



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:37 AM UTC

PDB ID : 8A7E / pdb_00008a7e
EMDB ID : EMD-15221
Title : PAPP-A dimer in complex with its inhibitor STC2
Authors : Kobbero, S.D.; Gajhede, M.; Mirza, O.A.; Boesen, T.; Oxvig, C.
Deposited on : 2022-06-20
Resolution : 5.02 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

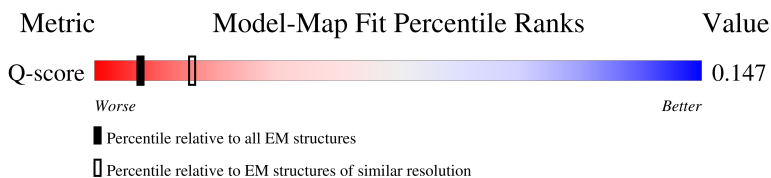
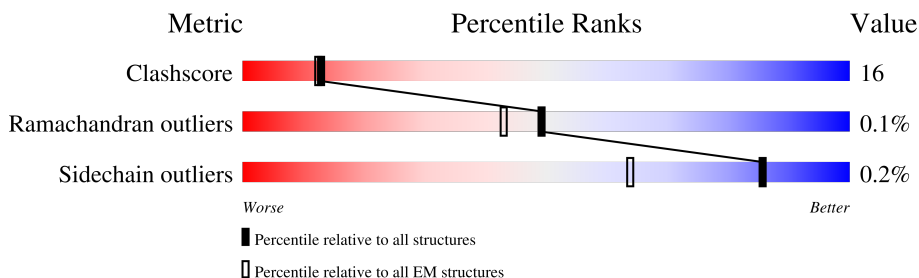
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.02 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	855 (4.52 - 5.51)

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	168	67% (Green), 33% (Yellow)
1	P	168	58% (Green), 42% (Yellow)
2	C	1536	64% (Green), 35% (Yellow), . (Grey)
2	Q	1536	65% (Green), 35% (Yellow), . (Grey)

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 26442 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 Stanniocalcin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	P	168	Total	C	N	O	S	0	0
			1315	822	237	239	17		
1	A	168	Total	C	N	O	S	0	0
			1315	822	237	239	17		

- Molecule 2 is a protein called Pappalysin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1524	Total	C	N	O	S	0	0
			11897	7436	2062	2294	105		
2	Q	1524	Total	C	N	O	S	0	0
			11897	7436	2062	2294	105		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	563	GLN	GLU	engineered mutation	UNP Q13219
Q	563	GLN	GLU	engineered mutation	UNP Q13219

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total	Zn	0
			1	1	
3	Q	1	Total	Zn	0
			1	1	

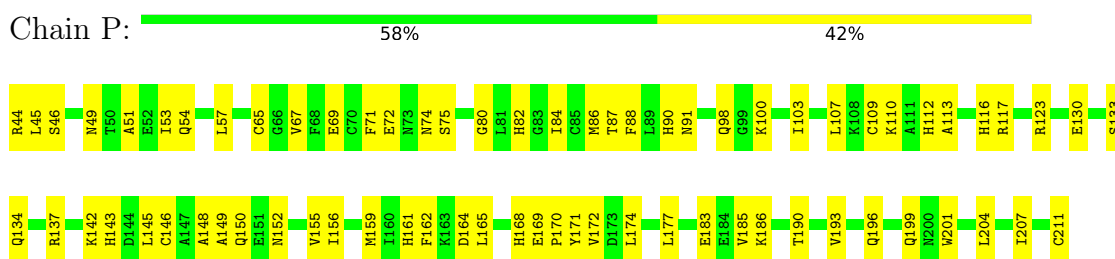
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	C	8	Total 8	Ca 8	0
4	Q	8	Total 8	Ca 8	0

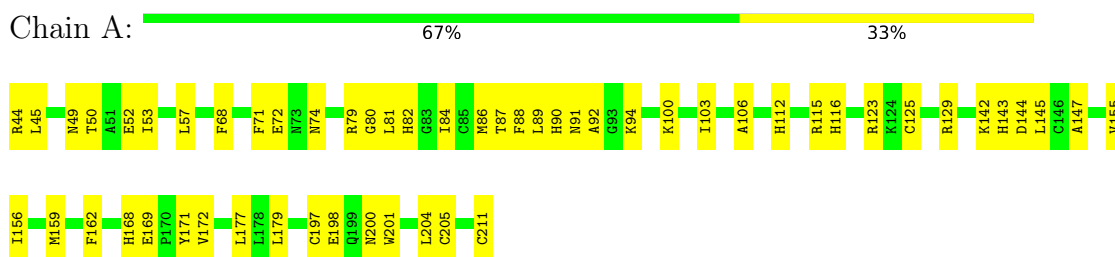
3 Residue-property plots

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

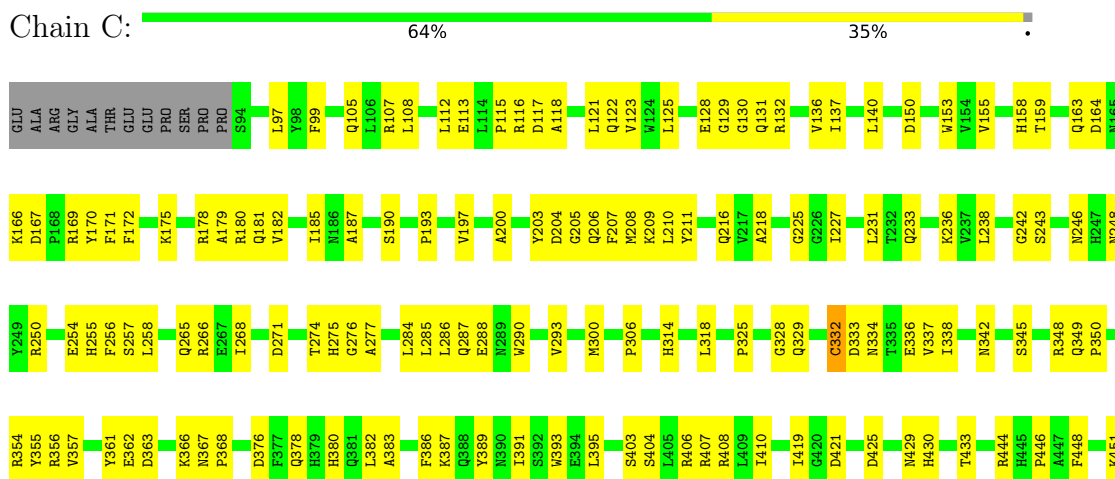
- Molecule 1: Stanniocalcin-2



- Molecule 1: Stanniocalcin-2



- Molecule 2: Pappalysin-1



D488	D489	C461	M462	F466	D469	E579	E580	M480	T484	C485	F486	D487	P488	R493	A494	Y495	M498	M499	K502	L505	K506	L507	D508	G509	L513	M514	I515	L525	M533	D534	K535	E536	A537	M539	H540	L541	T557	H558	T559	M560	I561	H562	H566	S567	L568																																										
G569	L570	Y571	H572	R575	G576	I577	S578	E579	E580	M581	S582	P592	G597	D598	L599	M604	P605	H609	K610	S611	D620	G623	F624	H625	S626	F627	N629	M633	M634	F635	D641	D642	C643	T644	D645	F647	T648	Q651	V652	A653	R654	I655	H656	L659	L661																																										
Y662	Y663	W666	Q667	P668	K671	P672	L677	L682	W693	I697	F702	S708	A709	C710	H711	L712	C713	L714	E715	G716	R717	I718	A723	S724	N725	F628	A726	S727	S728	P729	M730	P731	G736	H737	W738	S739	P740	R741	E744	G745	Q751	A653	P752	C753	K754	T759	N763																																								
V766	H769	P772	P773	A774	C775	F776	F777	Q779	C780	F781	Y782	L791	C975	V1101	P793	L796	T797	V803	V803	G716	D806	W807	G811	A812	V813	N814	D815	I816	K817	L818	L819	A820	M825	I826	P740	G829	Q831	M832	V833	D836	V837	P838	L839	T840	L843																																										
W850	I853	Q854	Y855	T857	L858	E859	E860	D865	L869	T870	S871	R872	C878	P883	Y886	V889	R890	D891	P892	P893	L894	V898	A899	S900	H903	L904	N905	R906	V918	Y921	W922	I924	E930	E931	S932	P934	A937	I941	Y946	D949	G950	I951	Q953	K954	D955	Q956	G957	E958	D961	N964	K965	I966	N967	G968	D969	F974	C975	R976	C983	P987	S988	R989	C990	D994	C999	Q1004	S1007	P1016	Q1017	G1018	F1019	L1020	W1023	A1024	I1041	I1042	G1043	Q1044	P934	S1048	K1054	L1058	G1061				
Q1064	Y1074	P1075	Q1078	L1079	L1086	F1090	S1091	Q1092	P1093	M1094	V1095	A1096	A1097	V1099	I1100	V1101	H1102	L1103	V1104	T1105	T1108	Y1109	Y1110	Q1115	I1118	S1119	V1120	Q1121	L1122	D1124	Q1128	L1137	R1140	M1141	M1142	V1148	V1149	H1150	F1156	Y1157	S1164	S1165	F1166	Q1064	Y1074	P1075	Q1078	L1079	L1086	F1090	S1091	Q1092	P1093	M1094	V1095	A1096	A1097	V1099	I1100	V1101	H1102	L1103	V1104	T1105	T1108	Y1109	Y1110	Q1115	I1118	S1119	V1120	Q1121	L1122	D1124	Q1128	L1137	R1140	M1141	M1142	V1148	V1149	H1150	F1156	Y1157	S1164	S1165	F1166
P1189	I1173	S1174	G1175	V1176	A1177	L1178	R1179	S1180	F1181	D1182	M1183	F1184	D1185	P1186	V1187	T1188	L1189	R1194	G1195	E1196	E1202	Q1203	S1204	C1205	V1206	H1207	C1210	E1211	D1214	C1227	S1230	D1231	H1234	Q1237	C1238	T1239	V1240	L1248	Q1249	I1250	R1251	D1254	E1255	L1256	I1257	K1258	S1259																																								
V1265	T1266	T1268	E1271	G1272	K1273	W1274	M1275	K1276	S1277	V1278	V1283	S1286	H1291	A1296	F1306	Q1309	A1318	K1321	G1322	H1323	M1324	S1325	L1326	L1327	T1328	L1334	W1335	P1338	E1339	A1340	L1341	C1342	L1357	C1362	R1363	E1364	H1367	G1380	V1381	H1382	V1383																																														
S1386	K1392	R1393	A1394	F1395	Q1398	C1399	T1400	Q1401	D1402	V1413	P1420	H1423	G1424	L1425	R1439	I1440	A1447	S1448	Q1449	G1450	V1455	T1456	H1457	C1458	R1459	C1478	S1479	L1484	N1485	L1488	K1489	L1490	Y1496	A1497	I1498	E1501	T1504	N1510	S1513	I1514	I1515	K1258	L1516	P1517																																											
M1518	T1521	D1524	I1525	P1531	T1532	R1533	Q1534	E1535	R1536	V1537	A1541	G1542	W1545	Y1546	P1547	H1548	L1551	I1552	H1553	G1557	C1558	F1561	N1565	D1568	M1571	N1572	R1573	A1574	F1575	C1584	T1587	V1588	K1589	T1590	K1591	K1592	P1595	F1596	P1597	M1598	D1601	C1606	A1607																																												
C1608	H1616	S1617																																																																																					

• Molecule 2: Pappalysin-1



GLU	ALA	ARG	GLY	ALA	THR	GLU	PRO	SER	PRO	PRO	S94	L97	I98	Y98	F99	L106	L107	L108	R109	L114	P115	R116	D117	A118	F119	T120	L121	Q122	V123	R126	A127	E128	G129	G130	Q131	G139	L140	V141	D142	R149	V153	V154	H158	T159	F1596	P1597	M1598	D1601	H165	K166	D167
Y170	F171	F172	K175	R176	A179	R180	Q181	V182	T183	I184	I185	N186	A187	H188	R189	W196	Y197	L199	A200	A201	T202	Y203	D204	G205	L211	F207	L210	Y211	Q216	E222	Q223	I227	L238	G242	N246	N248	Y249	R250	G251	Y252	L253	E254	H255	F256	S257	L258					

G1542	D1402	T1266	P1169	Q1049	A937	D836	P762	L661	R575	C461	R354	W259
W1545	Q1406	V1267	I1173	V1050	I941	V837	N763	V682	G576	M462	Y355	K260
Y1546	V1413	T1268	A1177	C1051	I941	P838	S764	Y663	I577	R356	R356	Q265
H1546	T1414	E1271	L1178	K1054	C947	L839	A765	W666	V766	F466	V357	R266
L1551	D1416	K1273	R1179	L1058	Q953	L843	N767	W667	S579	D469	Y361	L269
I1552	F1181	W1274	F1181	S1077	Q956	V850	T770	P586	P586	C473	E362	S270
H1553	L1425	N1275	D1182	Q1078	N964	K854	P772	C587	C587	N480	D363	D271
C1554	F1184	K1276	N1183	L1079	K965	I855	P773	P592	P592	N480	K366	T274
G1557	D1185	Q1277	F1184	W1085	D969	T857	A774	G597	G597	T484	N367	H275
C1558	P1186	C1285	D1185	L1086	G970	L888	F776	D598	D598	C485	P368	A277
E1559	Y1187	P1288	Y1089	F1090	F974	D859	E777	L599	L599	P488	D377	H278
F1561	L1188	T1188	F1090	F1090	F974	E660	P778	N604	N604	P488	F377	L281
N1571	S1191	L1189	V1095	V1095	F981	H861	Q779	P605	P605	R493	Q378	L281
N1572	C1192	S1190	A1096	A1096	F981	L862	G780	P605	P605	R493	H379	P282
R1573	G1195	G1195	A1097	A1097	F981	L862	C781	H609	H609	A494	H380	Q283
A1574	E1196	E1196	I1100	I1100	F981	L862	Y782	R610	R610	Y495	Q381	L284
F1575	A1201	E1202	L1103	L1103	F981	L862	L783	S611	S611	N499	L382	L285
C1584	E1202	Q1203	V1104	V1104	F981	L862	E786	P615	P615	K502	F386	Q287
T1587	Q1203	S1204	T1105	T1105	F981	L862	S708	D620	D620	G509	Y389	E288
K1591	C1205	C1205	T1108	T1108	F981	L862	A709	G623	G623	L513	N390	N289
P1595	W1206	W1206	Y1109	Y1109	F981	L862	C710	F624	F624	M514	N390	W290
P1597	H1207	H1207	F1109	F1109	F981	L862	H711	H625	H625	M514	I391	V293
M1598	C1210	C1210	Q1115	Q1115	F981	L862	C713	F626	F626	M514	D396	K294
L1602	E1211	E1211	I1118	I1118	F981	L862	R717	F627	F627	M514	S403	W297
C1608	K1212	K1212	L1118	L1118	F981	L862	I718	F628	F628	M514	L404	M300
H1616	D1214	D1214	L1122	L1122	F981	L862	I718	N629	N629	M514	L405	R407
S1617	A1223	A1223	D1124	D1124	F981	L862	L719	T630	T630	M514	R407	P306
L1507	C1227	C1227	Q1128	Q1128	F981	L862	N725	Y632	Y632	M514	L408	L318
I1514	H1230	H1230	L1132	L1132	F981	L862	A726	N633	N633	M514	L409	L318
I1515	H1234	H1234	L1137	L1137	F981	L862	S727	M634	M634	M514	I410	L318
L1516	Q1237	Q1237	R1140	R1140	F981	L862	E744	M636	M636	M514	C414	P324
P1517	C1238	C1238	N1141	N1141	F981	L862	G745	H540	H540	M514	D415	P325
M1518	T1239	T1239	M1142	M1142	F981	L862	H746	M636	M636	M514	N429	L326
T1521	R1243	R1243	D1151	D1151	F981	L862	P747	D641	D641	M514	H430	C327
D1524	R1251	R1251	L1152	L1152	F981	L862	W738	G542	G542	M514	I419	G328
I1525	R1252	R1252	L1157	L1157	F981	L862	S739	C643	C643	M514	D425	C332
L1529	D1253	D1253	H1158	H1158	F981	L862	P740	T644	T644	M514	N334	D333
R1533	E1254	E1254	V1162	V1162	F981	L862	E744	D645	D645	M514	T559	N334
V1534	L1256	L1256	Q1044	Q1044	F981	L862	G745	S646	S646	M514	C428	T335
V1537	K1258	K1258	F1166	F1166	F981	L862	H746	F647	F647	M514	N429	E336
					F981	L862	A820	Q651	Q651	M514	H430	V337
					F981	L862	N825	V652	V652	M514	T433	I338
					F981	L862	D815	A653	A653	M514	N342	N342
					F981	L862	I816	R654	R654	M514	R444	N342
					F981	L862	K817	M655	M655	M514	H445	S345
					F981	L862	L818	M656	M656	M514	P446	S345
					F981	L862	I819	L668	L668	M514	A447	R348
					F981	L862	A820	S755	S755	M514	F448	Q349
					F981	L862	N825	W760	W760	M514	L458	P350
					F981	L862	P1037	S761	S761	M514	D458	K351

