



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:51 AM UTC

PDB ID : 8C8R / pdb_00008c8r
EMDB ID : EMD-16492
Title : In situ structure of the Nitrosopumilus maritimus S-layer - Composite map between C2 and C6
Authors : von Kuegelgen, A.; Bharat, T.
Deposited on : 2023-01-20
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

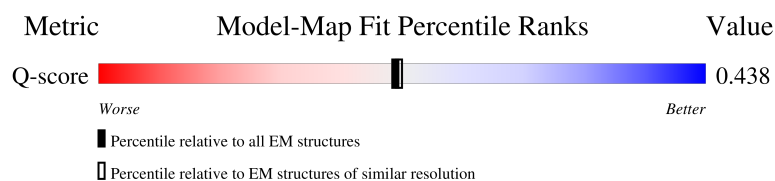
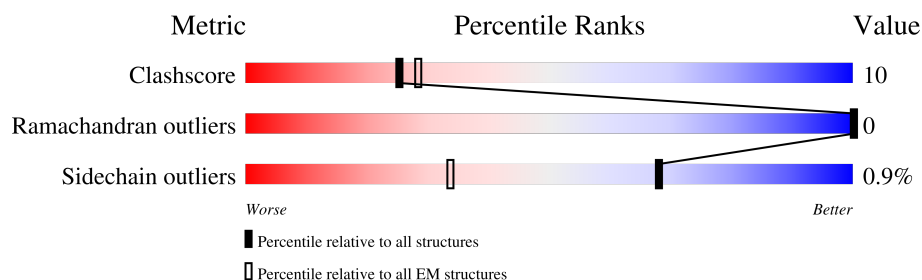
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	1734	
1	B	1734	
1	C	1734	
1	D	1734	

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Mol	Chain	Length	Quality of chain
1	E	1734	 7% 67% 17% 16%
1	F	1734	 7% 66% 18% 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 65154 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.

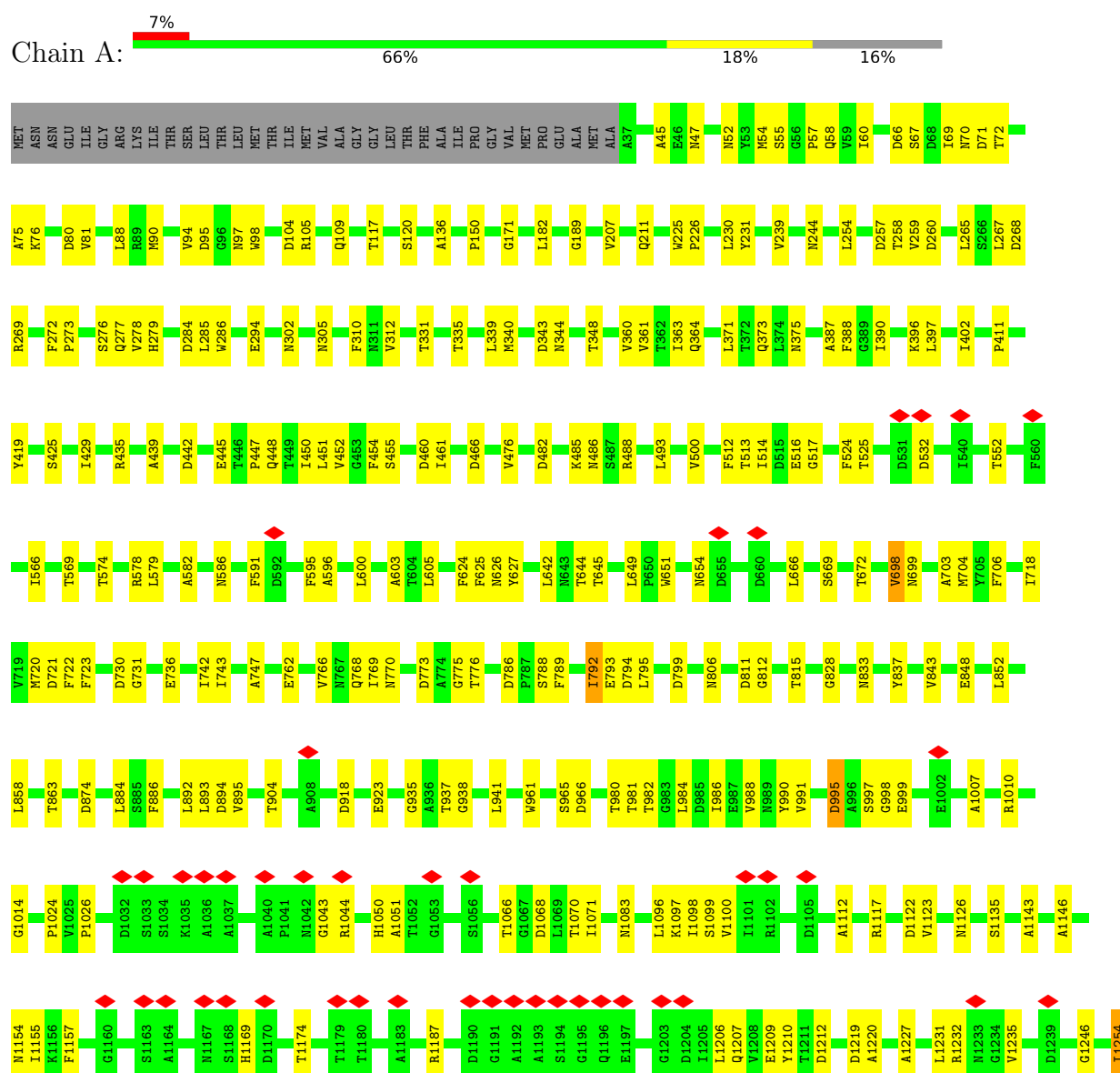
- Molecule 1 is a protein called Cell surface protein.

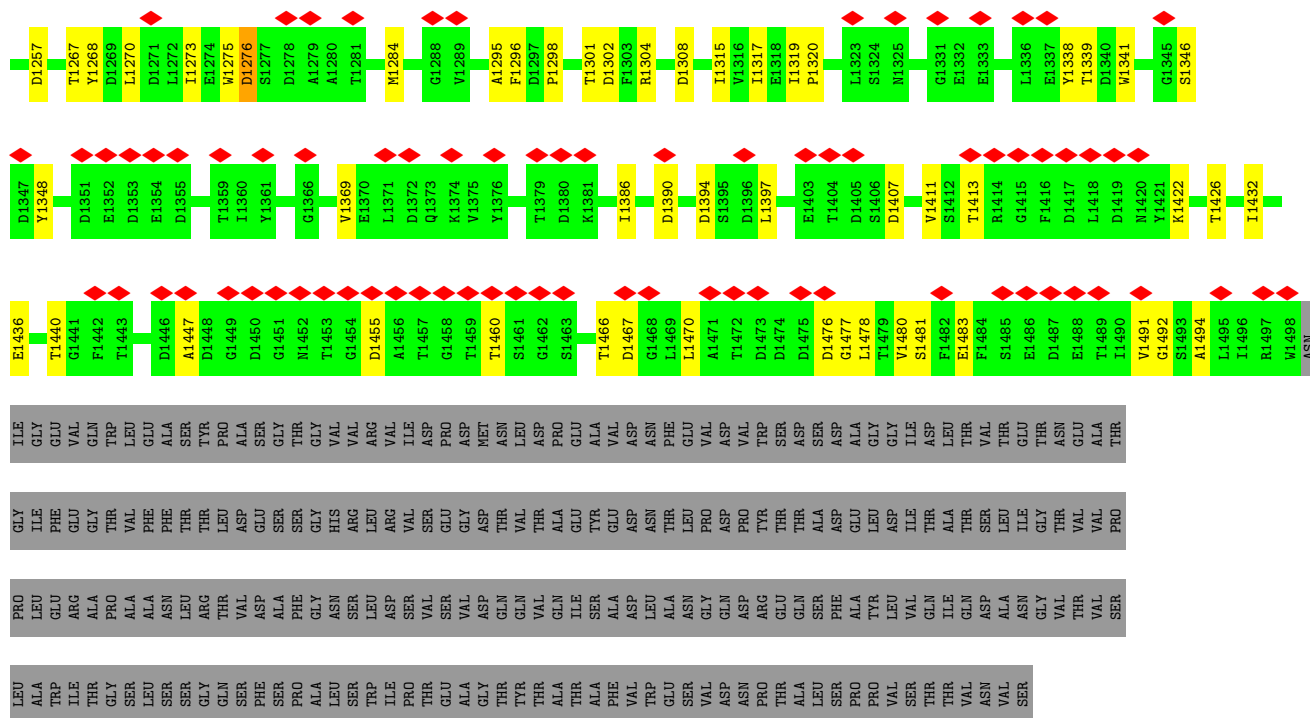
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	B	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	C	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	D	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	E	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	F	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		

3 Residue-property plots

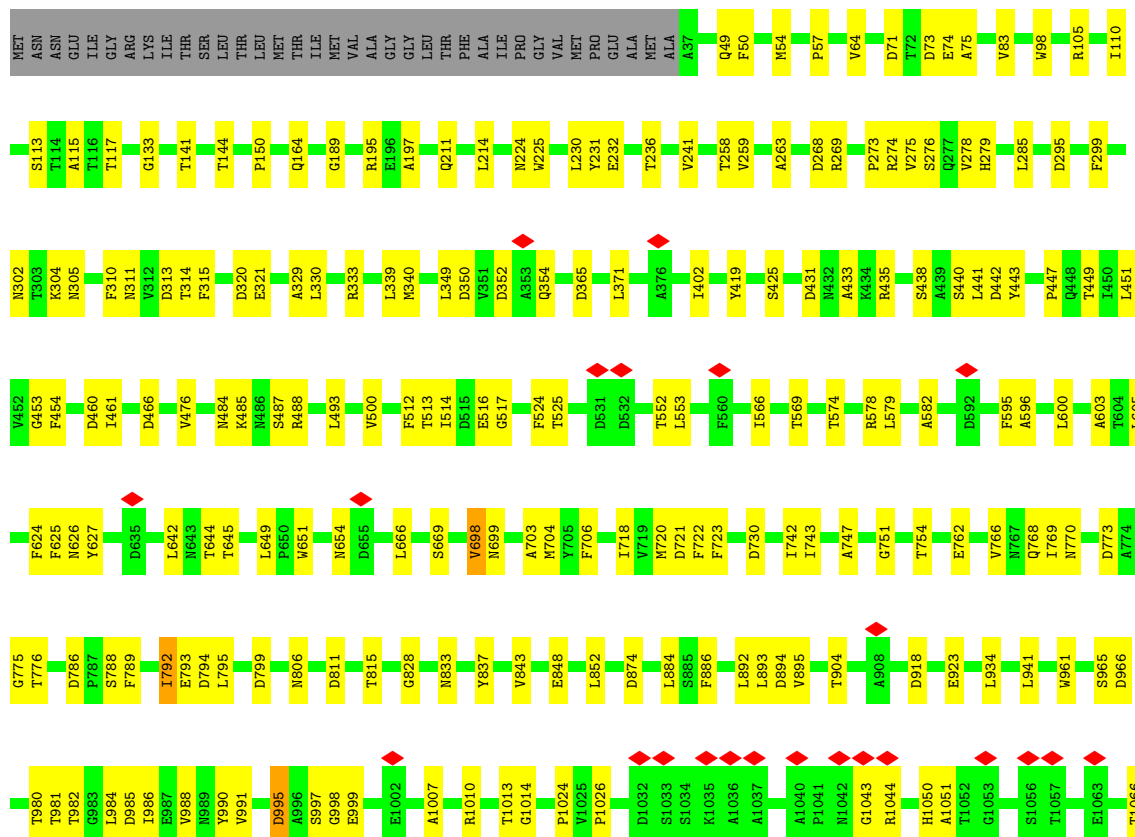
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



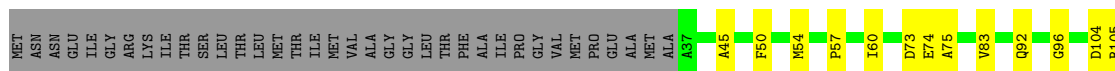


● Molecule 1: Cell surface protein



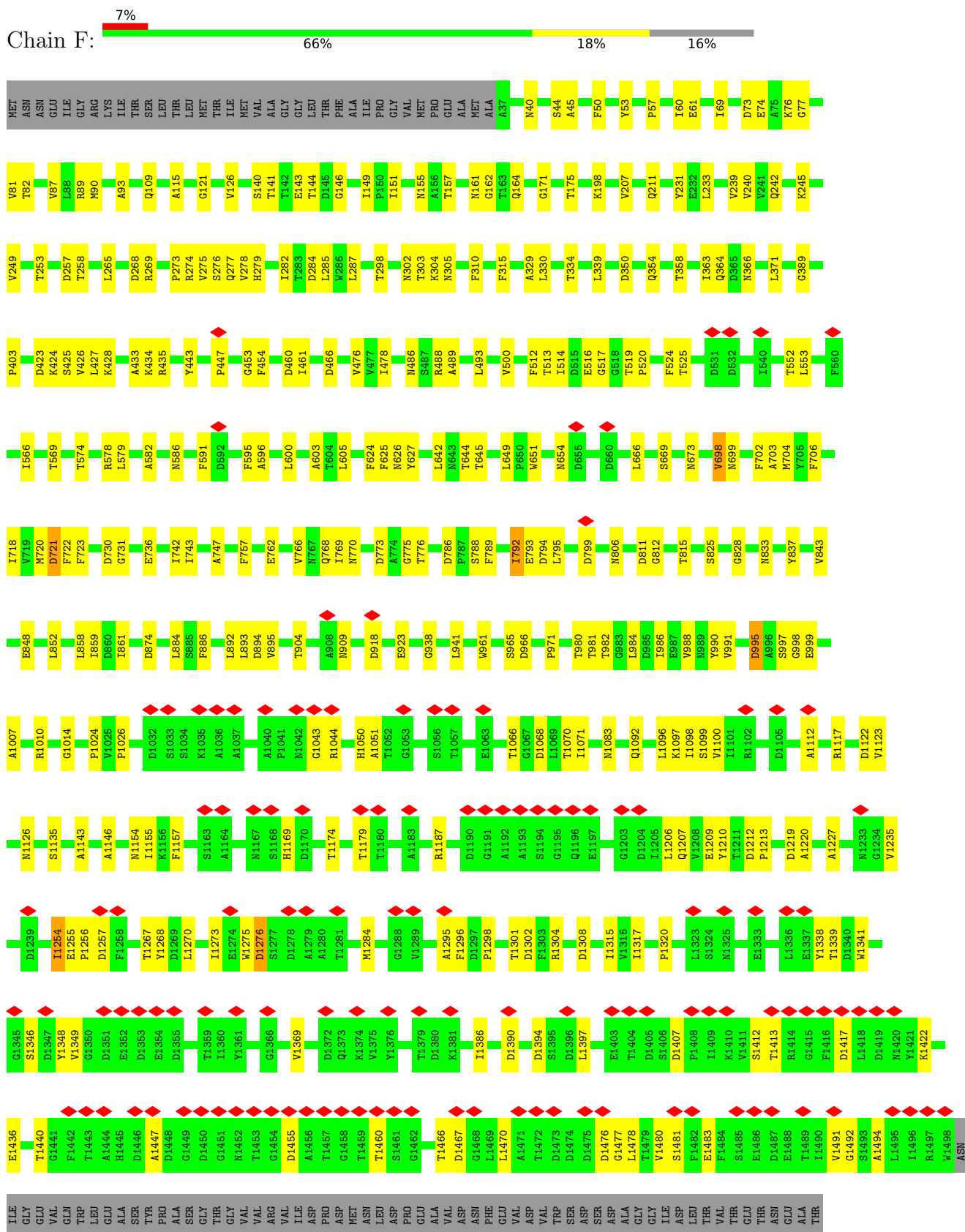


V278	H279	E294	N302	K303	K304	N305	F310	N311	V312	T335	L339	D343	N344	T348	L349	D350	V360	V361	T362	L363	Q364	L371	F388	G399	L390	L397	I402	E408	P411	Y419	D420	S421	S422	S425	I429	R435	A439	D442									
V94	D95	G96	N97	V98	D104	R105	Q109	T117	S120	A136	E143	P150	Q164	G171	L182	G189	V207	Q211	N216	P223	N224	W225	P226	L230	Y231	N244	D257	T258	V269	D260	L265	D268	R269	P273	S276	O277											
ASN	ASN	GLU	GLY	GLY	LYS	ILE	SER	LEU	THR	LEU	MET	THR	ILE	VAL	GLY	LEU	THR	PHE	ALA	ILE	PRO	GLY	VAL	MET	PRO	GLU	ALA	ALA	MET	ALA	ASP	N47	N52	P57	D66	S67	D68	I69	N70	D71	T72	K76	D80	V87	L88	P89	W90



D106	Q277	D460	A603	N770	E923	G1053	T1179	D1276	Y1361	M1452	GLY	GLU	PHE	ASP
I110	V278	I461	T604	D773	L934	S1056	T1180	S1277	G1366	T1453	THR	SER	SER	SER
T114	H279	D466	L605	A774	L941	E1063	A1183	D1278	Y1369	G1454	GLY	SER	ALA	ALA
A115	L285	V476	F624	T775	G953	E1066	R1187	A1279	D1372	D1455	VAL	ASN	LEU	LEU
T116	D295	I477	N626	T776	Q953	T1066	D1190	T1281	Q1373	A1456	ARG	VAL	LEU	TRP
T117	F299	V478	N627	D786	Q953	G1067	G1191	G1284	Q1377	T1457	VAL	ARG	ASP	ASP
S120	N302	N484	D635	F787	W961	D1068	A1192	G1288	S1375	G1458	ILE	VAL	VAL	THR
G121	K485	W486	L642	F788	S965	L1069	A1193	V1289	Y1376	T1459	ASP	GLY	ASP	GLY
G133	N311	S487	N643	F789	D966	T1070	A1194	A1295	W1377	T1460	PRO	ASP	ALA	ALA
T141	V312	R488	T644	D794	T980	N1083	G1195	D1296	S1378	G1462	LEU	ASP	GLN	THR
F315	D313	T314	T645	L795	T981	Q1092	Q1196	F1297	W1379	S1463	ASP	THR	VAL	TYR
I149	F315	L493	L649	D799	G983	Q1092	E1197	F1298	D1380	T1466	PRO	ALA	GLN	ALA
P150	A329	V500	W651	N806	L984	L1096	G1197	P1298	K1381	D1467	GLU	GLU	ILE	THR
I151	L330	F512	N654	N806	D985	K1097	D1203	T1301	I1386	D1468	ALA	ALA	SER	ALA
Q164	R333	I513	N654	D811	E987	I1098	G1204	D1302	Y1390	L1469	VAL	GLY	PHE	PHE
G189	L339	I514	D855	T915	V988	S1099	I1205	F1303	D1394	A1470	ASP	ASP	THR	VAL
R195	M340	D515	V659	S825	N989	V1100	L1206	R1304	S1395	T1472	VAL	LEU	ASN	SER
E196	L349	E516	D660	G828	Y991	I1101	Q1207	D1308	S1396	D1473	ASP	PRO	GLY	VAL
A197	L349	G517	L666	N933	D995	R1102	E1208	I1315	L1397	D1474	THR	ASP	GLN	ASP
A203	A353	T525	S669	N833	A996	D1105	Y1210	I1316	D1407	D1475	TRP	VAL	ASP	ASP
V209	Q364	D531	V698	Y837	S997	A1112	T1211	I1317	P1408	G1476	SER	GLY	THR	THR
Q211	D365	D632	N699	V843	G998	A1112	D1212	E1318	L1409	L1478	ASP	ALA	ALA	ALA
L214	L371	I540	A703	I945	E999	R1117	P1213	P1320	D1405	T1479	SER	GLU	SER	PHE
N224	A376	F560	M704	E948	E1002	D1122	D1219	L1323	D1406	V1480	ASP	GLU	ALA	PRO
W225	I402	I566	F705	L852	A1007	V1123	A1220	S1324	D1407	S1481	GLY	LEU	TYR	PRO
L230	S425	T569	F706	D874	R1010	N1126	A1227	N1325	P1408	F1482	ILE	ILE	THR	VAL
E232	K428	T574	I718	L884	G1014	S1135	L1231	G1331	L1409	F1484	ASP	THR	ALA	GLN
T236	R435	T574	V719	S885	P1024	A1143	R1232	E1332	K1410	S1485	LEU	LEU	THR	THR
V241	S438	R578	M720	F886	P1026	A1146	G1234	E1333	V1411	E1486	VAL	SER	ALA	ASN
K245	A439	L579	D721	F886	D1032	E1150	G1235	L1336	S1412	D1487	THR	ILE	LEU	ASN
S440	S440	A582	F722	L892	S1033	I1155	V1235	E1337	T1413	T1488	THR	GLY	GLY	GLY
L441	L441	A582	F723	D894	S1034	K1156	S1238	Y1338	R1414	T1489	THR	VAL	VAL	VAL
T288	D442	N586	D730	V895	K1035	F1157	D1239	T1339	G1415	I1490	ASN	VAL	VAL	THR
V259	P447	F591	A747	D998	A1036	T1158	E1238	D1340	F1416	V1491	GLY	VAL	VAL	THR
D268	Q448	D592	F757	T904	A1037	D1159	D1239	W1341	D1417	G1492	THR	VAL	VAL	THR
R269	T449	I450	E762	A908	A1040	A1164	E1254	G1345	L1418	S1493	ILE	ALA	ALA	ALA
P273	I450	L451	V766	D918	P1041	N1167	E1255	S1346	D1419	A1494	THR	ALA	ALA	ALA
R274	V275	G453	Q768	A908	N1042	S1168	E1256	D1347	N1420	L1495	THR	ARG	THR	THR
S276	F454	L500	I769	D918	G1043	H1169	F1258	Y1348	Y1421	T1496	THR	THR	THR	THR
					R1044	D1170	L1270	V1348	K1422	R1497	ASP	VAL	VAL	VAL
					H1050	T1174	I1273	G1350	E1436	W1498	THR	VAL	VAL	THR
					A1051		E1274	P1350	T1440	ASN	THR	VAL	VAL	THR
					T1052		W1275	D1351	G1441	ILE	THR	VAL	VAL	THR
								E1352	F1442	GLY	THR	VAL	VAL	THR
								S1168	T1443	GLY	THR	VAL	VAL	THR
								H1169	T1443	GLY	THR	VAL	VAL	THR
								D1170	T1443	GLY	THR	VAL	VAL	THR
								T1174	T1443	GLY	THR	VAL	VAL	THR
									T1446	LEU	THR	VAL	VAL	THR
									A1447	GLU	THR	VAL	VAL	THR
									D1448	ALA	THR	VAL	VAL	THR
									G1449	SER	THR	VAL	VAL	THR
									T1359	TYR	THR	VAL	VAL	THR
									G1451	PRO	THR	VAL	VAL	THR
										ALA	THR	VAL	VAL	THR

