR	K1713	G1722	THR	THR	THR	GLN	ASP	L1167	V758	D608	S507	M231	M231	THR
ASP	G1722	G1722	ASP	THR	THR	ASN	T1169	L1167	L762	V612	S507	M231	M231	ASP
VAL	D1729	D1729	VAL	THR	THR	ASN	K1176	L1169	E763	V612	N510	L410	L237	VAL
THR	S1739	S1739	THR	THR	THR	CYS	T1178	L1169	E763	V612	N510	L410	L237	THR
ALA	L1766	L1766	ALA	LYS	TRP	LYS	T1181	L1169	S768	I637	P522	G417	F268	ALA
PHE	F1767	F1767	PHE	LYS	ILE	TYR	GLY	L1181	T790	I637	P522	G417	F268	PHE
GLU	F1768	F1768	GLU	ARG	PRO	GLY	ASN	ASN	D797	E535	E534	S418	P273	GLU
ASP	W1769	W1769	ASP	LYS	ILE	GLY	SER	SER	A798	I536	I536	Y421	E280	ASP
GLY	E1770	E1770	GLY	ASP	ALA	LEU	D1058	LYS	V811	D537	D537	A422	E280	GLY
LYS	F1771	F1771	LYS	ASP	LYS	ASP	A1059	ASP	N812	L538	L538	K425	K283	LYS
ALA	Y1773	Y1773	ALA	ASP	ARG	ASP	Q1062	GLY	N812	N539	N539	K425	K283	ALA
LEU	Y1774	Y1774	LEU	THR	SER	PHE	L1069	Y1188	L822	S540	S540	Y434	L293	LEU
GLY	R1782	R1782	GLY	THR	LEU	ILE	L1069	Y1188	L822	H676	R547	Y434	L293	GLY
GLN	L1783	L1783	GLN	THR	THR	ILE	N1070	T1192	L830	G577	R547	L438	A300	GLN
ASN	E1786	E1786	ASN	THR	ALA	THR	A1071	L1200	L835	L678	K552	N441	F303	ASN
PRO	Q1787	Q1787	PRO	THR	ALA	LEU	D1072	L1200	A836	L679	R547	K442	F303	PRO
THR	M1788	M1788	THR	THR	ALA	GLY	T1073	R1204	L836	L679	R547	K442	F303	THR
ALA	F1789	F1789	ALA	THR	ALA	GLY	Y1081	K1220	D842	M692	I557	R445	N337	ALA
PRO	D1790	D1790	PRO	THR	VAL	VAL	V1093	K1220	L846	A693	D558	R445	A338	PRO
THR	E1791	E1791	THR	THR	ASP	ASP	Y1239	R1230	L847	P694	D559	R445	A338	THR
LEU	A1792	A1792	LEU	THR	GLY	ASN	Y1239	R1230	Q848	A698	V560	S453	Y339	LEU
LYS	M1793	M1793	LYS	THR	THR	ASN	Y1239	R1230	Q848	A698	V560	S453	Y339	LYS
VAL	R1794	R1794	VAL	THR	THR	SER	E1242	D1243	Q892	L702	L565	E458	Q340	VAL
SER	K1797	K1797	SER	THR	THR	ASN	T1244	T1244	V898	S703	L566	G459	I460	SER
THR			THR	THR	SER	ASN				S704	K567	N352	N352	THR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	230785	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.447	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	425.92, 425.92, 425.92	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/17247	0.42	0/23428
1	B	0.15	0/17247	0.42	0/23428
1	C	0.15	0/17247	0.42	0/23428
1	D	0.15	0/17247	0.42	0/23428
1	E	0.15	0/17247	0.42	0/23428
All	All	0.15	0/86235	0.42	0/117140