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	3	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58, 59	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	25.960	Depositor
Minimum map value	-13.178	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.939	Depositor
Recommended contour level	1.7	Depositor
Map size (Å)	303.59998, 303.59998, 303.59998	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1859374, 1.1859374, 1.1859374	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/1337	0.32	0/1799
1	P	0.15	0/1337	0.36	0/1799
2	C	0.10	0/12217	0.31	0/16633
2	Q	0.10	0/12217	0.31	0/16633
All	All	0.11	0/27108	0.32	0/36864

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	1315	0	1290	39	0
1	P	1315	0	1290	52	0
2	C	11897	0	11211	389	0
2	Q	11897	0	11213	398	0
3	C	1	0	0	0	0
3	Q	1	0	0	0	0
4	C	8	0	0	0	0
4	Q	8	0	0	0	0
All	All	26442	0	25004	847	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 16.

All (847) 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)
2:Q:984:ILE:O	2:Q:988:SER:HA	1.69	0.90
1:A:88:PHE:HB3	1:A:103:ILE:HD11	1.54	0.87
2:Q:332:CYS:CB	2:Q:657:CYS:SG	2.64	0.86
2:C:562:HIS:CD2	2:C:566:HIS:NE2	2.45	0.83
2:C:488:PRO:HA	2:C:493:ARG:HD3	1.62	0.81
2:C:1254:ASP:HB2	2:Q:1202:GLU:HB3	1.63	0.81
2:Q:488:PRO:HA	2:Q:493:ARG:HD3	1.64	0.79
2:Q:1318:ALA:HA	2:Q:1343:GLU:O	1.81	0.79
2:C:266:ARG:HH12	2:C:987:PRO:HG2	1.49	0.77
2:C:1210:CYS:SG	2:C:1211:GLU:N	2.58	0.77
2:C:562:HIS:CD2	2:C:566:HIS:HE2	1.97	0.76
2:C:1565:ASN:HD21	2:C:1589:LYS:HG2	1.50	0.75
2:C:535:LYS:HD3	2:C:745:GLY:HA3	1.68	0.74
2:Q:572:HIS:ND1	2:Q:579:GLU:OE2	2.19	0.73
2:Q:1210:CYS:SG	2:Q:1211:GLU:N	2.60	0.73
2:C:1150:HIS:HB2	2:Q:1152:LEU:HD12	1.70	0.72
2:C:1098:ALA:HB3	2:C:1179:ARG:HD2	1.71	0.72
2:Q:153:TRP:HB2	2:Q:172:PHE:HE1	1.55	0.72
2:C:1210:CYS:O	2:C:1211:GLU:HG3	1.90	0.72
2:C:266:ARG:HH21	2:C:989:ARG:HB3	1.55	0.72
2:C:921:TYR:O	2:C:937:ALA:HA	1.90	0.71
2:C:1420:PRO:O	2:C:1423:HIS:ND1	2.21	0.71
2:Q:1210:CYS:O	2:Q:1211:GLU:HG3	1.90	0.71
2:Q:1595:PRO:HG2	2:Q:1598:MET:HA	1.72	0.71
2:Q:378:GLN:HG3	2:Q:560:MET:HE2	1.71	0.71
2:C:1322:GLY:HA3	2:C:1340:ALA:HA	1.74	0.70
1:A:68:PHE:HB3	1:A:81:LEU:HB3	1.74	0.70
2:Q:246:ASN:OD1	2:Q:248:ASN:ND2	2.25	0.70
2:C:122:GLN:HG3	2:C:257:SER:HB3	1.74	0.69
2:C:817:LYS:HB2	2:C:854:GLN:HB2	1.73	0.69
2:C:123:VAL:HG12	2:C:256:PHE:HA	1.74	0.69
2:Q:999:CYS:SG	2:Q:1004:GLN:NE2	2.65	0.69
2:C:1595:PRO:HG2	2:C:1598:MET:HA	1.72	0.69
1:P:155:VAL:HG12	1:P:159:MET:HE1	1.75	0.69
2:C:1184:PHE:H	2:C:1203:GLN:HE21	1.41	0.69
2:C:1202:GLU:HB3	2:Q:1254:ASP:HB2	1.74	0.69
2:C:246:ASN:OD1	2:C:248:ASN:ND2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:GLN:NE2	2:C:248:ASN:OD1	2.26	0.69
2:C:730:MET:HE3	2:C:738:TRP:HB2	1.74	0.68
2:Q:1096:ALA:HA	2:Q:1180:SER:HA	1.74	0.68
1:A:86:MET:HE3	1:A:90:HIS:CE1	2.29	0.68
2:C:153:TRP:HB2	2:C:172:PHE:HE1	1.58	0.68
2:Q:717:ARG:NH1	2:Q:878:CYS:O	2.26	0.68
2:C:717:ARG:NH1	2:C:878:CYS:O	2.25	0.68
2:C:1095:VAL:HG21	2:C:1156:PHE:HB3	1.76	0.68
2:Q:921:TYR:O	2:Q:937:ALA:HA	1.94	0.68
1:A:197:CYS:O	1:A:201:TRP:HB2	1.93	0.68
2:Q:1100:ILE:HB	2:Q:1177:ALA:HB3	1.75	0.67
1:P:145:LEU:HD23	1:P:177:LEU:HD23	1.76	0.67
2:Q:918:VAL:HG22	2:Q:941:ILE:HG12	1.77	0.67
2:Q:1118:ILE:HG22	2:Q:1166:PHE:HB3	1.76	0.67
2:Q:1547:PRO:HB2	2:Q:1552:ILE:HD11	1.75	0.67
2:C:572:HIS:ND1	2:C:579:GLU:OE2	2.28	0.67
2:C:1258:LYS:NZ	2:Q:1020:LEU:O	2.27	0.67
2:C:107:ARG:HG3	2:C:300:MET:HE1	1.75	0.66
2:Q:107:ARG:HG3	2:Q:300:MET:HE1	1.77	0.66
2:Q:181:GLN:NE2	2:Q:1048:SER:OG	2.28	0.66
2:Q:661:LEU:HD13	2:Q:697:ILE:HG13	1.78	0.66
2:Q:1518:MET:HE1	2:Q:1551:LEU:HD22	1.77	0.66
2:C:577:ILE:HD13	2:C:627:PHE:HE1	1.60	0.66
2:C:886:TYR:HB2	2:C:903:HIS:HB2	1.78	0.66
2:C:378:GLN:HG3	2:C:560:MET:HE2	1.78	0.66
2:C:179:ALA:HA	2:Q:1334:LEU:HD11	1.78	0.65
2:Q:777:GLU:O	2:Q:779:GLN:N	2.27	0.65
1:P:109:CYS:SG	1:P:142:LYS:NZ	2.64	0.65
1:P:130:GLU:O	1:P:134:GLN:NE2	2.30	0.65
1:P:201:TRP:HB3	1:P:204:LEU:HB2	1.77	0.65
2:C:567:SER:O	2:C:663:TYR:OH	2.15	0.65
2:C:659:LEU:HD23	2:C:663:TYR:HD2	1.61	0.65
2:Q:164:ASP:O	2:Q:166:LYS:NZ	2.28	0.65
2:C:231:LEU:HD11	2:Q:1341:LEU:HD23	1.79	0.65
2:Q:1382:HIS:HD2	2:Q:1413:VAL:HG22	1.61	0.65
2:Q:1364:GLU:O	2:Q:1367:HIS:NE2	2.30	0.65
2:Q:1251:ARG:HG2	2:Q:1257:ILE:HG12	1.77	0.64
2:C:1547:PRO:HB2	2:C:1552:ILE:HD11	1.77	0.64
2:Q:833:VAL:HG22	2:Q:839:LEU:HD11	1.79	0.64
2:C:777:GLU:O	2:C:779:GLN:N	2.27	0.64
2:C:163:GLN:O	2:C:1140:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:169:ARG:HB3	2:C:187:ALA:HB3	1.79	0.64
2:Q:1388:ARG:NH1	2:Q:1416:ASP:OD1	2.29	0.64
1:P:88:PHE:HB3	1:P:103:ILE:HD11	1.79	0.64
2:C:803:VAL:HG21	2:C:833:VAL:HG11	1.80	0.64
1:A:155:VAL:HG12	1:A:159:MET:HE1	1.79	0.64
2:Q:568:LEU:HD13	2:Q:663:TYR:HE2	1.61	0.64
2:C:129:GLY:O	2:C:250:ARG:NH2	2.31	0.63
2:Q:348:ARG:O	2:Q:390:ASN:ND2	2.31	0.63
2:C:1382:HIS:HD2	2:C:1413:VAL:HG22	1.62	0.63
1:P:87:THR:O	1:P:91:ASN:ND2	2.26	0.63
2:C:731:PRO:HG3	2:C:766:VAL:HG12	1.81	0.63
2:Q:1251:ARG:O	2:Q:1277:GLN:HB2	1.98	0.63
2:C:974:PHE:HB2	2:C:976:ARG:HH21	1.63	0.63
2:Q:129:GLY:O	2:Q:250:ARG:NH2	2.31	0.63
2:Q:566:HIS:CE1	2:Q:572:HIS:NE2	2.66	0.63
2:C:113:GLU:OE2	2:C:233:GLN:NE2	2.31	0.63
2:C:820:ALA:HA	2:C:850:VAL:HA	1.81	0.63
2:Q:139:GLY:HA3	2:Q:154:VAL:HG12	1.81	0.63
2:C:731:PRO:HB2	2:C:773:PRO:HG2	1.81	0.62
2:C:1334:LEU:HD11	2:Q:179:ALA:HA	1.80	0.62
2:Q:123:VAL:HG12	2:Q:256:PHE:HA	1.81	0.62
2:C:1097:ALA:N	2:C:1179:ARG:O	2.32	0.62
2:C:592:PRO:HG3	2:C:604:ASN:HA	1.81	0.62
2:C:207:PHE:HB3	2:C:209:LYS:HE3	1.82	0.62
2:C:635:PHE:HA	2:C:644:THR:HB	1.82	0.62
2:C:1273:LYS:NZ	2:C:1274:TRP:O	2.29	0.62
2:C:1590:THR:O	2:C:1592:LYS:NZ	2.33	0.62
2:C:1364:GLU:O	2:C:1367:HIS:NE2	2.33	0.61
2:Q:730:MET:HE3	2:Q:738:TRP:CG	2.36	0.61
2:Q:271:ASP:O	2:Q:274:THR:OG1	2.16	0.61
2:C:1096:ALA:HA	2:C:1180:SER:HA	1.82	0.61
2:Q:730:MET:HE1	2:Q:765:ALA:HB1	1.81	0.61
1:P:65:CYS:O	1:P:69:GLU:N	2.33	0.61
2:C:132:ARG:NH1	2:C:246:ASN:OD1	2.34	0.61
2:C:1079:LEU:HD22	2:C:1169:PRO:HG3	1.82	0.61
2:Q:970:GLY:HA2	2:Q:981:PHE:HD2	1.65	0.61
2:C:661:LEU:HD13	2:C:697:ILE:HG13	1.82	0.60
2:C:1118:ILE:HG22	2:C:1166:PHE:HB3	1.81	0.60
1:P:107:LEU:HA	1:P:110:LYS:HZ3	1.65	0.60
1:A:145:LEU:HD23	1:A:177:LEU:HD23	1.82	0.60
2:Q:158:HIS:HD2	2:Q:171:PHE:CG	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:818:LEU:HA	2:C:853:ILE:HD12	1.84	0.60
2:Q:277:ALA:O	2:Q:287:GLN:NE2	2.34	0.60
2:Q:345:SER:HA	2:Q:348:ARG:HE	1.65	0.60
2:C:818:LEU:HB3	2:C:826:ILE:HB	1.82	0.60
2:C:108:LEU:HD22	2:C:238:LEU:HD23	1.83	0.60
2:C:334:ASN:HB3	2:C:337:VAL:HG12	1.84	0.60
2:C:1196:GLU:HB2	2:C:1207:HIS:HA	1.84	0.60
2:C:1214:ASP:N	2:C:1272:GLY:O	2.35	0.59
2:C:1291:HIS:CG	2:Q:180:ARG:HH12	2.20	0.59
2:Q:570:LEU:HD23	2:Q:654:ARG:HE	1.66	0.59
2:Q:816:ILE:HB	2:Q:828:LEU:HB2	1.83	0.59
1:A:45:LEU:O	1:A:123:ARG:NE	2.31	0.59
2:Q:809:SER:O	2:Q:832:ASN:ND2	2.35	0.59
1:P:67:VAL:HG12	1:P:71:PHE:HE2	1.68	0.59
2:C:140:LEU:HD11	2:C:236:LYS:HB3	1.83	0.59
2:Q:351:LYS:HZ2	2:Q:659:LEU:HB2	1.67	0.59
2:Q:1214:ASP:N	2:Q:1272:GLY:O	2.36	0.59
2:C:118:ALA:HA	2:C:203:TYR:O	2.02	0.59
1:P:67:VAL:HG12	1:P:71:PHE:CE2	2.37	0.59
2:C:751:GLN:HE22	2:C:754:LYS:HB2	1.67	0.59
2:Q:318:LEU:HD21	2:Q:692:GLU:HB2	1.84	0.59
2:Q:1416:ASP:O	2:Q:1464:TRP:NE1	2.31	0.59
2:Q:558:HIS:ND1	2:Q:644:THR:O	2.36	0.59
2:Q:947:CYS:O	2:Q:965:LYS:NZ	2.33	0.59
2:Q:1188:THR:HG22	2:Q:1205:CYS:HB3	1.85	0.59
1:P:146:CYS:O	1:P:150:GLN:NE2	2.36	0.58
2:Q:389:TYR:OH	2:Q:647:PHE:N	2.31	0.58
2:Q:1196:GLU:HB2	2:Q:1207:HIS:HA	1.84	0.58
2:C:116:ARG:O	2:C:227:ILE:N	2.34	0.58
2:Q:376:ASP:O	2:Q:380:HIS:ND1	2.31	0.58
2:C:536:GLU:HA	2:C:539:MET:HB3	1.85	0.58
2:C:1184:PHE:HB3	2:Q:1189:LEU:HB3	1.85	0.58
2:Q:363:ASP:H	2:Q:403:SER:HB3	1.67	0.58
2:Q:569:GLY:O	2:Q:654:ARG:NH2	2.36	0.58
2:C:536:GLU:OE2	2:C:536:GLU:N	2.31	0.58
2:C:818:LEU:HD22	2:C:826:ILE:HD12	1.85	0.58
2:Q:751:GLN:NE2	2:Q:752:PRO:O	2.36	0.58
2:C:539:MET:HE3	2:C:540:HIS:ND1	2.19	0.58
2:C:169:ARG:HG2	2:C:190:SER:HA	1.86	0.58
2:C:964:ASN:ND2	2:C:969:ASP:OD2	2.37	0.58
2:Q:163:GLN:O	2:Q:1140:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:493:ARG:NH1	2:Q:495:TYR:O	2.36	0.58
2:C:999:CYS:SG	2:C:1004:GLN:NE2	2.77	0.58
2:Q:183:THR:OG1	2:Q:222:GLU:OE1	2.21	0.58
2:C:609:HIS:NE2	2:C:611:SER:OG	2.36	0.58
2:Q:354:ARG:HG3	2:Q:668:PRO:HD3	1.86	0.58
2:C:499:ASN:HA	2:C:502:LYS:HD2	1.85	0.57
2:C:983:CYS:HB3	2:C:990:CYS:HA	1.85	0.57
2:C:1514:ILE:HG22	2:C:1533:ARG:HA	1.86	0.57
2:Q:258:LEU:HD23	2:Q:285:LEU:HD23	1.86	0.57
2:Q:1330:MET:HE1	2:Q:1336:SER:HA	1.85	0.57
2:C:354:ARG:HG3	2:C:668:PRO:HD3	1.85	0.57
2:C:672:PRO:HD3	2:C:930:GLU:HB3	1.86	0.57
2:C:566:HIS:HE1	2:C:572:HIS:NE2	2.02	0.57
2:C:918:VAL:HG22	2:C:941:ILE:HG12	1.86	0.57
2:C:811:GLY:HA2	2:C:833:VAL:HG12	1.87	0.57
1:P:71:PHE:O	1:P:74:ASN:ND2	2.37	0.57
1:P:130:GLU:CD	1:P:134:GLN:HE22	2.13	0.57
2:C:153:TRP:HB2	2:C:172:PHE:CE1	2.39	0.57
2:Q:128:GLU:O	2:Q:131:GLN:NE2	2.34	0.57
2:C:558:HIS:ND1	2:C:641:ASP:O	2.37	0.57
2:C:558:HIS:ND1	2:C:644:THR:O	2.37	0.57
2:Q:730:MET:HE3	2:Q:738:TRP:CD1	2.40	0.57
2:Q:1486:SER:O	2:Q:1489:LYS:NZ	2.38	0.57
2:C:386:PHE:HD1	2:C:393:TRP:HE1	1.53	0.57
2:C:592:PRO:HG3	2:C:605:PRO:HD3	1.87	0.56
2:C:728:SER:HG	2:C:738:TRP:CD1	2.22	0.56
2:C:807:TRP:HH2	2:C:859:ASP:HA	1.70	0.56
2:C:1149:VAL:HG13	2:Q:1151:ASP:HA	1.86	0.56
2:Q:260:LYS:HG2	2:Q:285:LEU:HB2	1.86	0.56
2:Q:338:ILE:O	2:Q:342:ASN:ND2	2.37	0.56
2:Q:536:GLU:HG2	2:Q:541:LEU:HD23	1.87	0.56
2:Q:558:HIS:ND1	2:Q:641:ASP:O	2.38	0.56
2:Q:1479:SER:O	2:Q:1545:TRP:NE1	2.38	0.56
2:Q:1537:VAL:HG12	2:Q:1547:PRO:HD2	1.87	0.56
1:P:86:MET:O	1:P:90:HIS:ND1	2.29	0.56
2:C:117:ASP:OD1	2:C:118:ALA:N	2.38	0.56
2:C:751:GLN:NE2	2:C:752:PRO:O	2.38	0.56
2:Q:795:SER:HG	2:Q:870:THR:HG1	1.34	0.56
