



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:36 PM UTC

PDB ID : 8C8M / pdb_00008c8m
EMDB ID : EMD-16484
Title : In vitro structure of the Nitrosopumilus maritimus S-layer - Composite map
between two and six-fold symmetrised
Authors : von Kuegelgen, A.; Bharat, T.
Deposited on : 2023-01-20
Resolution : 2.87 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:

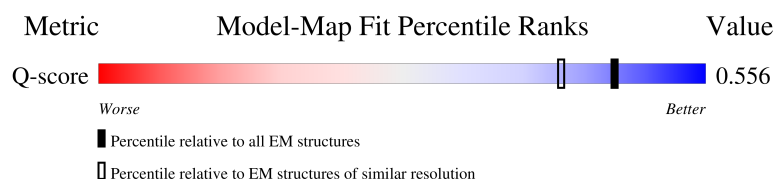
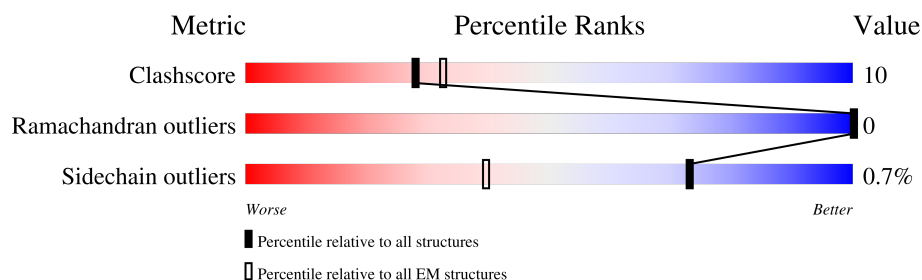
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.87 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	12062 (2.37 - 3.37)

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	72% 19% 9%
1	F	1734	72% 19% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 70506 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.

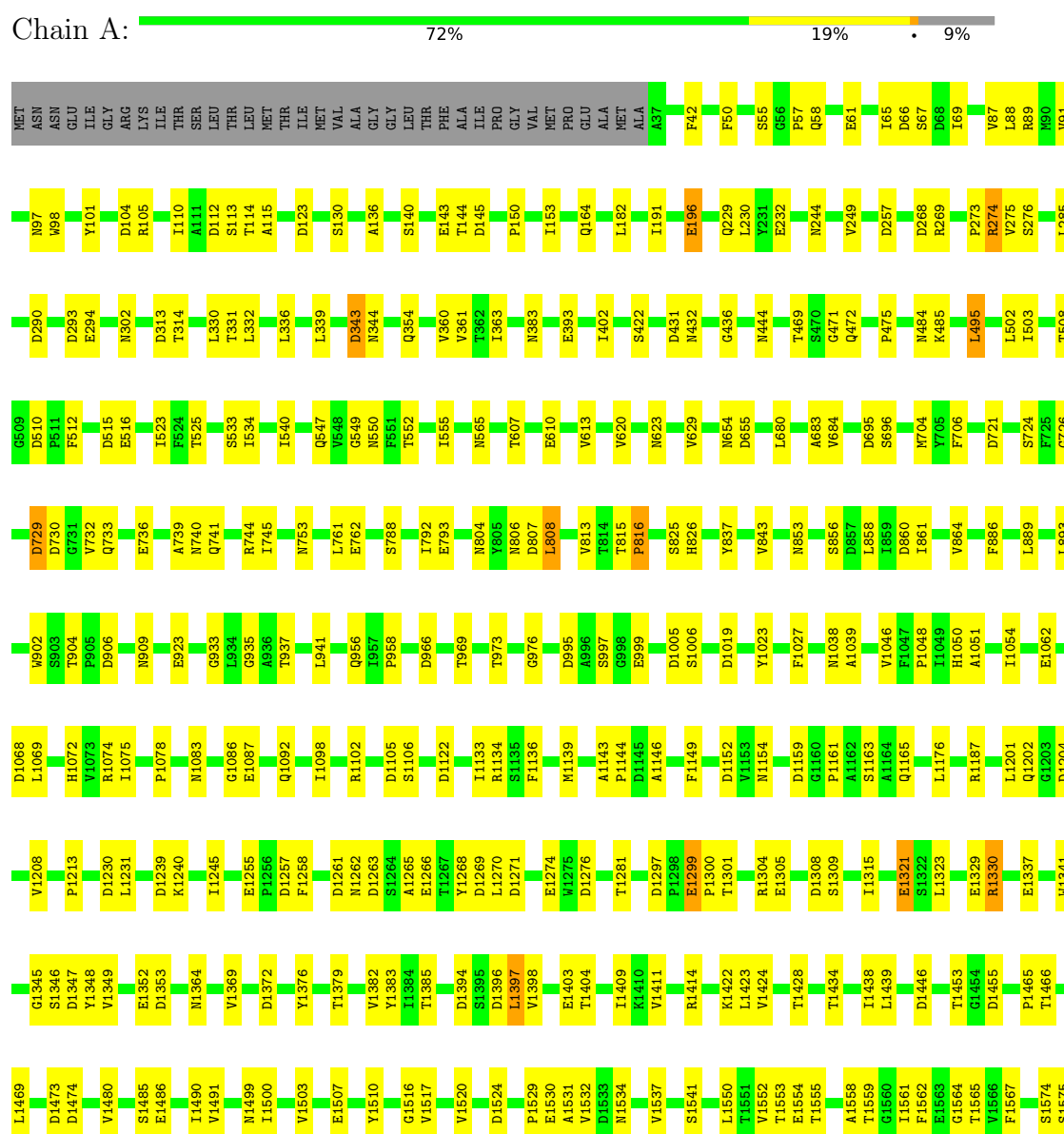
- Molecule 1 is a protein called Cell surface protein.

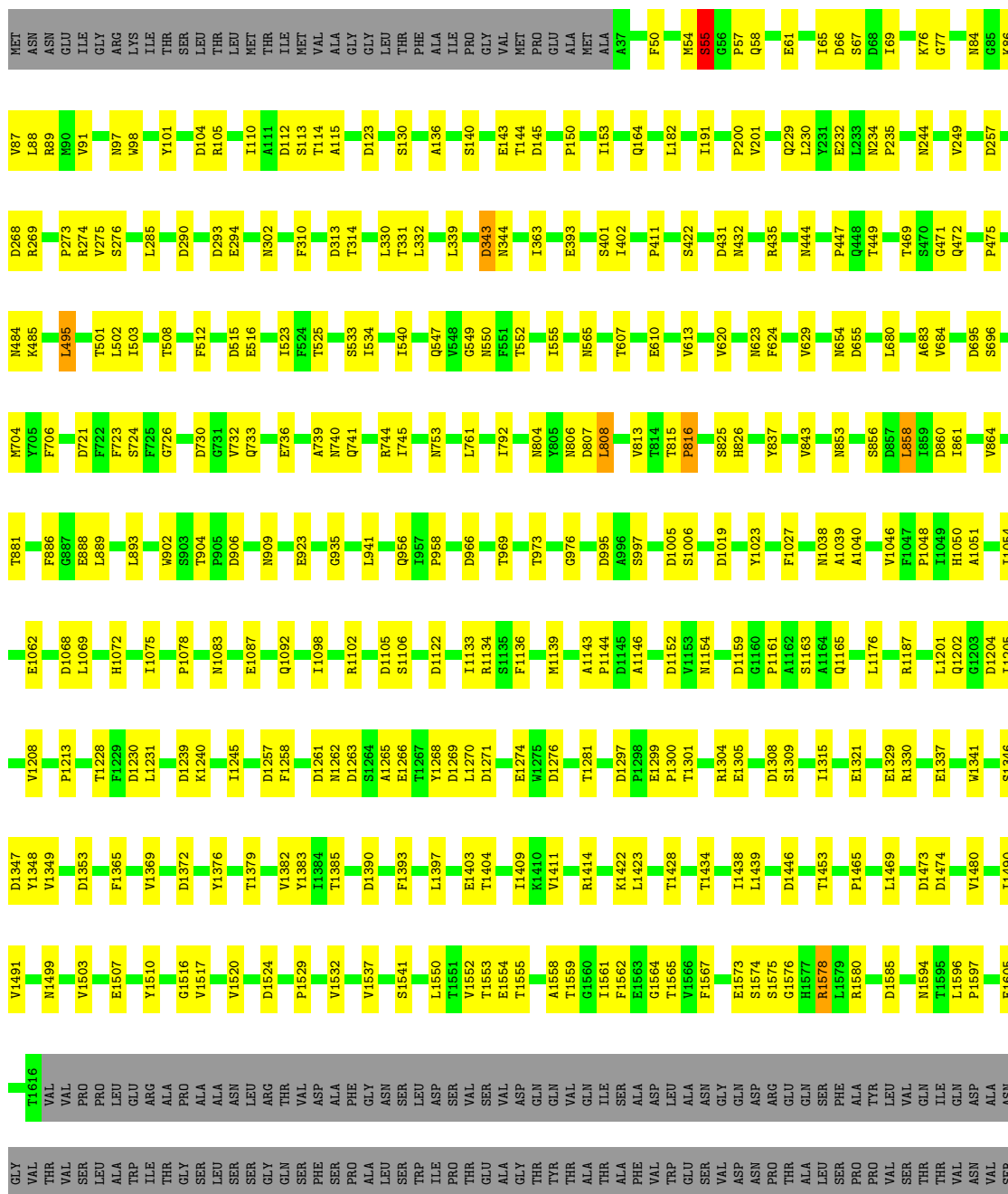
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1580	Total	C	N	O	S	0	0
			11751	7234	1888	2610	19		
1	B	1580	Total	C	N	O	S	0	0
			11751	7234	1888	2610	19		
1	C	1580	Total	C	N	O	S	0	0
			11751	7234	1888	2610	19		
1	D	1580	Total	C	N	O	S	0	0
			11751	7234	1888	2610	19		
1	E	1580	Total	C	N	O	S	0	0
			11751	7234	1888	2610	19		
1	F	1580	Total	C	N	O	S	0	0
			11751	7234	1888	2610	19		

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.

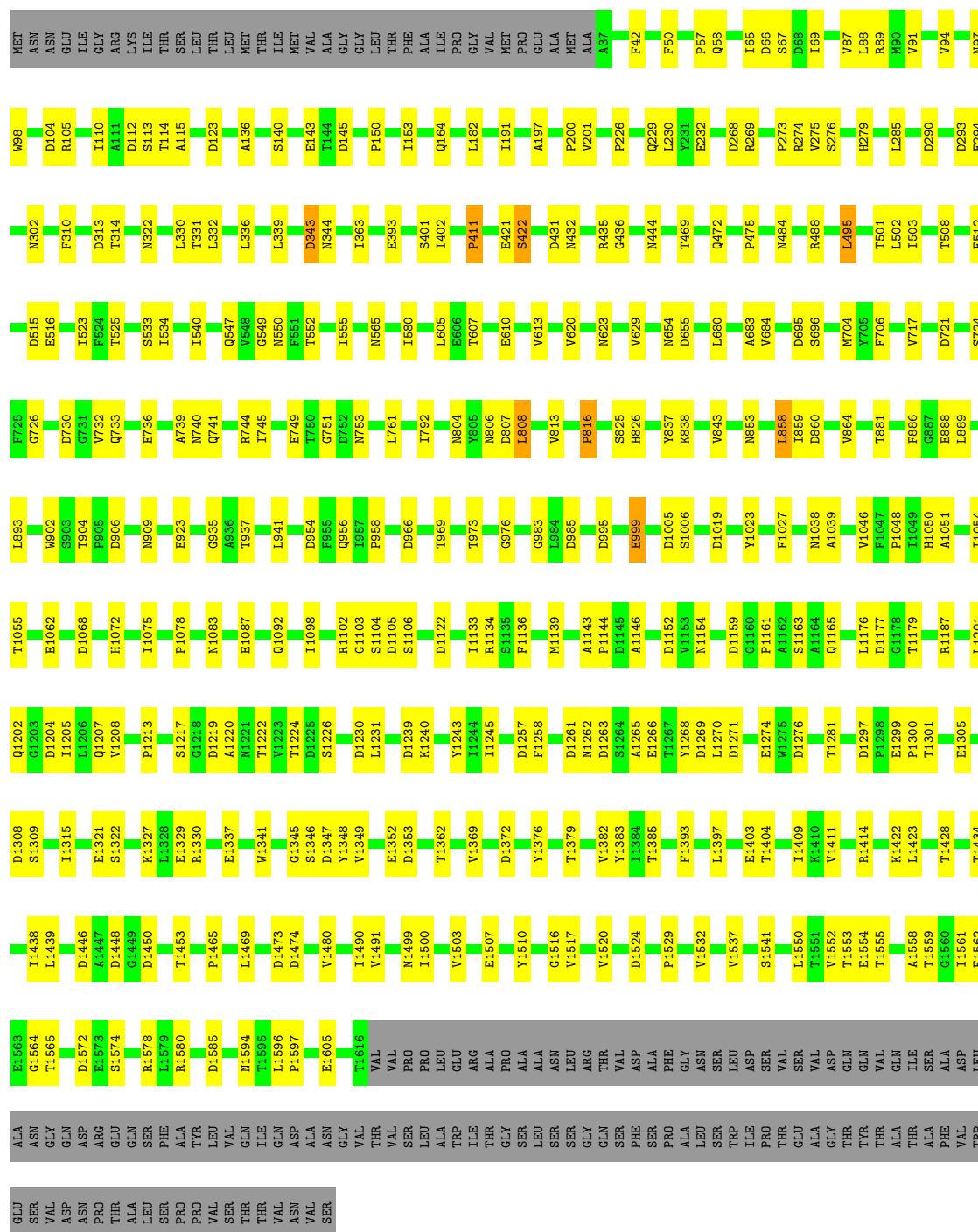
• Molecule 1: Cell surface protein





• Molecule 1: Cell surface protein

Chain C:  72% 19% 9%



• Molecule 1: Cell surface protein

Chain D:  72% 19% 9%

V275	L495	D721	F986	E1062	D1204	Y1348	D1473	N1594	GLN	THR
S276	T501	F722	L889	D1068	V1208	V1349	D1474	T1595	ILE	THR
L285	L502	F723	L893	L1069	P1213	E1352	V1480	L1596	GLN	THR
D290	I503	S724	F902	H1072	D1230	D1353	V1491	P1597	ASP	ASN
D293	T508	F725	S903	I1073	L1231	F1365	V1499	E1605	ALA	VAL
E294	F512	G726	T904	A1074	L1231	V1369	N1499	T1616	GLY	GLY
N302	D515	G731	P905	I1075	D1239	V1369	N1499	VAL	THR	VAL
F310	E516	G732	D906	P1078	K1240	D1372	V1500	PRO	THR	THR
D313	I523	Q733	N909	N1083	I1245	Y1376	V1503	PRO	LEU	LEU
T314	F524	E736	E923	E1087	D1257	T1379	E1507	GLU	THR	THR
T331	T525	A739	G935	Q1092	F1258	Y1510	Y1510	ARG	ILE	THR
L332	S533	N740	L941	I1098	D1261	V1382	G1516	ALA	ALA	ALA
L336	I534	Q741	L941	I1098	N1262	Y1384	V1517	ALA	ALA	ALA
L339	I540	R744	Q956	R1102	D1263	T1385	V1520	ASN	ALA	ALA
D343	Q547	I745	P957	D1105	S1264	D1390	D1524	LEU	LEU	LEU
N344	G549	E762	P958	S1106	E1265	F1393	P1529	THR	THR	THR
I363	N550	S788	T969	D1122	T1267	L1397	V1532	VAL	THR	THR
N383	F551	T972	T973	I1133	D1270	V1398	V1537	ASP	THR	THR
E393	I555	N804	G976	S1135	E1274	E1403	S1541	ALA	THR	THR
S401	T607	Y805	D995	F1136	D1276	T1404	L1550	LEU	THR	THR
I402	E610	N806	E999	D1145	T1281	V1411	T1551	VAL	THR	THR
P411	V613	D807	I1000	A1146	D1297	R1414	V1552	GLN	THR	THR
S422	V620	L808	D1005	A1146	PH298	E1554	T1553	ASP	THR	THR
D431	N623	T814	S1006	F1149	E1299	K1422	E1558	GLN	THR	THR
N432	F624	T815	D1019	N1154	T1301	L1423	G1560	VAL	THR	THR
R435	V629	P816	Y1023	N1154	R1304	T1428	I1561	ILE	THR	THR
N444	N654	S825	F1027	D1159	E1308	T1434	F1562	SER	THR	THR
P447	D655	H826	N1038	Q1165	S1309	D1438	E1563	ALA	THR	THR
Q448	L680	Y837	A1039	L1176	E1321	L1439	G1564	ASP	THR	THR
T449	A683	V843	A1040	L1176	E1321	D1446	V1566	VAL	THR	THR
T469	V684	N853	V1046	Q1165	E1329	A1447	F1567	GLN	THR	THR
S470	P684	S856	F1047	Q1165	R1330	D1448	S1574	ASP	THR	THR
G471	D695	D857	P1048	L1176	E1337	G1449	S1575	ARG	THR	THR
P475	S696	L858	I1049	L1176	E1337	D1450	G1576	GLU	THR	THR
N485	T704	D860	H1050	R1187	W1341	T1453	H1577	GLN	THR	THR
K485	T706	I861	A1051	L1201	S1346	P1465	L1579	ALA	THR	THR
		V864	T1055	Q1202	S1346	L1469	D1585	TYR	THR	THR
				G1203	D1347			VAL	THR	THR

● Molecule 1: Cell surface protein

Chain F: 72% 19% 9%

MET	W98	D290	F512	MET	ASN	THR
ASN	D104	D293	D515	ASN	ASN	THR
GLU	R105	E294	E516	GLU	GLU	THR
ILE	I110	N302	I523	ILE	ILE	THR
ASN	A111	F310	F524	ASN	ASN	THR
GLY	D112	D313	T525	GLY	GLY	THR
ARG	S113	T314	S533	ARG	ARG	THR
LYS	A115	N322	I534	LYS	LYS	THR
THR	D123	L330	I540	THR	THR	THR
LEU	S130	T331	Q547	LEU	LEU	THR
THR	A136	R332	V548	THR	THR	THR
LEU	S140	R333	G549	LEU	LEU	THR
ALA	E143	T334	N550	ALA	ALA	THR
GLY	T335	T336	F551	GLY	GLY	THR
GLY	D144	T336	T552	GLY	GLY	THR
GLY	D145	D343	I555	GLY	GLY	THR
THR	P150	N344	N565	THR	THR	THR
PHE	T153	I363	I580	PHE	PHE	THR
ALA	Q164	E393	T607	ALA	ALA	THR
ALA	L182	S401	E610	ALA	ALA	THR
THR	T191	I402	V613	THR	THR	THR
PRO	A197	P411	V620	PRO	PRO	THR
ALA	P200	E421	N623	ALA	ALA	THR
ALA	V201	S422	V629	ALA	ALA	THR
ALA	P226	D431	N654	ALA	ALA	THR
ALA	Q229	M432	D655	ALA	ALA	THR
ALA	L230	R435	L680	ALA	ALA	THR
ALA	Y231	C436	A683	ALA	ALA	THR
THR	E232	M444	V684	THR	THR	THR
THR	S251	T469	D695	THR	THR	THR
THR	D268	Q472	S696	THR	THR	THR
THR	R269	P475	M704	THR	THR	THR
THR	P273	M484	Y705	THR	THR	THR
THR	R274	R488	F706	THR	THR	THR
THR	V275	L495	V717	THR	THR	THR
THR	S276	T501	D721	THR	THR	THR
THR	H279	L502	S724	THR	THR	THR
THR	L285	I503		THR	THR	THR
THR	N97			THR	THR	THR