- Molecule 1: Cell surface protein



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	108621	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; PseudoSubtomograms as described in Zivanov 2022 (https://elifesciences.org/articles/83724)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	121	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	12.055	Depositor
Minimum map value	-6.789	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.582	Depositor
Recommended contour level	1.45621	Depositor
Map size ($\text{\AA}$)	265.4, 265.4, 265.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.327, 1.327, 1.327	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/11032	0.29	0/15089
1	B	0.12	0/11032	0.29	0/15089
1	C	0.13	0/11032	0.29	0/15089
1	D	0.12	0/11032	0.29	0/15089
1	E	0.13	0/11032	0.29	0/15089
1	F	0.13	0/11032	0.29	0/15089
All	All	0.13	0/66192	0.29	0/90534

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10859	0	10131	266	0
1	B	10859	0	10136	209	0
1	C	10859	0	10136	242	0
1	D	10859	0	10130	255	0
1	E	10859	0	10135	220	0
1	F	10859	0	10136	241	0
All	All	65154	0	60804	1314	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 10.

All (1314) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HH12	1:A:485:LYS:C	0.98	1.52
1:C:435:ARG:NH1	1:C:812:GLY:HA3	1.24	1.44
1:A:269:ARG:NH1	1:A:485:LYS:C	1.76	1.39
1:A:269:ARG:HH12	1:A:486:ASN:N	1.17	1.38
1:B:354:GLN:NE2	1:C:861:ILE:HD11	1.37	1.36
1:E:354:GLN:NE2	1:F:861:ILE:HD11	1.42	1.32
1:F:435:ARG:NH1	1:F:812:GLY:CA	1.88	1.32
1:F:435:ARG:NH1	1:F:812:GLY:HA3	0.97	1.28
1:A:276:SER:HB2	1:A:485:LYS:O	1.34	1.25
1:D:435:ARG:NH2	1:D:811:ASP:O	1.73	1.21
1:D:276:SER:HB2	1:D:485:LYS:O	1.45	1.15
1:A:435:ARG:NH2	1:A:811:ASP:O	1.79	1.14
1:C:435:ARG:NH1	1:C:812:GLY:CA	2.10	1.14
1:D:268:ASP:OD2	1:D:488:ARG:NH1	1.81	1.13
1:A:269:ARG:NH1	1:A:486:ASN:N	1.90	1.10
1:D:269:ARG:HG3	1:D:487:SER:HB3	1.31	1.10
1:F:435:ARG:HH12	1:F:812:GLY:CA	1.50	1.10
1:B:275:VAL:HG12	1:B:485:LYS:HD3	1.33	1.06
1:F:423:ASP:OD2	1:F:486:ASN:ND2	1.88	1.05
1:E:275:VAL:HG12	1:E:485:LYS:HD3	1.36	1.04
1:A:435:ARG:NH1	1:A:812:GLY:HA3	1.74	1.01
1:C:435:ARG:CZ	1:C:812:GLY:HA3	1.92	0.99
1:B:354:GLN:NE2	1:C:861:ILE:CD1	2.27	0.97
1:D:273:PRO:CG	1:D:485:LYS:HG2	1.95	0.97
1:F:435:ARG:HH11	1:F:812:GLY:HA3	1.23	0.96
1:E:268:ASP:OD2	1:E:488:ARG:NH1	1.99	0.96
1:F:279:HIS:CD2	1:F:488:ARG:HH22	1.83	0.95
1:B:449:THR:CG2	1:C:858:LEU:HG	1.96	0.95
1:C:435:ARG:HH12	1:C:812:GLY:HA3	1.23	0.94
1:A:863:THR:HG21	1:F:354:GLN:CD	1.93	0.93
1:A:273:PRO:CG	1:A:485:LYS:HG2	1.99	0.93
1:A:435:ARG:HH12	1:A:812:GLY:HA3	1.34	0.93
1:A:279:HIS:H	1:A:488:ARG:HH22	1.16	0.92
1:D:268:ASP:CG	1:D:488:ARG:NH1	2.28	0.91
1:E:354:GLN:NE2	1:F:861:ILE:CD1	2.33	0.91
1:E:275:VAL:CG1	1:E:485:LYS:HD3	2.01	0.91
1:A:276:SER:CB	1:A:485:LYS:O	2.20	0.90
1:D:273:PRO:HG2	1:D:485:LYS:HG2	1.53	0.90
1:B:449:THR:HG22	1:C:858:LEU:HG	1.55	0.89
1:B:268:ASP:OD2	1:B:488:ARG:NH1	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:435:ARG:CZ	1:F:812:GLY:HA3	2.02	0.88
1:C:435:ARG:HH12	1:C:812:GLY:CA	1.77	0.88
1:E:449:THR:CG2	1:F:858:LEU:HG	2.05	0.87
1:A:858:LEU:HD11	1:F:447:PRO:O	1.75	0.86
1:B:354:GLN:HE22	1:C:861:ILE:HD11	1.38	0.86
1:D:279:HIS:H	1:D:488:ARG:HH22	1.19	0.85
1:C:279:HIS:CD2	1:C:488:ARG:HH22	1.94	0.85
1:E:354:GLN:HE22	1:F:861:ILE:HD11	1.36	0.85
1:B:275:VAL:CG1	1:B:485:LYS:HD3	2.05	0.85
1:C:435:ARG:HG3	1:D:938:GLY:HA3	1.59	0.85
1:A:935:GLY:O	1:F:434:LYS:NZ	2.10	0.85
1:C:423:ASP:OD2	1:C:486:ASN:ND2	2.09	0.85
1:A:273:PRO:HG2	1:A:485:LYS:HG2	1.55	0.84
1:E:435:ARG:NH2	1:E:811:ASP:O	2.12	0.83
1:E:275:VAL:HG12	1:E:485:LYS:CD	2.09	0.83
1:B:105:ARG:HA	1:B:230:LEU:HD12	1.60	0.83
1:B:275:VAL:HG12	1:B:485:LYS:CD	2.08	0.83
1:F:279:HIS:CD2	1:F:488:ARG:NH2	2.46	0.83
1:A:81:VAL:HG11	1:A:90:MET:HE2	1.60	0.82
1:A:269:ARG:NH1	1:A:485:LYS:O	2.10	0.82
1:E:105:ARG:HA	1:E:230:LEU:HD12	1.60	0.81
1:A:435:ARG:CZ	1:A:811:ASP:O	2.27	0.81
1:A:938:GLY:HA3	1:F:435:ARG:HG3	1.62	0.81
1:A:435:ARG:NH1	1:A:812:GLY:CA	2.44	0.80
1:A:269:ARG:NH1	1:A:486:ASN:CA	2.44	0.80
1:D:999:GLU:OE1	1:E:1304:ARG:NH1	2.15	0.80
1:A:268:ASP:OD2	1:A:488:ARG:NH1	2.15	0.80
1:A:279:HIS:N	1:A:488:ARG:NH2	2.24	0.80
1:B:268:ASP:OD2	1:B:487:SER:OG	2.01	0.79
1:C:434:LYS:NZ	1:D:935:GLY:O	2.13	0.79
1:D:279:HIS:N	1:D:488:ARG:HH22	1.78	0.79
1:D:273:PRO:HB2	1:D:485:LYS:NZ	1.98	0.79
1:E:449:THR:HG22	1:F:858:LEU:HG	1.62	0.79
1:A:279:HIS:N	1:A:488:ARG:HH22	1.77	0.79
1:A:999:GLU:OE1	1:B:1304:ARG:NH1	2.16	0.78
1:C:354:GLN:CD	1:D:863:THR:HG21	2.08	0.78
1:B:999:GLU:OE1	1:C:1304:ARG:NH1	2.17	0.78
1:C:999:GLU:OE1	1:D:1304:ARG:NH1	2.17	0.78
1:A:1304:ARG:NH1	1:F:999:GLU:OE1	2.17	0.78
1:E:999:GLU:OE1	1:F:1304:ARG:NH1	2.17	0.78
1:C:447:PRO:O	1:D:858:LEU:HD11	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:ASP:OD2	1:E:487:SER:OG	2.02	0.77
1:A:276:SER:CB	1:A:485:LYS:HB3	2.15	0.76
1:A:273:PRO:HG2	1:A:485:LYS:HA	1.68	0.76
1:A:273:PRO:HB2	1:A:485:LYS:NZ	2.01	0.76
1:F:435:ARG:HH12	1:F:812:GLY:HA3	0.97	0.75
1:F:435:ARG:HH12	1:F:812:GLY:N	1.85	0.75
1:A:276:SER:HB3	1:A:485:LYS:HB3	1.70	0.74
1:B:768:GLN:HE21	1:B:991:VAL:HG12	1.53	0.74
1:D:105:ARG:HA	1:D:230:LEU:HD12	1.70	0.74
1:C:279:HIS:CD2	1:C:488:ARG:NH2	2.56	0.74
1:A:302:ASN:HB2	1:A:402:ILE:H	1.53	0.73
1:A:768:GLN:HE21	1:A:991:VAL:HG12	1.53	0.73
1:E:768:GLN:HE21	1:E:991:VAL:HG12	1.53	0.73
1:A:672:THR:HG21	1:F:334:THR:HG22	1.69	0.73
1:C:768:GLN:HE21	1:C:991:VAL:HG12	1.53	0.73
1:D:768:GLN:HE21	1:D:991:VAL:HG12	1.53	0.73
1:D:273:PRO:HB2	1:D:485:LYS:HZ2	1.51	0.73
1:F:768:GLN:HE21	1:F:991:VAL:HG12	1.53	0.72
1:A:863:THR:HG21	1:F:354:GLN:CG	2.18	0.72
1:D:302:ASN:HB2	1:D:402:ILE:H	1.53	0.72
1:D:269:ARG:NH1	1:D:485:LYS:CA	2.43	0.72
1:A:276:SER:CA	1:A:485:LYS:HB3	2.18	0.72
1:A:276:SER:HB2	1:A:485:LYS:C	2.14	0.72
1:C:354:GLN:HG2	1:D:863:THR:HG21	1.70	0.72
1:D:276:SER:CB	1:D:485:LYS:HB3	2.19	0.71
1:B:274:ARG:NH1	1:B:433:ALA:O	2.24	0.71
1:C:155:ASN:O	1:C:161:ASN:ND2	2.24	0.71
1:E:269:ARG:NH2	1:E:484:ASN:O	2.24	0.71
1:A:863:THR:HG21	1:F:354:GLN:HG2	1.72	0.71
1:D:276:SER:CB	1:D:485:LYS:O	2.34	0.70
1:D:279:HIS:N	1:D:488:ARG:NH2	2.28	0.70
1:E:275:VAL:CG1	1:E:485:LYS:CD	2.68	0.70
1:C:334:THR:HG22	1:D:672:THR:HG21	1.71	0.70
1:A:863:THR:OG1	1:F:354:GLN:HG2	1.91	0.70
1:D:276:SER:CA	1:D:485:LYS:HB3	2.22	0.70
1:A:105:ARG:HA	1:A:230:LEU:HD12	1.74	0.70
1:D:268:ASP:CG	1:D:488:ARG:HH12	1.97	0.69
1:F:155:ASN:O	1:F:161:ASN:ND2	2.25	0.69
1:D:273:PRO:HG2	1:D:485:LYS:HA	1.75	0.69
1:B:236:THR:OG1	1:C:489:ALA:HB2	1.93	0.69
1:A:863:THR:HG23	1:F:354:GLN:NE2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:LEU:O	1:D:448:GLN:NE2	2.26	0.69
1:B:259:VAL:HG11	1:B:285:LEU:HD22	1.75	0.68
1:C:273:PRO:HG2	1:C:276:SER:HB2	1.75	0.68
1:E:105:ARG:NH2	1:E:232:GLU:OE2	2.27	0.68
1:B:435:ARG:NH1	1:B:811:ASP:O	2.27	0.68
1:A:279:HIS:NE2	1:A:486:ASN:ND2	2.42	0.67
1:A:411:PRO:HG2	1:F:249:VAL:HG11	1.76	0.67
1:D:269:ARG:CG	1:D:487:SER:HB3	2.18	0.67
1:D:273:PRO:HG2	1:D:276:SER:HB3	1.75	0.67
1:D:279:HIS:NE2	1:D:486:ASN:ND2	2.42	0.67
1:A:273:PRO:HG2	1:A:276:SER:HB3	1.76	0.67
1:A:273:PRO:CG	1:A:485:LYS:HA	2.24	0.67
1:E:259:VAL:HG11	1:E:285:LEU:HD22	1.76	0.67
1:E:743:ILE:HG13	1:E:789:PHE:HB3	1.77	0.67
1:A:268:ASP:CG	1:A:488:ARG:NH1	2.53	0.67
1:C:354:GLN:CG	1:D:863:THR:HG21	2.24	0.67
1:D:743:ILE:HG13	1:D:789:PHE:HB3	1.77	0.67
1:B:574:THR:OG1	1:B:806:ASN:ND2	2.29	0.66
1:C:574:THR:OG1	1:C:806:ASN:ND2	2.29	0.66
1:C:354:GLN:NE2	1:D:863:THR:HG23	2.09	0.66
1:D:574:THR:OG1	1:D:806:ASN:ND2	2.29	0.66
1:E:574:THR:OG1	1:E:806:ASN:ND2	2.29	0.66
1:F:574:THR:OG1	1:F:806:ASN:ND2	2.29	0.66
1:F:743:ILE:HG13	1:F:789:PHE:HB3	1.77	0.66
1:C:743:ILE:HG13	1:C:789:PHE:HB3	1.77	0.66
1:D:1220:ALA:O	1:E:1466:THR:OG1	2.13	0.66
1:A:863:THR:CG2	1:F:354:GLN:NE2	2.59	0.66
1:F:240:VAL:HG22	1:F:253:THR:HG22	1.78	0.66
1:A:276:SER:HB3	1:A:485:LYS:CB	2.25	0.66
1:A:574:THR:OG1	1:A:806:ASN:ND2	2.29	0.66
1:D:294:GLU:HB2	1:D:408:GLU:HB3	1.77	0.66
1:A:1220:ALA:O	1:B:1466:THR:OG1	2.13	0.66
1:A:743:ILE:HG13	1:A:789:PHE:HB3	1.77	0.65
1:C:354:GLN:NE2	1:D:863:THR:CG2	2.59	0.65
1:B:743:ILE:HG13	1:B:789:PHE:HB3	1.77	0.65
1:B:766:VAL:HG11	1:B:792:ILE:HD12	1.78	0.65
1:A:1097:LYS:HB3	1:A:1209:GLU:HB3	1.79	0.65
1:B:1097:LYS:HB3	1:B:1209:GLU:HB3	1.79	0.65
1:C:364:GLN:OE1	1:C:364:GLN:N	2.29	0.65
1:C:766:VAL:HG11	1:C:792:ILE:HD12	1.78	0.65
1:A:373:GLN:HE22	1:A:387:ALA:HB1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:SER:HA	1:D:485:LYS:HB3	1.78	0.65
1:B:354:GLN:CD	1:C:861:ILE:HD11	2.19	0.65
1:E:236:THR:OG1	1:F:489:ALA:HB2	1.96	0.65
1:C:1097:LYS:HB3	1:C:1209:GLU:HB3	1.79	0.65
1:D:454:PHE:HA	1:D:482:ASP:OD1	1.97	0.65
1:F:1097:LYS:HB3	1:F:1209:GLU:HB3	1.79	0.65
1:E:1394:ASP:HB3	1:E:1397:LEU:HB3	1.79	0.64
1:A:1394:ASP:HB3	1:A:1397:LEU:HB3	1.79	0.64
1:E:512:PHE:HB3	1:E:722:PHE:HB2	1.80	0.64
1:A:273:PRO:HB2	1:A:485:LYS:HZ2	1.62	0.64
1:A:863:THR:CG2	1:F:354:GLN:CD	2.68	0.64
1:D:71:ASP:OD2	1:D:76:LYS:NZ	2.30	0.64
1:D:269:ARG:NH1	1:D:486:ASN:N	2.35	0.64
1:F:512:PHE:HB3	1:F:722:PHE:HB2	1.80	0.64
1:A:766:VAL:HG11	1:A:792:ILE:HD12	1.78	0.64
1:B:269:ARG:NH2	1:B:484:ASN:O	2.31	0.64
1:B:1394:ASP:HB3	1:B:1397:LEU:HB3	1.79	0.64
1:C:249:VAL:HG11	1:D:411:PRO:HG2	1.80	0.64
1:D:273:PRO:HG2	1:D:485:LYS:CG	2.26	0.64
1:D:1097:LYS:HB3	1:D:1209:GLU:HB3	1.79	0.64
1:E:1097:LYS:HB3	1:E:1209:GLU:HB3	1.79	0.64
1:F:435:ARG:HH12	1:F:811:ASP:C	1.97	0.64
1:F:1394:ASP:HB3	1:F:1397:LEU:HB3	1.79	0.64
1:F:766:VAL:HG11	1:F:792:ILE:HD12	1.78	0.64
1:D:1394:ASP:HB3	1:D:1397:LEU:HB3	1.80	0.64
1:A:276:SER:HA	1:A:485:LYS:HB3	1.80	0.64
1:D:512:PHE:HB3	1:D:722:PHE:HB2	1.80	0.64
1:A:55:SER:O	1:A:58:GLN:NE2	2.28	0.64
1:A:265:LEU:O	1:A:448:GLN:NE2	2.31	0.64
1:A:273:PRO:HG2	1:A:485:LYS:CG	2.28	0.64
1:A:331:THR:HG22	1:A:396:LYS:HE2	1.80	0.64
1:D:766:VAL:HG11	1:D:792:ILE:HD12	1.78	0.64
1:A:512:PHE:HB3	1:A:722:PHE:HB2	1.80	0.63
1:C:1394:ASP:HB3	1:C:1397:LEU:HB3	1.79	0.63
1:D:273:PRO:CG	1:D:485:LYS:HA	2.29	0.63
1:E:766:VAL:HG11	1:E:792:ILE:HD12	1.78	0.63
1:E:1220:ALA:O	1:F:1466:THR:OG1	2.16	0.63
1:A:455:SER:N	1:A:482:ASP:OD1	2.30	0.63
1:C:435:ARG:CG	1:D:938:GLY:HA3	2.29	0.63
1:C:512:PHE:HB3	1:C:722:PHE:HB2	1.80	0.63
1:D:268:ASP:OD2	1:D:488:ARG:CZ	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1220:ALA:O	1:D:1466:THR:OG1	2.17	0.63
1:D:276:SER:HB3	1:D:485:LYS:HB3	1.80	0.63
1:E:1050:HIS:HD2	1:E:1051:ALA:N	1.97	0.63
1:D:1050:HIS:HD2	1:D:1051:ALA:N	1.97	0.62
1:B:1295:ALA:HB1	1:B:1320:PRO:HB3	1.81	0.62
1:C:1050:HIS:HD2	1:C:1051:ALA:N	1.97	0.62
1:F:1050:HIS:HD2	1:F:1051:ALA:N	1.97	0.62
1:A:1050:HIS:HD2	1:A:1051:ALA:N	1.97	0.62
1:B:269:ARG:NH1	1:B:276:SER:OG	2.32	0.62
1:B:273:PRO:HG2	1:B:276:SER:HB2	1.82	0.62
1:B:512:PHE:HB3	1:B:722:PHE:HB2	1.80	0.62
1:B:1050:HIS:HD2	1:B:1051:ALA:N	1.97	0.62
1:F:366:ASN:ND2	1:F:424:LYS:O	2.32	0.62
1:C:354:GLN:HG2	1:D:863:THR:OG1	1.99	0.62
1:C:1295:ALA:HB1	1:C:1320:PRO:HB3	1.81	0.62
1:D:276:SER:HB2	1:D:485:LYS:C	2.25	0.62
1:B:1436:GLU:N	1:B:1436:GLU:OE2	2.33	0.62
1:A:1295:ALA:HB1	1:A:1320:PRO:HB3	1.81	0.62
1:B:449:THR:HG21	1:C:859:ILE:H	1.64	0.62
1:F:1436:GLU:OE2	1:F:1436:GLU:N	2.33	0.62
1:A:1436:GLU:OE2	1:A:1436:GLU:N	2.33	0.62
1:E:1436:GLU:OE2	1:E:1436:GLU:N	2.33	0.62
1:C:1066:THR:OG1	1:C:1068:ASP:OD1	2.17	0.61
1:A:71:ASP:OD2	1:A:76:LYS:NZ	2.32	0.61
1:F:284:ASP:OD2	1:F:443:TYR:OH	2.16	0.61
1:A:863:THR:CB	1:F:354:GLN:HG2	2.31	0.61
1:A:257:ASP:OD1	1:A:258:THR:N	2.33	0.61
1:A:863:THR:CG2	1:F:354:GLN:HG2	2.30	0.61
1:C:1436:GLU:OE2	1:C:1436:GLU:N	2.33	0.61
1:C:87:VAL:O	1:C:231:TYR:OH	2.19	0.61
1:A:886:PHE:HA	1:B:1301:THR:HG21	1.83	0.61
1:D:1295:ALA:HB1	1:D:1320:PRO:HB3	1.81	0.61
1:E:886:PHE:HA	1:F:1301:THR:HG21	1.82	0.61
1:E:1476:ASP:OD1	1:E:1477:GLY:N	2.31	0.61
1:A:1066:THR:OG1	1:A:1068:ASP:OD1	2.17	0.61
1:B:1066:THR:OG1	1:B:1068:ASP:OD1	2.17	0.61
1:C:1476:ASP:OD1	1:C:1477:GLY:N	2.31	0.61
1:D:1122:ASP:OD1	1:D:1126:ASN:ND2	2.34	0.61
1:F:1295:ALA:HB1	1:F:1320:PRO:HB3	1.81	0.61
1:C:126:VAL:HG22	1:C:164:GLN:HA	1.83	0.60
1:D:1436:GLU:N	1:D:1436:GLU:OE2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1481:SER:HB3	1:D:1491:VAL:HG12	1.83	0.60
1:E:449:THR:HG21	1:F:859:ILE:H	1.64	0.60
1:E:115:ALA:HA	1:E:330:LEU:HD13	1.83	0.60
1:E:1066:THR:OG1	1:E:1068:ASP:OD1	2.17	0.60
1:D:87:VAL:O	1:D:231:TYR:OH	2.19	0.60
1:E:1122:ASP:OD1	1:E:1126:ASN:ND2	2.34	0.60
1:B:886:PHE:HA	1:C:1301:THR:HG21	1.83	0.60
1:C:1122:ASP:OD1	1:C:1126:ASN:ND2	2.34	0.60
1:F:126:VAL:HG22	1:F:164:GLN:HA	1.82	0.60
1:E:1295:ALA:HB1	1:E:1320:PRO:HB3	1.81	0.60
1:A:90:MET:HB3	1:A:98:TRP:HB3	1.82	0.60
1:A:284:ASP:OD1	1:A:286:TRP:N	2.33	0.60
1:A:1466:THR:OG1	1:F:1220:ALA:O	2.18	0.60
1:B:1481:SER:HB3	1:B:1491:VAL:HG12	1.83	0.60
1:E:1481:SER:HB3	1:E:1491:VAL:HG12	1.83	0.60
1:C:354:GLN:HG2	1:D:863:THR:CG2	2.32	0.60
1:C:240:VAL:HG22	1:C:253:THR:HG22	1.82	0.60
1:A:1122:ASP:OD1	1:A:1126:ASN:ND2	2.34	0.60
1:A:858:LEU:HD21	1:F:447:PRO:HB2	1.84	0.60
1:C:1481:SER:HB3	1:C:1491:VAL:HG12	1.82	0.60
1:F:144:THR:HG23	1:F:146:GLY:H	1.67	0.59
1:A:273:PRO:CB	1:A:485:LYS:HG2	2.31	0.59
1:C:303:THR:HG23	1:C:304:LYS:HG3	1.84	0.59
1:D:886:PHE:HA	1:E:1301:THR:HG21	1.83	0.59
1:F:1122:ASP:OD1	1:F:1126:ASN:ND2	2.34	0.59
1:D:273:PRO:CB	1:D:485:LYS:HG2	2.32	0.59
1:D:279:HIS:HD1	1:D:425:SER:HB2	1.67	0.59
1:B:1220:ALA:O	1:C:1466:THR:OG1	2.16	0.59
1:C:886:PHE:HA	1:D:1301:THR:HG21	1.84	0.59
1:F:1481:SER:HB3	1:F:1491:VAL:HG12	1.82	0.59
1:B:1122:ASP:OD1	1:B:1126:ASN:ND2	2.34	0.59
1:A:1481:SER:HB3	1:A:1491:VAL:HG12	1.83	0.59
1:E:273:PRO:HG2	1:E:276:SER:HB2	1.85	0.59
1:F:1476:ASP:OD1	1:F:1477:GLY:N	2.31	0.59
1:E:364:GLN:HE21	1:E:428:LYS:HB2	1.68	0.59
1:C:625:PHE:HE1	1:C:627:TYR:HB3	1.69	0.58
1:E:74:GLU:O	1:E:211:GLN:NE2	2.36	0.58
1:B:1476:ASP:OD1	1:B:1477:GLY:N	2.31	0.58
1:D:625:PHE:HE1	1:D:627:TYR:HB3	1.69	0.58
1:F:569:THR:HB	1:F:582:ALA:HB3	1.86	0.58
1:A:273:PRO:HG2	1:A:485:LYS:CA	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:PRO:HG3	1:D:339:LEU:HD22	1.85	0.58
1:A:569:THR:HB	1:A:582:ALA:HB3	1.85	0.58
1:A:937:THR:O	1:F:435:ARG:NE	2.37	0.58
1:A:1301:THR:HG21	1:F:886:PHE:HA	1.84	0.58
1:B:625:PHE:HE1	1:B:627:TYR:HB3	1.69	0.58
1:F:257:ASP:OD1	1:F:258:THR:N	2.36	0.58
1:D:257:ASP:OD1	1:D:258:THR:N	2.37	0.58
1:F:89:ARG:NH1	1:F:140:SER:O	2.36	0.58
1:E:569:THR:HB	1:E:582:ALA:HB3	1.85	0.58
1:F:109:GLN:NE2	1:F:171:GLY:O	2.31	0.58
1:A:1308:ASP:OD1	1:A:1308:ASP:N	2.37	0.58
1:A:1476:ASP:OD1	1:A:1477:GLY:N	2.31	0.57
1:D:569:THR:HB	1:D:582:ALA:HB3	1.85	0.57
1:E:625:PHE:HE1	1:E:627:TYR:HB3	1.69	0.57
1:F:87:VAL:O	1:F:231:TYR:OH	2.21	0.57
1:F:278:VAL:HB	1:F:427:LEU:HB2	1.86	0.57
1:E:1206:LEU:N	1:E:1227:ALA:O	2.32	0.57
1:D:279:HIS:ND1	1:D:425:SER:HB2	2.19	0.57
1:A:625:PHE:HE1	1:A:627:TYR:HB3	1.68	0.57
1:D:260:ASP:HA	1:D:344:ASN:HD22	1.70	0.57
1:A:80:ASP:OD2	1:A:244:ASN:ND2	2.35	0.57
1:E:624:PHE:HB2	1:E:723:PHE:HB2	1.87	0.57
1:B:214:LEU:HD22	1:B:224:ASN:HB3	1.85	0.57
1:C:1308:ASP:N	1:C:1308:ASP:OD1	2.37	0.57
1:B:569:THR:HB	1:B:582:ALA:HB3	1.85	0.57