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16884	0	16507	289	0
1	B	16884	0	16507	291	0
1	C	16884	0	16507	281	0
1	D	16884	0	16507	284	0
1	E	16884	0	16507	290	0
All	All	84420	0	82535	1282	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 (1282) 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:B:341:MET:HE1	1:B:410:LEU:HD22	1.49	0.95
1:C:341:MET:HE1	1:C:410:LEU:HD22	1.49	0.93
1:A:341:MET:HE1	1:A:410:LEU:HD22	1.50	0.93
1:D:341:MET:HE1	1:D:410:LEU:HD22	1.50	0.91
1:E:341:MET:HE1	1:E:410:LEU:HD22	1.49	0.91
1:B:689:LEU:HD11	1:B:712:LEU:HB3	1.62	0.82
1:C:1296:THR:HG23	1:C:1301:ARG:HH12	1.46	0.81
1:C:689:LEU:HD11	1:C:712:LEU:HB3	1.61	0.81
1:E:689:LEU:HD11	1:E:712:LEU:HB3	1.62	0.81
1:D:1296:THR:HG23	1:D:1301:ARG:HH12	1.45	0.81
1:A:1296:THR:HG23	1:A:1301:ARG:HH12	1.46	0.80
1:B:1296:THR:HG23	1:B:1301:ARG:HH12	1.46	0.80
1:A:689:LEU:HD11	1:A:712:LEU:HB3	1.62	0.79
1:A:2445:CYS:SG	1:B:2327:ARG:NH1	2.56	0.79
1:D:2445:CYS:SG	1:E:2327:ARG:NH1	2.56	0.79
1:A:2327:ARG:NH1	1:E:2445:CYS:SG	2.55	0.79
1:B:2445:CYS:SG	1:C:2327:ARG:NH1	2.56	0.78
1:E:1296:THR:HG23	1:E:1301:ARG:HH12	1.46	0.78
1:D:689:LEU:HD11	1:D:712:LEU:HB3	1.63	0.78
1:C:2445:CYS:SG	1:D:2327:ARG:NH1	2.57	0.78
1:E:1108:THR:HG1	1:E:1128:HIS:HE2	1.31	0.77
1:C:1059:ALA:HA	1:C:1062:GLN:HE21	1.50	0.75
1:E:1059:ALA:HA	1:E:1062:GLN:HE21	1.50	0.75
1:B:1797:LYS:HG3	1:B:1801:SER:HB2	1.69	0.74
1:B:1059:ALA:HA	1:B:1062:GLN:HE21	1.51	0.74
1:D:1059:ALA:HA	1:D:1062:GLN:HE21	1.51	0.74
1:A:1059:ALA:HA	1:A:1062:GLN:HE21	1.51	0.74
1:C:1108:THR:HG1	1:C:1128:HIS:HE2	1.34	0.73
1:C:1797:LYS:HG3	1:C:1801:SER:HB2	1.70	0.73
1:D:1093:VAL:HG21	1:D:1605:LEU:HD23	1.70	0.73
1:B:341:MET:HE3	1:B:422:ALA:HB3	1.71	0.73
1:D:1797:LYS:HG3	1:D:1801:SER:HB2	1.68	0.73
1:E:1797:LYS:HG3	1:E:1801:SER:HB2	1.69	0.73
1:B:1093:VAL:HG21	1:B:1605:LEU:HD23	1.70	0.72
1:C:341:MET:HE3	1:C:422:ALA:HB3	1.71	0.72
1:C:460:ILE:HG12	1:C:496:LEU:HD21	1.70	0.72
1:B:460:ILE:HG12	1:B:496:LEU:HD21	1.71	0.72
1:D:460:ILE:HG12	1:D:496:LEU:HD21	1.69	0.72
1:A:460:ILE:HG12	1:A:496:LEU:HD21	1.71	0.72
1:C:210:VAL:HG11	1:C:922:LEU:HB3	1.72	0.72
1:E:341:MET:HE3	1:E:422:ALA:HB3	1.71	0.72
1:A:1797:LYS:HG3	1:A:1801:SER:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:MET:HE3	1:A:422:ALA:HB3	1.72	0.72
1:C:1093:VAL:HG21	1:C:1605:LEU:HD23	1.71	0.72
1:E:460:ILE:HG12	1:E:496:LEU:HD21	1.70	0.71
1:D:1163:TYR:HB2	1:D:1245:LEU:HD21	1.72	0.71
1:C:462:ARG:HH11	1:C:506:ARG:HH11	1.37	0.71
1:E:1163:TYR:HB2	1:E:1245:LEU:HD21	1.72	0.71
1:A:300:ALA:HA	1:A:303:PHE:CD2	2.26	0.70
1:B:300:ALA:HA	1:B:303:PHE:CD2	2.27	0.70
1:D:300:ALA:HA	1:D:303:PHE:CD2	2.27	0.70
1:E:210:VAL:HG11	1:E:922:LEU:HB3	1.74	0.70
1:A:698:ALA:HB1	1:B:2253:TRP:HA	1.71	0.70
1:C:300:ALA:HA	1:C:303:PHE:CD2	2.26	0.70
1:C:698:ALA:HB1	1:D:2253:TRP:HA	1.73	0.70
1:D:341:MET:HE3	1:D:422:ALA:HB3	1.72	0.70
1:B:698:ALA:HB1	1:C:2253:TRP:HA	1.72	0.70
1:C:1163:TYR:HB2	1:C:1245:LEU:HD21	1.72	0.70
1:E:1093:VAL:HG21	1:E:1605:LEU:HD23	1.72	0.70
1:A:462:ARG:HH11	1:A:506:ARG:HH11	1.39	0.70
1:A:1093:VAL:HG21	1:A:1605:LEU:HD23	1.73	0.70
1:A:210:VAL:HG11	1:A:922:LEU:HB3	1.73	0.69
1:D:462:ARG:HH11	1:D:506:ARG:HH11	1.40	0.69
1:B:210:VAL:HG11	1:B:922:LEU:HB3	1.74	0.69
1:B:1163:TYR:HB2	1:B:1245:LEU:HD21	1.72	0.69
1:D:210:VAL:HG11	1:D:922:LEU:HB3	1.73	0.69
1:E:300:ALA:HA	1:E:303:PHE:CD2	2.27	0.69
1:A:1108:THR:HG1	1:A:1128:HIS:HE2	1.40	0.69
1:A:2253:TRP:HA	1:E:698:ALA:HB1	1.75	0.69
1:B:746:VAL:HB	1:B:749:GLN:HB2	1.74	0.69
1:E:462:ARG:HH11	1:E:506:ARG:HH11	1.41	0.69
1:E:746:VAL:HB	1:E:749:GLN:HB2	1.75	0.69
1:A:1163:TYR:HB2	1:A:1245:LEU:HD21	1.73	0.69
1:D:746:VAL:HB	1:D:749:GLN:HB2	1.74	0.69
1:B:462:ARG:HH11	1:B:506:ARG:HH11	1.41	0.68
1:A:746:VAL:HB	1:A:749:GLN:HB2	1.76	0.68
1:C:746:VAL:HB	1:C:749:GLN:HB2	1.73	0.67
1:C:2356:GLU:HA	1:C:2359:LYS:HG2	1.76	0.66
1:E:2356:GLU:HA	1:E:2359:LYS:HG2	1.77	0.66
1:B:2356:GLU:HA	1:B:2359:LYS:HG2	1.77	0.66
1:C:505:GLN:HE22	1:C:582:LEU:HD13	1.61	0.66
1:D:121:GLU:HG2	1:D:124:ARG:HH21	1.61	0.66
1:D:2356:GLU:HA	1:D:2359:LYS:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:GLU:HG2	1:C:124:ARG:HH21	1.61	0.65
1:E:2068:LEU:HD22	1:E:2227:LEU:HG	1.78	0.65
1:C:1069:LEU:HD23	1:C:1786:GLU:HG3	1.78	0.65
1:A:2255:ARG:NH2	1:E:703:SER:O	2.27	0.65
1:D:698:ALA:HB1	1:E:2253:TRP:HA	1.79	0.65
1:A:121:GLU:HG2	1:A:124:ARG:HH21	1.62	0.64
1:A:659:TYR:HB2	1:A:754:GLN:HG2	1.79	0.64
1:B:703:SER:O	1:C:2255:ARG:NH2	2.28	0.64
1:D:2068:LEU:HD22	1:D:2227:LEU:HG	1.79	0.64
1:A:2068:LEU:HD22	1:A:2227:LEU:HG	1.78	0.64
1:D:659:TYR:HB2	1:D:754:GLN:HG2	1.78	0.64
1:A:703:SER:O	1:B:2255:ARG:NH2	2.28	0.64
1:D:698:ALA:HB2	1:E:2256:GLY:HA3	1.79	0.64
1:A:2356:GLU:HA	1:A:2359:LYS:HG2	1.78	0.64
1:A:91:GLY:N	1:A:94:ASN:HD22	1.96	0.63
1:A:505:GLN:HE22	1:A:582:LEU:HD13	1.64	0.63
1:B:2068:LEU:HD22	1:B:2227:LEU:HG	1.79	0.63
1:B:659:TYR:HB2	1:B:754:GLN:HG2	1.80	0.63
1:E:91:GLY:N	1:E:94:ASN:HD22	1.96	0.63
1:C:703:SER:O	1:D:2255:ARG:NH2	2.29	0.63
1:E:568:ILE:HD11	1:E:606:ASP:HB2	1.81	0.63
1:A:519:PHE:O	1:A:553:ARG:NH2	2.31	0.63
1:A:1069:LEU:HD23	1:A:1786:GLU:HG3	1.80	0.63
1:B:121:GLU:HG2	1:B:124:ARG:HH21	1.64	0.63
1:D:505:GLN:HE22	1:D:582:LEU:HD13	1.64	0.63
1:E:2025:ASN:OD1	1:E:2272:ARG:NH1	2.30	0.63
1:D:1864:GLY:HA3	1:D:1883:TYR:CE1	2.34	0.63
1:E:121:GLU:HG2	1:E:124:ARG:HH21	1.62	0.63
1:E:519:PHE:O	1:E:553:ARG:NH2	2.31	0.63
1:C:670:LEU:HA	1:C:699:THR:HG21	1.81	0.62
1:A:1864:GLY:HA3	1:A:1883:TYR:CE1	2.34	0.62
1:A:368:LEU:N	1:A:381:THR:O	2.27	0.62
1:C:698:ALA:HB2	1:D:2256:GLY:HA3	1.81	0.62
1:D:703:SER:O	1:E:2255:ARG:NH2	2.28	0.62
1:E:1069:LEU:HD23	1:E:1786:GLU:HG3	1.81	0.62
1:B:2277:GLU:HA	1:B:2317:MET:HE1	1.81	0.62
1:C:91:GLY:N	1:C:94:ASN:HD22	1.97	0.62
1:C:659:TYR:HB2	1:C:754:GLN:HG2	1.80	0.62
1:E:1783:LEU:HD12	1:E:1788:ASN:HB3	1.81	0.62
1:B:368:LEU:N	1:B:381:THR:O	2.27	0.62
1:B:505:GLN:HE22	1:B:582:LEU:HD13	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1864:GLY:HA3	1:E:1883:TYR:CE1	2.34	0.62
1:A:698:ALA:HB2	1:B:2256:GLY:HA3	1.81	0.62
1:B:1885:GLN:HA	1:B:1888:HIS:CE1	2.35	0.62
1:A:2277:GLU:HA	1:A:2317:MET:HE1	1.82	0.62
1:C:568:ILE:HD11	1:C:606:ASP:HB2	1.82	0.62
1:D:2277:GLU:HA	1:D:2317:MET:HE1	1.82	0.62
1:A:1164:LYS:HE2	1:B:1611:ARG:HG2	1.81	0.61
1:A:2256:GLY:HA3	1:E:698:ALA:HB2	1.81	0.61
1:B:1864:GLY:HA3	1:B:1883:TYR:CE1	2.34	0.61
1:B:2067:ASN:HB3	1:B:2227:LEU:HD21	1.82	0.61
1:D:1069:LEU:HD23	1:D:1786:GLU:HG3	1.81	0.61
1:A:458:GLU:OE2	1:A:506:ARG:NH1	2.30	0.61
1:B:1783:LEU:HD12	1:B:1788:ASN:HB3	1.81	0.61
1:A:1885:GLN:HA	1:A:1888:HIS:CE1	2.35	0.61
1:B:2016:LEU:O	1:C:2327:ARG:NH2	2.34	0.61
1:E:505:GLN:HE22	1:E:582:LEU:HD13	1.66	0.61
1:C:2068:LEU:HD22	1:C:2227:LEU:HG	1.80	0.61
1:D:1783:LEU:HD12	1:D:1788:ASN:HB3	1.82	0.61
1:C:1783:LEU:HD12	1:C:1788:ASN:HB3	1.82	0.61
1:B:91:GLY:N	1:B:94:ASN:HD22	1.97	0.61
1:B:2153:ARG:NH1	1:B:2159:GLU:OE1	2.31	0.61
1:D:1885:GLN:HA	1:D:1888:HIS:CE1	2.35	0.61
1:D:2438:LYS:HG3	1:D:2446:GLU:HG3	1.83	0.61
1:E:2504:LEU:HD21	1:E:2507:ILE:HD11	1.82	0.61
1:C:2016:LEU:O	1:D:2327:ARG:NH2	2.34	0.61
1:C:2504:LEU:HD21	1:C:2507:ILE:HD11	1.82	0.61
1:C:1864:GLY:HA3	1:C:1883:TYR:CE1	2.35	0.61
1:C:2218:GLU:OE1	1:D:2073:LYS:NZ	2.34	0.61
1:A:568:ILE:HD11	1:A:606:ASP:HB2	1.83	0.61
1:B:2438:LYS:HG3	1:B:2446:GLU:HG3	1.83	0.61
1:B:2504:LEU:HD21	1:B:2507:ILE:HD11	1.81	0.61
1:C:519:PHE:O	1:C:553:ARG:NH2	2.34	0.61
1:E:1885:GLN:HA	1:E:1888:HIS:CE1	2.35	0.61
1:B:568:ILE:HD11	1:B:606:ASP:HB2	1.81	0.60
1:A:1611:ARG:HG2	1:E:1164:LYS:HE2	1.83	0.60
1:D:2504:LEU:HD21	1:D:2507:ILE:HD11	1.83	0.60
1:E:2393:PHE:HA	1:E:2396:LEU:HD12	1.83	0.60
1:A:1783:LEU:HD12	1:A:1788:ASN:HB3	1.83	0.60
1:B:2460:PHE:CE1	1:C:2330:GLU:HB3	2.36	0.60
1:D:670:LEU:HA	1:D:699:THR:HG21	1.84	0.60
1:D:2025:ASN:OD1	1:D:2272:ARG:NH1	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2330:GLU:HB3	1:E:2460:PHE:CE1	2.36	0.60
1:B:698:ALA:HB2	1:C:2256:GLY:HA3	1.82	0.60
1:B:830:LEU:HD21	1:B:835:LEU:HD12	1.84	0.60
1:D:1794:ARG:NH2	1:D:1798:TYR:OH	2.35	0.60
1:D:2393:PHE:HA	1:D:2396:LEU:HD12	1.82	0.60
1:E:2438:LYS:HG3	1:E:2446:GLU:HG3	1.82	0.60
1:B:458:GLU:OE2	1:B:506:ARG:NH1	2.31	0.60
1:C:1885:GLN:HA	1:C:1888:HIS:CE1	2.36	0.60
1:D:2218:GLU:OE1	1:E:2073:LYS:NZ	2.34	0.60
1:E:659:TYR:HB2	1:E:754:GLN:HG2	1.83	0.60
1:E:830:LEU:HD21	1:E:835:LEU:HD12	1.83	0.60
1:B:2393:PHE:HA	1:B:2396:LEU:HD12	1.83	0.60
1:C:2025:ASN:OD1	1:C:2272:ARG:NH1	2.32	0.60
1:C:2438:LYS:HG3	1:C:2446:GLU:HG3	1.82	0.60
1:D:2460:PHE:CE1	1:E:2330:GLU:HB3	2.37	0.60
1:A:2460:PHE:CE1	1:B:2330:GLU:HB3	2.37	0.60
1:B:1069:LEU:HD23	1:B:1786:GLU:HG3	1.83	0.60
1:C:2460:PHE:CE1	1:D:2330:GLU:HB3	2.37	0.60
1:D:519:PHE:O	1:D:553:ARG:NH2	2.34	0.60
1:D:1607:THR:HG21	1:D:1768:PHE:HZ	1.66	0.60
1:B:670:LEU:HA	1:B:699:THR:HG21	1.82	0.60
1:D:568:ILE:HD11	1:D:606:ASP:HB2	1.83	0.60
1:A:2504:LEU:HD21	1:A:2507:ILE:HD11	1.82	0.59
1:C:337:ASN:ND2	1:C:421:TYR:O	2.25	0.59
1:B:2218:GLU:OE1	1:C:2073:LYS:NZ	2.33	0.59
1:D:91:GLY:N	1:D:94:ASN:HD22	2.00	0.59
1:A:2073:LYS:NZ	1:E:2218:GLU:OE1	2.34	0.59
1:A:830:LEU:HD21	1:A:835:LEU:HD12	1.84	0.59
1:A:2016:LEU:O	1:B:2327:ARG:NH2	2.35	0.59
1:C:741:GLY:HA2	1:E:2005:GLY:HA2	1.85	0.59
1:D:830:LEU:HD21	1:D:835:LEU:HD12	1.83	0.59
1:A:670:LEU:HA	1:A:699:THR:HG21	1.83	0.59
1:E:2277:GLU:HA	1:E:2317:MET:HE1	1.85	0.59
1:D:2016:LEU:O	1:E:2327:ARG:NH2	2.34	0.59
1:A:2005:GLY:HA2	1:D:741:GLY:HA2	1.85	0.59
1:A:2393:PHE:HA	1:A:2396:LEU:HD12	1.85	0.59
1:A:2218:GLU:OE1	1:B:2073:LYS:NZ	2.35	0.58
1:C:540:SER:HB2	1:D:848:GLN:NE2	2.18	0.58
1:E:368:LEU:N	1:E:381:THR:O	2.27	0.58
1:A:741:GLY:HA2	1:C:2005:GLY:HA2	1.86	0.58
1:B:540:SER:HB2	1:C:848:GLN:NE2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2067:ASN:HB3	1:C:2227:LEU:HD21	1.84	0.58
1:C:2277:GLU:HA	1:C:2317:MET:HE1	1.85	0.58
1:E:337:ASN:ND2	1:E:421:TYR:O	2.25	0.58
1:A:848:GLN:NE2	1:E:540:SER:HB2	2.18	0.58
1:B:2005:GLY:HA2	1:E:741:GLY:HA2	1.85	0.58
1:E:1607:THR:HG21	1:E:1768:PHE:HZ	1.67	0.58
1:C:830:LEU:HD21	1:C:835:LEU:HD12	1.84	0.58
1:C:1607:THR:HG21	1:C:1768:PHE:HZ	1.67	0.58
1:D:540:SER:HB2	1:E:848:GLN:NE2	2.18	0.58
1:A:2438:LYS:HG3	1:A:2446:GLU:HG3	1.86	0.58
1:B:741:GLY:HA2	1:D:2005:GLY:HA2	1.86	0.58
1:E:198:THR:O	1:E:445:ARG:NH1	2.37	0.58
1:A:540:SER:HB2	1:B:848:GLN:NE2	2.18	0.58
1:B:1607:THR:HG21	1:B:1768:PHE:HZ	1.67	0.58
1:C:2219:ALA:HA	1:D:2073:LYS:HZ1	1.68	0.58
1:D:2246:SER:HA	1:D:2250:LEU:HD23	1.85	0.58
1:A:2112:ASN:HA	1:A:2115:MET:HG2	1.86	0.58
1:C:2393:PHE:HA	1:C:2396:LEU:HD12	1.84	0.58
1:A:110:SER:HG	1:A:1902:TRP:CD1	2.22	0.58
1:A:1607:THR:HG21	1:A:1768:PHE:HZ	1.69	0.58
1:B:519:PHE:O	1:B:553:ARG:NH2	2.37	0.58
1:B:2246:SER:HA	1:B:2250:LEU:HD23	1.85	0.58
1:E:458:GLU:OE2	1:E:506:ARG:NH1	2.30	0.58
1:E:2040:LEU:O	1:E:2044:ILE:HG12	2.04	0.58
1:A:2327:ARG:NH2	1:E:2016:LEU:O	2.36	0.58
1:B:1794:ARG:NH2	1:B:1798:TYR:OH	2.37	0.58
1:C:505:GLN:NE2	1:C:582:LEU:HD13	2.19	0.58
1:D:2153:ARG:NH1	1:D:2159:GLU:OE1	2.32	0.57
1:C:458:GLU:OE2	1:C:506:ARG:NH1	2.31	0.57
1:C:1966:ARG:HD2	1:C:1976:ILE:HG13	1.86	0.57
1:D:612:VAL:HG22	1:D:637:ILE:HD12	1.86	0.57
1:D:2067:ASN:HB3	1:D:2227:LEU:HD21	1.86	0.57
1:D:2112:ASN:HA	1:D:2115:MET:HG2	1.86	0.57
1:A:2246:SER:HA	1:A:2250:LEU:HD23	1.85	0.57
1:B:505:GLN:NE2	1:B:582:LEU:HD13	2.19	0.57
1:B:2040:LEU:O	1:B:2044:ILE:HG12	2.05	0.57
1:C:2246:SER:HA	1:C:2250:LEU:HD23	1.84	0.57
1:D:505:GLN:NE2	1:D:582:LEU:HD13	2.20	0.57
1:E:670:LEU:HA	1:E:699:THR:HG21	1.85	0.57
1:E:2246:SER:HA	1:E:2250:LEU:HD23	1.86	0.57
1:A:2040:LEU:O	1:A:2044:ILE:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2353:LEU:HD23	1:B:2357:ILE:HD11	1.87	0.57
1:C:141:ARG:HH22	1:C:1005:GLU:CD	2.13	0.57
1:C:1220:LYS:HE2	1:C:1267:LEU:HB3	1.85	0.57
1:C:2040:LEU:O	1:C:2044:ILE:HG12	2.05	0.57
1:C:2112:ASN:HA	1:C:2115:MET:HG2	1.85	0.57
1:C:2153:ARG:NH1	1:C:2159:GLU:OE1	2.32	0.57
1:E:2067:ASN:HB3	1:E:2227:LEU:HD21	1.87	0.57
1:E:2112:ASN:HA	1:E:2115:MET:HG2	1.85	0.57
1:B:797:ASP:OD1	1:B:798:ALA:N	2.38	0.57
1:B:2112:ASN:HA	1:B:2115:MET:HG2	1.87	0.57
1:A:2353:LEU:HD23	1:A:2357:ILE:HD11	1.87	0.56
1:B:646:TRP:CZ2	1:B:768:SER:HB3	2.40	0.56
1:D:2040:LEU:O	1:D:2044:ILE:HG12	2.05	0.56
1:A:836:ALA:HB2	1:A:846:LEU:HD12	1.87	0.56
1:A:2153:ARG:NH1	1:A:2159:GLU:OE1	2.32	0.56
1:C:2353:LEU:HD23	1:C:2357:ILE:HD11	1.88	0.56
1:D:337:ASN:ND2	1:D:421:TYR:O	2.25	0.56
1:D:458:GLU:OE2	1:D:506:ARG:NH1	2.32	0.56
1:D:646:TRP:CZ2	1:D:768:SER:HB3	2.40	0.56
1:D:797:ASP:OD1	1:D:798:ALA:N	2.38	0.56
1:D:1164:LYS:HE2	1:E:1611:ARG:HG2	1.85	0.56
1:D:2353:LEU:HD23	1:D:2357:ILE:HD11	1.87	0.56
1:E:1072:ASP:OD1	1:E:1073:THR:N	2.38	0.56
1:E:2353:LEU:HD23	1:E:2357:ILE:HD11	1.87	0.56
1:A:1966:ARG:HD2	1:A:1976:ILE:HG13	1.87	0.56
1:B:1072:ASP:OD1	1:B:1073:THR:N	2.38	0.56
1:E:836:ALA:HB2	1:E:846:LEU:HD12	1.87	0.56
1:B:1966:ARG:HD2	1:B:1976:ILE:HG13	1.87	0.56
1:E:797:ASP:OD1	1:E:798:ALA:N	2.38	0.56
1:E:2153:ARG:NH1	1:E:2159:GLU:OE1	2.33	0.56
1:C:797:ASP:OD1	1:C:798:ALA:N	2.38	0.56
1:C:2103:TYR:CE1	1:C:2189:ARG:HG2	2.40	0.56
1:D:836:ALA:HB2	1:D:846:LEU:HD12	1.88	0.56
1:A:337:ASN:ND2	1:A:421:TYR:O	2.25	0.56
1:B:836:ALA:HB2	1:B:846:LEU:HD12	1.88	0.56
1:B:2433:LEU:HA	1:B:2484:LEU:HA	1.88	0.56
1:D:1072:ASP:OD1	1:D:1073:THR:N	2.39	0.56
1:D:2219:ALA:HA	1:E:2073:LYS:HZ1	1.71	0.56
1:A:646:TRP:CZ2	1:A:768:SER:HB3	2.41	0.56
1:A:2067:ASN:HB3	1:A:2227:LEU:HD21	1.87	0.56
1:A:141:ARG:HH22	1:A:1005:GLU:CD	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ASN:ND2	1:B:421:TYR:O	2.25	0.56
1:C:646:TRP:CZ2	1:C:768:SER:HB3	2.41	0.56
1:D:1271:ALA:HB1	1:E:1611:ARG:HD3	1.88	0.56
1:A:797:ASP:OD1	1:A:798:ALA:N	2.38	0.56
1:A:1024:TYR:O	1:A:1030:THR:OG1	2.23	0.56
1:B:141:ARG:HH22	1:B:1005:GLU:CD	2.13	0.56
1:C:612:VAL:HG22	1:C:637:ILE:HD12	1.88	0.56
1:A:505:GLN:NE2	1:A:582:LEU:HD13	2.20	0.55
1:C:836:ALA:HB2	1:C:846:LEU:HD12	1.88	0.55
1:C:2341:TYR:OH	1:C:2390:SER:O	2.20	0.55
1:D:2433:LEU:HA	1:D:2484:LEU:HA	1.88	0.55
1:E:141:ARG:HH22	1:E:1005:GLU:CD	2.14	0.55
1:E:646:TRP:CZ2	1:E:768:SER:HB3	2.41	0.55
1:C:1164:LYS:HE2	1:D:1611:ARG:HG2	1.87	0.55
1:D:2204:LYS:HG2	1:E:2087:LYS:HD2	1.88	0.55
1:E:2433:LEU:HA	1:E:2484:LEU:HA	1.87	0.55
1:A:1252:GLN:HB3	1:A:1297:ASN:OD1	2.06	0.55
1:E:557:ILE:HB	1:E:561:SER:OG	2.07	0.55
1:E:1966:ARG:HD2	1:E:1976:ILE:HG13	1.87	0.55
1:A:2025:ASN:OD1	1:A:2272:ARG:NH1	2.33	0.55
1:B:1058:ASP:O	1:B:1062:GLN:HG3	2.06	0.55
1:E:505:GLN:NE2	1:E:582:LEU:HD13	2.20	0.55
1:A:1072:ASP:OD1	1:A:1073:THR:N	2.39	0.55
1:C:198:THR:O	1:C:445:ARG:NH1	2.39	0.55
1:D:141:ARG:HH22	1:D:1005:GLU:CD	2.13	0.55
1:D:1117:ASP:OD1	1:D:1118:ALA:N	2.38	0.55
1:A:612:VAL:HG22	1:A:637:ILE:HD12	1.87	0.55
1:E:120:THR:O	1:E:124:ARG:HG3	2.07	0.55
1:A:2103:TYR:CE1	1:A:2189:ARG:HG2	2.42	0.55
1:B:253:GLU:O	1:B:442:LYS:NZ	2.29	0.55
1:B:1164:LYS:HE2	1:C:1611:ARG:HG2	1.87	0.55
1:B:1252:GLN:HB3	1:B:1297:ASN:OD1	2.07	0.55