LEU	SER	R1578	D1450	K1327	I1205	E1062	L893	F725
SER	PHE	L1579	T1453	R1330	L1206	D1068	W902	G726
PRO	ALA	R1580	P1465	E1337	Q1207	L1069	S903	D730
PRO	TYR	D1585	L1469	W1341	V1208	T904	T904	G731
VAL	LEU	N1594	D1473	G1345	P1213	H1072	P905	V732
THR	GLN	T1595	D1474	D1347	S1217	I1075	D906	Q733
THR	ILE	L1596	V1480	Y1348	G1218	P1078	N909	E736
VAL	ASP	P1597	I1490	V1349	D1219	E923	A739	A739
ASN	ALA	E1605	V1491	E1352	A1220	N1083	N740	N740
GLY	ASN	T1616	N1499	D1353	N1221	E1087	G935	R744
VAL	VAL	VAL	I1500	V1369	V1223	Q1092	A936	I745
THR	VAL	PRO	V1503	D1372	T1224	Q1092	T937	E749
SER	PRO	LEU	E1507	Y1376	S1226	I1098	L941	T750
THR	ALA	ALA	Y1510	T1379	D1230	R1102	D954	G751
LEU	ALA	ASN	G1516	V1382	L1231	Q956	F955	D752
SER	ASN	LEU	V1517	Y1383	D1239	S1103	N957	N753
SER	SER	GLY	V1520	T1385	K1240	S1104	P958	L761
GLY	GLN	THR	D1524	F1393	I1245	D1105	D966	E762
THR	THR	VAL	P1529	L1397	D1257	S1106	T969	S788
ASP	PHE	ALA	V1532	D1399	F1258	R1134	T973	I792
PRO	PRO	ALA	V1537	E1403	D1261	F1135	G976	N804
THR	ASP	ASP	S1541	T1404	N1262	F1136	G983	Y805
GLU	ALA	GLY	L1550	K1409	S1264	M1139	D985	N806
ALA	VAL	ASP	T1551	T1410	E1265	A1143	D995	D807
ASP	ASP	VAL	V1552	V1411	T1267	P1144	T999	L808
GLN	GLN	THR	T1553	R1414	E1269	D1145	E999	V813
THR	VAL	VAL	E1554	K1422	L1270	A1146	D1005	T814
THR	ILE	ILE	T1555	L1423	D1271	S1006	S1006	T815
ALA	ALA	SER	A1558	T1428	E1274	N1154	D1019	P816
PHE	ALA	ALA	G1560	T1434	V1275	D1152	Y1023	N853
VAL	VAL	ASP	I1561	T1438	D1297	D1159	F1027	L858
THR	LEU	LEU	F1562	L1439	E1299	G1160	N1038	I859
GLU	ALA	ASN	E1563	D1446	P1300	P1161	A1039	D860
SER	ASN	GLY	T1565	A1447	T1301	A1162	V1046	V864
VAL	GLN	GLN	V1566	D1448	D1308	Q1165	F1047	F886
ASN	ASP	ASP	F1567	G1449	S1309	L1176	T1049	L889
THR	THR	THR	S1574		I1315	R1187	H1050	
PRO	PRO	GLU			E1321	L1201	A1051	
ALA	ALA	GLN			S1322	Q1202	T1054	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	354860	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; RELION refinement with in-built CTF correction. The function is similar to a Wiener filter, so amplitude correction included.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.5	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	10.250	Depositor
Minimum map value	-4.662	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.422	Depositor
Recommended contour level	1.05514	Depositor
Map size ($\text{\AA}$)	349.44, 349.44, 349.44	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.092, 1.092, 1.092	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	1.02	13/11941 (0.1%)	1.13	20/16339 (0.1%)
1	B	1.01	9/11941 (0.1%)	1.11	14/16339 (0.1%)
1	C	1.01	8/11941 (0.1%)	1.11	15/16339 (0.1%)
1	D	0.99	6/11941 (0.1%)	1.11	15/16339 (0.1%)
1	E	1.01	9/11941 (0.1%)	1.11	12/16339 (0.1%)
1	F	1.01	9/11941 (0.1%)	1.11	15/16339 (0.1%)
All	All	1.01	54/71646 (0.1%)	1.11	91/98034 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	858	LEU	C-O	-13.63	1.07	1.23
1	C	858	LEU	C-O	-13.58	1.07	1.23
1	D	858	LEU	C-O	-12.68	1.08	1.23
1	A	858	LEU	C-O	-12.51	1.08	1.23
1	B	858	LEU	C-O	-12.04	1.09	1.23
1	E	858	LEU	C-O	-11.98	1.09	1.23
1	C	808	LEU	C-O	-9.51	1.12	1.24
1	A	793	GLU	CD-OE2	9.44	1.43	1.25
1	F	808	LEU	C-O	-9.40	1.12	1.24
1	A	1255	GLU	CD-OE1	-8.75	1.08	1.25
1	E	808	LEU	C-O	-8.72	1.13	1.24
1	B	808	LEU	C-O	-8.63	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1428	THR	C-O	-8.59	1.13	1.24
1	D	808	LEU	C-O	-8.51	1.13	1.24
1	A	808	LEU	C-O	-8.48	1.13	1.24
1	E	1397	LEU	C-O	-8.34	1.14	1.23
1	B	1397	LEU	C-O	-8.19	1.14	1.23
1	D	1428	THR	C-O	-7.97	1.14	1.24
1	F	1397	LEU	C-O	-7.76	1.14	1.23
1	C	1428	THR	C-O	-7.62	1.15	1.24
1	A	793	GLU	CD-OE1	-7.57	1.10	1.25
1	A	1397	LEU	C-O	-7.20	1.15	1.23
1	C	1397	LEU	C-O	-7.19	1.15	1.23
1	F	1144	PRO	C-O	-7.03	1.15	1.24
1	C	1144	PRO	C-O	-6.99	1.15	1.24
1	B	1144	PRO	C-O	-6.68	1.15	1.24
1	D	1144	PRO	C-O	-6.64	1.15	1.24
1	E	1144	PRO	C-O	-6.63	1.15	1.24
1	A	1144	PRO	C-O	-6.61	1.15	1.24
1	F	1399	ASP	CG-OD1	-6.55	1.12	1.25
1	D	1397	LEU	C-O	-6.44	1.16	1.23
1	E	201	VAL	C-O	-6.24	1.17	1.24
1	B	201	VAL	C-O	-6.18	1.17	1.24
1	A	196	GLU	CD-OE1	-6.13	1.13	1.25
1	F	475	PRO	C-O	-6.13	1.16	1.23
1	C	475	PRO	C-O	-6.04	1.17	1.23
1	F	1428	THR	C-O	-5.88	1.17	1.24
1	A	1299	GLU	CD-OE1	-5.61	1.14	1.25
1	D	1086	GLY	C-O	-5.59	1.17	1.24
1	E	235	PRO	C-O	-5.53	1.16	1.23
1	B	1428	THR	C-O	-5.51	1.17	1.24
1	E	1399	ASP	CG-OD1	-5.48	1.15	1.25
1	B	235	PRO	C-O	-5.47	1.17	1.23
1	A	1086	GLY	C-O	-5.45	1.17	1.24
1	A	997	SER	C-O	5.34	1.31	1.24
1	F	411	PRO	C-O	-5.27	1.17	1.24
1	C	411	PRO	C-O	-5.26	1.17	1.24
1	A	510	ASP	CG-OD1	-5.25	1.15	1.25
1	E	411	PRO	C-O	-5.08	1.17	1.24
1	B	997	SER	C-O	5.07	1.31	1.24
1	C	201	VAL	C-O	-5.07	1.19	1.24
1	F	201	VAL	C-O	-5.07	1.19	1.24
1	E	1428	THR	C-O	-5.05	1.18	1.24
1	B	411	PRO	C-O	-5.03	1.17	1.24

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	ASP	CA-CB-CG	18.17	130.77	112.60
1	D	58	GLN	CB-CA-C	-8.51	96.00	109.70
1	A	58	GLN	CB-CA-C	-8.49	96.03	109.70
1	C	58	GLN	CB-CA-C	-8.39	96.20	109.70
1	B	58	GLN	CB-CA-C	-7.88	97.01	109.70
1	C	475	PRO	CB-CA-C	-7.70	100.89	110.98
1	F	475	PRO	CB-CA-C	-7.69	100.91	110.98
1	E	58	GLN	CB-CA-C	-7.40	97.78	109.70
1	C	858	LEU	CA-C-O	-7.28	112.93	121.16
1	F	858	LEU	CA-C-O	-7.24	112.98	121.16
1	D	1257	ASP	CA-CB-CG	7.06	119.66	112.60
1	D	475	PRO	CB-CA-C	-7.06	100.54	110.63
1	A	475	PRO	CB-CA-C	-7.05	100.55	110.63
1	A	793	GLU	CG-CD-OE2	7.02	134.55	118.40
1	F	1257	ASP	CA-CB-CG	6.99	119.59	112.60
1	B	858	LEU	CA-C-O	-6.97	113.28	121.16
1	B	1257	ASP	CA-CB-CG	6.96	119.56	112.60
1	E	858	LEU	CA-C-O	-6.95	113.31	121.16
1	F	38	ASN	CB-CA-C	6.94	124.22	110.42
1	E	1257	ASP	CA-CB-CG	6.93	119.53	112.60
1	E	475	PRO	CB-CA-C	-6.84	100.85	110.63
1	B	475	PRO	CB-CA-C	-6.82	100.89	110.63
1	C	1257	ASP	CA-CB-CG	6.75	119.35	112.60
1	D	858	LEU	CA-C-O	-6.67	113.63	121.16
1	A	858	LEU	CA-C-O	-6.66	113.64	121.16
1	F	200	PRO	CA-C-N	6.62	129.63	120.49
1	F	200	PRO	C-N-CA	6.62	129.63	120.49
1	C	200	PRO	CA-C-N	6.60	129.60	120.49
1	C	200	PRO	C-N-CA	6.60	129.60	120.49
1	E	200	PRO	CA-C-N	6.49	129.45	120.49
1	E	200	PRO	C-N-CA	6.49	129.45	120.49
1	B	200	PRO	CA-C-N	6.48	129.43	120.49
1	B	200	PRO	C-N-CA	6.48	129.43	120.49
1	D	999	GLU	CB-CG-CD	6.40	123.48	112.60
1	B	393	GLU	CB-CA-C	-6.01	103.01	111.85
1	E	393	GLU	CB-CA-C	-5.99	103.04	111.85
1	A	729	ASP	CB-CG-OD1	5.98	132.16	118.40
1	C	816	PRO	CB-CA-C	-5.98	103.57	111.23
1	E	816	PRO	CB-CA-C	-5.88	103.70	111.23
1	B	816	PRO	CB-CA-C	-5.86	103.72	111.23
1	A	1257	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	393	GLU	CB-CA-C	-5.72	103.44	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	393	GLU	CB-CA-C	-5.72	103.44	111.85
1	C	393	GLU	CB-CA-C	-5.69	103.49	111.85
1	F	393	GLU	CB-CA-C	-5.68	103.50	111.85
1	F	816	PRO	CB-CA-C	-5.62	103.61	110.98
1	D	343	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	343	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	793	GLU	CG-CD-OE1	-5.49	105.78	118.40
1	A	1321	GLU	CB-CA-C	5.43	118.74	109.24
1	F	501	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	816	PRO	CB-CA-C	-5.39	103.92	110.98
1	F	58	GLN	CB-CA-C	5.39	118.67	109.72
1	C	501	THR	CA-CB-OG1	-5.38	101.53	109.60
1	D	816	PRO	CB-CA-C	-5.35	103.97	110.98
1	E	1078	PRO	CB-CA-C	-5.34	104.27	111.85
1	B	1078	PRO	CB-CA-C	-5.32	104.30	111.85
1	C	550	ASN	CB-CA-C	5.32	120.83	110.30
1	F	550	ASN	CB-CA-C	5.31	120.82	110.30
1	C	343	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	274	ARG	CA-C-O	-5.30	114.80	120.42
1	F	343	ASP	CA-CB-CG	5.29	117.89	112.60
1	D	274	ARG	CA-C-O	-5.27	114.83	120.42
1	D	550	ASN	CB-CA-C	5.27	120.73	110.30
1	A	550	ASN	CB-CA-C	5.26	120.71	110.30
1	A	1321	GLU	CA-C-O	-5.25	113.47	119.41
1	B	1578	ARG	CG-CD-NE	-5.22	100.52	112.00
1	B	550	ASN	CB-CA-C	5.21	120.62	110.30
1	A	91	VAL	CA-C-O	-5.21	114.80	120.84
1	D	91	VAL	CA-C-O	-5.21	114.80	120.84
1	E	550	ASN	CB-CA-C	5.20	120.60	110.30
1	D	1078	PRO	CB-CA-C	-5.19	104.48	111.85
1	C	1362	THR	CB-CA-C	5.19	118.52	109.65
1	A	1078	PRO	CB-CA-C	-5.18	104.49	111.85
1	E	343	ASP	CA-CB-CG	5.11	117.71	112.60
1	C	91	VAL	CA-C-O	-5.11	114.91	120.84
1	C	838	LYS	CA-C-O	-5.11	115.66	121.58
1	D	933	GLY	CA-C-O	-5.10	116.59	121.38
1	A	1323	LEU	CA-C-O	-5.10	115.45	120.80
1	F	91	VAL	CA-C-O	-5.10	114.93	120.84
1	D	1340	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	91	VAL	CA-C-O	-5.07	114.96	120.84
1	C	1078	PRO	CB-CA-C	-5.07	104.65	111.85
1	F	1078	PRO	CB-CA-C	-5.07	104.65	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	1578	ARG	CG-CD-NE	-5.07	100.85	112.00
1	B	55	SER	CA-C-O	-5.05	115.33	120.89
1	A	1578	ARG	CG-CD-NE	-5.05	100.89	112.00
1	B	91	VAL	CA-C-O	-5.04	114.99	120.84
1	F	838	LYS	CA-C-O	-5.04	115.73	121.58
1	A	933	GLY	CA-C-O	-5.04	116.64	121.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	GLU	Sidechain
1	A	729	ASP	Sidechain
1	B	55	SER	Mainchain