1:D:624:PHE:HB2	1:D:723:PHE:HB2	1.87	0.57
1:D:995:ASP:OD2	1:D:997:SER:N	2.38	0.57
1:A:279:HIS:HD1	1:A:425:SER:HB2	1.69	0.57
1:C:995:ASP:OD2	1:C:997:SER:N	2.38	0.57
1:D:304:LYS:NZ	1:D:350:ASP:OD2	2.37	0.57
1:F:1308:ASP:OD1	1:F:1308:ASP:N	2.37	0.57
1:B:236:THR:HG21	1:C:489:ALA:HB1	1.86	0.56
1:C:569:THR:HB	1:C:582:ALA:HB3	1.85	0.56
1:A:276:SER:HB3	1:A:485:LYS:CA	2.35	0.56
1:A:524:PHE:HB2	1:A:566:ILE:HB	1.88	0.56
1:E:995:ASP:OD2	1:E:997:SER:N	2.38	0.56
1:A:442:ASP:HA	1:A:447:PRO:HA	1.86	0.56
1:C:524:PHE:HB2	1:C:566:ILE:HB	1.88	0.56
1:D:442:ASP:HA	1:D:447:PRO:HA	1.86	0.56
1:F:624:PHE:HB2	1:F:723:PHE:HB2	1.87	0.56
1:F:995:ASP:OD2	1:F:997:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:PRO:HG2	1:F:276:SER:HB2	1.88	0.56
1:B:524:PHE:HB2	1:B:566:ILE:HB	1.88	0.56
1:B:624:PHE:HB2	1:B:723:PHE:HB2	1.87	0.56
1:C:144:THR:HG23	1:C:146:GLY:H	1.68	0.56
1:D:524:PHE:HB2	1:D:566:ILE:HB	1.88	0.56
1:F:524:PHE:HB2	1:F:566:ILE:HB	1.88	0.56
1:B:1206:LEU:N	1:B:1227:ALA:O	2.32	0.56
1:F:625:PHE:HE1	1:F:627:TYR:HB3	1.68	0.56
1:B:995:ASP:OD2	1:B:997:SER:N	2.38	0.56
1:C:105:ARG:NH2	1:C:232:GLU:OE2	2.38	0.56
1:D:1066:THR:OG1	1:D:1068:ASP:OD1	2.17	0.56
1:A:995:ASP:OD2	1:A:997:SER:N	2.38	0.56
1:A:1206:LEU:N	1:A:1227:ALA:O	2.32	0.56
1:D:1206:LEU:N	1:D:1227:ALA:O	2.32	0.56
1:E:195:ARG:NH2	1:E:295:ASP:OD1	2.36	0.56
1:F:837:TYR:O	1:F:1010:ARG:N	2.39	0.56
1:F:1206:LEU:N	1:F:1227:ALA:O	2.32	0.56
1:C:624:PHE:HB2	1:C:723:PHE:HB2	1.87	0.55
1:E:524:PHE:HB2	1:E:566:ILE:HB	1.88	0.55
1:F:45:ALA:HB2	1:F:60:ILE:HD12	1.87	0.55
1:B:837:TYR:O	1:B:1010:ARG:N	2.40	0.55
1:C:89:ARG:NH1	1:C:140:SER:O	2.39	0.55
1:F:1066:THR:OG1	1:F:1068:ASP:OD1	2.17	0.55
1:B:83:VAL:HG12	1:B:241:VAL:HG22	1.89	0.55
1:E:302:ASN:HB2	1:E:402:ILE:H	1.71	0.55
1:E:1308:ASP:N	1:E:1308:ASP:OD1	2.37	0.55
1:B:275:VAL:CG1	1:B:485:LYS:CD	2.76	0.55
1:B:313:ASP:OD1	1:B:314:THR:N	2.39	0.55
1:B:1308:ASP:OD1	1:B:1308:ASP:N	2.37	0.55
1:D:1308:ASP:OD1	1:D:1308:ASP:N	2.37	0.55
1:A:624:PHE:HB2	1:A:723:PHE:HB2	1.87	0.55
1:B:236:THR:OG1	1:C:489:ALA:CB	2.55	0.55
1:E:313:ASP:OD1	1:E:314:THR:N	2.40	0.55
1:A:279:HIS:ND1	1:A:425:SER:HB2	2.21	0.55
1:C:435:ARG:NE	1:D:937:THR:O	2.40	0.55
1:D:837:TYR:O	1:D:1010:ARG:N	2.39	0.55
1:A:150:PRO:HB2	1:A:189:GLY:HA2	1.89	0.54
1:A:837:TYR:O	1:A:1010:ARG:N	2.40	0.54
1:B:195:ARG:NH2	1:B:295:ASP:OD1	2.35	0.54
1:F:278:VAL:O	1:F:425:SER:OG	2.25	0.54
1:B:278:VAL:O	1:B:425:SER:OG	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:965:SER:OG	1:F:966:ASP:OD1	2.26	0.54
1:C:965:SER:OG	1:C:966:ASP:OD1	2.26	0.54
1:E:277:GLN:HE22	1:E:364:GLN:HE22	1.56	0.54
1:B:117:THR:HG22	1:B:330:LEU:HD21	1.89	0.54
1:B:449:THR:HG23	1:C:858:LEU:HG	1.86	0.54
1:D:360:VAL:HB	1:D:439:ALA:HB2	1.90	0.54
1:E:105:ARG:NH1	1:E:106:ASP:OD1	2.40	0.54
1:E:1096:LEU:HB3	1:E:1112:ALA:HB3	1.89	0.54
1:A:938:GLY:HA3	1:F:435:ARG:CG	2.34	0.54
1:C:1096:LEU:HB3	1:C:1112:ALA:HB3	1.89	0.54
1:C:837:TYR:O	1:C:1010:ARG:N	2.40	0.54
1:D:1476:ASP:OD1	1:D:1477:GLY:N	2.31	0.54
1:A:965:SER:OG	1:A:966:ASP:OD1	2.26	0.54
1:C:966:ASP:OD1	1:C:966:ASP:N	2.41	0.54
1:E:965:SER:OG	1:E:966:ASP:OD1	2.26	0.54
1:C:354:GLN:HG2	1:D:863:THR:CB	2.38	0.54
1:C:435:ARG:NH1	1:C:812:GLY:C	2.64	0.54
1:D:150:PRO:HB2	1:D:189:GLY:HA2	1.89	0.54
1:D:419:TYR:HA	1:D:425:SER:HA	1.90	0.54
1:A:1096:LEU:HB3	1:A:1112:ALA:HB3	1.89	0.53
1:B:1096:LEU:HB3	1:B:1112:ALA:HB3	1.89	0.53
1:C:45:ALA:HB2	1:C:60:ILE:HD12	1.89	0.53
1:E:214:LEU:HD22	1:E:224:ASN:HB3	1.89	0.53
1:E:1050:HIS:CD2	1:E:1051:ALA:N	2.77	0.53
1:F:1044:ARG:HA	1:F:1169:HIS:HB3	1.91	0.53
1:A:1044:ARG:HA	1:A:1169:HIS:HB3	1.91	0.53
1:B:320:ASP:OD1	1:B:321:GLU:N	2.42	0.53
1:B:500:VAL:O	1:B:578:ARG:NH2	2.40	0.53
1:C:144:THR:HA	1:C:231:TYR:HE1	1.73	0.53
1:C:1206:LEU:N	1:C:1227:ALA:O	2.32	0.53
1:D:642:LEU:HD11	1:D:703:ALA:HB2	1.91	0.53
1:F:1096:LEU:HB3	1:F:1112:ALA:HB3	1.89	0.53
1:A:273:PRO:HB2	1:A:485:LYS:HZ3	1.72	0.53
1:C:447:PRO:HB2	1:D:858:LEU:HD21	1.90	0.53
1:C:642:LEU:HD11	1:C:703:ALA:HB2	1.91	0.53
1:D:966:ASP:OD1	1:D:966:ASP:N	2.41	0.53
1:E:83:VAL:HG12	1:E:241:VAL:HG22	1.90	0.53
1:E:837:TYR:O	1:E:1010:ARG:N	2.39	0.53
1:E:1296:PHE:HB3	1:E:1317:ILE:HG23	1.91	0.53
1:A:1098:ILE:HD11	1:A:1206:LEU:HD11	1.91	0.53
1:B:642:LEU:HD11	1:B:703:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1098:ILE:HD11	1:C:1206:LEU:HD11	1.91	0.53
1:D:269:ARG:HH12	1:D:486:ASN:N	2.06	0.53
1:D:769:ILE:HD11	1:D:892:LEU:HB2	1.91	0.53
1:D:1050:HIS:CD2	1:D:1051:ALA:N	2.77	0.53
1:D:1096:LEU:HB3	1:D:1112:ALA:HB3	1.89	0.53
1:A:268:ASP:CG	1:A:488:ARG:HH12	2.17	0.53
1:A:769:ILE:HD11	1:A:892:LEU:HB2	1.91	0.53
1:C:109:GLN:NE2	1:C:171:GLY:O	2.36	0.53
1:C:1478:LEU:HB3	1:C:1494:ALA:HB3	1.91	0.53
1:A:642:LEU:HD11	1:A:703:ALA:HB2	1.91	0.53
1:B:596:ALA:HB3	1:B:704:MET:HB2	1.91	0.53
1:D:815:THR:OG1	1:E:1083:ASN:OD1	2.27	0.53
1:E:1044:ARG:HA	1:E:1169:HIS:HB3	1.91	0.53
1:A:269:ARG:NH1	1:A:485:LYS:CA	2.68	0.53
1:B:236:THR:CB	1:C:489:ALA:HA	2.39	0.53
1:E:236:THR:HG21	1:F:489:ALA:HB1	1.91	0.53
1:E:435:ARG:CZ	1:E:811:ASP:O	2.57	0.53
1:E:500:VAL:O	1:E:578:ARG:NH2	2.40	0.53
1:F:666:LEU:HD21	1:F:669:SER:HB2	1.91	0.53
1:F:1050:HIS:CD2	1:F:1051:ALA:N	2.77	0.53
1:A:419:TYR:HA	1:A:425:SER:HA	1.91	0.52
1:A:645:THR:HA	1:A:698:VAL:HA	1.91	0.52
1:A:768:GLN:NE2	1:A:991:VAL:HG12	2.23	0.52
1:A:1296:PHE:HB3	1:A:1317:ILE:HG23	1.91	0.52
1:B:1044:ARG:HA	1:B:1169:HIS:HB3	1.91	0.52
1:C:645:THR:HA	1:C:698:VAL:HA	1.92	0.52
1:D:109:GLN:NE2	1:D:171:GLY:O	2.38	0.52
1:D:273:PRO:HG2	1:D:485:LYS:CA	2.39	0.52
1:E:596:ALA:HB3	1:E:704:MET:HB2	1.91	0.52
1:F:596:ALA:HB3	1:F:704:MET:HB2	1.91	0.52
1:B:1478:LEU:HB3	1:B:1494:ALA:HB3	1.91	0.52
1:C:389:GLY:HA2	1:C:403:PRO:HG3	1.91	0.52
1:C:1050:HIS:CD2	1:C:1051:ALA:N	2.77	0.52
1:E:642:LEU:HD11	1:E:703:ALA:HB2	1.91	0.52
1:B:302:ASN:HB2	1:B:402:ILE:H	1.73	0.52
1:B:769:ILE:HD11	1:B:892:LEU:HB2	1.91	0.52
1:B:1296:PHE:HB3	1:B:1317:ILE:HG23	1.91	0.52
1:C:1296:PHE:HB3	1:C:1317:ILE:HG23	1.91	0.52
1:D:965:SER:OG	1:D:966:ASP:OD1	2.26	0.52
1:D:1478:LEU:HB3	1:D:1494:ALA:HB3	1.91	0.52
1:E:311:ASN:ND2	1:E:333:ARG:HD3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1296:PHE:HB3	1:F:1317:ILE:HG23	1.91	0.52
1:A:294:GLU:OE2	1:F:242:GLN:NE2	2.42	0.52
1:B:645:THR:HA	1:B:698:VAL:HA	1.92	0.52
1:E:769:ILE:HD11	1:E:892:LEU:HB2	1.91	0.52
1:E:966:ASP:OD1	1:E:966:ASP:N	2.41	0.52
1:A:1440:THR:N	1:A:1470:LEU:O	2.40	0.52
1:C:769:ILE:HD11	1:C:892:LEU:HB2	1.91	0.52
1:D:207:VAL:HG13	1:D:211:GLN:HG2	1.90	0.52
1:F:642:LEU:HD11	1:F:703:ALA:HB2	1.91	0.52
1:A:1050:HIS:CD2	1:A:1051:ALA:N	2.77	0.52
1:F:1478:LEU:HB3	1:F:1494:ALA:HB3	1.91	0.52
1:B:768:GLN:NE2	1:B:991:VAL:HG12	2.23	0.52
1:B:1050:HIS:CD2	1:B:1051:ALA:N	2.77	0.52
1:C:82:THR:HG22	1:C:87:VAL:HA	1.91	0.52
1:E:961:TRP:CD1	1:E:981:THR:HG22	2.45	0.52
1:E:1478:LEU:HB3	1:E:1494:ALA:HB3	1.91	0.52
1:F:1098:ILE:HD11	1:F:1206:LEU:HD11	1.91	0.52
1:A:596:ALA:HB3	1:A:704:MET:HB2	1.91	0.52
1:B:1098:ILE:HD11	1:B:1206:LEU:HD11	1.91	0.52
1:C:596:ALA:HB3	1:C:704:MET:HB2	1.91	0.52
1:C:961:TRP:CD1	1:C:981:THR:HG22	2.45	0.52
1:C:1044:ARG:HA	1:C:1169:HIS:HB3	1.91	0.52
1:D:645:THR:HA	1:D:698:VAL:HA	1.92	0.52
1:D:1044:ARG:HA	1:D:1169:HIS:HB3	1.91	0.52
1:F:768:GLN:NE2	1:F:991:VAL:HG12	2.23	0.52
1:A:72:THR:OG1	1:F:74:GLU:OE1	2.26	0.52
1:A:267:LEU:HD21	1:A:450:ILE:HG12	1.91	0.52
1:A:454:PHE:HA	1:A:482:ASP:OD1	2.10	0.52
1:A:966:ASP:OD1	1:A:966:ASP:N	2.41	0.52
1:A:1467:ASP:OD1	1:A:1467:ASP:N	2.43	0.52
1:B:815:THR:OG1	1:C:1083:ASN:OD1	2.28	0.52
1:B:1050:HIS:HD2	1:B:1051:ALA:H	1.58	0.52
1:B:1235:VAL:HG13	1:B:1254:ILE:HG23	1.92	0.52
1:D:596:ALA:HB3	1:D:704:MET:HB2	1.91	0.52
1:D:1050:HIS:HD2	1:D:1051:ALA:H	1.58	0.52
1:D:1296:PHE:HB3	1:D:1317:ILE:HG23	1.91	0.52
1:E:1174:THR:OG1	1:E:1187:ARG:NH1	2.43	0.52
1:F:769:ILE:HD11	1:F:892:LEU:HB2	1.91	0.52
1:C:40:ASN:OD1	1:C:245:LYS:NZ	2.40	0.52
1:C:815:THR:OG1	1:D:1083:ASN:OD1	2.28	0.52
1:D:666:LEU:HD21	1:D:669:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:645:THR:HA	1:F:698:VAL:HA	1.91	0.52
1:F:961:TRP:CD1	1:F:981:THR:HG22	2.45	0.52
1:F:966:ASP:OD1	1:F:966:ASP:N	2.41	0.52
1:A:273:PRO:HB2	1:A:485:LYS:HG2	1.91	0.51
1:A:666:LEU:HD21	1:A:669:SER:HB2	1.91	0.51
1:A:815:THR:OG1	1:B:1083:ASN:OD1	2.28	0.51
1:B:1174:THR:OG1	1:B:1187:ARG:NH1	2.43	0.51
1:F:466:ASP:OD2	1:F:466:ASP:N	2.43	0.51
1:A:961:TRP:CD1	1:A:981:THR:HG22	2.45	0.51
1:B:64:VAL:HB	1:B:98:TRP:HB2	1.92	0.51
1:B:517:GLY:HA3	1:B:603:ALA:HB2	1.93	0.51
1:D:961:TRP:CD1	1:D:981:THR:HG22	2.45	0.51
1:D:1098:ILE:HD11	1:D:1206:LEU:HD11	1.91	0.51
1:E:349:LEU:HD13	1:E:441:LEU:HD13	1.91	0.51
1:E:645:THR:HA	1:E:698:VAL:HA	1.91	0.51
1:E:666:LEU:HD21	1:E:669:SER:HB2	1.91	0.51
1:A:1174:THR:OG1	1:A:1187:ARG:NH1	2.43	0.51
1:C:1174:THR:OG1	1:C:1187:ARG:NH1	2.43	0.51
1:F:517:GLY:HA3	1:F:603:ALA:HB2	1.93	0.51
1:F:1467:ASP:OD1	1:F:1467:ASP:N	2.43	0.51
1:A:517:GLY:HA3	1:A:603:ALA:HB2	1.93	0.51
1:B:1467:ASP:OD1	1:B:1467:ASP:N	2.43	0.51
1:D:276:SER:HB3	1:D:485:LYS:CB	2.39	0.51
1:F:1235:VAL:HG13	1:F:1254:ILE:HG23	1.92	0.51
1:B:961:TRP:CD1	1:B:981:THR:HG22	2.45	0.51
1:B:966:ASP:N	1:B:966:ASP:OD1	2.41	0.51
1:C:768:GLN:NE2	1:C:991:VAL:HG12	2.23	0.51
1:D:500:VAL:O	1:D:578:ARG:NH2	2.40	0.51
1:E:815:THR:OG1	1:F:1083:ASN:OD1	2.27	0.51
1:A:1478:LEU:HB3	1:A:1494:ALA:HB3	1.91	0.51
1:E:435:ARG:NH1	1:F:938:GLY:O	2.43	0.51
1:F:1174:THR:OG1	1:F:1187:ARG:NH1	2.43	0.51
1:C:284:ASP:HB3	1:C:287:LEU:HD12	1.93	0.51
1:C:666:LEU:HD21	1:C:669:SER:HB2	1.91	0.51
1:E:1071:ILE:HG12	1:E:1155:ILE:HD11	1.93	0.51
1:E:1098:ILE:HD11	1:E:1206:LEU:HD11	1.91	0.51
1:F:284:ASP:HB3	1:F:287:LEU:HD12	1.92	0.51
1:B:1071:ILE:HG12	1:B:1155:ILE:HD11	1.93	0.51
1:D:1219:ASP:OD2	1:E:1422:LYS:NZ	2.34	0.51
1:E:315:PHE:CD2	1:E:329:ALA:HB1	2.46	0.51
1:B:965:SER:OG	1:B:966:ASP:OD1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ARG:HD3	1:D:937:THR:O	2.11	0.51
1:E:768:GLN:NE2	1:E:991:VAL:HG12	2.23	0.51
1:F:40:ASN:OD1	1:F:245:LYS:NZ	2.40	0.51
1:F:1050:HIS:HD2	1:F:1051:ALA:H	1.58	0.51
1:A:260:ASP:HA	1:A:344:ASN:HD22	1.77	0.50
1:A:269:ARG:NH1	1:A:486:ASN:HA	2.26	0.50
1:B:666:LEU:HD21	1:B:669:SER:HB2	1.91	0.50
1:C:517:GLY:HA3	1:C:603:ALA:HB2	1.93	0.50
1:C:1467:ASP:N	1:C:1467:ASP:OD1	2.43	0.50
1:D:768:GLN:NE2	1:D:991:VAL:HG12	2.23	0.50
1:F:1071:ILE:HG12	1:F:1155:ILE:HD11	1.93	0.50
1:A:1235:VAL:HG13	1:A:1254:ILE:HG23	1.92	0.50
1:C:121:GLY:HA3	1:C:330:LEU:HD12	1.92	0.50
1:E:236:THR:CB	1:F:489:ALA:HA	2.42	0.50
1:E:517:GLY:HA3	1:E:603:ALA:HB2	1.93	0.50
1:E:1235:VAL:HG13	1:E:1254:ILE:HG23	1.92	0.50
1:E:1467:ASP:N	1:E:1467:ASP:OD1	2.43	0.50
1:B:105:ARG:NH1	1:B:232:GLU:OE2	2.42	0.50
1:C:57:PRO:HG3	1:C:339:LEU:HD22	1.93	0.50
1:C:115:ALA:HA	1:C:330:LEU:HD13	1.93	0.50
1:C:1235:VAL:HG13	1:C:1254:ILE:HG23	1.92	0.50
1:D:1235:VAL:HG13	1:D:1254:ILE:HG23	1.92	0.50
1:D:1467:ASP:OD1	1:D:1467:ASP:N	2.43	0.50
1:A:360:VAL:HB	1:A:439:ALA:HB2	1.94	0.50
1:C:354:GLN:NE2	1:D:863:THR:HG21	2.26	0.50
1:D:1174:THR:OG1	1:D:1187:ARG:NH1	2.43	0.50
1:E:197:ALA:HB1	1:E:225:TRP:NE1	2.27	0.50
1:E:236:THR:OG1	1:F:489:ALA:CB	2.58	0.50
1:F:82:THR:HG22	1:F:87:VAL:HA	1.94	0.50
1:A:276:SER:CB	1:A:485:LYS:CA	2.90	0.50
1:A:277:GLN:OE1	1:A:364:GLN:NE2	2.43	0.50
1:A:1050:HIS:HD2	1:A:1051:ALA:H	1.58	0.50
1:C:918:ASP:HB3	1:C:923:GLU:HG3	1.94	0.50
1:C:1050:HIS:HD2	1:C:1051:ALA:H	1.58	0.50
1:C:1071:ILE:HG12	1:C:1155:ILE:HD11	1.93	0.50
1:D:517:GLY:HA3	1:D:603:ALA:HB2	1.93	0.50
1:F:121:GLY:HA3	1:F:330:LEU:HD12	1.94	0.50
1:A:500:VAL:O	1:A:578:ARG:NH2	2.40	0.50
1:D:277:GLN:OE1	1:D:364:GLN:NE2	2.45	0.50
1:B:349:LEU:HD13	1:B:441:LEU:HD13	1.94	0.50
1:E:1050:HIS:HD2	1:E:1051:ALA:H	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:PRO:HG3	1:F:339:LEU:HD22	1.94	0.50
1:D:1071:ILE:HG12	1:D:1155:ILE:HD11	1.93	0.50
1:D:1440:THR:N	1:D:1470:LEU:O	2.40	0.50
1:E:1440:THR:N	1:E:1470:LEU:O	2.40	0.50
1:A:937:THR:O	1:F:435:ARG:HD3	2.11	0.49
1:C:1298:PRO:HB2	1:C:1301:THR:HA	1.94	0.49
1:D:513:THR:OG1	1:D:514:ILE:N	2.45	0.49
1:F:918:ASP:HB3	1:F:923:GLU:HG3	1.94	0.49
1:A:269:ARG:CZ	1:A:485:LYS:C	2.72	0.49
1:A:642:LEU:HD22	1:A:651:TRP:CZ2	2.47	0.49
1:A:1071:ILE:HG12	1:A:1155:ILE:HD11	1.93	0.49
1:B:642:LEU:HD22	1:B:651:TRP:CZ2	2.47	0.49
1:C:1440:THR:N	1:C:1470:LEU:O	2.40	0.49
1:D:642:LEU:HD22	1:D:651:TRP:CZ2	2.47	0.49
1:D:1339:THR:OG1	1:D:1341:TRP:NE1	2.46	0.49
1:E:513:THR:OG1	1:E:514:ILE:N	2.45	0.49
1:E:918:ASP:HB3	1:E:923:GLU:HG3	1.94	0.49
1:F:513:THR:OG1	1:F:514:ILE:N	2.45	0.49
1:A:373:GLN:NE2	1:A:375:ASN:O	2.42	0.49
1:A:1298:PRO:HB2	1:A:1301:THR:HA	1.94	0.49
1:A:1339:THR:OG1	1:A:1341:TRP:NE1	2.46	0.49
1:D:466:ASP:OD2	1:D:466:ASP:N	2.44	0.49
1:D:80:ASP:HB3	1:D:244:ASN:HB2	1.94	0.49
1:E:466:ASP:OD2	1:E:466:ASP:N	2.44	0.49
1:B:1298:PRO:HB2	1:B:1301:THR:HA	1.94	0.49
1:C:513:THR:OG1	1:C:514:ILE:N	2.45	0.49
1:D:1298:PRO:HB2	1:D:1301:THR:HA	1.94	0.49
1:F:157:THR:H	1:F:161:ASN:HD22	1.60	0.49
1:F:642:LEU:HD22	1:F:651:TRP:CZ2	2.47	0.49
1:F:1339:THR:OG1	1:F:1341:TRP:NE1	2.46	0.49
1:C:207:VAL:HG13	1:C:211:GLN:HG2	1.95	0.49
1:C:1270:LEU:HD12	1:C:1315:ILE:HD13	1.95	0.49
1:D:312:VAL:HG11	1:D:348:THR:HG22	1.94	0.49
1:D:918:ASP:HB3	1:D:923:GLU:HG3	1.94	0.49
1:E:1043:GLY:O	1:E:1348:TYR:OH	2.31	0.49
1:F:1270:LEU:HD12	1:F:1315:ILE:HD13	1.95	0.49
1:A:980:THR:HG22	1:A:982:THR:H	1.78	0.49
1:A:995:ASP:N	1:A:999:GLU:O	2.45	0.49
1:B:315:PHE:CD2	1:B:329:ALA:HB1	2.48	0.49
1:C:893:LEU:HD23	1:C:941:LEU:HD21	1.95	0.49
1:A:513:THR:OG1	1:A:514:ILE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:HA	1:B:1397:LEU:HD13	1.94	0.49
1:B:980:THR:HG22	1:B:982:THR:H	1.78	0.49
1:B:1339:THR:OG1	1:B:1341:TRP:NE1	2.46	0.49
1:C:1339:THR:OG1	1:C:1341:TRP:NE1	2.46	0.49
1:E:278:VAL:O	1:E:425:SER:OG	2.22	0.49
1:E:642:LEU:HD22	1:E:651:TRP:CZ2	2.47	0.49
1:E:893:LEU:HD23	1:E:941:LEU:HD21	1.95	0.49
1:F:980:THR:HG22	1:F:982:THR:H	1.78	0.49
1:A:837:TYR:CZ	1:A:843:VAL:HG23	2.48	0.49
1:A:1043:GLY:O	1:A:1348:TYR:OH	2.31	0.49
1:A:1270:LEU:HD12	1:A:1315:ILE:HD13	1.95	0.49
1:B:918:ASP:HB3	1:B:923:GLU:HG3	1.94	0.49
1:A:1083:ASN:OD1	1:F:815:THR:OG1	2.28	0.48
1:D:893:LEU:HD23	1:D:941:LEU:HD21	1.95	0.48
1:D:1270:LEU:HD12	1:D:1315:ILE:HD13	1.95	0.48
1:E:1339:THR:OG1	1:E:1341:TRP:NE1	2.46	0.48
1:A:67:SER:HA	1:A:70:ASN:ND2	2.29	0.48
1:A:918:ASP:HB3	1:A:923:GLU:HG3	1.94	0.48
1:B:75:ALA:HA	1:B:211:GLN:HE22	1.78	0.48
1:C:642:LEU:HD22	1:C:651:TRP:CZ2	2.47	0.48
1:C:980:THR:HG22	1:C:982:THR:H	1.78	0.48
1:A:109:GLN:NE2	1:A:171:GLY:O	2.38	0.48
1:A:278:VAL:O	1:A:425:SER:OG	2.24	0.48
1:B:513:THR:OG1	1:B:514:ILE:N	2.45	0.48
1:B:837:TYR:CZ	1:B:843:VAL:HG23	2.48	0.48
1:B:893:LEU:HD23	1:B:941:LEU:HD21	1.95	0.48
1:B:1270:LEU:HD12	1:B:1315:ILE:HD13	1.95	0.48
1:C:1117:ARG:HG2	1:C:1135:SER:HB3	1.95	0.48
1:E:1117:ARG:HG2	1:E:1135:SER:HB3	1.95	0.48
1:E:1270:LEU:HD12	1:E:1315:ILE:HD13	1.95	0.48
1:E:1298:PRO:HB2	1:E:1301:THR:HA	1.94	0.48
1:F:1298:PRO:HB2	1:F:1301:THR:HA	1.94	0.48
1:A:273:PRO:HG2	1:A:485:LYS:CB	2.43	0.48
1:A:893:LEU:HD23	1:A:941:LEU:HD21	1.95	0.48
1:B:164:GLN:O	1:B:164:GLN:NE2	2.46	0.48
1:B:274:ARG:HD2	1:B:431:ASP:O	2.14	0.48