1:D:368:LEU:N	1:D:381:THR:O	2.27	0.55
1:B:1868:TYR:HB3	1:B:1976:ILE:HD12	1.89	0.55
1:C:120:THR:O	1:C:124:ARG:HG3	2.07	0.55
1:C:368:LEU:HG	1:C:370:ILE:HD11	1.89	0.55
1:A:2433:LEU:HA	1:A:2484:LEU:HA	1.88	0.55
1:C:1252:GLN:HB3	1:C:1297:ASN:OD1	2.07	0.55
1:D:1630:GLN:HG2	1:D:1772:PHE:CE2	2.42	0.55
1:A:557:ILE:HB	1:A:561:SER:OG	2.07	0.54
1:B:2025:ASN:OD1	1:B:2272:ARG:NH1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2103:TYR:CE1	1:B:2189:ARG:HG2	2.43	0.54
1:C:2103:TYR:CE1	1:C:2193:GLU:HG2	2.43	0.54
1:D:1966:ARG:HD2	1:D:1976:ILE:HG13	1.87	0.54
1:A:811:VAL:HG22	1:A:822:LEU:HD21	1.89	0.54
1:B:120:THR:O	1:B:124:ARG:HG3	2.07	0.54
1:C:368:LEU:N	1:C:381:THR:O	2.27	0.54
1:D:120:THR:O	1:D:124:ARG:HG3	2.06	0.54
1:D:1058:ASP:O	1:D:1062:GLN:HG3	2.07	0.54
1:A:120:THR:O	1:A:124:ARG:HG3	2.07	0.54
1:A:368:LEU:HG	1:A:370:ILE:HD11	1.89	0.54
1:A:1794:ARG:NH2	1:A:1798:TYR:OH	2.39	0.54
1:A:2073:LYS:HZ1	1:E:2219:ALA:HA	1.72	0.54
1:C:1072:ASP:OD1	1:C:1073:THR:N	2.39	0.54
1:C:2337:LEU:HB3	1:C:2507:ILE:HB	1.89	0.54
1:D:1252:GLN:HB3	1:D:1297:ASN:OD1	2.07	0.54
1:E:300:ALA:HA	1:E:303:PHE:HD2	1.73	0.54
1:E:612:VAL:HG22	1:E:637:ILE:HD12	1.88	0.54
1:A:1630:GLN:HG2	1:A:1772:PHE:CE2	2.42	0.54
1:E:1252:GLN:HB3	1:E:1297:ASN:OD1	2.07	0.54
1:B:510:ASN:OD1	1:C:153:GLN:NE2	2.38	0.54
1:C:2433:LEU:HA	1:C:2484:LEU:HA	1.88	0.54
1:B:198:THR:O	1:B:445:ARG:NH1	2.41	0.54
1:B:368:LEU:HG	1:B:370:ILE:HD11	1.89	0.54
1:D:2426:TYR:HB3	1:E:2334:THR:HG21	1.88	0.54
1:A:195:SER:HB3	1:A:198:THR:OG1	2.08	0.54
1:A:300:ALA:HA	1:A:303:PHE:HD2	1.72	0.54
1:A:848:GLN:HE22	1:E:540:SER:HB2	1.73	0.54
1:C:195:SER:HB3	1:C:198:THR:OG1	2.08	0.54
1:E:1630:GLN:HG2	1:E:1772:PHE:CE2	2.42	0.54
1:A:198:THR:O	1:A:445:ARG:NH1	2.40	0.54
1:A:1271:ALA:HB1	1:B:1611:ARG:HD3	1.90	0.54
1:D:368:LEU:HG	1:D:370:ILE:HD11	1.89	0.54
1:D:811:VAL:HG22	1:D:822:LEU:HD21	1.89	0.54
1:A:1058:ASP:O	1:A:1062:GLN:HG3	2.06	0.54
1:C:557:ILE:HB	1:C:561:SER:OG	2.07	0.54
1:D:557:ILE:HB	1:D:561:SER:OG	2.07	0.54
1:E:2337:LEU:HB3	1:E:2507:ILE:HB	1.90	0.54
1:A:2103:TYR:CE1	1:A:2193:GLU:HG2	2.43	0.53
1:B:612:VAL:HG22	1:B:637:ILE:HD12	1.89	0.53
1:C:2053:ASN:ND2	1:C:2241:LEU:HD11	2.23	0.53
1:D:2141:VAL:HG21	1:E:1175:LYS:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2103:TYR:CE1	1:E:2189:ARG:HG2	2.44	0.53
1:C:300:ALA:HA	1:C:303:PHE:HD2	1.72	0.53
1:E:197:ALA:N	1:E:948:THR:HG21	2.23	0.53
1:A:1071:ALA:HB2	1:A:1791:GLU:OE2	2.09	0.53
1:C:2426:TYR:HB3	1:D:2334:THR:HG21	1.90	0.53
1:E:195:SER:HB3	1:E:198:THR:OG1	2.08	0.53
1:E:368:LEU:HG	1:E:370:ILE:HD11	1.89	0.53
1:E:811:VAL:HG22	1:E:822:LEU:HD21	1.90	0.53
1:B:557:ILE:HB	1:B:561:SER:OG	2.07	0.53
1:C:268:PHE:HZ	1:C:441:ASN:HB2	1.74	0.53
1:C:1058:ASP:O	1:C:1062:GLN:HG3	2.09	0.53
1:C:1271:ALA:HB1	1:D:1611:ARG:HD3	1.90	0.53
1:D:198:THR:O	1:D:445:ARG:NH1	2.41	0.53
1:D:540:SER:HB2	1:E:848:GLN:HE22	1.74	0.53
1:D:1220:LYS:HE2	1:D:1267:LEU:HB3	1.91	0.53
1:E:2341:TYR:OH	1:E:2390:SER:O	2.21	0.53
1:C:926:LEU:HD22	1:C:930:GLN:HB3	1.91	0.53
1:D:1790:ASP:OD1	1:D:1791:GLU:N	2.42	0.53
1:D:2103:TYR:CE1	1:D:2189:ARG:HG2	2.43	0.53
1:A:197:ALA:N	1:A:948:THR:HG21	2.24	0.53
1:B:540:SER:HB2	1:C:848:GLN:HE22	1.73	0.53
1:B:719:GLN:HB3	1:B:724:ALA:HB1	1.90	0.53
1:B:2141:VAL:HG21	1:C:1175:LYS:HE2	1.91	0.53
1:B:2426:TYR:HB3	1:C:2334:THR:HG21	1.89	0.53
1:C:540:SER:HB2	1:D:848:GLN:HE22	1.74	0.53
1:B:1271:ALA:HB1	1:C:1611:ARG:HD3	1.90	0.53
1:D:197:ALA:N	1:D:948:THR:HG21	2.23	0.53
1:D:300:ALA:HA	1:D:303:PHE:HD2	1.73	0.53
1:E:2122:ALA:HA	1:E:2171:VAL:HG23	1.91	0.53
1:B:195:SER:HB3	1:B:198:THR:OG1	2.08	0.53
1:B:1790:ASP:OD1	1:B:1791:GLU:N	2.42	0.53
1:B:2204:LYS:HG2	1:C:2087:LYS:HD2	1.90	0.53
1:E:671:LEU:HD22	1:E:734:LEU:HD21	1.90	0.53
1:A:1220:LYS:HE2	1:A:1267:LEU:HB3	1.90	0.53
1:C:510:ASN:OD1	1:D:153:GLN:NE2	2.39	0.53
1:C:671:LEU:HD22	1:C:734:LEU:HD21	1.90	0.53
1:E:253:GLU:O	1:E:442:LYS:NZ	2.30	0.53
1:E:1058:ASP:O	1:E:1062:GLN:HG3	2.08	0.53
1:A:540:SER:HB2	1:B:848:GLN:HE22	1.74	0.53
1:A:1611:ARG:HD3	1:E:1271:ALA:HB1	1.91	0.53
1:B:1108:THR:OG1	1:B:1128:HIS:NE2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:462:ARG:NH1	1:E:506:ARG:HH11	2.07	0.53
1:A:2426:TYR:HB3	1:B:2334:THR:HG21	1.91	0.52
1:B:197:ALA:N	1:B:948:THR:HG21	2.23	0.52
1:C:1071:ALA:HB2	1:C:1791:GLU:OE2	2.09	0.52
1:D:195:SER:HB3	1:D:198:THR:OG1	2.08	0.52
1:D:1868:TYR:HB3	1:D:1976:ILE:HD12	1.91	0.52
1:A:2219:ALA:HA	1:B:2073:LYS:HZ1	1.73	0.52
1:B:268:PHE:HZ	1:B:441:ASN:HB2	1.75	0.52
1:B:300:ALA:HA	1:B:303:PHE:HD2	1.73	0.52
1:B:671:LEU:HD22	1:B:734:LEU:HD21	1.90	0.52
1:C:1790:ASP:OD1	1:C:1791:GLU:N	2.42	0.52
1:E:601:THR:HG22	1:E:604:GLU:OE1	2.10	0.52
1:E:1220:LYS:HE2	1:E:1267:LEU:HB3	1.91	0.52
1:E:1722:GLY:O	1:E:1739:SER:HB2	2.10	0.52
1:A:1790:ASP:OD1	1:A:1791:GLU:N	2.42	0.52
1:B:2053:ASN:ND2	1:B:2241:LEU:HD11	2.24	0.52
1:B:2122:ALA:HA	1:B:2171:VAL:HG23	1.91	0.52
1:B:2341:TYR:OH	1:B:2390:SER:O	2.22	0.52
1:D:671:LEU:HD22	1:D:734:LEU:HD21	1.90	0.52
1:D:812:ASN:HA	1:E:1998:ALA:HB2	1.91	0.52
1:E:2053:ASN:ND2	1:E:2241:LEU:HD11	2.24	0.52
1:B:2219:ALA:HA	1:C:2073:LYS:HZ1	1.73	0.52
1:C:1794:ARG:NH2	1:C:1798:TYR:OH	2.42	0.52
1:D:268:PHE:HZ	1:D:441:ASN:HB2	1.74	0.52
1:D:1878:GLU:HA	1:D:1881:MET:HG3	1.91	0.52
1:E:1878:GLU:HA	1:E:1881:MET:HG3	1.90	0.52
1:A:2334:THR:HG21	1:E:2426:TYR:HB3	1.90	0.52
1:B:1117:ASP:OD1	1:B:1118:ALA:N	2.39	0.52
1:B:1630:GLN:HG2	1:B:1772:PHE:CE2	2.44	0.52
1:C:197:ALA:N	1:C:948:THR:HG21	2.24	0.52
1:E:1117:ASP:OD1	1:E:1118:ALA:N	2.39	0.52
1:C:811:VAL:HG22	1:C:822:LEU:HD21	1.91	0.52
1:E:926:LEU:HD22	1:E:930:GLN:HB3	1.92	0.52
1:A:719:GLN:HB3	1:A:724:ALA:HB1	1.90	0.52
1:A:812:ASN:HA	1:B:1998:ALA:HB2	1.91	0.52
1:B:237:LEU:HD11	1:B:483:TYR:HB2	1.91	0.52
1:B:1230:ARG:NH2	1:B:1251:ASN:OD1	2.43	0.52
1:D:462:ARG:NH1	1:D:506:ARG:HH11	2.07	0.52
1:A:2141:VAL:HG21	1:B:1175:LYS:HE2	1.92	0.52
1:B:462:ARG:NH1	1:B:506:ARG:HH11	2.08	0.52
1:C:462:ARG:NH1	1:C:506:ARG:HH11	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:THR:HG22	1:C:604:GLU:OE1	2.10	0.52
1:E:719:GLN:HB3	1:E:724:ALA:HB1	1.89	0.52
1:E:2103:TYR:CE1	1:E:2193:GLU:HG2	2.45	0.52
1:A:268:PHE:HZ	1:A:441:ASN:HB2	1.75	0.52
1:A:601:THR:HG22	1:A:604:GLU:OE1	2.10	0.52
1:C:1630:GLN:HG2	1:C:1772:PHE:CE2	2.45	0.52
1:C:1878:GLU:HA	1:C:1881:MET:HG3	1.91	0.52
1:E:497:ILE:HG21	1:E:589:TYR:HD2	1.74	0.52
1:A:237:LEU:HD11	1:A:483:TYR:HB2	1.92	0.52
1:A:926:LEU:HD22	1:A:930:GLN:HB3	1.92	0.52
1:A:1878:GLU:HA	1:A:1881:MET:HG3	1.91	0.52
1:B:601:THR:HG22	1:B:604:GLU:OE1	2.10	0.52
1:B:678:LEU:HD11	1:B:692:MET:HA	1.92	0.52
1:B:811:VAL:HG22	1:B:822:LEU:HD21	1.91	0.52
1:B:2266:TYR:CZ	1:B:2297:TRP:HB2	2.45	0.52
1:B:1722:GLY:O	1:B:1739:SER:HB2	2.11	0.51
1:C:1146:LYS:NZ	1:C:1147:ILE:O	2.40	0.51
1:C:1722:GLY:O	1:C:1739:SER:HB2	2.10	0.51
1:D:1071:ALA:HB2	1:D:1791:GLU:OE2	2.10	0.51
1:A:671:LEU:HD22	1:A:734:LEU:HD21	1.92	0.51
1:A:1614:VAL:O	1:A:1618:THR:HG23	2.11	0.51
1:B:537:ASP:HA	1:B:577:LYS:HA	1.91	0.51
1:B:564:ARG:NH2	1:C:842:ASP:OD1	2.43	0.51
1:B:2337:LEU:HB3	1:B:2507:ILE:HB	1.93	0.51
1:C:2338:ALA:HA	1:C:2353:LEU:HD13	1.92	0.51
1:E:1794:ARG:NH2	1:E:1798:TYR:OH	2.43	0.51
1:A:537:ASP:HA	1:A:577:LYS:HA	1.92	0.51
1:A:1722:GLY:O	1:A:1739:SER:HB2	2.10	0.51
1:B:1614:VAL:O	1:B:1618:THR:HG23	2.11	0.51
1:A:678:LEU:HD11	1:A:692:MET:HA	1.92	0.51
1:C:2004:GLN:H	1:C:2300:THR:HG22	1.76	0.51
1:D:2341:TYR:OH	1:D:2390:SER:O	2.22	0.51
1:E:1071:ALA:HB2	1:E:1791:GLU:OE2	2.11	0.51
1:A:2204:LYS:HG2	1:B:2087:LYS:HD2	1.92	0.51
1:D:601:THR:HG22	1:D:604:GLU:OE1	2.10	0.51
1:E:1230:ARG:NH2	1:E:1251:ASN:OD1	2.43	0.51
1:A:2053:ASN:ND2	1:A:2241:LEU:HD11	2.25	0.51
1:A:2266:TYR:CZ	1:A:2297:TRP:HB2	2.46	0.51
1:B:536:ILE:HD13	1:B:547:ARG:HB2	1.93	0.51
1:C:1868:TYR:HB3	1:C:1976:ILE:HD12	1.93	0.51
1:D:237:LEU:HD11	1:D:483:TYR:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:ASP:OD1	1:E:564:ARG:NH2	2.44	0.51
1:A:153:GLN:NE2	1:E:510:ASN:OD1	2.39	0.51
1:A:724:ALA:O	1:A:729:LYS:NZ	2.32	0.51
1:B:1878:GLU:HA	1:B:1881:MET:HG3	1.92	0.51
1:B:2132:ARG:HH11	1:B:2163:TYR:HB3	1.76	0.51
1:D:926:LEU:HD22	1:D:930:GLN:HB3	1.93	0.51
1:D:2122:ALA:HA	1:D:2171:VAL:HG23	1.93	0.51
1:E:268:PHE:HZ	1:E:441:ASN:HB2	1.74	0.51
1:E:2266:TYR:CZ	1:E:2297:TRP:HB2	2.45	0.51
1:B:2103:TYR:CE1	1:B:2193:GLU:HG2	2.45	0.51
1:D:2337:LEU:HB3	1:D:2507:ILE:HB	1.92	0.51
1:E:370:ILE:HG13	1:E:410:LEU:HG	1.93	0.51
1:E:1790:ASP:OD1	1:E:1791:GLU:N	2.43	0.51
1:A:253:GLU:O	1:A:442:LYS:NZ	2.28	0.51
1:A:2122:ALA:HA	1:A:2171:VAL:HG23	1.93	0.51
1:C:719:GLN:HB3	1:C:724:ALA:HB1	1.92	0.51
1:D:2103:TYR:CE1	1:D:2193:GLU:HG2	2.46	0.51
1:A:453:SER:HB3	1:A:456:ILE:HG12	1.93	0.50
1:A:462:ARG:NH1	1:A:506:ARG:HH11	2.06	0.50
1:A:2087:LYS:HD2	1:E:2204:LYS:HG2	1.92	0.50
1:D:1722:GLY:O	1:D:1739:SER:HB2	2.10	0.50
1:D:2053:ASN:ND2	1:D:2241:LEU:HD11	2.26	0.50
1:D:2266:TYR:CZ	1:D:2297:TRP:HB2	2.47	0.50
1:A:2341:TYR:OH	1:A:2390:SER:O	2.21	0.50
1:B:497:ILE:HG21	1:B:589:TYR:HD2	1.76	0.50
1:C:370:ILE:HG13	1:C:410:LEU:HG	1.94	0.50
1:D:537:ASP:HA	1:D:577:LYS:HA	1.94	0.50
1:E:1291:TYR:HA	1:E:1294:PHE:CE2	2.47	0.50
1:C:536:ILE:HD13	1:C:547:ARG:HB2	1.94	0.50
1:D:702:LEU:HD22	1:D:708:ALA:HB2	1.93	0.50
1:C:678:LEU:HD11	1:C:692:MET:HA	1.94	0.50
1:D:1230:ARG:NH2	1:D:1251:ASN:OD1	2.45	0.50
1:B:460:ILE:HG21	1:B:478:VAL:HG12	1.94	0.50
1:D:370:ILE:HG13	1:D:410:LEU:HG	1.94	0.50
1:D:1291:TYR:HA	1:D:1294:PHE:CE2	2.47	0.50
1:E:470:ILE:HA	1:E:474:VAL:HG11	1.93	0.50
1:E:1614:VAL:O	1:E:1618:THR:HG23	2.11	0.50
1:B:1291:TYR:HA	1:B:1294:PHE:CE2	2.47	0.50
1:B:2033:LEU:HD11	1:B:2266:TYR:HA	1.94	0.50
1:C:812:ASN:HA	1:D:1998:ALA:HB2	1.93	0.50
1:C:1230:ARG:NH2	1:C:1251:ASN:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ASN:OD1	1:B:153:GLN:NE2	2.40	0.50
1:A:1291:TYR:HA	1:A:1294:PHE:CE2	2.47	0.50
1:A:1998:ALA:HB2	1:E:812:ASN:HA	1.92	0.50
1:A:2337:LEU:HB3	1:A:2507:ILE:HB	1.93	0.50
1:C:470:ILE:HA	1:C:474:VAL:HG11	1.94	0.50
1:C:702:LEU:HD22	1:C:708:ALA:HB2	1.93	0.50
1:B:926:LEU:HD22	1:B:930:GLN:HB3	1.93	0.50
1:C:2122:ALA:HA	1:C:2171:VAL:HG23	1.94	0.50
1:C:2204:LYS:HG2	1:D:2087:LYS:HD2	1.93	0.50
1:E:471:ASN:H	1:E:474:VAL:HG12	1.76	0.50
1:A:371:LYS:HG2	1:A:377:GLU:HA	1.94	0.50
1:A:2004:GLN:H	1:A:2300:THR:HG22	1.76	0.50
1:B:370:ILE:HG13	1:B:410:LEU:HG	1.93	0.50
1:C:497:ILE:HG21	1:C:589:TYR:HD2	1.76	0.50
1:D:2393:PHE:HE1	1:D:2482:LEU:HB2	1.77	0.50
1:E:198:THR:HB	1:E:199:PRO:HA	1.94	0.50
1:E:453:SER:HB3	1:E:456:ILE:HG12	1.94	0.50
1:B:1220:LYS:HE2	1:B:1267:LEU:HB3	1.93	0.49
1:D:371:LYS:HG2	1:D:377:GLU:HA	1.93	0.49
1:E:210:VAL:HG22	1:E:926:LEU:HD11	1.94	0.49
1:E:702:LEU:HD22	1:E:708:ALA:HB2	1.93	0.49
1:A:470:ILE:HA	1:A:474:VAL:HG11	1.93	0.49
1:B:470:ILE:HA	1:B:474:VAL:HG11	1.94	0.49
1:C:522:PRO:O	1:C:553:ARG:NH1	2.45	0.49
1:C:564:ARG:NH2	1:D:842:ASP:OD1	2.45	0.49
1:C:2266:TYR:CZ	1:C:2297:TRP:HB2	2.48	0.49
1:E:2393:PHE:HE1	1:E:2482:LEU:HB2	1.77	0.49
1:A:1230:ARG:NH2	1:A:1251:ASN:OD1	2.45	0.49
1:A:1962:THR:OG1	1:A:1966:ARG:NH2	2.45	0.49
1:C:471:ASN:H	1:C:474:VAL:HG12	1.77	0.49
1:D:471:ASN:H	1:D:474:VAL:HG12	1.77	0.49
1:A:702:LEU:HD22	1:A:708:ALA:HB2	1.93	0.49
1:A:1098:HIS:HE1	1:A:1100:ASN:HB3	1.78	0.49
1:B:1071:ALA:HB2	1:B:1791:GLU:OE2	2.11	0.49
1:C:537:ASP:HA	1:C:577:LYS:HA	1.93	0.49
1:D:470:ILE:HA	1:D:474:VAL:HG11	1.93	0.49
1:A:1175:LYS:HE2	1:E:2141:VAL:HG21	1.94	0.49
1:B:1098:HIS:HE1	1:B:1100:ASN:HB3	1.78	0.49
1:C:1614:VAL:O	1:C:1618:THR:HG23	2.11	0.49
1:D:198:THR:HB	1:D:199:PRO:HA	1.94	0.49
1:D:460:ILE:HG21	1:D:478:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:GLU:HA	1:E:425:LYS:HA	1.94	0.49
1:A:1117:ASP:OD1	1:A:1118:ALA:N	2.38	0.49
1:A:2099:TYR:CE2	1:A:2195:GLN:HB3	2.48	0.49
1:B:371:LYS:HG2	1:B:377:GLU:HA	1.93	0.49
1:D:1614:VAL:O	1:D:1618:THR:HG23	2.11	0.49
1:A:370:ILE:HG13	1:A:410:LEU:HG	1.94	0.49
1:A:714:TRP:CZ3	1:A:762:LEU:HD22	2.48	0.49
1:A:1268:TYR:CD1	1:A:1278:MET:HE2	2.48	0.49
1:C:371:LYS:HG2	1:C:377:GLU:HA	1.93	0.49
1:C:1291:TYR:HA	1:C:1294:PHE:CE2	2.47	0.49
1:D:1108:THR:OG1	1:D:1128:HIS:NE2	2.37	0.49
1:E:371:LYS:HG2	1:E:377:GLU:HA	1.93	0.49
1:E:1146:LYS:NZ	1:E:1147:ILE:O	2.42	0.49
1:A:2132:ARG:HH11	1:A:2163:TYR:HB3	1.77	0.49
1:B:453:SER:HB3	1:B:456:ILE:HG12	1.94	0.49
1:D:536:ILE:HD13	1:D:547:ARG:HB2	1.94	0.49
1:D:1962:THR:OG1	1:D:1966:ARG:NH2	2.46	0.49
1:E:237:LEU:HD11	1:E:483:TYR:HB2	1.95	0.49
1:E:678:LEU:HD11	1:E:692:MET:HA	1.93	0.49
1:A:497:ILE:HG21	1:A:589:TYR:HD2	1.77	0.49
1:A:564:ARG:NH2	1:B:842:ASP:OD1	2.46	0.49
1:B:198:THR:HB	1:B:199:PRO:HA	1.94	0.49
1:C:453:SER:HB3	1:C:456:ILE:HG12	1.94	0.49
1:D:453:SER:HB3	1:D:456:ILE:HG12	1.93	0.49
1:D:564:ARG:NH2	1:E:842:ASP:OD1	2.46	0.49
1:A:2338:ALA:HA	1:A:2353:LEU:HD13	1.94	0.49
1:B:471:ASN:H	1:B:474:VAL:HG12	1.77	0.49
1:C:210:VAL:HG22	1:C:926:LEU:HD11	1.95	0.49
1:E:2099:TYR:CE2	1:E:2195:GLN:HB3	2.48	0.49
1:A:92:TYR:CD1	1:A:1956:MET:HE2	2.49	0.48
1:A:536:ILE:HD13	1:A:547:ARG:HB2	1.94	0.48
1:B:702:LEU:HD22	1:B:708:ALA:HB2	1.94	0.48
1:B:1962:THR:OG1	1:B:1966:ARG:NH2	2.46	0.48
1:D:2235:GLN:HG3	1:E:1995:LEU:HB2	1.96	0.48
1:E:1868:TYR:HB3	1:E:1976:ILE:HD12	1.95	0.48
1:A:471:ASN:H	1:A:474:VAL:HG12	1.78	0.48
1:B:2338:ALA:HA	1:B:2353:LEU:HD13	1.95	0.48
1:C:714:TRP:CZ3	1:C:762:LEU:HD22	2.48	0.48
1:D:110:SER:HG	1:D:1902:TRP:CD1	2.32	0.48
1:D:2099:TYR:CE2	1:D:2195:GLN:HB3	2.49	0.48
1:C:1098:HIS:HE1	1:C:1100:ASN:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2393:PHE:HE1	1:C:2482:LEU:HB2	1.78	0.48
1:D:92:TYR:CD1	1:D:1956:MET:HE2	2.49	0.48
1:D:1098:HIS:HE1	1:D:1100:ASN:HB3	1.79	0.48
1:E:537:ASP:HA	1:E:577:LYS:HA	1.95	0.48
1:A:198:THR:HB	1:A:199:PRO:HA	1.95	0.48
1:B:2393:PHE:HE1	1:B:2482:LEU:HB2	1.78	0.48
1:C:2132:ARG:HH11	1:C:2163:TYR:HB3	1.79	0.48
1:D:719:GLN:HB3	1:D:724:ALA:HB1	1.95	0.48
1:E:1098:HIS:HE1	1:E:1100:ASN:HB3	1.78	0.48
1:A:407:GLU:HA	1:A:425:LYS:HA	1.94	0.48
1:B:2099:TYR:CE2	1:B:2195:GLN:HB3	2.48	0.48
1:C:198:THR:HB	1:C:199:PRO:HA	1.94	0.48
1:C:460:ILE:HG21	1:C:478:VAL:HG12	1.96	0.48
1:D:678:LEU:HD11	1:D:692:MET:HA	1.95	0.48
1:D:2004:GLN:H	1:D:2300:THR:HG22	1.78	0.48
1:E:460:ILE:HG21	1:E:478:VAL:HG12	1.96	0.48
1:A:2393:PHE:HE1	1:A:2482:LEU:HB2	1.77	0.48
1:C:1024:TYR:O	1:C:1030:THR:OG1	2.26	0.48
1:D:210:VAL:HG22	1:D:926:LEU:HD11	1.96	0.48
1:E:497:ILE:HG21	1:E:589:TYR:CD2	2.49	0.48
1:A:160:SER:HA	1:A:982:LYS:HA	1.96	0.48
1:A:1124:ARG:HD2	1:A:1144:TRP:CE2	2.49	0.48
1:D:510:ASN:OD1	1:E:153:GLN:NE2	2.40	0.48
1:D:1124:ARG:HD2	1:D:1144:TRP:CE2	2.49	0.48
1:E:1124:ARG:HD2	1:E:1144:TRP:CE2	2.49	0.48
1:E:1268:TYR:CD1	1:E:1278:MET:HE2	2.49	0.48
1:A:464:VAL:HG21	1:A:474:VAL:HA	1.96	0.48
1:B:197:ALA:H	1:B:948:THR:HG21	1.79	0.47
1:D:2338:ALA:HA	1:D:2353:LEU:HD13	1.95	0.47
1:A:460:ILE:HG21	1:A:478:VAL:HG12	1.96	0.47
1:C:1268:TYR:CD1	1:C:1278:MET:HE2	2.48	0.47
1:D:464:VAL:HG21	1:D:474:VAL:HA	1.97	0.47
1:A:522:PRO:O	1:A:553:ARG:NH1	2.46	0.47