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	11751	0	10951	253	0
1	B	11751	0	10951	228	0
1	C	11751	0	10951	259	0
1	D	11751	0	10951	265	0
1	E	11751	0	10949	230	0
1	F	11751	0	10951	256	0
All	All	70506	0	65704	1301	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 (1301) 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:C:1217:SER:CB	1:D:1424:VAL:HG21	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:VAL:HG21	1:F:1217:SER:CB	1.65	1.24
1:C:816:PRO:HD2	1:D:1083:ASN:HD21	1.01	1.14
1:A:1424:VAL:CG2	1:F:1217:SER:HB2	1.82	1.09
1:C:1217:SER:HB2	1:D:1424:VAL:CG2	1.83	1.08
1:D:1330:ARG:HB2	1:D:1364:ASN:OD1	1.53	1.06
1:C:816:PRO:HD2	1:D:1083:ASN:ND2	1.72	1.03
1:C:816:PRO:CD	1:D:1083:ASN:HD21	1.75	1.00
1:A:1329:GLU:OE1	1:A:1486:GLU:OE2	1.78	0.99
1:D:1321:GLU:OE1	1:D:1393:PHE:CZ	2.16	0.99
1:A:1329:GLU:OE1	1:A:1486:GLU:CD	2.06	0.98
1:C:1217:SER:HB2	1:D:1424:VAL:HG21	1.01	0.98
1:D:1363:SER:HB3	1:D:1390:ASP:OD1	1.62	0.98
1:A:1424:VAL:HG21	1:F:1217:SER:HB2	0.99	0.96
1:B:1075:ILE:HD12	1:B:1139:MET:HE1	1.48	0.95
1:E:1075:ILE:HD12	1:E:1139:MET:HE1	1.48	0.94
1:C:985:ASP:OD1	1:D:1394:ASP:OD2	1.85	0.94
1:B:1567:PHE:HD2	1:B:1578:ARG:HG3	1.32	0.93
1:C:1075:ILE:HD12	1:C:1139:MET:HE1	1.50	0.93
1:A:1075:ILE:HD12	1:A:1139:MET:HE1	1.51	0.93
1:A:1394:ASP:OD2	1:F:985:ASP:OD1	1.87	0.92
1:D:1075:ILE:HD12	1:D:1139:MET:HE1	1.51	0.92
1:F:1075:ILE:HD12	1:F:1139:MET:HE1	1.50	0.92
1:D:57:PRO:HG3	1:D:339:LEU:HD22	1.54	0.90
1:C:57:PRO:HG3	1:C:339:LEU:HD22	1.53	0.90
1:C:886:PHE:O	1:D:1301:THR:HG21	1.71	0.90
1:A:57:PRO:HG3	1:A:339:LEU:HD22	1.54	0.90
1:B:57:PRO:HG3	1:B:339:LEU:HD22	1.54	0.90
1:A:1301:THR:HG21	1:F:886:PHE:O	1.72	0.89
1:E:57:PRO:HG3	1:E:339:LEU:HD22	1.54	0.88
1:D:886:PHE:O	1:E:1301:THR:HG21	1.76	0.86
1:D:1321:GLU:OE1	1:D:1393:PHE:CE1	2.28	0.86
1:E:1567:PHE:HD2	1:E:1578:ARG:HG2	1.41	0.85
1:A:1329:GLU:OE1	1:A:1486:GLU:OE1	1.93	0.84
1:A:1567:PHE:HD2	1:A:1578:ARG:HG2	1.42	0.84
1:A:886:PHE:O	1:B:1301:THR:HG21	1.76	0.84
1:D:1567:PHE:HD2	1:D:1578:ARG:HG2	1.42	0.82
1:C:1261:ASP:O	1:C:1266:GLU:OE2	1.98	0.82
1:F:1261:ASP:O	1:F:1266:GLU:OE2	1.98	0.82
1:E:1567:PHE:CD2	1:E:1578:ARG:HG2	2.15	0.81
1:A:1261:ASP:O	1:A:1266:GLU:OE2	1.99	0.81
1:B:1261:ASP:O	1:B:1266:GLU:OE2	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1261:ASP:O	1:E:1266:GLU:OE2	1.99	0.81
1:C:1068:ASP:HB3	1:C:1154:ASN:HD21	1.46	0.80
1:F:1068:ASP:HB3	1:F:1154:ASN:HD21	1.46	0.80
1:B:363:ILE:HD13	1:B:402:ILE:HG23	1.64	0.80
1:D:1261:ASP:O	1:D:1266:GLU:OE2	1.98	0.80
1:D:1567:PHE:CD2	1:D:1578:ARG:HG2	2.16	0.80
1:C:363:ILE:HD13	1:C:402:ILE:HG23	1.63	0.80
1:A:1567:PHE:CD2	1:A:1578:ARG:HG2	2.16	0.80
1:E:1068:ASP:HB3	1:E:1154:ASN:HD21	1.47	0.80
1:A:1352:GLU:OE2	1:B:1578:ARG:CZ	2.30	0.79
1:B:234:ASN:CB	1:C:422:SER:HB3	2.12	0.79
1:F:363:ILE:HD13	1:F:402:ILE:HG23	1.63	0.79
1:D:1068:ASP:HB3	1:D:1154:ASN:HD21	1.48	0.79
1:B:1068:ASP:HB3	1:B:1154:ASN:HD21	1.47	0.79
1:E:363:ILE:HD13	1:E:402:ILE:HG23	1.63	0.79
1:E:234:ASN:CB	1:F:422:SER:HB3	2.13	0.78
1:A:1397:LEU:HD12	1:F:985:ASP:H	1.48	0.78
1:A:1068:ASP:HB3	1:A:1154:ASN:HD21	1.48	0.78
1:C:985:ASP:H	1:D:1397:LEU:HD12	1.49	0.78
1:D:1345:GLY:CA	1:E:1578:ARG:HG3	2.14	0.78
1:A:1330:ARG:HB3	1:A:1364:ASN:HA	1.65	0.77
1:A:363:ILE:HD13	1:A:402:ILE:HG23	1.65	0.77
1:D:363:ILE:HD13	1:D:402:ILE:HG23	1.65	0.77
1:D:1321:GLU:OE2	1:D:1393:PHE:CG	2.37	0.77
1:A:956:GLN:NE2	1:F:813:VAL:HG11	2.01	0.76
1:F:1567:PHE:CD2	1:F:1578:ARG:HG2	2.21	0.76
1:B:449:THR:HG21	1:C:859:ILE:HB	1.68	0.75
1:E:449:THR:HG21	1:F:859:ILE:HB	1.68	0.75
1:B:886:PHE:O	1:C:1301:THR:HG21	1.88	0.74
1:E:886:PHE:O	1:F:1301:THR:HG21	1.86	0.74
1:D:1330:ARG:CB	1:D:1364:ASN:OD1	2.34	0.74
1:F:1567:PHE:HD2	1:F:1578:ARG:HG2	1.52	0.73
1:F:1046:VAL:HG23	1:F:1048:PRO:HD3	1.71	0.73
1:A:815:THR:HG23	1:B:1083:ASN:OD1	1.89	0.73
1:C:813:VAL:HG11	1:D:956:GLN:NE2	2.03	0.73
1:D:825:SER:OG	1:D:995:ASP:O	2.07	0.73
1:F:825:SER:OG	1:F:995:ASP:O	2.06	0.73
1:A:1532:VAL:HB	1:F:1226:SER:OG	1.89	0.72
1:C:816:PRO:CD	1:D:1083:ASN:ND2	2.41	0.72
1:C:825:SER:OG	1:C:995:ASP:O	2.06	0.72
1:C:1046:VAL:HG23	1:C:1048:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:815:THR:HG23	1:E:1083:ASN:OD1	1.89	0.72
1:E:825:SER:OG	1:E:995:ASP:O	2.07	0.72
1:C:1226:SER:OG	1:D:1532:VAL:HB	1.89	0.72
1:D:1596:LEU:HD12	1:D:1597:PRO:HD2	1.72	0.72
1:A:1083:ASN:ND2	1:F:816:PRO:HD2	2.05	0.72
1:B:1046:VAL:HG23	1:B:1048:PRO:HD3	1.72	0.72
1:C:1596:LEU:HD12	1:C:1597:PRO:HD2	1.72	0.72
1:F:1596:LEU:HD12	1:F:1597:PRO:HD2	1.72	0.72
1:B:816:PRO:HD2	1:C:1083:ASN:ND2	2.05	0.72
1:B:1596:LEU:HD12	1:B:1597:PRO:HD2	1.72	0.72
1:A:1596:LEU:HD12	1:A:1597:PRO:HD2	1.72	0.72
1:E:1596:LEU:HD12	1:E:1597:PRO:HD2	1.72	0.72
1:B:825:SER:OG	1:B:995:ASP:O	2.07	0.71
1:A:825:SER:OG	1:A:995:ASP:O	2.07	0.71
1:E:816:PRO:HD2	1:F:1083:ASN:ND2	2.05	0.71
1:D:816:PRO:HD2	1:E:1083:ASN:ND2	2.06	0.71
1:D:1244:ILE:HA	1:D:1363:SER:OG	1.90	0.70
1:A:1046:VAL:HG23	1:A:1048:PRO:HD3	1.72	0.70
1:A:1424:VAL:CG2	1:F:1217:SER:CB	2.54	0.70
1:C:985:ASP:HB3	1:D:1396:ASP:O	1.91	0.70
1:D:1330:ARG:HB3	1:D:1364:ASN:HA	1.71	0.70
1:A:816:PRO:HD2	1:B:1083:ASN:ND2	2.06	0.70
1:A:1297:ASP:OD2	1:A:1299:GLU:OE2	2.09	0.69
1:E:1046:VAL:HG23	1:E:1048:PRO:HD3	1.72	0.69
1:B:435:ARG:NH1	1:C:937:THR:O	2.26	0.69
1:C:816:PRO:HG2	1:D:1083:ASN:ND2	2.07	0.69
1:D:1046:VAL:HG23	1:D:1048:PRO:HD3	1.72	0.69
1:E:435:ARG:NH1	1:F:937:THR:O	2.25	0.69
1:E:1517:VAL:HG22	1:E:1565:THR:HG22	1.74	0.69
1:B:1567:PHE:CD2	1:B:1578:ARG:HG3	2.23	0.69
1:F:1517:VAL:HG22	1:F:1565:THR:HG22	1.75	0.69
1:A:1517:VAL:HG22	1:A:1565:THR:HG22	1.74	0.69
1:A:1396:ASP:O	1:F:985:ASP:HB3	1.93	0.69
1:C:1217:SER:CB	1:D:1424:VAL:CG2	2.54	0.69
1:D:1517:VAL:HG22	1:D:1565:THR:HG22	1.74	0.69
1:E:813:VAL:HG11	1:F:956:GLN:NE2	2.09	0.69
1:A:1398:VAL:HG22	1:F:983:GLY:CA	2.23	0.68
1:B:813:VAL:HG11	1:C:956:GLN:NE2	2.08	0.68
1:C:1345:GLY:HA3	1:D:1578:ARG:HE	1.58	0.68
1:D:1363:SER:CB	1:D:1390:ASP:OD1	2.39	0.68
1:A:1530:GLU:O	1:F:1224:THR:HB	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ASP:O	1:B:444:ASN:HA	1.94	0.68
1:D:1072:HIS:ND1	1:D:1152:ASP:OD1	2.27	0.68
1:E:721:ASP:OD2	1:E:744:ARG:NH2	2.27	0.68
1:B:721:ASP:OD2	1:B:744:ARG:NH2	2.27	0.68
1:C:983:GLY:CA	1:D:1398:VAL:HG22	2.22	0.67
1:B:1517:VAL:HG22	1:B:1565:THR:HG22	1.75	0.67
1:C:1517:VAL:HG22	1:C:1565:THR:HG22	1.75	0.67
1:E:343:ASP:O	1:E:444:ASN:HA	1.94	0.67
1:E:816:PRO:HD2	1:F:1083:ASN:HD21	1.60	0.67
1:C:1224:THR:HB	1:D:1530:GLU:O	1.94	0.67
1:C:1345:GLY:O	1:D:1576:GLY:HA3	1.95	0.67
1:D:721:ASP:OD2	1:D:744:ARG:NH2	2.27	0.67
1:F:629:VAL:HG11	1:F:704:MET:HE1	1.77	0.67
1:A:1531:ALA:CB	1:F:1207:GLN:OE1	2.44	0.66
1:E:1072:HIS:ND1	1:E:1152:ASP:OD1	2.28	0.66
1:A:1072:HIS:ND1	1:A:1152:ASP:OD1	2.27	0.66
1:F:721:ASP:OD2	1:F:744:ARG:NH2	2.28	0.66
1:F:1072:HIS:ND1	1:F:1152:ASP:OD1	2.28	0.66
1:B:84:ASN:HD22	1:C:421:GLU:CB	2.09	0.66
1:C:1072:HIS:ND1	1:C:1152:ASP:OD1	2.28	0.66
1:D:1345:GLY:HA3	1:E:1578:ARG:HG3	1.78	0.66
1:B:886:PHE:HA	1:C:1301:THR:HG21	1.77	0.66
1:A:343:ASP:O	1:A:444:ASN:HA	1.96	0.66
1:A:1578:ARG:HE	1:F:1345:GLY:HA3	1.59	0.66
1:B:1072:HIS:ND1	1:B:1152:ASP:OD1	2.28	0.66
1:A:721:ASP:OD2	1:A:744:ARG:NH2	2.27	0.66
1:B:816:PRO:HD2	1:C:1083:ASN:HD21	1.60	0.65
1:B:923:GLU:OE1	1:B:976:GLY:O	2.15	0.65
1:C:721:ASP:OD2	1:C:744:ARG:NH2	2.28	0.65
1:C:923:GLU:OE1	1:C:976:GLY:O	2.15	0.65
1:E:886:PHE:HA	1:F:1301:THR:HG21	1.78	0.65
1:C:343:ASP:O	1:C:444:ASN:HA	1.96	0.65
1:C:1207:GLN:OE1	1:D:1531:ALA:CB	2.44	0.65
1:C:629:VAL:HG11	1:C:704:MET:HE1	1.78	0.65
1:C:864:VAL:HG11	1:C:935:GLY:HA2	1.79	0.65
1:F:343:ASP:O	1:F:444:ASN:HA	1.96	0.65
1:F:923:GLU:OE1	1:F:976:GLY:O	2.15	0.65
1:A:923:GLU:OE1	1:A:976:GLY:O	2.15	0.65
1:E:84:ASN:HD22	1:F:421:GLU:CB	2.09	0.65
1:A:1576:GLY:HA3	1:F:1345:GLY:O	1.96	0.65
1:D:105:ARG:HA	1:D:230:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:923:GLU:OE1	1:E:976:GLY:O	2.15	0.65
1:A:105:ARG:HA	1:A:230:LEU:HD12	1.78	0.65
1:F:864:VAL:HG11	1:F:935:GLY:HA2	1.79	0.65
1:A:275:VAL:HG12	1:A:275:VAL:O	1.97	0.65
1:B:105:ARG:HA	1:B:230:LEU:HD12	1.79	0.65
1:C:1550:LEU:HD21	1:C:1564:GLY:HA3	1.79	0.65
1:B:275:VAL:HG12	1:B:275:VAL:O	1.97	0.64
1:D:1550:LEU:HD21	1:D:1564:GLY:HA3	1.80	0.64
1:A:1531:ALA:HB2	1:F:1207:GLN:OE1	1.98	0.64
1:B:1550:LEU:HD21	1:B:1564:GLY:HA3	1.79	0.64
1:F:1550:LEU:HD21	1:F:1564:GLY:HA3	1.79	0.64
1:C:1207:GLN:OE1	1:D:1531:ALA:HB2	1.98	0.64
1:D:275:VAL:HG12	1:D:275:VAL:O	1.97	0.64
1:D:343:ASP:O	1:D:444:ASN:HA	1.96	0.64
1:D:629:VAL:HG11	1:D:704:MET:HE1	1.79	0.64
1:D:923:GLU:OE1	1:D:976:GLY:O	2.15	0.64
1:A:1550:LEU:HD21	1:A:1564:GLY:HA3	1.80	0.64
1:C:105:ARG:HA	1:C:230:LEU:HD12	1.80	0.64
1:E:105:ARG:HA	1:E:230:LEU:HD12	1.80	0.64
1:E:1550:LEU:HD21	1:E:1564:GLY:HA3	1.80	0.64
1:A:145:ASP:OD2	1:A:232:GLU:N	2.31	0.63
1:E:145:ASP:OD2	1:E:232:GLU:N	2.32	0.63
1:E:275:VAL:O	1:E:275:VAL:HG12	1.97	0.63
1:F:909:ASN:HB3	1:F:973:THR:HG22	1.81	0.63
1:A:813:VAL:HG11	1:B:956:GLN:NE2	2.14	0.63
1:A:864:VAL:HG11	1:A:935:GLY:HA2	1.80	0.63
1:C:495:LEU:HD12	1:C:503:ILE:HD13	1.81	0.63
1:A:629:VAL:HG11	1:A:704:MET:HE1	1.79	0.63
1:B:86:LYS:HG2	1:C:322:ASN:HB2	1.80	0.63
1:B:629:VAL:HG11	1:B:704:MET:HE1	1.81	0.63
1:B:909:ASN:HB3	1:B:973:THR:HG22	1.81	0.63
1:B:864:VAL:HG11	1:B:935:GLY:HA2	1.81	0.63
1:C:275:VAL:HG12	1:C:275:VAL:O	1.99	0.63
1:D:864:VAL:HG11	1:D:935:GLY:HA2	1.80	0.63
1:C:909:ASN:HB3	1:C:973:THR:HG22	1.81	0.63
1:E:864:VAL:HG11	1:E:935:GLY:HA2	1.81	0.63
1:E:86:LYS:HG2	1:F:322:ASN:HB2	1.80	0.62
1:D:613:VAL:HG22	1:D:623:ASN:HD21	1.64	0.62
1:F:275:VAL:HG12	1:F:275:VAL:O	1.99	0.62
1:A:909:ASN:HB3	1:A:973:THR:HG22	1.81	0.62
1:D:813:VAL:HG11	1:E:956:GLN:NE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:ARG:HA	1:F:230:LEU:HD12	1.80	0.62
1:C:816:PRO:CG	1:D:1083:ASN:ND2	2.62	0.62
1:D:1345:GLY:O	1:E:1576:GLY:HA3	2.00	0.62
1:A:1329:GLU:HG3	1:A:1485:SER:HB2	1.81	0.62
1:A:1083:ASN:OD1	1:F:815:THR:HG23	1.99	0.62
1:D:1329:GLU:HG3	1:D:1485:SER:HB2	1.81	0.62
1:A:613:VAL:HG22	1:A:623:ASN:HD21	1.64	0.61
1:B:145:ASP:OD2	1:B:232:GLU:N	2.32	0.61
1:D:495:LEU:HD12	1:D:503:ILE:HD13	1.81	0.61
1:D:1330:ARG:HB3	1:D:1363:SER:O	1.99	0.61
1:A:1466:THR:OG1	1:F:1220:ALA:O	2.18	0.61
1:E:234:ASN:HB2	1:F:422:SER:HB3	1.83	0.61
1:E:909:ASN:HB3	1:E:973:THR:HG22	1.81	0.61
1:A:495:LEU:HD12	1:A:503:ILE:HD13	1.81	0.61
1:E:629:VAL:HG11	1:E:704:MET:HE1	1.81	0.61
1:F:613:VAL:HG22	1:F:623:ASN:HD21	1.66	0.61
1:C:1104:SER:CB	1:D:1455:ASP:OD1	2.48	0.61
1:F:495:LEU:HD12	1:F:503:ILE:HD13	1.81	0.61
1:D:909:ASN:HB3	1:D:973:THR:HG22	1.81	0.61
1:F:1341:TRP:CZ3	1:F:1353:ASP:HB3	2.36	0.61
1:B:1341:TRP:CZ3	1:B:1353:ASP:HB3	2.36	0.60
1:D:145:ASP:OD2	1:D:232:GLU:N	2.31	0.60
1:E:613:VAL:HG22	1:E:623:ASN:HD21	1.66	0.60
1:B:495:LEU:HD12	1:B:503:ILE:HD13	1.83	0.60
1:C:145:ASP:OD2	1:C:232:GLU:N	2.32	0.60
1:E:1341:TRP:CZ3	1:E:1353:ASP:HB3	2.36	0.60
1:A:1341:TRP:CZ3	1:A:1353:ASP:HB3	2.36	0.60
1:C:1341:TRP:CZ3	1:C:1353:ASP:HB3	2.36	0.60
1:C:613:VAL:HG22	1:C:623:ASN:HD21	1.66	0.60
1:E:495:LEU:HD12	1:E:503:ILE:HD13	1.83	0.60
1:D:1341:TRP:CZ3	1:D:1353:ASP:HB3	2.36	0.60
1:B:234:ASN:HB2	1:C:422:SER:HB3	1.83	0.60
1:C:1220:ALA:O	1:D:1466:THR:OG1	2.18	0.60
1:B:87:VAL:HG12	1:B:143:GLU:HB2	1.84	0.60
1:B:1567:PHE:HD2	1:B:1578:ARG:CG	2.11	0.59
1:F:145:ASP:OD2	1:F:232:GLU:N	2.31	0.59
1:F:1269:ASP:OD2	1:F:1271:ASP:OD2	2.21	0.59
1:B:613:VAL:HG22	1:B:623:ASN:HD21	1.67	0.59
1:E:1269:ASP:OD2	1:E:1271:ASP:OD2	2.21	0.59
1:A:1269:ASP:OD2	1:A:1271:ASP:OD2	2.21	0.59
1:B:1269:ASP:OD2	1:B:1271:ASP:OD2	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1455:ASP:OD1	1:F:1104:SER:CB	2.51	0.59
1:D:1321:GLU:CD	1:D:1393:PHE:CG	2.81	0.59
1:E:1352:GLU:OE2	1:F:1578:ARG:NH2	2.35	0.59
1:D:1269:ASP:OD2	1:D:1271:ASP:OD2	2.21	0.58
1:E:87:VAL:HG12	1:E:143:GLU:HB2	1.84	0.58
1:B:739:ALA:HB2	1:B:792:ILE:CG1	2.34	0.58
1:C:1201:LEU:HD12	1:C:1347:ASP:HB3	1.86	0.58
1:C:1269:ASP:OD2	1:C:1271:ASP:OD2	2.21	0.58
1:B:1102:ARG:NH2	1:B:1161:PRO:O	2.37	0.58
1:F:1102:ARG:NH2	1:F:1161:PRO:O	2.37	0.58
1:F:1201:LEU:HD12	1:F:1347:ASP:HB3	1.85	0.58
1:C:1438:ILE:HB	1:C:1469:LEU:HD23	1.85	0.58
1:A:1102:ARG:NH2	1:A:1161:PRO:O	2.37	0.58
1:B:1438:ILE:HB	1:B:1469:LEU:HD23	1.85	0.58
1:C:302:ASN:HB2	1:C:402:ILE:HD12	1.86	0.58
1:F:302:ASN:HB2	1:F:402:ILE:HD12	1.86	0.58
1:B:540:ILE:HA	1:B:547:GLN:OE1	2.04	0.58
1:D:1321:GLU:OE1	1:D:1393:PHE:CE2	2.55	0.58
1:D:540:ILE:HA	1:D:547:GLN:OE1	2.04	0.58
1:A:540:ILE:HA	1:A:547:GLN:OE1	2.04	0.57
1:B:1201:LEU:HD12	1:B:1347:ASP:HB3	1.86	0.57
1:E:77:GLY:H	1:F:94:VAL:HG21	1.69	0.57
1:F:1019:ASP:OD1	1:F:1262:ASN:ND2	2.37	0.57
1:D:1321:GLU:CD	1:D:1393:PHE:CD1	2.82	0.57
1:E:1102:ARG:NH2	1:E:1161:PRO:O	2.37	0.57
1:F:540:ILE:HA	1:F:547:GLN:OE1	2.04	0.57
1:D:302:ASN:HB2	1:D:402:ILE:HD12	1.85	0.57
1:E:1201:LEU:HD12	1:E:1347:ASP:HB3	1.86	0.57
1:C:1102:ARG:NH2	1:C:1161:PRO:O	2.37	0.57
1:D:1438:ILE:HB	1:D:1469:LEU:HD23	1.85	0.57
1:C:739:ALA:HB2	1:C:792:ILE:CG1	2.35	0.57
1:A:302:ASN:HB2	1:A:402:ILE:HD12	1.85	0.57
1:A:816:PRO:HD2	1:B:1083:ASN:HD21	1.69	0.57
1:C:1019:ASP:OD1	1:C:1262:ASN:ND2	2.37	0.57
1:E:302:ASN:HB2	1:E:402:ILE:HD12	1.87	0.57
1:F:279:HIS:CE1	1:F:488:ARG:HD3	2.40	0.57
1:F:1092:GLN:HG2	1:F:1213:PRO:HG3	1.87	0.57
1:A:1019:ASP:OD1	1:A:1262:ASN:ND2	2.38	0.57
1:A:1201:LEU:HD12	1:A:1347:ASP:HB3	1.86	0.57
1:A:1438:ILE:HB	1:A:1469:LEU:HD23	1.86	0.57
1:C:1499:ASN:N	1:C:1524:ASP:OD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1102:ARG:NH2	1:D:1161:PRO:O	2.37	0.57
1:D:1537:VAL:O	1:D:1550:LEU:N	2.38	0.57
1:F:1438:ILE:HB	1:F:1469:LEU:HD23	1.85	0.57
1:A:739:ALA:HB2	1:A:792:ILE:CG1	2.35	0.56
1:B:1019:ASP:OD1	1:B:1262:ASN:ND2	2.38	0.56
1:E:540:ILE:HA	1:E:547:GLN:OE1	2.04	0.56
1:B:77:GLY:H	1:C:94:VAL:HG21	1.69	0.56
1:B:302:ASN:HB2	1:B:402:ILE:HD12	1.86	0.56
1:C:1537:VAL:O	1:C:1550:LEU:N	2.38	0.56
1:D:739:ALA:HB2	1:D:792:ILE:CG1	2.35	0.56
1:E:1537:VAL:O	1:E:1550:LEU:N	2.38	0.56
1:F:1537:VAL:O	1:F:1550:LEU:N	2.38	0.56
1:C:540:ILE:HA	1:C:547:GLN:OE1	2.04	0.56
1:F:739:ALA:HB2	1:F:792:ILE:CG1	2.35	0.56
1:A:1092:GLN:HG2	1:A:1213:PRO:HG3	1.87	0.56
1:A:1537:VAL:O	1:A:1550:LEU:N	2.38	0.56
1:E:739:ALA:HB2	1:E:792:ILE:CG1	2.34	0.56
1:B:886:PHE:CA	1:C:1301:THR:HG21	2.36	0.56
1:E:1438:ILE:HB	1:E:1469:LEU:HD23	1.85	0.56
1:D:1019:ASP:OD1	1:D:1262:ASN:ND2	2.38	0.56
1:E:1092:GLN:HG2	1:E:1213:PRO:HG3	1.88	0.56
1:C:1092:GLN:HG2	1:C:1213:PRO:HG3	1.87	0.56
1:E:1019:ASP:OD1	1:E:1262:ASN:ND2	2.37	0.56
1:E:1376:TYR:CE1	1:E:1382:VAL:HG12	2.41	0.56
1:D:1201:LEU:HD12	1:D:1347:ASP:HB3	1.86	0.56
1:D:1369:VAL:HG23	1:D:1490:ILE:HD12	1.87	0.56
1:A:1376:TYR:CE1	1:A:1382:VAL:HG12	2.41	0.56
1:B:1019:ASP:HB3	1:B:1023:TYR:OH	2.06	0.56
1:B:1376:TYR:CE1	1:B:1382:VAL:HG12	2.41	0.56
1:F:1376:TYR:CE1	1:F:1382:VAL:HG12	2.41	0.56
1:B:1499:ASN:N	1:B:1524:ASP:OD2	2.34	0.56
1:F:1019:ASP:HB3	1:F:1023:TYR:OH	2.06	0.56
1:D:1376:TYR:CE1	1:D:1382:VAL:HG12	2.41	0.55
1:D:1499:ASN:N	1:D:1524:ASP:OD2	2.35	0.55
1:E:1019:ASP:HB3	1:E:1023:TYR:OH	2.06	0.55
1:F:1369:VAL:HG23	1:F:1490:ILE:HD12	1.88	0.55
1:C:1376:TYR:CE1	1:C:1382:VAL:HG12	2.41	0.55
1:E:435:ARG:NH2	1:F:954:ASP:O	2.37	0.55
1:F:322:ASN:C	1:F:322:ASN:OD1	2.48	0.55
1:F:1098:ILE:HG13	1:F:1208:VAL:HG12	1.88	0.55
1:C:322:ASN:OD1	1:C:322:ASN:C	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:886:PHE:CA	1:F:1301:THR:HG21	2.36	0.55
1:E:1098:ILE:HG13	1:E:1208:VAL:HG12	1.88	0.55
1:C:279:HIS:CE1	1:C:488:ARG:HD3	2.40	0.55
1:C:1019:ASP:HB3	1:C:1023:TYR:OH	2.06	0.55
1:B:1369:VAL:HG23	1:B:1490:ILE:HD12	1.88	0.55
1:D:816:PRO:HD2	1:E:1083:ASN:HD21	1.69	0.55
1:B:1098:ILE:HG13	1:B:1208:VAL:HG12	1.88	0.55
1:D:1321:GLU:OE2	1:D:1393:PHE:CD2	2.59	0.55
1:A:1098:ILE:HG13	1:A:1208:VAL:HG12	1.88	0.55
1:D:1019:ASP:HB3	1:D:1023:TYR:OH	2.06	0.55
1:B:1092:GLN:HG2	1:B:1213:PRO:HG3	1.88	0.55
1:B:1537:VAL:O	1:B:1550:LEU:N	2.38	0.55
1:C:1098:ILE:HG13	1:C:1208:VAL:HG12	1.88	0.55
1:B:435:ARG:NH2	1:C:954:ASP:O	2.37	0.55
1:C:1369:VAL:HG23	1:C:1490:ILE:HD12	1.88	0.55
1:A:1369:VAL:HG23	1:A:1490:ILE:HD12	1.89	0.54
1:B:534:ILE:HD13	1:B:549:GLY:HA3	1.89	0.54
1:D:1092:GLN:HG2	1:D:1213:PRO:HG3	1.87	0.54
1:E:1369:VAL:HG23	1:E:1490:ILE:HD12	1.88	0.54
1:A:1019:ASP:HB3	1:A:1023:TYR:OH	2.06	0.54
1:C:150:PRO:HB3	1:C:191:ILE:HG13	1.89	0.54
1:D:1098:ILE:HG13	1:D:1208:VAL:HG12	1.88	0.54
1:D:1269:ASP:OD1	1:D:1270:LEU:N	2.41	0.54
1:C:1269:ASP:OD1	1:C:1270:LEU:N	2.40	0.54
1:A:1269:ASP:OD1	1:A:1270:LEU:N	2.41	0.54
1:C:1297:ASP:OD2	1:C:1299:GLU:OE2	2.26	0.54
1:D:969:THR:HG21	1:D:973:THR:HG23	1.89	0.54
1:A:534:ILE:HD13	1:A:549:GLY:HA3	1.90	0.54
1:B:1269:ASP:OD1	1:B:1270:LEU:N	2.40	0.54
1:F:533:SER:OG	1:F:552:THR:O	2.25	0.54
1:A:1422:LYS:O	1:A:1423:LEU:HD12	2.08	0.54
1:B:547:GLN:HG3	1:B:683:ALA:HB3	1.90	0.54
1:B:1422:LYS:O	1:B:1423:LEU:HD12	2.08	0.54
1:E:534:ILE:HD13	1:E:549:GLY:HA3	1.89	0.54
1:B:150:PRO:HB3	1:B:191:ILE:HG13	1.90	0.54
1:D:1297:ASP:OD2	1:D:1299:GLU:OE2	2.26	0.54
1:D:1422:LYS:O	1:D:1423:LEU:HD12	2.08	0.54
1:C:1422:LYS:O	1:C:1423:LEU:HD12	2.08	0.54
1:E:533:SER:OG	1:E:552:THR:O	2.25	0.54
1:E:1269:ASP:OD1	1:E:1270:LEU:N	2.40	0.54
1:F:150:PRO:HB3	1:F:191:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:813:VAL:HG11	1:F:956:GLN:CD	2.33	0.54
1:A:1398:VAL:HG22	1:F:983:GLY:HA3	1.91	0.53
1:B:1297:ASP:OD2	1:B:1299:GLU:OE2	2.26	0.53
1:E:1265:ALA:HA	1:E:1305:GLU:OE2	2.08	0.53
1:F:534:ILE:HD13	1:F:549:GLY:HA3	1.90	0.53
1:F:1422:LYS:O	1:F:1423:LEU:HD12	2.08	0.53
1:A:1499:ASN:N	1:A:1524:ASP:OD2	2.35	0.53
1:F:1269:ASP:OD1	1:F:1270:LEU:N	2.40	0.53
1:D:436:GLY:O	1:E:861:ILE:HD13	2.08	0.53
1:E:1422:LYS:O	1:E:1423:LEU:HD12	2.08	0.53
1:B:813:VAL:HG11	1:C:956:GLN:CD	2.33	0.53
1:B:1573:GLU:O	1:B:1578:ARG:NH1	2.42	0.53
1:C:525:THR:HG21	1:C:555:ILE:HD13	1.91	0.53
1:E:249:VAL:HG11	1:F:411:PRO:HG2	1.90	0.53
1:E:813:VAL:HG13	1:E:815:THR:HG23	1.91	0.53
1:E:1297:ASP:OD2	1:E:1299:GLU:OE2	2.26	0.53
1:B:1372:ASP:OD2	1:B:1383:TYR:HD2	1.92	0.53
1:C:534:ILE:HD13	1:C:549:GLY:HA3	1.90	0.53
1:D:534:ILE:HD13	1:D:549:GLY:HA3	1.90	0.53
1:E:1499:ASN:N	1:E:1524:ASP:OD2	2.35	0.53
1:C:969:THR:HG21	1:C:973:THR:HG23	1.90	0.53
1:D:1265:ALA:HA	1:D:1305:GLU:OE2	2.08	0.53
1:F:969:THR:HG21	1:F:973:THR:HG23	1.90	0.53
1:A:969:THR:HG21	1:A:973:THR:HG23	1.89	0.53
1:B:813:VAL:HG13	1:B:815:THR:HG23	1.91	0.53
1:B:1532:VAL:HG13	1:B:1554:GLU:HB3	1.91	0.53
1:C:1163:SER:OG	1:C:1165:GLN:OE1	2.21	0.53
1:C:1265:ALA:HA	1:C:1305:GLU:OE2	2.08	0.53
1:C:1372:ASP:OD2	1:C:1383:TYR:HD2	1.92	0.53
1:D:1345:GLY:HA2	1:E:1578:ARG:HG3	1.88	0.53
1:E:150:PRO:HB3	1:E:191:ILE:HG13	1.90	0.53
1:F:1499:ASN:N	1:F:1524:ASP:OD2	2.34	0.53
1:A:1345:GLY:O	1:B:1576:GLY:HA3	2.08	0.53
1:B:249:VAL:HG11	1:C:411:PRO:HG2	1.90	0.53
1:C:436:GLY:O	1:D:861:ILE:HD13	2.09	0.53
1:A:533:SER:OG	1:A:552:THR:O	2.25	0.53
1:A:1102:ARG:NH1	1:A:1204:ASP:OD2	2.42	0.53
1:B:1102:ARG:NH1	1:B:1204:ASP:OD2	2.42	0.53
1:C:401:SER:O	1:C:401:SER:OG	2.22	0.53
1:C:1532:VAL:HG13	1:C:1554:GLU:HB3	1.90	0.53
1:D:1262:ASN:HB2	1:D:1309:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1269:ASP:CG	1:D:1271:ASP:OD2	2.52	0.53
1:D:1372:ASP:OD2	1:D:1383:TYR:HD2	1.92	0.53
1:E:1532:VAL:HG13	1:E:1554:GLU:HB3	1.91	0.53
1:F:704:MET:HE2	1:F:706:PHE:HE1	1.74	0.53
1:A:436:GLY:O	1:B:861:ILE:HD13	2.08	0.52
1:A:1083:ASN:HD21	1:F:816:PRO:HD2	1.73	0.52
1:A:1372:ASP:OD2	1:A:1383:TYR:HD2	1.92	0.52
1:B:739:ALA:HB2	1:B:792:ILE:HG13	1.91	0.52
1:B:1269:ASP:CG	1:B:1271:ASP:OD2	2.52	0.52
1:D:1102:ARG:NH1	1:D:1204:ASP:OD2	2.42	0.52
1:D:1510:TYR:CE1	1:D:1516:GLY:HA2	2.45	0.52
1:E:401:SER:O	1:E:401:SER:OG	2.23	0.52
1:E:547:GLN:HG3	1:E:683:ALA:HB3	1.90	0.52
1:E:704:MET:HE2	1:E:706:PHE:HE1	1.74	0.52
1:E:1269:ASP:CG	1:E:1271:ASP:OD2	2.52	0.52
1:A:1262:ASN:HB2	1:A:1309:SER:OG	2.09	0.52
1:B:1265:ALA:HA	1:B:1305:GLU:OE2	2.08	0.52
1:C:435:ARG:NH1	1:D:937:THR:O	2.42	0.52
1:E:1510:TYR:CE1	1:E:1516:GLY:HA2	2.44	0.52