1:B:1043:GLY:O	1:B:1348:TYR:OH	2.31	0.48
1:E:837:TYR:CZ	1:E:843:VAL:HG23	2.48	0.48
1:E:274:ARG:HG2	1:E:454:PHE:HE1	1.78	0.48
1:B:833:ASN:OD1	1:B:833:ASN:N	2.46	0.48
1:B:1275:TRP:HB2	1:B:1284:MET:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ARG:CZ	1:D:937:THR:O	2.62	0.48
1:C:837:TYR:CZ	1:C:843:VAL:HG23	2.48	0.48
1:D:273:PRO:HG2	1:D:485:LYS:CB	2.44	0.48
1:D:1407:ASP:HA	1:D:1483:GLU:OE2	2.14	0.48
1:E:279:HIS:CE1	1:E:488:ARG:NE	2.62	0.48
1:F:837:TYR:CZ	1:F:843:VAL:HG23	2.48	0.48
1:F:893:LEU:HD23	1:F:941:LEU:HD21	1.95	0.48
1:A:276:SER:HB3	1:A:485:LYS:HA	1.96	0.48
1:C:1275:TRP:HB2	1:C:1284:MET:HG2	1.96	0.48
1:D:273:PRO:HB2	1:D:485:LYS:HZ3	1.77	0.48
1:D:837:TYR:CZ	1:D:843:VAL:HG23	2.48	0.48
1:E:268:ASP:CG	1:E:487:SER:OG	2.57	0.48
1:E:1407:ASP:HA	1:E:1483:GLU:OE2	2.14	0.48
1:F:1407:ASP:HA	1:F:1483:GLU:OE2	2.14	0.48
1:A:512:PHE:HA	1:A:516:GLU:HG3	1.96	0.48
1:C:1407:ASP:HA	1:C:1483:GLU:OE2	2.14	0.48
1:D:343:ASP:HB2	1:D:445:GLU:CD	2.39	0.48
1:D:980:THR:HG22	1:D:982:THR:H	1.78	0.48
1:D:1117:ARG:HG2	1:D:1135:SER:HB3	1.95	0.48
1:E:980:THR:HG22	1:E:982:THR:H	1.78	0.48
1:F:207:VAL:HG13	1:F:211:GLN:HG2	1.96	0.48
1:F:1275:TRP:HB2	1:F:1284:MET:HG2	1.96	0.48
1:A:1407:ASP:HA	1:A:1483:GLU:OE2	2.14	0.48
1:B:1440:THR:N	1:B:1470:LEU:O	2.40	0.48
1:C:512:PHE:HA	1:C:516:GLU:HG3	1.96	0.48
1:D:66:ASP:HB3	1:D:69:ILE:HG12	1.96	0.48
1:A:863:THR:CG2	1:F:354:GLN:CG	2.89	0.47
1:A:1275:TRP:HB2	1:A:1284:MET:HG2	1.96	0.47
1:B:512:PHE:HA	1:B:516:GLU:HG3	1.96	0.47
1:B:751:GLY:H	1:B:754:THR:HG1	1.62	0.47
1:B:1407:ASP:HA	1:B:1483:GLU:OE2	2.14	0.47
1:C:466:ASP:N	1:C:466:ASP:OD2	2.43	0.47
1:C:500:VAL:O	1:C:578:ARG:NH2	2.40	0.47
1:D:984:LEU:HA	1:E:1397:LEU:HD13	1.94	0.47
1:D:995:ASP:N	1:D:999:GLU:O	2.45	0.47
1:F:552:THR:HG22	1:F:654:ASN:H	1.79	0.47
1:A:644:THR:O	1:A:699:ASN:N	2.45	0.47
1:F:1440:THR:N	1:F:1470:LEU:O	2.40	0.47
1:A:207:VAL:HG13	1:A:211:GLN:HG2	1.96	0.47
1:A:552:THR:HG22	1:A:654:ASN:H	1.79	0.47
1:B:110:ILE:O	1:B:113:SER:OG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:ARG:HG2	1:B:1135:SER:HB3	1.95	0.47
1:C:833:ASN:OD1	1:C:833:ASN:N	2.46	0.47
1:E:203:ALA:HB2	1:E:209:VAL:HG23	1.96	0.47
1:E:365:ASP:HB2	1:E:371:LEU:HB3	1.96	0.47
1:E:984:LEU:HA	1:F:1397:LEU:HD13	1.96	0.47
1:F:512:PHE:HA	1:F:516:GLU:HG3	1.96	0.47
1:A:312:VAL:HG11	1:A:348:THR:HG22	1.95	0.47
1:B:644:THR:O	1:B:699:ASN:N	2.45	0.47
1:F:87:VAL:HG12	1:F:143:GLU:HB2	1.96	0.47
1:A:833:ASN:OD1	1:A:833:ASN:N	2.46	0.47
1:D:80:ASP:OD2	1:D:244:ASN:ND2	2.41	0.47
1:D:512:PHE:HA	1:D:516:GLU:HG3	1.96	0.47
1:E:121:GLY:HA3	1:E:330:LEU:HD12	1.97	0.47
1:F:704:MET:HB3	1:F:706:PHE:CE2	2.50	0.47
1:A:75:ALA:HB3	1:B:73:ASP:HB3	1.97	0.47
1:A:863:THR:OG1	1:F:354:GLN:CG	2.59	0.47
1:A:1117:ARG:HG2	1:A:1135:SER:HB3	1.95	0.47
1:B:236:THR:HB	1:C:489:ALA:HA	1.97	0.47
1:B:1447:ALA:N	1:B:1455:ASP:OD2	2.48	0.47
1:C:40:ASN:HD22	1:C:66:ASP:HA	1.80	0.47
1:C:44:SER:OG	1:C:61:GLU:HB3	2.14	0.47
1:D:67:SER:HA	1:D:70:ASN:ND2	2.30	0.47
1:D:164:GLN:O	1:D:164:GLN:NE2	2.46	0.47
1:E:1099:SER:OG	1:E:1207:GLN:NE2	2.46	0.47
1:F:81:VAL:HG11	1:F:90:MET:HE2	1.96	0.47
1:F:435:ARG:NH1	1:F:812:GLY:C	2.67	0.47
1:F:1044:ARG:HG2	1:F:1169:HIS:HB3	1.97	0.47
1:A:335:THR:HG22	1:A:339:LEU:HG	1.97	0.47
1:D:1447:ALA:N	1:D:1455:ASP:OD2	2.48	0.47
1:E:1044:ARG:HG2	1:E:1169:HIS:HB3	1.97	0.47
1:E:1447:ALA:N	1:E:1455:ASP:OD2	2.48	0.47
1:F:1099:SER:OG	1:F:1207:GLN:NE2	2.46	0.47
1:A:45:ALA:HB2	1:A:60:ILE:HD12	1.97	0.47
1:A:704:MET:HB3	1:A:706:PHE:CE2	2.50	0.47
1:A:1447:ALA:N	1:A:1455:ASP:OD2	2.48	0.47
1:B:704:MET:HB3	1:B:706:PHE:CE2	2.50	0.47
1:C:1044:ARG:HG2	1:C:1169:HIS:HB3	1.97	0.47
1:D:360:VAL:HG12	1:D:361:VAL:HG13	1.96	0.47
1:F:1447:ALA:N	1:F:1455:ASP:OD2	2.48	0.47
1:A:269:ARG:CZ	1:A:486:ASN:N	2.70	0.47
1:C:1447:ALA:N	1:C:1455:ASP:OD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:HIS:HD1	1:D:419:TYR:HB3	1.80	0.47
1:E:258:THR:HG22	1:E:340:MET:HB3	1.97	0.47
1:E:552:THR:HG22	1:E:654:ASN:H	1.79	0.47
1:E:1275:TRP:HB2	1:E:1284:MET:HG2	1.96	0.47
1:F:303:THR:HG23	1:F:304:LYS:HG3	1.97	0.47
1:B:552:THR:HG22	1:B:654:ASN:H	1.79	0.46
1:E:442:ASP:HA	1:E:447:PRO:HA	1.96	0.46
1:E:453:GLY:C	1:E:454:PHE:CG	2.93	0.46
1:F:1117:ARG:HG2	1:F:1135:SER:HB3	1.95	0.46
1:B:1044:ARG:HG2	1:B:1169:HIS:HB3	1.97	0.46
1:D:1099:SER:OG	1:D:1207:GLN:NE2	2.46	0.46
1:E:512:PHE:HA	1:E:516:GLU:HG3	1.96	0.46
1:F:274:ARG:NH1	1:F:433:ALA:O	2.49	0.46
1:A:57:PRO:HG3	1:A:339:LEU:HD22	1.97	0.46
1:A:279:HIS:HD1	1:A:419:TYR:HB3	1.79	0.46
1:A:1099:SER:OG	1:A:1207:GLN:NE2	2.46	0.46
1:C:786:ASP:OD1	1:C:786:ASP:N	2.49	0.46
1:E:625:PHE:CE1	1:E:627:TYR:HB3	2.50	0.46
1:F:358:THR:HG21	1:F:434:LYS:H	1.79	0.46
1:B:995:ASP:N	1:B:999:GLU:O	2.45	0.46
1:D:704:MET:HB3	1:D:706:PHE:CE2	2.50	0.46
1:D:1044:ARG:HG2	1:D:1169:HIS:HB3	1.97	0.46
1:D:1275:TRP:HB2	1:D:1284:MET:HG2	1.96	0.46
1:E:794:ASP:OD1	1:E:998:GLY:HA3	2.16	0.46
1:F:1270:LEU:HD21	1:F:1284:MET:HB2	1.98	0.46
1:A:360:VAL:HG12	1:A:361:VAL:HG13	1.98	0.46
1:B:133:GLY:HA3	1:B:141:THR:HG22	1.98	0.46
1:B:626:ASN:O	1:B:720:MET:HA	2.16	0.46
1:C:773:ASP:OD2	1:C:775:GLY:N	2.43	0.46
1:D:1238:SER:HG	1:D:1243:TYR:HH	1.58	0.46
1:E:995:ASP:N	1:E:999:GLU:O	2.45	0.46
1:E:1050:HIS:CD2	1:E:1051:ALA:H	2.33	0.46
1:F:500:VAL:O	1:F:578:ARG:NH2	2.40	0.46
1:F:605:LEU:HD13	1:F:698:VAL:HG13	1.98	0.46
1:A:66:ASP:HB3	1:A:69:ILE:HG12	1.97	0.46
1:A:1397:LEU:HD13	1:F:984:LEU:HA	1.98	0.46
1:B:625:PHE:CE1	1:B:627:TYR:HB3	2.50	0.46
1:C:704:MET:HB3	1:C:706:PHE:CE2	2.50	0.46
1:D:1050:HIS:CD2	1:D:1051:ALA:H	2.34	0.46
1:E:1238:SER:HG	1:E:1243:TYR:HH	1.61	0.46
1:E:1270:LEU:HD21	1:E:1284:MET:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:HE21	1:A:375:ASN:C	2.23	0.46
1:A:770:ASN:HB2	1:A:776:THR:HG21	1.98	0.46
1:C:71:ASP:OD1	1:C:76:LYS:HE2	2.16	0.46
1:C:278:VAL:O	1:C:425:SER:OG	2.24	0.46
1:C:552:THR:HG22	1:C:654:ASN:H	1.79	0.46
1:C:644:THR:O	1:C:699:ASN:N	2.45	0.46
1:D:552:THR:HG22	1:D:654:ASN:H	1.79	0.46
1:E:449:THR:HG23	1:F:858:LEU:HG	1.93	0.46
1:F:1050:HIS:CD2	1:F:1051:ALA:H	2.33	0.46
1:A:1050:HIS:CD2	1:A:1051:ALA:H	2.33	0.46
1:B:453:GLY:C	1:B:454:PHE:CG	2.93	0.46
1:B:730:ASP:HA	1:B:884:LEU:HD23	1.98	0.46
1:C:77:GLY:H	1:D:94:VAL:HG21	1.81	0.46
1:C:626:ASN:O	1:C:720:MET:HA	2.16	0.46
1:D:90:MET:HB3	1:D:98:TRP:HB3	1.98	0.46
1:E:704:MET:HB3	1:E:706:PHE:CE2	2.50	0.46
1:F:389:GLY:HA2	1:F:403:PRO:HG3	1.98	0.46
1:F:644:THR:O	1:F:699:ASN:N	2.45	0.46
1:A:1044:ARG:HG2	1:A:1169:HIS:HB3	1.97	0.46
1:B:984:LEU:HA	1:C:1397:LEU:HD13	1.97	0.46
1:C:180:ASN:OD1	1:C:181:THR:N	2.49	0.46
1:C:730:ASP:HA	1:C:884:LEU:HD23	1.98	0.46
1:C:1050:HIS:CD2	1:C:1051:ALA:H	2.33	0.46
1:D:136:ALA:O	1:D:182:LEU:HD11	2.16	0.46
1:D:143:GLU:HB2	1:E:196:GLU:OE2	2.16	0.46
1:E:605:LEU:HD13	1:E:698:VAL:HG13	1.98	0.46
1:A:626:ASN:O	1:A:720:MET:HA	2.16	0.45
1:B:786:ASP:OD1	1:B:786:ASP:N	2.49	0.45
1:C:1369:VAL:HG22	1:C:1386:ILE:HG12	1.98	0.45
1:D:895:VAL:HG12	1:D:988:VAL:HG12	1.98	0.45
1:F:115:ALA:HA	1:F:330:LEU:HD13	1.98	0.45
1:F:794:ASP:OD1	1:F:998:GLY:HA3	2.16	0.45
1:A:1206:LEU:O	1:A:1227:ALA:N	2.40	0.45
1:B:299:PHE:CE1	1:B:314:THR:HG23	2.51	0.45
1:C:275:VAL:HG12	1:C:275:VAL:O	2.16	0.45
1:D:794:ASP:OD1	1:D:998:GLY:HA3	2.16	0.45
1:E:626:ASN:O	1:E:720:MET:HA	2.16	0.45
1:C:794:ASP:OD1	1:C:998:GLY:HA3	2.16	0.45
1:C:984:LEU:HA	1:D:1397:LEU:HD13	1.97	0.45
1:D:1043:GLY:O	1:D:1348:TYR:OH	2.31	0.45
1:E:92:GLN:OE1	1:E:211:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:ASP:OD1	1:A:998:GLY:HA3	2.16	0.45
1:B:794:ASP:OD1	1:B:998:GLY:HA3	2.16	0.45
1:B:795:LEU:HB3	1:B:799:ASP:O	2.17	0.45
1:B:1270:LEU:HD21	1:B:1284:MET:HB2	1.98	0.45
1:C:1270:LEU:HD21	1:C:1284:MET:HB2	1.98	0.45
1:E:439:ALA:HB3	1:E:450:ILE:HD12	1.98	0.45
1:F:315:PHE:CD2	1:F:329:ALA:HB1	2.52	0.45
1:F:833:ASN:OD1	1:F:833:ASN:N	2.46	0.45
1:A:605:LEU:HD13	1:A:698:VAL:HG13	1.98	0.45
1:B:723:PHE:HE1	1:B:742:ILE:HG22	1.82	0.45
1:B:770:ASN:HB2	1:B:776:THR:HG21	1.98	0.45
1:B:1050:HIS:CD2	1:B:1051:ALA:H	2.33	0.45
1:C:770:ASN:HB2	1:C:776:THR:HG21	1.98	0.45
1:E:75:ALA:HA	1:E:211:GLN:HE22	1.82	0.45
1:E:299:PHE:CE1	1:E:314:THR:HG23	2.51	0.45
1:E:723:PHE:HE1	1:E:742:ILE:HG22	1.82	0.45
1:E:773:ASP:OD2	1:E:775:GLY:N	2.43	0.45
1:F:69:ILE:HA	1:F:76:LYS:HE3	1.97	0.45
1:F:625:PHE:CE1	1:F:627:TYR:HB3	2.50	0.45
1:A:363:ILE:HD11	1:A:388:PHE:HB2	1.97	0.45
1:B:1014:GLY:N	1:B:1212:ASP:OD2	2.50	0.45
1:C:848:GLU:O	1:C:848:GLU:HG3	2.17	0.45
1:D:273:PRO:HB2	1:D:485:LYS:HG2	1.97	0.45
1:D:605:LEU:HD13	1:D:698:VAL:HG13	1.98	0.45
1:D:770:ASN:HB2	1:D:776:THR:HG21	1.98	0.45
1:D:848:GLU:HG3	1:D:848:GLU:O	2.17	0.45
1:F:461:ILE:HG12	1:F:476:VAL:HG22	1.98	0.45
1:A:343:ASP:HB2	1:A:445:GLU:CD	2.41	0.45
1:A:1270:LEU:O	1:A:1273:ILE:HG22	2.17	0.45
1:C:53:TYR:O	1:C:285:LEU:HD11	2.17	0.45
1:D:1014:GLY:N	1:D:1212:ASP:OD2	2.50	0.45
1:D:1369:VAL:HG22	1:D:1386:ILE:HG12	1.98	0.45
1:E:1369:VAL:HG22	1:E:1386:ILE:HG12	1.98	0.45
1:F:302:ASN:ND2	1:F:305:ASN:HB2	2.32	0.45
1:F:1369:VAL:HG22	1:F:1386:ILE:HG12	1.98	0.45
1:A:272:PHE:HB3	1:A:429:ILE:HG13	1.99	0.45
1:B:311:ASN:ND2	1:B:333:ARG:HD3	2.31	0.45
1:C:354:GLN:HE21	1:D:863:THR:HG23	1.79	0.45
1:C:895:VAL:HG12	1:C:988:VAL:HG12	1.98	0.45
1:D:1270:LEU:HD21	1:D:1284:MET:HB2	1.98	0.45
1:E:895:VAL:HG12	1:E:988:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:995:ASP:OD2	1:E:995:ASP:C	2.60	0.45
1:F:995:ASP:OD2	1:F:995:ASP:C	2.60	0.45
1:F:1270:LEU:O	1:F:1273:ILE:HG22	2.17	0.45
1:A:625:PHE:CE1	1:A:627:TYR:HB3	2.50	0.45
1:A:1369:VAL:HG22	1:A:1386:ILE:HG12	1.98	0.45
1:B:258:THR:HG22	1:B:340:MET:HB3	1.99	0.45
1:B:466:ASP:OD2	1:B:466:ASP:N	2.43	0.45
1:B:605:LEU:HD13	1:B:698:VAL:HG13	1.98	0.45
1:C:304:LYS:NZ	1:C:350:ASP:OD1	2.49	0.45
1:C:315:PHE:CD2	1:C:329:ALA:HB1	2.52	0.45
1:C:795:LEU:HB3	1:C:799:ASP:O	2.17	0.45
1:C:1068:ASP:OD2	1:C:1156:LYS:NZ	2.34	0.45
1:D:67:SER:HA	1:D:70:ASN:HD21	1.82	0.45
1:D:626:ASN:O	1:D:720:MET:HA	2.16	0.45
1:E:92:GLN:HE21	1:E:96:GLY:HA2	1.82	0.45
1:A:723:PHE:HE1	1:A:742:ILE:HG22	1.82	0.45
1:A:795:LEU:HB3	1:A:799:ASP:O	2.17	0.45
1:A:995:ASP:OD2	1:A:995:ASP:C	2.60	0.45
1:B:115:ALA:HA	1:B:330:LEU:HD22	1.99	0.45
1:C:366:ASN:ND2	1:C:424:LYS:O	2.50	0.45
1:E:104:ASP:OD1	1:E:105:ARG:N	2.50	0.45
1:F:626:ASN:O	1:F:720:MET:HA	2.16	0.45
1:A:730:ASP:HA	1:A:884:LEU:HD23	1.98	0.44
1:B:268:ASP:CG	1:B:487:SER:OG	2.59	0.44
1:B:1369:VAL:HG22	1:B:1386:ILE:HG12	1.98	0.44
1:C:723:PHE:HE1	1:C:742:ILE:HG22	1.82	0.44
1:D:1270:LEU:O	1:D:1273:ILE:HG22	2.17	0.44
1:E:133:GLY:HA3	1:E:141:THR:HG22	1.99	0.44
1:C:302:ASN:ND2	1:C:305:ASN:HB2	2.32	0.44
1:C:460:ASP:OD2	1:C:461:ILE:N	2.50	0.44
1:C:1099:SER:OG	1:C:1207:GLN:NE2	2.46	0.44
1:C:1270:LEU:O	1:C:1273:ILE:HG22	2.17	0.44
1:D:723:PHE:HE1	1:D:742:ILE:HG22	1.82	0.44
1:E:461:ILE:HG12	1:E:476:VAL:HG22	1.99	0.44
1:F:44:SER:OG	1:F:61:GLU:HB3	2.16	0.44
1:A:95:ASP:CG	1:A:97:ASN:HD22	2.26	0.44
1:C:605:LEU:HD13	1:C:698:VAL:HG13	1.98	0.44
1:D:730:ASP:HA	1:D:884:LEU:HD23	1.98	0.44
1:E:57:PRO:HG3	1:E:339:LEU:HD22	1.99	0.44
1:F:848:GLU:O	1:F:848:GLU:HG3	2.17	0.44
1:A:461:ILE:HG12	1:A:476:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ASP:OD1	1:A:786:ASP:N	2.49	0.44
1:A:1270:LEU:HD21	1:A:1284:MET:HB2	1.98	0.44
1:B:1270:LEU:O	1:B:1273:ILE:HG22	2.17	0.44
1:C:751:GLY:H	1:C:754:THR:HG1	1.65	0.44
1:C:1014:GLY:N	1:C:1212:ASP:OD2	2.50	0.44
1:D:47:ASN:N	1:D:52:ASN:OD1	2.49	0.44
1:A:258:THR:HG22	1:A:340:MET:HG2	1.99	0.44
1:B:57:PRO:HG3	1:B:339:LEU:HD22	1.99	0.44
1:B:1273:ILE:HD12	1:B:1273:ILE:HA	1.85	0.44
1:C:162:GLY:HA2	1:C:175:THR:HB	2.00	0.44
1:D:269:ARG:NH1	1:D:485:LYS:HA	2.32	0.44
1:D:460:ASP:OD2	1:D:461:ILE:N	2.51	0.44
1:D:995:ASP:OD2	1:D:995:ASP:C	2.60	0.44
1:E:770:ASN:HB2	1:E:776:THR:HG21	1.98	0.44
1:E:1270:LEU:O	1:E:1273:ILE:HG22	2.17	0.44
1:F:730:ASP:HA	1:F:884:LEU:HD23	1.98	0.44
1:A:848:GLU:O	1:A:848:GLU:HG3	2.17	0.44
1:A:937:THR:O	1:F:435:ARG:CD	2.65	0.44
1:C:233:LEU:HD13	1:C:239:VAL:HG21	2.00	0.44
1:D:95:ASP:CG	1:D:97:ASN:HD22	2.24	0.44
1:D:795:LEU:HB3	1:D:799:ASP:O	2.17	0.44
1:E:730:ASP:HA	1:E:884:LEU:HD23	1.98	0.44
1:A:55:SER:H	1:A:58:GLN:NE2	2.16	0.44
1:A:136:ALA:O	1:A:182:LEU:HD11	2.17	0.44
1:A:1026:PRO:HG2	1:A:1157:PHE:HA	2.00	0.44
1:B:848:GLU:HG3	1:B:848:GLU:O	2.17	0.44
1:C:157:THR:H	1:C:161:ASN:HD22	1.64	0.44
1:C:1143:ALA:HB3	1:C:1146:ALA:HB2	2.00	0.44
1:D:390:ILE:HD12	1:D:397:LEU:HD13	2.00	0.44
1:E:795:LEU:HB3	1:E:799:ASP:O	2.17	0.44
1:E:1096:LEU:HD12	1:E:1210:TYR:HB2	2.00	0.44
1:F:770:ASN:HB2	1:F:776:THR:HG21	1.98	0.44
1:A:1267:THR:HB	1:A:1304:ARG:HH12	1.83	0.44
1:B:1026:PRO:HG2	1:B:1157:PHE:HA	2.00	0.44
1:D:751:GLY:H	1:D:754:THR:HG1	1.63	0.44
1:E:644:THR:O	1:E:699:ASN:N	2.45	0.44
1:E:848:GLU:O	1:E:848:GLU:HG3	2.17	0.44
1:E:1014:GLY:N	1:E:1212:ASP:OD2	2.50	0.44
1:A:390:ILE:HD12	1:A:397:LEU:HD13	2.00	0.44
1:B:460:ASP:OD2	1:B:461:ILE:N	2.50	0.44
1:B:995:ASP:OD2	1:B:995:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:VAL:N	1:C:254:LEU:O	2.28	0.44
1:D:88:LEU:HD13	1:D:231:TYR:HE2	1.83	0.44
1:D:644:THR:O	1:D:699:ASN:N	2.45	0.44
1:E:460:ASP:OD2	1:E:461:ILE:N	2.50	0.44
1:F:460:ASP:OD2	1:F:461:ILE:N	2.50	0.44
1:F:1267:THR:HB	1:F:1304:ARG:HH12	1.83	0.44
1:C:41:LEU:HD13	1:C:243:TYR:HB2	2.00	0.43
1:C:461:ILE:HG12	1:C:476:VAL:HG22	1.99	0.43
1:D:1143:ALA:HB3	1:D:1146:ALA:HB2	2.00	0.43
1:E:493:LEU:HD22	1:E:747:ALA:HB3	2.00	0.43
1:E:786:ASP:OD1	1:E:786:ASP:N	2.49	0.43
1:F:723:PHE:HE1	1:F:742:ILE:HG22	1.82	0.43
1:F:1026:PRO:HG2	1:F:1157:PHE:HA	2.00	0.43
1:B:442:ASP:HA	1:B:447:PRO:HA	1.99	0.43
1:B:447:PRO:HB2	1:C:858:LEU:HD11	2.00	0.43
1:B:895:VAL:HG12	1:B:988:VAL:HG12	1.98	0.43
1:B:1143:ALA:HB3	1:B:1146:ALA:HB2	2.00	0.43
1:C:74:GLU:OE1	1:D:72:THR:OG1	2.35	0.43
1:D:461:ILE:HG12	1:D:476:VAL:HG22	1.99	0.43
1:D:786:ASP:OD1	1:D:786:ASP:N	2.49	0.43
1:E:435:ARG:NH2	1:E:811:ASP:C	2.75	0.43
1:F:493:LEU:HD22	1:F:747:ALA:HB3	2.00	0.43
1:F:795:LEU:HB3	1:F:799:ASP:O	2.17	0.43
1:F:895:VAL:HG12	1:F:988:VAL:HG12	1.98	0.43
1:A:451:LEU:HD23	1:A:452:VAL:O	2.18	0.43
1:A:1096:LEU:HD12	1:A:1210:TYR:HB2	2.00	0.43
1:A:1422:LYS:NZ	1:F:1219:ASP:OD2	2.33	0.43
1:E:75:ALA:HB3	1:F:73:ASP:HB3	1.99	0.43
1:E:110:ILE:O	1:E:113:SER:OG	2.28	0.43
1:E:164:GLN:O	1:E:164:GLN:NE2	2.48	0.43
1:E:447:PRO:HB2	1:F:858:LEU:HD11	2.01	0.43
1:E:1267:THR:HB	1:E:1304:ARG:HH12	1.83	0.43
1:F:1143:ALA:HB3	1:F:1146:ALA:HB2	2.00	0.43
1:A:1122:ASP:OD1	1:A:1123:VAL:N	2.52	0.43
1:B:461:ILE:HG12	1:B:476:VAL:HG22	1.99	0.43
1:C:81:VAL:HG11	1:C:90:MET:HE2	1.99	0.43
1:C:349:LEU:HD23	1:C:402:ILE:HG21	2.00	0.43
1:C:1206:LEU:O	1:C:1227:ALA:N	2.40	0.43
1:D:269:ARG:NH2	1:D:276:SER:HB2	2.31	0.43
1:E:149:ILE:HG13	1:E:151:ILE:HG12	2.01	0.43
1:F:233:LEU:HD13	1:F:239:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1014:GLY:N	1:F:1212:ASP:OD2	2.50	0.43
1:A:460:ASP:OD2	1:A:461:ILE:N	2.50	0.43
1:A:532:ASP:O	1:A:552:THR:OG1	2.35	0.43
1:B:493:LEU:HD22	1:B:747:ALA:HB3	2.00	0.43
1:B:1267:THR:HB	1:B:1304:ARG:HH12	1.83	0.43
1:C:435:ARG:CD	1:D:937:THR:O	2.67	0.43
1:C:995:ASP:OD2	1:C:995:ASP:C	2.60	0.43
1:F:786:ASP:OD1	1:F:786:ASP:N	2.49	0.43
1:F:1273:ILE:HD12	1:F:1273:ILE:HA	1.85	0.43