2:Q:1024:ALA:O	2:Q:1043:GLY:N	2.38	0.56
2:C:671:LYS:NZ	2:C:931:GLU:O	2.38	0.56
2:C:493:ARG:NH1	2:C:495:TYR:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:723:ALA:HB1	2:C:785:LEU:HD12	1.87	0.56
2:C:796:LEU:HB2	2:C:843:LEU:HD11	1.87	0.56
2:C:812:ALA:HB1	2:C:859:ASP:HB2	1.88	0.56
2:Q:334:ASN:HB3	2:Q:337:VAL:HG22	1.87	0.56
2:Q:804:SER:OG	2:Q:807:TRP:NE1	2.38	0.56
2:Q:812:ALA:HB1	2:Q:859:ASP:HB2	1.88	0.56
2:Q:106:LEU:HD12	2:Q:297:TRP:HB3	1.88	0.56
2:Q:1514:ILE:HG22	2:Q:1533:ARG:HA	1.86	0.56
2:C:814:ASN:N	2:C:856:TYR:O	2.39	0.56
2:Q:1079:LEU:HD22	2:Q:1169:PRO:HG3	1.89	0.56
2:Q:1398:GLN:H	2:Q:1406:GLN:HG2	1.71	0.56
2:C:1485:ASN:HB2	2:C:1488:LEU:HB3	1.87	0.55
2:Q:1273:LYS:NZ	2:Q:1274:TRP:O	2.29	0.55
2:C:535:LYS:NZ	2:C:744:GLU:O	2.25	0.55
2:Q:332:CYS:HB3	2:Q:657:CYS:SG	2.45	0.55
2:C:778:PRO:HA	2:C:858:LEU:HD21	1.89	0.55
2:Q:461:CYS:HA	2:Q:466:PHE:HD2	1.69	0.55
2:Q:708:SER:O	2:Q:711:HIS:ND1	2.39	0.55
1:P:44:ARG:N	1:P:123:ARG:O	2.38	0.55
2:C:1234:HIS:HB3	2:C:1271:GLU:HA	1.87	0.55
2:C:1513:SER:OG	2:C:1533:ARG:NH1	2.40	0.55
2:Q:172:PHE:HB3	2:Q:210:LEU:HD11	1.88	0.55
2:Q:609:HIS:NE2	2:Q:611:SER:OG	2.39	0.55
2:Q:635:PHE:HA	2:Q:644:THR:HB	1.87	0.55
2:C:211:TYR:CD1	2:C:216:GLN:HA	2.42	0.55
1:P:152:ASN:HB3	1:P:155:VAL:HB	1.88	0.55
2:C:159:THR:HA	2:C:167:ASP:O	2.07	0.55
2:C:376:ASP:O	2:C:380:HIS:ND1	2.33	0.55
2:Q:763:ASN:ND2	2:Q:860:GLU:O	2.32	0.55
2:Q:890:ARG:NE	2:Q:892:PRO:O	2.30	0.55
1:A:89:LEU:HD22	2:Q:1598:MET:HE3	1.89	0.55
2:Q:754:LYS:NZ	2:Q:755:SER:O	2.39	0.55
2:C:1439:ARG:HG2	2:C:1455:VAL:HG13	1.87	0.55
2:C:164:ASP:O	2:C:166:LYS:HG3	2.06	0.55
2:Q:480:ASN:O	2:Q:484:THR:OG1	2.19	0.55
1:P:201:TRP:HE3	1:P:204:LEU:HB3	1.72	0.54
2:C:158:HIS:HD2	2:C:171:PHE:CG	2.25	0.54
2:C:271:ASP:O	2:C:274:THR:OG1	2.22	0.54
2:C:1020:LEU:HB3	2:Q:1258:LYS:HD3	1.88	0.54
2:C:604:ASN:ND2	2:C:629:ASN:O	2.40	0.54
2:C:738:TRP:CD1	2:C:740:PRO:HD3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:410:ILE:HG23	2:Q:518:ALA:HA	1.89	0.54
2:Q:539:MET:HE3	2:Q:540:HIS:HD2	1.71	0.54
2:Q:1345:MET:HB3	2:Q:1366:LYS:HZ3	1.73	0.54
2:Q:1548:HIS:HB3	2:Q:1551:LEU:HG	1.89	0.54
2:C:702:PHE:HA	2:C:883:PRO:HA	1.89	0.54
2:C:1400:THR:OG1	2:C:1402:ASP:OD1	2.19	0.54
2:Q:985:ASP:OD1	2:Q:986:GLU:N	2.39	0.54
1:P:45:LEU:O	1:P:123:ARG:NE	2.36	0.54
2:C:277:ALA:O	2:C:287:GLN:NE2	2.39	0.54
2:C:1533:ARG:NH1	2:C:1534:VAL:O	2.39	0.54
2:C:1362:CYS:HA	2:C:1367:HIS:CE1	2.42	0.54
1:A:94:LYS:HE2	1:A:155:VAL:HG13	1.88	0.54
2:Q:404:SER:O	2:Q:407:ARG:NH1	2.41	0.54
2:Q:1186:PRO:HA	2:Q:1189:LEU:HB2	1.89	0.54
2:Q:1377:CYS:N	2:Q:1393:ARG:O	2.37	0.54
2:Q:1400:THR:OG1	2:Q:1402:ASP:OD1	2.20	0.54
1:P:207:ILE:HD12	1:A:179:LEU:HD12	1.89	0.54
2:C:1324:ASN:ND2	2:C:1326:LEU:O	2.41	0.54
2:Q:625:HIS:ND1	2:Q:626:SER:O	2.41	0.54
2:C:448:PHE:HB2	2:C:466:PHE:HE2	1.72	0.54
2:C:1024:ALA:O	2:C:1043:GLY:N	2.39	0.54
2:C:854:GLN:HB3	2:C:856:TYR:HE1	1.72	0.54
1:P:165:LEU:HD23	1:P:171:TYR:HB3	1.89	0.54
1:A:168:HIS:HB2	1:A:171:TYR:HD1	1.72	0.54
2:Q:728:SER:HB3	2:Q:783:LEU:HD12	1.89	0.54
2:Q:1256:LEU:HD23	2:Q:1258:LYS:HE3	1.90	0.54
1:P:183:GLU:HA	1:P:186:LYS:HE3	1.89	0.54
2:C:672:PRO:HG2	2:C:932:SER:HB3	1.90	0.54
2:C:1237:GLN:HG2	2:C:1268:THR:HG23	1.89	0.54
2:Q:181:GLN:O	2:Q:223:GLN:NE2	2.41	0.54
2:Q:356:ARG:HA	2:Q:396:ASP:O	2.08	0.54
2:C:382:LEU:HD13	2:C:560:MET:HE1	1.89	0.53
2:C:448:PHE:HB3	2:C:451:LYS:HD2	1.89	0.53
2:C:1100:ILE:HB	2:C:1177:ALA:HB3	1.89	0.53
2:Q:564:ILE:HG23	2:Q:568:LEU:HD23	1.90	0.53
2:C:459:MET:HE1	2:C:486:PHE:HE2	1.73	0.53
2:C:509:GLY:O	2:C:666:TRP:NE1	2.33	0.53
2:C:1531:PRO:HD2	2:C:1575:PHE:HD2	1.72	0.53
2:Q:356:ARG:NH1	2:Q:514:ASN:OD1	2.40	0.53
2:C:158:HIS:HD2	2:C:171:PHE:CD1	2.26	0.53
2:C:461:CYS:HA	2:C:466:PHE:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1521:THR:H	2:C:1524:ASP:HB2	1.74	0.53
2:C:569:GLY:O	2:C:654:ARG:NH2	2.41	0.53
2:Q:767:ASN:ND2	2:Q:770:THR:OG1	2.41	0.53
2:Q:1557:GLY:HA2	2:Q:1573:ARG:HH22	1.73	0.53
2:C:817:LYS:HE3	2:C:825:ASN:HB2	1.91	0.53
2:C:951:ILE:O	2:C:953:GLN:NE2	2.42	0.53
2:C:682:LEU:HA	2:C:965:LYS:HE3	1.91	0.53
2:C:121:LEU:O	2:C:200:ALA:HA	2.09	0.53
2:C:185:ILE:HG12	2:C:218:ALA:HB1	1.90	0.53
1:P:72:GLU:HG3	1:P:82:HIS:HB2	1.91	0.53
2:C:242:GLY:HA3	2:C:248:ASN:HA	1.91	0.53
2:C:1240:VAL:HG21	2:C:1278:VAL:HG21	1.90	0.53
2:Q:566:HIS:HE1	2:Q:572:HIS:NE2	2.04	0.53
2:Q:1237:GLN:HG2	2:Q:1268:THR:HG23	1.90	0.53
2:C:336:GLU:HG2	2:C:974:PHE:HE2	1.74	0.53
2:Q:796:LEU:HB2	2:Q:843:LEU:HD11	1.90	0.53
2:C:254:GLU:HA	2:C:290:TRP:HE1	1.74	0.53
2:Q:1214:ASP:HB3	2:Q:1273:LYS:HD3	1.90	0.52
2:Q:797:THR:HA	2:Q:839:LEU:O	2.10	0.52
2:Q:671:LYS:NZ	2:Q:931:GLU:O	2.41	0.52
2:Q:672:PRO:HD3	2:Q:930:GLU:HB3	1.92	0.52
2:Q:814:ASN:N	2:Q:856:TYR:O	2.41	0.52
2:C:389:TYR:OH	2:C:647:PHE:N	2.36	0.52
2:Q:284:LEU:HD21	2:Q:287:GLN:HB2	1.90	0.52
2:Q:367:ASN:O	2:Q:406:ARG:NE	2.42	0.52
2:Q:818:LEU:HD22	2:Q:826:ILE:HD12	1.91	0.52
2:Q:1023:TRP:NE1	2:Q:1044:GLN:OE1	2.43	0.52
2:C:1227:CYS:HA	2:C:1238:CYS:HA	1.91	0.52
2:C:1510:ASN:O	2:C:1557:GLY:N	2.41	0.52
2:Q:448:PHE:HB2	2:Q:466:PHE:HE2	1.74	0.52
2:Q:752:PRO:HA	2:Q:801:THR:HG23	1.92	0.52
2:Q:1525:ILE:HG23	2:Q:1529:LEU:HD23	1.92	0.52
2:C:577:ILE:HD13	2:C:627:PHE:CE1	2.44	0.52
2:Q:122:GLN:HE22	2:Q:259:TRP:NE1	2.08	0.52
2:Q:738:TRP:CD1	2:Q:740:PRO:HD3	2.45	0.52
2:C:994:ASP:OD1	2:C:1007:SER:OG	2.27	0.52
2:C:715:GLU:O	2:C:718:ILE:HG12	2.09	0.52
1:A:156:ILE:HA	1:A:159:MET:HE2	1.92	0.52
2:Q:1021:ASP:OD2	2:Q:1179:ARG:NH2	2.43	0.52
2:C:625:HIS:ND1	2:C:626:SER:O	2.42	0.51
2:C:1124:ASP:HB3	2:C:1157:TYR:HD1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1484:LEU:HD21	2:C:1490:LEU:HG	1.93	0.51
2:Q:604:ASN:ND2	2:Q:629:ASN:O	2.43	0.51
2:C:1398:GLN:NE2	2:C:1399:CYS:O	2.44	0.51
2:C:1558:CYS:HB2	2:C:1571:ASN:HA	1.91	0.51
2:Q:290:TRP:HE3	2:Q:293:VAL:HG22	1.76	0.51
2:Q:351:LYS:HG3	2:Q:656:HIS:HD2	1.75	0.51
2:Q:567:SER:O	2:Q:663:TYR:OH	2.28	0.51
2:Q:818:LEU:HB3	2:Q:826:ILE:HB	1.92	0.51
2:C:633:ASN:O	2:C:645:ASP:N	2.32	0.51
2:C:1054:LYS:HB3	2:C:1110:TYR:HA	1.92	0.51
2:C:815:ASP:OD1	2:C:829:GLY:N	2.41	0.51
2:C:1120:VAL:HG12	2:C:1164:VAL:HG22	1.92	0.51
2:C:1504:THR:HG1	2:C:1513:SER:HG	1.58	0.51
2:Q:116:ARG:O	2:Q:227:ILE:N	2.39	0.51
2:Q:175:LYS:HB2	2:Q:182:VAL:HG22	1.93	0.51
2:Q:332:CYS:HA	2:Q:657:CYS:SG	2.50	0.51
2:Q:672:PRO:HG2	2:Q:932:SER:HB3	1.93	0.51
2:C:1016:PRO:HB2	2:Q:1190:SER:HB3	1.92	0.51
2:C:1561:PHE:HB2	2:C:1571:ASN:HD21	1.75	0.51
2:C:1608:CYS:O	2:C:1616:HIS:NE2	2.37	0.51
2:Q:409:LEU:HD21	2:Q:519:LYS:HZ3	1.76	0.51
2:Q:766:VAL:HG11	2:Q:773:PRO:HD2	1.92	0.51
2:Q:1559:GLU:N	2:Q:1571:ASN:OD1	2.44	0.51
2:C:180:ARG:HH22	2:Q:1292:GLN:HB2	1.75	0.51
1:A:87:THR:O	1:A:91:ASN:ND2	2.33	0.51
2:Q:97:LEU:HD12	2:Q:306:PRO:HG2	1.93	0.51
2:C:131:GLN:HE22	2:C:250:ARG:HB3	1.75	0.51
2:C:1122:LEU:HB3	2:C:1157:TYR:HE1	1.75	0.51
1:A:80:GLY:O	1:A:84:ILE:N	2.31	0.51
2:Q:382:LEU:HD13	2:Q:560:MET:HE1	1.93	0.51
2:Q:833:VAL:HG22	2:Q:839:LEU:HD21	1.93	0.51
1:P:211:CYS:HB3	1:A:211:CYS:C	2.36	0.50
1:A:49:ASN:O	1:A:53:ILE:HG12	2.11	0.50
2:C:1254:ASP:CG	2:Q:1204:SER:HB2	2.35	0.50
2:Q:121:LEU:O	2:Q:200:ALA:HA	2.10	0.50
2:Q:729:PRO:HG3	2:Q:782:TYR:CE1	2.46	0.50
2:Q:817:LYS:HE3	2:Q:825:ASN:HB2	1.93	0.50
2:C:570:LEU:HA	2:C:654:ARG:HH21	1.76	0.50
2:C:708:SER:O	2:C:711:HIS:ND1	2.42	0.50
2:C:1058:LEU:HD22	2:C:1105:THR:HG21	1.94	0.50
2:C:1558:CYS:H	2:C:1573:ARG:NH2	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:1487:ASN:HB3	2:Q:1554:CYS:HB2	1.94	0.50
2:Q:719:LEU:HD23	2:Q:791:LEU:HD13	1.92	0.50
2:Q:1362:CYS:HA	2:Q:1367:HIS:CE1	2.47	0.50
2:C:1183:ASN:HB2	2:Q:1189:LEU:O	2.11	0.50
2:Q:288:GLU:HG3	2:Q:290:TRP:H	1.75	0.50
2:C:210:LEU:HB3	2:C:218:ALA:HB3	1.94	0.50
2:C:329:GLN:N	2:C:333:ASP:OD2	2.41	0.50
2:Q:266:ARG:HA	2:Q:269:LEU:HD12	1.94	0.50
2:Q:509:GLY:O	2:Q:666:TRP:NE1	2.29	0.50
2:C:265:GLN:HA	2:C:268:ILE:HG12	1.93	0.50
2:C:290:TRP:HE3	2:C:293:VAL:HG22	1.76	0.50
2:C:332:CYS:SG	2:C:657:CYS:C	2.95	0.50
2:C:1318:ALA:HB1	2:C:1342:CYS:HB3	1.94	0.50
2:Q:118:ALA:HA	2:Q:203:TYR:O	2.12	0.50
2:C:562:HIS:HE1	2:C:572:HIS:CD2	2.30	0.49
2:Q:389:TYR:HB3	2:Q:652:VAL:HG13	1.94	0.49
2:Q:562:HIS:CD2	2:Q:566:HIS:NE2	2.79	0.49
2:Q:1234:HIS:HB3	2:Q:1271:GLU:HA	1.93	0.49
2:C:338:ILE:O	2:C:342:ASN:ND2	2.42	0.49
2:Q:461:CYS:O	2:Q:469:ASP:N	2.46	0.49
1:P:149:ALA:HB1	1:P:185:VAL:HG11	1.94	0.49
2:C:136:VAL:HG21	2:C:243:SER:HB3	1.94	0.49
2:C:983:CYS:CB	2:C:990:CYS:HA	2.43	0.49
2:C:1537:VAL:HG12	2:C:1547:PRO:HD2	1.95	0.49
2:Q:120:THR:HA	2:Q:201:ALA:O	2.11	0.49
2:Q:160:ILE:HG12	2:Q:167:ASP:HB3	1.93	0.49
2:Q:170:TYR:O	2:Q:187:ALA:N	2.44	0.49
2:Q:254:GLU:HA	2:Q:290:TRP:HE1	1.77	0.49
2:C:890:ARG:NE	2:C:892:PRO:O	2.30	0.49
2:C:1357:LEU:HD23	2:C:1363:ARG:HE	1.77	0.49
2:C:1188:THR:HG22	2:C:1205:CYS:HB3	1.94	0.49
2:C:1568:ASP:OD2	2:C:1571:ASN:ND2	2.45	0.49
2:Q:718:ILE:HG22	2:Q:873:ALA:HA	1.95	0.49
1:A:92:ALA:HB3	2:Q:1596:PHE:HE1	1.78	0.49
2:Q:894:LEU:HD13	2:Q:898:VAL:HB	1.95	0.49
2:Q:1124:ASP:OD1	2:Q:1128:GLN:N	2.45	0.49
2:C:204:ASP:OD2	2:C:206:GLN:NE2	2.46	0.49
2:C:345:SER:HA	2:C:348:ARG:HE	1.77	0.49
2:C:728:SER:HB3	2:C:783:LEU:HD12	1.94	0.49
2:C:1103:LEU:HD23	2:C:1173:ILE:HG12	1.93	0.49
2:Q:1086:LEU:HD21	2:Q:1173:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:HG13	1:A:171:TYR:CZ	2.48	0.49
1:A:86:MET:HE3	1:A:90:HIS:HE1	1.73	0.49
2:Q:260:LYS:HE3	2:Q:285:LEU:HD22	1.94	0.49
2:Q:1122:LEU:HD12	2:Q:1132:LEU:HD21	1.95	0.49
2:Q:1329:CYS:HB2	2:Q:1335:TRP:CZ3	2.48	0.49
1:P:133:SER:OG	1:P:137:ARG:NH1	2.44	0.49
2:C:1103:LEU:O	2:C:1142:ASN:ND2	2.46	0.49
2:Q:1285:CYS:SG	2:Q:1334:LEU:N	2.86	0.49
2:C:1518:MET:HE1	2:C:1551:LEU:HD22	1.93	0.48
2:Q:1239:THR:HA	2:Q:1266:THR:HA	1.95	0.48
2:C:386:PHE:HB3	2:C:391:ILE:HB	1.94	0.48