1:F:1102:ARG:NH1	1:F:1204:ASP:OD2	2.42	0.52
1:F:1574:SER:OG	1:F:1580:ARG:N	2.26	0.52
1:A:999:GLU:HB3	1:B:1304:ARG:NH1	2.25	0.52
1:A:1269:ASP:CG	1:A:1271:ASP:OD2	2.52	0.52
1:B:704:MET:HE2	1:B:706:PHE:HE1	1.74	0.52
1:C:704:MET:HE2	1:C:706:PHE:HE1	1.74	0.52
1:C:1102:ARG:NH1	1:C:1204:ASP:OD2	2.42	0.52
1:C:1104:SER:HB3	1:D:1455:ASP:OD1	2.08	0.52
1:C:1503:VAL:HG22	1:C:1520:VAL:HG23	1.91	0.52
1:D:533:SER:OG	1:D:552:THR:O	2.25	0.52
1:D:1503:VAL:HG22	1:D:1520:VAL:HG23	1.91	0.52
1:F:1297:ASP:OD2	1:F:1299:GLU:OE2	2.26	0.52
1:B:76:LYS:HD2	1:C:94:VAL:O	2.10	0.52
1:C:1262:ASN:HB2	1:C:1309:SER:OG	2.10	0.52
1:A:150:PRO:HB3	1:A:191:ILE:HG13	1.90	0.52
1:A:937:THR:O	1:F:435:ARG:NH1	2.42	0.52
1:A:1265:ALA:HA	1:A:1305:GLU:OE2	2.08	0.52
1:A:1465:PRO:CG	1:F:1219:ASP:HB2	2.39	0.52
1:C:1510:TYR:CE1	1:C:1516:GLY:HA2	2.44	0.52
1:D:150:PRO:HB3	1:D:191:ILE:HG13	1.90	0.52
1:A:547:GLN:HG3	1:A:683:ALA:HB3	1.91	0.52
1:A:1532:VAL:HG13	1:A:1554:GLU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1534:ASN:CG	1:F:1205:ILE:HG12	2.34	0.52
1:B:969:THR:HG21	1:B:973:THR:HG23	1.91	0.52
1:E:502:LEU:HD13	1:E:806:ASN:O	2.10	0.52
1:E:807:ASP:OD1	1:E:808:LEU:N	2.43	0.52
1:E:969:THR:HG21	1:E:973:THR:HG23	1.91	0.52
1:E:1262:ASN:HB2	1:E:1309:SER:OG	2.10	0.52
1:A:1503:VAL:HG22	1:A:1520:VAL:HG23	1.91	0.52
1:C:547:GLN:HG3	1:C:683:ALA:HB3	1.92	0.52
1:C:1269:ASP:CG	1:C:1271:ASP:OD2	2.52	0.52
1:E:1372:ASP:OD2	1:E:1383:TYR:HD2	1.92	0.52
1:A:112:ASP:OD1	1:A:123:ASP:OD2	2.28	0.52
1:B:1411:VAL:HG12	1:B:1480:VAL:HG22	1.92	0.52
1:C:807:ASP:OD1	1:C:808:LEU:N	2.43	0.52
1:D:704:MET:HE2	1:D:706:PHE:HE1	1.75	0.52
1:D:739:ALA:HB2	1:D:792:ILE:HG13	1.92	0.52
1:F:525:THR:HG21	1:F:555:ILE:HD13	1.91	0.52
1:F:1262:ASN:HB2	1:F:1309:SER:OG	2.10	0.52
1:F:1510:TYR:CE1	1:F:1516:GLY:HA2	2.44	0.52
1:A:739:ALA:HB2	1:A:792:ILE:HG13	1.92	0.52
1:E:739:ALA:HB2	1:E:792:ILE:HG13	1.92	0.52
1:F:1372:ASP:OD2	1:F:1383:TYR:HD2	1.92	0.52
1:F:1503:VAL:HG22	1:F:1520:VAL:HG23	1.91	0.52
1:B:807:ASP:OD1	1:B:808:LEU:N	2.43	0.52
1:B:1510:TYR:CE1	1:B:1516:GLY:HA2	2.45	0.52
1:C:1205:ILE:HG12	1:D:1534:ASN:CG	2.34	0.52
1:C:1510:TYR:HE1	1:C:1516:GLY:HA2	1.75	0.52
1:E:1102:ARG:NH1	1:E:1204:ASP:OD2	2.42	0.52
1:F:807:ASP:OD1	1:F:808:LEU:N	2.43	0.52
1:C:1219:ASP:HB2	1:D:1465:PRO:CG	2.39	0.51
1:C:1411:VAL:HG12	1:C:1480:VAL:HG22	1.92	0.51
1:C:1473:ASP:OD1	1:C:1474:ASP:N	2.42	0.51
1:E:525:THR:HG21	1:E:555:ILE:HD13	1.92	0.51
1:F:1532:VAL:HG13	1:F:1554:GLU:HB3	1.90	0.51
1:A:695:ASP:OD2	1:A:696:SER:N	2.43	0.51
1:A:704:MET:HE2	1:A:706:PHE:HE1	1.75	0.51
1:A:861:ILE:HD13	1:F:436:GLY:O	2.10	0.51
1:B:502:LEU:HD13	1:B:806:ASN:O	2.10	0.51
1:C:816:PRO:CG	1:D:1083:ASN:HD21	2.18	0.51
1:C:1055:THR:OG1	1:C:1062:GLU:OE2	2.22	0.51
1:E:886:PHE:C	1:F:1301:THR:HG21	2.36	0.51
1:F:1269:ASP:CG	1:F:1271:ASP:OD2	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:ASN:ND2	1:F:816:PRO:HG2	2.25	0.51
1:D:547:GLN:HG3	1:D:683:ALA:HB3	1.92	0.51
1:E:1163:SER:OG	1:E:1165:GLN:OE1	2.22	0.51
1:B:88:LEU:HD12	1:B:229:GLN:OE1	2.10	0.51
1:B:1503:VAL:HG22	1:B:1520:VAL:HG23	1.91	0.51
1:D:1532:VAL:HG13	1:D:1554:GLU:HB3	1.91	0.51
1:A:956:GLN:CD	1:F:813:VAL:HG11	2.35	0.51
1:A:1446:ASP:OD1	1:A:1453:THR:HA	2.11	0.51
1:A:1578:ARG:HG3	1:F:1345:GLY:CA	2.40	0.51
1:A:724:SER:OG	1:A:740:ASN:ND2	2.44	0.51
1:A:807:ASP:OD1	1:A:808:LEU:N	2.44	0.51
1:A:1411:VAL:HG12	1:A:1480:VAL:HG22	1.92	0.51
1:A:1510:TYR:CE1	1:A:1516:GLY:HA2	2.44	0.51
1:A:1532:VAL:CG2	1:F:1226:SER:HB3	2.41	0.51
1:D:1446:ASP:OD1	1:D:1453:THR:HA	2.11	0.51
1:F:547:GLN:HG3	1:F:683:ALA:HB3	1.92	0.51
1:B:401:SER:O	1:B:401:SER:OG	2.23	0.51
1:B:533:SER:OG	1:B:552:THR:O	2.25	0.51
1:C:739:ALA:HB2	1:C:792:ILE:HG13	1.92	0.51
1:E:1262:ASN:O	1:E:1308:ASP:HB3	2.11	0.51
1:E:1446:ASP:OD1	1:E:1453:THR:HA	2.11	0.51
1:F:695:ASP:OD2	1:F:696:SER:N	2.44	0.51
1:B:525:THR:HG21	1:B:555:ILE:HD13	1.92	0.51
1:B:1262:ASN:HB2	1:B:1309:SER:OG	2.10	0.51
1:D:502:LEU:HD13	1:D:806:ASN:O	2.11	0.51
1:D:695:ASP:OD2	1:D:696:SER:N	2.43	0.51
1:D:1510:TYR:HE1	1:D:1516:GLY:HA2	1.76	0.51
1:D:1574:SER:OG	1:D:1580:ARG:N	2.26	0.51
1:E:76:LYS:HD2	1:F:94:VAL:O	2.10	0.51
1:E:88:LEU:HD12	1:E:229:GLN:OE1	2.10	0.51
1:E:1055:THR:OG1	1:E:1062:GLU:OE2	2.22	0.51
1:E:1503:VAL:HG22	1:E:1520:VAL:HG23	1.91	0.51
1:E:1574:SER:OG	1:E:1580:ARG:N	2.26	0.51
1:F:88:LEU:HD12	1:F:229:GLN:OE1	2.11	0.51
1:A:525:THR:HG21	1:A:555:ILE:HD13	1.93	0.51
1:A:1345:GLY:HA2	1:B:1578:ARG:HB2	1.92	0.51
1:B:695:ASP:OD2	1:B:696:SER:N	2.43	0.51
1:C:695:ASP:OD2	1:C:696:SER:N	2.44	0.51
1:C:1345:GLY:CA	1:D:1578:ARG:HG3	2.41	0.51
1:D:807:ASP:OD1	1:D:808:LEU:N	2.44	0.51
1:D:893:LEU:HD13	1:D:941:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:739:ALA:HB2	1:F:792:ILE:HG13	1.92	0.51
1:F:1411:VAL:HG12	1:F:1480:VAL:HG22	1.92	0.51
1:C:1446:ASP:OD1	1:C:1453:THR:HA	2.11	0.51
1:F:37:ALA:HB2	1:F:251:SER:O	2.11	0.51
1:F:1262:ASN:O	1:F:1308:ASP:HB3	2.11	0.51
1:D:525:THR:HG21	1:D:555:ILE:HD13	1.94	0.50
1:D:1262:ASN:O	1:D:1308:ASP:HB3	2.11	0.50
1:E:695:ASP:OD2	1:E:696:SER:N	2.43	0.50
1:A:88:LEU:HD12	1:A:229:GLN:OE1	2.11	0.50
1:A:502:LEU:HD13	1:A:806:ASN:O	2.11	0.50
1:D:1411:VAL:HG12	1:D:1480:VAL:HG22	1.92	0.50
1:F:1050:HIS:NE2	1:F:1274:GLU:OE1	2.45	0.50
1:B:1446:ASP:OD1	1:B:1453:THR:HA	2.11	0.50
1:E:1050:HIS:NE2	1:E:1274:GLU:OE1	2.45	0.50
1:F:1446:ASP:OD1	1:F:1453:THR:HA	2.11	0.50
1:F:1510:TYR:HE1	1:F:1516:GLY:HA2	1.75	0.50
1:C:1262:ASN:O	1:C:1308:ASP:HB3	2.11	0.50
1:F:502:LEU:HD13	1:F:806:ASN:O	2.12	0.50
1:A:1050:HIS:NE2	1:A:1274:GLU:OE1	2.45	0.50
1:A:1473:ASP:OD1	1:A:1474:ASP:N	2.42	0.50
1:B:1262:ASN:O	1:B:1308:ASP:HB3	2.10	0.50
1:C:1050:HIS:NE2	1:C:1274:GLU:OE1	2.45	0.50
1:D:724:SER:OG	1:D:740:ASN:ND2	2.44	0.50
1:D:1050:HIS:NE2	1:D:1274:GLU:OE1	2.45	0.50
1:A:1163:SER:OG	1:A:1165:GLN:OE1	2.21	0.50
1:A:1262:ASN:O	1:A:1308:ASP:HB3	2.11	0.50
1:B:724:SER:OG	1:B:740:ASN:ND2	2.45	0.50
1:B:1050:HIS:NE2	1:B:1274:GLU:OE1	2.45	0.50
1:C:88:LEU:HD12	1:C:229:GLN:OE1	2.11	0.50
1:C:1385:THR:HG22	1:C:1434:THR:HG22	1.94	0.50
1:D:999:GLU:HG2	1:E:1304:ARG:NH1	2.27	0.50
1:E:1510:TYR:HE1	1:E:1516:GLY:HA2	1.75	0.50
1:F:724:SER:OG	1:F:740:ASN:ND2	2.44	0.50
1:A:1510:TYR:HE1	1:A:1516:GLY:HA2	1.76	0.50
1:B:1385:THR:HG22	1:B:1434:THR:HG22	1.94	0.50
1:C:502:LEU:HD13	1:C:806:ASN:O	2.12	0.50
1:E:1411:VAL:HG12	1:E:1480:VAL:HG22	1.92	0.50
1:C:724:SER:OG	1:C:740:ASN:ND2	2.44	0.50
1:C:1226:SER:HB3	1:D:1532:VAL:CG2	2.41	0.50
1:D:88:LEU:HD12	1:D:229:GLN:OE1	2.11	0.50
1:E:1473:ASP:OD1	1:E:1474:ASP:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1226:SER:HB3	1:D:1532:VAL:HG23	1.94	0.49
1:C:533:SER:OG	1:C:552:THR:O	2.25	0.49
1:D:1385:THR:HG22	1:D:1434:THR:HG22	1.94	0.49
1:E:84:ASN:ND2	1:F:421:GLU:HB3	2.27	0.49
1:F:1438:ILE:HD12	1:F:1529:PRO:HG2	1.95	0.49
1:A:1574:SER:OG	1:A:1580:ARG:N	2.27	0.49
1:B:1163:SER:OG	1:B:1165:GLN:OE1	2.21	0.49
1:B:1510:TYR:HE1	1:B:1516:GLY:HA2	1.76	0.49
1:C:813:VAL:HG11	1:D:956:GLN:CD	2.37	0.49
1:E:893:LEU:HD13	1:E:941:LEU:HD11	1.95	0.49
1:B:84:ASN:ND2	1:C:421:GLU:CB	2.75	0.49
1:B:1276:ASP:HB3	1:B:1281:THR:HG23	1.95	0.49
1:B:1438:ILE:HD12	1:B:1529:PRO:HG2	1.95	0.49
1:C:983:GLY:HA3	1:D:1398:VAL:HG22	1.91	0.49
1:C:1438:ILE:HD12	1:C:1529:PRO:HG2	1.94	0.49
1:E:724:SER:OG	1:E:740:ASN:ND2	2.45	0.49
1:F:1276:ASP:HB3	1:F:1281:THR:HG23	1.95	0.49
1:A:745:ILE:HD11	1:A:761:LEU:HD21	1.94	0.49
1:A:1385:THR:HG22	1:A:1434:THR:HG22	1.94	0.49
1:A:1455:ASP:OD1	1:F:1104:SER:HB3	2.12	0.49
1:A:1578:ARG:CZ	1:F:1352:GLU:OE2	2.61	0.49
1:E:512:PHE:HA	1:E:516:GLU:HG3	1.95	0.49
1:E:745:ILE:HD11	1:E:761:LEU:HD21	1.94	0.49
1:A:512:PHE:HA	1:A:516:GLU:HG3	1.94	0.49
1:B:112:ASP:OD1	1:B:123:ASP:OD2	2.31	0.49
1:C:1122:ASP:HB2	1:C:1133:ILE:HD12	1.95	0.49
1:A:275:VAL:HB	1:A:485:LYS:HE3	1.94	0.49
1:A:893:LEU:HD13	1:A:941:LEU:HD11	1.93	0.49
1:A:1122:ASP:HB2	1:A:1133:ILE:HD12	1.95	0.49
1:B:275:VAL:HB	1:B:485:LYS:HE3	1.95	0.49
1:B:512:PHE:HA	1:B:516:GLU:HG3	1.95	0.49
1:B:745:ILE:HD11	1:B:761:LEU:HD21	1.94	0.49
1:C:512:PHE:HA	1:C:516:GLU:HG3	1.95	0.49
1:C:1276:ASP:HB3	1:C:1281:THR:HG23	1.95	0.49
1:D:512:PHE:HA	1:D:516:GLU:HG3	1.94	0.49
1:D:745:ILE:HD11	1:D:761:LEU:HD21	1.94	0.49
1:F:512:PHE:HA	1:F:516:GLU:HG3	1.95	0.49
1:E:84:ASN:ND2	1:F:421:GLU:CB	2.75	0.49
1:E:730:ASP:HB2	1:E:732:VAL:HG23	1.95	0.49
1:B:1051:ALA:HA	1:B:1054:ILE:HD12	1.95	0.49
1:A:804:ASN:HD21	1:B:1087:GLU:HG3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1276:ASP:HB3	1:A:1281:THR:HG23	1.95	0.49
1:A:1532:VAL:HG23	1:F:1226:SER:HB3	1.94	0.49
1:B:84:ASN:ND2	1:C:421:GLU:HB3	2.27	0.49
1:B:1122:ASP:HB2	1:B:1133:ILE:HD12	1.95	0.49
1:D:1122:ASP:HB2	1:D:1133:ILE:HD12	1.95	0.49
1:B:886:PHE:C	1:C:1301:THR:HG21	2.37	0.48
1:D:275:VAL:HB	1:D:485:LYS:HE3	1.94	0.48
1:D:804:ASN:HD21	1:E:1087:GLU:HG3	1.77	0.48
1:E:902:TRP:CZ2	1:E:958:PRO:HG3	2.48	0.48
1:E:1239:ASP:OD1	1:E:1240:LYS:N	2.46	0.48
1:A:1051:ALA:HA	1:A:1054:ILE:HD12	1.95	0.48
1:D:112:ASP:OD1	1:D:123:ASP:OD2	2.30	0.48
1:E:1051:ALA:HA	1:E:1054:ILE:HD12	1.95	0.48
1:E:1385:THR:HG22	1:E:1434:THR:HG22	1.94	0.48
1:E:1438:ILE:HD12	1:E:1529:PRO:HG2	1.94	0.48
1:A:354:GLN:NE2	1:B:861:ILE:HD12	2.28	0.48
1:A:1075:ILE:CD1	1:A:1139:MET:HE1	2.35	0.48
1:E:1276:ASP:HB3	1:E:1281:THR:HG23	1.95	0.48
1:E:1346:SER:OG	1:E:1348:TYR:O	2.30	0.48
1:F:89:ARG:NH1	1:F:140:SER:O	2.46	0.48
1:F:1385:THR:HG22	1:F:1434:THR:HG22	1.94	0.48
1:B:293:ASP:OD1	1:B:294:GLU:OE1	2.31	0.48
1:B:902:TRP:CZ2	1:B:958:PRO:HG3	2.48	0.48
1:A:1438:ILE:HD12	1:A:1529:PRO:HG2	1.95	0.48
1:D:730:ASP:HB2	1:D:732:VAL:HG23	1.95	0.48
1:D:1163:SER:OG	1:D:1165:GLN:OE1	2.21	0.48
1:D:1346:SER:OG	1:D:1348:TYR:O	2.30	0.48
1:E:275:VAL:HB	1:E:485:LYS:HE3	1.95	0.48
1:F:112:ASP:OD1	1:F:123:ASP:OD2	2.31	0.48
1:F:1239:ASP:OD1	1:F:1240:LYS:N	2.46	0.48
1:A:273:PRO:HG2	1:A:276:SER:OG	2.14	0.48
1:B:1559:THR:HG23	1:B:1561:ILE:H	1.78	0.48
1:C:89:ARG:NH1	1:C:140:SER:O	2.46	0.48
1:E:112:ASP:OD1	1:E:123:ASP:OD2	2.31	0.48
1:A:1087:GLU:HG3	1:F:804:ASN:HD21	1.79	0.48
1:A:1143:ALA:HB3	1:A:1146:ALA:HB2	1.96	0.48
1:A:1352:GLU:CD	1:B:1578:ARG:CZ	2.85	0.48
1:A:1559:THR:HG23	1:A:1561:ILE:H	1.78	0.48
1:F:275:VAL:O	1:F:275:VAL:CG1	2.62	0.48
1:F:1143:ALA:HB3	1:F:1146:ALA:HB2	1.96	0.48
1:F:1346:SER:OG	1:F:1348:TYR:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1559:THR:HG23	1:F:1561:ILE:H	1.78	0.48
1:A:813:VAL:HG11	1:B:956:GLN:CD	2.39	0.48
1:B:893:LEU:HD13	1:B:941:LEU:HD11	1.95	0.48
1:B:1258:PHE:HB3	1:B:1268:TYR:CE2	2.49	0.48
1:C:273:PRO:HG2	1:C:276:SER:OG	2.14	0.48
1:C:902:TRP:CZ2	1:C:958:PRO:HG3	2.49	0.48
1:C:1352:GLU:OE2	1:D:1578:ARG:CZ	2.62	0.48
1:C:1559:THR:HG23	1:C:1561:ILE:H	1.78	0.48
1:D:354:GLN:NE2	1:E:861:ILE:HD12	2.28	0.48
1:D:902:TRP:CZ2	1:D:958:PRO:HG3	2.49	0.48
1:D:1559:THR:HG23	1:D:1561:ILE:H	1.78	0.48
1:E:804:ASN:HD21	1:F:1087:GLU:HG3	1.79	0.48
1:F:902:TRP:CZ2	1:F:958:PRO:HG3	2.49	0.48
1:A:275:VAL:O	1:A:275:VAL:CG1	2.62	0.48
1:A:902:TRP:CZ2	1:A:958:PRO:HG3	2.49	0.48
1:B:730:ASP:HB2	1:B:732:VAL:HG23	1.95	0.48
1:C:112:ASP:OD1	1:C:123:ASP:OD2	2.31	0.48
1:D:110:ILE:O	1:D:113:SER:OG	2.30	0.48
1:D:273:PRO:HG2	1:D:276:SER:OG	2.14	0.48
1:D:1473:ASP:OD1	1:D:1474:ASP:N	2.42	0.48
1:E:89:ARG:NH1	1:E:140:SER:O	2.47	0.48
1:E:1245:ILE:HD12	1:E:1245:ILE:H	1.79	0.48
1:F:1122:ASP:HB2	1:F:1133:ILE:HD12	1.95	0.48
1:C:804:ASN:HD21	1:D:1087:GLU:HG3	1.78	0.48
1:C:1258:PHE:HB3	1:C:1268:TYR:CE2	2.49	0.48
1:D:813:VAL:HG11	1:E:956:GLN:CD	2.39	0.48
1:D:1051:ALA:HA	1:D:1054:ILE:HD12	1.95	0.48
1:A:730:ASP:HB2	1:A:732:VAL:HG23	1.94	0.47
1:B:1143:ALA:HB3	1:B:1146:ALA:HB2	1.95	0.47
1:B:1245:ILE:HD12	1:B:1245:ILE:H	1.79	0.47
1:C:730:ASP:HB2	1:C:732:VAL:HG23	1.95	0.47
1:D:1239:ASP:OD1	1:D:1240:LYS:N	2.46	0.47
1:E:293:ASP:OD1	1:E:294:GLU:OE1	2.31	0.47
1:E:1559:THR:HG23	1:E:1561:ILE:H	1.78	0.47
1:F:1048:PRO:HD2	1:F:1341:TRP:CD1	2.49	0.47
1:C:275:VAL:O	1:C:275:VAL:CG1	2.62	0.47
1:C:1239:ASP:OD1	1:C:1240:LYS:N	2.46	0.47
1:D:1321:GLU:CD	1:D:1393:PHE:CE1	2.92	0.47
1:D:1438:ILE:HD12	1:D:1529:PRO:HG2	1.95	0.47
1:D:1555:THR:OG1	1:D:1559:THR:HG21	2.14	0.47
1:F:293:ASP:OD1	1:F:294:GLU:OE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:VAL:O	1:B:275:VAL:CG1	2.62	0.47
1:B:290:ASP:OD2	1:B:293:ASP:N	2.46	0.47
1:F:273:PRO:HG2	1:F:276:SER:OG	2.14	0.47
1:A:293:ASP:OD1	1:A:294:GLU:OE1	2.32	0.47
1:A:1239:ASP:OD1	1:A:1240:LYS:N	2.46	0.47
1:B:1473:ASP:OD1	1:B:1474:ASP:N	2.42	0.47
1:D:1276:ASP:HB3	1:D:1281:THR:HG23	1.95	0.47
1:D:1403:GLU:HG2	1:D:1404:THR:HG23	1.97	0.47
1:E:1122:ASP:HB2	1:E:1133:ILE:HD12	1.95	0.47
1:F:730:ASP:HB2	1:F:732:VAL:HG23	1.96	0.47
1:F:1051:ALA:HA	1:F:1054:ILE:HD12	1.96	0.47
1:A:89:ARG:NH1	1:A:140:SER:O	2.47	0.47
1:A:104:ASP:OD2	1:A:105:ARG:N	2.48	0.47
1:B:89:ARG:NH1	1:B:140:SER:O	2.47	0.47
1:C:1507:GLU:HB2	1:C:1510:TYR:CE2	2.50	0.47
1:D:1507:GLU:HB2	1:D:1510:TYR:CE2	2.50	0.47
1:E:275:VAL:O	1:E:275:VAL:CG1	2.62	0.47
1:E:1403:GLU:HG2	1:E:1404:THR:HG23	1.97	0.47
1:E:1555:THR:OG1	1:E:1559:THR:HG21	2.14	0.47
1:F:1258:PHE:HB3	1:F:1268:TYR:CE2	2.49	0.47
1:F:1555:THR:OG1	1:F:1559:THR:HG21	2.14	0.47
1:A:1258:PHE:HB3	1:A:1268:TYR:CE2	2.50	0.47
1:B:1239:ASP:OD1	1:B:1240:LYS:N	2.46	0.47
1:C:104:ASP:OD2	1:C:105:ARG:N	2.48	0.47
1:C:1048:PRO:HD2	1:C:1341:TRP:CD1	2.49	0.47
1:C:1245:ILE:HD12	1:C:1245:ILE:H	1.79	0.47
1:C:1555:THR:OG1	1:C:1559:THR:HG21	2.14	0.47
1:F:104:ASP:OD2	1:F:105:ARG:N	2.48	0.47
1:F:290:ASP:OD2	1:F:293:ASP:N	2.47	0.47
1:A:1069:LEU:O	1:A:1154:ASN:ND2	2.47	0.47
1:B:1048:PRO:HD2	1:B:1341:TRP:CD1	2.49	0.47
1:C:525:THR:HG21	1:C:555:ILE:CD1	2.45	0.47
1:C:733:GLN:HB2	1:C:736:GLU:OE2	2.15	0.47
1:C:1143:ALA:HB3	1:C:1146:ALA:HB2	1.96	0.47
1:C:1205:ILE:HG12	1:D:1534:ASN:ND2	2.29	0.47
1:D:1143:ALA:HB3	1:D:1146:ALA:HB2	1.96	0.47
1:D:1596:LEU:HD12	1:D:1597:PRO:CD	2.44	0.47
1:E:234:ASN:HB3	1:F:422:SER:HB3	1.94	0.47
1:E:1507:GLU:HB2	1:E:1510:TYR:CE2	2.50	0.47
1:F:1507:GLU:HB2	1:F:1510:TYR:CE2	2.50	0.47
1:A:607:THR:O	1:A:610:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASN:HB3	1:C:422:SER:HB3	1.94	0.47
1:B:484:ASN:HD21	1:B:753:ASN:HA	1.80	0.47
1:B:1069:LEU:O	1:B:1154:ASN:ND2	2.47	0.47
1:C:1051:ALA:HA	1:C:1054:ILE:HD12	1.96	0.47
1:D:89:ARG:NH1	1:D:140:SER:O	2.47	0.47
1:D:1048:PRO:HD2	1:D:1341:TRP:CD1	2.49	0.47
1:D:1322:SER:HB2	1:D:1327:LYS:HG2	1.96	0.47
1:E:273:PRO:HG2	1:E:276:SER:OG	2.15	0.47
1:B:804:ASN:HD21	1:C:1087:GLU:HG3	1.79	0.47
1:D:104:ASP:OD2	1:D:105:ARG:N	2.48	0.47
1:D:293:ASP:OD1	1:D:294:GLU:OE1	2.32	0.47
1:D:1258:PHE:HB3	1:D:1268:TYR:CE2	2.50	0.47
1:E:1048:PRO:HD2	1:E:1341:TRP:CD1	2.50	0.47
1:E:1258:PHE:HB3	1:E:1268:TYR:CE2	2.49	0.47
1:C:290:ASP:OD2	1:C:293:ASP:N	2.47	0.47
1:C:293:ASP:OD1	1:C:294:GLU:OE1	2.32	0.47
1:C:1322:SER:HB2	1:C:1327:LYS:HG2	1.97	0.47
1:E:607:THR:O	1:E:610:GLU:HG2	2.15	0.47
1:A:290:ASP:OD2	1:A:293:ASP:N	2.46	0.46
1:A:1048:PRO:HD2	1:A:1341:TRP:CD1	2.50	0.46
1:A:1534:ASN:ND2	1:F:1205:ILE:HG12	2.30	0.46
1:B:607:THR:O	1:B:610:GLU:HG2	2.15	0.46
1:B:1507:GLU:HB2	1:B:1510:TYR:CE2	2.50	0.46
1:B:1555:THR:OG1	1:B:1559:THR:HG21	2.14	0.46
1:C:1075:ILE:CD1	1:C:1139:MET:HE1	2.36	0.46
1:D:290:ASP:OD2	1:D:293:ASP:N	2.46	0.46
1:E:84:ASN:HD22	1:F:421:GLU:HB3	1.80	0.46
1:E:104:ASP:OD2	1:E:105:ARG:N	2.48	0.46
1:E:1409:ILE:CD1	1:E:1423:LEU:HD13	2.46	0.46
1:F:525:THR:HG21	1:F:555:ILE:CD1	2.45	0.46
1:F:1403:GLU:HG2	1:F:1404:THR:HG23	1.97	0.46
1:A:1507:GLU:HB2	1:A:1510:TYR:CE2	2.50	0.46
1:B:733:GLN:HB2	1:B:736:GLU:OE2	2.15	0.46
1:C:1403:GLU:HG2	1:C:1404:THR:HG23	1.97	0.46
1:E:733:GLN:HB2	1:E:736:GLU:OE2	2.15	0.46
1:E:1143:ALA:HB3	1:E:1146:ALA:HB2	1.95	0.46
1:F:607:THR:O	1:F:610:GLU:HG2	2.16	0.46
1:A:733:GLN:HB2	1:A:736:GLU:OE2	2.16	0.46
1:A:1409:ILE:CD1	1:A:1423:LEU:HD13	2.45	0.46
1:B:273:PRO:HG2	1:B:276:SER:OG	2.15	0.46
1:C:484:ASN:HD21	1:C:753:ASN:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1596:LEU:HD12	1:C:1597:PRO:CD	2.44	0.46
1:F:401:SER:O	1:F:401:SER:OG	2.22	0.46
1:F:484:ASN:HD21	1:F:753:ASN:HA	1.80	0.46
1:A:1555:THR:OG1	1:A:1559:THR:HG21	2.14	0.46
1:B:104:ASP:OD2	1:B:105:ARG:N	2.48	0.46
1:B:680:LEU:HD13	1:B:684:VAL:HG11	1.98	0.46
1:D:733:GLN:HB2	1:D:736:GLU:OE2	2.15	0.46
1:D:881:THR:OG1	1:D:888:GLU:OE2	2.25	0.46
1:F:1245:ILE:HD12	1:F:1245:ILE:H	1.79	0.46
1:B:1346:SER:OG	1:B:1348:TYR:O	2.31	0.46
1:F:733:GLN:HB2	1:F:736:GLU:OE2	2.14	0.46
1:A:1578:ARG:NH2	1:F:1352:GLU:OE2	2.49	0.46
1:C:607:THR:O	1:C:610:GLU:HG2	2.16	0.46
1:C:1352:GLU:OE2	1:D:1578:ARG:NH2	2.49	0.46
1:D:275:VAL:O	1:D:275:VAL:CG1	2.62	0.46
1:E:484:ASN:HD21	1:E:753:ASN:HA	1.80	0.46
1:F:1409:ILE:CD1	1:F:1423:LEU:HD13	2.46	0.46
1:B:65:ILE:HG12	1:B:97:ASN:CG	2.41	0.46
1:B:739:ALA:HB2	1:B:792:ILE:HG12	1.97	0.46
1:B:1300:PRO:O	1:B:1315:ILE:HD11	2.16	0.46
1:B:1403:GLU:HG2	1:B:1404:THR:HG23	1.97	0.46
1:C:1104:SER:HB2	1:D:1455:ASP:OD1	2.16	0.46
1:C:1574:SER:OG	1:C:1580:ARG:N	2.27	0.46
1:D:87:VAL:HG12	1:D:143:GLU:HB3	1.98	0.46
1:D:1409:ILE:CD1	1:D:1423:LEU:HD13	2.45	0.46
1:F:1300:PRO:O	1:F:1315:ILE:HD11	2.16	0.46
1:F:1322:SER:HB2	1:F:1327:LYS:HG2	1.97	0.46
1:A:1403:GLU:HG2	1:A:1404:THR:HG23	1.97	0.46
1:D:484:ASN:HD21	1:D:753:ASN:HA	1.81	0.46
1:D:739:ALA:HB2	1:D:792:ILE:HG12	1.98	0.46
1:D:1300:PRO:O	1:D:1315:ILE:HD11	2.16	0.46
1:E:1069:LEU:O	1:E:1154:ASN:ND2	2.47	0.46
1:F:65:ILE:HG12	1:F:97:ASN:CG	2.41	0.46
1:F:1027:PHE:HB3	1:F:1349:VAL:HB	1.98	0.46
1:A:65:ILE:HG12	1:A:97:ASN:CG	2.41	0.46
1:A:1269:ASP:OD1	1:A:1271:ASP:OD2	2.34	0.46
1:B:525:THR:HG21	1:B:555:ILE:CD1	2.46	0.46
1:D:1269:ASP:OD1	1:D:1271:ASP:OD2	2.34	0.46
1:F:893:LEU:HD13	1:F:941:LEU:HD11	1.98	0.46
1:B:84:ASN:HD22	1:C:421:GLU:HB3	1.80	0.46
1:E:290:ASP:OD2	1:E:293:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1596:LEU:HD12	1:E:1597:PRO:CD	2.44	0.46
1:F:704:MET:HE2	1:F:706:PHE:CE1	2.51	0.46
1:A:1300:PRO:O	1:A:1315:ILE:HD11	2.16	0.45
1:B:502:LEU:HD22	1:B:806:ASN:HB3	1.98	0.45
1:C:739:ALA:HB2	1:C:792:ILE:HG12	1.98	0.45
1:C:1300:PRO:O	1:C:1315:ILE:HD11	2.16	0.45
1:D:680:LEU:HD13	1:D:684:VAL:HG11	1.98	0.45
1:D:704:MET:HE2	1:D:706:PHE:CE1	2.52	0.45
1:F:745:ILE:HD11	1:F:761:LEU:HD21	1.98	0.45
1:F:1596:LEU:HD12	1:F:1597:PRO:CD	2.44	0.45
1:A:110:ILE:O	1:A:113:SER:OG	2.30	0.45
1:A:904:THR:OG1	1:A:906:ASP:OD2	2.34	0.45
1:A:1027:PHE:HB3	1:A:1349:VAL:HB	1.98	0.45
1:A:1346:SER:OG	1:A:1348:TYR:O	2.30	0.45
1:B:1575:SER:HB3	1:B:1578:ARG:HH21	1.81	0.45
1:C:1409:ILE:CD1	1:C:1423:LEU:HD13	2.46	0.45
1:D:1075:ILE:CD1	1:D:1139:MET:HE1	2.36	0.45
1:E:66:ASP:OD1	1:E:67:SER:N	2.50	0.45
1:E:1300:PRO:O	1:E:1315:ILE:HD11	2.16	0.45
1:A:680:LEU:HD13	1:A:684:VAL:HG11	1.97	0.45
1:B:904:THR:OG1	1:B:906:ASP:OD2	2.35	0.45
1:C:893:LEU:HD13	1:C:941:LEU:HD11	1.98	0.45
1:C:1269:ASP:OD1	1:C:1271:ASP:OD2	2.35	0.45
1:D:607:THR:O	1:D:610:GLU:HG2	2.15	0.45
1:E:704:MET:HE2	1:E:706:PHE:CE1	2.51	0.45
1:B:66:ASP:OD1	1:B:67:SER:N	2.50	0.45
1:C:66:ASP:OD1	1:C:67:SER:N	2.49	0.45
1:C:87:VAL:HG12	1:C:143:GLU:HB3	1.99	0.45
1:D:66:ASP:OD1	1:D:67:SER:N	2.50	0.45
1:B:1409:ILE:CD1	1:B:1423:LEU:HD13	2.46	0.45
1:C:1222:THR:O	1:D:1530:GLU:OE1	2.35	0.45
1:D:65:ILE:HG12	1:D:97:ASN:CG	2.41	0.45
1:D:1027:PHE:HB3	1:D:1349:VAL:HB	1.99	0.45
1:D:1330:ARG:CB	1:D:1364:ASN:HA	2.43	0.45
1:F:1473:ASP:OD1	1:F:1474:ASP:N	2.42	0.45
1:A:87:VAL:HG12	1:A:143:GLU:HB3	1.98	0.45
1:A:704:MET:HE2	1:A:706:PHE:CE1	2.52	0.45
1:C:704:MET:HE2	1:C:706:PHE:CE1	2.51	0.45
1:C:904:THR:OG1	1:C:906:ASP:OD2	2.35	0.45
1:C:1346:SER:OG	1:C:1348:TYR:O	2.30	0.45
1:D:1245:ILE:H	1:D:1245:ILE:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:THR:HG21	1:E:555:ILE:CD1	2.46	0.45
1:F:110:ILE:O	1:F:113:SER:OG	2.31	0.45
1:A:739:ALA:HB2	1:A:792:ILE:HG12	1.98	0.45
1:B:704:MET:HE2	1:B:706:PHE:CE1	2.51	0.45
1:C:502:LEU:HD22	1:C:806:ASN:HB3	1.98	0.45
1:C:1027:PHE:HB3	1:C:1349:VAL:HB	1.98	0.45
1:D:1345:GLY:HA3	1:E:1578:ARG:CG	2.45	0.45
1:E:65:ILE:HG12	1:E:97:ASN:CG	2.41	0.45