1:A:47:ASN:N	1:A:52:ASN:OD1	2.51	0.43
1:A:117:THR:HG23	1:A:120:SER:HB2	1.99	0.43
1:A:1014:GLY:N	1:A:1212:ASP:OD2	2.50	0.43
1:C:435:ARG:HH12	1:C:812:GLY:C	2.23	0.43
1:C:435:ARG:CD	1:D:938:GLY:HA3	2.48	0.43
1:C:1026:PRO:HG2	1:C:1157:PHE:HA	2.00	0.43
1:E:269:ARG:NH1	1:E:276:SER:OG	2.52	0.43
1:E:279:HIS:ND1	1:E:425:SER:HB2	2.33	0.43
1:E:1026:PRO:HG2	1:E:1157:PHE:HA	2.00	0.43
1:F:162:GLY:HA2	1:F:175:THR:HB	2.00	0.43
1:F:1122:ASP:OD1	1:F:1123:VAL:N	2.52	0.43
1:B:75:ALA:HB3	1:C:73:ASP:HB3	2.00	0.43
1:C:493:LEU:HD22	1:C:747:ALA:HB3	2.00	0.43
1:C:1219:ASP:OD2	1:D:1422:LYS:NZ	2.33	0.43
1:D:1096:LEU:HD12	1:D:1210:TYR:HB2	2.00	0.43
1:E:333:ARG:NH2	1:F:673:ASN:OD1	2.51	0.43
1:A:895:VAL:HG12	1:A:988:VAL:HG12	1.98	0.43
1:B:986:ILE:N	1:B:1007:ALA:O	2.52	0.43
1:B:1096:LEU:HD12	1:B:1210:TYR:HB2	2.00	0.43
1:C:141:THR:O	1:C:144:THR:HG22	2.19	0.43
1:D:104:ASP:OD1	1:D:105:ARG:N	2.52	0.43
1:F:995:ASP:N	1:F:999:GLU:O	2.45	0.43
1:F:1043:GLY:O	1:F:1348:TYR:OH	2.31	0.43
1:D:442:ASP:HB2	1:D:447:PRO:HB3	2.01	0.43
1:D:986:ILE:N	1:D:1007:ALA:O	2.52	0.43
1:E:833:ASN:OD1	1:E:833:ASN:N	2.46	0.43
1:F:93:ALA:HB1	1:F:198:LYS:HB3	2.01	0.43
1:F:265:LEU:HD12	1:F:282:ILE:HG12	2.00	0.43
1:A:1143:ALA:HB3	1:A:1146:ALA:HB2	2.00	0.43
1:B:985:ASP:OD1	1:B:985:ASP:N	2.49	0.43
1:B:1122:ASP:OD1	1:B:1123:VAL:N	2.52	0.43
1:E:209:VAL:HG12	1:E:214:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:986:ILE:N	1:E:1007:ALA:O	2.52	0.43
1:F:275:VAL:HG12	1:F:275:VAL:O	2.19	0.43
1:F:986:ILE:N	1:F:1007:ALA:O	2.52	0.43
1:F:1480:VAL:O	1:F:1492:GLY:N	2.42	0.43
1:C:361:VAL:HG11	1:C:427:LEU:HD23	2.00	0.42
1:C:1024:PRO:HB3	1:C:1257:ASP:HA	2.01	0.42
1:C:1096:LEU:HD12	1:C:1210:TYR:HB2	2.00	0.42
1:D:1122:ASP:OD1	1:D:1123:VAL:N	2.52	0.42
1:E:236:THR:HB	1:F:489:ALA:HA	2.00	0.42
1:E:874:ASP:OD2	1:E:904:THR:HG22	2.20	0.42
1:F:363:ILE:HA	1:F:426:VAL:O	2.19	0.42
1:A:466:ASP:OD2	1:A:466:ASP:N	2.44	0.42
1:A:986:ILE:N	1:A:1007:ALA:O	2.52	0.42
1:B:71:ASP:OD1	1:B:74:GLU:HB2	2.19	0.42
1:C:122:LEU:HD23	1:C:316:TYR:CD2	2.54	0.42
1:C:874:ASP:OD2	1:C:904:THR:HG22	2.19	0.42
1:C:1436:GLU:OE1	1:C:1466:THR:HG22	2.19	0.42
1:F:1096:LEU:HD12	1:F:1210:TYR:HB2	2.00	0.42
1:A:279:HIS:H	1:A:488:ARG:NH2	1.83	0.42
1:C:111:ALA:HB1	1:C:122:LEU:HB3	2.00	0.42
1:C:1122:ASP:OD1	1:C:1123:VAL:N	2.52	0.42
1:D:1024:PRO:HB3	1:D:1257:ASP:HA	2.01	0.42
1:D:1267:THR:HB	1:D:1304:ARG:HH12	1.83	0.42
1:E:1143:ALA:HB3	1:E:1146:ALA:HB2	2.00	0.42
1:F:773:ASP:OD2	1:F:775:GLY:N	2.43	0.42
1:A:259:VAL:HG21	1:A:285:LEU:HB2	2.01	0.42
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.91	0.42
1:A:1024:PRO:HB3	1:A:1257:ASP:HA	2.01	0.42
1:A:1268:TYR:O	1:A:1302:ASP:HB3	2.20	0.42
1:B:1024:PRO:HB3	1:B:1257:ASP:HA	2.01	0.42
1:B:1436:GLU:OE1	1:B:1466:THR:HG22	2.19	0.42
1:C:347:LEU:HD11	1:C:441:LEU:HD21	2.02	0.42
1:D:420:ASP:OD2	1:D:422:SER:OG	2.38	0.42
1:F:1024:PRO:HB3	1:F:1257:ASP:HA	2.01	0.42
1:A:94:VAL:HG21	1:F:77:GLY:H	1.85	0.42
1:A:493:LEU:HD22	1:A:747:ALA:HB3	2.00	0.42
1:B:305:ASN:HB3	1:B:310:PHE:CE2	2.54	0.42
1:B:419:TYR:HA	1:B:425:SER:HA	2.00	0.42
1:B:874:ASP:OD2	1:B:904:THR:HG22	2.19	0.42
1:C:249:VAL:HG21	1:D:411:PRO:HD2	2.02	0.42
1:D:1268:TYR:O	1:D:1302:ASP:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ALA:HB2	1:E:60:ILE:HD12	2.01	0.42
1:E:1122:ASP:OD1	1:E:1123:VAL:N	2.52	0.42
1:F:364:GLN:C	1:F:371:LEU:HD23	2.44	0.42
1:F:1268:TYR:O	1:F:1302:ASP:HB3	2.20	0.42
1:A:239:VAL:O	1:A:254:LEU:N	2.48	0.42
1:B:721:ASP:N	1:B:721:ASP:OD1	2.53	0.42
1:B:1099:SER:OG	1:B:1207:GLN:NE2	2.46	0.42
1:C:298:THR:HB	1:C:315:PHE:HB2	2.01	0.42
1:C:364:GLN:NE2	1:C:428:LYS:HD2	2.34	0.42
1:C:995:ASP:N	1:C:999:GLU:O	2.45	0.42
1:D:493:LEU:HD22	1:D:747:ALA:HB3	2.00	0.42
1:D:514:ILE:O	1:D:600:LEU:HD12	2.20	0.42
1:D:1026:PRO:HG2	1:D:1157:PHE:HA	2.00	0.42
1:E:435:ARG:HB3	1:E:454:PHE:HE2	1.84	0.42
1:E:1268:TYR:O	1:E:1302:ASP:HB3	2.20	0.42
1:F:909:ASN:ND2	1:F:971:PRO:O	2.46	0.42
1:A:514:ILE:O	1:A:600:LEU:HD12	2.20	0.42
1:B:579:LEU:HD22	1:B:718:ILE:HB	2.02	0.42
1:B:773:ASP:OD2	1:B:775:GLY:N	2.43	0.42
1:C:305:ASN:HB3	1:C:310:PHE:CE2	2.54	0.42
1:C:579:LEU:HD22	1:C:718:ILE:HB	2.02	0.42
1:D:104:ASP:HA	1:D:231:TYR:O	2.20	0.42
1:D:833:ASN:OD1	1:D:833:ASN:N	2.46	0.42
1:E:50:PHE:CD2	1:E:285:LEU:HD12	2.55	0.42
1:F:514:ILE:O	1:F:600:LEU:HD12	2.20	0.42
1:F:721:ASP:OD1	1:F:721:ASP:N	2.53	0.42
1:A:54:MET:HE2	1:A:60:ILE:HG13	2.02	0.42
1:A:874:ASP:OD2	1:A:904:THR:HG22	2.20	0.42
1:C:514:ILE:O	1:C:600:LEU:HD12	2.20	0.42
1:C:595:PHE:N	1:C:595:PHE:CD2	2.88	0.42
1:C:1267:THR:HB	1:C:1304:ARG:HH12	1.83	0.42
1:F:305:ASN:HB3	1:F:310:PHE:CE2	2.55	0.42
1:F:762:GLU:O	1:F:788:SER:HA	2.20	0.42
1:F:1255:GLU:HA	1:F:1256:PRO:HD3	1.89	0.42
1:A:852:LEU:HD11	1:A:990:TYR:OH	2.20	0.42
1:A:1273:ILE:HD12	1:A:1273:ILE:HA	1.85	0.42
1:B:54:MET:HA	1:B:285:LEU:HD21	2.01	0.42
1:B:279:HIS:ND1	1:B:425:SER:HB2	2.34	0.42
1:C:364:GLN:NE2	1:C:425:SER:O	2.53	0.42
1:C:986:ILE:N	1:C:1007:ALA:O	2.52	0.42
1:C:1268:TYR:O	1:C:1302:ASP:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:VAL:O	1:D:425:SER:OG	2.26	0.42
1:D:721:ASP:OD1	1:D:721:ASP:N	2.53	0.42
1:D:893:LEU:HD12	1:D:894:ASP:N	2.35	0.42
1:E:54:MET:HA	1:E:285:LEU:HD21	2.02	0.42
1:F:874:ASP:OD2	1:F:904:THR:HG22	2.19	0.42
1:A:273:PRO:HB3	1:A:482:ASP:O	2.20	0.42
1:A:595:PHE:N	1:A:595:PHE:CD2	2.88	0.42
1:A:762:GLU:O	1:A:788:SER:HA	2.20	0.42
1:A:828:GLY:HA3	1:A:990:TYR:HE2	1.85	0.42
1:A:1100:VAL:HG22	1:A:1206:LEU:HD13	2.02	0.42
1:B:595:PHE:N	1:B:595:PHE:CD2	2.88	0.42
1:B:893:LEU:HD12	1:B:894:ASP:N	2.35	0.42
1:C:893:LEU:HD12	1:C:894:ASP:N	2.35	0.42
1:D:276:SER:CB	1:D:485:LYS:CB	2.94	0.42
1:E:595:PHE:N	1:E:595:PHE:CD2	2.88	0.42
1:D:371:LEU:HD12	1:D:371:LEU:HA	1.92	0.41
1:D:1436:GLU:OE1	1:D:1466:THR:HG22	2.19	0.41
1:E:1276:ASP:OD2	1:E:1276:ASP:C	2.63	0.41
1:B:197:ALA:HB1	1:B:225:TRP:NE1	2.35	0.41
1:B:304:LYS:NZ	1:B:352:ASP:O	2.53	0.41
1:B:1268:TYR:O	1:B:1302:ASP:HB3	2.20	0.41
1:C:1070:THR:HG22	1:C:1154:ASN:HB3	2.02	0.41
1:D:625:PHE:CE1	1:D:627:TYR:HB3	2.51	0.41
1:D:874:ASP:OD2	1:D:904:THR:HG22	2.19	0.41
1:D:1100:VAL:HG22	1:D:1206:LEU:HD13	2.02	0.41
1:E:721:ASP:OD1	1:E:721:ASP:N	2.53	0.41
1:F:1346:SER:OG	1:F:1348:TYR:O	2.38	0.41
1:C:1346:SER:OG	1:C:1348:TYR:O	2.38	0.41
1:D:595:PHE:CD2	1:D:595:PHE:N	2.88	0.41
1:D:1070:THR:HG22	1:D:1154:ASN:HB3	2.02	0.41
1:E:762:GLU:O	1:E:788:SER:HA	2.20	0.41
1:E:852:LEU:HD11	1:E:990:TYR:OH	2.20	0.41
1:E:893:LEU:HD12	1:E:894:ASP:N	2.35	0.41
1:E:1100:VAL:HG22	1:E:1206:LEU:HD13	2.02	0.41
1:F:277:GLN:OE1	1:F:428:LYS:HG2	2.20	0.41
1:F:852:LEU:HD11	1:F:990:TYR:OH	2.20	0.41
1:A:104:ASP:HA	1:A:231:TYR:O	2.20	0.41
1:B:50:PHE:CD2	1:B:285:LEU:HD12	2.55	0.41
1:B:365:ASP:HB2	1:B:371:LEU:HB3	2.01	0.41
1:B:762:GLU:O	1:B:788:SER:HA	2.20	0.41
1:C:149:ILE:HG13	1:C:151:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:852:LEU:HD11	1:C:990:TYR:OH	2.20	0.41
1:D:117:THR:HG23	1:D:120:SER:HB2	2.03	0.41
1:E:1436:GLU:OE1	1:E:1466:THR:HG22	2.20	0.41
1:F:50:PHE:O	1:F:53:TYR:HD1	2.03	0.41
1:F:519:THR:HA	1:F:520:PRO:HD3	1.94	0.41
1:A:893:LEU:HD12	1:A:894:ASP:N	2.35	0.41
1:B:144:THR:HA	1:B:231:TYR:HE2	1.86	0.41
1:B:514:ILE:O	1:B:600:LEU:HD12	2.20	0.41
1:B:828:GLY:HA3	1:B:990:TYR:HE2	1.85	0.41
1:C:895:VAL:HG22	1:C:934:LEU:HD22	2.03	0.41
1:C:1100:VAL:HG22	1:C:1206:LEU:HD13	2.02	0.41
1:D:361:VAL:HG12	1:D:429:ILE:HD13	2.03	0.41
1:D:852:LEU:HD11	1:D:990:TYR:OH	2.20	0.41
1:D:895:VAL:HG22	1:D:934:LEU:HD22	2.03	0.41
1:E:73:ASP:OD1	1:E:73:ASP:N	2.45	0.41
1:F:268:ASP:OD1	1:F:269:ARG:N	2.54	0.41
1:F:277:GLN:HB3	1:F:425:SER:HB3	2.02	0.41
1:F:595:PHE:N	1:F:595:PHE:CD2	2.88	0.41
1:F:1276:ASP:OD2	1:F:1276:ASP:C	2.64	0.41
1:A:225:TRP:CE3	1:A:226:PRO:HA	2.56	0.41
1:A:525:THR:HB	1:A:595:PHE:HB2	2.03	0.41
1:A:1219:ASP:OD2	1:B:1422:LYS:NZ	2.35	0.41
1:A:1436:GLU:OE1	1:A:1466:THR:HG22	2.20	0.41
1:C:553:LEU:HB2	1:C:595:PHE:HE1	1.85	0.41
1:C:721:ASP:OD1	1:C:721:ASP:N	2.53	0.41
1:D:1077:ASP:OD2	1:D:1210:TYR:OH	2.38	0.41
1:E:514:ILE:O	1:E:600:LEU:HD12	2.20	0.41
1:E:828:GLY:HA3	1:E:990:TYR:HE2	1.85	0.41
1:B:49:GLN:HG2	1:B:50:PHE:CE1	2.56	0.41
1:B:354:GLN:HE21	1:C:861:ILE:CD1	2.26	0.41
1:C:525:THR:HB	1:C:595:PHE:HB2	2.03	0.41
1:C:1412:SER:HA	1:C:1417:ASP:HA	2.03	0.41
1:D:825:SER:HB3	1:D:995:ASP:O	2.21	0.41
1:D:828:GLY:HA3	1:D:990:TYR:HE2	1.85	0.41
1:D:1276:ASP:OD2	1:D:1276:ASP:C	2.64	0.41
1:E:845:ILE:N	1:E:953:GLY:O	2.35	0.41
1:E:1068:ASP:OD2	1:E:1156:LYS:NZ	2.34	0.41
1:E:1231:LEU:C	1:E:1232:ARG:HD3	2.46	0.41
1:E:1480:VAL:O	1:E:1492:GLY:N	2.42	0.41
1:F:149:ILE:HG13	1:F:151:ILE:HG12	2.01	0.41
1:F:304:LYS:NZ	1:F:350:ASP:OD1	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1460:THR:HG23	1:F:1470:LEU:HD12	2.02	0.41
1:B:1070:THR:HG22	1:B:1154:ASN:HB3	2.02	0.41
1:B:1276:ASP:OD2	1:B:1276:ASP:C	2.64	0.41
1:C:1077:ASP:OD2	1:C:1210:TYR:OH	2.38	0.41
1:D:335:THR:HG22	1:D:339:LEU:HG	2.03	0.41
1:D:363:ILE:HD11	1:D:388:PHE:HB2	2.02	0.41
1:D:363:ILE:HD13	1:D:402:ILE:HG23	2.02	0.41
1:D:553:LEU:HB2	1:D:595:PHE:HE1	1.86	0.41
1:D:1092:GLN:NE2	1:D:1213:PRO:HB3	2.36	0.41
1:D:1231:LEU:C	1:D:1232:ARG:HD3	2.46	0.41
1:F:453:GLY:C	1:F:454:PHE:CG	2.99	0.41
1:F:478:ILE:O	1:F:757:PHE:N	2.44	0.41
1:F:828:GLY:HA3	1:F:990:TYR:HE2	1.85	0.41
1:F:1100:VAL:HG22	1:F:1206:LEU:HD13	2.02	0.41
1:F:1436:GLU:OE1	1:F:1466:THR:HG22	2.20	0.41
1:A:305:ASN:HB3	1:A:310:PHE:CD2	2.56	0.41
1:A:586:ASN:HB3	1:A:591:PHE:CE1	2.56	0.41
1:A:721:ASP:OD1	1:A:721:ASP:N	2.53	0.41
1:A:773:ASP:OD2	1:A:775:GLY:N	2.43	0.41
1:A:793:GLU:O	1:A:795:LEU:N	2.54	0.41
1:A:1231:LEU:C	1:A:1232:ARG:HD3	2.46	0.41
1:A:1276:ASP:OD2	1:A:1276:ASP:C	2.63	0.41
1:A:1480:VAL:O	1:A:1492:GLY:N	2.43	0.41
1:B:279:HIS:CE1	1:B:425:SER:HB2	2.56	0.41
1:B:525:THR:HB	1:B:595:PHE:HB2	2.03	0.41
1:B:793:GLU:O	1:B:795:LEU:N	2.54	0.41
1:B:852:LEU:HD11	1:B:990:TYR:OH	2.20	0.41
1:B:1231:LEU:C	1:B:1232:ARG:HD3	2.46	0.41
1:B:1412:SER:HA	1:B:1417:ASP:HA	2.03	0.41
1:B:1460:THR:HG23	1:B:1470:LEU:HD12	2.02	0.41
1:C:1013:THR:HG22	1:C:1215:ASP:HB2	2.03	0.41
1:D:525:THR:HB	1:D:595:PHE:HB2	2.03	0.41
1:D:762:GLU:O	1:D:788:SER:HA	2.20	0.41
1:D:1013:THR:HG22	1:D:1215:ASP:HB2	2.03	0.41
1:D:1460:THR:HG23	1:D:1470:LEU:HD12	2.02	0.41
1:E:150:PRO:HB2	1:E:189:GLY:HA2	2.02	0.41
1:E:279:HIS:CE1	1:E:425:SER:HB2	2.56	0.41
1:E:586:ASN:HB3	1:E:591:PHE:CE1	2.56	0.41
1:E:825:SER:HB3	1:E:995:ASP:O	2.21	0.41
1:E:1024:PRO:HB3	1:E:1257:ASP:HA	2.01	0.41
1:E:1092:GLN:NE2	1:E:1213:PRO:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1255:GLU:HA	1:E:1256:PRO:HD3	1.89	0.41
1:F:141:THR:O	1:F:144:THR:HG22	2.21	0.41
1:F:579:LEU:HD22	1:F:718:ILE:HB	2.02	0.41
1:F:586:ASN:HB3	1:F:591:PHE:CE1	2.56	0.41
1:F:793:GLU:O	1:F:795:LEU:N	2.54	0.41
1:F:893:LEU:HD12	1:F:894:ASP:N	2.35	0.41
1:F:1070:THR:HG22	1:F:1154:ASN:HB3	2.02	0.41
1:A:269:ARG:NH2	1:A:485:LYS:CA	2.82	0.41
1:B:263:ALA:HB1	1:B:443:TYR:HE2	1.86	0.41
1:B:1100:VAL:HG22	1:B:1206:LEU:HD13	2.02	0.41
1:B:1219:ASP:OD2	1:C:1422:LYS:NZ	2.35	0.41
1:B:1346:SER:OG	1:B:1348:TYR:O	2.38	0.41
1:B:1411:VAL:HG23	1:B:1480:VAL:HG22	2.03	0.41
1:C:87:VAL:HG12	1:C:143:GLU:HB2	2.03	0.41
1:C:762:GLU:O	1:C:788:SER:HA	2.20	0.41
1:C:828:GLY:HA3	1:C:990:TYR:HE2	1.85	0.41
1:C:1276:ASP:OD2	1:C:1276:ASP:C	2.64	0.41
1:D:225:TRP:CE3	1:D:226:PRO:HA	2.56	0.41
1:D:305:ASN:HB3	1:D:310:PHE:CD2	2.56	0.41
1:D:793:GLU:O	1:D:795:LEU:N	2.54	0.41
1:D:1335:ILE:HD13	1:D:1335:ILE:HA	1.93	0.41
1:D:1411:VAL:HG23	1:D:1480:VAL:HG22	2.03	0.41
1:E:438:SER:HB3	1:E:451:LEU:HD12	2.03	0.41
1:F:525:THR:HB	1:F:595:PHE:HB2	2.03	0.41
1:F:553:LEU:HB2	1:F:595:PHE:HE1	1.85	0.41
1:A:1426:THR:HG22	1:A:1432:ILE:O	2.22	0.40
1:C:216:ASN:HB3	1:C:223:PRO:HD2	2.02	0.40
1:C:793:GLU:O	1:C:795:LEU:N	2.54	0.40
1:D:1246:GLY:H	1:D:1319:ILE:HB	1.86	0.40
1:E:312:VAL:O	1:E:333:ARG:HD2	2.21	0.40
1:E:540:ILE:HD13	1:E:540:ILE:HA	1.84	0.40
1:E:1070:THR:HG22	1:E:1154:ASN:HB3	2.02	0.40
1:E:1246:GLY:H	1:E:1319:ILE:HB	1.86	0.40
1:E:1412:SER:HA	1:E:1417:ASP:HA	2.03	0.40
1:E:1460:THR:HG23	1:E:1470:LEU:HD12	2.02	0.40
1:F:731:GLY:HA2	1:F:736:GLU:HG3	2.03	0.40
1:A:579:LEU:HD22	1:A:718:ILE:HB	2.02	0.40
1:A:1246:GLY:H	1:A:1319:ILE:HB	1.86	0.40
1:A:1460:THR:HG23	1:A:1470:LEU:HD12	2.02	0.40
1:B:150:PRO:HB2	1:B:189:GLY:HA2	2.02	0.40
1:B:438:SER:HB3	1:B:451:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:LEU:HB2	1:B:595:PHE:HE1	1.86	0.40
1:B:1013:THR:HG22	1:B:1215:ASP:HB2	2.03	0.40
1:B:1202:GLN:NE2	1:B:1346:SER:O	2.54	0.40
1:C:731:GLY:HA2	1:C:736:GLU:HG3	2.03	0.40
1:D:731:GLY:HA2	1:D:736:GLU:HG3	2.03	0.40
1:D:1390:ASP:N	1:D:1390:ASP:OD1	2.54	0.40
1:E:579:LEU:HD22	1:E:718:ILE:HB	2.02	0.40
1:E:895:VAL:HG22	1:E:934:LEU:HD22	2.03	0.40
1:E:1219:ASP:OD2	1:F:1422:LYS:NZ	2.34	0.40
1:F:53:TYR:O	1:F:285:LEU:HD11	2.20	0.40
1:F:298:THR:HB	1:F:315:PHE:HB2	2.02	0.40
1:F:1092:GLN:NE2	1:F:1213:PRO:HB3	2.36	0.40
1:B:895:VAL:HG22	1:B:934:LEU:HD22	2.03	0.40
1:B:1246:GLY:H	1:B:1319:ILE:HB	1.86	0.40
1:C:701:GLY:C	1:C:702:PHE:HD1	2.30	0.40
1:C:825:SER:HB3	1:C:995:ASP:O	2.21	0.40
1:C:1411:VAL:HG23	1:C:1480:VAL:HG22	2.03	0.40
1:D:1346:SER:OG	1:D:1348:TYR:O	2.38	0.40
1:E:117:THR:HG23	1:E:120:SER:HB2	2.03	0.40
1:F:1412:SER:HA	1:F:1417:ASP:HA	2.03	0.40
1:A:81:VAL:HG13	1:A:88:LEU:HB3	2.04	0.40
1:A:731:GLY:HA2	1:A:736:GLU:HG3	2.03	0.40
1:A:1070:THR:HG22	1:A:1154:ASN:HB3	2.02	0.40
1:B:350:ASP:HB3	1:B:440:SER:OG	2.21	0.40
1:B:1426:THR:HG22	1:B:1432:ILE:O	2.22	0.40
1:C:1092:GLN:NE2	1:C:1213:PRO:HB3	2.36	0.40
1:C:1231:LEU:C	1:C:1232:ARG:HD3	2.46	0.40
1:D:736:GLU:H	1:D:736:GLU:HG2	1.65	0.40
1:D:1302:ASP:C	1:D:1315:ILE:HD12	2.47	0.40
1:E:245:LYS:HE3	1:E:245:LYS:HB2	1.93	0.40
1:E:478:ILE:O	1:E:757:PHE:N	2.44	0.40
1:E:1273:ILE:HD12	1:E:1273:ILE:HA	1.85	0.40
1:F:702:PHE:CZ	1:F:722:PHE:HE2	2.40	0.40
1:A:442:ASP:HB2	1:A:447:PRO:HB3	2.03	0.40
1:A:1346:SER:OG	1:A:1348:TYR:O	2.38	0.40
1:A:1411:VAL:HG23	1:A:1480:VAL:HG22	2.03	0.40
1:C:625:PHE:CE1	1:C:627:TYR:HB3	2.50	0.40
1:C:1411:VAL:CG1	1:C:1418:LEU:HB2	2.52	0.40
1:C:1421:TYR:CZ	1:C:1437:VAL:HG22	2.57	0.40
1:D:216:ASN:HB3	1:D:223:PRO:HD2	2.02	0.40
1:D:934:LEU:HD12	1:D:934:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:THR:HB	1:E:595:PHE:HB2	2.03	0.40
1:E:793:GLU:O	1:E:795:LEU:N	2.54	0.40
1:F:825:SER:HB3	1:F:995:ASP:O	2.21	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	1460/1734 (84%)	1418 (97%)	42 (3%)	0	100	100
1	B	1460/1734 (84%)	1415 (97%)	45 (3%)	0	100	100
1	C	1460/1734 (84%)	1414 (97%)	46 (3%)	0	100	100
1	D	1460/1734 (84%)	1421 (97%)	39 (3%)	0	100	100
1	E	1460/1734 (84%)	1414 (97%)	46 (3%)	0	100	100
1	F	1460/1734 (84%)	1412 (97%)	48 (3%)	0	100	100
All	All	8760/10404 (84%)	8494 (97%)	266 (3%)	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	1212/1438 (84%)	1203 (99%)	9 (1%)	76	78
1	B	1212/1438 (84%)	1200 (99%)	12 (1%)	68	75
1	C	1212/1438 (84%)	1201 (99%)	11 (1%)	70	76
1	D	1212/1438 (84%)	1202 (99%)	10 (1%)	73	77
1	E	1212/1438 (84%)	1199 (99%)	13 (1%)	65	74
1	F	1212/1438 (84%)	1200 (99%)	12 (1%)	68	75
All	All	7272/8628 (84%)	7205 (99%)	67 (1%)	68	76