2:Q:142:ASP:O	2:Q:149:ARG:NH1	2.41	0.48
2:Q:351:LYS:NZ	2:Q:656:HIS:O	2.46	0.48
2:Q:462:ASN:ND2	2:Q:484:THR:O	2.28	0.48
2:C:1086:LEU:HD21	2:C:1173:ILE:HD12	1.95	0.48
2:Q:389:TYR:CZ	2:Q:647:PHE:HB2	2.48	0.48
2:Q:592:PRO:HG3	2:Q:605:PRO:HD3	1.93	0.48
2:C:181:GLN:NE2	2:C:1048:SER:OG	2.45	0.48
2:C:1573:ARG:NE	2:C:1575:PHE:HB3	2.28	0.48
2:Q:361:TYR:CZ	2:Q:368:PRO:HB3	2.49	0.48
1:P:156:ILE:HA	1:P:159:MET:HE2	1.95	0.48
2:C:710:CYS:HA	2:C:713:CYS:SG	2.53	0.48
2:Q:536:GLU:HA	2:Q:539:MET:HB3	1.95	0.48
2:Q:793:PRO:HB2	2:Q:843:LEU:HD12	1.94	0.48
2:Q:1425:LEU:HD23	2:Q:1440:ILE:HD11	1.95	0.48
2:C:538:LEU:H	2:C:538:LEU:HD23	1.78	0.48
2:C:1094:MET:HE2	2:C:1203:GLN:OE1	2.14	0.48
2:Q:126:ARG:HG3	2:Q:196:TRP:CD2	2.49	0.48
2:Q:1345:MET:HB2	2:Q:1367:HIS:H	1.77	0.48
2:Q:1608:CYS:O	2:Q:1616:HIS:NE2	2.33	0.48
2:C:378:GLN:HE22	2:C:557:THR:HB	1.79	0.48
2:C:815:ASP:OD1	2:C:816:ILE:N	2.47	0.48
2:C:1098:ALA:HA	2:C:1148:VAL:HG23	1.95	0.48
1:A:71:PHE:O	1:A:74:ASN:ND2	2.47	0.48
2:Q:175:LYS:HB2	2:Q:182:VAL:HA	1.96	0.48
2:Q:336:GLU:HG2	2:Q:974:PHE:HE2	1.78	0.48
2:Q:659:LEU:HD23	2:Q:663:TYR:HD2	1.78	0.48
2:C:361:TYR:CZ	2:C:368:PRO:HB3	2.49	0.48
2:Q:1097:ALA:N	2:Q:1179:ARG:O	2.47	0.48
2:C:175:LYS:HB2	2:C:182:VAL:HG22	1.94	0.48
2:C:404:SER:O	2:C:408:ARG:NE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:332:CYS:CA	2:Q:657:CYS:SG	3.01	0.48
2:Q:886:TYR:C	2:Q:903:HIS:HD1	2.20	0.48
2:Q:1561:PHE:HB2	2:Q:1571:ASN:HD21	1.79	0.48
1:P:98:GLN:HE22	1:P:148:ALA:HA	1.79	0.48
1:P:130:GLU:OE2	1:P:134:GLN:NE2	2.47	0.48
2:C:1023:TRP:NE1	2:C:1044:GLN:OE1	2.46	0.48
2:C:1334:LEU:HD21	2:Q:178:ARG:HB3	1.96	0.48
2:Q:575:ARG:NH1	2:Q:597:GLY:O	2.38	0.48
2:C:288:GLU:HG3	2:C:290:TRP:H	1.79	0.47
2:Q:1124:ASP:HB3	2:Q:1157:TYR:HB2	1.96	0.47
2:C:785:LEU:HB2	2:C:853:ILE:HG22	1.96	0.47
2:C:1478:CYS:N	2:C:1496:TYR:O	2.38	0.47
2:Q:415:ASP:HB2	2:Q:418:LYS:HG3	1.96	0.47
2:Q:1017:GLN:HG2	2:Q:1017:GLN:O	2.14	0.47
2:C:362:GLU:HG3	2:C:366:LYS:HG3	1.96	0.47
2:Q:458:ASP:HB2	2:Q:461:CYS:HB2	1.96	0.47
2:Q:876:PRO:HA	2:Q:879:LEU:HD23	1.95	0.47
2:Q:900:SER:HB2	2:Q:903:HIS:HE1	1.78	0.47
2:Q:211:TYR:CD1	2:Q:216:GLN:HA	2.50	0.47
2:Q:265:GLN:OE1	2:Q:989:ARG:NH2	2.46	0.47
1:P:168:HIS:HB2	1:P:171:TYR:CD1	2.48	0.47
2:C:599:LEU:HD12	2:C:654:ARG:HH12	1.79	0.47
2:Q:1026:ASN:O	2:Q:1089:TYR:N	2.45	0.47
2:Q:1095:VAL:HG23	2:Q:1158:HIS:HD2	1.80	0.47
2:Q:726:ALA:C	2:Q:740:PRO:HD2	2.39	0.47
2:C:383:ALA:O	2:C:387:LYS:HG2	2.14	0.47
2:C:389:TYR:HB3	2:C:652:VAL:HG13	1.96	0.47
2:C:1568:ASP:HB3	2:C:1596:PHE:HD2	1.79	0.47
2:Q:153:TRP:HB2	2:Q:172:PHE:CE1	2.42	0.47
2:Q:642:ASP:OD1	2:Q:643:CYS:N	2.47	0.47
2:Q:775:CYS:HB3	2:Q:781:CYS:HB2	1.70	0.47
2:Q:1054:LYS:HB3	2:Q:1110:TYR:HA	1.97	0.47
1:P:162:PHE:HB2	1:P:196:GLN:HB3	1.97	0.47
2:C:150:ASP:N	2:C:150:ASP:OD1	2.47	0.47
2:C:1251:ARG:HG2	2:C:1257:ILE:HG12	1.97	0.47
2:Q:351:LYS:HE3	2:Q:656:HIS:HD2	1.80	0.47
2:Q:1017:GLN:OE1	2:Q:1017:GLN:N	2.45	0.47
2:C:275:HIS:O	2:C:314:HIS:ND1	2.39	0.47
2:C:642:ASP:OD1	2:C:643:CYS:N	2.47	0.47
2:Q:1003:GLU:HB3	2:Q:1007:SER:OG	2.15	0.47
2:Q:1185:ASP:CB	2:Q:1203:GLN:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:1227:CYS:HA	2:Q:1238:CYS:HA	1.96	0.47
2:C:172:PHE:CD2	2:C:208:MET:HE3	2.50	0.46
2:C:386:PHE:HD1	2:C:393:TRP:NE1	2.12	0.46
2:C:1250:ILE:HD13	2:C:1276:LYS:HD3	1.96	0.46
2:C:1309:GLN:HB3	2:C:1326:LEU:HD22	1.96	0.46
2:Q:122:GLN:HE22	2:Q:259:TRP:CD1	2.33	0.46
2:Q:242:GLY:HA3	2:Q:248:ASN:HA	1.98	0.46
2:Q:1030:SER:HB3	2:Q:1085:TRP:H	1.80	0.46
2:Q:1103:LEU:HD23	2:Q:1173:ILE:HG12	1.95	0.46
2:Q:1124:ASP:CB	2:Q:1157:TYR:HB2	2.45	0.46
2:C:791:LEU:HD12	2:C:871:SER:HB3	1.95	0.46
2:C:1074:TYR:HA	2:C:1079:LEU:HD21	1.97	0.46
2:C:1124:ASP:HB3	2:C:1157:TYR:CD1	2.51	0.46
2:Q:766:VAL:HG21	2:Q:772:PRO:HB3	1.97	0.46
2:Q:1185:ASP:HB2	2:Q:1203:GLN:HB3	1.96	0.46
2:C:814:ASN:H	2:C:857:THR:HA	1.80	0.46
2:C:1204:SER:HB2	2:Q:1254:ASP:CG	2.41	0.46
2:C:1248:LEU:O	2:C:1259:SER:OG	2.25	0.46
2:Q:820:ALA:HA	2:Q:850:VAL:HA	1.98	0.46
2:Q:1015:THR:HB	2:Q:1019:PHE:CE2	2.50	0.46
2:Q:1037:PRO:HG2	2:Q:1040:VAL:HG13	1.97	0.46
2:Q:1558:CYS:HB2	2:Q:1571:ASN:HA	1.96	0.46
2:C:791:LEU:HD21	2:C:869:LEU:HD22	1.97	0.46
1:P:44:ARG:NH2	1:P:75:SER:O	2.37	0.46
2:C:180:ARG:NH2	2:Q:1289:ASP:H	2.13	0.46
2:C:205:GLY:O	2:C:225:GLY:N	2.47	0.46
2:C:728:SER:HG	2:C:738:TRP:HD1	1.63	0.46
2:C:836:ASP:OD1	2:C:837:VAL:N	2.46	0.46
2:Q:538:LEU:HD23	2:Q:538:LEU:H	1.79	0.46
1:P:80:GLY:O	1:P:84:ILE:N	2.36	0.46
2:C:967:ASN:OD1	2:C:968:GLY:N	2.49	0.46
2:Q:791:LEU:HD21	2:Q:869:LEU:HD22	1.96	0.46
2:C:677:LEU:HD23	2:C:677:LEU:HA	1.85	0.46
2:Q:615:PRO:HG2	2:Q:627:PHE:HB2	1.98	0.46
2:Q:1457:HIS:N	2:Q:1465:ASN:OD1	2.44	0.46
2:C:255:HIS:CD2	2:C:276:GLY:HA2	2.51	0.46
2:Q:516:PHE:HE2	2:Q:543:GLY:HA3	1.80	0.46
2:Q:818:LEU:HD21	2:Q:850:VAL:HG22	1.96	0.46
2:Q:886:TYR:O	2:Q:903:HIS:ND1	2.42	0.46
2:Q:1183:ASN:HD22	2:Q:1201:ALA:HA	1.81	0.46
2:C:819:LEU:HD11	2:C:854:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1386:SER:HB3	2:C:1392:LYS:H	1.81	0.46
2:Q:473:CYS:HB3	2:Q:484:THR:HB	1.97	0.46
2:Q:891:ASP:HB2	2:Q:922:TRP:HH2	1.80	0.46
2:C:533:TRP:CD1	2:C:533:TRP:H	2.34	0.45
2:C:1327:LEU:HD21	2:C:1338:PRO:HA	1.98	0.45
2:Q:357:VAL:HA	2:Q:515:ILE:HB	1.97	0.45
2:Q:577:ILE:HD13	2:Q:627:PHE:CE1	2.51	0.45
2:Q:1515:ILE:HG13	2:Q:1534:VAL:HG21	1.98	0.45
2:Q:1595:PRO:HD3	2:Q:1602:LEU:HD21	1.98	0.45
2:C:284:LEU:HD21	2:C:287:GLN:HB2	1.99	0.45
2:C:1041:ILE:HG23	2:C:1175:GLY:HA2	1.98	0.45
2:Q:351:LYS:HE3	2:Q:656:HIS:CD2	2.52	0.45
1:P:57:LEU:HD21	1:P:71:PHE:CZ	2.51	0.45
2:Q:249:TYR:OH	2:Q:252:TYR:N	2.50	0.45
2:Q:777:GLU:HB3	2:Q:778:PRO:HD2	1.99	0.45
2:Q:1521:THR:H	2:Q:1524:ASP:HB2	1.82	0.45
2:C:97:LEU:HD12	2:C:306:PRO:HG2	1.98	0.45
2:C:112:LEU:HD13	2:C:286:LEU:HD12	1.98	0.45
2:C:444:ARG:HH12	2:C:446:PRO:HB2	1.81	0.45
2:C:780:GLY:HA3	2:C:856:TYR:HD2	1.82	0.45
1:A:84:ILE:O	1:A:88:PHE:HD2	2.00	0.45
2:Q:204:ASP:OD1	2:Q:207:PHE:N	2.46	0.45
2:C:357:VAL:HA	2:C:515:ILE:HB	1.99	0.45
2:C:580:ILE:HD12	2:C:582:SER:O	2.15	0.45
2:C:1189:LEU:O	2:Q:1183:ASN:HB2	2.16	0.45
2:C:1309:GLN:HG2	2:C:1328:THR:HA	1.98	0.45
2:C:1380:GLY:H	2:C:1393:ARG:NH2	2.14	0.45
2:C:1382:HIS:ND1	2:C:1383:VAL:O	2.50	0.45
1:A:49:ASN:O	1:A:52:GLU:HG2	2.16	0.45
2:Q:260:LYS:HE3	2:Q:285:LEU:HD13	1.98	0.45
2:Q:631:PRO:HB2	2:Q:634:ASN:HB2	1.98	0.45
2:C:125:LEU:HD23	2:C:197:VAL:O	2.17	0.45
2:C:170:TYR:O	2:C:187:ALA:N	2.49	0.45
2:C:363:ASP:H	2:C:403:SER:HB3	1.82	0.45
2:C:956:GLN:HB2	2:C:958:GLU:HG3	1.99	0.45
2:C:1584:CYS:HB2	2:C:1587:THR:OG1	2.17	0.45
2:Q:859:ASP:HB3	2:Q:862:LEU:HB2	1.99	0.45
2:Q:1386:SER:HB3	2:Q:1392:LYS:H	1.81	0.45
1:P:196:GLN:HA	1:P:199:GLN:HG2	1.99	0.45
2:Q:108:LEU:HD22	2:Q:238:LEU:HD23	1.99	0.45
2:Q:692:GLU:HG2	2:Q:907:LYS:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:795:SER:OG	2:Q:870:THR:OG1	2.15	0.45
2:Q:1223:ALA:O	2:Q:1243:ARG:NH2	2.50	0.45
2:C:178:ARG:NH1	2:C:225:GLY:HA3	2.32	0.45
2:C:730:MET:H	2:C:736:GLY:HA3	1.81	0.45
2:C:777:GLU:HB3	2:C:778:PRO:HD2	1.99	0.45
2:C:1382:HIS:CD2	2:C:1413:VAL:HG22	2.47	0.45
2:Q:259:TRP:HH2	2:Q:281:LEU:HD22	1.81	0.45
2:Q:652:VAL:HG12	2:Q:656:HIS:CE1	2.52	0.45
2:C:900:SER:HB2	2:C:903:HIS:HE1	1.82	0.45
2:Q:278:HIS:NE2	2:Q:289:ASN:HB3	2.32	0.45
2:Q:1021:ASP:OD1	2:Q:1179:ARG:NE	2.50	0.45
1:P:172:VAL:HG21	1:A:204:LEU:HD22	1.99	0.44
2:Q:572:HIS:CD2	2:Q:636:MET:HE3	2.51	0.44
2:Q:703:GLU:HB2	2:Q:882:LYS:HE3	1.98	0.44
2:Q:854:GLN:HB3	2:Q:856:TYR:HE1	1.81	0.44
2:Q:1051:CYS:HB2	2:Q:1142:ASN:HD22	1.83	0.44
2:C:1102:HIS:HD1	2:C:1174:SER:HG	1.65	0.44
1:A:106:ALA:HA	1:A:143:HIS:HD2	1.82	0.44
2:Q:332:CYS:CB	2:Q:657:CYS:HG	2.23	0.44
2:Q:679:PRO:HB3	2:Q:693:TRP:HB3	1.99	0.44
2:Q:1108:THR:HG22	2:Q:1115:GLN:HA	1.98	0.44
2:C:206:GLN:HE21	2:C:207:PHE:HD2	1.66	0.44
2:C:410:ILE:HD11	2:C:498:VAL:HA	1.99	0.44
2:C:485:CYS:SG	2:C:493:ARG:HA	2.57	0.44
2:C:894:LEU:HD13	2:C:898:VAL:HB	2.00	0.44
2:C:1095:VAL:HG22	2:C:1157:TYR:O	2.17	0.44
2:C:1256:LEU:HD11	2:C:1258:LYS:HE2	1.99	0.44
2:Q:122:GLN:HE22	2:Q:259:TRP:HE1	1.65	0.44
2:Q:255:HIS:CD2	2:Q:276:GLY:HA2	2.53	0.44
2:Q:259:TRP:CE2	2:Q:284:LEU:HD13	2.52	0.44
2:Q:900:SER:HB2	2:Q:903:HIS:CE1	2.53	0.44
2:Q:1196:GLU:CB	2:Q:1207:HIS:HA	2.48	0.44
2:C:859:ASP:OD1	2:C:860:GLU:N	2.49	0.44
2:Q:318:LEU:O	2:Q:318:LEU:HD12	2.18	0.44
2:Q:710:CYS:HA	2:Q:713:CYS:SG	2.58	0.44
2:Q:812:ALA:O	2:Q:857:THR:OG1	2.27	0.44
1:P:168:HIS:HB2	1:P:171:TYR:HD1	1.83	0.44
2:C:575:ARG:NH1	2:C:597:GLY:O	2.41	0.44
2:C:924:ILE:HG13	2:C:934:PRO:HA	1.99	0.44
2:C:1321:LYS:N	2:C:1341:LEU:O	2.50	0.44
2:C:1516:LEU:HD11	2:C:1525:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:122:GLN:HG3	2:Q:198:TYR:OH	2.17	0.44
2:Q:140:LEU:N	2:Q:153:TRP:O	2.42	0.44
2:Q:274:THR:HB	2:Q:277:ALA:HB3	1.99	0.44
2:C:407:ARG:HE	2:C:407:ARG:HB2	1.66	0.44
2:C:726:ALA:C	2:C:740:PRO:HD2	2.42	0.44
2:C:950:GLY:N	2:C:961:ASP:OD1	2.45	0.44
2:C:1425:LEU:HD23	2:C:1440:ILE:HD11	1.99	0.44
2:Q:126:ARG:O	2:Q:249:TYR:OH	2.33	0.44
2:Q:762:PRO:HB3	2:Q:775:CYS:SG	2.58	0.44
2:C:115:PRO:HD3	2:C:285:LEU:HD22	2.00	0.44
2:C:356:ARG:HD2	2:C:514:ASN:OD1	2.18	0.44
2:C:389:TYR:CZ	2:C:647:PHE:HB2	2.53	0.44
2:C:480:ASN:O	2:C:484:THR:OG1	2.31	0.44
2:C:1214:ASP:HB3	2:C:1273:LYS:HD3	2.00	0.44
2:Q:682:LEU:HB2	2:Q:690:THR:HB	1.99	0.44
2:Q:725:ASN:HB3	2:Q:786:GLU:HB2	1.99	0.44
2:Q:1214:ASP:H	2:Q:1273:LYS:HB2	1.82	0.44
2:Q:1382:HIS:CD2	2:Q:1413:VAL:HG22	2.48	0.44
2:C:367:ASN:O	2:C:406:ARG:NE	2.44	0.44
2:C:536:GLU:H	2:C:536:GLU:CD	2.23	0.44
2:C:1108:THR:HG22	2:C:1115:GLN:HA	2.00	0.44
2:Q:389:TYR:CE2	2:Q:647:PHE:HB2	2.53	0.44
2:Q:983:CYS:HB3	2:Q:988:SER:HB3	2.00	0.44
2:Q:1483:GLU:O	2:Q:1483:GLU:HG2	2.18	0.44
1:P:113:ALA:HA	1:P:117:ARG:HH11	1.83	0.44
2:C:178:ARG:HB3	2:Q:1334:LEU:HD21	1.99	0.44