1:E:680:LEU:HD13	1:E:684:VAL:HG11	1.98	0.45
1:F:654:ASN:OD1	1:F:655:ASP:N	2.50	0.45
1:F:1069:LEU:O	1:F:1154:ASN:ND2	2.47	0.45
1:B:837:TYR:CZ	1:B:843:VAL:HG23	2.52	0.45
1:B:1027:PHE:HB3	1:B:1349:VAL:HB	1.99	0.45
1:B:1269:ASP:OD1	1:B:1271:ASP:OD2	2.35	0.45
1:C:816:PRO:HG2	1:D:1083:ASN:HD22	1.79	0.45
1:E:654:ASN:OD1	1:E:655:ASP:N	2.50	0.45
1:E:837:TYR:CZ	1:E:843:VAL:HG23	2.52	0.45
1:F:66:ASP:OD1	1:F:67:SER:N	2.49	0.45
1:F:739:ALA:HB2	1:F:792:ILE:HG12	1.98	0.45
1:E:999:GLU:OE1	1:F:1265:ALA:HB3	2.17	0.45
1:F:837:TYR:CZ	1:F:843:VAL:HG23	2.52	0.45
1:A:502:LEU:HD22	1:A:806:ASN:HB3	1.99	0.45
1:A:654:ASN:OD1	1:A:655:ASP:N	2.50	0.45
1:C:745:ILE:HD11	1:C:761:LEU:HD21	1.98	0.45
1:C:837:TYR:CZ	1:C:843:VAL:HG23	2.52	0.45
1:C:881:THR:OG1	1:C:888:GLU:OE2	2.25	0.45
1:A:66:ASP:OD1	1:A:67:SER:N	2.50	0.44
1:A:484:ASN:HD21	1:A:753:ASN:HA	1.81	0.44
1:A:1530:GLU:OE1	1:F:1222:THR:O	2.35	0.44
1:C:110:ILE:O	1:C:113:SER:OG	2.31	0.44
1:F:1269:ASP:OD1	1:F:1271:ASP:OD2	2.35	0.44
1:A:313:ASP:OD1	1:A:314:THR:N	2.47	0.44
1:A:525:THR:HG21	1:A:555:ILE:CD1	2.47	0.44
1:A:1534:ASN:O	1:F:1103:GLY:HA2	2.18	0.44
1:A:1596:LEU:HD12	1:A:1597:PRO:CD	2.44	0.44
1:B:1274:GLU:HB3	1:B:1337:GLU:HB3	2.00	0.44
1:C:65:ILE:HG12	1:C:97:ASN:CG	2.41	0.44
1:C:313:ASP:OD1	1:C:314:THR:N	2.47	0.44
1:D:904:THR:OG1	1:D:906:ASP:OD2	2.35	0.44
1:E:110:ILE:O	1:E:113:SER:OG	2.30	0.44
1:E:515:ASP:C	1:E:515:ASP:OD2	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:739:ALA:HB2	1:E:792:ILE:HG12	1.97	0.44
1:E:1027:PHE:HB3	1:E:1349:VAL:HB	1.99	0.44
1:B:654:ASN:OD1	1:B:655:ASP:N	2.50	0.44
1:D:502:LEU:HD22	1:D:806:ASN:HB3	1.99	0.44
1:F:1163:SER:OG	1:F:1165:GLN:OE1	2.21	0.44
1:A:886:PHE:C	1:B:1301:THR:HG21	2.42	0.44
1:A:1005:ASP:OD2	1:A:1006:SER:N	2.51	0.44
1:B:1005:ASP:OD2	1:B:1006:SER:N	2.51	0.44
1:C:1202:GLN:HG2	1:C:1230:ASP:HA	1.99	0.44
1:E:447:PRO:HG2	1:F:858:LEU:HG	2.00	0.44
1:E:1202:GLN:HG2	1:E:1230:ASP:HA	1.99	0.44
1:F:313:ASP:OD1	1:F:314:THR:N	2.47	0.44
1:A:1202:GLN:HG2	1:A:1230:ASP:HA	1.99	0.44
1:A:1396:ASP:C	1:F:985:ASP:HB3	2.42	0.44
1:B:515:ASP:OD2	1:B:515:ASP:C	2.61	0.44
1:C:515:ASP:OD2	1:C:515:ASP:C	2.60	0.44
1:C:1005:ASP:OD2	1:C:1006:SER:N	2.51	0.44
1:D:515:ASP:OD2	1:D:515:ASP:C	2.61	0.44
1:F:904:THR:OG1	1:F:906:ASP:OD2	2.35	0.44
1:A:130:SER:OG	1:A:144:THR:O	2.27	0.44
1:A:153:ILE:HD13	1:A:164:GLN:HB2	2.00	0.44
1:A:837:TYR:CZ	1:A:843:VAL:HG23	2.52	0.44
1:A:1274:GLU:HB3	1:A:1337:GLU:HB3	1.99	0.44
1:C:985:ASP:HB3	1:D:1396:ASP:C	2.43	0.44
1:D:401:SER:O	1:D:401:SER:OG	2.23	0.44
1:E:1269:ASP:OD1	1:E:1271:ASP:OD2	2.35	0.44
1:B:1596:LEU:HD12	1:B:1597:PRO:CD	2.44	0.44
1:C:1594:ASN:HA	1:C:1605:GLU:OE1	2.18	0.44
1:D:837:TYR:CZ	1:D:843:VAL:HG23	2.52	0.44
1:D:1594:ASN:HA	1:D:1605:GLU:OE1	2.18	0.44
1:F:502:LEU:HD22	1:F:806:ASN:HB3	1.98	0.44
1:B:344:ASN:HB3	1:B:444:ASN:OD1	2.18	0.44
1:B:1594:ASN:HA	1:B:1605:GLU:OE1	2.18	0.44
1:C:469:THR:HG22	1:C:826:HIS:CE1	2.53	0.44
1:E:904:THR:OG1	1:E:906:ASP:OD2	2.35	0.44
1:A:1352:GLU:OE2	1:B:1578:ARG:NH1	2.51	0.44
1:C:654:ASN:OD1	1:C:655:ASP:N	2.50	0.44
1:C:985:ASP:CG	1:D:1394:ASP:OD2	2.58	0.44
1:C:1321:GLU:OE1	1:C:1393:PHE:CE1	2.71	0.44
1:F:515:ASP:OD2	1:F:515:ASP:C	2.60	0.44
1:A:1465:PRO:CD	1:F:1219:ASP:CB	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASP:OD1	1:B:314:THR:N	2.47	0.43
1:E:344:ASN:HB3	1:E:444:ASN:OD1	2.18	0.43
1:E:620:VAL:O	1:E:726:GLY:HA3	2.18	0.43
1:E:1274:GLU:HB3	1:E:1337:GLU:HB3	2.00	0.43
1:F:1005:ASP:OD2	1:F:1006:SER:N	2.51	0.43
1:A:1345:GLY:CA	1:B:1578:ARG:HB2	2.49	0.43
1:A:1532:VAL:HB	1:F:1226:SER:CB	2.49	0.43
1:B:1202:GLN:HG2	1:B:1230:ASP:HA	2.00	0.43
1:D:153:ILE:HD13	1:D:164:GLN:HB2	2.00	0.43
1:D:1363:SER:HB3	1:D:1390:ASP:CG	2.39	0.43
1:B:1379:THR:HA	1:B:1439:LEU:O	2.19	0.43
1:C:1103:GLY:HA2	1:D:1534:ASN:O	2.18	0.43
1:C:1572:ASP:HB3	1:C:1578:ARG:HH12	1.83	0.43
1:E:313:ASP:OD1	1:E:314:THR:N	2.47	0.43
1:E:502:LEU:HD22	1:E:806:ASN:HB3	1.98	0.43
1:F:1321:GLU:OE1	1:F:1393:PHE:CE1	2.71	0.43
1:F:1517:VAL:HA	1:F:1564:GLY:O	2.18	0.43
1:A:1594:ASN:HA	1:A:1605:GLU:OE1	2.18	0.43
1:C:1379:THR:HA	1:C:1439:LEU:O	2.19	0.43
1:D:130:SER:OG	1:D:144:THR:O	2.27	0.43
1:D:654:ASN:OD1	1:D:655:ASP:N	2.50	0.43
1:D:1005:ASP:OD2	1:D:1006:SER:N	2.51	0.43
1:D:1202:GLN:HG2	1:D:1230:ASP:HA	1.99	0.43
1:D:1379:THR:HA	1:D:1439:LEU:O	2.19	0.43
1:E:1005:ASP:OD2	1:E:1006:SER:N	2.51	0.43
1:E:1379:THR:HA	1:E:1439:LEU:O	2.19	0.43
1:F:1159:ASP:CG	1:F:1187:ARG:HH21	2.26	0.43
1:F:1541:SER:OG	1:F:1585:ASP:OD1	2.37	0.43
1:B:1574:SER:OG	1:B:1580:ARG:N	2.27	0.43
1:C:629:VAL:HG11	1:C:704:MET:CE	2.48	0.43
1:D:431:ASP:OD1	1:D:432:ASN:N	2.52	0.43
1:D:1262:ASN:OD1	1:D:1263:ASP:N	2.52	0.43
1:E:1329:GLU:N	1:E:1329:GLU:OE2	2.52	0.43
1:A:115:ALA:HA	1:A:330:LEU:HD13	2.00	0.43
1:B:447:PRO:HG2	1:C:858:LEU:HG	2.00	0.43
1:C:1207:GLN:OE1	1:D:1531:ALA:HB1	2.18	0.43
1:C:1230:ASP:OD1	1:C:1231:LEU:N	2.52	0.43
1:D:136:ALA:O	1:D:182:LEU:HD11	2.19	0.43
1:F:1202:GLN:HG2	1:F:1230:ASP:HA	1.99	0.43
1:F:1567:PHE:HB3	1:F:1578:ARG:HG2	1.99	0.43
1:F:1594:ASN:HA	1:F:1605:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1455:ASP:OD1	1:F:1104:SER:HB2	2.19	0.43
1:A:1517:VAL:HA	1:A:1564:GLY:O	2.18	0.43
1:C:605:LEU:HD23	1:C:605:LEU:HA	1.89	0.43
1:C:1177:ASP:OD1	1:C:1179:THR:OG1	2.34	0.43
1:C:1226:SER:CB	1:D:1532:VAL:HB	2.49	0.43
1:D:471:GLY:O	1:D:856:SER:HB3	2.19	0.43
1:E:1262:ASN:OD1	1:E:1263:ASP:N	2.52	0.43
1:E:1517:VAL:HA	1:E:1564:GLY:O	2.18	0.43
1:F:620:VAL:O	1:F:726:GLY:HA3	2.19	0.43
1:A:471:GLY:O	1:A:856:SER:HB3	2.19	0.43
1:B:1422:LYS:O	1:B:1465:PRO:HA	2.19	0.43
1:C:431:ASP:OD1	1:C:432:ASN:N	2.52	0.43
1:C:1159:ASP:CG	1:C:1187:ARG:HH21	2.26	0.43
1:D:1274:GLU:HB3	1:D:1337:GLU:HB3	2.00	0.43
1:F:42:PHE:CE1	1:F:65:ILE:HD12	2.54	0.43
1:F:431:ASP:OD1	1:F:432:ASN:N	2.52	0.43
1:F:1379:THR:HA	1:F:1439:LEU:O	2.19	0.43
1:A:620:VAL:O	1:A:726:GLY:HA3	2.19	0.43
1:A:1245:ILE:HD12	1:A:1245:ILE:H	1.83	0.43
1:B:471:GLY:O	1:B:856:SER:HB3	2.19	0.43
1:B:620:VAL:O	1:B:726:GLY:HA3	2.18	0.43
1:E:1159:ASP:CG	1:E:1187:ARG:HH21	2.26	0.43
1:E:1541:SER:OG	1:E:1585:ASP:OD1	2.37	0.43
1:A:1230:ASP:OD1	1:A:1231:LEU:N	2.52	0.43
1:B:1262:ASN:OD1	1:B:1263:ASP:N	2.52	0.43
1:B:1329:GLU:N	1:B:1329:GLU:OE2	2.52	0.43
1:B:1550:LEU:HD22	1:B:1552:VAL:HG13	2.01	0.43
1:C:886:PHE:HZ	1:C:889:LEU:HD13	1.84	0.43
1:C:1219:ASP:CB	1:D:1465:PRO:CD	2.96	0.43
1:C:1262:ASN:OD1	1:C:1263:ASP:N	2.52	0.43
1:C:1541:SER:OG	1:C:1585:ASP:OD1	2.37	0.43
1:D:313:ASP:OD1	1:D:314:THR:N	2.47	0.43
1:D:525:THR:HG21	1:D:555:ILE:CD1	2.48	0.43
1:D:886:PHE:HZ	1:D:889:LEU:HD13	1.84	0.43
1:F:469:THR:HG22	1:F:826:HIS:CE1	2.53	0.43
1:F:1134:ARG:HH11	1:F:1176:LEU:HD21	1.84	0.43
1:A:431:ASP:OD1	1:A:432:ASN:N	2.52	0.42
1:A:1537:VAL:N	1:A:1550:LEU:O	2.47	0.42
1:A:1550:LEU:HD22	1:A:1552:VAL:HG13	2.01	0.42
1:B:431:ASP:OD1	1:B:432:ASN:N	2.52	0.42
1:B:1230:ASP:OD1	1:B:1231:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:PHE:HB3	1:C:285:LEU:HD12	2.00	0.42
1:D:115:ALA:HA	1:D:330:LEU:HD13	2.00	0.42
1:D:1517:VAL:HA	1:D:1564:GLY:O	2.18	0.42
1:E:886:PHE:HZ	1:E:889:LEU:HD13	1.84	0.42
1:F:87:VAL:HG12	1:F:143:GLU:HB3	2.01	0.42
1:C:1274:GLU:HB3	1:C:1337:GLU:HB3	2.01	0.42
1:D:469:THR:HG22	1:D:826:HIS:CE1	2.55	0.42
1:D:620:VAL:O	1:D:726:GLY:HA3	2.19	0.42
1:D:1159:ASP:CG	1:D:1187:ARG:HH21	2.27	0.42
1:E:431:ASP:OD1	1:E:432:ASN:N	2.52	0.42
1:E:1134:ARG:HH11	1:E:1176:LEU:HD21	1.84	0.42
1:E:1594:ASN:HA	1:E:1605:GLU:OE1	2.18	0.42
1:F:1262:ASN:OD1	1:F:1263:ASP:N	2.52	0.42
1:A:1379:THR:HA	1:A:1439:LEU:O	2.19	0.42
1:A:1422:LYS:O	1:A:1465:PRO:HA	2.19	0.42
1:A:1541:SER:OG	1:A:1585:ASP:OD1	2.37	0.42
1:B:110:ILE:O	1:B:113:SER:OG	2.30	0.42
1:B:886:PHE:O	1:C:1301:THR:CG2	2.64	0.42
1:B:1541:SER:OG	1:B:1585:ASP:OD1	2.37	0.42
1:C:999:GLU:HG2	1:D:1304:ARG:NH1	2.34	0.42
1:F:1274:GLU:HB3	1:F:1337:GLU:HB3	2.01	0.42
1:A:136:ALA:O	1:A:182:LEU:HD11	2.19	0.42
1:A:886:PHE:HZ	1:A:889:LEU:HD13	1.84	0.42
1:A:1134:ARG:HH11	1:A:1176:LEU:HD21	1.85	0.42
1:B:1159:ASP:CG	1:B:1187:ARG:HH21	2.27	0.42
1:B:1321:GLU:OE1	1:B:1393:PHE:CE1	2.72	0.42
1:C:136:ALA:O	1:C:182:LEU:HD11	2.19	0.42
1:D:886:PHE:C	1:E:1301:THR:HG21	2.42	0.42
1:D:1134:ARG:HH11	1:D:1176:LEU:HD21	1.85	0.42
1:E:469:THR:HG22	1:E:826:HIS:CE1	2.54	0.42
1:E:1230:ASP:OD1	1:E:1231:LEU:N	2.52	0.42
1:A:1304:ARG:NH1	1:F:999:GLU:HB3	2.34	0.42
1:B:130:SER:OG	1:B:144:THR:O	2.28	0.42
1:B:886:PHE:HZ	1:B:889:LEU:HD13	1.84	0.42
1:C:1038:ASN:OD1	1:C:1039:ALA:N	2.53	0.42
1:C:1517:VAL:HA	1:C:1564:GLY:O	2.19	0.42
1:C:1550:LEU:HD22	1:C:1552:VAL:HG13	2.01	0.42
1:D:1038:ASN:OD1	1:D:1039:ALA:N	2.53	0.42
1:E:153:ILE:HD13	1:E:164:GLN:HB2	2.02	0.42
1:E:1422:LYS:O	1:E:1465:PRO:HA	2.19	0.42
1:A:1038:ASN:OD1	1:A:1039:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:ASN:OD1	1:A:1263:ASP:N	2.52	0.42
1:B:114:THR:HG21	1:B:332:LEU:HD23	2.02	0.42
1:B:268:ASP:OD1	1:B:268:ASP:N	2.52	0.42
1:B:1134:ARG:HH11	1:B:1176:LEU:HD21	1.84	0.42
1:C:344:ASN:HB3	1:C:444:ASN:OD1	2.19	0.42
1:C:680:LEU:HD13	1:C:684:VAL:HG11	2.01	0.42
1:D:1230:ASP:OD1	1:D:1231:LEU:N	2.52	0.42
1:D:1448:ASP:OD2	1:D:1450:ASP:CG	2.63	0.42
1:E:471:GLY:O	1:E:856:SER:HB3	2.19	0.42
1:E:1054:ILE:HG23	1:E:1062:GLU:OE1	2.20	0.42
1:F:268:ASP:OD1	1:F:268:ASP:N	2.53	0.42
1:F:886:PHE:HZ	1:F:889:LEU:HD13	1.84	0.42
1:A:1105:ASP:OD2	1:A:1106:SER:N	2.53	0.42
1:A:1159:ASP:CG	1:A:1187:ARG:HH21	2.27	0.42
1:B:153:ILE:HD13	1:B:164:GLN:HB2	2.02	0.42
1:D:1054:ILE:HG23	1:D:1062:GLU:OE1	2.20	0.42
1:D:1422:LYS:O	1:D:1465:PRO:HA	2.19	0.42
1:E:104:ASP:OD2	1:E:104:ASP:C	2.63	0.42
1:F:580:ILE:HG12	1:F:717:VAL:HG12	2.02	0.42
1:A:1321:GLU:OE1	1:A:1321:GLU:N	2.52	0.42
1:B:55:SER:HB2	1:B:257:ASP:O	2.20	0.42
1:B:966:ASP:HB3	1:B:973:THR:OG1	2.20	0.42
1:C:1422:LYS:O	1:C:1465:PRO:HA	2.19	0.42
1:E:1038:ASN:OD1	1:E:1039:ALA:N	2.53	0.42
1:A:515:ASP:OD2	1:A:515:ASP:C	2.60	0.42
1:A:1394:ASP:OD2	1:F:985:ASP:CG	2.60	0.42
1:B:1517:VAL:HA	1:B:1564:GLY:O	2.18	0.42
1:C:620:VAL:O	1:C:726:GLY:HA3	2.19	0.42
1:C:1134:ARG:HH11	1:C:1176:LEU:HD21	1.84	0.42
1:C:1448:ASP:OD2	1:C:1450:ASP:CG	2.63	0.42
1:D:344:ASN:HB3	1:D:444:ASN:OD1	2.20	0.42
1:D:815:THR:HG23	1:E:1083:ASN:CG	2.44	0.42
1:E:69:ILE:HD12	1:E:98:TRP:NE1	2.35	0.42
1:E:268:ASP:OD1	1:E:268:ASP:N	2.52	0.42
1:F:1038:ASN:OD1	1:F:1039:ALA:N	2.53	0.42
1:F:1054:ILE:HG23	1:F:1062:GLU:OE1	2.20	0.42
1:F:1230:ASP:OD1	1:F:1231:LEU:N	2.52	0.42
1:F:1422:LYS:O	1:F:1465:PRO:HA	2.19	0.42
1:A:995:ASP:OD2	1:A:999:GLU:N	2.48	0.42
1:B:136:ALA:O	1:B:182:LEU:HD11	2.19	0.42
1:C:966:ASP:HB3	1:C:973:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1098:ILE:HD13	1:D:1136:PHE:CE1	2.55	0.42
1:E:136:ALA:O	1:E:182:LEU:HD11	2.19	0.42
1:E:1105:ASP:OD2	1:E:1106:SER:N	2.53	0.42
1:F:629:VAL:HG11	1:F:704:MET:CE	2.48	0.42
1:F:680:LEU:HD13	1:F:684:VAL:HG11	2.01	0.42
1:F:966:ASP:HB3	1:F:973:THR:OG1	2.20	0.42
1:F:1105:ASP:OD2	1:F:1106:SER:N	2.53	0.42
1:A:114:THR:HG21	1:A:332:LEU:HD23	2.01	0.41
1:A:268:ASP:OD1	1:A:268:ASP:N	2.52	0.41
1:A:344:ASN:HB3	1:A:444:ASN:OD1	2.19	0.41
1:A:469:THR:HG22	1:A:826:HIS:CE1	2.54	0.41
1:A:1329:GLU:OE2	1:A:1329:GLU:N	2.52	0.41
1:A:1500:ILE:HG22	1:A:1596:LEU:CD1	2.50	0.41
1:B:469:THR:HG22	1:B:826:HIS:CE1	2.55	0.41
1:C:42:PHE:CE1	1:C:65:ILE:HD12	2.55	0.41
1:D:966:ASP:HB3	1:D:973:THR:OG1	2.20	0.41
1:D:1541:SER:OG	1:D:1585:ASP:OD1	2.37	0.41
1:D:1553:THR:O	1:D:1562:PHE:HA	2.20	0.41
1:E:1550:LEU:HD22	1:E:1552:VAL:HG13	2.01	0.41
1:F:153:ILE:HD13	1:F:164:GLN:HB2	2.02	0.41
1:F:344:ASN:HB3	1:F:444:ASN:OD1	2.20	0.41
1:F:1500:ILE:HG22	1:F:1596:LEU:CD1	2.50	0.41
1:F:1550:LEU:HD22	1:F:1552:VAL:HG13	2.02	0.41
1:A:104:ASP:OD2	1:A:104:ASP:C	2.63	0.41
1:B:1105:ASP:OD2	1:B:1106:SER:N	2.53	0.41
1:B:1321:GLU:OE1	1:B:1393:PHE:CD1	2.73	0.41
1:C:268:ASP:OD1	1:C:268:ASP:N	2.53	0.41
1:C:332:LEU:O	1:C:336:LEU:HG	2.20	0.41
1:D:104:ASP:OD2	1:D:104:ASP:C	2.63	0.41
1:D:268:ASP:OD1	1:D:268:ASP:N	2.52	0.41
1:E:1321:GLU:OE1	1:E:1393:PHE:CD1	2.73	0.41
1:E:1553:THR:O	1:E:1562:PHE:HA	2.20	0.41
1:F:50:PHE:HB3	1:F:285:LEU:HD12	2.00	0.41
1:F:104:ASP:OD2	1:F:104:ASP:C	2.63	0.41
1:A:332:LEU:O	1:A:336:LEU:HG	2.20	0.41
1:B:84:ASN:HD22	1:C:421:GLU:HG2	1.85	0.41
1:B:1038:ASN:OD1	1:B:1039:ALA:N	2.53	0.41
1:B:1075:ILE:CD1	1:B:1139:MET:HE1	2.34	0.41
1:B:1098:ILE:HD13	1:B:1136:PHE:CE1	2.55	0.41
1:C:983:GLY:HA2	1:D:1398:VAL:HG22	2.00	0.41
1:C:1105:ASP:OD2	1:C:1106:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1329:GLU:N	1:C:1329:GLU:OE2	2.52	0.41
1:D:1480:VAL:O	1:D:1491:VAL:HA	2.21	0.41
1:D:1550:LEU:HD22	1:D:1552:VAL:HG13	2.01	0.41
1:E:84:ASN:HD22	1:F:421:GLU:HG2	1.85	0.41
1:E:1098:ILE:HD13	1:E:1136:PHE:CE1	2.55	0.41
1:E:1537:VAL:N	1:E:1550:LEU:O	2.48	0.41
1:F:197:ALA:HB2	1:F:226:PRO:HG3	2.03	0.41
1:F:310:PHE:CE2	1:F:401:SER:HB2	2.56	0.41
1:A:1098:ILE:HD13	1:A:1136:PHE:CE1	2.55	0.41
1:B:50:PHE:HB3	1:B:285:LEU:HD12	2.02	0.41
1:C:104:ASP:OD2	1:C:104:ASP:C	2.63	0.41
1:C:1239:ASP:OD1	1:C:1243:TYR:OH	2.25	0.41
1:D:1329:GLU:OE2	1:D:1329:GLU:N	2.53	0.41
1:E:114:THR:HG21	1:E:332:LEU:HD23	2.02	0.41
1:E:313:ASP:OD2	1:E:331:THR:HG23	2.21	0.41
1:E:966:ASP:HB3	1:E:973:THR:OG1	2.20	0.41
1:E:1321:GLU:OE1	1:E:1393:PHE:CE1	2.72	0.41
1:E:1448:ASP:OD2	1:E:1450:ASP:CG	2.63	0.41
1:E:1500:ILE:HG22	1:E:1596:LEU:CD1	2.51	0.41
1:F:136:ALA:O	1:F:182:LEU:HD11	2.19	0.41
1:B:1038:ASN:OD1	1:B:1040:ALA:N	2.45	0.41
1:D:114:THR:HG21	1:D:332:LEU:HD23	2.01	0.41
1:D:1105:ASP:OD2	1:D:1106:SER:N	2.53	0.41
1:D:1500:ILE:HG22	1:D:1596:LEU:CD1	2.50	0.41
1:F:1448:ASP:OD2	1:F:1450:ASP:CG	2.63	0.41
1:A:42:PHE:CE1	1:A:65:ILE:HD12	2.56	0.41
1:A:966:ASP:HB3	1:A:973:THR:OG1	2.20	0.41
1:A:1553:THR:O	1:A:1562:PHE:HA	2.20	0.41
1:B:244:ASN:HA	1:B:249:VAL:HG12	2.03	0.41
1:C:69:ILE:HD12	1:C:98:TRP:NE1	2.36	0.41
1:C:749:GLU:HG2	1:C:751:GLY:O	2.21	0.41
1:C:1224:THR:CB	1:D:1530:GLU:O	2.66	0.41
1:D:853:ASN:HA	1:D:860:ASP:OD2	2.21	0.41
1:E:310:PHE:CE2	1:E:401:SER:HB2	2.55	0.41
1:E:853:ASN:HA	1:E:860:ASP:OD2	2.20	0.41
1:F:115:ALA:HA	1:F:330:LEU:HD13	2.02	0.41
1:F:1480:VAL:O	1:F:1491:VAL:HA	2.21	0.41
1:F:1553:THR:O	1:F:1562:PHE:HA	2.20	0.41
1:A:230:LEU:HD13	1:A:230:LEU:HA	1.94	0.41
1:A:762:GLU:O	1:A:788:SER:HA	2.21	0.41
1:A:1529:PRO:O	1:A:1558:ALA:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:PHE:CE2	1:B:401:SER:HB2	2.56	0.41
1:B:313:ASP:OD2	1:B:331:THR:HG23	2.21	0.41
1:B:1365:PHE:N	1:B:1390:ASP:OD2	2.53	0.41
1:C:310:PHE:CE2	1:C:401:SER:HB2	2.56	0.41
1:C:1537:VAL:N	1:C:1550:LEU:O	2.47	0.41
1:D:508:THR:OG1	1:D:741:GLN:HG2	2.21	0.41
1:E:1365:PHE:N	1:E:1390:ASP:OD2	2.53	0.41
1:F:762:GLU:O	1:F:788:SER:HA	2.21	0.41
1:A:55:SER:HB2	1:A:257:ASP:O	2.21	0.41
1:B:69:ILE:HD12	1:B:98:TRP:NE1	2.35	0.41
1:B:469:THR:OG1	1:B:472:GLN:OE1	2.39	0.41
1:B:1054:ILE:HG23	1:B:1062:GLU:OE1	2.20	0.41
1:B:1553:THR:O	1:B:1562:PHE:HA	2.20	0.41
1:C:197:ALA:HB2	1:C:226:PRO:HG3	2.03	0.41
1:C:1553:THR:O	1:C:1562:PHE:HA	2.20	0.41
1:D:69:ILE:HD12	1:D:98:TRP:NE1	2.36	0.41
1:D:1069:LEU:O	1:D:1154:ASN:ND2	2.47	0.41
1:E:50:PHE:HB3	1:E:285:LEU:HD12	2.02	0.41
1:E:130:SER:OG	1:E:144:THR:O	2.28	0.41
1:E:332:LEU:O	1:E:336:LEU:HG	2.20	0.41
1:F:469:THR:OG1	1:F:472:GLN:OE1	2.39	0.41
1:F:1529:PRO:O	1:F:1558:ALA:HB2	2.21	0.41
1:A:50:PHE:HB3	1:A:285:LEU:HD12	2.02	0.41
1:A:244:ASN:HA	1:A:249:VAL:HG12	2.03	0.41
1:A:360:VAL:HG12	1:A:361:VAL:HG23	2.03	0.41
1:A:508:THR:OG1	1:A:741:GLN:HG2	2.21	0.41
1:A:1398:VAL:HG22	1:F:983:GLY:HA2	2.02	0.41
1:A:1576:GLY:CA	1:F:1345:GLY:O	2.68	0.41
1:B:54:MET:HA	1:B:285:LEU:HD21	2.03	0.41
1:B:104:ASP:OD2	1:B:104:ASP:C	2.63	0.41
1:C:115:ALA:HA	1:C:330:LEU:HD13	2.02	0.41
1:C:313:ASP:OD2	1:C:331:THR:HG23	2.21	0.41
1:C:580:ILE:HG12	1:C:717:VAL:HG12	2.02	0.41
1:C:1098:ILE:HD13	1:C:1136:PHE:CE1	2.55	0.41
1:C:1480:VAL:O	1:C:1491:VAL:HA	2.21	0.41
1:D:55:SER:HB2	1:D:257:ASP:O	2.21	0.41
1:D:332:LEU:O	1:D:336:LEU:HG	2.20	0.41
1:D:469:THR:OG1	1:D:472:GLN:OE1	2.39	0.41
1:E:695:ASP:OD2	1:E:695:ASP:C	2.64	0.41
1:F:1098:ILE:HD13	1:F:1136:PHE:CE1	2.55	0.41
1:F:1341:TRP:CE3	1:F:1353:ASP:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ASP:OD2	1:A:331:THR:HG23	2.21	0.41
1:A:469:THR:OG1	1:A:472:GLN:OE1	2.39	0.41
1:B:1529:PRO:O	1:B:1558:ALA:HB2	2.21	0.41
1:C:853:ASN:HA	1:C:860:ASP:OD2	2.21	0.41
1:C:1054:ILE:HG23	1:C:1062:GLU:OE1	2.20	0.41
1:E:55:SER:HB2	1:E:257:ASP:O	2.21	0.41
1:F:114:THR:HG21	1:F:332:LEU:HD23	2.02	0.41
1:F:313:ASP:OD2	1:F:331:THR:HG23	2.21	0.41
1:A:1087:GLU:CG	1:F:804:ASN:HD21	2.34	0.40
1:B:508:THR:OG1	1:B:741:GLN:HG2	2.21	0.40
1:B:629:VAL:HG11	1:B:704:MET:CE	2.49	0.40
1:C:153:ILE:HD13	1:C:164:GLN:HB2	2.02	0.40
1:C:469:THR:OG1	1:C:472:GLN:OE1	2.39	0.40
1:D:605:LEU:HD23	1:D:605:LEU:HA	1.88	0.40
1:E:383:ASN:ND2	1:E:432:ASN:OD1	2.55	0.40
1:E:1038:ASN:OD1	1:E:1040:ALA:N	2.45	0.40
1:E:1529:PRO:O	1:E:1558:ALA:HB2	2.21	0.40
1:F:69:ILE:HD12	1:F:98:TRP:NE1	2.36	0.40
1:F:749:GLU:HG2	1:F:751:GLY:O	2.21	0.40
1:A:383:ASN:ND2	1:A:432:ASN:OD1	2.55	0.40
1:A:1074:ARG:HA	1:A:1149:PHE:O	2.21	0.40
1:A:1341:TRP:CE3	1:A:1353:ASP:HB3	2.56	0.40
1:B:881:THR:OG1	1:B:888:GLU:OE2	2.25	0.40
1:B:1341:TRP:CE3	1:B:1353:ASP:HB3	2.56	0.40
1:D:42:PHE:CE1	1:D:65:ILE:HD12	2.56	0.40
1:D:61:GLU:HG3	1:D:101:TYR:CE1	2.57	0.40
1:D:313:ASP:OD2	1:D:331:THR:HG23	2.21	0.40
1:D:1409:ILE:HD13	1:D:1423:LEU:HD13	2.04	0.40
1:E:1074:ARG:HA	1:E:1149:PHE:O	2.22	0.40
1:E:1341:TRP:CE3	1:E:1353:ASP:HB3	2.56	0.40
1:F:332:LEU:O	1:F:336:LEU:HG	2.20	0.40
1:A:69:ILE:HD12	1:A:98:TRP:NE1	2.36	0.40
1:A:695:ASP:OD2	1:A:695:ASP:C	2.64	0.40
1:A:853:ASN:HA	1:A:860:ASP:OD2	2.21	0.40
1:A:1480:VAL:O	1:A:1491:VAL:HA	2.21	0.40
1:A:1530:GLU:OE2	1:F:1222:THR:O	2.40	0.40
1:B:115:ALA:HA	1:B:330:LEU:HD13	2.03	0.40
1:B:1205:ILE:CD1	1:B:1228:THR:HG22	2.52	0.40
1:C:114:THR:HG21	1:C:332:LEU:HD23	2.02	0.40
1:C:1500:ILE:HG22	1:C:1596:LEU:CD1	2.50	0.40
1:C:1529:PRO:O	1:C:1558:ALA:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:PHE:HB3	1:D:285:LEU:HD12	2.02	0.40
1:D:1341:TRP:CE3	1:D:1353:ASP:HB3	2.56	0.40
1:E:54:MET:HA	1:E:285:LEU:HD21	2.03	0.40
1:E:508:THR:OG1	1:E:741:GLN:HG2	2.21	0.40
1:E:762:GLU:O	1:E:788:SER:HA	2.21	0.40
1:E:1075:ILE:CD1	1:E:1139:MET:HE1	2.34	0.40
1:F:130:SER:OG	1:F:144:THR:O	2.28	0.40
1:A:61:GLU:HG3	1:A:101:TYR:CE1	2.57	0.40
1:A:1054:ILE:HG23	1:A:1062:GLU:OE1	2.20	0.40
1:A:1530:GLU:O	1:F:1224:THR:CB	2.66	0.40
1:A:1531:ALA:HB1	1:F:1207:GLN:OE1	2.18	0.40
1:B:624:PHE:HB2	1:B:723:PHE:HB2	2.02	0.40
1:B:858:LEU:HD23	1:B:858:LEU:HA	1.93	0.40
1:C:508:THR:OG1	1:C:741:GLN:HG2	2.22	0.40
1:D:695:ASP:OD2	1:D:695:ASP:C	2.64	0.40
1:D:1529:PRO:O	1:D:1558:ALA:HB2	2.21	0.40
1:E:624:PHE:HB2	1:E:723:PHE:HB2	2.02	0.40
1:E:886:PHE:O	1:F:1301:THR:CG2	2.63	0.40
1:E:1409:ILE:HD13	1:E:1423:LEU:HD13	2.04	0.40
1:E:1480:VAL:O	1:E:1491:VAL:HA	2.21	0.40
1:F:333:ARG:HG3	1:F:334:THR:HG23	2.03	0.40
1:F:1019:ASP:OD2	1:F:1072:HIS:HD2	2.05	0.40
1:B:61:GLU:HG3	1:B:101:TYR:CE1	2.57	0.40
1:B:853:ASN:HA	1:B:860:ASP:OD2	2.21	0.40
1:B:1480:VAL:O	1:B:1491:VAL:HA	2.21	0.40
1:C:695:ASP:OD2	1:C:695:ASP:C	2.64	0.40
1:C:1217:SER:HB2	1:D:1424:VAL:CB	2.48	0.40
1:E:244:ASN:HA	1:E:249:VAL:HG12	2.03	0.40
1:F:853:ASN:HA	1:F:860:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1578/1734 (91%)	1517 (96%)	61 (4%)	0	100	100
1	B	1578/1734 (91%)	1518 (96%)	60 (4%)	0	100	100
1	C	1578/1734 (91%)	1520 (96%)	58 (4%)	0	100	100
1	D	1578/1734 (91%)	1518 (96%)	60 (4%)	0	100	100
1	E	1578/1734 (91%)	1518 (96%)	60 (4%)	0	100	100
1	F	1578/1734 (91%)	1520 (96%)	58 (4%)	0	100	100
All	All	9468/10404 (91%)	9111 (96%)	357 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	1312/1438 (91%)	1303 (99%)	9 (1%)	76	90
1	B	1312/1438 (91%)	1303 (99%)	9 (1%)	76	90
1	C	1312/1438 (91%)	1303 (99%)	9 (1%)	76	90
1	D	1312/1438 (91%)	1302 (99%)	10 (1%)	73	89
1	E	1312/1438 (91%)	1301 (99%)	11 (1%)	73	89
1	F	1312/1438 (91%)	1302 (99%)	10 (1%)	73	89
All	All	7872/8628 (91%)	7814 (99%)	58 (1%)	73	90