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	649	LEU
1	A	698	VAL
1	A	792	ILE
1	A	995	ASP
1	A	1254	ILE
1	A	1276	ASP
1	A	1338	TYR
1	A	1390	ASP
1	A	1413	THR
1	B	649	LEU
1	B	698	VAL
1	B	792	ILE
1	B	995	ASP
1	B	1179	THR
1	B	1254	ILE
1	B	1276	ASP
1	B	1338	TYR
1	B	1349	VAL
1	B	1375	VAL
1	B	1390	ASP
1	B	1413	THR
1	C	455	SER
1	C	649	LEU
1	C	698	VAL
1	C	792	ILE
1	C	995	ASP
1	C	1254	ILE
1	C	1276	ASP
1	C	1338	TYR
1	C	1349	VAL

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Mol	Chain	Res	Type
1	C	1390	ASP
1	C	1413	THR
1	D	649	LEU
1	D	698	VAL
1	D	792	ILE
1	D	995	ASP
1	D	1179	THR
1	D	1254	ILE
1	D	1338	TYR
1	D	1349	VAL
1	D	1390	ASP
1	D	1413	THR
1	E	649	LEU
1	E	698	VAL
1	E	792	ILE
1	E	995	ASP
1	E	1155	ILE
1	E	1179	THR
1	E	1254	ILE
1	E	1276	ASP
1	E	1338	TYR
1	E	1349	VAL
1	E	1375	VAL
1	E	1390	ASP
1	E	1413	THR
1	F	649	LEU
1	F	698	VAL
1	F	721	ASP
1	F	792	ILE
1	F	995	ASP
1	F	1179	THR
1	F	1254	ILE
1	F	1276	ASP
1	F	1338	TYR
1	F	1349	VAL
1	F	1390	ASP
1	F	1413	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN

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Mol	Chain	Res	Type
1	A	211	GLN
1	A	311	ASN
1	A	373	GLN
1	A	643	ASN
1	A	806	ASN
1	A	853	ASN
1	A	1050	HIS
1	A	1127	ASN
1	B	38	ASN
1	B	40	ASN
1	B	161	ASN
1	B	288	ASN
1	B	379	ASN
1	B	806	ASN
1	B	853	ASN
1	B	956	GLN
1	B	1050	HIS
1	C	242	GLN
1	C	279	HIS
1	C	311	ASN
1	C	317	GLN
1	C	322	ASN
1	C	366	ASN
1	C	409	GLN
1	C	444	ASN
1	C	643	ASN
1	C	806	ASN
1	C	853	ASN
1	C	1050	HIS
1	C	1127	ASN
1	D	47	ASN
1	D	70	ASN
1	D	164	GLN
1	D	211	GLN
1	D	311	ASN
1	D	643	ASN
1	D	806	ASN
1	D	853	ASN
1	D	956	GLN
1	D	1050	HIS
1	D	1127	ASN
1	D	1391	HIS

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Mol	Chain	Res	Type
1	E	161	ASN
1	E	180	ASN
1	E	277	GLN
1	E	288	ASN
1	E	643	ASN
1	E	806	ASN
1	E	853	ASN
1	E	989	ASN
1	E	1050	HIS
1	F	279	HIS
1	F	317	GLN
1	F	322	ASN
1	F	409	GLN
1	F	444	ASN
1	F	806	ASN
1	F	853	ASN
1	F	956	GLN
1	F	1050	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

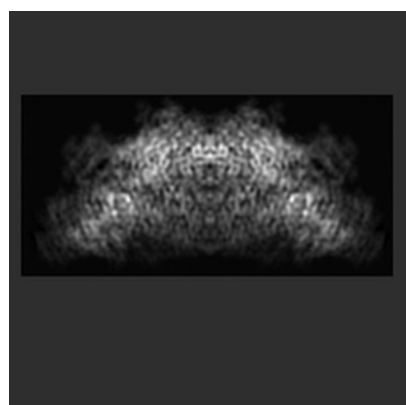
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16492. These allow visual inspection of the internal detail of the map and identification of artifacts.

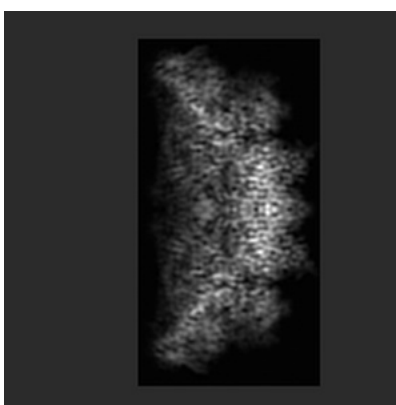
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

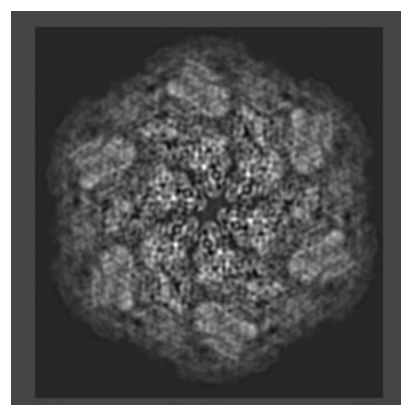
6.1.1 Primary map



X



Y



Z

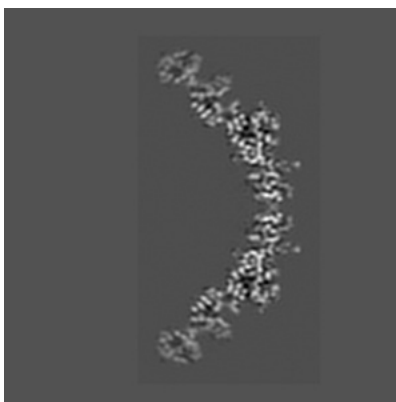
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

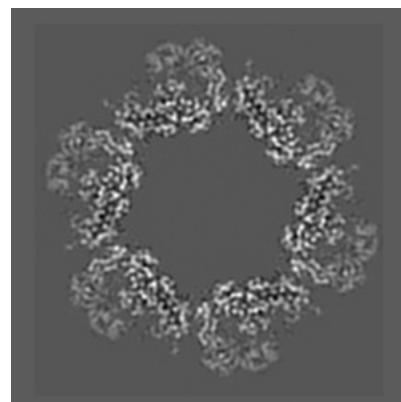
6.2.1 Primary map



X Index: 100



Y Index: 100

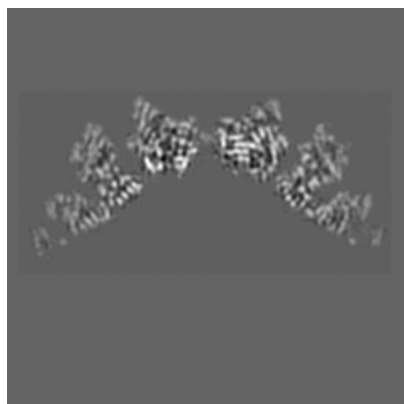


Z Index: 100

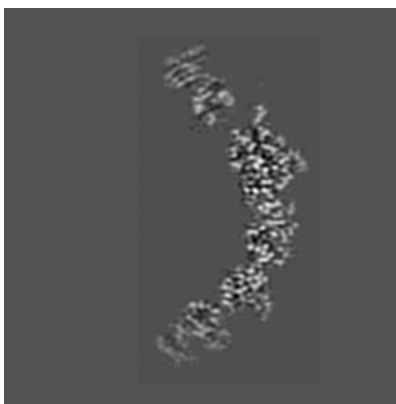
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

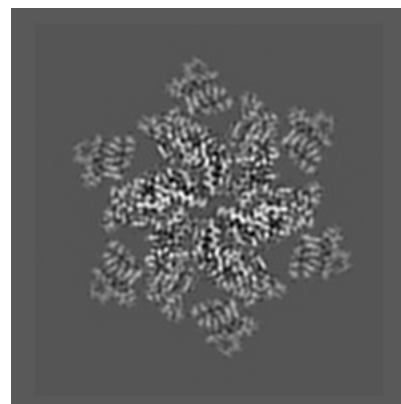
6.3.1 Primary map



X Index: 99



Y Index: 92

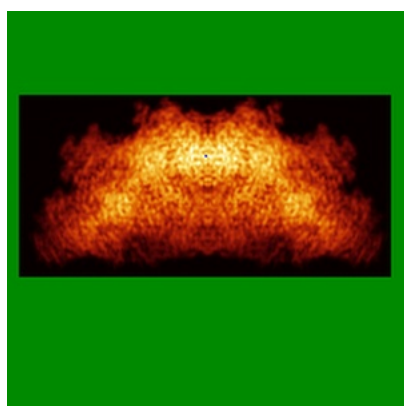


Z Index: 127

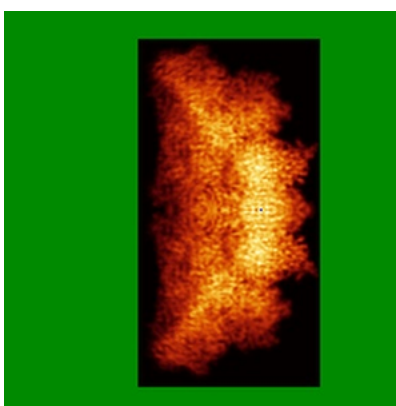
The images above show the largest variance slices of the map in three orthogonal directions.