1:C:92:TYR:CD1	1:C:1956:MET:HE2	2.49	0.47
1:C:2033:LEU:HD11	1:C:2266:TYR:HA	1.96	0.47
1:D:348:PHE:CE1	1:D:352:ASN:HB3	2.50	0.47
1:D:407:GLU:HA	1:D:425:LYS:HA	1.96	0.47
1:D:497:ILE:HG21	1:D:589:TYR:HD2	1.79	0.47
1:E:2338:ALA:HA	1:E:2353:LEU:HD13	1.95	0.47
1:B:1268:TYR:CD1	1:B:1278:MET:HE2	2.49	0.47
1:C:1117:ASP:OD1	1:C:1118:ALA:N	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ARG:HG3	1:D:127:ARG:HH11	1.79	0.47
1:E:714:TRP:CZ3	1:E:762:LEU:HD22	2.49	0.47
1:A:1868:TYR:HB3	1:A:1976:ILE:HD12	1.96	0.47
1:B:2004:GLN:H	1:B:2300:THR:HG22	1.79	0.47
1:B:92:TYR:CD1	1:B:1956:MET:HE2	2.49	0.47
1:B:1124:ARG:HD2	1:B:1144:TRP:CE2	2.50	0.47
1:B:1975:SER:OG	1:B:1977:ASP:OD1	2.32	0.47
1:B:2469:PHE:H	1:C:2327:ARG:NH2	2.13	0.47
1:C:2078:LEU:HD13	1:C:2217:ARG:HA	1.97	0.47
1:E:92:TYR:CD1	1:E:1956:MET:HE2	2.49	0.47
1:E:127:ARG:HG3	1:E:127:ARG:HH11	1.79	0.47
1:E:2132:ARG:HH11	1:E:2163:TYR:HB3	1.79	0.47
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.80	0.47
1:A:2469:PHE:H	1:B:2327:ARG:NH2	2.13	0.47
1:D:1268:TYR:CD1	1:D:1278:MET:HE2	2.49	0.47
1:D:2033:LEU:HD11	1:D:2266:TYR:HA	1.96	0.47
1:E:536:ILE:HD13	1:E:547:ARG:HB2	1.96	0.47
1:A:2033:LEU:HD11	1:A:2266:TYR:HA	1.96	0.47
1:B:538:LEU:HB2	1:B:566:LEU:HD22	1.97	0.47
1:C:160:SER:HA	1:C:982:LYS:HA	1.97	0.47
1:C:1962:THR:OG1	1:C:1966:ARG:NH2	2.47	0.47
1:E:2004:GLN:H	1:E:2300:THR:HG22	1.79	0.47
1:A:348:PHE:CE1	1:A:352:ASN:HB3	2.50	0.47
1:B:407:GLU:HA	1:B:425:LYS:HA	1.97	0.47
1:B:714:TRP:CZ3	1:B:762:LEU:HD22	2.50	0.47
1:B:812:ASN:HA	1:C:1998:ALA:HB2	1.96	0.47
1:C:2469:PHE:H	1:D:2327:ARG:NH2	2.13	0.47
1:A:1001:LEU:HD23	1:A:1013:ILE:HD12	1.97	0.46
1:C:497:ILE:HG21	1:C:589:TYR:CD2	2.50	0.46
1:C:1617:ALA:HA	1:C:1624:ILE:HD11	1.97	0.46
1:D:1617:ALA:HA	1:D:1624:ILE:HD11	1.97	0.46
1:B:1244:THR:HG21	1:B:1268:TYR:CD1	2.50	0.46
1:D:1001:LEU:HD23	1:D:1013:ILE:HD12	1.96	0.46
1:E:110:SER:HG	1:E:1902:TRP:CD1	2.33	0.46
1:A:1617:ALA:HA	1:A:1624:ILE:HD11	1.97	0.46
1:A:730:PHE:HE1	1:A:752:ILE:HG23	1.81	0.46
1:D:593:LEU:O	1:D:597:ILE:HG12	2.16	0.46
1:E:348:PHE:CE1	1:E:352:ASN:HB3	2.50	0.46
1:B:127:ARG:HG3	1:B:127:ARG:HH11	1.80	0.46
1:B:2321:HIS:NE2	1:B:2325:ASP:OD2	2.49	0.46
1:D:522:PRO:O	1:D:553:ARG:NH1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2033:LEU:HD11	1:E:2266:TYR:HA	1.96	0.46
1:B:474:VAL:O	1:B:478:VAL:HG13	2.16	0.46
1:C:348:PHE:CE1	1:C:352:ASN:HB3	2.50	0.46
1:D:1244:THR:HG21	1:D:1268:TYR:CD1	2.50	0.46
1:D:2132:ARG:HH11	1:D:2163:TYR:HB3	1.80	0.46
1:E:1617:ALA:HA	1:E:1624:ILE:HD11	1.98	0.46
1:B:593:LEU:O	1:B:597:ILE:HG12	2.16	0.46
1:B:1146:LYS:NZ	1:B:1147:ILE:O	2.43	0.46
1:C:237:LEU:HD11	1:C:483:TYR:HB2	1.98	0.46
1:C:407:GLU:HA	1:C:425:LYS:HA	1.96	0.46
1:D:1146:LYS:NZ	1:D:1147:ILE:O	2.42	0.46
1:E:174:LYS:HG2	1:E:185:VAL:HG21	1.96	0.46
1:E:370:ILE:HD13	1:E:379:VAL:HG13	1.98	0.46
1:E:1024:TYR:O	1:E:1030:THR:OG1	2.25	0.46
1:B:210:VAL:HG22	1:B:926:LEU:HD11	1.98	0.46
1:B:497:ILE:HG21	1:B:589:TYR:CD2	2.50	0.46
1:C:127:ARG:HG3	1:C:127:ARG:HH11	1.79	0.46
1:A:1118:ALA:O	1:D:2133:LEU:HD22	2.16	0.46
1:A:1244:THR:HG21	1:A:1268:TYR:CD1	2.51	0.46
1:B:2009:LEU:HG	1:B:2294:PRO:HB3	1.98	0.46
1:C:1113:LEU:HD11	1:C:1119:GLY:HA3	1.98	0.46
1:D:969:GLN:HB3	1:D:999:ARG:NH1	2.31	0.46
1:B:348:PHE:CE1	1:B:352:ASN:HB3	2.50	0.46
1:B:1617:ALA:HA	1:B:1624:ILE:HD11	1.97	0.46
1:C:1124:ARG:NE	1:C:1142:SER:O	2.48	0.46
1:C:2321:HIS:NE2	1:C:2325:ASP:OD2	2.49	0.46
1:E:522:PRO:O	1:E:553:ARG:NH1	2.48	0.46
1:A:497:ILE:HG21	1:A:589:TYR:CD2	2.51	0.45
1:B:357:TYR:CE2	1:B:391:TYR:HB2	2.51	0.45
1:C:1168:TYR:HD2	1:C:1200:LEU:HD11	1.81	0.45
1:C:2099:TYR:CE2	1:C:2195:GLN:HB3	2.50	0.45
1:D:357:TYR:CE2	1:D:391:TYR:HB2	2.51	0.45
1:A:2337:LEU:HD23	1:A:2507:ILE:HG13	1.99	0.45
1:C:1001:LEU:HD23	1:C:1013:ILE:HD12	1.98	0.45
1:C:2441:LEU:HG	1:C:2445:CYS:HB2	1.98	0.45
1:D:534:GLU:OE2	1:D:580:ASN:ND2	2.49	0.45
1:D:2469:PHE:H	1:E:2327:ARG:NH2	2.15	0.45
1:A:255:ILE:HD12	1:A:438:LEU:HD13	1.99	0.45
1:B:1024:TYR:CD1	1:B:1034:VAL:HG21	2.52	0.45
1:B:1797:LYS:O	1:B:1805:TYR:OH	2.34	0.45
1:C:174:LYS:HG2	1:C:185:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:ILE:HD13	1:C:379:VAL:HG13	1.99	0.45
1:C:1892:ASP:OD1	1:C:1892:ASP:N	2.50	0.45
1:D:1711:PHE:CE2	1:D:1713:LYS:HB3	2.52	0.45
1:E:197:ALA:H	1:E:948:THR:HG21	1.79	0.45
1:A:593:LEU:O	1:A:597:ILE:HG12	2.16	0.45
1:B:370:ILE:HD13	1:B:379:VAL:HG13	1.99	0.45
1:B:1711:PHE:CE2	1:B:1713:LYS:HB3	2.52	0.45
1:C:464:VAL:HG21	1:C:474:VAL:HA	1.98	0.45
1:D:1024:TYR:CG	1:D:1034:VAL:HG21	2.52	0.45
1:E:969:GLN:HB3	1:E:999:ARG:NH1	2.31	0.45
1:E:2441:LEU:HG	1:E:2445:CYS:HB2	1.98	0.45
1:A:370:ILE:HD13	1:A:379:VAL:HG13	1.99	0.45
1:A:1975:SER:OG	1:A:1977:ASP:OD1	2.33	0.45
1:B:1001:LEU:HD23	1:B:1013:ILE:HD12	1.99	0.45
1:C:1147:ILE:HD13	1:C:1169:LEU:HD11	1.99	0.45
1:D:174:LYS:HG2	1:D:185:VAL:HG21	1.98	0.45
1:D:370:ILE:HD13	1:D:379:VAL:HG13	1.99	0.45
1:E:1244:THR:HG21	1:E:1268:TYR:CD1	2.51	0.45
1:E:2337:LEU:HD23	1:E:2507:ILE:HG13	1.99	0.45
1:A:500:ASN:HB2	1:A:627:LEU:HD13	1.98	0.45
1:A:1024:TYR:CG	1:A:1034:VAL:HG21	2.52	0.45
1:A:1711:PHE:CE2	1:A:1713:LYS:HB3	2.51	0.45
1:A:2393:PHE:CE1	1:A:2482:LEU:HB2	2.52	0.45
1:B:1113:LEU:HD11	1:B:1119:GLY:HA3	1.99	0.45
1:B:1124:ARG:NE	1:B:1142:SER:O	2.49	0.45
1:B:1178:THR:HG22	1:B:1192:THR:HG23	1.99	0.45
1:C:2141:VAL:HG21	1:D:1175:LYS:HE2	1.99	0.45
1:D:1892:ASP:OD1	1:D:1892:ASP:N	2.50	0.45
1:B:181:ASN:HD21	1:B:184:LYS:HG2	1.82	0.45
1:B:2235:GLN:HG3	1:C:1995:LEU:HB2	1.98	0.45
1:C:969:GLN:HB3	1:C:999:ARG:NH1	2.31	0.45
1:C:1244:THR:HG21	1:C:1268:TYR:CD1	2.51	0.45
1:C:2393:PHE:HB3	1:C:2477:ILE:O	2.17	0.45
1:E:1711:PHE:CE2	1:E:1713:LYS:HB3	2.52	0.45
1:A:2441:LEU:HG	1:A:2445:CYS:HB2	1.98	0.45
1:B:730:PHE:HE1	1:B:752:ILE:HG23	1.82	0.45
1:B:969:GLN:HB3	1:B:999:ARG:NH1	2.32	0.45
1:B:2441:LEU:HG	1:B:2445:CYS:HB2	1.98	0.45
1:C:2393:PHE:CE1	1:C:2482:LEU:HB2	2.52	0.45
1:D:2393:PHE:HB3	1:D:2477:ILE:O	2.17	0.45
1:E:464:VAL:HG21	1:E:474:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:CE2	1:A:391:TYR:HB2	2.52	0.45
1:D:197:ALA:H	1:D:948:THR:HG21	1.81	0.45
1:E:200:TYR:CE1	1:E:941:SER:HB3	2.52	0.45
1:E:1024:TYR:CD1	1:E:1034:VAL:HG21	2.51	0.45
1:A:2147:PHE:CD1	1:E:2147:PHE:HB3	2.52	0.45
1:B:1236:CYS:H	1:B:1303:ASN:ND2	2.15	0.45
1:B:1892:ASP:OD1	1:B:1892:ASP:N	2.50	0.45
1:C:357:TYR:CE2	1:C:391:TYR:HB2	2.52	0.45
1:C:724:ALA:O	1:C:729:LYS:NZ	2.32	0.45
1:C:1024:TYR:CG	1:C:1034:VAL:HG21	2.52	0.45
1:D:507:SER:HB3	1:D:513:SER:HB2	1.99	0.45
1:D:2441:LEU:HG	1:D:2445:CYS:HB2	1.99	0.45
1:E:474:VAL:O	1:E:478:VAL:HG13	2.17	0.45
1:E:2393:PHE:CE1	1:E:2482:LEU:HB2	2.52	0.45
1:A:181:ASN:HD21	1:A:184:LYS:HG2	1.82	0.44
1:B:522:PRO:O	1:B:553:ARG:NH1	2.50	0.44
1:B:659:TYR:CE2	1:B:758:ALA:HB2	2.52	0.44
1:C:593:LEU:O	1:C:597:ILE:HG12	2.17	0.44
1:C:1124:ARG:HD2	1:C:1144:TRP:CE2	2.52	0.44
1:C:1711:PHE:CE2	1:C:1713:LYS:HB3	2.52	0.44
1:C:2133:LEU:HD22	1:E:1118:ALA:O	2.16	0.44
1:E:141:ARG:NH2	1:E:1005:GLU:OE2	2.44	0.44
1:E:507:SER:HB3	1:E:513:SER:HB2	2.00	0.44
1:E:593:LEU:O	1:E:597:ILE:HG12	2.16	0.44
1:A:210:VAL:HG22	1:A:926:LEU:HD11	1.99	0.44
1:B:340:GLN:OE1	1:B:412:ARG:NH2	2.50	0.44
1:B:1766:LEU:O	1:B:1770:GLU:HB2	2.17	0.44
1:B:2133:LEU:HD22	1:D:1118:ALA:O	2.17	0.44
1:C:2219:ALA:HA	1:D:2073:LYS:NZ	2.33	0.44
1:D:2393:PHE:CE1	1:D:2482:LEU:HB2	2.52	0.44
1:E:1056:MET:HG3	1:E:1081:TYR:CE1	2.52	0.44
1:E:1135:LYS:HA	1:E:1135:LYS:HD3	1.81	0.44
1:A:1146:LYS:NZ	1:A:1147:ILE:O	2.48	0.44
1:B:534:GLU:OE2	1:B:580:ASN:ND2	2.50	0.44
1:B:1147:ILE:HD13	1:B:1169:LEU:HD11	1.99	0.44
1:B:2129:GLN:NE2	1:D:1120:GLU:OE2	2.51	0.44
1:C:251:LEU:HD13	1:C:446:LEU:HD13	1.99	0.44
1:C:2360:LEU:HB3	1:C:2377:PHE:HE1	1.82	0.44
1:D:538:LEU:HB2	1:D:566:LEU:HD22	1.99	0.44
1:E:2018:ARG:NH2	1:E:2473:GLU:OE2	2.51	0.44
1:A:1056:MET:HG3	1:A:1081:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:SER:HA	1:B:982:LYS:HA	1.98	0.44
1:B:1056:MET:HG3	1:B:1081:TYR:CE1	2.53	0.44
1:B:2393:PHE:CE1	1:B:2482:LEU:HB2	2.53	0.44
1:E:160:SER:HA	1:E:982:LYS:HA	1.98	0.44
1:E:195:SER:OG	1:E:948:THR:HG22	2.18	0.44
1:A:2207:ASP:O	1:A:2211:LYS:HG2	2.18	0.44
1:A:2393:PHE:HB3	1:A:2477:ILE:O	2.18	0.44
1:B:110:SER:HG	1:B:1902:TRP:CD1	2.35	0.44
1:B:1024:TYR:O	1:B:1030:THR:OG1	2.27	0.44
1:B:2078:LEU:HD13	1:B:2217:ARG:HA	2.00	0.44
1:B:2219:ALA:HA	1:C:2073:LYS:NZ	2.33	0.44
1:E:181:ASN:HD21	1:E:184:LYS:HG2	1.83	0.44
1:E:1001:LEU:HD23	1:E:1013:ILE:HD12	1.99	0.44
1:A:197:ALA:H	1:A:948:THR:HG21	1.82	0.44
1:A:2219:ALA:HA	1:B:2073:LYS:NZ	2.32	0.44
1:E:1962:THR:OG1	1:E:1966:ARG:NH2	2.50	0.44
1:B:142:ARG:HE	1:B:973:ILE:HD11	1.82	0.44
1:B:784:GLU:HG3	1:B:790:THR:HA	1.98	0.44
1:B:2147:PHE:HB3	1:C:2147:PHE:CD1	2.52	0.44
1:C:197:ALA:H	1:C:948:THR:HG21	1.82	0.44
1:C:255:ILE:HD12	1:C:438:LEU:HD13	1.99	0.44
1:C:2207:ASP:O	1:C:2211:LYS:HG2	2.18	0.44
1:D:2030:VAL:O	1:D:2034:THR:HG23	2.18	0.44
1:D:2147:PHE:HB3	1:E:2147:PHE:CD1	2.52	0.44
1:D:2219:ALA:HA	1:E:2073:LYS:NZ	2.33	0.44
1:E:357:TYR:CE2	1:E:391:TYR:HB2	2.52	0.44
1:E:2078:LEU:HD13	1:E:2217:ARG:HA	2.00	0.44
1:A:474:VAL:O	1:A:478:VAL:HG13	2.18	0.44
1:B:174:LYS:HG2	1:B:185:VAL:HG21	2.00	0.44
1:C:507:SER:HB3	1:C:513:SER:HB2	2.00	0.44
1:D:784:GLU:HG3	1:D:790:THR:HA	1.99	0.44
1:D:2078:LEU:HD13	1:D:2217:ARG:HA	2.00	0.44
1:D:2321:HIS:NE2	1:D:2325:ASP:OD2	2.51	0.44
1:A:507:SER:HB3	1:A:513:SER:HB2	2.00	0.44
1:A:2235:GLN:HG3	1:B:1995:LEU:HB2	2.00	0.44
1:B:124:ARG:HG2	1:B:1911:ALA:HB1	2.00	0.44
1:C:273:PRO:HG3	1:C:434:TYR:CE1	2.52	0.44
1:C:1178:THR:HG22	1:C:1192:THR:HG23	2.00	0.44
1:C:2129:GLN:NE2	1:E:1120:GLU:OE2	2.51	0.44
1:E:1124:ARG:NE	1:E:1142:SER:O	2.51	0.44
1:E:1892:ASP:OD1	1:E:1892:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2207:ASP:O	1:E:2211:LYS:HG2	2.18	0.44
1:A:784:GLU:HG3	1:A:790:THR:HA	2.00	0.43
1:A:969:GLN:HB3	1:A:999:ARG:NH1	2.32	0.43
1:A:1113:LEU:HD11	1:A:1119:GLY:HA3	2.00	0.43
1:A:2133:LEU:HD22	1:C:1118:ALA:O	2.17	0.43
1:B:273:PRO:HG3	1:B:434:TYR:CE1	2.53	0.43
1:B:2360:LEU:HB3	1:B:2377:PHE:HE1	1.83	0.43
1:C:255:ILE:HG12	1:C:442:LYS:HE3	2.00	0.43
1:C:474:VAL:O	1:C:478:VAL:HG13	2.18	0.43
1:D:659:TYR:CE2	1:D:758:ALA:HB2	2.53	0.43
1:D:1002:GLU:OE1	1:E:1888:HIS:NE2	2.50	0.43
1:E:487:ARG:HE	1:E:635:ASN:HD21	1.66	0.43
1:A:174:LYS:HG2	1:A:185:VAL:HG21	1.99	0.43
1:B:464:VAL:HG21	1:B:474:VAL:HA	2.01	0.43
1:D:1975:SER:OG	1:D:1977:ASP:OD1	2.34	0.43
1:E:730:PHE:HE1	1:E:752:ILE:HG23	1.83	0.43
1:E:2009:LEU:HG	1:E:2294:PRO:HB3	1.99	0.43
1:A:490:ILE:HD12	1:A:494:THR:HG22	2.00	0.43
1:A:2030:VAL:O	1:A:2034:THR:HG23	2.18	0.43
1:A:2327:ARG:NH2	1:E:2469:PHE:H	2.16	0.43
1:C:1135:LYS:HA	1:C:1135:LYS:HD3	1.82	0.43
1:C:1766:LEU:O	1:C:1770:GLU:HB2	2.17	0.43
1:D:255:ILE:HG12	1:D:442:LYS:HE3	2.00	0.43
1:D:1773:TYR:HD2	1:D:1774:TYR:CD1	2.36	0.43
1:D:2337:LEU:HD23	1:D:2507:ILE:HG13	1.99	0.43
1:E:2321:HIS:NE2	1:E:2325:ASP:OD2	2.51	0.43
1:E:2393:PHE:HB3	1:E:2477:ILE:O	2.19	0.43
1:A:1178:THR:HG22	1:A:1192:THR:HG23	2.01	0.43
1:A:1236:CYS:H	1:A:1303:ASN:ND2	2.17	0.43
1:A:2321:HIS:NE2	1:A:2325:ASP:OD2	2.52	0.43
1:A:2452:HIS:CE1	1:A:2456:ASP:HB2	2.54	0.43
1:B:195:SER:OG	1:B:948:THR:HG22	2.18	0.43
1:C:534:GLU:OE2	1:C:580:ASN:ND2	2.51	0.43
1:C:2337:LEU:HD23	1:C:2507:ILE:HG13	2.00	0.43
1:D:474:VAL:O	1:D:478:VAL:HG13	2.18	0.43
1:E:255:ILE:HG12	1:E:442:LYS:HE3	2.00	0.43
1:A:280:GLU:OE2	1:B:1895:TYR:HB2	2.19	0.43
1:A:534:GLU:OE2	1:A:580:ASN:ND2	2.51	0.43
1:A:2073:LYS:NZ	1:E:2219:ALA:HA	2.33	0.43
1:B:1048:THR:HG23	1:B:1061:LEU:HD11	2.00	0.43
1:B:2030:VAL:O	1:B:2034:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2147:PHE:HB3	1:D:2147:PHE:CD1	2.52	0.43
1:D:1053:GLN:HE21	1:D:1057:MET:HG3	1.83	0.43
1:D:1159:ARG:HD3	1:D:1303:ASN:ND2	2.33	0.43
1:D:1769:TRP:CD1	1:D:1842:GLN:HE22	2.36	0.43
1:E:659:TYR:CE2	1:E:758:ALA:HB2	2.53	0.43
1:A:1766:LEU:O	1:A:1770:GLU:HB2	2.18	0.43
1:B:280:GLU:OE2	1:C:1895:TYR:HB2	2.18	0.43
1:B:487:ARG:HE	1:B:635:ASN:HD21	1.66	0.43
1:B:2452:HIS:CE1	1:B:2456:ASP:HB2	2.54	0.43
1:D:181:ASN:HD21	1:D:184:LYS:HG2	1.83	0.43
1:D:497:ILE:HG21	1:D:589:TYR:CD2	2.54	0.43
1:D:2360:LEU:HB3	1:D:2377:PHE:HE1	1.83	0.43
1:D:2448:LEU:HB2	1:D:2458:GLY:HA3	2.00	0.43
1:E:255:ILE:HD12	1:E:438:LEU:HD13	1.99	0.43
1:E:569:THR:HG21	1:E:587:ASN:HB3	2.01	0.43
1:E:1168:TYR:HD2	1:E:1200:LEU:HD11	1.83	0.43
1:A:1773:TYR:HD2	1:A:1774:TYR:CD1	2.37	0.43
1:A:1895:TYR:HB2	1:E:280:GLU:OE2	2.19	0.43
1:B:2207:ASP:O	1:B:2211:LYS:HG2	2.18	0.43
1:C:124:ARG:HD3	1:C:1914:THR:OG1	2.18	0.43
1:C:280:GLU:OE2	1:D:1895:TYR:HB2	2.19	0.43
1:C:730:PHE:HE1	1:C:752:ILE:HG23	1.82	0.43
1:C:1236:CYS:H	1:C:1303:ASN:ND2	2.16	0.43
1:D:1236:CYS:H	1:D:1303:ASN:ND2	2.16	0.43
1:D:1887:LEU:HD12	1:D:1887:LEU:HA	1.90	0.43
1:E:694:PRO:HA	1:E:705:GLU:OE1	2.19	0.43
1:A:659:TYR:CE2	1:A:758:ALA:HB2	2.53	0.43
1:A:1159:ARG:HD3	1:A:1303:ASN:ND2	2.33	0.43
1:A:1793:ASN:O	1:A:1797:LYS:HB2	2.19	0.43
1:A:2078:LEU:HD13	1:A:2217:ARG:HA	2.01	0.43
1:B:1118:ALA:O	1:E:2133:LEU:HD22	2.18	0.43
1:C:142:ARG:HE	1:C:973:ILE:HD11	1.84	0.43
1:C:659:TYR:CE2	1:C:758:ALA:HB2	2.53	0.43
1:C:1166:ARG:HB2	1:D:1614:VAL:HG11	2.01	0.43
1:C:2009:LEU:HG	1:C:2294:PRO:HB3	2.01	0.43
1:C:2452:HIS:CE1	1:C:2456:ASP:HB2	2.54	0.43
1:D:340:GLN:OE1	1:D:412:ARG:NH2	2.51	0.43
1:D:1168:TYR:HD2	1:D:1200:LEU:HD11	1.83	0.43
1:E:490:ILE:HD12	1:E:494:THR:HG22	2.01	0.43
1:E:558:ASP:OD1	1:E:558:ASP:N	2.47	0.43
1:E:1766:LEU:O	1:E:1770:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2030:VAL:O	1:E:2034:THR:HG23	2.18	0.43
1:A:273:PRO:HG3	1:A:434:TYR:CE1	2.54	0.43
1:A:340:GLN:OE1	1:A:412:ARG:NH2	2.52	0.43
1:A:1024:TYR:CD1	1:A:1034:VAL:HG21	2.54	0.43
1:A:2009:LEU:HG	1:A:2294:PRO:HB3	2.00	0.43
1:B:116:ALA:O	1:B:120:THR:HG23	2.19	0.43
1:B:2393:PHE:HB3	1:B:2477:ILE:O	2.18	0.43
1:C:2030:VAL:O	1:C:2034:THR:HG23	2.18	0.43
1:D:1124:ARG:NE	1:D:1142:SER:O	2.51	0.43
1:D:1124:ARG:NH2	1:D:1763:ALA:O	2.50	0.43
1:E:534:GLU:OE2	1:E:580:ASN:ND2	2.52	0.43
1:E:1178:THR:HG22	1:E:1192:THR:HG23	2.00	0.43
1:E:2416:SER:HB2	1:E:2510:HIS:HB2	2.00	0.43
1:A:1614:VAL:HG11	1:E:1166:ARG:HB2	2.01	0.43
1:B:251:LEU:HD13	1:B:446:LEU:HD13	2.01	0.43
1:C:253:GLU:O	1:C:442:LYS:NZ	2.28	0.43
1:D:280:GLU:OE2	1:E:1895:TYR:HB2	2.19	0.43
1:D:397:LEU:HD13	1:D:406:PHE:CZ	2.54	0.43
1:D:2207:ASP:O	1:D:2211:LYS:HG2	2.19	0.43
1:A:195:SER:OG	1:A:948:THR:HG22	2.19	0.42
1:A:343:VAL:HG23	1:A:357:TYR:HB3	2.01	0.42
1:A:1135:LYS:HA	1:A:1135:LYS:HD3	1.81	0.42
1:B:1162:ILE:HD13	1:B:1167:LEU:HA	2.01	0.42
1:B:2337:LEU:HD23	1:B:2507:ILE:HG13	2.01	0.42
1:D:1147:ILE:HD13	1:D:1169:LEU:HD11	2.01	0.42
1:E:1773:TYR:HD2	1:E:1774:TYR:CD1	2.37	0.42
1:A:538:LEU:HB2	1:A:566:LEU:HD22	2.01	0.42
1:A:848:GLN:OE1	1:A:892:GLN:NE2	2.53	0.42
1:A:2355:GLN:HG2	1:A:2356:GLU:OE1	2.19	0.42
1:C:569:THR:HG21	1:C:587:ASN:HB3	2.01	0.42
1:D:141:ARG:NH2	1:D:1005:GLU:OE2	2.44	0.42
1:E:124:ARG:HG2	1:E:1911:ALA:HB1	2.00	0.42