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	ARG
1	A	274	ARG
1	A	422	SER
1	A	495	LEU
1	A	523	ILE
1	A	565	ASN
1	A	1330	ARG

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Mol	Chain	Res	Type
1	A	1414	ARG
1	A	1575	SER
1	B	269	ARG
1	B	274	ARG
1	B	422	SER
1	B	495	LEU
1	B	501	THR
1	B	523	ILE
1	B	565	ASN
1	B	1330	ARG
1	B	1414	ARG
1	C	269	ARG
1	C	274	ARG
1	C	422	SER
1	C	495	LEU
1	C	523	ILE
1	C	565	ASN
1	C	999	GLU
1	C	1330	ARG
1	C	1414	ARG
1	D	269	ARG
1	D	274	ARG
1	D	422	SER
1	D	495	LEU
1	D	501	THR
1	D	523	ILE
1	D	565	ASN
1	D	1330	ARG
1	D	1414	ARG
1	D	1575	SER
1	E	269	ARG
1	E	274	ARG
1	E	422	SER
1	E	495	LEU
1	E	501	THR
1	E	523	ILE
1	E	565	ASN
1	E	999	GLU
1	E	1000	ILE
1	E	1330	ARG
1	E	1414	ARG
1	F	38	ASN

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Mol	Chain	Res	Type
1	F	58	GLN
1	F	269	ARG
1	F	274	ARG
1	F	422	SER
1	F	495	LEU
1	F	523	ILE
1	F	565	ASN
1	F	1330	ARG
1	F	1414	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	40	ASN
1	A	58	GLN
1	A	84	ASN
1	A	92	GLN
1	A	211	GLN
1	A	383	ASN
1	A	484	ASN
1	A	623	ASN
1	A	643	ASN
1	A	662	ASN
1	A	682	ASN
1	A	733	GLN
1	A	740	ASN
1	A	804	ASN
1	A	909	ASN
1	A	956	GLN
1	A	1083	ASN
1	A	1094	ASN
1	A	1154	ASN
1	B	38	ASN
1	B	40	ASN
1	B	58	GLN
1	B	84	ASN
1	B	92	GLN
1	B	224	ASN
1	B	234	ASN
1	B	383	ASN
1	B	484	ASN