2:Q:1017:GLN:OE1	2:Q:1182:ASP:HA	2.18	0.44
2:Q:1195:GLY:HA2	2:Q:1212:LYS:NZ	2.33	0.44
1:P:112:HIS:CE1	1:P:117:ARG:HH12	2.35	0.43
2:C:793:PRO:HB3	2:C:869:LEU:HD11	2.00	0.43
2:C:1501:GLU:HG2	2:C:1536:ARG:HB2	1.99	0.43
1:A:44:ARG:N	1:A:123:ARG:O	2.51	0.43
2:Q:1516:LEU:HD11	2:Q:1525:ILE:HD11	1.99	0.43
2:C:128:GLU:O	2:C:131:GLN:NE2	2.34	0.43
2:C:797:THR:HG23	2:C:840:THR:HG22	2.00	0.43
2:C:891:ASP:HB2	2:C:922:TRP:HH2	1.83	0.43
1:A:72:GLU:HG3	1:A:82:HIS:HB3	2.00	0.43
2:Q:1345:MET:SD	2:Q:1345:MET:N	2.90	0.43
1:P:51:ALA:O	1:P:54:GLN:HG3	2.18	0.43
2:C:693:TRP:CZ2	2:C:906:ARG:HA	2.53	0.43
2:C:1383:VAL:HG21	2:C:1395:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:131:GLN:HE22	2:Q:250:ARG:HB3	1.82	0.43
2:Q:181:GLN:NE2	2:Q:1049:GLN:HG2	2.33	0.43
2:Q:259:TRP:CH2	2:Q:281:LEU:HD22	2.53	0.43
1:P:109:CYS:HB2	1:P:143:HIS:NE2	2.33	0.43
2:C:153:TRP:HZ3	2:C:155:VAL:HG22	1.83	0.43
2:C:797:THR:HA	2:C:839:LEU:O	2.17	0.43
2:C:1023:TRP:HB3	2:C:1043:GLY:HA2	2.01	0.43
2:C:1479:SER:O	2:C:1545:TRP:NE1	2.47	0.43
1:A:169:GLU:O	1:A:172:VAL:HB	2.18	0.43
2:Q:1005:LYS:HA	2:Q:1014:TYR:CD1	2.53	0.43
2:Q:1016:PRO:HA	2:Q:1017:GLN:HA	1.48	0.43
2:Q:1095:VAL:HG22	2:Q:1157:TYR:O	2.18	0.43
2:Q:1252:ARG:NE	2:Q:1276:LYS:HG2	2.34	0.43
2:C:1090:PHE:CZ	2:C:1178:LEU:HG	2.53	0.43
2:C:1194:ARG:CZ	2:Q:1201:ALA:HB2	2.48	0.43
2:Q:122:GLN:HA	2:Q:199:LEU:O	2.19	0.43
2:Q:620:ASP:HB3	2:Q:623:GLY:HA2	2.00	0.43
2:Q:635:PHE:N	2:Q:646:SER:O	2.36	0.43
2:Q:815:ASP:OD1	2:Q:816:ILE:N	2.51	0.43
2:Q:1288:PRO:HB2	2:Q:1298:PHE:CD2	2.53	0.43
2:C:258:LEU:HD23	2:C:285:LEU:HD23	1.99	0.43
2:C:421:ASP:HA	2:C:769:HIS:NE2	2.34	0.43
2:C:1098:ALA:HB3	2:C:1179:ARG:HH11	1.83	0.43
2:C:1515:ILE:HG13	2:C:1534:VAL:HG21	1.99	0.43
2:Q:953:GLN:HB3	2:Q:956:GLN:HG2	2.01	0.43
2:Q:1591:LYS:HD3	2:Q:1591:LYS:HA	1.79	0.43
2:C:458:ASP:HB2	2:C:461:CYS:HB2	2.00	0.43
2:C:1075:PRO:HG2	2:C:1078:GLN:HB2	2.00	0.43
2:C:193:PRO:HG3	2:C:837:VAL:HG13	1.99	0.43
2:C:462:ASN:ND2	2:C:484:THR:O	2.33	0.43
2:C:819:LEU:HD21	2:C:854:GLN:HG3	1.99	0.43
2:C:1283:VAL:O	2:C:1306:PHE:N	2.52	0.43
2:Q:836:ASP:OD1	2:Q:837:VAL:N	2.52	0.43
2:C:97:LEU:HB3	2:C:99:PHE:CE1	2.54	0.43
2:C:209:LYS:HB3	2:C:211:TYR:CZ	2.54	0.43
2:C:816:ILE:HD12	2:C:855:ILE:HG12	2.01	0.43
2:C:1061:GLY:HA2	2:C:1064:GLN:NE2	2.34	0.43
1:A:100:LYS:HA	1:A:103:ILE:HG22	2.01	0.43
2:Q:886:TYR:HB2	2:Q:903:HIS:HB2	2.01	0.43
2:Q:1122:LEU:HD23	2:Q:1162:VAL:HG22	2.00	0.43
2:Q:1252:ARG:HE	2:Q:1276:LYS:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:137:ILE:HG13	2:C:155:VAL:HG23	2.00	0.43
2:C:1239:THR:HA	2:C:1266:THR:HA	2.00	0.43
2:Q:325:PRO:HD2	2:Q:328:GLY:HA3	2.00	0.43
1:P:49:ASN:HD21	1:P:74:ASN:HA	1.84	0.42
2:C:318:LEU:HD12	2:C:318:LEU:O	2.18	0.42
1:A:162:PHE:HD2	1:A:200:ASN:HB2	1.84	0.42
2:Q:259:TRP:HA	2:Q:284:LEU:HA	2.00	0.42
2:Q:568:LEU:HD13	2:Q:663:TYR:CE2	2.49	0.42
1:P:164:ASP:OD1	1:P:168:HIS:ND1	2.52	0.42
1:P:169:GLU:N	1:P:170:PRO:HD2	2.34	0.42
2:C:572:HIS:O	2:C:598:ASP:HB3	2.19	0.42
2:C:806:ASP:N	2:C:806:ASP:OD1	2.49	0.42
2:C:1548:HIS:HB3	2:C:1551:LEU:HG	2.00	0.42
2:Q:349:GLN:O	2:Q:350:PRO:C	2.62	0.42
2:Q:633:ASN:O	2:Q:645:ASP:N	2.32	0.42
2:C:793:PRO:HB2	2:C:843:LEU:HD12	2.02	0.42
2:Q:188:HIS:NE2	2:Q:189:ARG:HG2	2.33	0.42
2:Q:286:LEU:HD21	2:Q:288:GLU:HB2	1.99	0.42
2:Q:326:LEU:HD21	2:Q:586:PRO:HG2	2.02	0.42
2:C:1156:PHE:HE1	2:Q:1152:LEU:HD22	1.84	0.42
2:C:1498:ILE:HD13	2:C:1541:ALA:HA	2.00	0.42
1:A:112:HIS:O	1:A:116:HIS:ND1	2.51	0.42
2:Q:362:GLU:HG3	2:Q:366:LYS:HG3	2.01	0.42
2:C:425:ASP:O	2:C:429:ASN:N	2.52	0.42
2:C:505:LEU:HB3	2:C:507:LEU:HG	2.02	0.42
2:Q:430:HIS:HB3	2:Q:433:THR:HG23	2.02	0.42
2:Q:444:ARG:HH12	2:Q:446:PRO:HB2	1.83	0.42
2:Q:535:LYS:HD3	2:Q:745:GLY:HA3	2.02	0.42
2:C:1018:GLY:N	2:C:1182:ASP:HB2	2.34	0.42
2:C:1516:LEU:HD12	2:C:1553:HIS:NE2	2.33	0.42
2:Q:185:ILE:HD12	2:Q:185:ILE:HA	1.93	0.42
2:Q:572:HIS:O	2:Q:598:ASP:HB3	2.19	0.42
2:Q:1090:PHE:CZ	2:Q:1178:LEU:HG	2.54	0.42
1:P:161:HIS:O	1:P:165:LEU:HG	2.20	0.42
2:C:634:ASN:HD21	2:C:651:GLN:CD	2.26	0.42
2:C:1092:GLN:OE1	2:Q:1257:ILE:HG13	2.20	0.42
2:C:1457:HIS:HB3	2:C:1459:ARG:HH21	1.85	0.42
2:Q:599:LEU:HB2	2:Q:654:ARG:NH1	2.35	0.42
2:Q:1561:PHE:HB2	2:Q:1571:ASN:ND2	2.34	0.42
1:P:65:CYS:O	1:P:69:GLU:HG2	2.19	0.42
2:C:724:SER:HG	2:C:786:GLU:C	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:889:VAL:HB	2:C:922:TRP:NE1	2.35	0.42
2:C:955:ASP:N	2:C:955:ASP:OD1	2.52	0.42
2:C:1592:LYS:HE2	2:C:1592:LYS:HB2	1.85	0.42
2:Q:180:ARG:O	2:Q:180:ARG:NE	2.52	0.42
2:C:1096:ALA:HB2	2:C:1178:LEU:HB3	2.02	0.42
2:C:1184:PHE:CD2	2:Q:1186:PRO:HB3	2.54	0.42
2:Q:386:PHE:HB3	2:Q:391:ILE:HB	2.02	0.42
2:Q:516:PHE:CE2	2:Q:543:GLY:HA3	2.55	0.42
2:C:286:LEU:HD21	2:C:288:GLU:HB2	2.02	0.42
2:C:430:HIS:HB3	2:C:433:THR:HG23	2.02	0.42
2:C:620:ASP:HB3	2:C:623:GLY:HA2	2.01	0.42
2:Q:592:PRO:HG3	2:Q:604:ASN:HA	2.02	0.42
2:Q:1328:THR:O	2:Q:1336:SER:N	2.53	0.42
2:C:718:ILE:HG22	2:C:872:THR:O	2.20	0.41
2:C:1186:PRO:HB3	2:Q:1184:PHE:CG	2.55	0.41
2:C:1248:LEU:HD21	2:C:1265:VAL:HG12	2.01	0.41
2:Q:1267:VAL:HG12	2:Q:1276:LYS:HE2	2.02	0.41
2:Q:1584:CYS:HB2	2:Q:1587:THR:OG1	2.20	0.41
2:C:1122:LEU:HD23	2:C:1122:LEU:HA	1.94	0.41
2:Q:324:PRO:HA	2:Q:325:PRO:HD3	1.95	0.41
2:Q:499:ASN:HA	2:Q:502:LYS:HD2	2.02	0.41
2:Q:791:LEU:HD12	2:Q:871:SER:HB3	2.01	0.41
2:Q:1573:ARG:NE	2:Q:1575:PHE:HB3	2.34	0.41
2:C:775:CYS:HB3	2:C:781:CYS:HB2	1.69	0.41
2:C:1124:ASP:OD1	2:C:1128:GLN:N	2.53	0.41
1:A:144:ASP:OD2	1:A:147:ALA:HB3	2.20	0.41
2:Q:702:PHE:HA	2:Q:883:PRO:HA	2.02	0.41
2:C:1557:GLY:HA2	2:C:1573:ARG:HH12	1.85	0.41
1:A:49:ASN:ND2	1:A:52:GLU:OE2	2.53	0.41
2:Q:99:PHE:CE2	2:Q:306:PRO:HG3	2.56	0.41
2:Q:513:LEU:HB2	2:Q:666:TRP:CZ3	2.56	0.41
2:Q:682:LEU:HD13	2:Q:690:THR:HG22	2.03	0.41
1:P:100:LYS:HA	1:P:103:ILE:HG22	2.03	0.41
2:C:766:VAL:HG21	2:C:772:PRO:HB3	2.01	0.41
1:A:79:ARG:HB2	1:A:168:HIS:CD2	2.56	0.41
1:A:142:LYS:HG3	1:A:143:HIS:CE1	2.56	0.41
2:Q:114:LEU:HD13	2:Q:140:LEU:HD11	2.02	0.41
2:Q:170:TYR:HB2	2:Q:187:ALA:HB2	2.03	0.41
1:P:46:SER:HB3	1:P:49:ASN:HB2	2.03	0.41
1:P:53:ILE:O	1:P:57:LEU:HD23	2.20	0.41
2:C:714:LEU:HB2	2:C:718:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1286:SER:O	2:C:1335:TRP:NE1	2.48	0.41
1:A:72:GLU:OE2	1:A:81:LEU:N	2.50	0.41
2:Q:108:LEU:HB3	2:Q:238:LEU:HB3	2.03	0.41
2:C:158:HIS:CD2	2:C:171:PHE:CG	3.07	0.41
2:C:729:PRO:HA	2:C:736:GLY:HA3	2.03	0.41
2:C:759:THR:HG22	2:C:865:ASP:HA	2.03	0.41
2:C:772:PRO:HD2	1:A:50:THR:HG21	2.03	0.41
2:C:777:GLU:HB3	2:C:778:PRO:CD	2.51	0.41
2:Q:206:GLN:HE21	2:Q:207:PHE:HD2	1.68	0.41
2:Q:760:TRP:CD2	2:Q:783:LEU:HD22	2.56	0.41
2:Q:1058:LEU:HD22	2:Q:1105:THR:HG21	2.02	0.41
2:C:541:LEU:HD21	2:C:741:ARG:HH12	1.85	0.41
2:C:1196:GLU:CB	2:C:1207:HIS:HA	2.49	0.41
2:C:1601:ASP:O	2:C:1606:CYS:HB2	2.21	0.41
2:Q:425:ASP:O	2:Q:429:ASN:N	2.54	0.41
2:Q:485:CYS:SG	2:Q:493:ARG:HA	2.61	0.41
2:Q:807:TRP:CZ2	2:Q:812:ALA:HA	2.56	0.41
1:P:112:HIS:O	1:P:116:HIS:ND1	2.53	0.41
1:P:190:THR:HA	1:P:193:VAL:HG12	2.02	0.41
2:C:158:HIS:CD2	2:C:171:PHE:CD1	3.08	0.41
2:C:648:THR:O	2:C:652:VAL:HG23	2.20	0.41
2:C:763:ASN:O	2:C:766:VAL:HG22	2.21	0.41
2:C:1296:ALA:HB2	2:C:1342:CYS:SG	2.60	0.41
2:C:1504:THR:OG1	2:C:1534:VAL:O	2.37	0.41
2:Q:122:GLN:NE2	2:Q:259:TRP:HE1	2.18	0.41
2:Q:270:SER:O	2:Q:274:THR:HG23	2.20	0.41
2:Q:570:LEU:HA	2:Q:654:ARG:HH21	1.86	0.41
2:Q:651:GLN:O	2:Q:655:MET:HG2	2.21	0.41
2:Q:898:VAL:HG12	2:Q:900:SER:H	1.86	0.41
2:Q:913:LEU:HD23	2:Q:913:LEU:HA	1.94	0.41
2:Q:964:ASN:ND2	2:Q:969:ASP:OD2	2.53	0.41
2:Q:1534:VAL:HG11	2:Q:1552:ILE:HD13	2.03	0.41
2:C:459:MET:HE1	2:C:486:PHE:CE2	2.53	0.41
2:C:946:TYR:CE1	2:C:949:ASP:HB3	2.55	0.41
2:C:1150:HIS:CD2	2:C:1157:TYR:HH	2.35	0.41
2:Q:726:ALA:HB1	2:Q:740:PRO:HG2	2.02	0.41
2:Q:859:ASP:OD1	2:Q:860:GLU:N	2.54	0.41
2:Q:1026:ASN:HB3	2:Q:1089:TYR:HB2	2.03	0.41
2:Q:1452:GLY:HA3	2:Q:1469:HIS:CD2	2.56	0.41
2:Q:1485:ASN:ND2	2:Q:1552:ILE:O	2.54	0.41
2:C:1309:GLN:HA	2:C:1327:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HD23	1:A:115:ARG:HA	2.03	0.40
2:Q:1489:LYS:HE2	2:Q:1507:LEU:HD21	2.03	0.40
1:P:171:TYR:HA	1:P:174:LEU:HD12	2.04	0.40
2:C:130:GLY:O	2:C:832:ASN:HB2	2.21	0.40
2:Q:570:LEU:HG	2:Q:655:MET:HE3	2.03	0.40
2:Q:726:ALA:HB2	2:Q:744:GLU:HG3	2.04	0.40
2:C:325:PRO:HD2	2:C:328:GLY:HA3	2.03	0.40
2:C:349:GLN:O	2:C:350:PRO:C	2.64	0.40
2:C:355:TYR:CZ	2:C:395:LEU:HD13	2.57	0.40
2:C:461:CYS:O	2:C:469:ASP:N	2.54	0.40
2:C:813:VAL:HG13	2:C:831:GLN:H	1.85	0.40
2:C:883:PRO:HG2	2:C:904:LEU:HD23	2.02	0.40
2:C:964:ASN:HD21	2:C:966:ILE:HB	1.86	0.40
2:C:1534:VAL:HG11	2:C:1552:ILE:HD13	2.03	0.40
2:Q:747:PRO:HG3	2:Q:799:TRP:CE2	2.56	0.40
2:Q:1122:LEU:HB3	2:Q:1157:TYR:HE2	1.86	0.40
2:Q:1192:CYS:HA	2:Q:1196:GLU:OE2	2.21	0.40
2:Q:1255:GLU:C	2:Q:1256:LEU:HD12	2.46	0.40
2:Q:1414:THR:HG23	2:Q:1432:PHE:HB2	2.03	0.40
2:C:513:LEU:HB2	2:C:666:TRP:CZ3	2.56	0.40
2:C:525:LEU:HD23	2:C:525:LEU:HA	1.95	0.40
2:C:724:SER:OG	2:C:725:ASN:N	2.54	0.40
2:C:1103:LEU:HD11	2:C:1137:LEU:HD22	2.04	0.40
1:A:198:GLU:HG3	1:A:205:CYS:HB3	2.02	0.40
2:Q:109:ARG:HH21	2:Q:294:LYS:HG2	1.87	0.40
2:Q:854:GLN:HB3	2:Q:856:TYR:CE1	2.56	0.40
2:Q:1118:ILE:HD13	2:Q:1137:LEU:HD21	2.03	0.40
2:C:1186:PRO:HA	2:C:1189:LEU:HB2	2.03	0.40
1:A:125:CYS:O	1:A:129:ARG:HG3	2.21	0.40
2:Q:259:TRP:HE3	2:Q:283:GLN:HB2	1.87	0.40
2:Q:1007:SER:OG	2:Q:1007:SER:O	2.38	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	166/168 (99%)	162 (98%)	4 (2%)	0	100	100
1	P	166/168 (99%)	163 (98%)	3 (2%)	0	100	100
2	C	1522/1536 (99%)	1422 (93%)	98 (6%)	2 (0%)	48	83
2	Q	1522/1536 (99%)	1427 (94%)	93 (6%)	2 (0%)	48	83
All	All	3376/3408 (99%)	3174 (94%)	198 (6%)	4 (0%)	49	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1413	VAL
2	Q	1413	VAL
2	C	419	ILE
2	Q	419	ILE