1:E:538:LEU:HB2	1:E:566:LEU:HD22	2.01	0.42
1:E:2355:GLN:HG2	1:E:2356:GLU:OE1	2.19	0.42
1:A:1892:ASP:OD1	1:A:1892:ASP:N	2.50	0.42
1:C:181:ASN:HD21	1:C:184:LYS:HG2	1.84	0.42
1:D:2130:ALA:HB2	1:E:1204:ARG:HH22	1.82	0.42
1:E:540:SER:OG	1:E:560:VAL:HA	2.20	0.42
1:E:2360:LEU:HB3	1:E:2377:PHE:HE1	1.84	0.42
1:A:1295:ASP:CG	1:A:1301:ARG:H	2.27	0.42
1:A:1797:LYS:O	1:A:1805:TYR:OH	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1872:GLU:OE2	1:A:1875:THR:OG1	2.34	0.42
1:B:507:SER:HB3	1:B:513:SER:HB2	2.00	0.42
1:C:1769:TRP:NE1	1:C:1842:GLN:HE22	2.17	0.42
1:C:2018:ARG:N	1:C:2467:GLY:O	2.52	0.42
1:C:2369:GLY:HA3	1:C:2374:ASN:HA	2.01	0.42
1:D:160:SER:HA	1:D:982:LYS:HA	2.00	0.42
1:D:730:PHE:HE1	1:D:752:ILE:HG23	1.83	0.42
1:D:2009:LEU:HG	1:D:2294:PRO:HB3	2.01	0.42
1:E:273:PRO:HG3	1:E:434:TYR:CE1	2.53	0.42
1:E:340:GLN:OE1	1:E:412:ARG:NH2	2.51	0.42
1:E:1800:TRP:CZ2	1:E:1802:PRO:HG3	2.54	0.42
1:E:2372:ASN:HB2	1:E:2392:SER:HB2	2.02	0.42
1:A:1168:TYR:HD2	1:A:1200:LEU:HD11	1.85	0.42
1:A:1995:LEU:HB2	1:E:2235:GLN:HG3	2.01	0.42
1:A:2360:LEU:HB3	1:A:2377:PHE:HE1	1.85	0.42
1:C:110:SER:HG	1:C:1902:TRP:CD1	2.37	0.42
1:C:116:ALA:O	1:C:120:THR:HG23	2.19	0.42
1:C:340:GLN:OE1	1:C:412:ARG:NH2	2.52	0.42
1:D:1002:GLU:CD	1:E:1888:HIS:HE2	2.28	0.42
1:D:1800:TRP:CZ2	1:D:1802:PRO:HG3	2.54	0.42
1:E:579:LYS:HG3	1:E:581:ASN:H	1.85	0.42
1:A:124:ARG:HD3	1:A:1914:THR:OG1	2.20	0.42
1:A:579:LYS:HG3	1:A:581:ASN:H	1.84	0.42
1:A:1166:ARG:HB2	1:B:1614:VAL:HG11	2.02	0.42
1:A:2295:GLY:HA3	1:D:676:HIS:CD2	2.54	0.42
1:B:2355:GLN:HG2	1:B:2356:GLU:OE1	2.19	0.42
1:C:538:LEU:HB2	1:C:566:LEU:HD22	2.00	0.42
1:D:1056:MET:HG3	1:D:1081:TYR:CE1	2.54	0.42
1:D:2452:HIS:CE1	1:D:2456:ASP:HB2	2.54	0.42
1:E:1609:PHE:CZ	1:E:1613:LEU:HD13	2.55	0.42
1:A:569:THR:HG21	1:A:587:ASN:HB3	2.00	0.42
1:A:2448:LEU:HB2	1:A:2458:GLY:HA3	2.02	0.42
1:B:255:ILE:HG12	1:B:442:LYS:HE3	2.01	0.42
1:B:1168:TYR:HD2	1:B:1200:LEU:HD11	1.84	0.42
1:C:154:ASN:HB3	1:C:986:ILE:HG13	2.02	0.42
1:C:579:LYS:HG3	1:C:581:ASN:H	1.84	0.42
1:D:1166:ARG:HB2	1:E:1614:VAL:HG11	2.02	0.42
1:D:2355:GLN:HG2	1:D:2356:GLU:OE1	2.20	0.42
1:E:2033:LEU:CD1	1:E:2266:TYR:HA	2.50	0.42
1:E:2328:ALA:HB2	1:E:2516:LYS:HB3	2.02	0.42
1:A:2033:LEU:CD1	1:A:2266:TYR:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:VAL:HG11	1:C:763:GLU:OE2	2.20	0.42
1:D:368:LEU:HG	1:D:370:ILE:CD1	2.50	0.42
1:E:397:LEU:HD13	1:E:406:PHE:CZ	2.55	0.42
1:E:1053:GLN:HE21	1:E:1057:MET:HG3	1.85	0.42
1:E:2228:LYS:HE3	1:E:2228:LYS:HB2	1.87	0.42
1:A:1049:MET:HE3	1:A:1049:MET:HB3	1.99	0.42
1:A:1239:TYR:CD1	1:A:1242:GLU:HB3	2.54	0.42
1:A:2004:GLN:N	1:A:2300:THR:HG22	2.34	0.42
1:A:2077:GLU:OE2	1:E:2216:ARG:NH2	2.52	0.42
1:A:2277:GLU:OE2	1:A:2291:PHE:HB2	2.20	0.42
1:B:1773:TYR:HD2	1:B:1774:TYR:CD1	2.37	0.42
1:B:1800:TRP:CZ2	1:B:1802:PRO:HG3	2.55	0.42
1:C:141:ARG:NH2	1:C:1005:GLU:OE2	2.43	0.42
1:C:368:LEU:HG	1:C:370:ILE:CD1	2.50	0.42
1:C:1793:ASN:O	1:C:1797:LYS:HB2	2.20	0.42
1:D:490:ILE:HD12	1:D:494:THR:HG22	2.01	0.42
1:D:579:LYS:HG3	1:D:581:ASN:H	1.85	0.42
1:D:1793:ASN:O	1:D:1797:LYS:HB2	2.20	0.42
1:E:1769:TRP:CD1	1:E:1842:GLN:HE22	2.38	0.42
1:E:1865:ASP:OD1	1:E:1883:TYR:OH	2.34	0.42
1:A:1607:THR:HG22	1:A:1609:PHE:H	1.84	0.42
1:A:1800:TRP:CZ2	1:A:1802:PRO:HG3	2.55	0.42
1:A:2022:MET:HE1	1:B:2322:LEU:HD11	2.02	0.42
1:B:2018:ARG:N	1:B:2467:GLY:O	2.50	0.42
1:C:195:SER:OG	1:C:948:THR:HG22	2.20	0.42
1:C:2355:GLN:HG2	1:C:2356:GLU:OE1	2.20	0.42
1:D:124:ARG:HG2	1:D:1911:ALA:HB1	2.02	0.42
1:D:1178:THR:HG22	1:D:1192:THR:HG23	2.01	0.42
1:E:711:VAL:HG11	1:E:763:GLU:OE2	2.20	0.42
1:A:116:ALA:O	1:A:120:THR:HG23	2.20	0.41
1:A:142:ARG:HE	1:A:973:ILE:HD11	1.84	0.41
1:A:1123:TRP:NE1	1:A:1145:HIS:HB2	2.35	0.41
1:A:1162:ILE:HD13	1:A:1167:LEU:HA	2.01	0.41
1:A:2275:MET:SD	1:B:2322:LEU:HD22	2.60	0.41
1:B:493:GLU:O	1:B:497:ILE:HG12	2.20	0.41
1:B:711:VAL:HG11	1:B:763:GLU:OE2	2.20	0.41
1:B:1024:TYR:CG	1:B:1034:VAL:HG21	2.55	0.41
1:C:1676:ILE:HD12	1:C:1690:LEU:HD13	2.02	0.41
1:C:1773:TYR:HD2	1:C:1774:TYR:CD1	2.38	0.41
1:C:2275:MET:SD	1:D:2322:LEU:HD22	2.60	0.41
1:E:2452:HIS:CE1	1:E:2456:ASP:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HD13	1:A:446:LEU:HD13	2.02	0.41
1:A:1769:TRP:CD1	1:A:1842:GLN:HE22	2.38	0.41
1:B:255:ILE:HD12	1:B:438:LEU:HD13	2.02	0.41
1:B:397:LEU:HD13	1:B:406:PHE:CZ	2.56	0.41
1:C:1098:HIS:CE1	1:C:1100:ASN:HB3	2.55	0.41
1:C:1159:ARG:HD3	1:C:1303:ASN:ND2	2.35	0.41
1:D:195:SER:OG	1:D:948:THR:HG22	2.20	0.41
1:D:663:LEU:HD22	1:D:749:GLN:NE2	2.35	0.41
1:D:1676:ILE:HD12	1:D:1690:LEU:HD13	2.02	0.41
1:E:1123:TRP:NE1	1:E:1145:HIS:HB2	2.35	0.41
1:A:255:ILE:HG12	1:A:442:LYS:HE3	2.01	0.41
1:A:1053:GLN:HE21	1:A:1057:MET:HG3	1.86	0.41
1:A:2322:LEU:HD22	1:E:2275:MET:SD	2.60	0.41
1:B:200:TYR:CE1	1:B:941:SER:HB3	2.54	0.41
1:B:493:GLU:OE2	1:B:517:ARG:NH1	2.34	0.41
1:B:2033:LEU:CD1	1:B:2266:TYR:HA	2.50	0.41
1:B:2433:LEU:HB3	1:B:2484:LEU:HD13	2.02	0.41
1:C:283:LYS:HB2	1:C:293:LEU:HD22	2.02	0.41
1:C:784:GLU:HG3	1:C:790:THR:HA	2.02	0.41
1:C:1024:TYR:CD1	1:C:1034:VAL:HG21	2.55	0.41
1:C:1162:ILE:HD13	1:C:1167:LEU:HA	2.02	0.41
1:C:2235:GLN:HG3	1:D:1995:LEU:HB2	2.01	0.41
1:A:1888:HIS:HE2	1:E:1002:GLU:CD	2.29	0.41
1:B:141:ARG:NH2	1:B:1005:GLU:OE2	2.45	0.41
1:B:368:LEU:HG	1:B:370:ILE:CD1	2.50	0.41
1:B:490:ILE:HD12	1:B:494:THR:HG22	2.01	0.41
1:B:533:ASP:HA	1:B:579:LYS:NZ	2.36	0.41
1:B:2046:ARG:HE	1:B:2251:TYR:HH	1.65	0.41
1:D:343:VAL:HG23	1:D:357:TYR:HB3	2.02	0.41
1:D:1766:LEU:O	1:D:1770:GLU:HB2	2.19	0.41
1:E:1024:TYR:CG	1:E:1034:VAL:HG21	2.55	0.41
1:E:1887:LEU:HD12	1:E:1887:LEU:HA	1.90	0.41
1:A:124:ARG:HG2	1:A:1911:ALA:HB1	2.03	0.41
1:B:579:LYS:HG3	1:B:581:ASN:H	1.84	0.41
1:B:1053:GLN:HE21	1:B:1057:MET:HG3	1.84	0.41
1:B:1120:GLU:OE2	1:E:2129:GLN:NE2	2.54	0.41
1:B:1782:ARG:HE	1:B:1782:ARG:HB3	1.76	0.41
1:C:694:PRO:HA	1:C:705:GLU:OE1	2.20	0.41
1:C:971:LEU:O	1:C:973:ILE:HG12	2.21	0.41
1:C:1053:GLN:HE21	1:C:1057:MET:HG3	1.85	0.41
1:D:694:PRO:HA	1:D:705:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1024:TYR:CD1	1:D:1034:VAL:HG21	2.56	0.41
1:D:1239:TYR:HD2	1:D:1246:LEU:HD11	1.85	0.41
1:E:124:ARG:HD3	1:E:1914:THR:OG1	2.20	0.41
1:E:1113:LEU:HD11	1:E:1119:GLY:HA3	2.02	0.41
1:E:1159:ARG:HD3	1:E:1303:ASN:ND2	2.34	0.41
1:A:1617:ALA:CA	1:A:1624:ILE:HD11	2.51	0.41
1:A:2018:ARG:N	1:A:2467:GLY:O	2.52	0.41
1:A:2097:ASP:OD1	1:A:2098:SER:N	2.54	0.41
1:A:2145:PHE:CE2	1:C:1180:GLN:HG3	2.56	0.41
1:B:231:MET:HE2	1:B:898:VAL:HA	2.02	0.41
1:B:1609:PHE:CZ	1:B:1613:LEU:HD13	2.56	0.41
1:B:2022:MET:HE1	1:C:2322:LEU:HD11	2.03	0.41
1:C:490:ILE:HD12	1:C:494:THR:HG22	2.02	0.41
1:D:116:ALA:O	1:D:120:THR:HG23	2.20	0.41
1:D:1295:ASP:CG	1:D:1301:ARG:H	2.28	0.41
1:E:1147:ILE:HD13	1:E:1169:LEU:HD11	2.02	0.41
1:A:200:TYR:CE1	1:A:941:SER:HB3	2.55	0.41
1:A:711:VAL:HG11	1:A:763:GLU:OE2	2.20	0.41
1:A:717:LYS:HB3	1:A:793:ALA:HB2	2.03	0.41
1:A:1124:ARG:NE	1:A:1142:SER:O	2.54	0.41
1:A:1769:TRP:NE1	1:A:1842:GLN:HE22	2.18	0.41
1:A:2147:PHE:HB3	1:B:2147:PHE:CD1	2.54	0.41
1:B:149:ALA:O	1:B:154:ASN:ND2	2.50	0.41
1:B:694:PRO:HA	1:B:705:GLU:OE1	2.20	0.41
1:B:938:LEU:HD23	1:B:938:LEU:HA	1.93	0.41
1:B:971:LEU:O	1:B:973:ILE:HG12	2.20	0.41
1:C:677:GLY:HA3	1:C:695:TYR:CZ	2.56	0.41
1:C:1248:MET:HE1	1:C:1283:SER:HB2	2.02	0.41
1:C:2448:LEU:HB2	1:C:2458:GLY:HA3	2.02	0.41
1:D:124:ARG:HD3	1:D:1914:THR:OG1	2.20	0.41
1:D:200:TYR:CE1	1:D:941:SER:HB3	2.56	0.41
1:D:461:VAL:HA	1:D:474:VAL:HG21	2.03	0.41
1:D:478:VAL:O	1:D:481:THR:HG22	2.21	0.41
1:D:1769:TRP:NE1	1:D:1842:GLN:HE22	2.18	0.41
1:E:142:ARG:HE	1:E:973:ILE:HD11	1.85	0.41
1:E:478:VAL:O	1:E:481:THR:HG22	2.21	0.41
1:E:493:GLU:O	1:E:497:ILE:HG12	2.21	0.41
1:E:784:GLU:HG3	1:E:790:THR:HA	2.02	0.41
1:E:1098:HIS:CE1	1:E:1100:ASN:HB3	2.55	0.41
1:E:1797:LYS:O	1:E:1805:TYR:OH	2.34	0.41
1:A:125:GLU:HG3	1:A:1017:PHE:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HD13	1:A:406:PHE:CZ	2.56	0.41
1:B:458:GLU:HA	1:B:461:VAL:HG12	2.03	0.41
1:B:1607:THR:HG22	1:B:1609:PHE:H	1.86	0.41
1:B:1676:ILE:HD12	1:B:1690:LEU:HD13	2.01	0.41
1:C:200:TYR:CE1	1:C:941:SER:HB3	2.54	0.41
1:C:1056:MET:HG3	1:C:1081:TYR:CE1	2.56	0.41
1:C:2216:ARG:NH2	1:D:2077:GLU:OE2	2.54	0.41
1:D:125:GLU:HG3	1:D:1017:PHE:CG	2.56	0.41
1:D:193:ARG:NH2	1:D:253:GLU:OE1	2.54	0.41
1:D:273:PRO:HG3	1:D:434:TYR:CE1	2.55	0.41
1:D:569:THR:HG21	1:D:587:ASN:HB3	2.02	0.41
1:D:711:VAL:HG11	1:D:763:GLU:OE2	2.20	0.41
1:D:1162:ILE:HD13	1:D:1167:LEU:HA	2.02	0.41
1:D:2033:LEU:CD1	1:D:2266:TYR:HA	2.51	0.41
1:E:1793:ASN:O	1:E:1797:LYS:HB2	2.20	0.41
1:E:2433:LEU:HB3	1:E:2484:LEU:HD13	2.03	0.41
1:A:595:ALA:HB1	1:A:600:LEU:O	2.21	0.41
1:A:971:LEU:O	1:A:973:ILE:HG12	2.21	0.41
1:A:1098:HIS:CE1	1:A:1100:ASN:HB3	2.55	0.41
1:A:1782:ARG:HE	1:A:1782:ARG:HB3	1.76	0.41
1:A:2168:SER:HA	1:A:2171:VAL:HG12	2.03	0.41
1:A:2226:SER:HB2	1:B:2066:THR:HG21	2.03	0.41
1:B:365:ALA:HB3	1:B:384:ALA:HA	2.03	0.41
1:B:663:LEU:HD22	1:B:749:GLN:NE2	2.35	0.41
1:B:1098:HIS:CE1	1:B:1100:ASN:HB3	2.55	0.41
1:B:1239:TYR:CD1	1:B:1242:GLU:HB3	2.55	0.41
1:C:257:GLU:OE1	1:C:431:TYR:OH	2.33	0.41
1:C:397:LEU:HD13	1:C:406:PHE:CZ	2.55	0.41
1:C:733:TRP:NE1	1:C:748:THR:HB	2.36	0.41
1:C:845:LEU:HD21	1:C:881:VAL:HG13	2.03	0.41
1:C:1002:GLU:CD	1:D:1888:HIS:HE2	2.29	0.41
1:C:1607:THR:HG22	1:C:1609:PHE:H	1.86	0.41
1:C:1769:TRP:CD1	1:C:1842:GLN:HE22	2.39	0.41
1:C:2033:LEU:CD1	1:C:2266:TYR:HA	2.50	0.41
1:D:971:LEU:O	1:D:973:ILE:HG12	2.20	0.41
1:D:1036:GLN:O	1:D:1040:TYR:N	2.42	0.41
1:D:1805:TYR:HD2	1:D:1814:TYR:CE1	2.39	0.41
1:D:2018:ARG:N	1:D:2467:GLY:O	2.52	0.41
1:D:2372:ASN:HB2	1:D:2392:SER:HB2	2.03	0.41
1:D:2433:LEU:HB3	1:D:2484:LEU:HD13	2.03	0.41
1:E:231:MET:HE2	1:E:898:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:LEU:HG	1:E:370:ILE:CD1	2.50	0.41
1:E:500:ASN:HB2	1:E:627:LEU:HD13	2.03	0.41
1:E:595:ALA:HB1	1:E:600:LEU:O	2.21	0.41
1:E:1049:MET:HE3	1:E:1049:MET:HB3	2.00	0.41
1:E:1239:TYR:CD1	1:E:1242:GLU:HB3	2.56	0.41
1:E:2369:GLY:HA3	1:E:2374:ASN:HA	2.03	0.41
1:A:1239:TYR:HD2	1:A:1246:LEU:HD11	1.86	0.41
1:A:1248:MET:HE1	1:A:1283:SER:HB2	2.02	0.41
1:A:1607:THR:HG21	1:A:1768:PHE:CZ	2.54	0.41
1:A:1676:ILE:HD12	1:A:1690:LEU:HD13	2.03	0.41
1:B:540:SER:OG	1:B:560:VAL:HA	2.21	0.41
1:B:2275:MET:SD	1:C:2322:LEU:HD22	2.61	0.41
1:C:1002:GLU:OE1	1:D:1888:HIS:NE2	2.52	0.41
1:D:142:ARG:HE	1:D:973:ILE:HD11	1.86	0.41
1:D:251:LEU:HD13	1:D:446:LEU:HD13	2.02	0.41
1:D:493:GLU:O	1:D:497:ILE:HG12	2.20	0.41
1:D:661:LYS:HB2	1:D:750:GLU:HB2	2.03	0.41
1:D:1113:LEU:HD11	1:D:1119:GLY:HA3	2.02	0.41
1:D:1239:TYR:CD1	1:D:1242:GLU:HB3	2.55	0.41
1:D:1797:LYS:O	1:D:1805:TYR:OH	2.36	0.41
1:E:552:LYS:NZ	1:E:558:ASP:HA	2.36	0.41
1:E:663:LEU:HD22	1:E:749:GLN:NE2	2.36	0.41
1:E:848:GLN:OE1	1:E:892:GLN:NE2	2.54	0.41
1:A:1124:ARG:NH2	1:A:1763:ALA:O	2.49	0.40
1:A:2046:ARG:HE	1:A:2251:TYR:HH	1.65	0.40
1:B:1130:LYS:HZ3	1:B:1139:ASN:C	2.28	0.40
1:B:1239:TYR:HD2	1:B:1246:LEU:HD11	1.86	0.40
1:B:1793:ASN:O	1:B:1797:LYS:HB2	2.20	0.40
1:B:2369:GLY:HA3	1:B:2374:ASN:HA	2.03	0.40
1:C:478:VAL:O	1:C:481:THR:HG22	2.20	0.40
1:C:533:ASP:HA	1:C:579:LYS:NZ	2.36	0.40
1:C:1609:PHE:CZ	1:C:1613:LEU:HD13	2.56	0.40
1:C:1711:PHE:HE2	1:C:1713:LYS:HB3	1.86	0.40
1:C:1800:TRP:CZ2	1:C:1802:PRO:HG3	2.56	0.40
1:D:2097:ASP:OD1	1:D:2098:SER:N	2.54	0.40
1:E:1248:MET:HE1	1:E:1283:SER:HB2	2.03	0.40
1:E:1769:TRP:NE1	1:E:1842:GLN:HE22	2.18	0.40
1:E:2018:ARG:N	1:E:2467:GLY:O	2.52	0.40
1:E:2097:ASP:OD1	1:E:2098:SER:N	2.54	0.40
1:E:2448:LEU:HB2	1:E:2458:GLY:HA3	2.04	0.40
1:A:663:LEU:HD22	1:A:749:GLN:NE2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2369:GLY:HA3	1:A:2374:ASN:HA	2.03	0.40
1:B:461:VAL:HA	1:B:474:VAL:HG21	2.03	0.40
1:B:733:TRP:NE1	1:B:748:THR:HB	2.36	0.40
1:B:2168:SER:HA	1:B:2171:VAL:HG12	2.04	0.40
1:C:663:LEU:HD22	1:C:749:GLN:NE2	2.36	0.40
1:C:1048:THR:HG23	1:C:1061:LEU:HD11	2.04	0.40
1:D:1042:GLU:HA	1:D:1045:ILE:HD12	2.03	0.40
1:D:1711:PHE:HE2	1:D:1713:LYS:HB3	1.87	0.40
1:D:2124:LEU:O	1:D:2128:VAL:HG12	2.22	0.40
1:E:971:LEU:O	1:E:973:ILE:HG12	2.21	0.40
1:A:487:ARG:HE	1:A:635:ASN:HD21	1.70	0.40
1:B:371:LYS:HA	1:B:377:GLU:HA	2.04	0.40
1:B:661:LYS:HB2	1:B:750:GLU:HB2	2.04	0.40
1:B:1607:THR:HG21	1:B:1768:PHE:CZ	2.52	0.40
1:B:1650:TYR:OH	1:B:1656:GLY:O	2.36	0.40
1:B:1769:TRP:CD1	1:B:1842:GLN:HE22	2.39	0.40
1:B:2097:ASP:OD1	1:B:2098:SER:N	2.54	0.40
1:C:2328:ALA:HB2	1:C:2516:LYS:HB3	2.03	0.40
1:D:540:SER:OG	1:D:560:VAL:HA	2.21	0.40
1:D:1607:THR:HG22	1:D:1609:PHE:H	1.86	0.40
1:D:1609:PHE:CZ	1:D:1613:LEU:HD13	2.57	0.40
1:D:2216:ARG:NH2	1:E:2077:GLU:OE2	2.53	0.40
1:D:2277:GLU:OE2	1:D:2291:PHE:HB2	2.21	0.40
1:D:2328:ALA:HB2	1:D:2516:LYS:HB3	2.03	0.40
1:E:116:ALA:O	1:E:120:THR:HG23	2.20	0.40
1:E:538:LEU:HD12	1:E:566:LEU:HD22	2.04	0.40
1:A:540:SER:OG	1:A:560:VAL:HA	2.22	0.40
1:A:733:TRP:NE1	1:A:748:THR:HB	2.36	0.40
1:A:2328:ALA:HB2	1:A:2516:LYS:HB3	2.04	0.40
1:B:1166:ARG:HB2	1:C:1614:VAL:HG11	2.04	0.40
1:B:1711:PHE:HE2	1:B:1713:LYS:HB3	1.87	0.40
1:B:2124:LEU:O	1:B:2128:VAL:HG12	2.22	0.40
1:B:2328:ALA:HB2	1:B:2516:LYS:HB3	2.04	0.40
1:B:2388:GLN:HA	1:B:2485:SER:HA	2.04	0.40
1:C:124:ARG:HG2	1:C:1911:ALA:HB1	2.03	0.40
1:C:456:ILE:O	1:C:460:ILE:HG13	2.21	0.40
1:C:676:HIS:CD2	1:E:2295:GLY:HA3	2.56	0.40
1:C:1094:ILE:HD11	1:C:1113:LEU:HB2	2.04	0.40
1:C:1120:GLU:HB3	1:C:1146:LYS:HE2	2.02	0.40
1:D:149:ALA:O	1:D:154:ASN:ND2	2.49	0.40
1:E:1676:ILE:HD12	1:E:1690:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2412:ILE:HD11	1:E:2477:ILE:HG12	2.02	0.40
1:A:458:GLU:HA	1:A:461:VAL:HG12	2.04	0.40
1:A:478:VAL:O	1:A:481:THR:HG22	2.21	0.40
1:B:456:ILE:O	1:B:460:ILE:HG13	2.22	0.40
1:B:569:THR:HG21	1:B:587:ASN:HB3	2.02	0.40
1:B:1050:ARG:O	1:B:1053:GLN:HB2	2.22	0.40
1:B:2295:GLY:HA3	1:E:676:HIS:CD2	2.56	0.40
1:C:500:ASN:HB2	1:C:627:LEU:HD13	2.04	0.40
1:E:283:LYS:HB2	1:E:293:LEU:HD22	2.04	0.40
1:E:1782:ARG:HE	1:E:1782:ARG:HB3	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	B	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	C	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	D	2114/2535 (83%)	2065 (98%)	49 (2%)	0	100	100
1	E	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
All	All	10570/12675 (83%)	10329 (98%)	241 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1816/2173 (84%)	1816 (100%)	0	100	100
1	B	1816/2173 (84%)	1816 (100%)	0	100	100
1	C	1816/2173 (84%)	1816 (100%)	0	100	100
1	D	1816/2173 (84%)	1816 (100%)	0	100	100
1	E	1816/2173 (84%)	1816 (100%)	0	100	100
All	All	9080/10865 (84%)	9080 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	302	ASN
1	A	310	ASN
1	A	520	ASN
1	A	556	ASN
1	A	852	GLN
1	A	855	ASN
1	A	892	GLN
1	A	969	GLN
1	A	1053	GLN
1	A	1090	ASN
1	A	1100	ASN
1	A	1145	HIS
1	A	1174	GLN
1	A	1282	GLN
1	A	1633	GLN
1	A	1636	GLN
1	A	1680	GLN
1	A	1812	GLN
1	A	1842	GLN
1	A	2004	GLN
1	A	2042	ASN
1	A	2057	GLN
1	A	2059	GLN
1	A	2071	GLN
1	A	2430	GLN