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Mol	Chain	Res	Type
1	B	623	ASN
1	B	643	ASN
1	B	662	ASN
1	B	682	ASN
1	B	740	ASN
1	B	804	ASN
1	B	909	ASN
1	B	956	GLN
1	B	1083	ASN
1	B	1094	ASN
1	B	1154	ASN
1	C	38	ASN
1	C	58	GLN
1	C	84	ASN
1	C	92	GLN
1	C	192	ASN
1	C	211	GLN
1	C	224	ASN
1	C	383	ASN
1	C	484	ASN
1	C	623	ASN
1	C	643	ASN
1	C	662	ASN
1	C	682	ASN
1	C	740	ASN
1	C	772	GLN
1	C	804	ASN
1	C	868	ASN
1	C	909	ASN
1	C	956	GLN
1	C	1083	ASN
1	C	1094	ASN
1	C	1154	ASN
1	D	38	ASN
1	D	40	ASN
1	D	58	GLN
1	D	84	ASN
1	D	92	GLN
1	D	192	ASN
1	D	211	GLN
1	D	224	ASN
1	D	383	ASN

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Mol	Chain	Res	Type
1	D	484	ASN
1	D	623	ASN
1	D	643	ASN
1	D	682	ASN
1	D	733	GLN
1	D	740	ASN
1	D	804	ASN
1	D	909	ASN
1	D	956	GLN
1	D	1083	ASN
1	D	1094	ASN
1	D	1154	ASN
1	E	38	ASN
1	E	58	GLN
1	E	84	ASN
1	E	92	GLN
1	E	211	GLN
1	E	224	ASN
1	E	383	ASN
1	E	484	ASN
1	E	623	ASN
1	E	643	ASN
1	E	682	ASN
1	E	740	ASN
1	E	804	ASN
1	E	909	ASN
1	E	956	GLN
1	E	1083	ASN
1	E	1094	ASN
1	E	1154	ASN
1	F	84	ASN
1	F	92	GLN
1	F	211	GLN
1	F	224	ASN
1	F	383	ASN
1	F	484	ASN
1	F	623	ASN
1	F	643	ASN
1	F	662	ASN
1	F	682	ASN
1	F	733	GLN
1	F	740	ASN

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Mol	Chain	Res	Type
1	F	772	GLN
1	F	804	ASN
1	F	909	ASN
1	F	956	GLN
1	F	1083	ASN
1	F	1094	ASN
1	F	1154	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

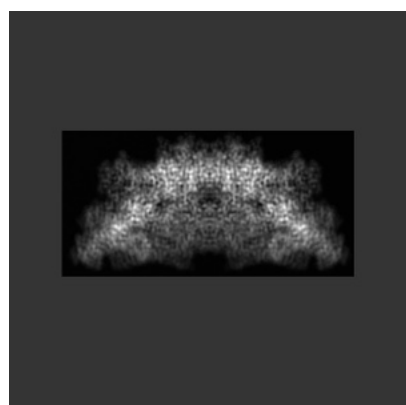
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16484. These allow visual inspection of the internal detail of the map and identification of artifacts.

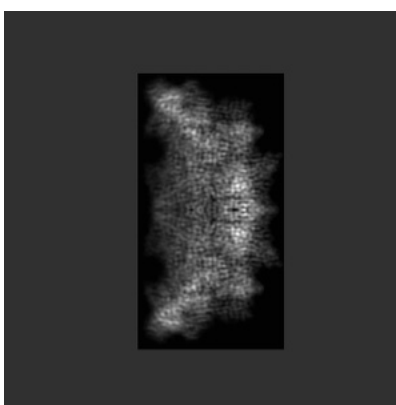
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

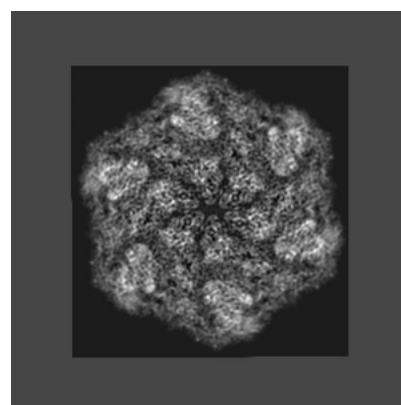
6.1.1 Primary map



X



Y

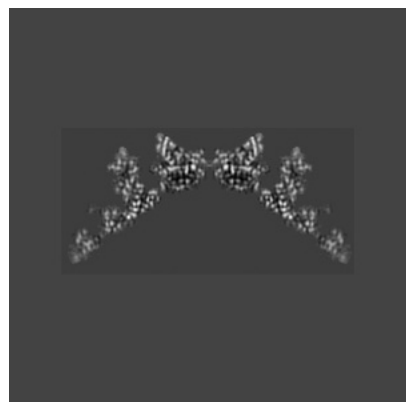


Z

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

6.2 Central slices [i](#)

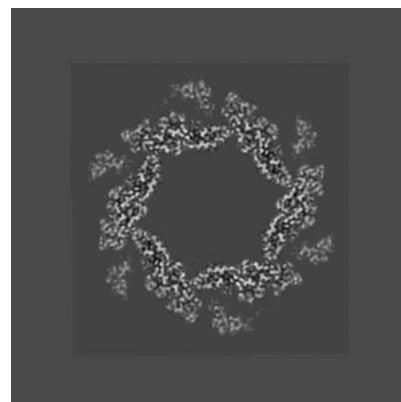
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

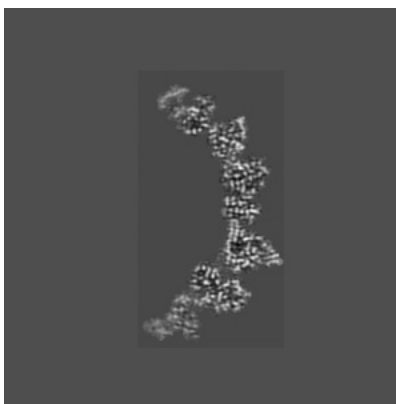
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 156



Y Index: 175

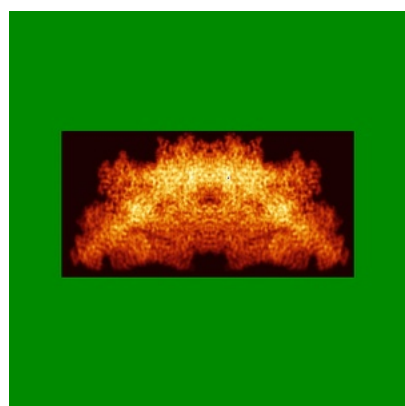


Z Index: 186

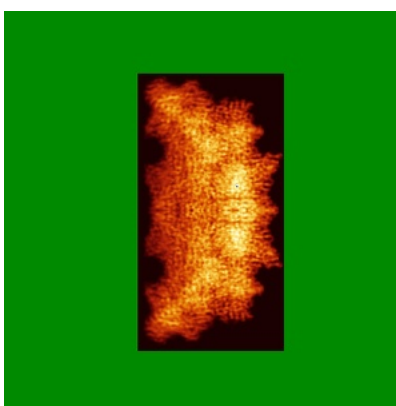
The images above show the largest variance slices of the map in three orthogonal directions.