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

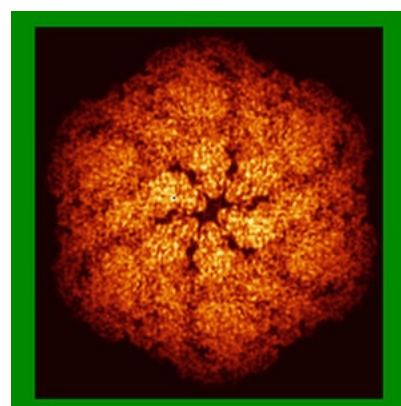
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

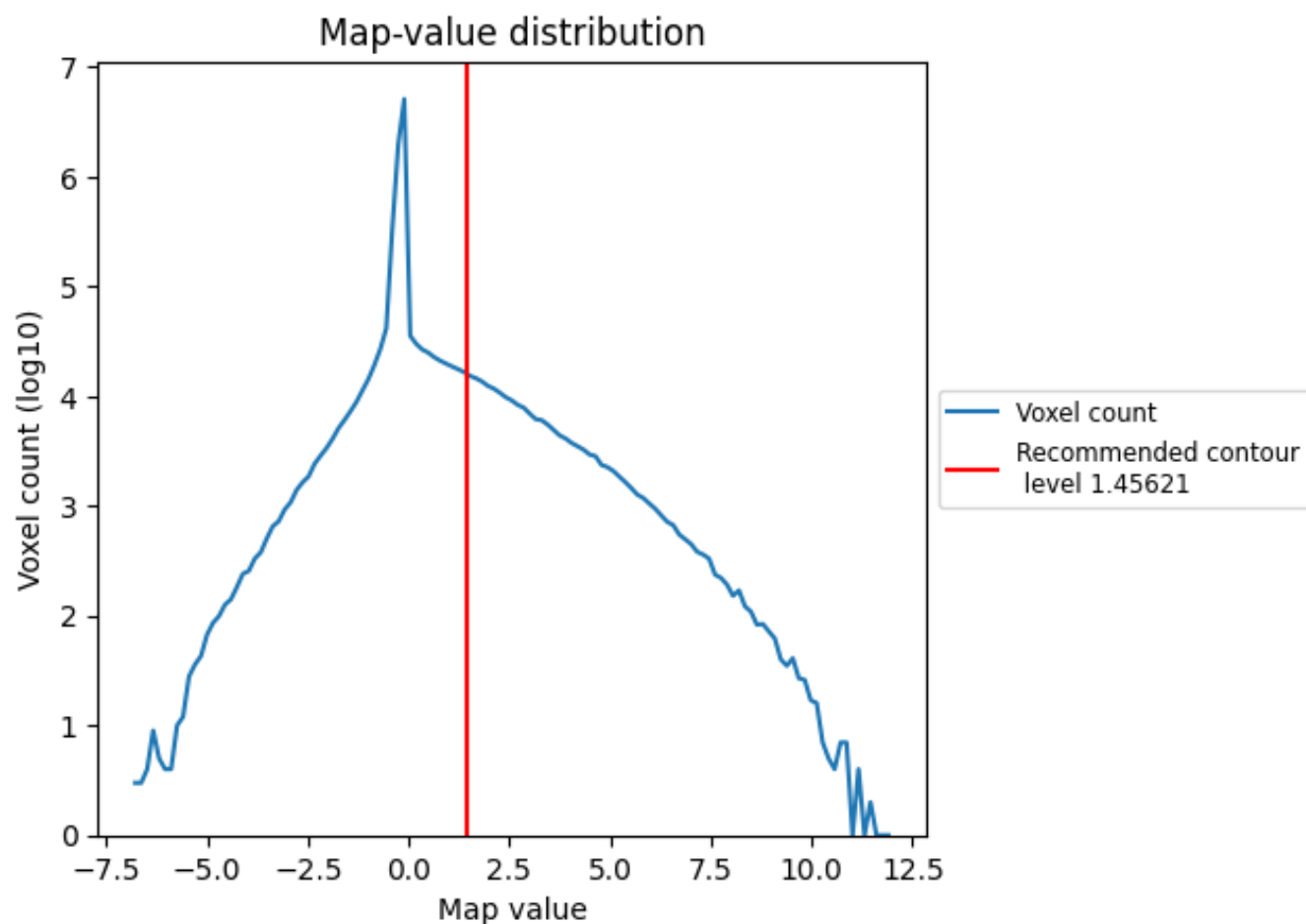
6.6 Mask visualisation

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

7 Map analysis [i](#)

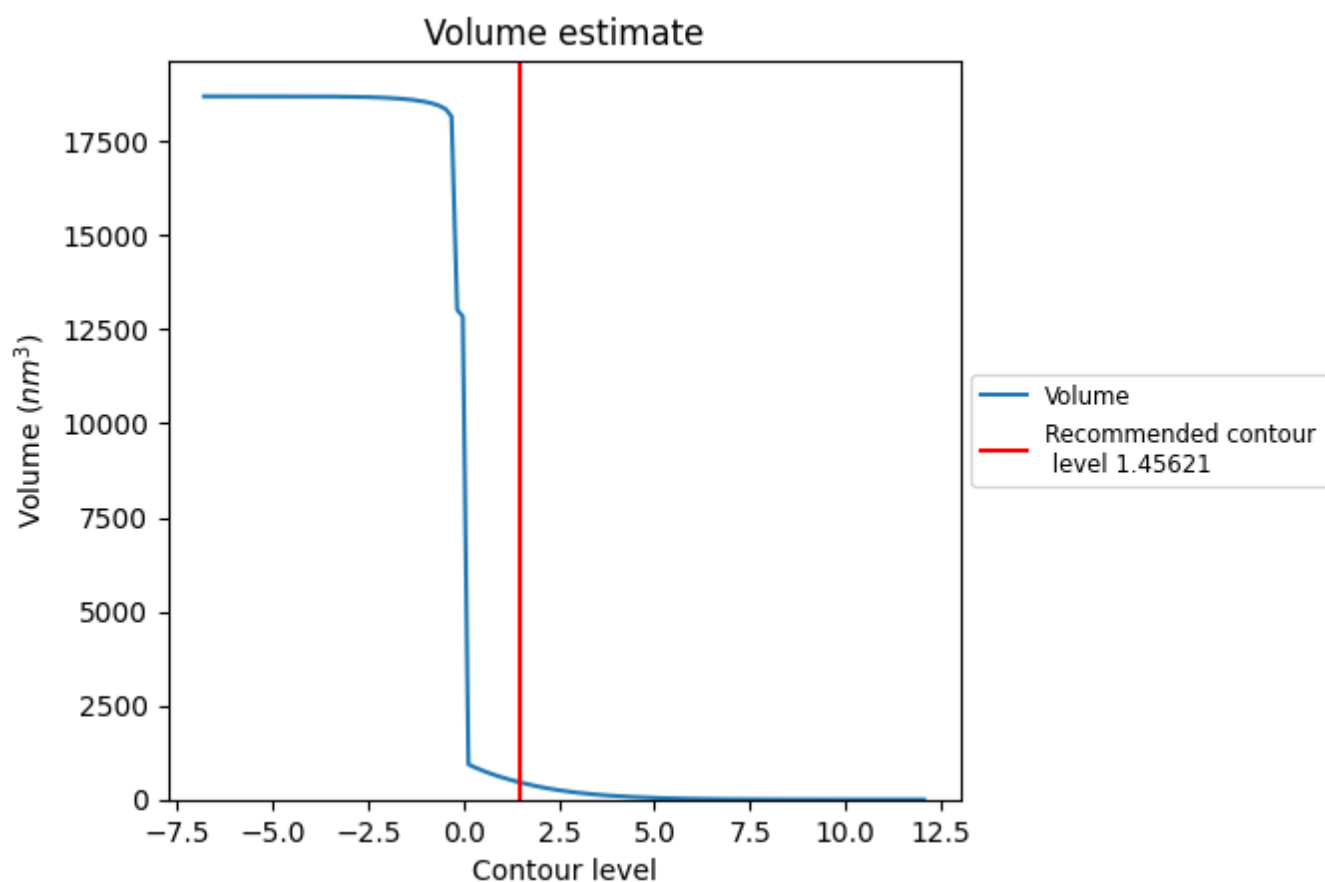
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

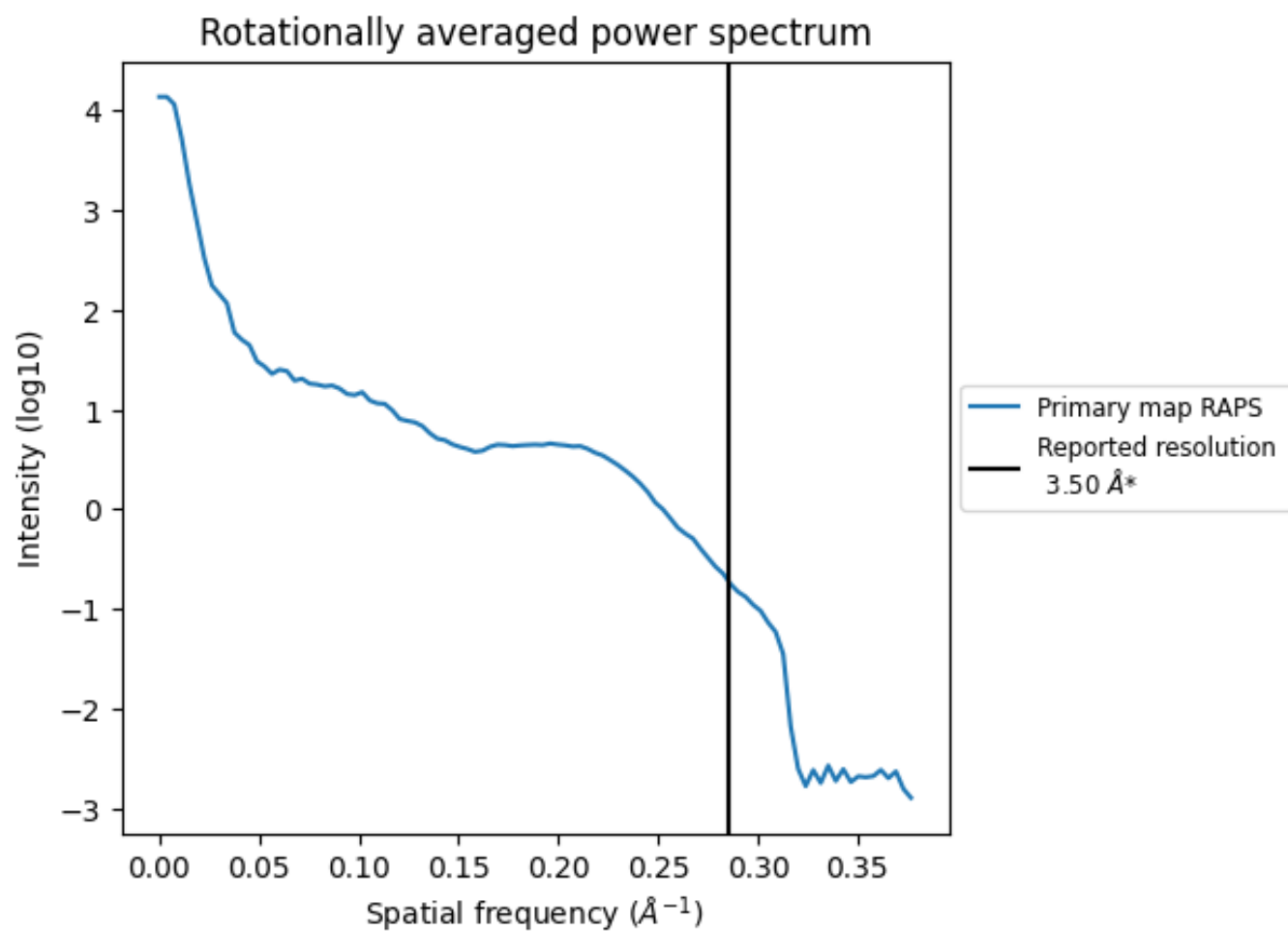
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 462 nm³; this corresponds to an approximate mass of 417 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 0.286 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

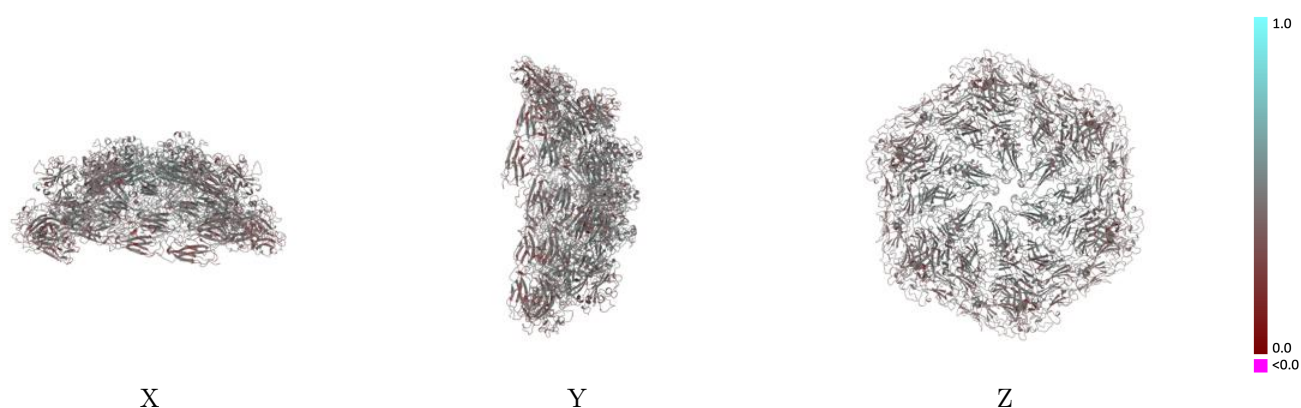
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16492 and PDB model 8C8R. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

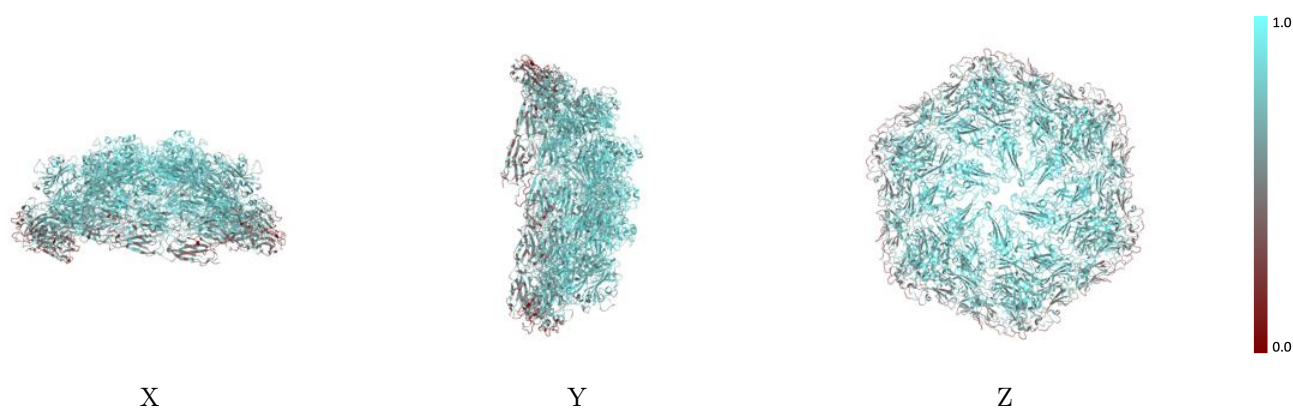
This section was not generated.

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



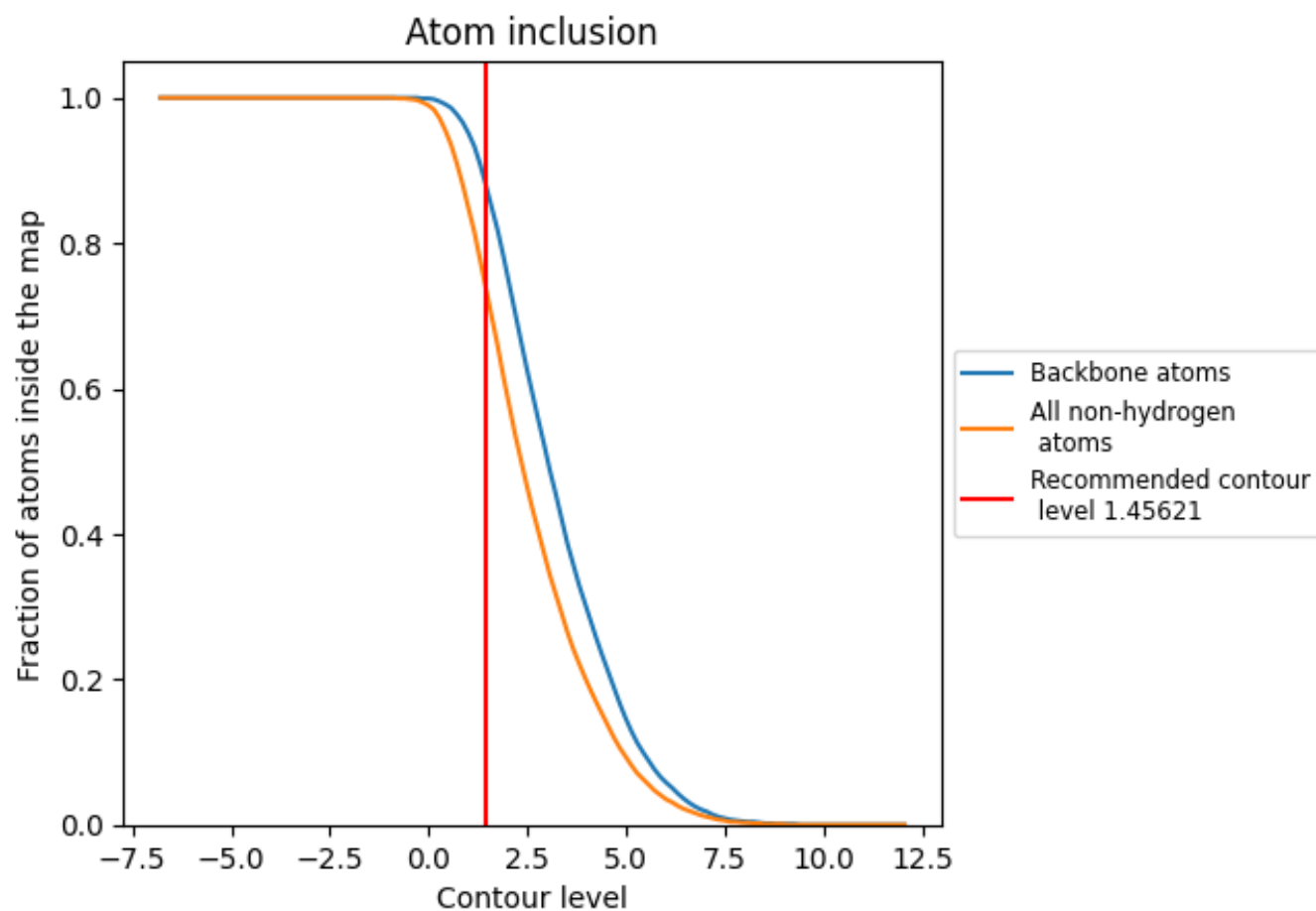
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.45621).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.45621) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.4380
A	0.7430	0.4440
B	0.7370	0.4350
C	0.7300	0.4350
D	0.7430	0.4440
E	0.7340	0.4360
F	0.7290	0.4350