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	146/146 (100%)	146 (100%)	0	100	100
1	P	146/146 (100%)	146 (100%)	0	100	100
2	C	1338/1347 (99%)	1336 (100%)	2 (0%)	88	88
2	Q	1338/1347 (99%)	1334 (100%)	4 (0%)	86	84
All	All	2968/2986 (99%)	2962 (100%)	6 (0%)	85	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	332	CYS
2	C	657	CYS
2	Q	414	CYS
2	Q	428	CYS

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Mol	Chain	Res	Type
2	Q	587	CYS
2	Q	657	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	49	ASN
1	P	98	GLN
1	P	112	HIS
1	P	134	GLN
1	P	150	GLN
1	P	200	ASN
2	C	233	GLN
2	C	255	HIS
2	C	566	HIS
2	C	601	ASN
2	C	751	GLN
2	C	832	ASN
2	C	920	GLN
2	C	1004	GLN
2	C	1022	GLN
2	C	1115	GLN
2	C	1130	HIS
2	C	1135	HIS
2	C	1290	HIS
2	C	1358	GLN
2	C	1398	GLN
2	C	1491	GLN
2	C	1572	ASN
1	A	48	GLN
1	A	112	HIS
1	A	191	HIS
2	Q	122	GLN
2	Q	181	GLN
2	Q	255	HIS
2	Q	650	ASN
2	Q	656	HIS
2	Q	1049	GLN
2	Q	1064	GLN
2	Q	1115	GLN
2	Q	1183	ASN
2	Q	1292	GLN