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

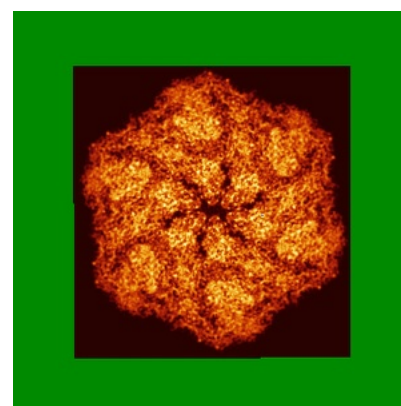
6.4.1 Primary map



X



Y

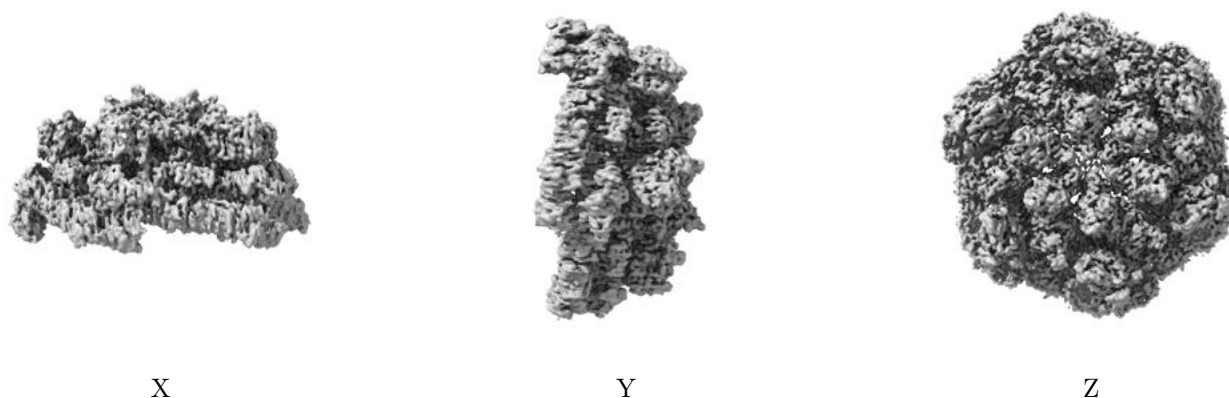


Z

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 1.05514. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

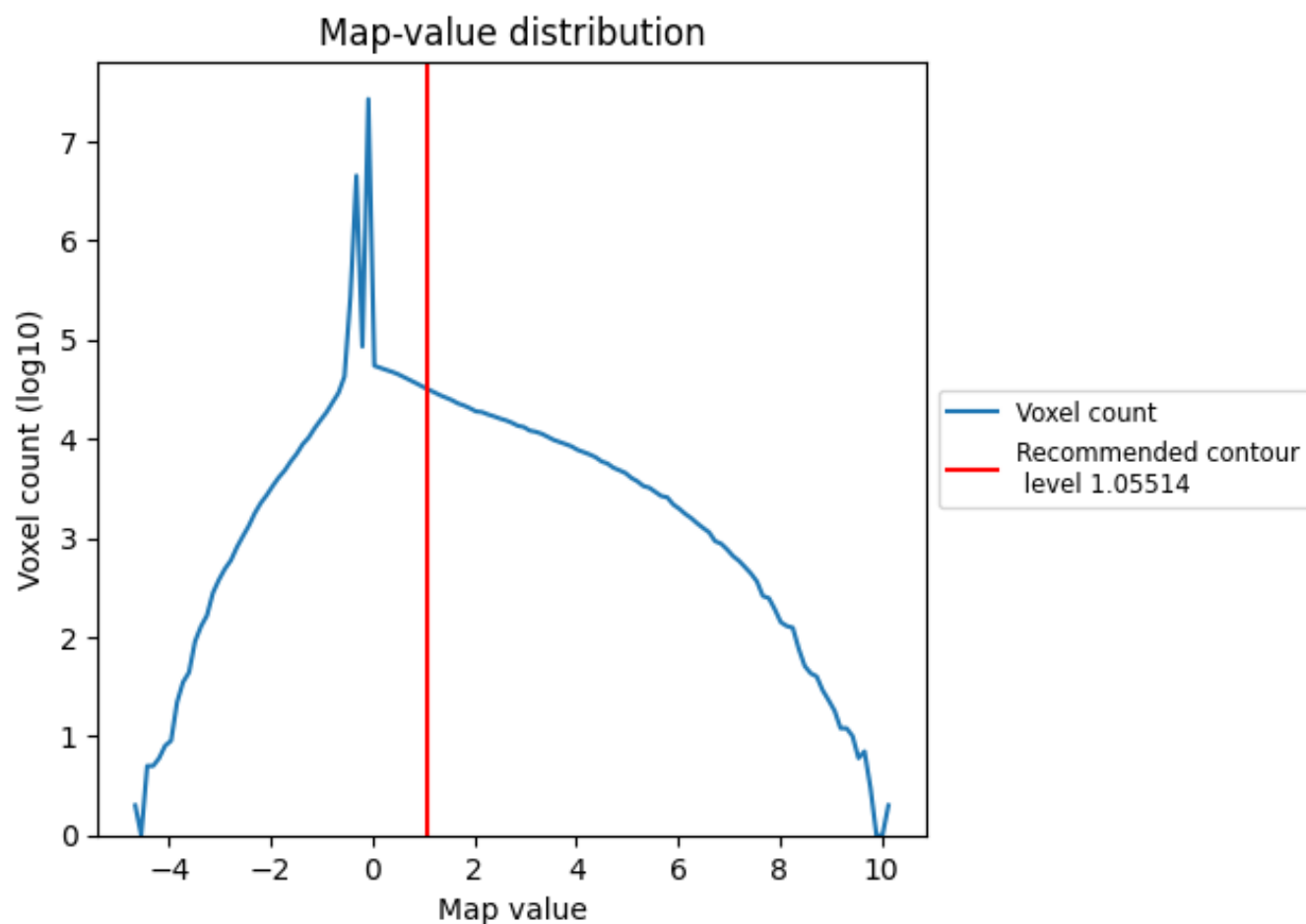
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

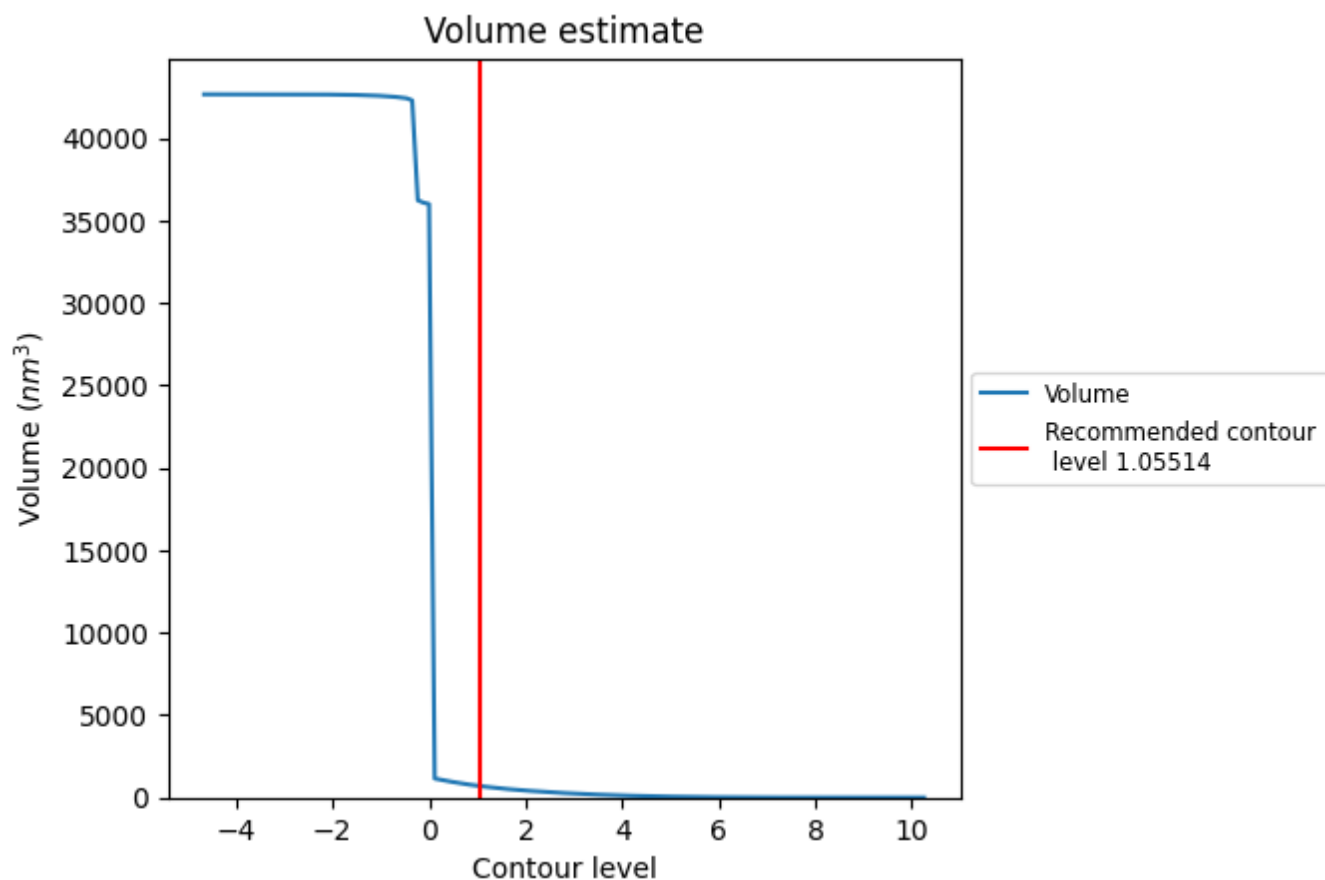
This section contains the results of statistical analysis of the map.

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.

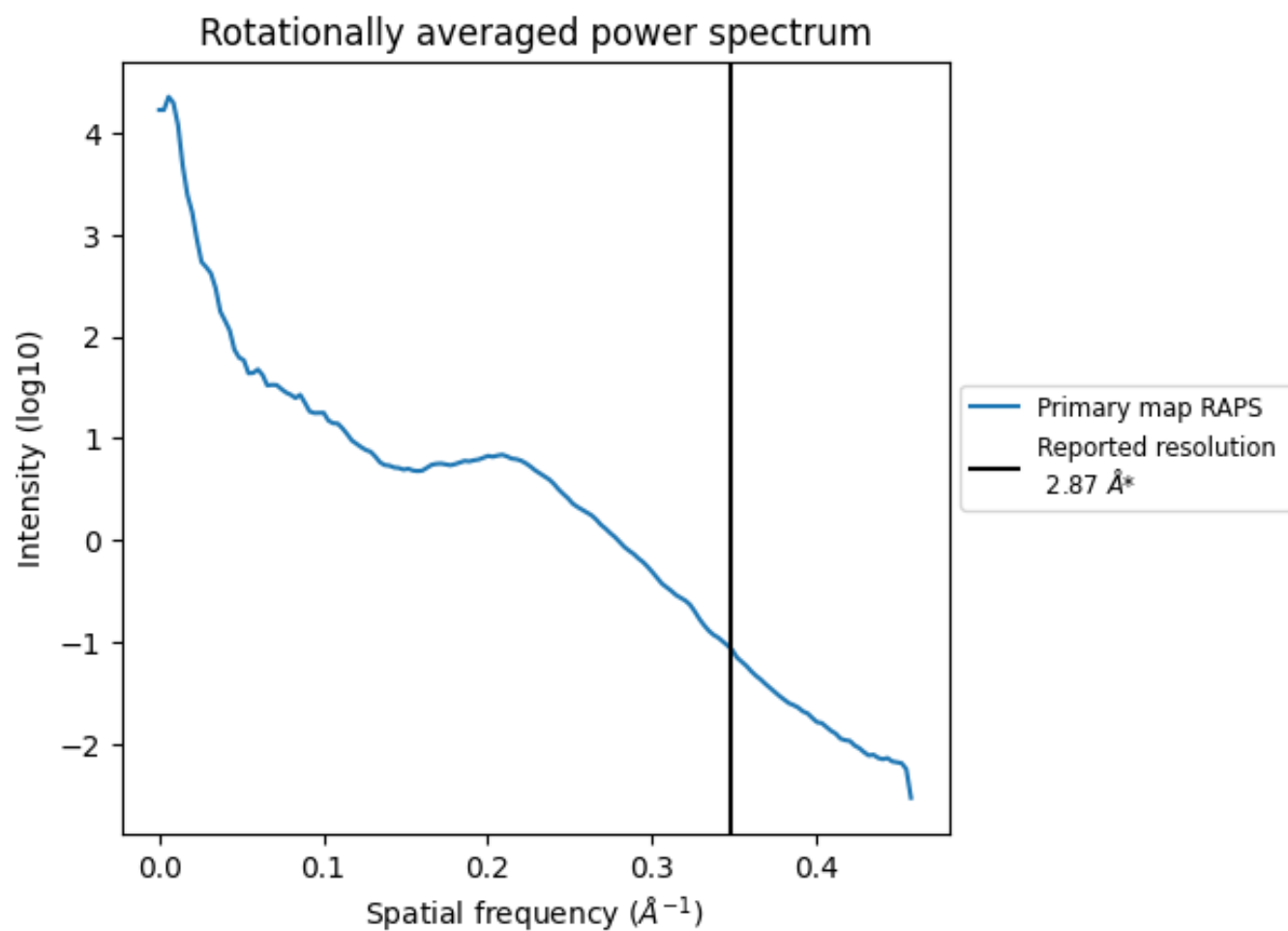
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 697 nm^3 ; this corresponds to an approximate mass of 630 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 0.348 Å⁻¹

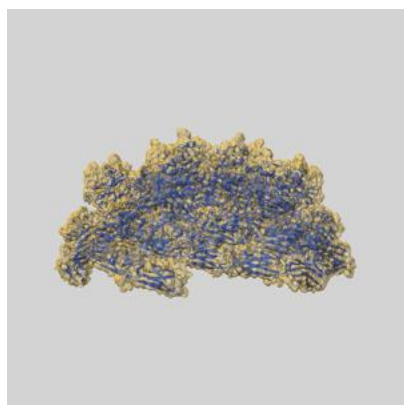
8 Fourier-Shell correlation ⓘ

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

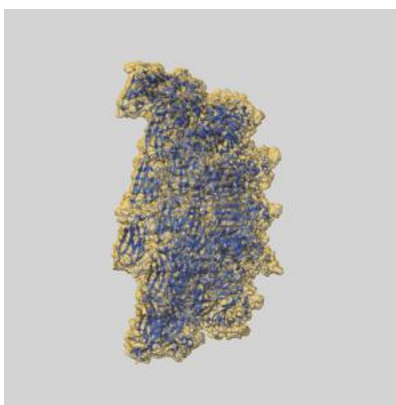
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16484 and PDB model 8C8M. Per-residue inclusion information can be found in section [3](#) on page [5](#).

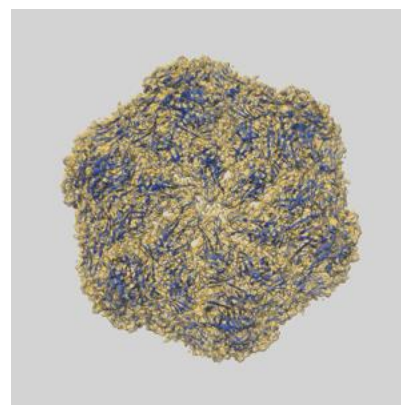
9.1 Map-model overlay [i](#)



X



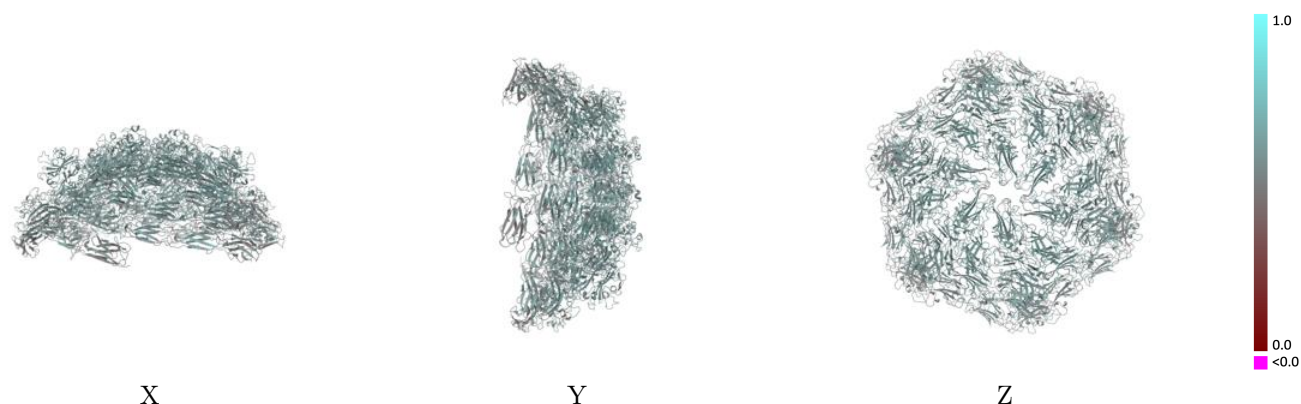
Y



Z

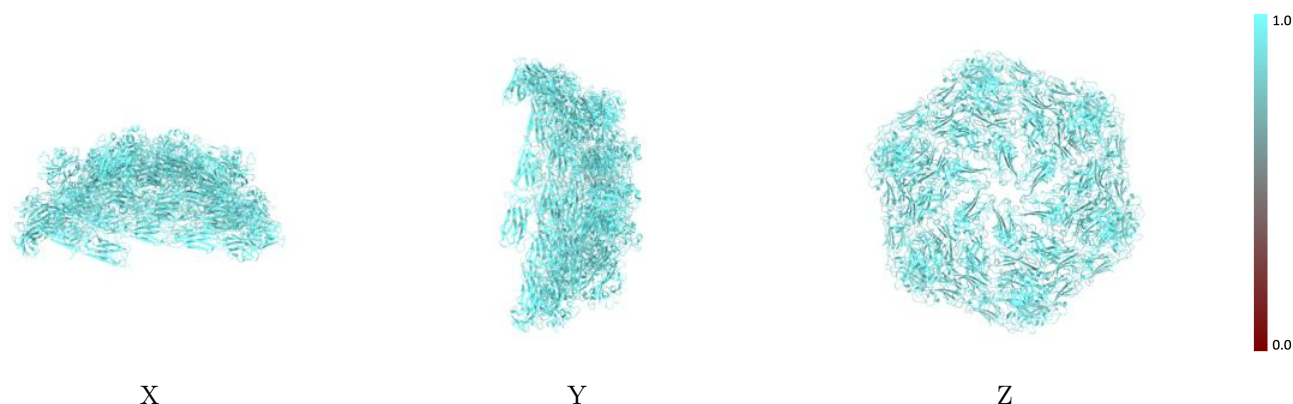
The images above show the 3D surface view of the map at the recommended contour level 1.05514 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



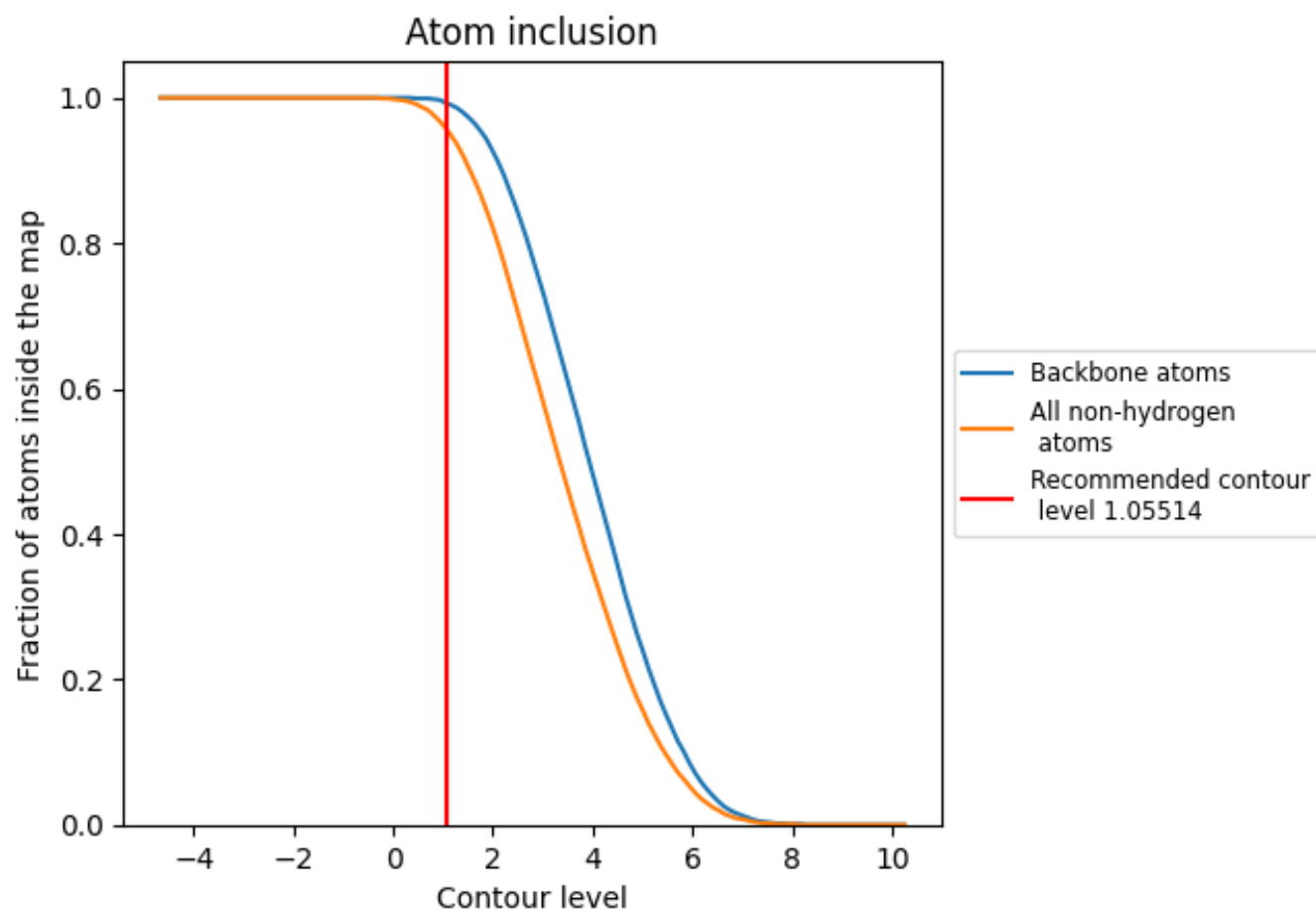
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.05514).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (1.05514) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.5560
A	0.9620	0.5630
B	0.9580	0.5530
C	0.9530	0.5520
D	0.9630	0.5620
E	0.9580	0.5530
F	0.9540	0.5520

1.0

0.0

<0.0