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Mol	Chain	Res	Type
1	B	302	ASN
1	B	310	ASN
1	B	556	ASN
1	B	852	GLN
1	B	855	ASN
1	B	892	GLN
1	B	969	GLN
1	B	1053	GLN
1	B	1090	ASN
1	B	1100	ASN
1	B	1145	HIS
1	B	1252	GLN
1	B	1282	GLN
1	B	1633	GLN
1	B	1636	GLN
1	B	1680	GLN
1	B	1812	GLN
1	B	1842	GLN
1	B	2004	GLN
1	B	2053	ASN
1	B	2057	GLN
1	B	2059	GLN
1	B	2430	GLN
1	C	302	ASN
1	C	556	ASN
1	C	852	GLN
1	C	855	ASN
1	C	892	GLN
1	C	969	GLN
1	C	1053	GLN
1	C	1090	ASN
1	C	1100	ASN
1	C	1252	GLN
1	C	1282	GLN
1	C	1633	GLN
1	C	1636	GLN
1	C	1680	GLN
1	C	1812	GLN
1	C	1842	GLN
1	C	2004	GLN
1	C	2042	ASN
1	C	2057	GLN

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Mol	Chain	Res	Type
1	C	2059	GLN
1	C	2071	GLN
1	C	2430	GLN
1	D	93	ASN
1	D	302	ASN
1	D	310	ASN
1	D	556	ASN
1	D	852	GLN
1	D	855	ASN
1	D	892	GLN
1	D	969	GLN
1	D	1053	GLN
1	D	1090	ASN
1	D	1282	GLN
1	D	1633	GLN
1	D	1636	GLN
1	D	1680	GLN
1	D	1812	GLN
1	D	1842	GLN
1	D	2004	GLN
1	D	2042	ASN
1	D	2059	GLN
1	D	2430	GLN
1	E	302	ASN
1	E	310	ASN
1	E	520	ASN
1	E	556	ASN
1	E	749	GLN
1	E	852	GLN
1	E	855	ASN
1	E	892	GLN
1	E	914	GLN
1	E	969	GLN
1	E	1053	GLN
1	E	1090	ASN
1	E	1100	ASN
1	E	1145	HIS
1	E	1282	GLN
1	E	1633	GLN
1	E	1636	GLN
1	E	1680	GLN
1	E	1812	GLN