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Mol	Chain	Res	Type
2	Q	1313	GLN
2	Q	1354	ASN
2	Q	1358	GLN
2	Q	1430	ASN
2	Q	1603	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

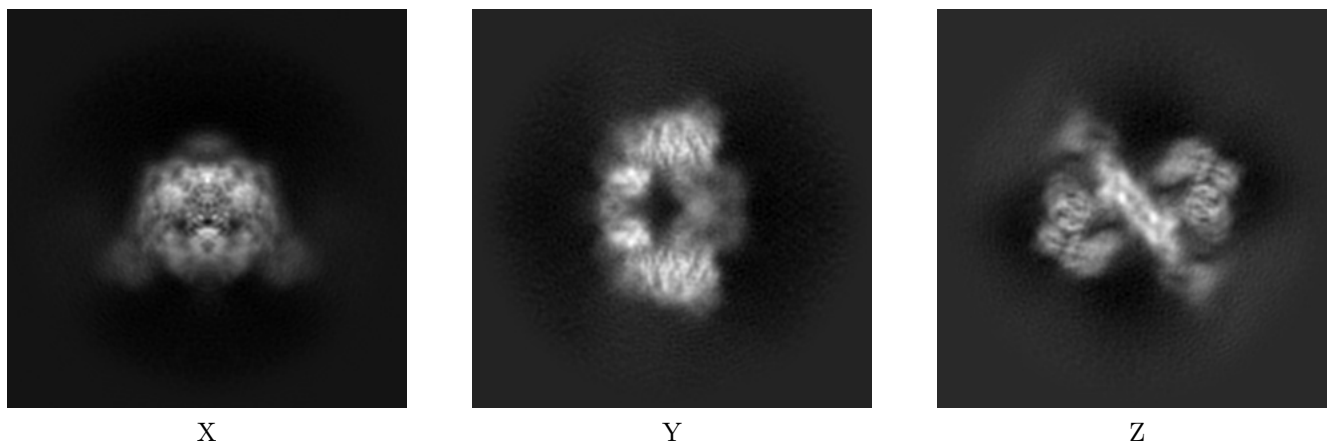
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15221. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

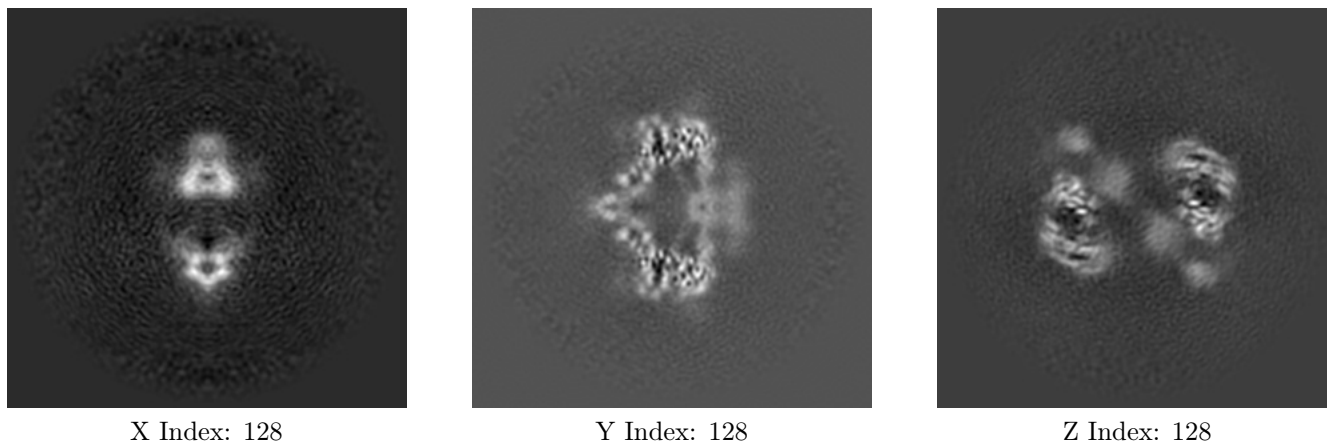
6.1.1 Primary map



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

6.2 Central slices [i](#)

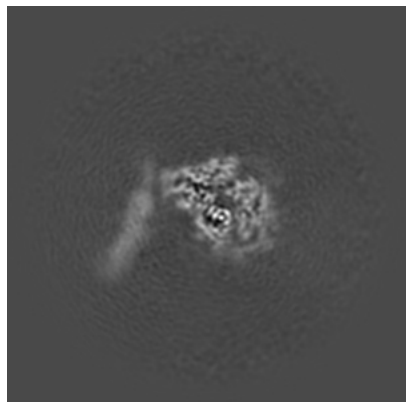
6.2.1 Primary map



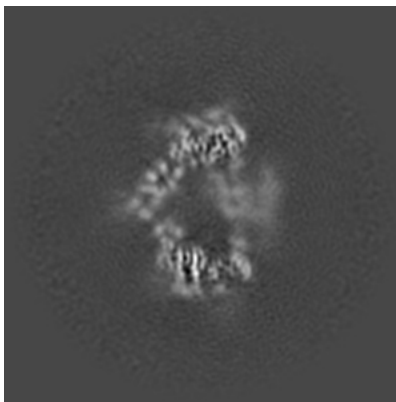
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

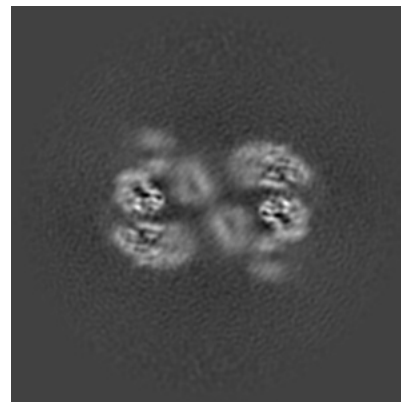
6.3.1 Primary map



X Index: 168



Y Index: 124

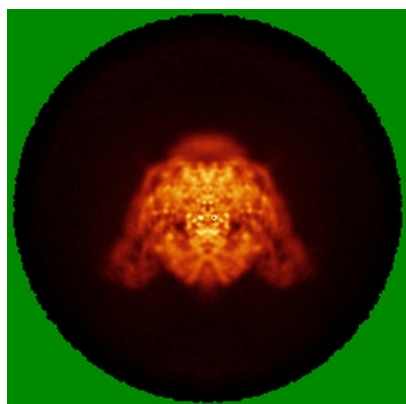


Z Index: 136

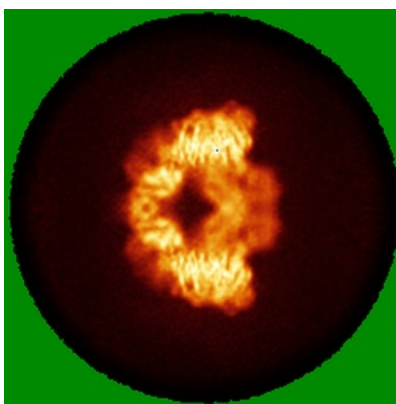
The images above show the largest variance slices of the map in three orthogonal directions.

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

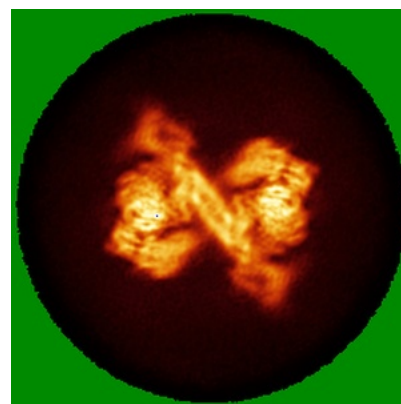
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

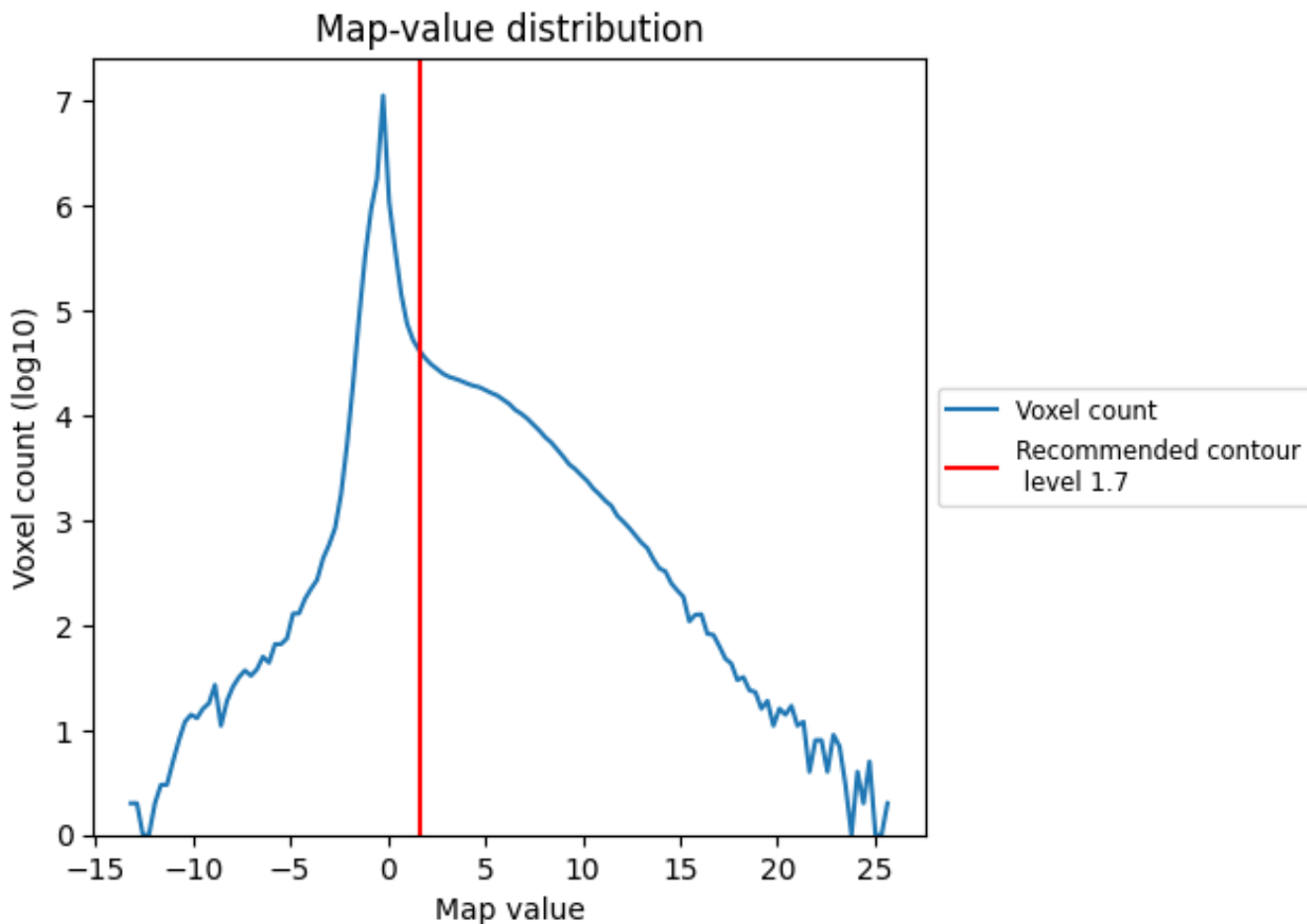
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