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Mol	Chain	Res	Type
1	E	1842	GLN
1	E	2004	GLN
1	E	2059	GLN
1	E	2071	GLN
1	E	2252	ASN
1	E	2430	GLN
1	E	2497	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16791. These allow visual inspection of the internal detail of the map and identification of artifacts.

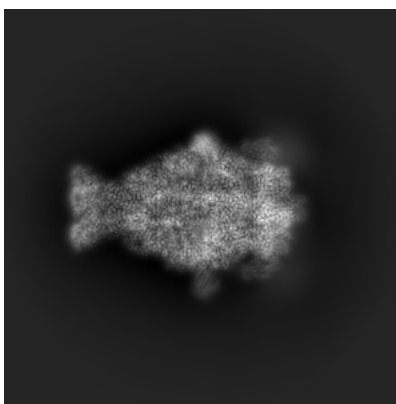
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

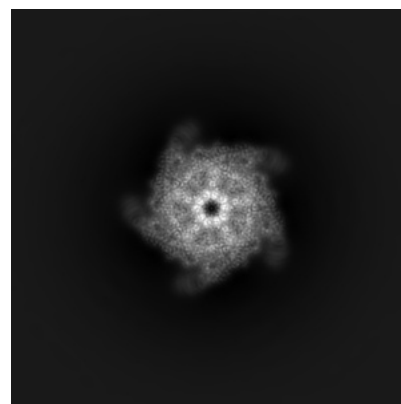
6.1.1 Primary map



X

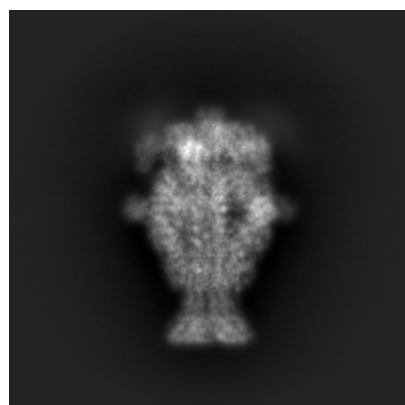


Y

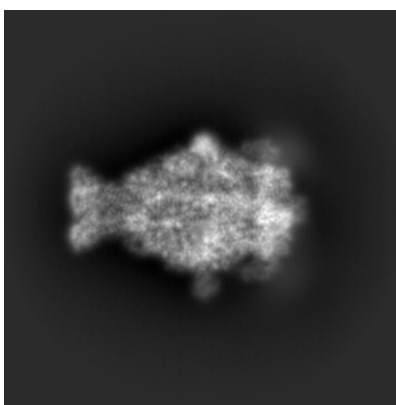


Z

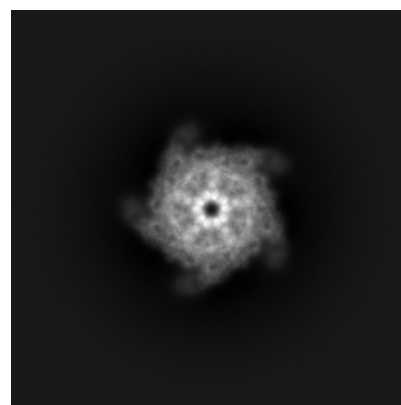
6.1.2 Raw map



X



Y



Z

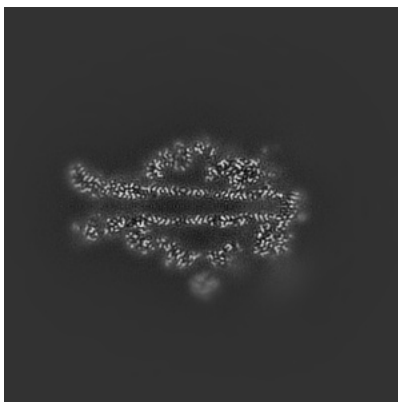
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

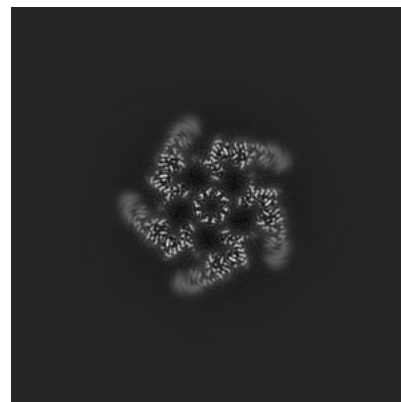
6.2.1 Primary map



X Index: 176

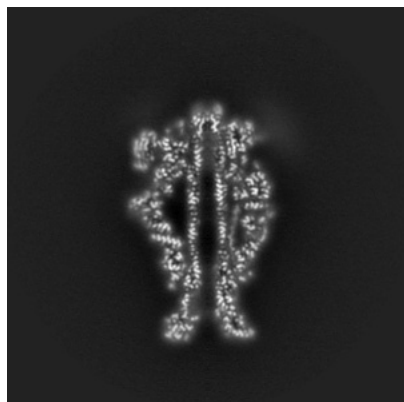


Y Index: 176

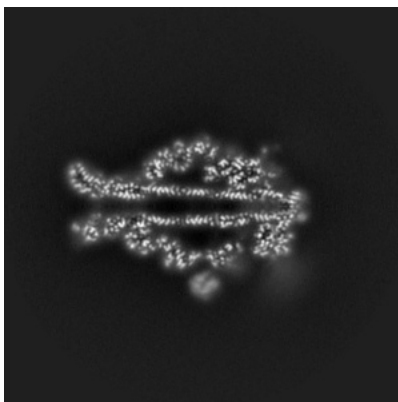


Z Index: 176

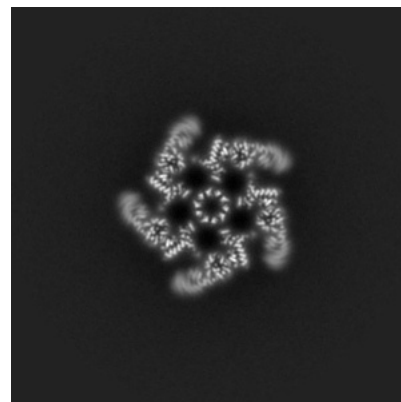
6.2.2 Raw map



X Index: 176



Y Index: 176

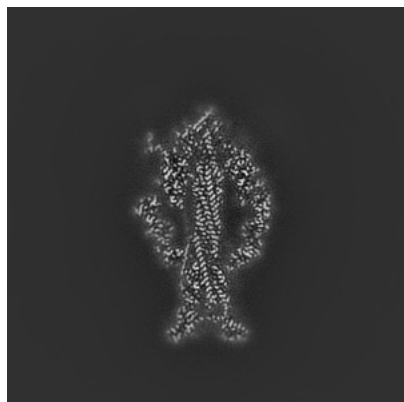


Z Index: 176

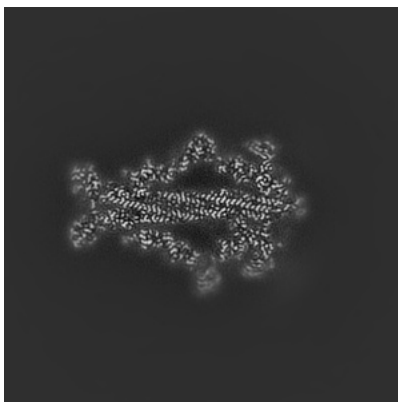
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

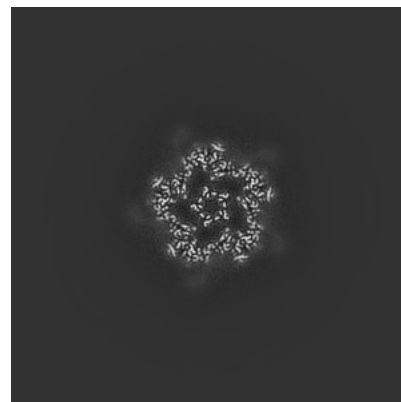
6.3.1 Primary map



X Index: 187

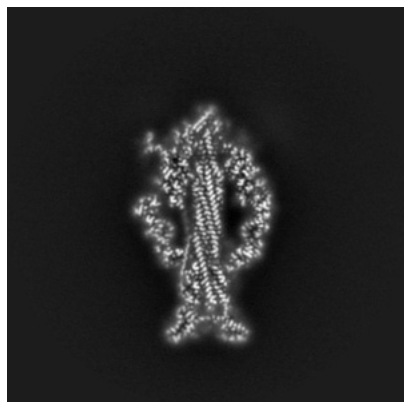


Y Index: 166

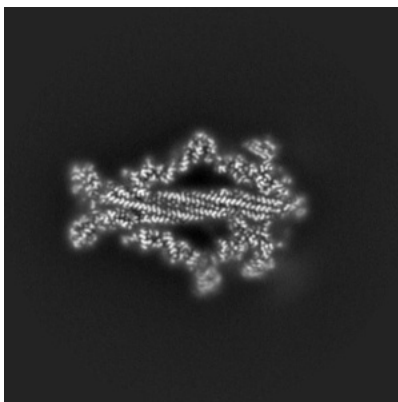


Z Index: 192

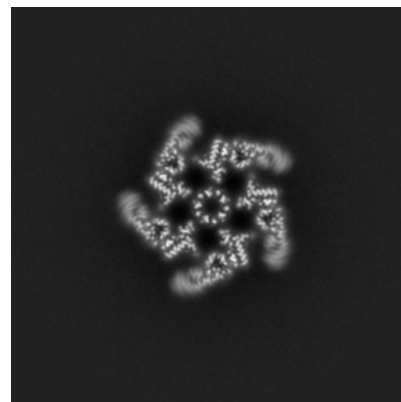
6.3.2 Raw map



X Index: 187



Y Index: 166

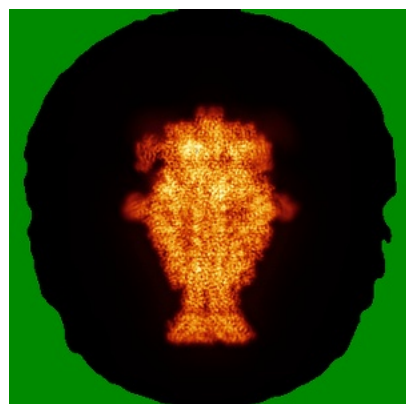


Z Index: 177

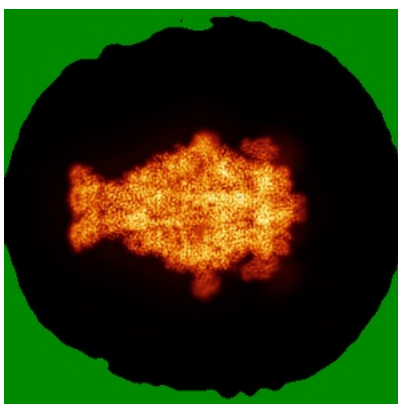
The images above show the largest variance slices of the map in three orthogonal directions.

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

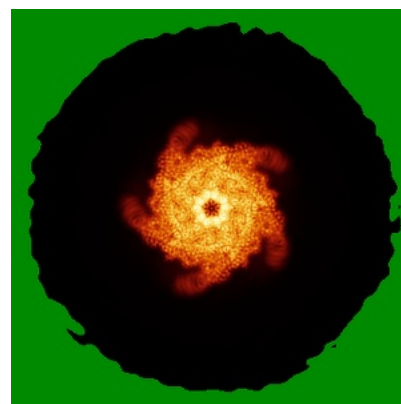
6.4.1 Primary map



X



Y

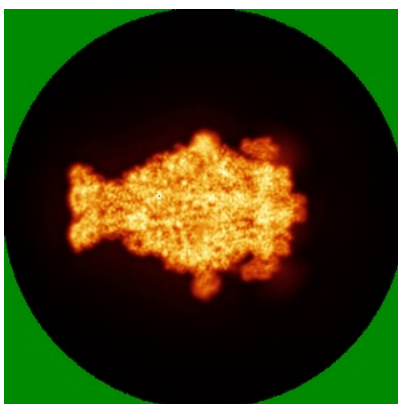


Z

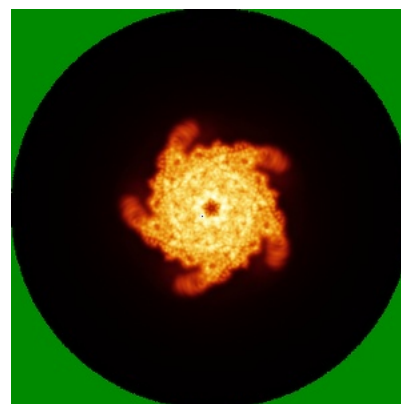
6.4.2 Raw map



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](#)

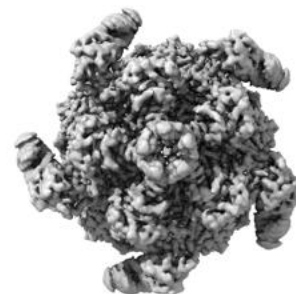
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

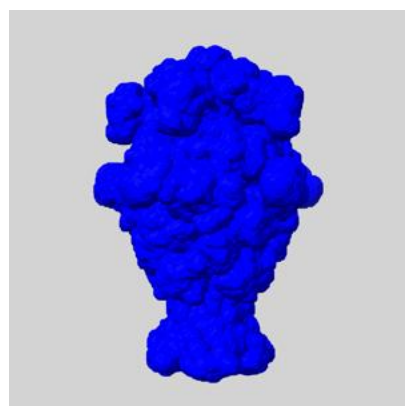
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

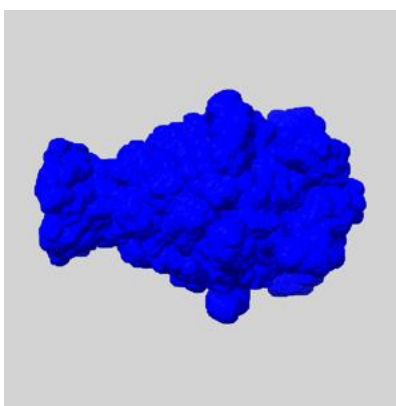
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

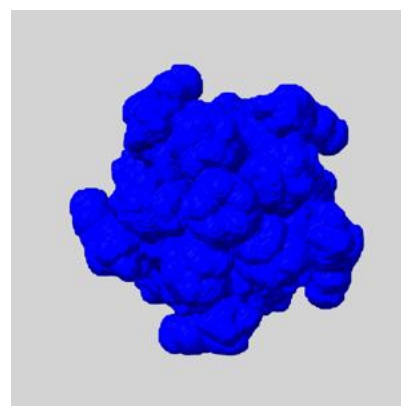
6.6.1 emd_16791_msk_1.map [i](#)