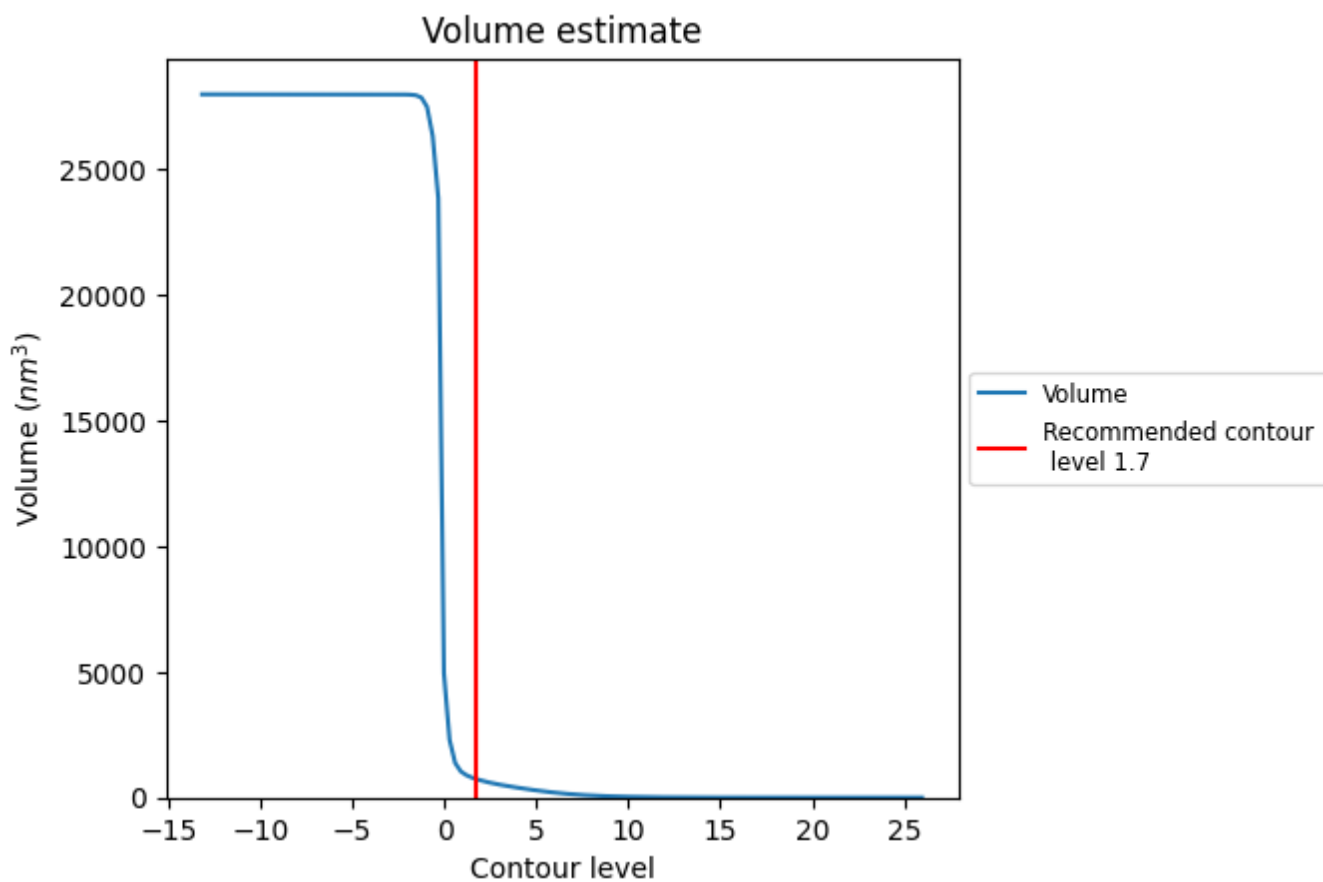
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

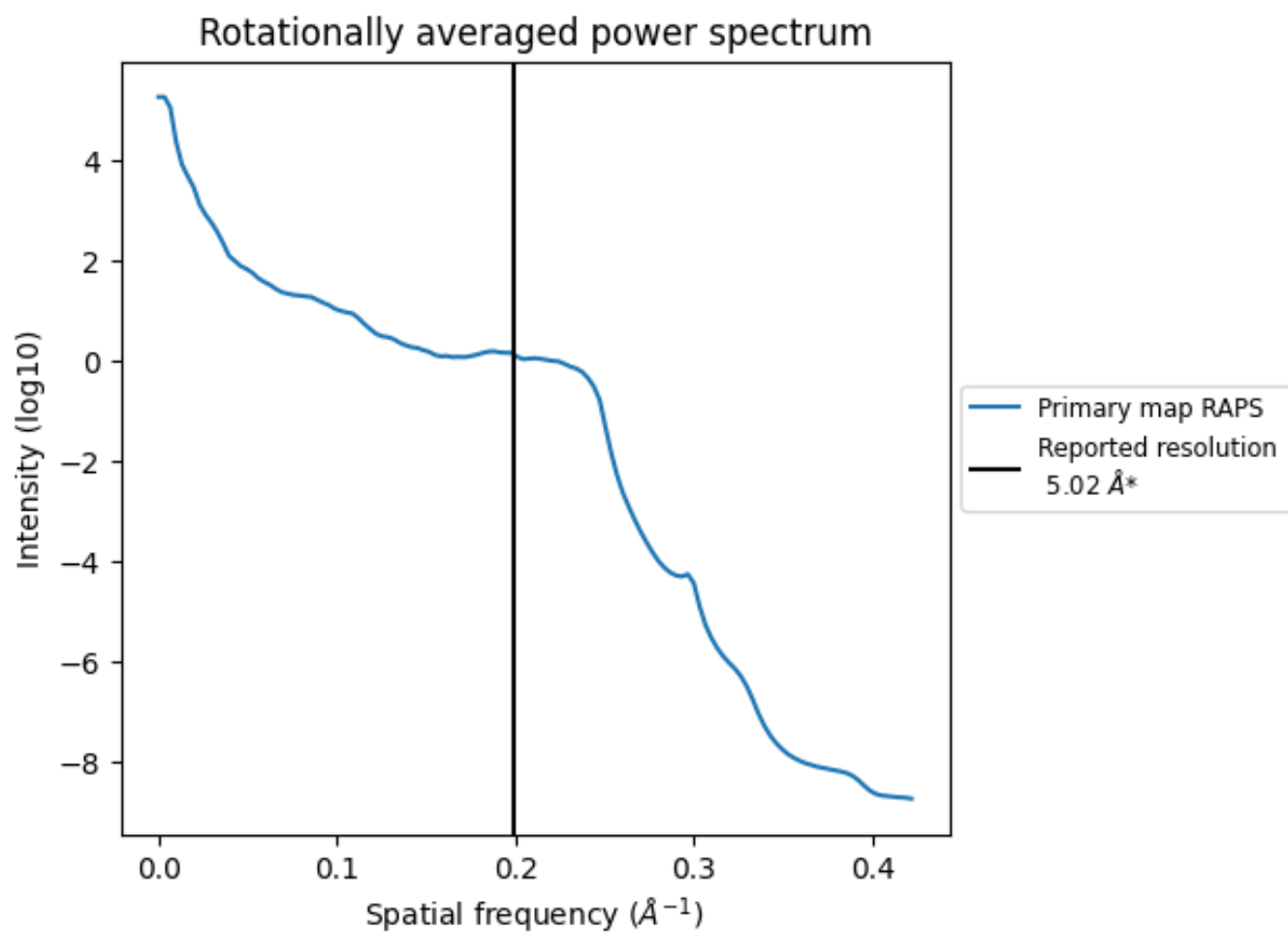
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 743 nm^3 ; this corresponds to an approximate mass of 671 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.199 Å⁻¹

8 Fourier-Shell correlation

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

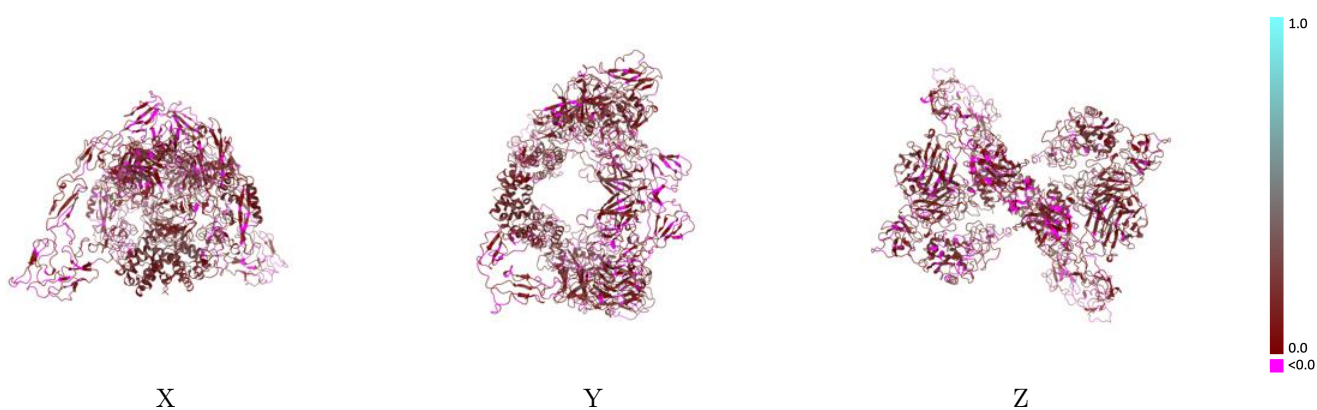
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15221 and PDB model 8A7E. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

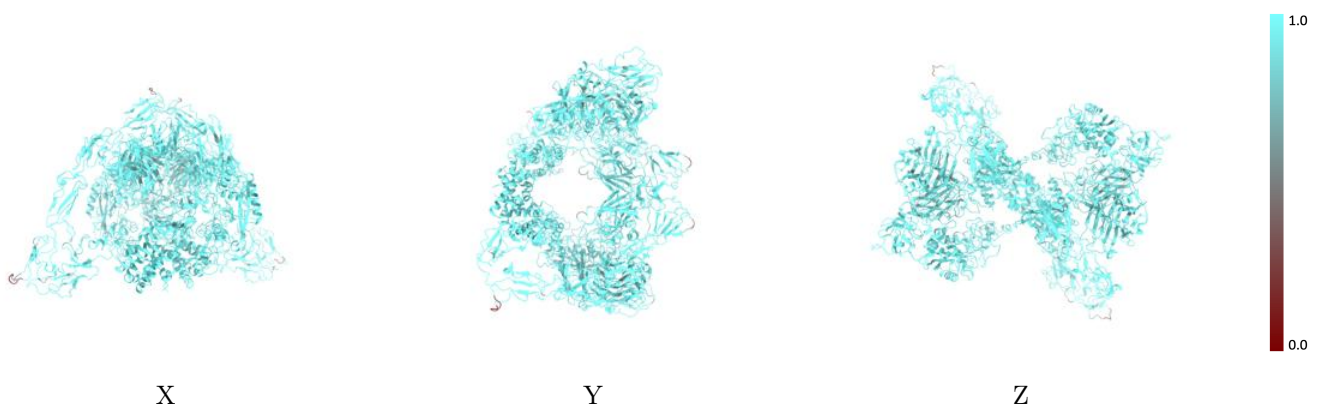
This section was not generated.

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



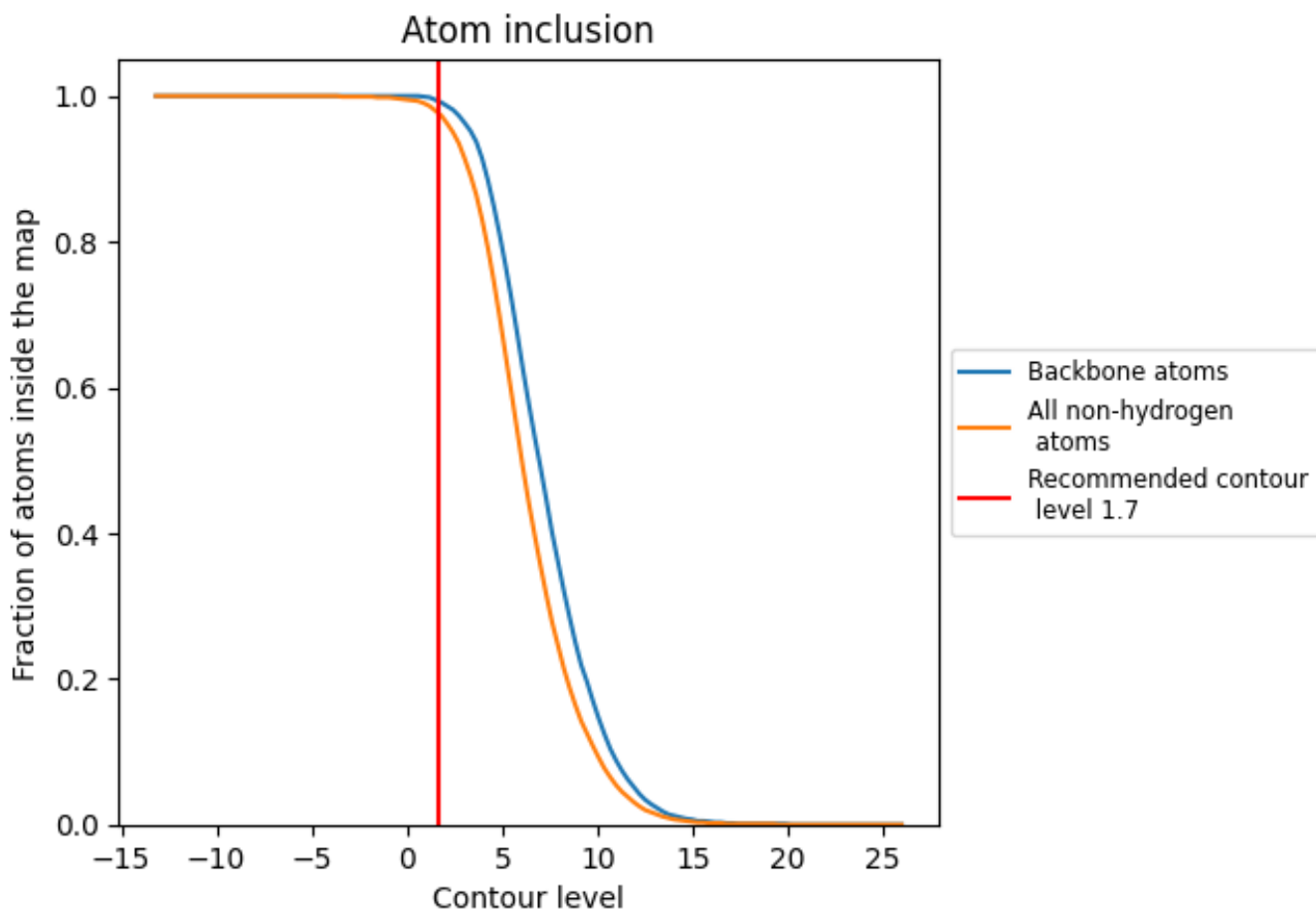
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.7).









9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (1.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.1470
A	 0.9930	 0.2210
C	 0.9710	 0.1300
P	 0.9960	 0.2160
Q	 0.9760	 0.1480