X



Y

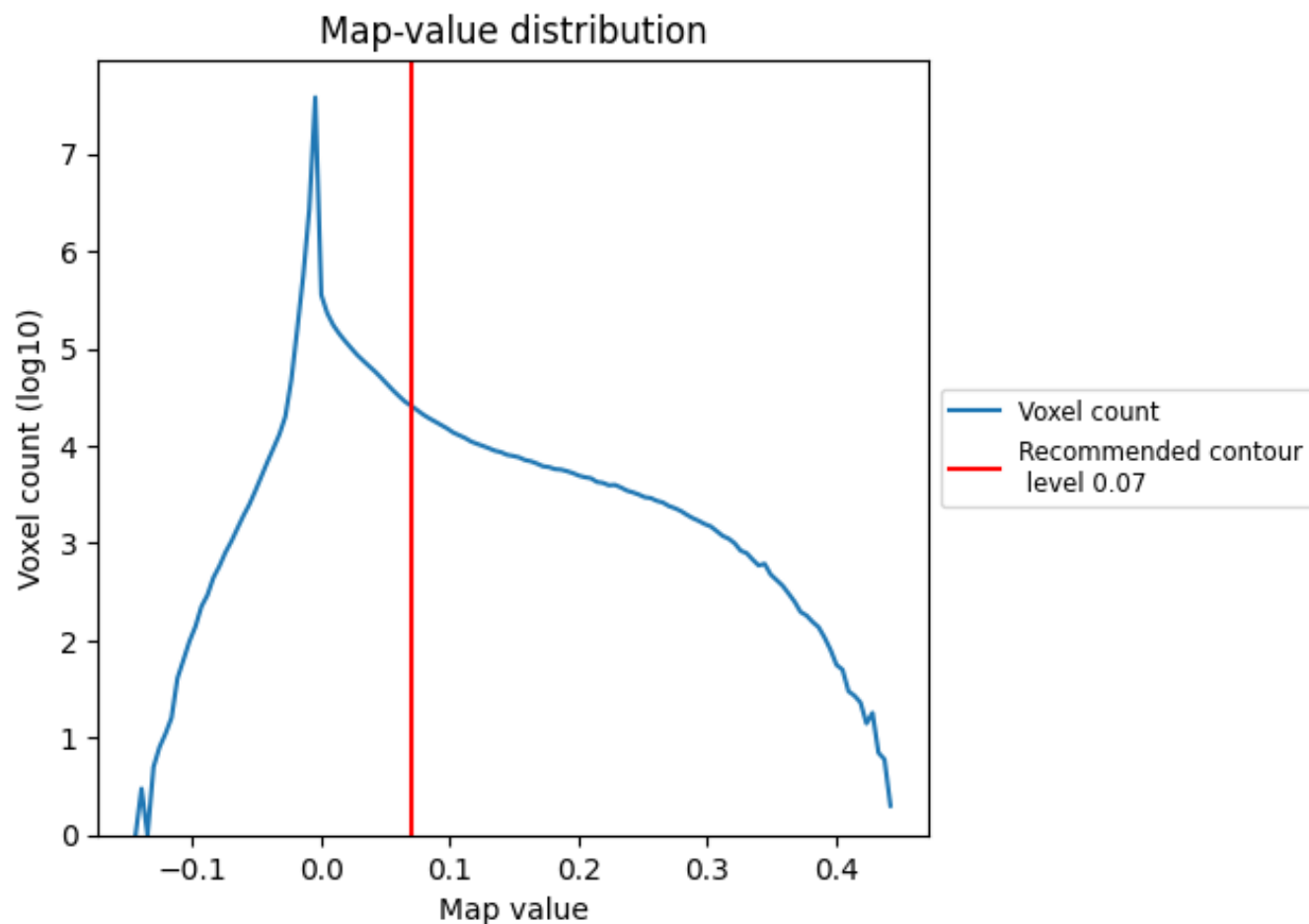


Z

7 Map analysis [i](#)

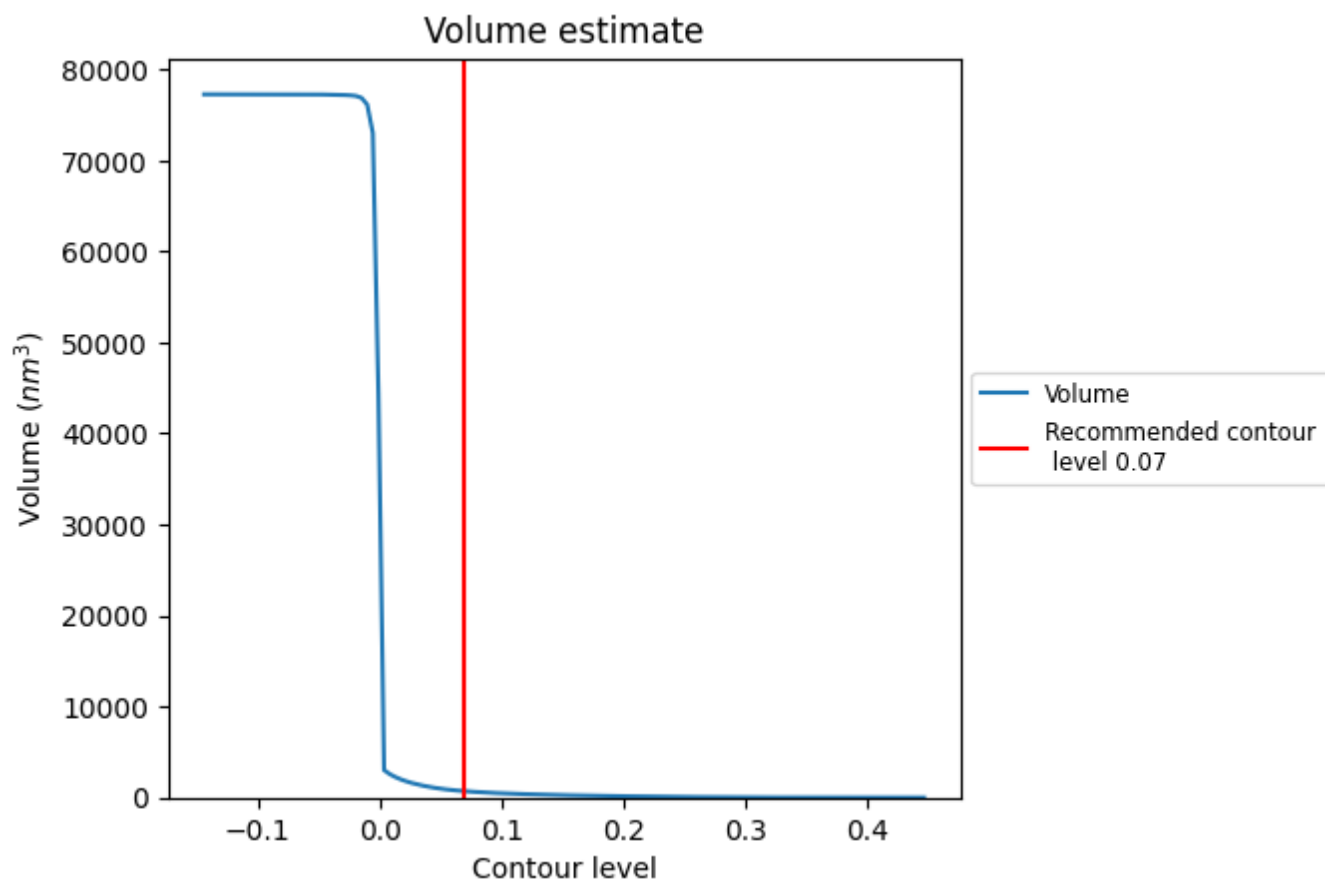
This section contains the results of statistical analysis of the map.

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.

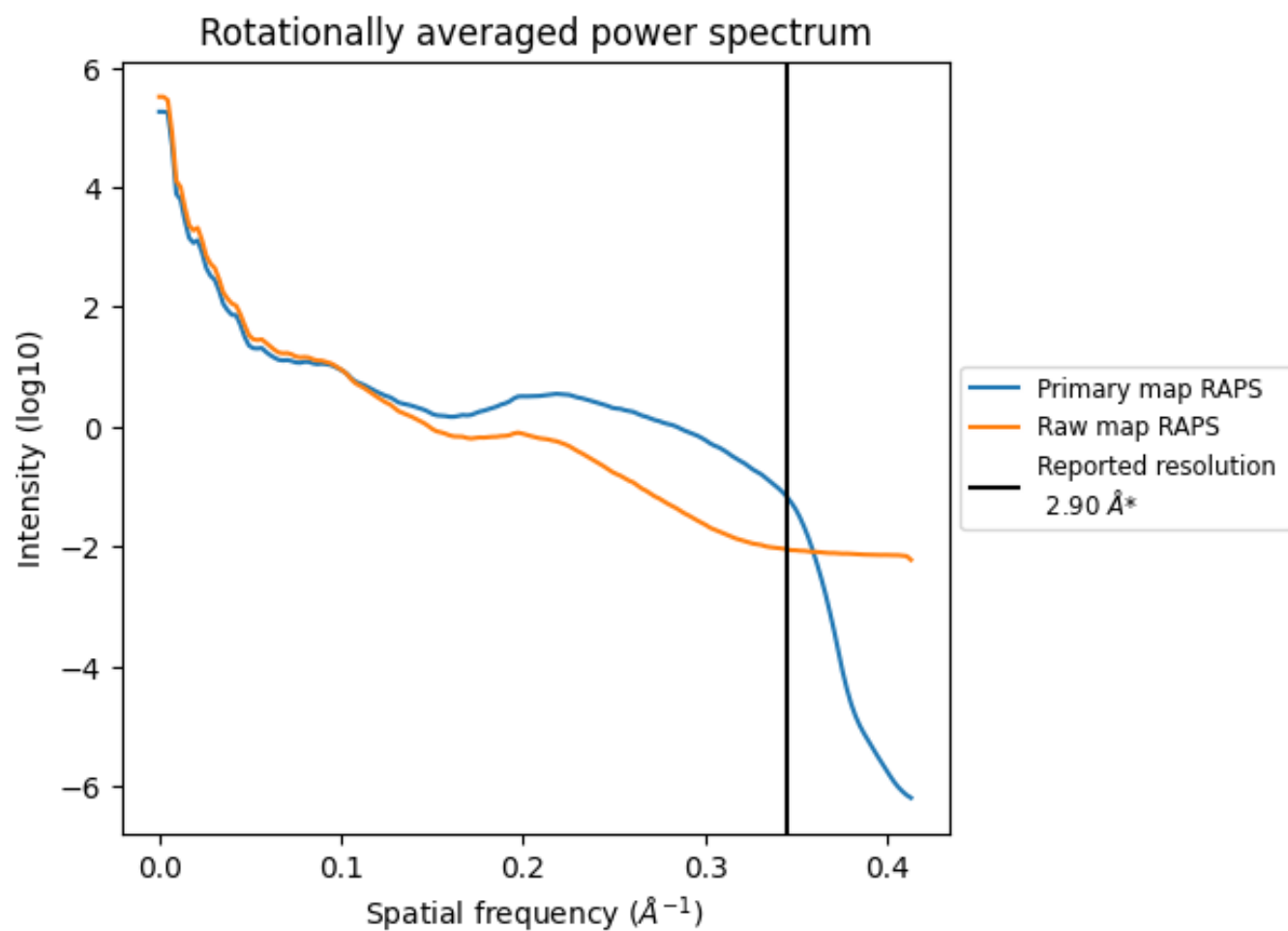
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 702 nm³; this corresponds to an approximate mass of 634 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 ⓘ

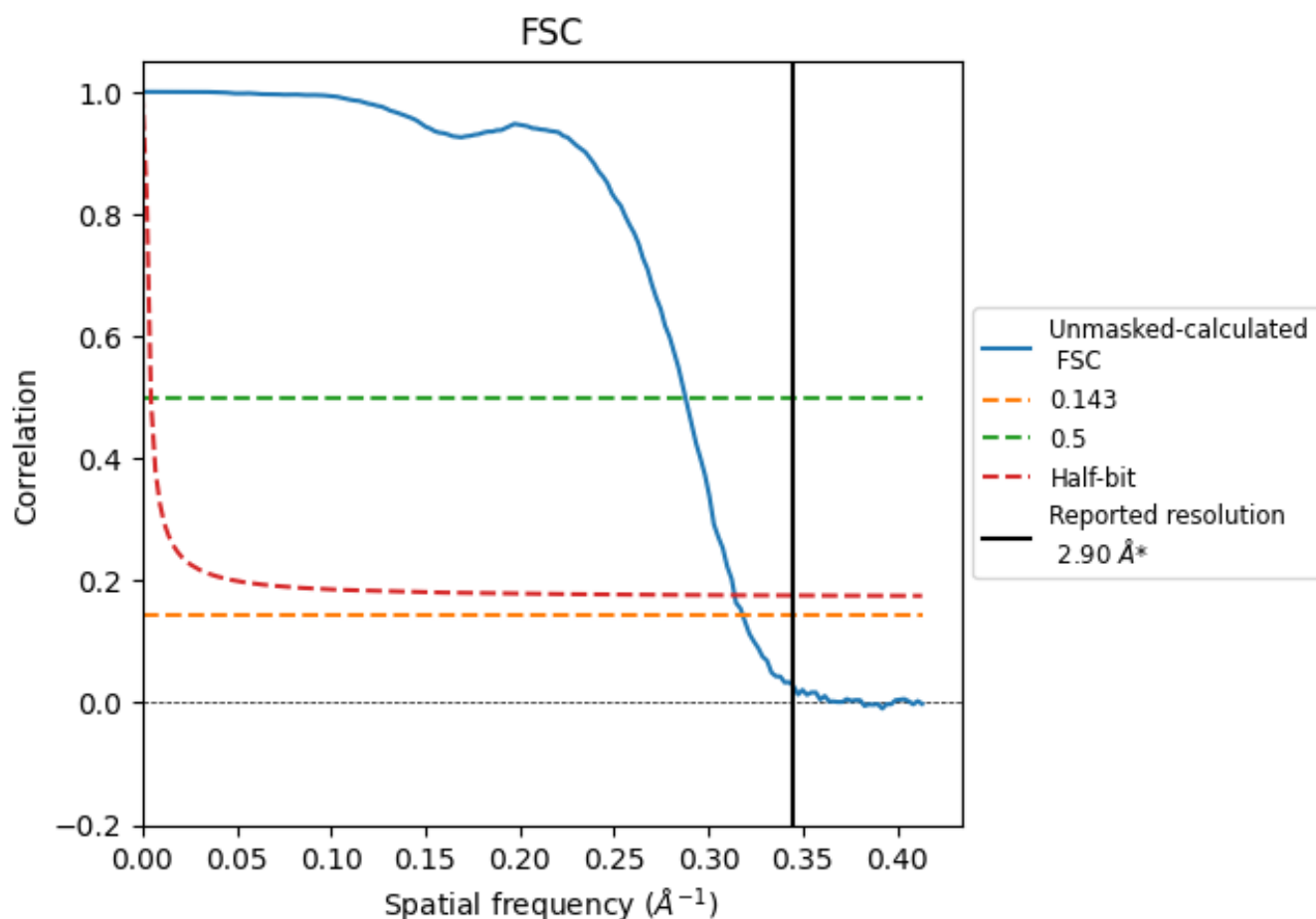


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

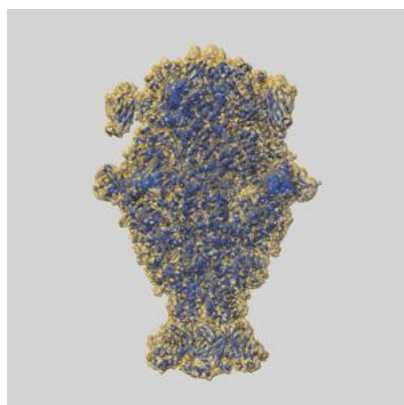
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.47	3.19

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

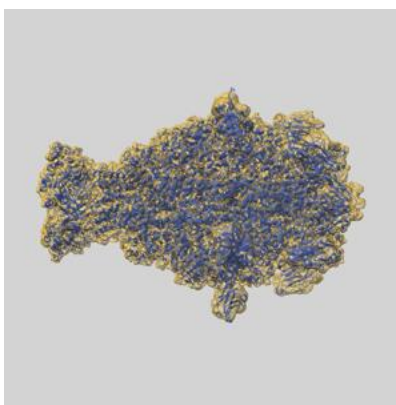
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16791 and PDB model 8CPZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

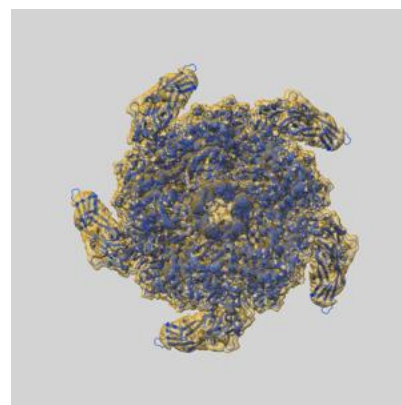
9.1 Map-model overlay [i](#)



X



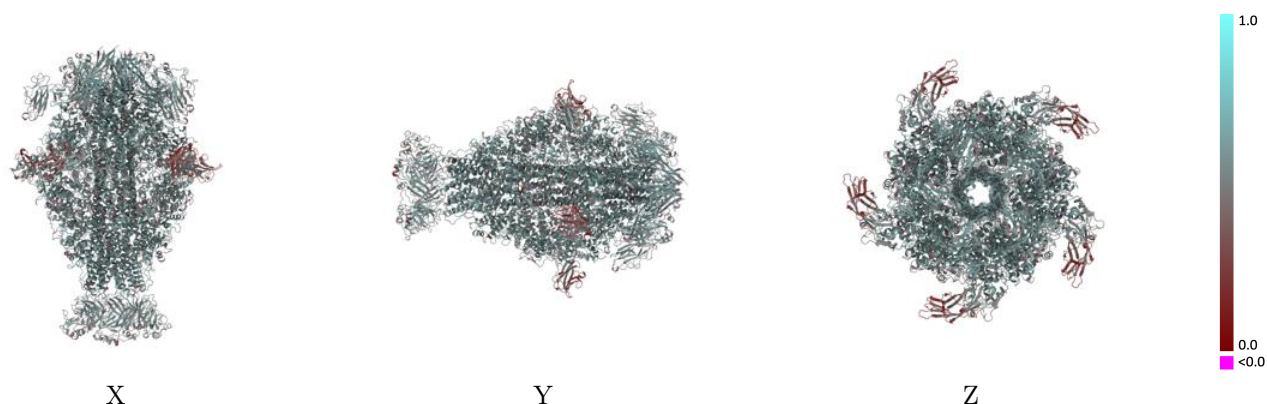
Y



Z

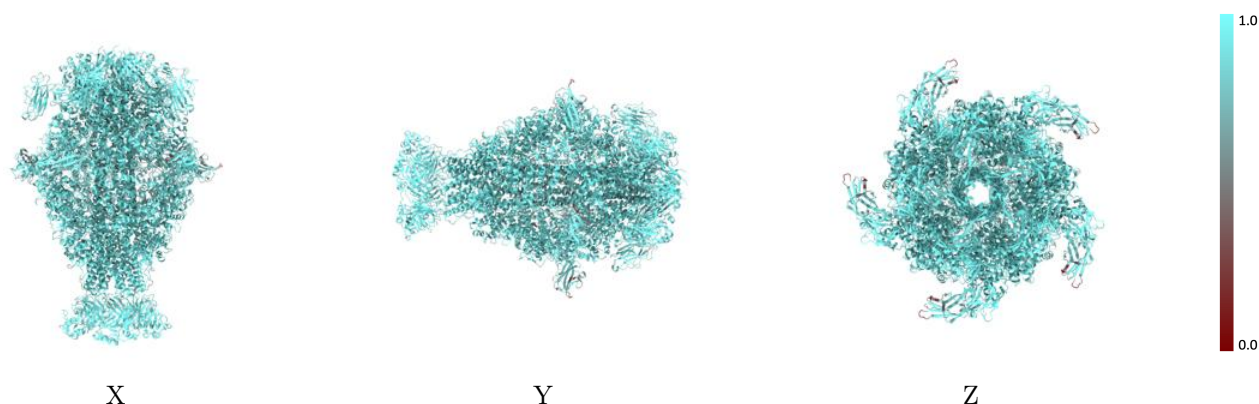
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



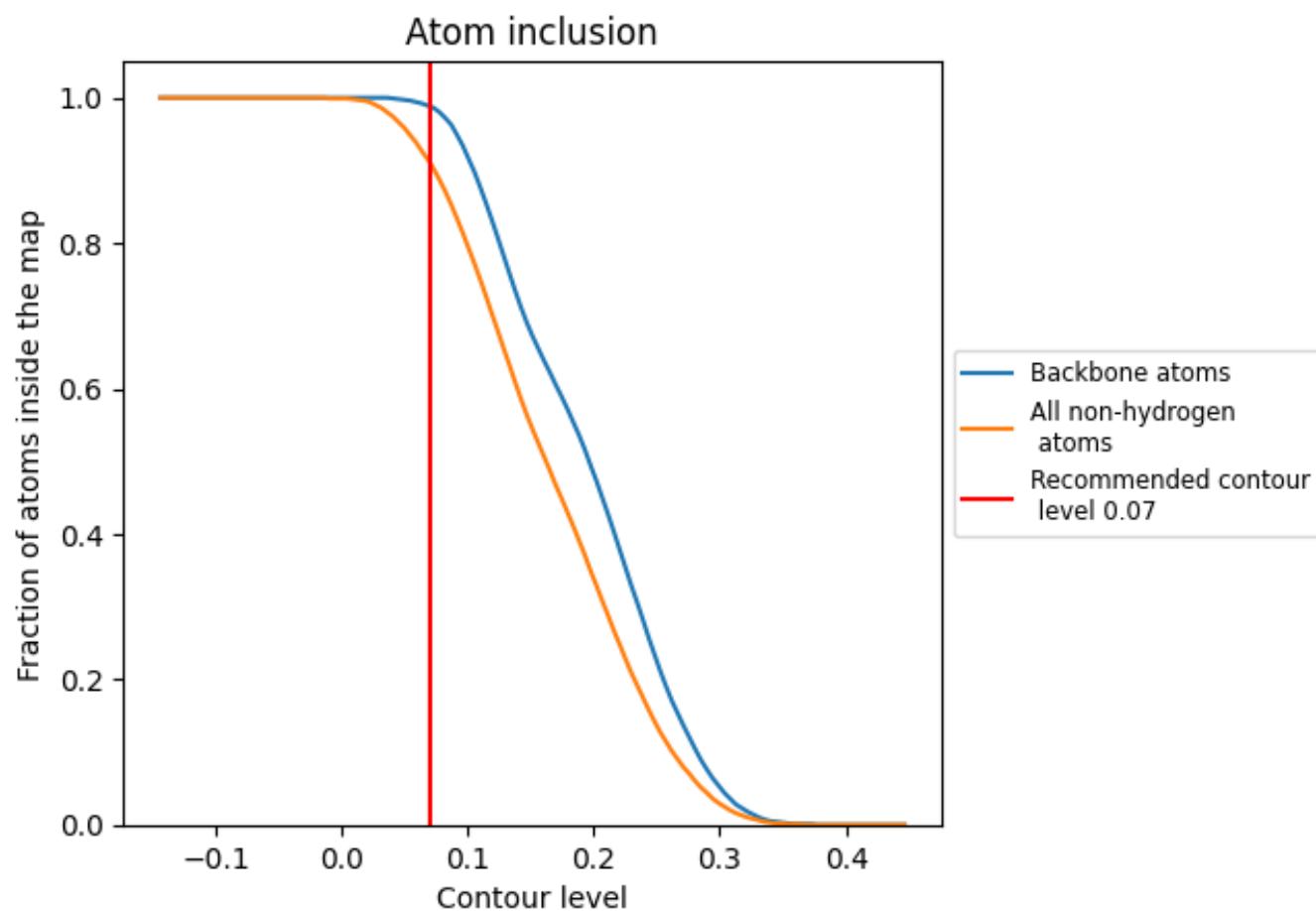
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 91% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.5260
A	0.9100	0.5260
B	0.9110	0.5270
C	0.9100	0.5270
D	0.9110	0.5260
E	0.9110	0.5260

